



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:20 AM UTC

PDB ID : 9HL9 / pdb\_00009hl9  
EMDB ID : EMD-52247  
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME  
WITH P/E-site tRNA AND mRNA : LM14Cs1H3 sKO STRAIN  
Authors : Rajan, K.S.; Yonath, A.  
Deposited on : 2024-12-04  
Resolution : 2.50 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](mailto: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>.

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

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

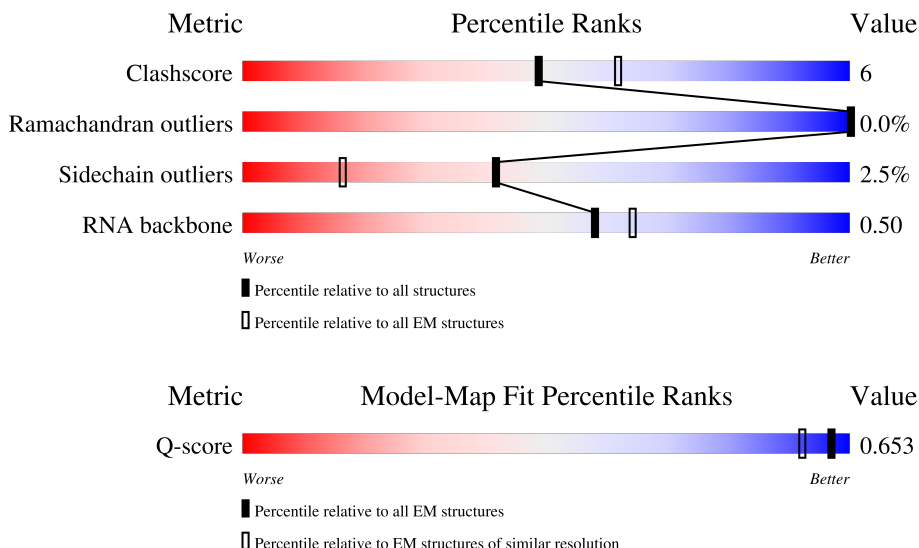
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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.





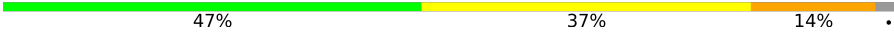







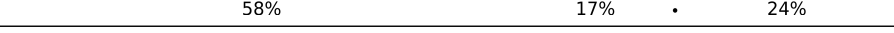
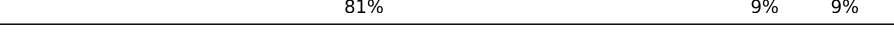
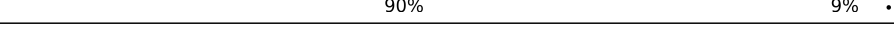


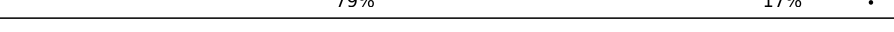









Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 ( 2.00 - 3.00 )

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  $\geq 3$ , 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	L1	1782	
2	L2	1526	
3	L3	216	


























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Mol	Chain	Length	Quality of chain
4	L4	184	
5	L5	135	
6	L6	73	
7	L7	171	
8	L8	124	
9	LA	260	
10	LB	419	
11	LC	373	
12	LD	188	
13	LE	190	
14	LF	195	
15	LG	264	
16	LH	222	
17	LI	220	
18	LJ	139	
19	LK	175	
20	LL	145	
21	LM	204	
22	LN	213	
23	LO	305	
24	LP	198	
25	LQ	254	
26	LR	179	
27	LS	159	
28	LT	166	


























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Mol	Chain	Length	Quality of chain
29	LU	129	 74% 19% 5%
30	LV	145	 74% 8% 18%
31	LW	143	 64% 21% 15%
32	LX	124	 64% 5% 31%
33	LY	134	 79% 20% 1%
34	LZ	147	 86% 12% 2%
35	La	127	 86% 11% 3%
36	Lb	70	 91% 6% 3%
37	Lc	252	 82% 8% 9%
38	Ld	104	 79% 11% 10%
39	Le	188	 92% 7% 1%
40	Lf	133	 80% 15% 5%
41	Lg	144	 83% 16% 1%
42	Lh	168	 65% 10% 24%
43	Li	105	 85% 11% 4%
44	Lj	83	 82% 16% 2%
45	Lk	83	 81% 11% 8%
46	Ll	51	 82% 16% 2%
47	Lm	128	 30% 9% 59%
48	Ln	34	 85% 9% 6%
49	Lo	92	 85% 11% 4%
50	Lp	106	 74% 17% 8%
51	S3	78	 51% 36% 6% 6%
52	S4	76	 33% 51% 13% 3%
53	S5	13	 46% 15% 8% 31%











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Mol	Chain	Length	Quality of chain
54	SA	264	
55	SB	246	
56	SC	219	
57	SD	190	
58	SE	273	
59	SF	265	
60	SG	249	
61	SH	190	
62	SI	200	
63	SJ	130	
64	SK	220	
65	SL	149	
66	SM	116	
67	SN	168	
68	SO	144	
69	SP	143	
70	SQ	141	
71	SR	153	
72	SS	57	
73	ST	151	
74	SU	173	
75	SV	143	
76	SW	152	
77	SX	161	
78	SY	164	

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Mol	Chain	Length	Quality of chain
79	SZ	137	 77%18%5%
80	Sa	120	 58%11%32%
81	Sb	112	 80%11%•7%
82	Sc	86	 70%29%•
83	Sd	87	 70%6%24%
84	Se	66	 74%18%8%
85	Sf	152	 23%6%71%
86	Sg	312	 70%25%••
87	Sh	235	 30%11%59%
88	S1	2204	 55%23%6%17%

## 2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 214618 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called LSUa\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1674	Total	C	N	O	P	1	0
			35924	16058	6567	11624	1675		

- Molecule 2 is a RNA chain called LSUb\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	1153	Total	C	N	O	P	1	0
			24694	11055	4451	8034	1154		

- Molecule 3 is a RNA chain called SR1\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	181	Total	C	N	O	P	0	0
			3834	1715	659	1279	181		

- Molecule 4 is a RNA chain called SR2\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L4	184	Total	C	N	O	P	0	0
			3937	1756	712	1285	184		

- Molecule 5 is a RNA chain called SR4\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	119	Total	C	N	O	P	0	0
			2533	1130	450	834	119		

- Molecule 6 is a RNA chain called SR6\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	71	Total	C	N	O	P	0	0
			1506	675	271	489	71		

- Molecule 7 is a RNA chain called 5.8S\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	165	Total	C	N	O	P	0	0
			3511	1573	621	1153	164		

- Molecule 8 is a RNA chain called 5S\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	120	Total	C	N	O	P	0	0
			2551	1141	454	836	120		

- Molecule 9 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	258	Total	C	N	O	S	0	0
			1962	1223	400	329	10		

- Molecule 10 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LB	404	Total	C	N	O	S	0	0
			3216	2024	638	541	13		

- Molecule 11 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	366	Total	C	N	O	S	0	0
			2820	1761	561	483	15		

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	175	Total	C	N	O	S	0	0
			1387	875	261	243	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	186	Total	C	N	O	S	0	0
			1477	936	273	262	6		

- Molecule 14 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LF	148	Total	C	N	O	S	0	0
			1144	726	215	201	2		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	239	Total	C	N	O	S	1	0
			1903	1198	377	321	7		

- Molecule 16 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	221	Total	C	N	O	S	0	0
			1767	1123	353	284	7		

- Molecule 17 is a protein called Putative 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	214	Total	C	N	O	S	0	0
			1695	1056	342	289	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	203	ARG	ASN	conflict	UNP E9AEA8

- Molecule 18 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	135	Total	C	N	O	S	0	0
			1012	638	191	177	6		

- Molecule 19 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	169	Total	C	N	O	S	0	0
			1336	833	264	231	8		

- Molecule 20 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	144	Total	C	N	O	S	0	0
			1124	707	226	185	6		

- Molecule 21 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	203	Total	C	N	O	S	0	0
			1711	1079	362	262	8		

- Molecule 22 is a protein called Putative 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	201	Total	C	N	O	S	0	0
			1634	1030	324	265	15		

- Molecule 23 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	298	Total	C	N	O	S	0	0
			2329	1480	437	406	6		

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	197	Total	C	N	O	S	0	0
			1539	968	307	258	6		

- Molecule 25 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	201	Total	C	N	O	S	0	0
			1682	1035	367	274	6		

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	178	Total	C	N	O	S	0	0
			1455	925	279	246	5		

- Molecule 27 is a protein called Putative 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LS	158	Total	C	N	O	S	0	0
			1261	803	245	209	4		

- Molecule 28 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	151	Total	C	N	O	S	0	0
			1211	757	240	203	11		

- Molecule 29 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	122	Total	C	N	O	S	0	0
			960	624	176	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LV	119	Total	C	N	O	S	0	0
			953	604	181	166	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LW	121	Total	C	N	O	S	0	0
			967	603	200	160	4		

- Molecule 32 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LX	85	Total	C	N	O	S	0	0
			714	461	140	109	4		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LY	133	Total	C	N	O	S	0	0
			1067	684	215	165	3		

- Molecule 34 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LZ	145	Total	C	N	O	S	0	0
			1117	685	238	189	5		

- Molecule 35 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	La	124	Total	C	N	O	S	0	0
			1032	644	214	170	4		

- Molecule 36 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lb	68	Total	C	N	O	S	0	0
			546	335	125	86			

- Molecule 37 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lc	229	Total	C	N	O	S	0	0
			1862	1185	358	308	11		

- Molecule 38 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ld	94	Total	C	N	O	S	0	0
			720	449	131	135	5		

- Molecule 39 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Le	186	Total	C	N	O	S	0	0
			1469	922	296	247	4		

- Molecule 40 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lf	128	Total	C	N	O	S	0	0
			1046	658	210	174	4		

- Molecule 41 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lg	143	Total	C	N	O	S	0	0
			1149	714	240	190	5		

- Molecule 42 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lh	127	Total	C	N	O	S	0	0
			1029	633	224	166	6		

- Molecule 43 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Li	101	Total	C	N	O	S	0	0
			799	503	162	132	2		

- Molecule 44 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lj	81	Total	C	N	O	S	0	0
			672	409	154	103	6		

- Molecule 45 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lk	76	Total	C	N	O	S	0	0
			595	376	116	100	3		

- Molecule 46 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Ll	50	Total	C	N	O	S	0	0
			446	288	94	63	1		

- Molecule 47 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lm	52	Total	C	N	O	S	0	0
			418	263	85	64	6		

- Molecule 48 is a protein called Putative 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ln	33	Total	C	N	O	S	0	0
			296	181	76	37	2		

- Molecule 49 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lo	89	Total	C	N	O	S	0	0
			693	431	143	113	6		

- Molecule 50 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lp	97	Total	C	N	O	S	0	0
			784	496	158	125	5		

- Molecule 51 is a RNA chain called P-site\_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S3	73	Total	C	N	O	P	0	0
			1556	694	282	507	73		

- Molecule 52 is a RNA chain called E-site\_tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S4	74	Total	C	N	O	P	0	0
			1574	703	280	518	73		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S5	9	Total	C	N	O	P	0	0
			187	84	30	64	9		

- Molecule 54 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SA	236	Total	C	N	O	S	0	0
			1898	1188	361	338	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	22	GLU	-	insertion	UNP Q4FX73
SA	?	-	ARG	deletion	UNP Q4FX73

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SB	211	Total	C	N	O	S	0	0
			1655	1052	300	292	11		

- Molecule 56 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SC	212	Total	C	N	O	S	1	0
			1646	1040	302	291	13		

- Molecule 57 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SD	183	Total	C	N	O	S	0	0
			1508	949	305	246	8		

- Molecule 58 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SE	260	Total	C	N	O	S	0	0
			2054	1301	393	351	9		

- Molecule 59 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SF	222	Total	C	N	O	S	0	0
			1708	1088	301	309	10		

- Molecule 60 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SG	229	Total	C	N	O	S	0	0
			1829	1140	375	311	3		

- Molecule 61 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SH	183	Total	C	N	O	S	0	0
			1447	899	279	262	7		

- Molecule 62 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SI	200	Total	C	N	O	S	0	0
			1649	1050	320	271	8		

- Molecule 63 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SJ	129	Total	C	N	O	S	0	0
			1021	646	188	179	8		

- Molecule 64 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SK	192	Total	C	N	O	S	0	0
			1546	964	319	261	2		

- Molecule 65 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SL	144	Total	C	N	O	S	0	0
			1140	731	210	196	3		

- Molecule 66 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SM	101	Total	C	N	O	S	0	0
			792	496	144	150	2		

- Molecule 67 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SN	99	Total	C	N	O	S	0	0
			813	522	142	142	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SO	137	Total	C	N	O	S	0	0
			1024	633	200	183	8		

- Molecule 69 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SP	141	Total	C	N	O	S	0	0
			1100	694	217	186	3		

- Molecule 70 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SQ	99	Total	C	N	O	S	0	0
			662	407	120	130	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SR	134	Total	C	N	O	S	0	0
			1077	681	211	181	4		

- Molecule 72 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SS	56	Total	C	N	O	S	0	0
			450	279	94	73	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
73	ST	143	Total	C	N	O	S	0	0
			1167	736	231	191	9		

- Molecule 74 is a protein called Ribosomal protein S17 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SU	144	Total	C	N	O	S	0	0
			1165	737	230	193	5		

- Molecule 75 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SV	122	Total	C	N	O	S	0	0
			992	619	193	175	5		

- Molecule 76 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SW	115	Total	C	N	O	S	0	0
			928	591	176	157	4		

- Molecule 77 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SX	152	Total	C	N	O	S	0	0
			1206	766	237	199	4		

- Molecule 78 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SY	88	Total	C	N	O	S	0	0
			663	409	121	129	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SZ	130	Total	C	N	O	S	0	0
			1051	675	204	169	3		

- Molecule 80 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sa	82	Total	C	N	O	S	0	0
			645	408	117	117	3		

- Molecule 81 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sb	104	Total	C	N	O	S	0	0
			825	511	177	130	7		

- Molecule 82 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sc	85	Total	C	N	O	S	0	0
			674	416	131	119	8		

- Molecule 83 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sd	66	Total	C	N	O	S	0	0
			492	299	99	90	4		

- Molecule 84 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Se	61	Total	C	N	O	S	0	0
			487	307	102	77	1		

- Molecule 85 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sf	44	Total	C	N	O	S	0	0
			359	229	67	62	1		

- Molecule 86 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Sg	302	Total	C	N	O	S	0	0
			2331	1462	415	441	13		

- Molecule 87 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Sh	96	Total	C	N	O	S	0	0
			768	486	146	133	3		

- Molecule 88 is a RNA chain called SSU\_rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	S1	1833	Total	C	N	O	P	1	0
			39229	17551	7079	12765	1834		

- Molecule 89 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
89	L1	9	Total 9	K 9	0
89	L2	4	Total 4	K 4	0
89	L4	3	Total 3	K 3	0
89	LA	2	Total 2	K 2	0
89	LN	1	Total 1	K 1	0
89	S5	1	Total 1	K 1	0
89	SO	1	Total 1	K 1	0
89	S1	7	Total 7	K 7	0

- Molecule 90 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
90	L1	9	Total 9	Na 9	0
90	L2	7	Total 7	Na 7	0
90	L4	1	Total 1	Na 1	0
90	SL	1	Total 1	Na 1	0
90	S1	7	Total 7	Na 7	0

- Molecule 91 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

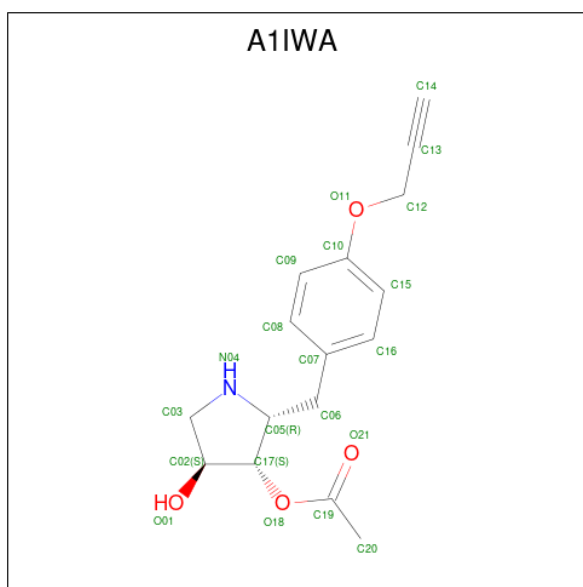
Mol	Chain	Residues	Atoms		AltConf
91	L1	187	Total 187	Mg 187	0
91	L2	96	Total 96	Mg 96	0
91	L3	1	Total 1	Mg 1	0
91	L4	2	Total 2	Mg 2	0
91	L7	5	Total 5	Mg 5	0

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Mol	Chain	Residues	Atoms		AltConf
91	L8	3	Total 3	Mg 3	0
91	LB	1	Total 1	Mg 1	0
91	LG	1	Total 1	Mg 1	0
91	LJ	1	Total 1	Mg 1	0
91	LM	1	Total 1	Mg 1	0
91	LN	1	Total 1	Mg 1	0
91	LS	1	Total 1	Mg 1	0
91	LT	2	Total 2	Mg 2	0
91	LV	1	Total 1	Mg 1	0
91	Lf	1	Total 1	Mg 1	0
91	Lh	2	Total 2	Mg 2	0
91	Ln	1	Total 1	Mg 1	0
91	S3	1	Total 1	Mg 1	0
91	SG	1	Total 1	Mg 1	0
91	SW	1	Total 1	Mg 1	0
91	S1	127	Total 127	Mg 127	0

- Molecule 92 is [(2R,3S,4S)-4-oxidanyl-2-[(4-prop-2-ynoxypheyl)methyl]pyrrolidin-3-yl] ethanoate (CCD ID: A1IWA) (formula: C<sub>16</sub>H<sub>19</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
92	L2	1	Total	C	N	O	0
			21	16	1	4	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	L1	280	Total	O	0
			280	280	
94	L2	365	Total	O	0
			365	365	
94	L3	12	Total	O	0
			12	12	

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Mol	Chain	Residues	Atoms		AltConf
94	L4	12	Total 12	O 12	0
94	L5	11	Total 11	O 11	0
94	L6	2	Total 2	O 2	0
94	L7	6	Total 6	O 6	0
94	L8	3	Total 3	O 3	0
94	LA	18	Total 18	O 18	0
94	LB	13	Total 13	O 13	0
94	LC	11	Total 11	O 11	0
94	LH	2	Total 2	O 2	0
94	LI	3	Total 3	O 3	0
94	LJ	2	Total 2	O 2	0
94	LL	3	Total 3	O 3	0
94	LM	10	Total 10	O 10	0
94	LN	1	Total 1	O 1	0
94	LO	1	Total 1	O 1	0
94	LQ	3	Total 3	O 3	0
94	LR	1	Total 1	O 1	0
94	LS	2	Total 2	O 2	0
94	LT	5	Total 5	O 5	0
94	LZ	1	Total 1	O 1	0
94	Lb	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
94	Lc	4	Total 4	O 4	0
94	Le	1	Total 1	O 1	0
94	Lf	3	Total 3	O 3	0
94	Lg	1	Total 1	O 1	0
94	Lh	2	Total 2	O 2	0
94	Lj	6	Total 6	O 6	0
94	Ll	2	Total 2	O 2	0
94	Ln	8	Total 8	O 8	0
94	Lo	4	Total 4	O 4	0
94	Lp	8	Total 8	O 8	0
94	S3	10	Total 10	O 10	0
94	S4	5	Total 5	O 5	0
94	S5	3	Total 3	O 3	0
94	SF	5	Total 5	O 5	0
94	SH	1	Total 1	O 1	0
94	SI	1	Total 1	O 1	0
94	SK	4	Total 4	O 4	0
94	SL	5	Total 5	O 5	0
94	SM	5	Total 5	O 5	0
94	SO	3	Total 3	O 3	0
94	SP	1	Total 1	O 1	0

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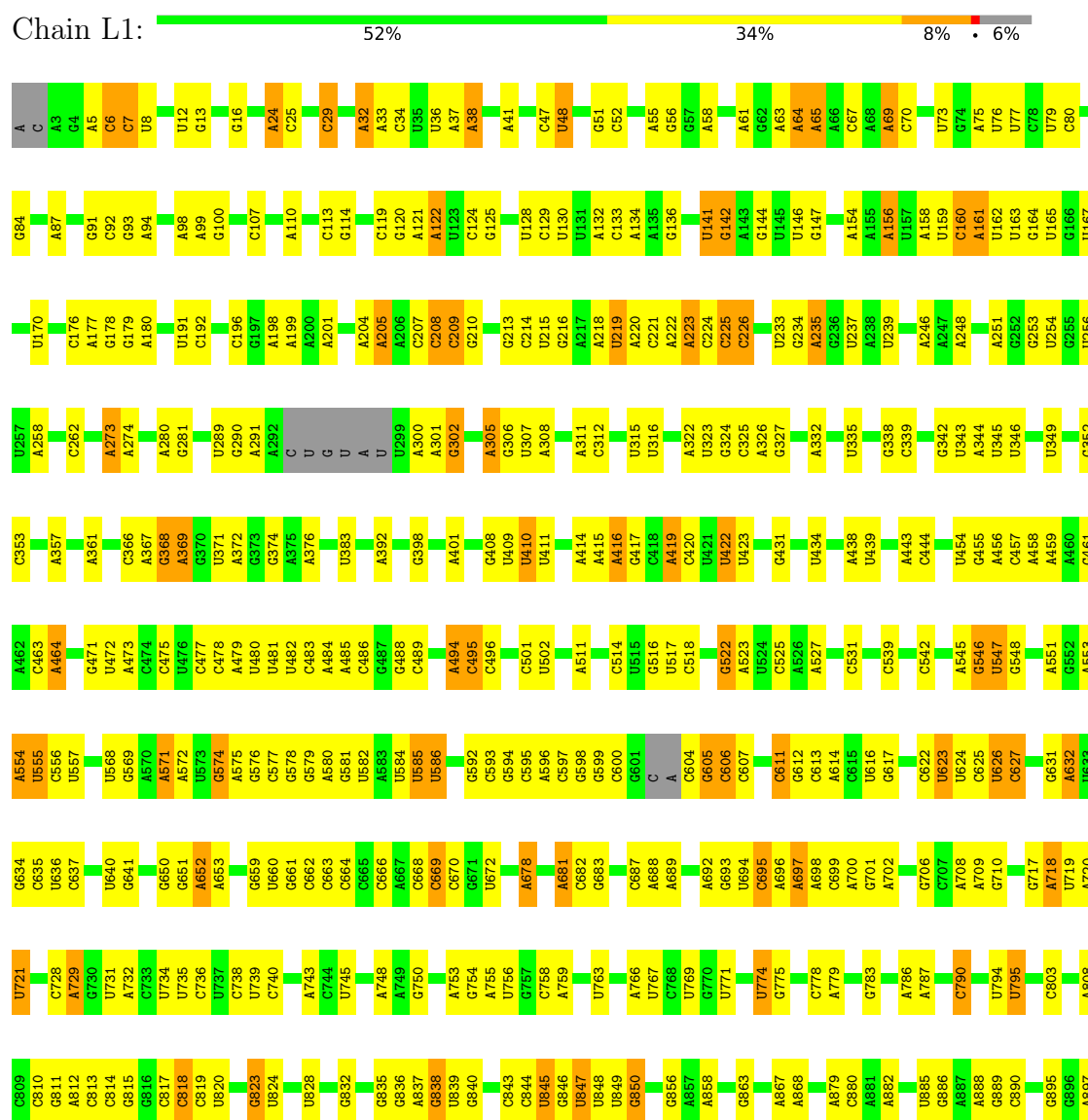
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Mol	Chain	Residues	Atoms		AltConf
94	SS	1	Total 1	O 1	0
94	ST	6	Total 6	O 6	0
94	SU	1	Total 1	O 1	0
94	SX	2	Total 2	O 2	0
94	Sb	9	Total 9	O 9	0
94	Sc	1	Total 1	O 1	0
94	S1	425	Total 425	O 425	0

### 3 Residue-property plots

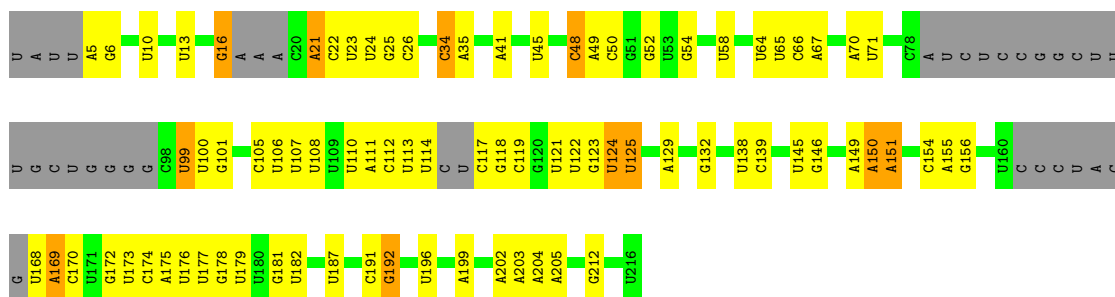
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: LSUa\_rRNA



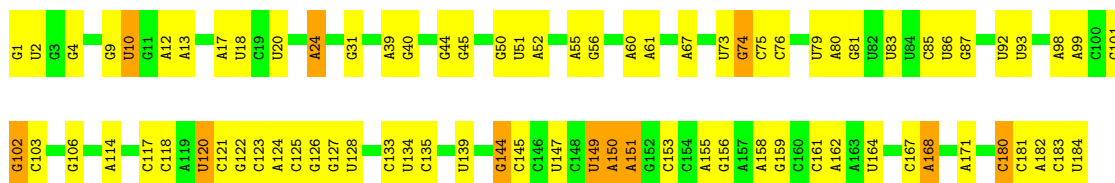
A898	G1008	U1092	U1172	U1270	A	G1416	G1612	C1706	U1707
A899	G1009	U1093	U1178	U1271	A	G1416	C1613	U1708	G1708
C900	G1010	U1094	U1182	U1272	C	G1420	G1626	U1709	C1709
G904	G1012	C1094	C1182	U1273	U	G1421	G1635	U1710	U1710
G911	A1013	A1097	U1185	G1274	C	G1422	U1627	U1715	U1715
C912	A1016	A1098	U1186	G1275	C	A1423	U1637	U1716	U1716
C913	U1017	A1099	U1187	G1276	C1341	A1424	U1638	U1717	U1717
U914	U1018	A1100	U1188	U1277	C1342	C1425	U1639	U1718	U1718
	A1019	U1101	U1189	U1278	C1343	A1426	U1640	U1719	U1719
	G1019	U1102	U1190	U1279	C1344	U1427	U1641	U1720	U1720
U925	C1020	A1105	G1197	U1280	C1345	U1428	U1642	U1721	U1721
G926	G1025	A1106	C1198	U1281	C1346	U1429	U1643	U1722	U1722
A927	U1025	U1107	U1199	U1282	C1347	U1430	U1644	U1723	U1723
U930	A1031	U1114	U1201	U1283	C1348	U1431	U1645	U1724	U1724
G938	U1036	C1115	U1202	U1284	C1349	U1432	U1646	U1725	U1725
A939	U1037	U1116	C1203	U1285	C1350	U1433	U1647	U1726	U1726
U940	U1038	U1117	U1204	U1286	C1351	U1434	U1648	U1727	U1727
U941	U1039	U1118	U1205	U1287	C1352	U1435	U1649	U1728	U1728
U945	G1044	U1119	U1206	U1288	C1353	U1436	U1650	U1729	U1729
G946	G1045	U1120	U1207	U1289	C1354	U1437	U1651	U1730	U1730
A947	U1050	U1121	U1208	U1290	C1355	U1438	U1652	U1731	U1731
G951	C1051	U1122	U1209	U1291	C1356	U1439	U1653	U1732	U1732
U954	A1052	U1123	U1210	U1292	C1357	U1440	U1654	U1733	U1733
A955	A1053	U1124	U1211	U1293	C1358	U1441	U1655	U1734	U1734
U956	G1061	U1125	U1212	U1294	C1359	U1442	U1656	U1735	U1735
C957	A1062	U1126	U1213	U1295	C1360	U1443	U1657	U1736	U1736
G958	G1063	U1127	U1214	U1296	C1361	U1444	U1658	U1737	U1737
G959	C1064	U1128	U1215	U1297	C1362	U1445	U1659	U1738	U1738
G963	C	U1129	U1216	U1298	C1363	U1446	U1660	U1739	U1739
A964	U	U1130	U1217	U1299	C1364	U1447	U1661	U1740	U1740
A965	U	U1131	U1218	U1300	C1365	U1448	U1662	U1741	U1741
A966	G	U1132	U1219	U1301	C1366	U1449	U1663	U1742	U1742
G967	G	U1133	U1220	U1302	C1367	U1450	U1664	U1743	U1743
A968	U	U1134	U1221	U1303	C1368	U1451	U1665	U1744	U1744
	U	U1135	U1222	U1304	C1369	U1452	U1666	U1745	U1745
	U	U1136	U1223	U1305	C1370	U1453	U1667	U1746	U1746
	U	U1137	U1224	U1306	C1371	U1454	U1668	U1747	U1747
	U	U1138	U1225	U1307	C1372	U1455	U1669	U1748	U1748
	U	U1139	U1226	U1308	C1373	U1456	U1670	U1749	U1749
	U	U1140	U1227	U1309	C1374	U1457	U1671	U1750	U1750
	U	U1141	U1228	U1310	C1375	U1458	U1672	U1751	U1751
	U	U1142	U1229	U1311	C1376	U1459	U1673	U1752	U1752
	U	U1143	U1230	U1312	C1377	U1460	U1674	U1753	U1753
	U	U1144	U1231	U1313	C1378	U1461	U1675	U1754	U1754
	U	U1145	U1232	U1314	C1379	U1462	U1676	U1755	U1755
	U	U1146	U1233	U1315	C1380	U1463	U1677	U1756	U1756
	U	U1147	U1234	U1316	C1381	U1464	U1678	U1757	U1757
	U	U1148	U1235	U1317	C1382	U1465	U1679	U1758	U1758
	U	U1149	U1236	U1318	C1383	U1466	U1680	U1759	U1759
	U	U1150	U1237	U1319	C1384	U1467	U1681	U1760	U1760
	U	U1151	U1238	U1320	C1385	U1468	U1682	U1761	U1761
	U	U1152	U1239	U1321	C1386	U1469	U1683	U1762	U1762
	U	U1153	U1240	U1322	C1387	U1470	U1684	U1763	U1763
	U	U1154	U1241	U1323	C1388	U1471	U1685	U1764	U1764
	U	U1155	U1242	U1324	C1389	U1472	U1686	U1765	U1765
	U	U1156	U1243	U1325	C1390	U1473	U1687	U1766	U1766
	U	U1157	U1244	U1326	C1391	U1474	U1688	U1767	U1767
	U	U1158	U1245	U1327	C1392	U1475	U1689	U1768	U1768
	U	U1159	U1246	U1328	C1393	U1476	U1690	U1769	U1769
	U	U1160	U1247	U1329	C1394	U1477	U1691	U1770	U1770
	U	U1161	U1248	U1330	C1395	U1478	U1692	U1771	U1771
	U	U1162	U1249	U1331	C1396	U1479	U1693	U1772	U1772
	U	U1163	U1250	U1332	C1397	U1480	U1694	U1773	U1773
	U	U1164	U1251	U1333	C1398	U1481	U1695	U1774	U1774
	U	U1165	U1252	U1334	C1399	U1482	U1696	U1775	U1775
	U	U1166	U1253	U1335	C1400	U1483	U1697	U1776	U1776
	U	U1167	U1254	U1336	C1401	U1484	U1698	U1777	U1777
	U	U1168	U1255	U1337	C1402	U1485	U1699	U1778	U1778
	U	U1169	U1256	U1338	C1403	U1486	U1700	U1779	U1779
	U	U1170	U1257	U1339	C1404	U1487	U1701	U1780	U1780
	U	U1171	U1258	U1340	C1405	U1488	U1702	U1781	U1781
	U	U1172	U1259	U1341	C1406	U1489	U1703	U1782	U1782
	U	U1173	U1260	U1342	C1407	U1490	U1704	U1783	U1783
	U	U1174	U1261	U1343	C1408	U1491	U1705	U1784	U1784
	U	U1175	U1262	U1344	C1409	U1492	U1706	U1785	U1785
	U	U1176	U1263	U1345	C1410	U1493	U1707	U1786	U1786
	U	U1177	U1264	U1346	C1411	U1494	U1708	U1787	U1787
	U	U1178	U1265	U1347	C1412	U1495	U1709	U1788	U1788
	U	U1179	U1266	U1348	C1413	U1496	U1710	U1789	U1789
	U	U1180	U1267	U1349	C1414	U1497	U1711	U1790	U1790
	U	U1181	U1268	U1350	C1415	U1498	U1712	U1791	U1791
	U	U1182	U1269	U1351	C1416	U1499	U1713	U1792	U1792
	U	U1183	U1270	U1352	C1417	U1500	U1714	U1793	U1793
	U	U1184	U1271	U1353	C1418	U1501	U1715	U1794	U1794
	U	U1185	U1272	U1354	C1419	U1502	U1716	U1795	U1795
	U	U1186	U1273	U1355	C1420	U1503	U1717	U1796	U1796
	U	U1187	U1274	U1356	C1421	U1504	U1718	U1797	U1797
	U	U1188	U1275	U1357	C1422	U1505	U1719	U1798	U1798
	U	U1189	U1276	U1358	C1423	U1506	U1720	U1799	U1799
	U	U1190	U1277	U1359	C1424	U1507	U1721	U1800	U1800
	U	U1191	U1278	U1360	C1425	U1508	U1722	U1801	U1801
	U	U1192	U1279	U1361	C1426	U1509	U1723	U1802	U1802
	U	U1193	U1280	U1362	C1427	U1510	U1724	U1803	U1803
	U	U1194	U1281	U1363	C1428	U1511	U1725	U1804	U1804
	U	U1195	U1282	U1364	C1429	U1512	U1726	U1805	U1805
	U	U1196	U1283	U1365	C1430	U1513	U1727	U1806	U1806
	U	U1197	U1284	U1366	C1431	U1514	U1728	U1807	U1807
	U	U1198	U1285	U1367	C1432	U1515	U1729	U1808	U1808
	U	U1199	U1286	U1368	C1433	U1516	U1730	U1809	U1809
	U	U1200	U1287	U1369	C1434	U1517	U1731	U1810	U1810
	U	U1201	U1288	U1370	C1435	U1518	U1732	U1811	U1811
	U	U1202	U1289	U1371	C1436	U1519	U1733	U1812	U1812
	U	U1203	U1290	U1372	C1437	U1520	U1734	U1813	U1813
	U	U1204	U1291	U1373	C1438	U1521	U1735	U1814	U1814
	U	U1205	U1292	U1374	C1439	U1522	U1736	U1815	U1815
	U	U1206	U1293	U1375	C1440	U1523	U1737	U1816	U1816
	U	U1207	U1294	U1376	C1441	U1524	U1738	U1817	U1817
	U	U1208	U1295	U1377	C1442	U1525	U1739	U1818	U1818
	U	U1209	U1296	U1378	C1443	U1526	U1740	U1819	U1819
	U	U1210	U1297	U1379	C1444	U1527	U1741	U1820	U1820
	U	U1211	U1298	U1380	C1445	U1528	U1742	U1821	U1821
	U	U1212	U1299	U1381	C1446	U1529	U1743	U1822	U1822
	U	U1213	U1300	U1382	C1447	U1530	U1744	U1823	U1823
	U	U1214	U1301	U1383	C1448	U1531	U1745	U1824	U1824
	U	U1215	U1302	U1384	C1449	U1532	U1746	U1825	U1825
	U	U1216	U1303	U1385	C1450	U1533	U1747	U1826	U1826
	U	U1217	U1304	U1386	C1451	U1534	U1748	U1827	U1827
	U	U1218	U1305	U1387	C1452	U1535	U1749	U1828	U1828
	U	U1219	U1306	U1388	C1453	U1536	U1750	U1829	U1829
	U	U1220	U1307	U1389	C1454	U1537	U1751	U1830	U1830
	U	U1221	U1308	U1390	C1455	U1538	U1752	U1831	U1831
	U	U1222	U1309	U1391	C1456	U1539	U1753	U1832	U1832
	U	U1223	U1310	U1392	C1457	U1540	U1754	U1833	U1833
	U	U1224	U1311	U1393	C1458	U1541	U1755	U1834	U1834
	U	U1225	U1312	U1394	C1459	U1542	U1756	U1835	U1835
	U	U1226	U1313	U1395	C1460	U1543	U1757	U1836	U1836
	U	U1227	U1314	U1396	C1461	U1544	U1758	U1837	U1837
	U	U1228	U1315	U1397	C1462	U1545	U1759	U1838	U1838
	U	U1229	U1316	U1398</					





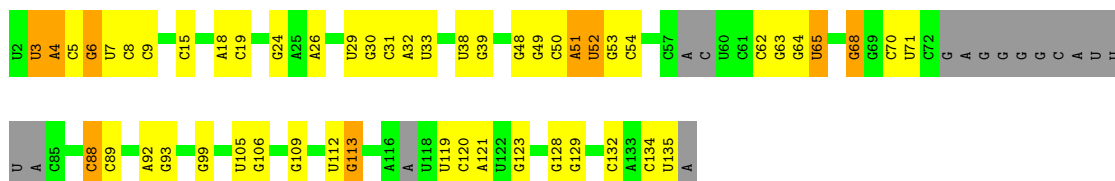
• Molecule 4: SR2\_rRNA

Chain L4: 56% 38% 6%



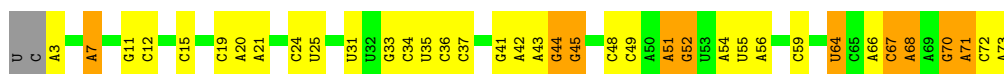
• Molecule 5: SR4\_rRNA

Chain L5: 50% 32% 7% 12%



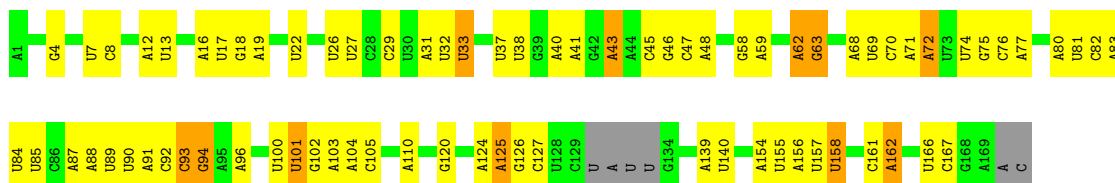
• Molecule 6: SR6\_rRNA

Chain L6: 47% 37% 14%



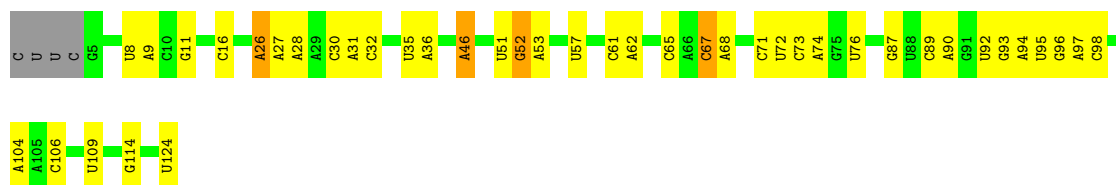
• Molecule 7: 5.8S\_rRNA

Chain L7: 52% 38% 6%



• Molecule 8: 5S\_rRNA

Chain L8: 63% 31% 6%



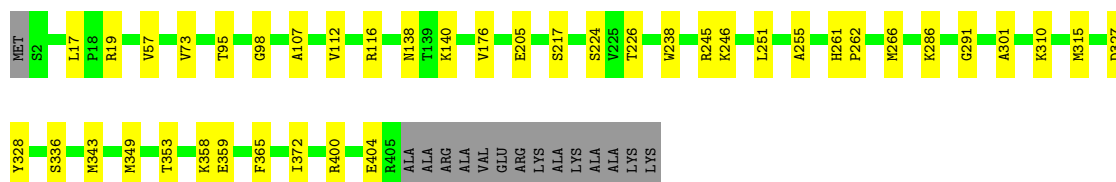
- Molecule 9: Putative 60S ribosomal protein L2

Chain LA: 89% 10% .



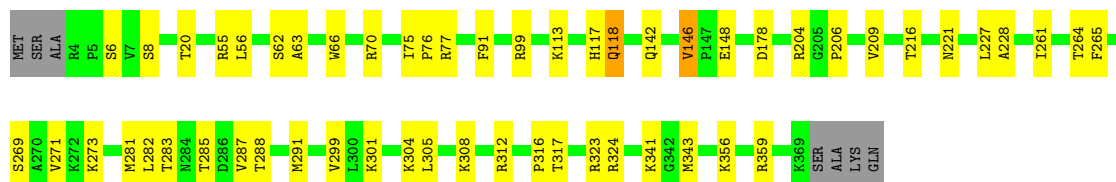
- Molecule 10: Putative ribosomal protein L3

Chain LB: 87% 10% .



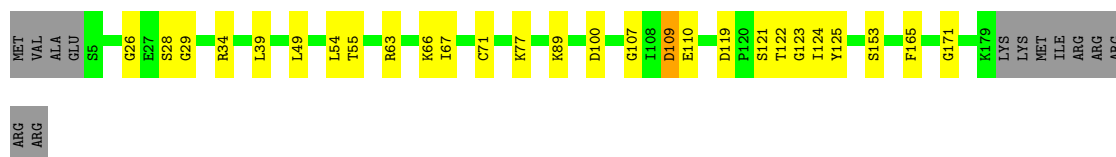
- Molecule 11: Putative ribosomal protein L1a

Chain LC: 83% 14% ..



- Molecule 12: 60S ribosomal protein L11

Chain LD: 79% 14% 7% .



- Molecule 13: Putative 60S ribosomal protein L9

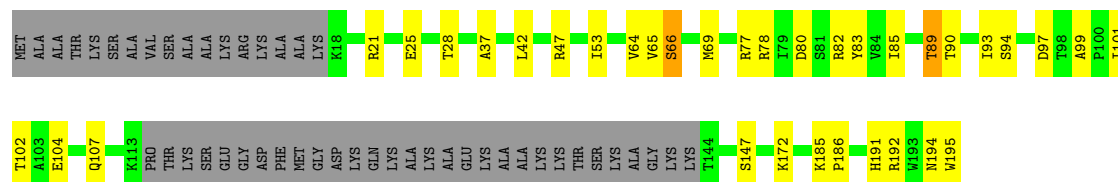
Chain LE: 78% 19% ..





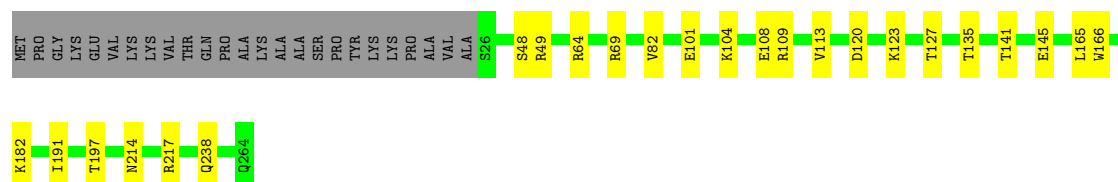
- Molecule 14: Putative 60S ribosomal protein L6

Chain LF: 58% 17% 24%



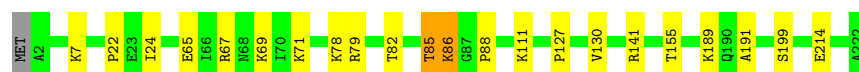
- Molecule 15: 60S ribosomal protein L7a

Chain LG: 81% 9% 9%



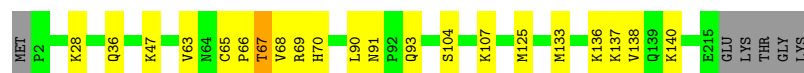
- Molecule 16: Putative 60S ribosomal protein L13a

Chain LH: 90% 9% .



- Molecule 17: Putative 60S ribosomal protein L13

Chain LI: 88% 9% .



- Molecule 18: Putative 60S ribosomal protein L23

Chain LJ: 86% 12% .



- Molecule 19: Putative 40S ribosomal protein L14

Chain LK: 79% 17% .



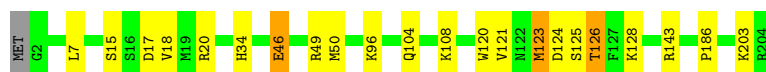
- Molecule 20: Putative 60S ribosomal protein L27A/L29

Chain LL: 86% 14% .



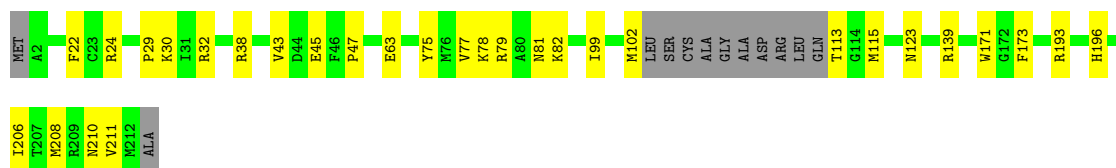
- Molecule 21: Ribosomal protein L15

Chain LM: 89% 9% .



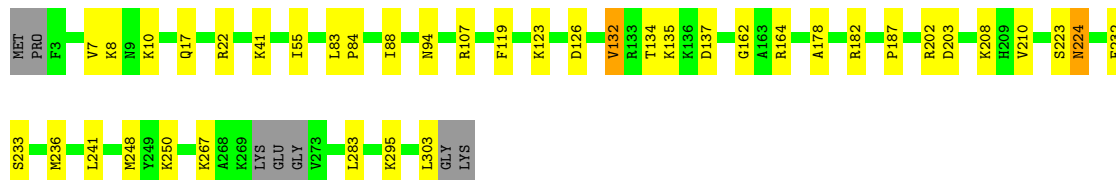
- Molecule 22: Putative 60S ribosomal protein L10

Chain LN: 80% 14% 6%



- Molecule 23: Putative 60S ribosomal protein L5

Chain LO: 85% 12% ..



- Molecule 24: 60S ribosomal protein L18

Chain LP: 90% 9% ..



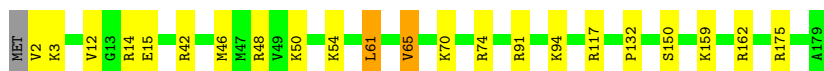
- Molecule 25: Putative 60S ribosomal protein L19

Chain LQ: 72% 7% 21%



- Molecule 26: 60S ribosomal protein L18a

Chain LR: 87% 11% ..



- Molecule 27: Putative 60S ribosomal protein L21

Chain LS: 87% 11% ..



- Molecule 28: Putative 60S ribosomal protein L17

Chain LT: 78% 12% 9%



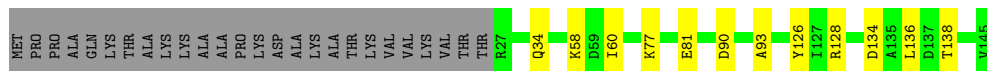
- Molecule 29: Putative 60S ribosomal protein L22

Chain LU: 74% 19% 5%



- Molecule 30: Putative 60S ribosomal protein L23a

Chain LV: 74% 8% 18%



- Molecule 31: Putative 60S ribosomal protein L26

Chain LW: 64% 21% 15%




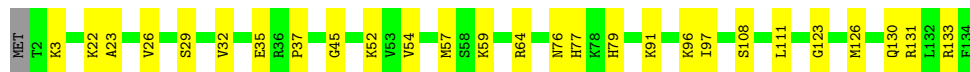
- Molecule 32: Putative ribosomal protein L24

Chain LX:  64% 5% 31%




- Molecule 33: 60S ribosomal protein L27

Chain LY:  79% 20%




- Molecule 34: Putative 60S ribosomal protein L28

Chain LZ:  86% 12%



- Molecule 35: Putative 60S ribosomal protein L35

Chain La:  86% 11%




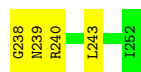
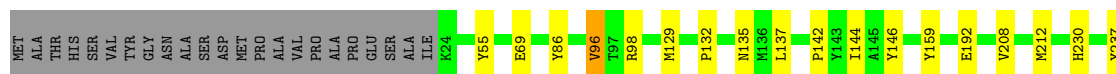
- Molecule 36: 60S ribosomal protein L29

Chain Lb:  91% 6%




- Molecule 37: Putative 60S ribosomal protein L7

Chain Lc:  82% 8% 9%



- Molecule 38: 60S ribosomal protein L30

Chain Ld:  79% 11% 10%



- Molecule 39: Putative 60S ribosomal subunit protein L31

Chain Le: 92% 7% .



- Molecule 40: 60S ribosomal protein L32

Chain Lf: 80% 15% . .



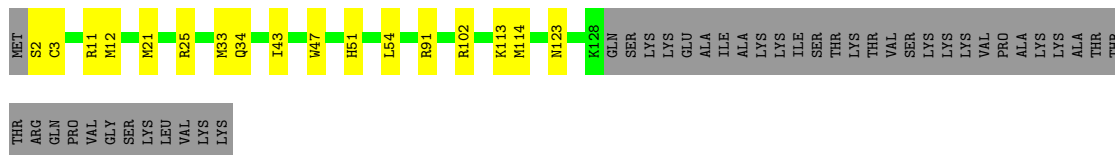
- Molecule 41: Putative ribosomal protein l35a

Chain Lg: 83% 16% . .



- Molecule 42: Putative 60S ribosomal protein L34

Chain Lh: 65% 10% 24%



- Molecule 43: Putative 60S Ribosomal protein L36

Chain Li: 85% 11% .




- Molecule 44: Ribosomal protein L37

Chain Lj: 82% 16% .




- Molecule 45: Putative ribosomal protein L38

Chain Lk:  81% 11% 8%



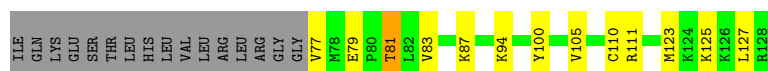
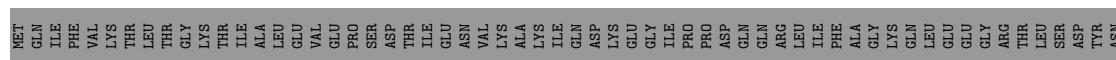
- Molecule 46: Putative 60S ribosomal protein L39

Chain Ll:  82% 16% .




- Molecule 47: Ubiquitin-60S ribosomal protein L40

Chain Lm:  30% 9% . 59%




- Molecule 48: Putative 60S ribosomal protein L41

Chain Ln:  85% 9% . .




- Molecule 49: 60S ribosomal protein L37a

Chain Lo:  85% 11% . .



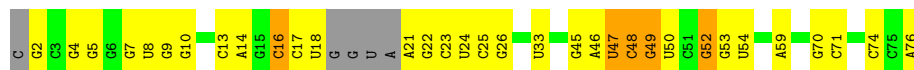
- Molecule 50: Putative 60S ribosomal protein L44

Chain Lp:  74% 17% . 8%



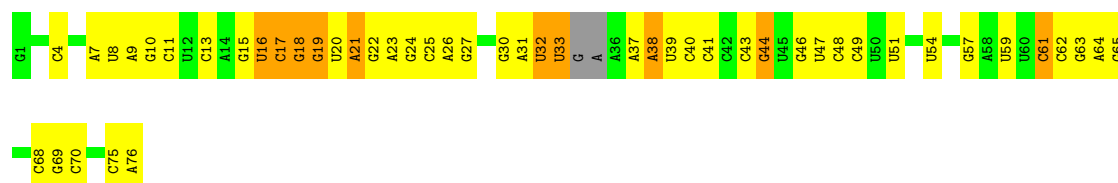
- Molecule 51: P-site\_tRNA

Chain S3:  51% 36% 6% 6%



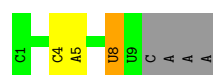
- Molecule 52: E-site\_tRNA

Chain S4:  33% 51% 13%




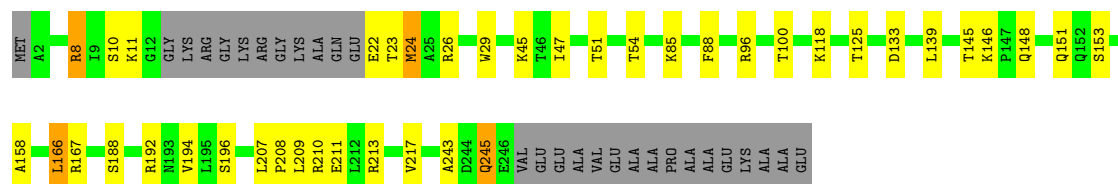
- Molecule 53: mRNA

Chain S5:  46% 15% 8% 31%



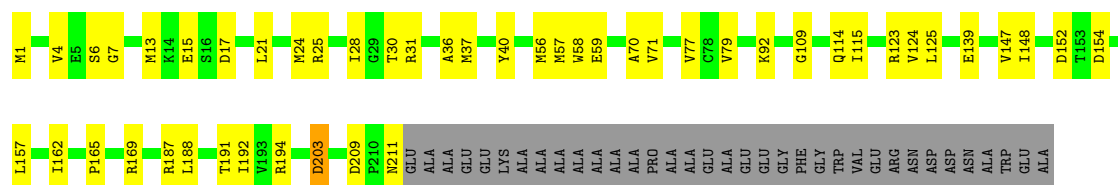
- Molecule 54: Small ribosomal subunit protein eS1

Chain SA:  74% 14% 11%




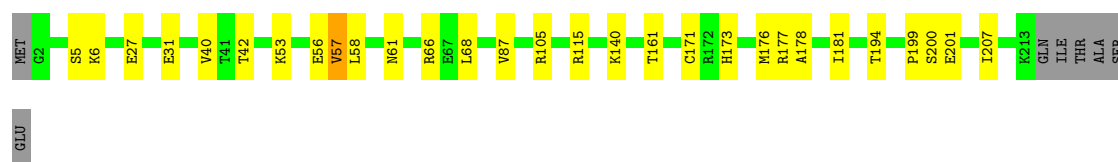
- Molecule 55: 40S ribosomal protein SA

Chain SB:  66% 19% 14%




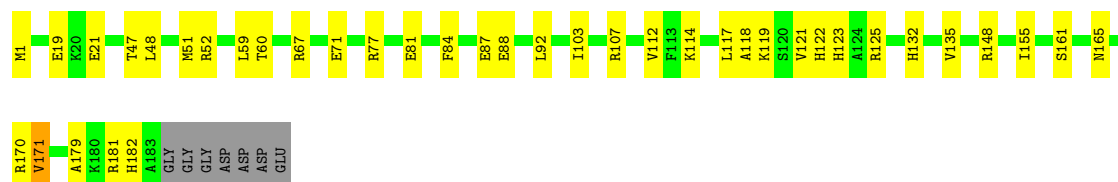
- Molecule 56: Putative 40S ribosomal protein S3

Chain SC:  84% 13%



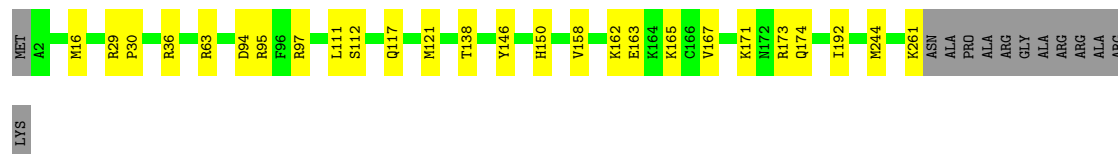
- Molecule 57: Putative 40S ribosomal protein S9

Chain SD:  76% 20%



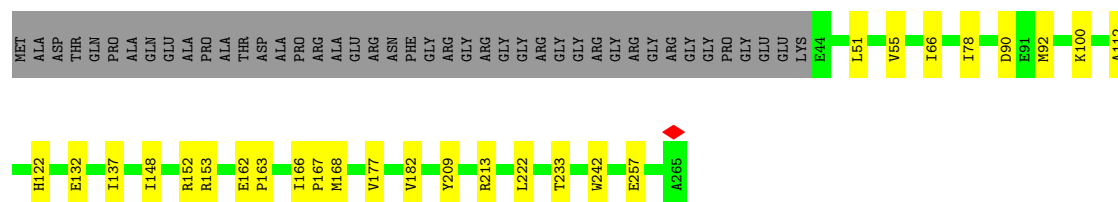
- Molecule 58: 40S ribosomal protein S4

Chain SE: 86% 10% 5%



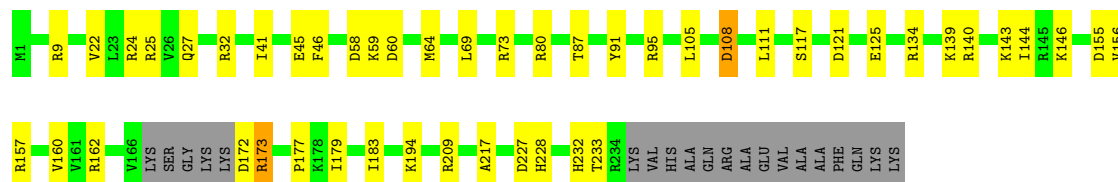
- Molecule 59: 40S ribosomal protein S2

Chain SF: 74% 10% 16%



- Molecule 60: 40S ribosomal protein S6

Chain SG: 73% 18% 8%



- Molecule 61: 40S ribosomal protein S5

Chain SH: 83% 13% 4%




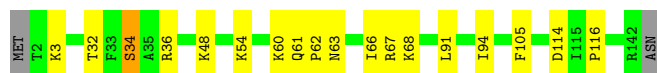
- Molecule 62: 40S ribosomal protein S7

Chain SI: 86% 14% 0%



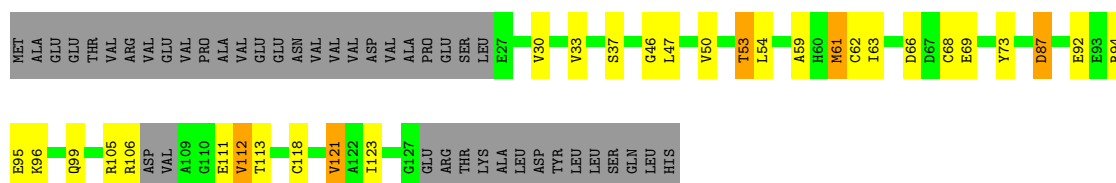


Chain SP:  86% 12% ..




- Molecule 70: 40S ribosomal protein S12

Chain SQ:  49% 18% • 30%




- Molecule 71: Putative 40S ribosomal protein S18

Chain SR:  76% 10% • 12%




- Molecule 72: Putative ribosomal protein S29

Chain SS:  86% 12% •




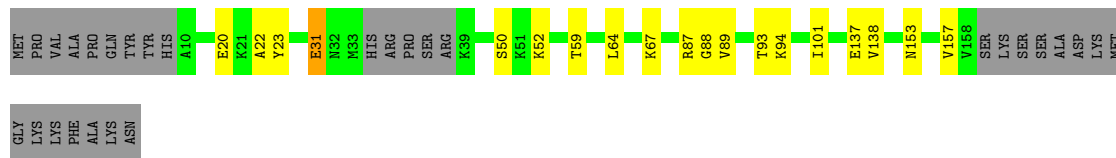
- Molecule 73: Putative 40S ribosomal protein S13

Chain ST:  77% 17% 5%



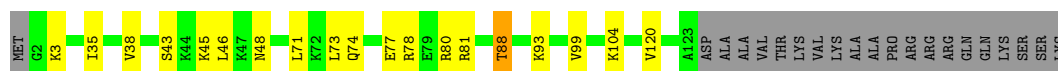
- Molecule 74: Ribosomal protein S17 family protein

Chain SU:  72% 10% • 17%

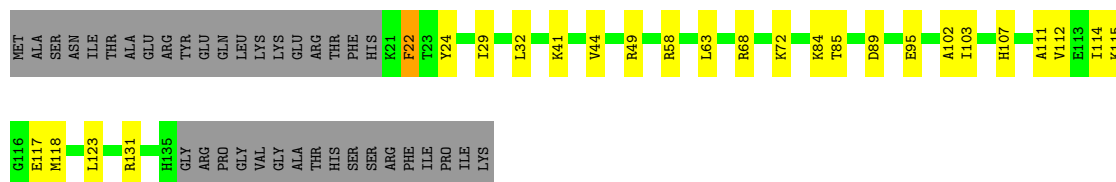


- Molecule 75: Putative 40S ribosomal protein S17

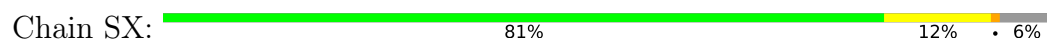
Chain SV:  72% 13% • 15%



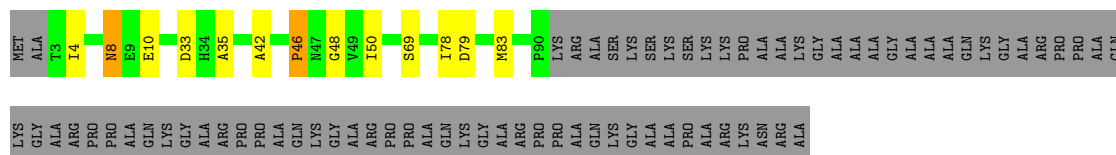
- Molecule 76: Putative 40S ribosomal protein S15



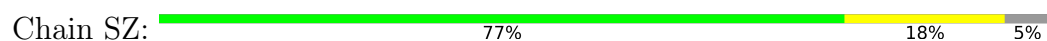
- Molecule 77: 40S ribosomal protein S19-like protein



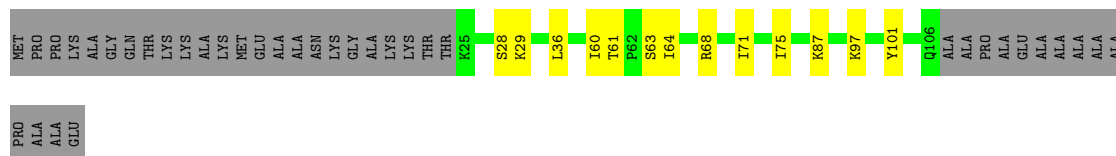
- Molecule 78: Putative 40S ribosomal protein S21



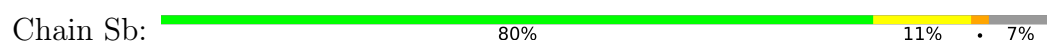
- Molecule 79: 40S ribosomal protein S24



- Molecule 80: 40S ribosomal protein S25



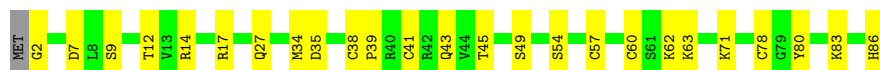
- Molecule 81: 40S ribosomal protein S26





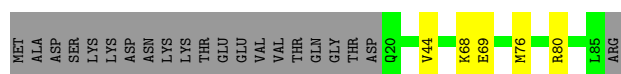
- Molecule 82: Putative 40S ribosomal protein S27-1

Chain Sc: 70% 29%



- Molecule 83: Putative 40S ribosomal protein S33

Chain Sd: 70% 6% 24%



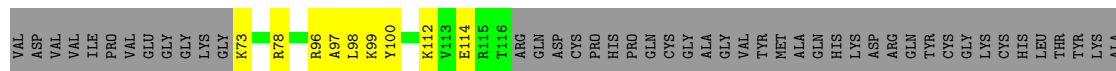
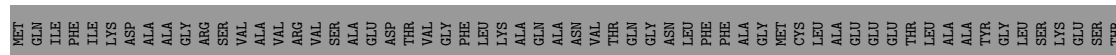
- Molecule 84: 40S ribosomal protein S30

Chain Se: 74% 18% 8%



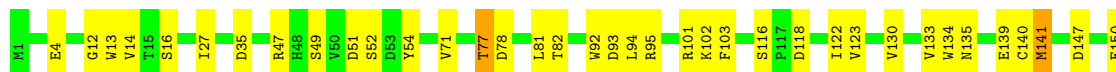
- Molecule 85: Ubiquitin-60S ribosomal protein L40

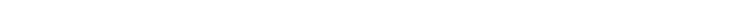
Chain Sf: 23% 6% 71%

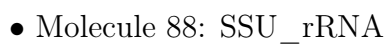


- Molecule 86: Guanine nucleotide-binding protein subunit beta-like protein

Chain Sg: 70% 25%



Chain Sh:  30% 11% 59%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138498	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 ( $e^-/\text{\AA}^2$ )	1.0018	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	527.68, 527.68, 527.68	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82449996, 0.82449996, 0.82449996	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, NA, OMC, A2M, OMG, OMU, K, 5MC, A1IWA, G7M, MA6, ZN, MG, PSU

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	L1	0.22	0/39257	0.32	0/61207
2	L2	0.24	3/26022 (0.0%)	0.32	0/40555
3	L3	0.19	0/4253	0.30	0/6611
4	L4	0.20	0/4376	0.31	0/6822
5	L5	0.19	0/2826	0.35	0/4395
6	L6	0.17	0/1683	0.34	0/2618
7	L7	0.22	0/3757	0.31	0/5850
8	L8	0.18	0/2851	0.29	0/4439
9	LA	0.15	0/2007	0.30	0/2696
10	LB	0.14	0/3283	0.27	0/4412
11	LC	0.14	0/2870	0.25	0/3861
12	LD	0.11	0/1410	0.23	0/1884
13	LE	0.14	0/1497	0.32	0/2017
14	LF	0.15	0/1165	0.33	0/1574
15	LG	0.17	0/1933	0.32	0/2599
16	LH	0.13	0/1803	0.25	0/2422
17	LI	0.14	0/1728	0.25	0/2313
18	LJ	0.15	0/1029	0.29	0/1388
19	LK	0.11	0/1355	0.22	0/1816
20	LL	0.14	0/1151	0.28	0/1538
21	LM	0.16	0/1751	0.27	0/2338
22	LN	0.14	0/1666	0.28	0/2227
23	LO	0.13	0/2370	0.27	0/3172
24	LP	0.14	0/1564	0.25	0/2092
25	LQ	0.12	0/1701	0.20	0/2250
26	LR	0.14	0/1489	0.24	0/2008
27	LS	0.15	0/1290	0.28	0/1736
28	LT	0.16	0/1235	0.29	0/1656
29	LU	0.12	0/976	0.27	0/1303
30	LV	0.13	0/968	0.24	0/1302
31	LW	0.13	0/981	0.24	0/1310
32	LX	0.13	0/735	0.25	0/989

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	LY	0.12	0/1088	0.23	0/1455
34	LZ	0.15	0/1133	0.23	0/1516
35	La	0.12	0/1042	0.24	0/1383
36	Lb	0.14	0/557	0.24	0/743
37	Lc	0.15	0/1896	0.28	0/2540
38	Ld	0.12	0/730	0.23	0/989
39	Le	0.12	0/1488	0.25	0/1979
40	Lf	0.14	0/1066	0.29	0/1424
41	Lg	0.15	0/1172	0.25	0/1573
42	Lh	0.13	0/1045	0.25	0/1390
43	Li	0.12	0/814	0.22	0/1089
44	Lj	0.16	0/686	0.28	0/915
45	Lk	0.12	0/604	0.23	0/810
46	Ll	0.13	0/459	0.23	0/613
47	Lm	0.13	0/424	0.30	0/564
48	Ln	0.24	0/300	0.32	0/390
49	Lo	0.16	0/705	0.36	0/940
50	Lp	0.16	0/797	0.28	0/1053
51	S3	0.15	0/1737	0.28	0/2703
52	S4	0.17	0/1757	0.34	0/2735
53	S5	0.18	0/207	0.32	0/319
54	SA	0.29	0/1922	0.40	0/2582
55	SB	0.14	0/1689	0.29	0/2285
56	SC	0.10	0/1674	0.21	0/2240
57	SD	0.12	0/1536	0.24	0/2059
58	SE	0.12	0/2092	0.26	0/2819
59	SF	0.14	0/1744	0.26	0/2362
60	SG	0.14	0/1851	0.28	0/2474
61	SH	0.12	0/1469	0.25	0/1970
62	SI	0.12	0/1679	0.25	0/2255
63	SJ	0.12	0/1038	0.23	0/1391
64	SK	0.12	0/1569	0.25	0/2103
65	SL	0.15	0/1161	0.26	0/1559
66	SM	0.12	0/802	0.23	0/1088
67	SN	0.60	2/837 (0.2%)	0.86	4/1134 (0.4%)
68	SO	0.35	0/1039	0.51	0/1395
69	SP	0.13	0/1120	0.26	0/1500
70	SQ	0.13	0/663	0.37	0/900
71	SR	0.12	0/1095	0.24	0/1468
72	SS	0.12	0/456	0.25	0/605
73	ST	0.16	0/1190	0.29	0/1594
74	SU	0.14	0/1188	0.27	0/1594
75	SV	0.10	0/1002	0.21	0/1334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	SW	0.14	0/948	0.31	0/1275
77	SX	0.13	0/1237	0.26	0/1661
78	SY	0.21	0/673	0.52	2/913 (0.2%)
79	SZ	0.11	0/1071	0.28	0/1425
80	Sa	0.13	0/652	0.27	0/876
81	Sb	0.20	0/842	0.29	0/1127
82	Sc	0.14	0/688	0.33	0/921
83	Sd	0.11	0/494	0.26	0/663
84	Se	0.16	0/496	0.31	0/658
85	Sf	0.13	0/366	0.30	0/487
86	Sg	0.15	0/2389	0.30	0/3247
87	Sh	0.10	0/783	0.26	0/1053
88	S1	0.17	0/42828	0.25	0/66714
All	All	0.19	5/224972 (0.0%)	0.29	6/330254 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	SN	100	PRO	CG-CD	-15.37	0.98	1.50
2	L2	527	A2M	O3'-P	5.25	1.61	1.56
67	SN	100	PRO	CA-CB	-5.22	1.43	1.53
2	L2	1384	A2M	O3'-P	5.07	1.61	1.56
2	L2	570	A2M	O3'-P	5.02	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	SN	100	PRO	N-CD-CG	-19.66	73.70	103.20
67	SN	100	PRO	CA-CB-CG	-15.52	75.02	104.50
78	SY	46	PRO	CA-N-CD	-11.81	95.46	112.00
67	SN	100	PRO	N-CA-CB	-9.83	92.19	103.00
78	SY	46	PRO	N-CD-CG	-5.47	94.99	103.20
67	SN	100	PRO	CA-N-CD	-5.13	104.82	112.00

There are no chirality outliers.

There are no planarity outliers.

## 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	L1	35924	0	18112	442	0
2	L2	24694	0	12519	290	0
3	L3	3834	0	1944	50	0
4	L4	3937	0	1987	43	0
5	L5	2533	0	1288	43	0
6	L6	1506	0	768	24	0
7	L7	3511	0	1780	38	0
8	L8	2551	0	1293	27	0
9	LA	1962	0	2011	19	0
10	LB	3216	0	3334	30	0
11	LC	2820	0	2926	40	0
12	LD	1387	0	1425	17	0
13	LE	1477	0	1558	20	0
14	LF	1144	0	1209	26	0
15	LG	1903	0	2039	15	0
16	LH	1767	0	1872	15	0
17	LI	1695	0	1764	16	0
18	LJ	1012	0	1057	10	0
19	LK	1336	0	1403	22	0
20	LL	1124	0	1151	17	0
21	LM	1711	0	1791	18	0
22	LN	1634	0	1705	18	0
23	LO	2329	0	2418	30	0
24	LP	1539	0	1648	14	0
25	LQ	1682	0	1801	16	0
26	LR	1455	0	1492	18	0
27	LS	1261	0	1311	13	0
28	LT	1211	0	1247	17	0
29	LU	960	0	987	13	0
30	LV	953	0	1016	8	0
31	LW	967	0	1040	18	0
32	LX	714	0	727	3	0
33	LY	1067	0	1140	19	0
34	LZ	1117	0	1165	13	0
35	La	1032	0	1132	11	0
36	Lb	546	0	575	3	0
37	Lc	1862	0	1959	15	0
38	Ld	720	0	739	7	0
39	Le	1469	0	1599	10	0
40	Lf	1046	0	1106	15	0
41	Lg	1149	0	1203	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	Lh	1029	0	1084	13	0
43	Li	799	0	853	7	0
44	Lj	672	0	684	9	0
45	Lk	595	0	630	6	0
46	Ll	446	0	472	6	0
47	Lm	418	0	449	9	0
48	Ln	296	0	342	7	0
49	Lo	693	0	712	10	0
50	Lp	784	0	841	12	0
51	S3	1556	0	794	19	0
52	S4	1574	0	801	41	0
53	S5	187	0	97	3	0
54	SA	1898	0	1987	24	0
55	SB	1655	0	1678	31	0
56	SC	1646	0	1716	16	0
57	SD	1508	0	1582	26	0
58	SE	2054	0	2148	17	0
59	SF	1708	0	1754	17	0
60	SG	1829	0	1942	37	0
61	SH	1447	0	1480	17	0
62	SI	1649	0	1752	22	0
63	SJ	1021	0	1050	5	0
64	SK	1546	0	1618	21	0
65	SL	1140	0	1197	10	0
66	SM	792	0	835	10	0
67	SN	813	0	802	12	0
68	SO	1024	0	1052	15	0
69	SP	1100	0	1146	12	0
70	SQ	662	0	597	20	0
71	SR	1077	0	1132	12	0
72	SS	450	0	455	6	0
73	ST	1167	0	1243	21	0
74	SU	1165	0	1209	10	0
75	SV	992	0	1065	13	0
76	SW	928	0	955	16	0
77	SX	1206	0	1231	17	0
78	SY	663	0	658	10	0
79	SZ	1051	0	1130	18	0
80	Sa	645	0	681	7	0
81	Sb	825	0	861	10	0
82	Sc	674	0	674	21	0
83	Sd	492	0	505	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Se	487	0	542	7	0
85	Sf	359	0	362	9	0
86	Sg	2331	0	2242	52	0
87	Sh	768	0	780	17	0
88	S1	39229	0	19821	289	0
89	L1	9	0	0	0	0
89	L2	4	0	0	0	0
89	L4	3	0	0	0	0
89	LA	2	0	0	0	0
89	LN	1	0	0	0	0
89	S1	7	0	0	0	0
89	S5	1	0	0	0	0
89	SO	1	0	0	0	0
90	L1	9	0	0	0	0
90	L2	7	0	0	0	0
90	L4	1	0	0	0	0
90	S1	7	0	0	0	0
90	SL	1	0	0	0	0
91	L1	187	0	0	0	0
91	L2	96	0	0	0	0
91	L3	1	0	0	0	0
91	L4	2	0	0	0	0
91	L7	5	0	0	0	0
91	L8	3	0	0	0	0
91	LB	1	0	0	0	0
91	LG	1	0	0	0	0
91	LJ	1	0	0	0	0
91	LM	1	0	0	0	0
91	LN	1	0	0	0	0
91	LS	1	0	0	0	0
91	LT	2	0	0	0	0
91	LV	1	0	0	0	0
91	Lf	1	0	0	0	0
91	Lh	2	0	0	0	0
91	Ln	1	0	0	0	0
91	S1	127	0	0	0	0
91	S3	1	0	0	0	0
91	SG	1	0	0	0	0
91	SW	1	0	0	0	0
92	L2	21	0	0	0	0
93	Lj	1	0	0	0	0
93	Lm	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	Lo	1	0	0	0	0
93	Lp	1	0	0	0	0
93	SS	1	0	0	0	0
94	L1	280	0	0	1	0
94	L2	365	0	0	1	0
94	L3	12	0	0	0	0
94	L4	12	0	0	0	0
94	L5	11	0	0	0	0
94	L6	2	0	0	0	0
94	L7	6	0	0	0	0
94	L8	3	0	0	0	0
94	LA	18	0	0	0	0
94	LB	13	0	0	0	0
94	LC	11	0	0	0	0
94	LH	2	0	0	0	0
94	LI	3	0	0	1	0
94	LJ	2	0	0	0	0
94	LL	3	0	0	0	0
94	LM	10	0	0	0	0
94	LN	1	0	0	0	0
94	LO	1	0	0	1	0
94	LQ	3	0	0	0	0
94	LR	1	0	0	0	0
94	LS	2	0	0	0	0
94	LT	5	0	0	0	0
94	LZ	1	0	0	0	0
94	Lb	1	0	0	0	0
94	Lc	4	0	0	0	0
94	Le	1	0	0	0	0
94	Lf	3	0	0	1	0
94	Lg	1	0	0	0	0
94	Lh	2	0	0	0	0
94	Lj	6	0	0	0	0
94	Ll	2	0	0	0	0
94	Ln	8	0	0	0	0
94	Lo	4	0	0	0	0
94	Lp	8	0	0	0	0
94	S1	425	0	0	0	0
94	S3	10	0	0	0	0
94	S4	5	0	0	0	0
94	S5	3	0	0	0	0
94	SF	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	SH	1	0	0	0	0
94	SI	1	0	0	0	0
94	SK	4	0	0	0	0
94	SL	5	0	0	0	0
94	SM	5	0	0	0	0
94	SO	3	0	0	0	0
94	SP	1	0	0	0	0
94	SS	1	0	0	0	0
94	ST	6	0	0	0	0
94	SU	1	0	0	0	0
94	SX	2	0	0	0	0
94	Sb	9	0	0	0	0
94	Sc	1	0	0	0	0
All	All	214618	0	156882	2063	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 6.

All (2063) 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)
78:SY:79:ASP:OD2	88:S1:1358:A:N6	1.99	0.95
1:L1:1683:C:H3'	1:L1:1684:G:H21	1.30	0.95
42:Lh:21:MET:HG3	42:Lh:33:MET:HE3	1.50	0.92
2:L2:1510:A:H61	10:LB:327:ASP:H	1.21	0.86
17:LI:67:THR:HG21	20:LL:66:ASN:HB3	1.58	0.86
1:L1:32:A:N7	1:L1:48:OMU:H5	1.90	0.85
17:LI:67:THR:HG22	17:LI:69:ARG:H	1.42	0.84
1:L1:696:A:H2'	1:L1:697:A2M:H8	1.59	0.84
88:S1:1659:U:H3	88:S1:1670:G:H22	1.24	0.83
61:SH:113:ARG:HE	61:SH:120:VAL:HG23	1.44	0.82
88:S1:1224:A:H62	88:S1:1271:C:H5	1.25	0.81
23:LO:224:ASN:O	23:LO:224:ASN:ND2	2.14	0.80
21:LM:17:ASP:OD1	21:LM:20:ARG:NH2	2.15	0.79
2:L2:695:G:H2'	2:L2:696:A:C8	2.18	0.79
51:S3:10:G:O6	51:S3:45:G:N2	2.17	0.78
13:LE:155:ARG:HA	13:LE:158:ALA:HB3	1.65	0.77
75:SV:48:ASN:HB3	88:S1:1788:U:H5'	1.64	0.77
5:L5:65:U:H3	5:L5:93:G:H1	1.32	0.77
58:SE:117:GLN:HG2	58:SE:162:LYS:HD3	1.67	0.77
1:L1:889:G:H21	3:L3:124:U:H5'	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SJ:2:THR:N	88:S1:1281:C:HO2'	1.83	0.76
1:L1:1588:G:O2'	1:L1:1590:G:OP2	2.04	0.76
1:L1:1253:OMU:H5	16:LH:71:LYS:HG2	1.68	0.76
88:S1:694:U:H3	88:S1:751:G:H1	1.30	0.76
4:L4:24:A:H5''	16:LH:7:LYS:HB2	1.67	0.76
1:L1:554:A:H5''	1:L1:555:U:H5	1.51	0.75
2:L2:569:G:O2'	2:L2:571:G:OP2	2.04	0.75
3:L3:176:U:OP1	29:LU:114:LYS:NZ	2.20	0.75
1:L1:1182:C:O2	1:L1:1190:OMG:N2	2.16	0.75
2:L2:1170:U:H2'	2:L2:1171:G:H8	1.52	0.74
60:SG:32:ARG:NH1	88:S1:2101:C:OP2	2.18	0.74
74:SU:87:ARG:NH2	74:SU:137:GLU:OE2	2.20	0.74
22:LN:208:MET:HE2	22:LN:208:MET:HA	1.69	0.74
1:L1:700:A:N1	1:L1:845:OMU:H5	2.02	0.74
2:L2:1078:OMG:N2	2:L2:1236:C:O2	2.13	0.73
52:S4:51:U:H3	52:S4:63:G:H1	1.35	0.73
4:L4:181:C:H4'	5:L5:3:U:H5	1.54	0.73
10:LB:224:SER:HB3	10:LB:343:MET:HG2	1.70	0.73
2:L2:683:G:H1	2:L2:756:C:H5	1.36	0.72
2:L2:1335:C:H5''	47:Lm:125:LYS:HG3	1.70	0.72
1:L1:594:G:H1	1:L1:613:C:H5	1.36	0.72
88:S1:1369:U:H3	88:S1:1401:G:H1	1.38	0.72
8:L8:67:C:N4	22:LN:210:ASN:O	2.20	0.72
79:SZ:5:LYS:NZ	88:S1:582:U:OP2	2.20	0.72
2:L2:590:U:H2'	2:L2:591:A2M:H8	1.71	0.71
86:Sg:255:GLU:OE2	86:Sg:255:GLU:N	2.17	0.71
88:S1:1114:G:H1	88:S1:1207:U:H3	1.37	0.71
3:L3:119:C:N4	3:L3:125:U:O4	2.20	0.71
34:LZ:113:ARG:NH1	40:Lf:87:VAL:O	2.24	0.71
13:LE:154:SER:O	13:LE:155:ARG:HG3	1.89	0.71
52:S4:16:U:H2'	52:S4:17:C:H4'	1.72	0.71
59:SF:92:MET:HE2	59:SF:137:ILE:HG12	1.72	0.71
83:Sd:69:GLU:OE2	83:Sd:69:GLU:N	2.24	0.71
86:Sg:147:ASP:O	86:Sg:177:LYS:NZ	2.23	0.71
59:SF:92:MET:HE1	59:SF:112:ALA:HB1	1.73	0.70
66:SM:48:HIS:HB2	66:SM:87:ASP:HB2	1.72	0.70
1:L1:954:U:H2'	1:L1:955:A2M:H8	1.72	0.70
77:SX:95:LYS:HD2	77:SX:103:GLU:HG3	1.73	0.70
1:L1:1540:OMG:N2	2:L2:600:C:O2	2.14	0.70
79:SZ:34:HIS:HB2	79:SZ:37:TRP:HB2	1.72	0.70
2:L2:974:G:O6	42:Lh:102:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1510:A:N6	10:LB:327:ASP:H	1.89	0.70
2:L2:984:G:H1	2:L2:1000:U:H3	1.37	0.70
88:S1:1980:U:H4'	88:S1:2019:C:H4'	1.74	0.70
52:S4:27:G:H1	52:S4:43:C:H42	1.39	0.69
88:S1:2136:A:O2'	88:S1:2137:U:O2	2.09	0.69
87:Sh:210:GLU:OE1	87:Sh:210:GLU:N	2.22	0.69
12:LD:49:LEU:HD23	12:LD:66:LYS:HD2	1.74	0.69
64:SK:160:ARG:HD2	64:SK:164:ARG:HH22	1.57	0.69
88:S1:2059:OMC:H5	88:S1:2166:A:H61	1.40	0.69
21:LM:15:SER:O	21:LM:20:ARG:NH1	2.26	0.69
60:SG:183:ILE:HD13	88:S1:146:U:H4'	1.75	0.69
1:L1:604:C:O2'	1:L1:605:G:O4'	2.11	0.68
2:L2:502[B]:A:H2	88:S1:2159:A:H3'	1.59	0.68
82:Sc:17:ARG:NH2	88:S1:1362:A:OP1	2.25	0.68
1:L1:415:A:H4'	1:L1:416:A:H5'	1.75	0.68
6:L6:67:C:OP1	41:Lg:96:ARG:NH2	2.27	0.68
15:LG:113:VAL:HG11	15:LG:127:THR:HG22	1.76	0.68
3:L3:45:U:OP1	42:Lh:25:ARG:NH2	2.26	0.68
15:LG:135:THR:HG21	15:LG:191:ILE:HD13	1.74	0.68
54:SA:8:ARG:HE	54:SA:11:LYS:HB2	1.57	0.68
88:S1:484:G:H1	88:S1:511:C:H5	1.39	0.68
82:Sc:60:CYS:HB3	82:Sc:62:LYS:HE3	1.76	0.68
2:L2:454:A:N6	2:L2:477:G:OP1	2.27	0.68
13:LE:121:ARG:HB3	13:LE:163:MET:HE3	1.76	0.68
1:L1:12:U:H2'	1:L1:13:G:H8	1.59	0.67
1:L1:1683:C:H3'	1:L1:1684:G:N2	2.06	0.67
48:Ln:25:ARG:NH2	88:S1:2152:A:OP1	2.27	0.67
79:SZ:106:ALA:O	88:S1:503:C:N4	2.24	0.67
88:S1:1767:G:N2	88:S1:1767:G:OP1	2.27	0.67
88:S1:309:G:O2'	88:S1:311:G:OP2	2.11	0.67
1:L1:1147:A:O2'	1:L1:1150:A:N1	2.27	0.67
27:LS:68:THR:HG22	27:LS:71:GLY:H	1.59	0.67
57:SD:125:ARG:HD2	84:Se:33:ARG:HD3	1.76	0.67
5:L5:123:G:O6	39:Le:70:ARG:NH2	2.28	0.67
27:LS:49:ARG:HA	27:LS:52:MET:HE2	1.75	0.67
1:L1:1352:C:H2'	1:L1:1353:A:C8	2.29	0.66
1:L1:1685:G:H22	1:L1:1707:U:H3	1.42	0.66
54:SA:10:SER:OG	88:S1:1160:A:OP1	2.13	0.66
1:L1:352:G:OP2	43:Li:25:ARG:NH2	2.27	0.66
21:LM:120:TRP:HE1	21:LM:123:MET:HG3	1.58	0.66
1:L1:1363:A:H4'	1:L1:1364:A:H5''	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1170:U:H2'	2:L2:1171:G:C8	2.30	0.66
4:L4:74:OMG:N2	4:L4:123:C:O2	2.20	0.66
86:Sg:12:GLY:H	86:Sg:35:ASP:HB3	1.60	0.66
14:LF:25:GLU:OE2	14:LF:25:GLU:N	2.29	0.66
14:LF:194:ASN:O	19:LK:110:ARG:NH2	2.28	0.66
22:LN:102:MET:HA	22:LN:102:MET:HE3	1.77	0.66
1:L1:1674:A:H2	1:L1:1726:G:H21	1.44	0.66
1:L1:1489:U:H2'	1:L1:1490:G:C8	2.31	0.66
64:SK:24:ARG:NH1	88:S1:435:G:OP1	2.28	0.66
76:SW:117:GLU:OE2	76:SW:117:GLU:N	2.27	0.65
86:Sg:150:GLU:OE1	86:Sg:150:GLU:N	2.29	0.65
20:LL:39:HIS:O	20:LL:40:HIS:ND1	2.28	0.65
62:SI:100:ARG:NH2	62:SI:131:ASP:OD2	2.30	0.65
5:L5:51:A:H1'	5:L5:52:U:H5''	1.77	0.65
1:L1:133:C:OP2	35:La:77:ARG:NH2	2.25	0.65
73:ST:142:GLU:OE1	73:ST:142:GLU:N	2.30	0.65
81:Sb:78:CYS:SG	81:Sb:81:CYS:N	2.67	0.65
1:L1:694:U:H2'	1:L1:695:OMC:C6	2.32	0.65
2:L2:1398:C:H2'	2:L2:1399:G:C8	2.31	0.65
82:Sc:41:CYS:O	82:Sc:43:GLN:NE2	2.29	0.65
1:L1:472:U:H2'	1:L1:473:A:C8	2.32	0.64
4:L4:4:G:H1	4:L4:20:U:H3	1.44	0.64
64:SK:57:ALA:HB2	64:SK:196:GLY:HA2	1.79	0.64
65:SL:99:PHE:HB3	65:SL:108:LYS:HB2	1.80	0.64
78:SY:8:ASN:N	78:SY:8:ASN:OD1	2.28	0.64
1:L1:368:G:OP2	11:LC:55:ARG:NH1	2.30	0.64
19:LK:43:ASP:HB3	19:LK:46:MET:HB2	1.78	0.64
31:LW:52:GLU:HB2	31:LW:105:LYS:HB3	1.78	0.64
60:SG:160:VAL:HG21	60:SG:179:ILE:HD11	1.79	0.64
62:SI:162:ARG:NH1	62:SI:166:GLU:OE2	2.30	0.64
88:S1:2098:G:H21	88:S1:2125:A:H2	1.43	0.64
73:ST:3:ARG:HB2	88:S1:1112:A:H5''	1.80	0.64
88:S1:695:G:H1	88:S1:750:U:H3	1.43	0.64
48:Ln:3:THR:HG22	88:S1:1273:A:H61	1.62	0.64
1:L1:1281:A:O2'	1:L1:1348:A:N6	2.29	0.64
2:L2:1407:A:N7	9:LA:215:ASN:ND2	2.45	0.64
1:L1:846:G:H2'	1:L1:847:OMU:H6	1.78	0.64
1:L1:687:C:H2'	1:L1:688:A:H8	1.61	0.64
56:SC:161:THR:HG23	88:S1:1820:G:H21	1.62	0.64
5:L5:64:G:OP2	5:L5:64:G:N2	2.28	0.63
2:L2:1282:C:H5	2:L2:1336:G:H22	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Sb:86:ARG:HG3	81:Sb:86:ARG:HH11	1.63	0.63
1:L1:1680:U:H2'	1:L1:1681:G:H8	1.62	0.63
5:L5:65:U:O2	5:L5:93:G:N2	2.24	0.63
8:L8:96:G:H2'	8:L8:97:A:C8	2.34	0.63
1:L1:454:U:H2'	1:L1:455:G:C8	2.34	0.63
1:L1:475:C:OP1	41:Lg:83:LYS:NZ	2.28	0.63
2:L2:1012:U:OP1	15:LG:49[B]:ARG:NH1	2.30	0.63
7:L7:93:C:O2'	7:L7:94:G:OP1	2.14	0.63
1:L1:179:G:H2'	1:L1:180:A:C8	2.33	0.63
1:L1:1176:C:H2'	1:L1:1177:PSU:H6	1.63	0.63
35:La:92:THR:HG22	35:La:95:ARG:H	1.62	0.63
58:SE:173:ARG:NH2	88:S1:789:G:OP2	2.31	0.63
2:L2:1124:A:H2'	2:L2:1125:G:C8	2.33	0.63
33:LY:97:ILE:HG22	33:LY:111:LEU:HD23	1.81	0.63
1:L1:795:U:OP1	11:LC:301:LYS:NZ	2.28	0.63
88:S1:814:G:N2	88:S1:819:G:O2'	2.32	0.63
61:SH:45:ARG:NH1	61:SH:45:ARG:HB2	2.14	0.63
33:LY:26:VAL:HG11	33:LY:97:ILE:HD11	1.81	0.62
60:SG:60:ASP:OD2	60:SG:73:ARG:NH2	2.32	0.62
79:SZ:19:VAL:HG22	79:SZ:26:LYS:HG2	1.81	0.62
1:L1:1684:G:H2'	1:L1:1685:G:C8	2.33	0.62
31:LW:35:GLU:OE2	31:LW:35:GLU:N	2.25	0.62
49:Lo:81:SER:HA	49:Lo:84:ARG:HH12	1.63	0.62
68:SO:136:LYS:NZ	88:S1:1256:U:OP2	2.33	0.62
50:Lp:17:CYS:SG	50:Lp:21:LYS:NZ	2.70	0.62
77:SX:55:GLY:HA2	77:SX:96:LYS:HD2	1.81	0.62
86:Sg:116:SER:OG	86:Sg:118:ASP:OD1	2.16	0.62
1:L1:141:U:H1'	1:L1:142:G:H5''	1.80	0.62
33:LY:97:ILE:HB	33:LY:108:SER:HB3	1.80	0.62
62:SI:106:PRO:HD2	62:SI:112:LEU:HD12	1.82	0.62
2:L2:5:A:H2'	2:L2:6:A:C8	2.35	0.62
23:LO:22:ARG:NH2	94:LO:401:HOH:O	2.31	0.62
88:S1:787:G:H8	88:S1:833:G:H1	1.45	0.62
1:L1:1680:U:H2'	1:L1:1681:G:C8	2.35	0.62
69:SP:32:THR:HG22	69:SP:34:SER:H	1.64	0.62
1:L1:1667:G:OP2	21:LM:34:HIS:NE2	2.32	0.62
8:L8:74:A:H61	8:L8:109:U:H3	1.46	0.62
52:S4:39:U:H2'	52:S4:40:C:C6	2.35	0.62
76:SW:115:LYS:H	76:SW:118:MET:HE2	1.64	0.62
2:L2:528:U:OP1	2:L2:1411:G:O2'	2.17	0.61
12:LD:26:GLY:HA2	12:LD:67:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:353:C:OP2	17:LI:107:LYS:NZ	2.33	0.61
1:L1:700:A:H2'	1:L1:701:G:C8	2.35	0.61
1:L1:1242:U:OP1	19:LK:17:ARG:NH2	2.32	0.61
2:L2:354:A:O2'	64:SK:89:GLU:OE1	2.17	0.61
2:L2:558:A:OP1	2:L2:560:OMU:H5	2.00	0.61
60:SG:155:ASP:OD2	60:SG:157:ARG:N	2.33	0.61
64:SK:76:VAL:HG12	64:SK:108:PRO:HG2	1.82	0.61
73:ST:16:LEU:HD12	88:S1:1108:A:H5''	1.83	0.61
77:SX:26:ARG:HH21	88:S1:1716:A:H61	1.47	0.61
1:L1:1687:G:H22	1:L1:1705:G:H1	1.46	0.61
38:Ld:43:LEU:HD22	38:Ld:102:ILE:HG21	1.83	0.61
62:SI:183:ARG:NH1	88:S1:747:C:OP1	2.33	0.61
1:L1:1287:A:OP2	1:L1:1347:G:N2	2.33	0.61
3:L3:204:A:H2'	3:L3:205:A:C8	2.34	0.61
40:Lf:10:ILE:HD13	40:Lf:64:THR:HB	1.83	0.61
1:L1:219:U:H5''	1:L1:220:A:H5'	1.81	0.61
1:L1:253:G:OP1	31:LW:13:ARG:NH1	2.31	0.61
2:L2:406:G:H2'	2:L2:407:C:C6	2.36	0.61
7:L7:93:C:H2'	7:L7:94:G:H5''	1.82	0.61
1:L1:1597:G:O6	46:LI:2:GLY:N	2.33	0.61
22:LN:38:ARG:NH1	22:LN:45:GLU:OE1	2.25	0.61
1:L1:494:A:OP1	14:LF:82:ARG:NE	2.32	0.61
3:L3:5:A:OP1	33:LY:64:ARG:NH2	2.33	0.61
2:L2:823:A:HO2'	2:L2:824:G:N2	1.99	0.61
2:L2:1339:G:O2'	4:L4:52:A:N1	2.34	0.60
1:L1:1571:C:H5	28:LT:85:ARG:HH21	1.47	0.60
2:L2:1335:C:H2'	2:L2:1337:C:H5'	1.83	0.60
8:L8:65:C:H5''	23:LO:283:LEU:HD12	1.83	0.60
29:LU:15:ARG:NH2	29:LU:16:GLN:O	2.34	0.60
1:L1:662:C:H2'	1:L1:663:C:C6	2.36	0.60
2:L2:1052:C:O2'	2:L2:1053:A:O5'	2.16	0.60
25:LQ:31:GLU:OE1	25:LQ:31:GLU:N	2.31	0.60
60:SG:32:ARG:HH12	88:S1:2101:C:P	2.23	0.60
88:S1:672:G:N1	88:S1:1217:A:OP1	2.26	0.60
1:L1:198:A:OP2	34:LZ:139:ARG:NH2	2.35	0.60
1:L1:687:C:H2'	1:L1:688:A:C8	2.37	0.60
1:L1:843:C:H2'	1:L1:844:C:C6	2.36	0.60
25:LQ:181:ARG:NH2	88:S1:972:A:OP1	2.32	0.60
86:Sg:229:LEU:HB3	86:Sg:230:PHE:HD1	1.66	0.60
1:L1:179:G:H2'	1:L1:180:A:H8	1.65	0.60
1:L1:1243:G:OP2	26:LR:2:VAL:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1292:G:H1	1:L1:1343:A:N6	2.00	0.60
66:SM:49:GLY:HA3	88:S1:1695:C:H5''	1.84	0.60
73:ST:55:ARG:HD3	88:S1:1207:U:H5'	1.83	0.60
4:L4:150:A:O2'	4:L4:151:A:H5'	2.01	0.60
23:LO:55:ILE:HG21	23:LO:164:ARG:HH21	1.66	0.60
74:SU:31:GLU:H	74:SU:31:GLU:CD	2.09	0.60
87:Sh:169:ARG:HB2	88:S1:263:G:H5'	1.84	0.60
1:L1:696:A:H2'	1:L1:697:A2M:C8	2.29	0.60
88:S1:788:A:H61	88:S1:832:C:H41	1.50	0.60
88:S1:876:G:H1	88:S1:885:C:H5	1.50	0.60
2:L2:1485:G:OP1	41:Lg:15:HIS:NE2	2.34	0.60
73:ST:36:MET:HE1	73:ST:58:MET:HG3	1.83	0.60
54:SA:118:LYS:HB2	88:S1:2202:PSU:H2'	1.84	0.60
1:L1:904:G:N7	49:Lo:2:ALA:N	2.50	0.59
9:LA:234:LYS:HG2	9:LA:238:ILE:HG12	1.84	0.59
15:LG:69:ARG:NH1	15:LG:238:GLN:O	2.35	0.59
25:LQ:189:ARG:HG2	25:LQ:190:ARG:HH12	1.68	0.59
73:ST:40:SER:HB3	73:ST:45:MET:HE3	1.83	0.59
88:S1:594:A:H61	88:S1:643:A:H5''	1.67	0.59
1:L1:165:U:H3	1:L1:290:G:H1	1.48	0.59
2:L2:823:A:O2'	2:L2:824:G:N2	2.35	0.59
2:L2:1136:U:H2'	2:L2:1137:G:C8	2.36	0.59
14:LF:42:LEU:HD11	14:LF:85:ILE:HG13	1.83	0.59
31:LW:80:ASP:OD1	31:LW:81:LYS:N	2.35	0.59
38:Ld:97:VAL:O	38:Ld:100:SER:OG	2.20	0.59
64:SK:207:GLU:HG3	74:SU:23:TYR:CD2	2.38	0.59
76:SW:41:LYS:HG2	76:SW:49:ARG:HG3	1.83	0.59
87:Sh:222:VAL:HA	87:Sh:225:ALA:HB3	1.85	0.59
1:L1:662:C:H2'	1:L1:663:C:H6	1.65	0.59
2:L2:652:C:H2'	2:L2:653:C:C6	2.38	0.59
3:L3:174:C:H2'	3:L3:175:A:N3	2.17	0.59
52:S4:23:A:H2'	52:S4:24:G:H8	1.66	0.59
68:SO:127:PRO:HB3	88:S1:1134:A:H5''	1.85	0.59
1:L1:1342:C:H2'	1:L1:1343:A:C8	2.37	0.59
43:Li:8:THR:HG23	43:Li:15:ASN:HB2	1.85	0.59
60:SG:134:ARG:NE	88:S1:171:C:OP1	2.26	0.59
2:L2:91:C:O2	10:LB:245:ARG:NH2	2.33	0.59
2:L2:560:OMU:H4'	2:L2:561:G:OP2	2.01	0.59
85:Sf:99:LYS:HA	85:Sf:99:LYS:HE3	1.84	0.59
2:L2:958:A:H2'	2:L2:959:A:H8	1.66	0.59
6:L6:49:C:N4	41:Lg:29:LYS:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SR:88:GLN:HA	71:SR:96:THR:HG23	1.84	0.59
1:L1:1773:C:O2'	7:L7:139:A:N3	2.32	0.59
70:SQ:87:ASP:OD1	70:SQ:87:ASP:N	2.31	0.59
88:S1:128:C:H4'	88:S1:129:U:O5'	2.01	0.59
1:L1:73:U:H5''	17:LI:63:VAL:HB	1.85	0.59
58:SE:150:HIS:O	58:SE:171:LYS:NZ	2.35	0.59
1:L1:945:U:OP1	94:L1:2101:HOH:O	2.16	0.59
2:L2:1398:C:H2'	2:L2:1399:G:H8	1.67	0.59
34:LZ:30:ASP:HB3	34:LZ:33:ASN:HB2	1.85	0.59
1:L1:1352:C:H2'	1:L1:1353:A:H8	1.67	0.58
56:SC:61:ASN:O	56:SC:66:ARG:NH2	2.36	0.58
57:SD:21:GLU:CD	57:SD:21:GLU:H	2.11	0.58
59:SF:182:VAL:HB	59:SF:209:TYR:HB2	1.85	0.58
73:ST:25:TRP:CD2	82:Sc:83:LYS:HE3	2.38	0.58
29:LU:40:SER:OG	29:LU:42:ASP:OD1	2.20	0.58
1:L1:326:A:H2'	1:L1:327:G:C8	2.38	0.58
1:L1:1017:PSU:OP1	20:LL:44:ASN:ND2	2.36	0.58
1:L1:1764:A:OP2	45:Lk:21:ARG:NH2	2.35	0.58
2:L2:619:A:N3	2:L2:1262:G:O2'	2.27	0.58
1:L1:699:C:H2'	1:L1:700:A:C8	2.38	0.58
38:Ld:50:CYS:O	38:Ld:55:ARG:NH2	2.37	0.58
53:S5:8:U:O2	88:S1:2159:A:C8	2.57	0.58
57:SD:1:MET:N	88:S1:40:A:OP1	2.33	0.58
73:ST:2:VAL:HG23	73:ST:3:ARG:H	1.69	0.58
88:S1:761:A:H62	88:S1:768:A:H61	1.50	0.58
24:LP:165:PRO:HB3	24:LP:193:LYS:HB2	1.84	0.58
60:SG:217:ALA:HB1	88:S1:286:G:H1'	1.86	0.58
1:L1:1602:C:H2'	1:L1:1603:G:C8	2.39	0.58
88:S1:1397:A:O2'	88:S1:1399:G:OP2	2.17	0.58
48:Ln:3:THR:CG2	88:S1:1273:A:H61	2.17	0.58
65:SL:56:GLU:OE1	65:SL:88:ARG:NH1	2.37	0.58
70:SQ:37:SER:HB3	70:SQ:123:ILE:HG23	1.86	0.58
88:S1:276:G:H4'	88:S1:277:U:OP1	2.04	0.58
2:L2:1024:U:H2'	2:L2:1025:G:C8	2.39	0.58
17:LI:28:LYS:NZ	94:LI:301:HOH:O	2.36	0.58
76:SW:68:ARG:NH1	76:SW:95:GLU:OE2	2.29	0.58
1:L1:1239:U:OP1	16:LH:141:ARG:NH1	2.37	0.58
1:L1:1265:A:H2'	1:L1:1266:A:C8	2.37	0.57
1:L1:1276:U:H5	1:L1:1353:A:N1	2.02	0.57
2:L2:975:A:OP1	42:Lh:91:ARG:NH2	2.35	0.57
71:SR:90:ASP:OD2	71:SR:107:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Sg:14:VAL:HG21	86:Sg:303:ILE:HG13	1.85	0.57
88:S1:972:A:H61	88:S1:1100:U:H2'	1.69	0.57
1:L1:699:C:H2'	1:L1:700:A:H8	1.70	0.57
2:L2:690:C:H2'	2:L2:691:A:H8	1.69	0.57
2:L2:974:G:O2'	2:L2:975:A:H8	1.87	0.57
16:LH:85:THR:O	16:LH:86:LYS:HG2	2.04	0.57
4:L4:181:C:H4'	5:L5:3:U:C5	2.38	0.57
29:LU:46:ASN:HA	29:LU:49:GLN:HB3	1.86	0.57
52:S4:17:C:H3'	52:S4:18:G:C2	2.40	0.57
1:L1:790:C:H41	11:LC:304:LYS:HB3	1.69	0.57
84:Se:29:GLN:HG3	84:Se:30:PRO:HD2	1.86	0.57
1:L1:1018:A:N3	27:LS:81:ARG:NH2	2.52	0.57
55:SB:109:GLY:N	55:SB:139:GLU:OE2	2.28	0.57
61:SH:45:ARG:HB2	61:SH:45:ARG:HH11	1.70	0.57
88:S1:1695:C:H5	88:S1:1780:C:H42	1.51	0.57
5:L5:38:U:H5''	10:LB:315:MET:HE2	1.86	0.57
1:L1:1255:G:H2'	1:L1:1256:A:C8	2.40	0.57
2:L2:1321:U:H2'	2:L2:1322:C:H6	1.68	0.57
64:SK:37:ARG:NE	64:SK:93:THR:O	2.35	0.57
1:L1:1090:U:H2'	1:L1:1091:A:C8	2.40	0.57
51:S3:47:U:O2'	51:S3:48:C:O5'	2.21	0.57
67:SN:84:ARG:NH1	67:SN:93:ALA:O	2.29	0.57
1:L1:29:C:H4'	21:LM:96:LYS:HE2	1.87	0.56
1:L1:1250:U:OP2	16:LH:67:ARG:NH1	2.37	0.56
64:SK:81:VAL:HG13	64:SK:94:LYS:HD3	1.87	0.56
1:L1:592:G:H2'	1:L1:593:C:C6	2.40	0.56
1:L1:1549:U:H2'	1:L1:1550:A:C8	2.39	0.56
1:L1:1775:U:H2'	1:L1:1776:G:C8	2.41	0.56
5:L5:6:G:H2'	5:L5:7:U:C6	2.41	0.56
88:S1:1896:G:H1	88:S1:1905:C:H5	1.52	0.56
1:L1:1654:A:OP1	21:LM:108:LYS:NZ	2.28	0.56
2:L2:653:C:H2'	2:L2:654:U:H6	1.70	0.56
2:L2:1383:G:O2'	2:L2:1386:C:OP2	2.23	0.56
71:SR:63:GLU:OE2	71:SR:63:GLU:N	2.29	0.56
73:ST:21:THR:OG1	82:Sc:86:HIS:NE2	2.33	0.56
86:Sg:246:ASN:OD1	86:Sg:247:ARG:N	2.38	0.56
88:S1:815:U:O2'	88:S1:817:A:OP2	2.21	0.56
3:L3:203:A:H2'	3:L3:204:A:C8	2.40	0.56
4:L4:73:U:OP1	10:LB:19:ARG:NH2	2.38	0.56
61:SH:39:SER:O	65:SL:128:ARG:NH2	2.38	0.56
86:Sg:4:GLU:O	86:Sg:47:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1522:U:H2'	2:L2:1523:C:C6	2.40	0.56
54:SA:125:THR:HG23	54:SA:167:ARG:HG3	1.87	0.56
2:L2:1087:C:H2'	2:L2:1088:G:H8	1.71	0.56
3:L3:99:U:H2'	3:L3:100:U:C6	2.41	0.56
4:L4:92:U:H2'	4:L4:93:U:C6	2.40	0.56
60:SG:173:ARG:NH2	88:S1:71:G:N7	2.52	0.56
61:SH:190:ARG:O	83:Sd:80:ARG:NH1	2.38	0.56
88:S1:934:U:H4'	88:S1:936:U:H3	1.71	0.56
2:L2:1157:U:H5	2:L2:1237:A:N1	2.04	0.56
51:S3:49:G:H2'	51:S3:50:U:H6	1.70	0.56
88:S1:809:C:O2'	88:S1:810:G:N7	2.35	0.56
1:L1:1405:U:H2'	1:L1:1406:C:C6	2.41	0.56
2:L2:603:A:H5'	28:LT:137:THR:HG23	1.87	0.56
11:LC:283:THR:H	24:LP:129:THR:HG21	1.71	0.56
26:LR:46:MET:HE3	26:LR:50:LYS:HG3	1.87	0.56
54:SA:211:GLU:OE2	54:SA:213:ARG:NH2	2.33	0.56
71:SR:130:LEU:HD22	88:S1:1860:C:H5'	1.88	0.56
71:SR:63:GLU:H	71:SR:63:GLU:CD	2.13	0.56
2:L2:996:C:H2'	2:L2:997:A:C8	2.41	0.55
2:L2:1151:U:H5	2:L2:1161:A:N1	2.04	0.55
5:L5:62:C:H3'	5:L5:63:G:N2	2.21	0.55
62:SI:75:ARG:HH12	62:SI:131:ASP:HA	1.70	0.55
2:L2:652:C:H2'	2:L2:653:C:H6	1.70	0.55
2:L2:1114:G:OP1	23:LO:8:LYS:NZ	2.37	0.55
2:L2:1262:G:H2'	2:L2:1263:C:H6	1.70	0.55
56:SC:105:ARG:NH1	56:SC:173:HIS:O	2.40	0.55
1:L1:315:U:H2'	1:L1:316:U:C6	2.41	0.55
1:L1:1686:C:H42	1:L1:1706:C:H42	1.54	0.55
2:L2:1365:C:H2'	2:L2:1366:C:C6	2.41	0.55
23:LO:224:ASN:HD22	23:LO:224:ASN:C	2.11	0.55
74:SU:94:LYS:HD3	88:S1:390:G:H5'	1.87	0.55
88:S1:324:U:H4'	88:S1:325:G:C4	2.41	0.55
1:L1:345:U:H2'	1:L1:346:U:C6	2.41	0.55
1:L1:1253:OMU:OP1	1:L1:1253:OMU:H4'	2.06	0.55
11:LC:113:LYS:HG2	21:LM:203:LYS:HB3	1.87	0.55
33:LY:23:ALA:HA	33:LY:45:GLY:HA2	1.87	0.55
37:Lc:96:VAL:HG13	37:Lc:146:TYR:HB3	1.87	0.55
57:SD:87:GLU:OE2	57:SD:87:GLU:N	2.22	0.55
61:SH:83:LEU:HD22	61:SH:94:PRO:HB2	1.89	0.55
1:L1:120:G:H1'	1:L1:122:A:H62	1.71	0.55
2:L2:622:G:H2'	2:L2:623:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L6:36:C:H2'	6:L6:37:C:H6	1.72	0.55
12:LD:109:ASP:N	12:LD:109:ASP:OD1	2.40	0.55
55:SB:77:VAL:HG22	55:SB:124:VAL:HB	1.87	0.55
1:L1:1402:U:H2'	1:L1:1403:A:H8	1.71	0.55
68:SO:96:VAL:HG12	68:SO:132:SER:HB2	1.88	0.55
1:L1:1749:G:H2'	1:L1:1751:A:N7	2.22	0.55
2:L2:958:A:H2'	2:L2:959:A:C8	2.41	0.55
2:L2:1006:G:H2'	2:L2:1007:U:C6	2.42	0.55
33:LY:96:LYS:HZ2	33:LY:111:LEU:HD22	1.72	0.55
55:SB:4:VAL:HG13	55:SB:7:GLY:H	1.72	0.55
60:SG:80:ARG:HG2	60:SG:87:THR:HA	1.89	0.55
61:SH:46:ARG:HD2	88:S1:2035:C:H2'	1.89	0.55
1:L1:700:A:C2	1:L1:845:OMU:H5	2.41	0.55
25:LQ:184:GLU:OE2	62:SI:10:LYS:NZ	2.40	0.55
56:SC:207:ILE:HD11	75:SV:46:LEU:HD13	1.88	0.55
88:S1:1646:G:O2'	88:S1:1673:A:N1	2.36	0.55
1:L1:739:U:H2'	1:L1:740:C:C6	2.42	0.55
1:L1:794:U:O2'	1:L1:795:U:H6	1.90	0.55
1:L1:70:C:H1'	17:LI:66:PRO:O	2.06	0.55
1:L1:1524:OMG:H5''	1:L1:1527:OMC:H5	1.71	0.55
2:L2:690:C:H2'	2:L2:691:A:C8	2.42	0.55
5:L5:128:G:H2'	5:L5:129:G:H8	1.72	0.55
51:S3:49:G:H2'	51:S3:50:U:C6	2.41	0.55
66:SM:77:PHE:HB3	72:SS:53:PHE:HB3	1.88	0.55
88:S1:629:A:O2'	88:S1:631:U:OP1	2.25	0.55
88:S1:2085:A:H2'	88:S1:2086:A:C8	2.42	0.55
1:L1:77:U:H5''	21:LM:186:PRO:HG3	1.88	0.54
2:L2:974:G:H4'	42:Lh:91:ARG:HG2	1.89	0.54
86:Sg:47:ARG:HD2	86:Sg:54:TYR:HA	1.89	0.54
1:L1:1238:C:OP2	26:LR:162:ARG:NH2	2.40	0.54
1:L1:1677:G:H1	1:L1:1715:U:H3	1.55	0.54
2:L2:1496:G:H2'	2:L2:1497:C:C6	2.42	0.54
2:L2:97:A:O2'	2:L2:366:C:O2	2.20	0.54
3:L3:48:C:OP1	25:LQ:60:ARG:NE	2.35	0.54
56:SC:115:ARG:NE	59:SF:132:GLU:OE1	2.35	0.54
79:SZ:112:LYS:O	79:SZ:116:GLU:HG2	2.07	0.54
1:L1:708:A:N7	24:LP:111:ARG:NH2	2.55	0.54
1:L1:1257[B]:U:N3	1:L1:1263:A:OP1	2.39	0.54
1:L1:1728:A:HO2'	1:L1:1729:A:H8	1.54	0.54
3:L3:118:G:H2'	3:L3:119:C:O2	2.07	0.54
5:L5:53:G:H22	5:L5:63:G:H8	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SA:8:ARG:NE	54:SA:11:LYS:HB2	2.22	0.54
1:L1:128:U:H2'	1:L1:129:C:C6	2.42	0.54
1:L1:844:C:H2'	1:L1:845:OMU:O2	2.07	0.54
2:L2:342:U:HO2'	2:L2:343:U:H6	1.52	0.54
2:L2:525:A:N7	2:L2:532:U:H5	2.06	0.54
2:L2:1456:C:H5	2:L2:1468:G:H1	1.55	0.54
55:SB:187:ARG:HD3	55:SB:194:ARG:HG3	1.89	0.54
60:SG:58:ASP:OD1	60:SG:59:LYS:N	2.39	0.54
78:SY:78:ILE:HD11	82:Sc:2:GLY:HA3	1.89	0.54
86:Sg:82:THR:HB	86:Sg:92:TRP:HE1	1.72	0.54
54:SA:24:MET:HG2	68:SO:77:ARG:HH22	1.73	0.54
55:SB:1:MET:N	55:SB:59:GLU:O	2.41	0.54
69:SP:60:LYS:HD2	69:SP:116:PRO:HA	1.90	0.54
86:Sg:81:LEU:HD11	86:Sg:122:ILE:HG12	1.89	0.54
86:Sg:135:ASN:HB2	86:Sg:141:MET:HE1	1.89	0.54
1:L1:160:C:O2'	1:L1:161:A:O5'	2.23	0.54
1:L1:472:U:H2'	1:L1:473:A:H8	1.72	0.54
13:LE:90:LYS:HB2	13:LE:182:THR:HB	1.90	0.54
56:SC:176:MET:HG3	56:SC:181:ILE:HD12	1.89	0.54
88:S1:756:C:H42	88:S1:772:A:H62	1.56	0.54
51:S3:7:G:OP1	51:S3:16:C:N4	2.41	0.54
57:SD:165:ASN:HD22	79:SZ:2:VAL:N	2.05	0.54
1:L1:547:U:HO2'	1:L1:548:G:H8	1.55	0.54
1:L1:1287:A:N6	1:L1:1348:A:H1'	2.23	0.54
2:L2:1089:A:H2'	2:L2:1090:G:C8	2.43	0.54
19:LK:136:PRO:HB3	19:LK:141:LYS:HB3	1.88	0.54
82:Sc:27:GLN:NE2	88:S1:1110:G:OP2	2.38	0.54
86:Sg:13:TRP:HB2	86:Sg:299:LYS:HA	1.90	0.54
88:S1:944:U:H5'	88:S1:945:G:H5''	1.90	0.54
88:S1:1523:A:H2'	88:S1:1524:G:C8	2.43	0.54
1:L1:571:A:OP1	11:LC:312:ARG:NH1	2.39	0.54
1:L1:1176:C:H2'	1:L1:1177:PSU:C6	2.43	0.54
26:LR:70:LYS:O	26:LR:74:ARG:NH2	2.41	0.54
82:Sc:34:MET:HE2	82:Sc:49:SER:HA	1.90	0.54
3:L3:24:U:O2'	3:L3:26:C:OP2	2.25	0.53
7:L7:161:C:H2'	7:L7:162:A2M:H8	1.90	0.53
8:L8:51:U:OP2	23:LO:164:ARG:HD2	2.08	0.53
50:Lp:55:LYS:NZ	52:S4:75:C:O2	2.41	0.53
88:S1:1652:A:H5'	88:S1:1653:U:OP2	2.07	0.53
11:LC:216:THR:HB	11:LC:227:LEU:HD13	1.90	0.53
52:S4:39:U:H2'	52:S4:40:C:H6	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S4:41:C:H4'	61:SH:184:ARG:HD2	1.89	0.53
88:S1:2124:A:H2'	88:S1:2125:A:H5''	1.90	0.53
1:L1:938:G:H2'	1:L1:939:C:C6	2.43	0.53
7:L7:70:C:H5''	31:LW:115:ILE:HD11	1.89	0.53
16:LH:199:SER:OG	19:LK:131:LYS:NZ	2.41	0.53
20:LL:134:ILE:HG21	20:LL:141:VAL:HG23	1.89	0.53
73:ST:133:LYS:HB2	88:S1:916:G:H22	1.74	0.53
1:L1:584:U:O2'	1:L1:585:U:O4'	2.25	0.53
15:LG:101:GLU:OE2	15:LG:109:ARG:NH2	2.41	0.53
1:L1:1292:G:H1	1:L1:1343:A:H61	1.55	0.53
7:L7:32:U:H5''	7:L7:33:U:OP2	2.09	0.53
10:LB:107:ALA:HB1	10:LB:205:GLU:HG3	1.91	0.53
66:SM:46:THR:HB	66:SM:89:HIS:HB2	1.90	0.53
2:L2:1318:PSU:H1'	10:LB:255:ALA:HB3	1.89	0.53
57:SD:107:ARG:HH22	57:SD:125:ARG:HH21	1.55	0.53
59:SF:257:GLU:H	59:SF:257:GLU:CD	2.17	0.53
82:Sc:39:PRO:HG3	82:Sc:78:CYS:HB3	1.90	0.53
2:L2:762:U:H2'	2:L2:763:C:H6	1.74	0.53
16:LH:65:GLU:HG2	16:LH:69:LYS:HD3	1.90	0.53
29:LU:91:LYS:HG3	29:LU:109:ILE:HD13	1.91	0.53
2:L2:1150:U:H2'	2:L2:1151:U:O2	2.08	0.53
3:L3:71:U:H5	3:L3:150:A:N7	2.06	0.53
55:SB:203:ASP:OD1	55:SB:203:ASP:N	2.42	0.53
60:SG:24:ARG:HB2	60:SG:25:ARG:HH11	1.74	0.53
1:L1:146:U:OP2	15:LG:197:THR:OG1	2.26	0.53
1:L1:517:U:H2'	1:L1:518:C:C6	2.44	0.53
1:L1:1479:A:H5''	1:L1:1481:G:O4'	2.07	0.53
2:L2:954:A:C5	42:Lh:114:MET:HE1	2.44	0.53
2:L2:1089:A:H2'	2:L2:1090:G:H8	1.74	0.53
5:L5:113:G:OP2	39:Le:64:ARG:N	2.30	0.53
64:SK:164:ARG:HA	64:SK:167:ARG:HE	1.73	0.53
1:L1:576:G:O6	11:LC:324:ARG:HG3	2.09	0.53
1:L1:1293:A:H61	1:L1:1342:C:H42	1.55	0.53
3:L3:10:U:O2'	33:LY:79:HIS:ND1	2.41	0.53
5:L5:7:U:H2'	5:L5:8:C:H6	1.73	0.53
5:L5:132:C:OP1	28:LT:43:LYS:NZ	2.33	0.53
11:LC:299:VAL:HG21	24:LP:138:PRO:HB2	1.89	0.53
51:S3:2:G:H1	51:S3:71:C:H42	1.57	0.53
55:SB:194:ARG:NH2	78:SY:48:GLY:O	2.40	0.53
78:SY:10:GLU:OE1	78:SY:10:GLU:N	2.42	0.53
2:L2:83:G:O2'	2:L2:580:U:O4	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L6:64:U:OP2	14:LF:78:ARG:NE	2.38	0.52
27:LS:137:ILE:HG12	37:Lc:86:TYR:HD1	1.74	0.52
50:Lp:2:VAL:N	50:Lp:90:HIS:O	2.42	0.52
54:SA:146:LYS:HB3	54:SA:210:ARG:HB2	1.91	0.52
84:Se:7:SER:HB3	84:Se:10:ARG:NH1	2.23	0.52
85:Sf:96:ARG:NH2	88:S1:1605:U:OP2	2.41	0.52
1:L1:636:U:H2'	1:L1:637:C:C6	2.43	0.52
1:L1:1240:U:OP1	26:LR:159:LYS:NZ	2.28	0.52
4:L4:51:U:H2'	4:L4:52:A:H8	1.73	0.52
8:L8:26:A:H2'	8:L8:27:A:C8	2.44	0.52
11:LC:6:SER:OG	11:LC:20:THR:OG1	2.27	0.52
29:LU:70:LEU:HD12	29:LU:79:ILE:HG23	1.91	0.52
88:S1:1521:G:N1	88:S1:1995:G7M:OP2	2.28	0.52
2:L2:1379:A:H5''	2:L2:1381:G:H4'	1.91	0.52
50:Lp:70:LEU:HD11	50:Lp:85:LEU:HD11	1.90	0.52
59:SF:122:HIS:HB3	59:SF:148:ILE:HD11	1.91	0.52
79:SZ:13:ARG:HB3	79:SZ:31:GLU:HB3	1.92	0.52
80:Sa:87:LYS:HE2	88:S1:1718:A:H4'	1.91	0.52
34:LZ:3:HIS:O	34:LZ:8:GLN:NE2	2.43	0.52
40:Lf:20:ARG:HD2	40:Lf:34:ARG:HB2	1.91	0.52
88:S1:322:C:H2'	88:S1:323:U:H2'	1.90	0.52
88:S1:1589:G:O6	88:S1:1590:A:N6	2.42	0.52
2:L2:1486:G:H2'	2:L2:1487:G:H8	1.73	0.52
2:L2:1521:A:H2'	2:L2:1522:U:C6	2.43	0.52
7:L7:43:A2M:N1	7:L7:100:U:H5	2.08	0.52
7:L7:94:G:OP2	44:Lj:73:ARG:NH1	2.43	0.52
9:LA:14:SER:OG	9:LA:15:VAL:N	2.31	0.52
88:S1:793:G:OP2	88:S1:793:G:N2	2.30	0.52
1:L1:79:U:H2'	1:L1:80:C:C6	2.45	0.52
1:L1:1391:U:C5	19:LK:19:PRO:HB2	2.44	0.52
4:L4:98:A:H2'	4:L4:99:A:H8	1.75	0.52
7:L7:31:A:O2'	7:L7:33:U:OP2	2.26	0.52
19:LK:25:GLY:HA2	19:LK:40:ASN:HB2	1.90	0.52
40:Lf:46:ARG:NH2	94:Lf:302:HOH:O	2.43	0.52
54:SA:133:ASP:OD1	54:SA:133:ASP:N	2.35	0.52
61:SH:8:LEU:HD21	61:SH:55:VAL:HG11	1.92	0.52
86:Sg:215:ASP:OD1	86:Sg:215:ASP:N	2.39	0.52
1:L1:882:A:N1	1:L1:914:U:H5	2.07	0.52
1:L1:1739:A:H4'	42:Lh:12:MET:HE2	1.91	0.52
58:SE:163:GLU:HB3	58:SE:165:LYS:HG2	1.91	0.52
68:SO:26:ILE:HB	68:SO:90:MET:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:847:U:H3	2:L2:951:G:H1	1.56	0.52
2:L2:1404:G:H5''	9:LA:220:GLY:HA3	1.91	0.52
6:L6:20:A:H2'	6:L6:21:A:C8	2.44	0.52
54:SA:151:GLN:HE21	54:SA:153:SER:HB2	1.74	0.52
59:SF:177:VAL:HG11	59:SF:222:LEU:HA	1.91	0.52
69:SP:68:LYS:HB3	69:SP:91:LEU:HD22	1.92	0.52
88:S1:955:A:H3'	88:S1:956:A:H8	1.74	0.52
1:L1:814:C:H2'	1:L1:815:G:H8	1.74	0.52
2:L2:565:OMU:H5	94:L2:1815:HOH:O	2.09	0.52
10:LB:266:MET:HG2	16:LH:82:THR:HG22	1.91	0.52
52:S4:61:C:H2'	52:S4:62:C:C6	2.45	0.52
75:SV:99:VAL:HB	75:SV:120:VAL:HG22	1.91	0.52
81:Sb:96:ARG:HB3	88:S1:2199:C:O2	2.10	0.52
1:L1:624:U:O2'	1:L1:625:C:H4'	2.10	0.52
2:L2:612:C:H2'	2:L2:613:A:H8	1.75	0.52
17:LI:67:THR:HG22	17:LI:69:ARG:N	2.21	0.52
22:LN:29:PRO:O	22:LN:32:ARG:NH1	2.42	0.52
54:SA:145:THR:HG21	54:SA:158:ALA:HB2	1.91	0.52
66:SM:96:LYS:O	66:SM:100:SER:OG	2.27	0.52
68:SO:27:PHE:HB3	68:SO:34:PHE:HB2	1.92	0.52
72:SS:33:ARG:NH1	88:S1:2016:C:OP2	2.42	0.52
76:SW:72:LYS:NZ	76:SW:72:LYS:HB3	2.25	0.52
88:S1:294:G:O2'	88:S1:295:A:OP1	2.24	0.52
1:L1:213:G:N7	34:LZ:143:ARG:NH2	2.56	0.51
1:L1:817:C:H2'	1:L1:818:C:O4'	2.10	0.51
1:L1:1374:C:H2'	1:L1:1375:G:O4'	2.10	0.51
2:L2:1175:A:H2'	2:L2:1176:A:C8	2.45	0.51
5:L5:112:U:H5	5:L5:121:A:N7	2.08	0.51
6:L6:45:G:N7	26:LR:175:ARG:NH2	2.57	0.51
33:LY:77:HIS:HB3	38:Ld:37:ARG:HD3	1.92	0.51
52:S4:61:C:H2'	52:S4:62:C:H6	1.75	0.51
58:SE:97:ARG:HB2	58:SE:111:LEU:HD11	1.92	0.51
64:SK:4:VAL:HG11	64:SK:24:ARG:HG2	1.92	0.51
68:SO:91:ARG:HA	68:SO:126:THR:HG22	1.91	0.51
69:SP:3:LYS:NZ	88:S1:661:OMU:OP2	2.42	0.51
76:SW:84:LYS:NZ	88:S1:1593:G:OP2	2.43	0.51
1:L1:1533:PSU:H2'	1:L1:1534:G:C8	2.45	0.51
4:L4:167:C:H2'	4:L4:168:A:O4'	2.10	0.51
5:L5:70:C:H41	5:L5:88:C:H42	1.58	0.51
8:L8:52:G:OP2	23:LO:94:ASN:HB3	2.10	0.51
27:LS:25:PRO:HG3	27:LS:94:GLU:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LZ:113:ARG:NH2	40:Lf:116:LEU:O	2.37	0.51
52:S4:23:A:H2'	52:S4:24:G:C8	2.44	0.51
64:SK:83:TYR:HB2	64:SK:215:LEU:HD21	1.91	0.51
75:SV:77:GLU:HG2	75:SV:80:ARG:HH21	1.75	0.51
88:S1:277:U:O4	88:S1:945:G:O2'	2.21	0.51
88:S1:1989:A:H2'	88:S1:1990:A:C8	2.44	0.51
1:L1:494:A:H3'	1:L1:495:C:H6	1.76	0.51
1:L1:688:A:H2'	1:L1:689:A:C8	2.45	0.51
2:L2:603:A:H2'	2:L2:604:A2M:H8	1.92	0.51
4:L4:75:C:H5'	10:LB:336:SER:HA	1.93	0.51
16:LH:79:ARG:HA	16:LH:88:PRO:HD2	1.91	0.51
29:LU:106:TRP:HB3	29:LU:107:ILE:HD12	1.92	0.51
45:Lk:73:SER:HB3	45:Lk:76:LYS:HG2	1.93	0.51
59:SF:153:ARG:HB3	59:SF:163:PRO:HB2	1.92	0.51
71:SR:134:GLY:HA3	88:S1:1978:A:H5''	1.91	0.51
33:LY:54:VAL:HG22	33:LY:57:MET:HE3	1.92	0.51
65:SL:32:GLN:NE2	77:SX:12:GLY:O	2.39	0.51
73:ST:130:LYS:NZ	73:ST:139:TRP:O	2.39	0.51
76:SW:24:TYR:HB3	76:SW:32:LEU:HD11	1.91	0.51
86:Sg:49:SER:OG	86:Sg:51:ASP:OD1	2.26	0.51
88:S1:777:A:H4'	88:S1:778:G:O5'	2.11	0.51
88:S1:2102:A:H61	88:S1:2121:C:H42	1.59	0.51
1:L1:1405:U:H2'	1:L1:1406:C:H6	1.76	0.51
1:L1:1602:C:H2'	1:L1:1603:G:H8	1.75	0.51
2:L2:590:U:H2'	2:L2:591:A2M:C8	2.38	0.51
2:L2:1321:U:H2'	2:L2:1322:C:C6	2.44	0.51
3:L3:172:G:OP2	3:L3:172:G:N2	2.33	0.51
6:L6:19:C:H2'	6:L6:20:A:C8	2.46	0.51
9:LA:36:GLU:HG3	9:LA:91:GLY:HA2	1.93	0.51
1:L1:93:G:H2'	1:L1:94:A:C8	2.46	0.51
1:L1:129:C:H2'	1:L1:130:U:H6	1.74	0.51
1:L1:478:C:H2'	1:L1:479:A:H8	1.76	0.51
1:L1:663:C:H2'	1:L1:664:C:O2	2.11	0.51
3:L3:105:C:H2'	3:L3:106:U:C6	2.45	0.51
48:Ln:3:THR:OG1	88:S1:2196:G:H5''	2.11	0.51
51:S3:23:C:H2'	51:S3:24:U:C6	2.45	0.51
52:S4:68:C:H2'	52:S4:69:G:H8	1.74	0.51
18:LJ:8:VAL:HB	18:LJ:127:LEU:HD13	1.92	0.51
20:LL:29:GLU:OE1	20:LL:29:GLU:N	2.34	0.51
31:LW:28:MET:HB3	31:LW:98:PRO:HG2	1.93	0.51
54:SA:188:SER:O	54:SA:192:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SG:95:ARG:O	88:S1:448:C:O2'	2.25	0.51
63:SJ:78:ARG:HB3	63:SJ:124:LYS:HB3	1.92	0.51
1:L1:593:C:H42	1:L1:614:A:H61	1.59	0.51
1:L1:996:A:H2'	1:L1:997:C:C6	2.45	0.51
1:L1:1750:G:N1	3:L3:170:C:H2'	2.25	0.51
2:L2:389:A:OP2	2:L2:570:A2M:H8	2.10	0.51
54:SA:23:THR:O	54:SA:26:ARG:HG2	2.11	0.51
73:ST:32:ASN:O	73:ST:36:MET:HG3	2.11	0.51
1:L1:913:C:H2'	1:L1:914:U:O2	2.11	0.51
2:L2:653:C:C2	2:L2:654:U:C5	2.99	0.51
7:L7:63:G:H22	7:L7:96:A:H2	1.58	0.51
26:LR:48:ARG:HG3	26:LR:54:LYS:HD3	1.92	0.51
76:SW:102:ALA:HA	76:SW:111:ALA:HA	1.93	0.51
1:L1:133:C:H5'	35:La:77:ARG:HH12	1.76	0.51
1:L1:1477:G:O2'	40:Lf:100:THR:HG22	2.10	0.51
5:L5:62:C:H3'	5:L5:63:G:H21	1.76	0.51
22:LN:30:LYS:HG2	22:LN:63:GLU:HG3	1.93	0.51
52:S4:22:G:H2'	52:S4:23:A:H8	1.76	0.51
88:S1:934:U:O2'	88:S1:936:U:O2	2.29	0.51
1:L1:611:C:OP2	11:LC:359:ARG:NH1	2.44	0.50
2:L2:436:U:OP1	49:Lo:21:ASN:ND2	2.43	0.50
2:L2:1137:G:H2'	2:L2:1138:C:C6	2.46	0.50
2:L2:1320:U:H2'	2:L2:1321:U:C6	2.45	0.50
3:L3:58:U:O4	29:LU:104:ARG:NE	2.30	0.50
4:L4:12:A:H2'	4:L4:13:A:C8	2.47	0.50
13:LE:152:GLN:O	13:LE:156:GLU:HG2	2.11	0.50
14:LF:104:GLU:H	14:LF:104:GLU:CD	2.19	0.50
88:S1:2132:C:H2'	88:S1:2133:G:O4'	2.11	0.50
1:L1:208:C:O2'	1:L1:209:C:OP1	2.28	0.50
1:L1:290:G:H2'	1:L1:291:A:C8	2.46	0.50
1:L1:408:G:O2'	1:L1:410:U:OP1	2.28	0.50
1:L1:1257[A]:U:H4'	1:L1:1258:A:O5'	2.10	0.50
1:L1:1438:A:OP2	34:LZ:41:ARG:NH2	2.40	0.50
1:L1:1603:G:H2'	1:L1:1604:U:C6	2.45	0.50
2:L2:1412:U:H2'	2:L2:1413:U:C6	2.46	0.50
3:L3:155:A:H61	3:L3:175:A:H62	1.60	0.50
35:La:69:ASN:O	35:La:72:MET:HE3	2.11	0.50
52:S4:31:A:H3'	52:S4:32:U:H5''	1.94	0.50
88:S1:32:U:O2'	88:S1:643:A:N1	2.43	0.50
88:S1:56:U:OP1	88:S1:446:A:N6	2.40	0.50
88:S1:1572:C:H5	88:S1:1615:G:H1	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:S1:1576:A:H61	88:S1:1611:C:N4	2.10	0.50
31:LW:54:ILE:HB	31:LW:64:GLU:HG2	1.92	0.50
49:Lo:81:SER:HA	49:Lo:84:ARG:NH1	2.23	0.50
52:S4:10:G:H2'	52:S4:11:C:C6	2.46	0.50
70:SQ:105:ARG:O	70:SQ:113:THR:OG1	2.25	0.50
79:SZ:91:ARG:O	88:S1:498:C:O2'	2.30	0.50
1:L1:159:U:O2'	1:L1:160:C:H5'	2.11	0.50
1:L1:478:C:H2'	1:L1:479:A:C8	2.47	0.50
1:L1:1627:U:OP1	30:LV:126:TYR:OH	2.24	0.50
3:L3:23:U:O2'	3:L3:25:G:OP1	2.29	0.50
70:SQ:50:VAL:O	70:SQ:54:LEU:N	2.43	0.50
88:S1:323:U:O2'	88:S1:325:G:N2	2.44	0.50
1:L1:434:U:H5	1:L1:438:A:N7	2.10	0.50
2:L2:750:U:HO2'	2:L2:751:U:H6	1.60	0.50
2:L2:996:C:H2'	2:L2:997:A:H8	1.77	0.50
2:L2:1336:G:OP2	2:L2:1337:C:H2'	2.12	0.50
4:L4:180:C:H1'	5:L5:5:C:H1'	1.93	0.50
8:L8:31:A:H2'	8:L8:32:C:C6	2.47	0.50
8:L8:61:C:H2'	8:L8:62:A:H8	1.77	0.50
48:Ln:6:ARG:HD2	48:Ln:8:ARG:HG2	1.94	0.50
70:SQ:94:ARG:HG2	70:SQ:94:ARG:HH11	1.76	0.50
86:Sg:77:THR:OG1	86:Sg:78:ASP:N	2.44	0.50
1:L1:1097:A:H2'	1:L1:1100:C:C5	2.47	0.50
5:L5:8:C:H2'	5:L5:9:C:H6	1.77	0.50
5:L5:26:A:OP2	10:LB:116:ARG:NH2	2.44	0.50
32:LX:93:TYR:O	32:LX:97:VAL:HG23	2.12	0.50
60:SG:162:ARG:NH2	88:S1:77:G:OP1	2.45	0.50
80:Sa:60:ILE:HB	80:Sa:101:TYR:HB2	1.93	0.50
87:Sh:148:THR:HG22	87:Sh:196:ARG:HH21	1.77	0.50
1:L1:12:U:H2'	1:L1:13:G:C8	2.44	0.50
1:L1:593:C:H2'	1:L1:594:G:C8	2.46	0.50
1:L1:650:G:O2'	1:L1:652:A:H5'	2.12	0.50
2:L2:815:G:H2'	2:L2:816:G:H8	1.77	0.50
5:L5:7:U:H2'	5:L5:8:C:C6	2.46	0.50
41:Lg:34:TYR:CE1	41:Lg:136:ARG:HG2	2.47	0.50
41:Lg:61:VAL:HG13	41:Lg:66:ASP:HB3	1.94	0.50
66:SM:17:VAL:HG11	66:SM:95:VAL:HG11	1.94	0.50
82:Sc:63:LYS:HE3	82:Sc:63:LYS:HA	1.93	0.50
85:Sf:73:LYS:HD3	88:S1:1848:U:H1'	1.93	0.50
1:L1:99:A:H3'	1:L1:100:G:H21	1.77	0.50
1:L1:888:A:H5'	49:Lo:9:GLY:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1201:U:H1'	1:L1:1202:G:C8	2.47	0.50
1:L1:1357:G:H2'	1:L1:1358:C:C6	2.46	0.50
2:L2:105:A:H2'	2:L2:106:A:C8	2.46	0.50
2:L2:1075:G:OP1	22:LN:24:ARG:NH2	2.42	0.50
3:L3:54:G:H4'	3:L3:156:G:H4'	1.94	0.50
7:L7:45:C:H5''	46:Ll:15:LYS:HD2	1.93	0.50
7:L7:154:A:H2'	7:L7:155:U:O4'	2.12	0.50
23:LO:94:ASN:HD22	23:LO:210:VAL:HG21	1.76	0.50
27:LS:41:ASP:OD1	27:LS:61:THR:OG1	2.26	0.50
54:SA:88:PHE:HB3	54:SA:100:THR:HB	1.93	0.50
57:SD:67:ARG:NH1	57:SD:71:GLU:OE1	2.44	0.50
75:SV:88:THR:O	75:SV:93:LYS:NZ	2.45	0.50
86:Sg:134:TRP:CE3	86:Sg:140:CYS:HB3	2.47	0.50
86:Sg:264:GLU:HA	86:Sg:264:GLU:OE2	2.12	0.50
88:S1:409:G:OP1	88:S1:859:G:O2'	2.26	0.50
88:S1:436:C:H2'	88:S1:437:C:C6	2.47	0.50
1:L1:531:C:H1'	26:LR:132:PRO:HG3	1.94	0.50
1:L1:1169:A:H2'	1:L1:1170:G:C8	2.47	0.50
1:L1:1776:G:H22	2:L2:6:A:H2	1.60	0.50
2:L2:464:G:H2'	2:L2:465:A:H8	1.77	0.50
2:L2:1038:U:H2'	2:L2:1039:U:C6	2.47	0.50
3:L3:173:U:H2'	3:L3:174:C:O4'	2.12	0.50
10:LB:226:THR:HG22	10:LB:336:SER:HB3	1.94	0.50
11:LC:282:LEU:HD11	24:LP:29:LEU:HG	1.93	0.50
15:LG:120:ASP:HB2	15:LG:123:LYS:HE2	1.92	0.50
62:Sl:164:ARG:HH22	88:S1:1018:G:H4'	1.77	0.50
66:SM:99:THR:O	66:SM:99:THR:OG1	2.28	0.50
67:SN:71:TYR:OH	88:S1:1836:G:O6	2.23	0.50
70:SQ:47:LEU:HD23	70:SQ:73:TYR:CE1	2.47	0.50
86:Sg:281:GLU:HB3	86:Sg:299:LYS:HD2	1.94	0.50
1:L1:626:U:HO2'	1:L1:627:C:H6	1.58	0.49
2:L2:1505:A:H2'	2:L2:1506:G:C8	2.47	0.49
7:L7:85:U:OP1	31:LW:111:HIS:NE2	2.38	0.49
21:LM:123:MET:HG2	21:LM:128:LYS:HG3	1.93	0.49
77:SX:6:ASN:O	77:SX:9:HIS:ND1	2.42	0.49
88:S1:1360:U:H4'	88:S1:1361:U:O5'	2.11	0.49
1:L1:1189:C:H2'	1:L1:1190:OMG:H8	1.78	0.49
42:Lh:47:TRP:HA	42:Lh:51:HIS:HB2	1.94	0.49
77:SX:8:ILE:HD11	88:S1:1714:C:H5''	1.94	0.49
1:L1:837:A:H4'	1:L1:838:G:O5'	2.12	0.49
1:L1:1038:U:OP1	37:Lc:135:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:746:A:O2'	2:L2:747:A:H5'	2.11	0.49
3:L3:154:C:H2'	3:L3:155:A:C8	2.47	0.49
4:L4:120:U:O2'	4:L4:122:G:OP2	2.26	0.49
4:L4:155:A:H2'	4:L4:156:G:O4'	2.12	0.49
9:LA:83:PHE:HB3	49:Lo:64:VAL:HG22	1.94	0.49
51:S3:53:G:H2'	51:S3:54:U:C6	2.47	0.49
55:SB:188:LEU:HD12	78:SY:50:ILE:HG22	1.94	0.49
60:SG:25:ARG:N	60:SG:25:ARG:HD2	2.27	0.49
76:SW:114:ILE:HA	76:SW:118:MET:HE2	1.94	0.49
1:L1:1613:C:OP1	28:LT:127:ARG:NH2	2.38	0.49
1:L1:1672:U:H2'	1:L1:1673:G:O4'	2.12	0.49
2:L2:1250:C:H2'	2:L2:1251:A:C8	2.48	0.49
13:LE:20:VAL:HG12	13:LE:25:VAL:HG22	1.94	0.49
22:LN:139:ARG:HD3	22:LN:173:PHE:CG	2.47	0.49
73:ST:14:SER:HB3	88:S1:1206:C:H5''	1.94	0.49
1:L1:1527:OMC:HM22	1:L1:1528:PSU:H5''	1.94	0.49
2:L2:1020:C:O2'	2:L2:1021:A:O5'	2.29	0.49
2:L2:1233:U:OP2	50:Lp:63:LYS:HG2	2.12	0.49
2:L2:1285:A:C4	2:L2:1286:G:C8	3.00	0.49
10:LB:301:ALA:HB3	10:LB:310:LYS:HB2	1.94	0.49
35:La:6:LYS:HB2	35:La:9:ASP:OD1	2.13	0.49
48:Ln:3:THR:HG21	88:S1:2174:G:H21	1.76	0.49
57:SD:135:VAL:HG22	57:SD:155:ILE:HG12	1.93	0.49
60:SG:144:ILE:HD13	60:SG:160:VAL:HG22	1.94	0.49
1:L1:547:U:H4'	26:LR:65:VAL:HG21	1.95	0.49
1:L1:885:U:H2'	1:L1:886:G:O4'	2.12	0.49
2:L2:694:U:N3	2:L2:695:G:C2	2.81	0.49
2:L2:1020:C:O2'	2:L2:1021:A:H8	1.96	0.49
6:L6:34:C:H2'	6:L6:35:U:C6	2.48	0.49
9:LA:80:GLU:HG2	49:Lo:76:ASN:CG	2.38	0.49
13:LE:46:ARG:NH2	19:LK:6:TYR:OH	2.46	0.49
17:LI:137:LYS:NZ	17:LI:138:VAL:O	2.45	0.49
42:Lh:43:ILE:HG22	42:Lh:54:LEU:HD12	1.95	0.49
52:S4:62:C:H2'	52:S4:63:G:C8	2.48	0.49
59:SF:55:VAL:HG21	59:SF:78:ILE:HG23	1.94	0.49
77:SX:27:TRP:HH2	77:SX:74:LEU:HD23	1.77	0.49
77:SX:45:ASN:H	88:S1:1919:C:H5	1.61	0.49
1:L1:129:C:H2'	1:L1:130:U:C6	2.48	0.49
1:L1:326:A:H2'	1:L1:327:G:H8	1.77	0.49
15:LG:82:VAL:HG21	15:LG:182:LYS:HD3	1.95	0.49
1:L1:622:C:O2'	1:L1:623:U:O5'	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1044:G:N3	2:L2:1064:A:H2'	2.28	0.49
2:L2:790:U:H2'	2:L2:791:A:C8	2.47	0.49
3:L3:16:G:N2	3:L3:21:A:OP1	2.42	0.49
11:LC:281:MET:HE1	24:LP:26:ILE:HG12	1.93	0.49
37:Lc:142:PRO:HA	37:Lc:237:TYR:CG	2.48	0.49
1:L1:622:C:HO2'	1:L1:623:U:C5'	2.25	0.49
1:L1:734:U:H2'	1:L1:735:U:C6	2.48	0.49
2:L2:473:C:H2'	2:L2:474:A:H8	1.77	0.49
3:L3:64:U:H2'	3:L3:65:U:C6	2.47	0.49
5:L5:19:C:O2'	28:LT:69:ARG:O	2.24	0.49
5:L5:32:A:H2'	5:L5:33:U:C6	2.48	0.49
7:L7:125:A:C2	7:L7:126:G:H1'	2.47	0.49
18:LJ:72:ARG:NH2	88:S1:2078:A:OP1	2.46	0.49
88:S1:1684:U:H3	88:S1:1820:G:H22	1.59	0.49
1:L1:811:G:H2'	1:L1:812:A:H8	1.78	0.49
1:L1:1410:U:H2'	1:L1:1411:G:C8	2.48	0.49
2:L2:665:A2M:H2'	2:L2:666:C:C6	2.48	0.49
2:L2:1101:A:O2'	2:L2:1102:C:OP1	2.28	0.49
39:Le:98:LYS:HB3	39:Le:98:LYS:HE3	1.68	0.49
69:SP:63:ASN:ND2	69:SP:114:ASP:OD2	2.35	0.49
88:S1:252:G:O6	88:S1:838:U:H4'	2.13	0.49
88:S1:1227:G:H4'	88:S1:2179:A:H4'	1.95	0.49
88:S1:1912:A:H61	88:S1:1927:U:H3	1.61	0.49
1:L1:156:A:OP1	17:LI:91:ASN:ND2	2.46	0.48
1:L1:204:A:OP1	40:Lf:84:TYR:OH	2.21	0.48
1:L1:811:G:H2'	1:L1:812:A:C8	2.48	0.48
2:L2:382:A2M:H8	2:L2:382:A2M:O5'	2.12	0.48
22:LN:113:THR:O	22:LN:113:THR:OG1	2.28	0.48
52:S4:68:C:H2'	52:S4:69:G:C8	2.48	0.48
57:SD:87:GLU:H	57:SD:87:GLU:CD	2.16	0.48
64:SK:41:ARG:NH2	88:S1:308:C:OP2	2.46	0.48
70:SQ:47:LEU:HD23	70:SQ:73:TYR:CZ	2.48	0.48
1:L1:700:A:H2'	1:L1:701:G:H8	1.76	0.48
1:L1:1122:U:H2'	1:L1:1122:U:O2	2.13	0.48
15:LG:214:ASN:OD1	15:LG:217:ARG:NH2	2.46	0.48
47:Lm:79:GLU:OE1	47:Lm:81:THR:HG23	2.13	0.48
51:S3:24:U:H2'	51:S3:25:C:H6	1.78	0.48
56:SC:200:SER:OG	56:SC:201:GLU:N	2.46	0.48
60:SG:24:ARG:HB2	60:SG:25:ARG:NH1	2.28	0.48
60:SG:64:MET:HE1	60:SG:105:LEU:HD23	1.94	0.48
60:SG:121:ASP:OD2	60:SG:121:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:S1:479:A2M:O5'	88:S1:479:A2M:H8	2.12	0.48
1:L1:669:C:C2	1:L1:670:C:C5	3.01	0.48
1:L1:1162:G:N7	24:LP:13:ARG:NH2	2.50	0.48
2:L2:1498:G:H4'	10:LB:138:ASN:HB3	1.95	0.48
5:L5:51:A:H8	5:L5:52:U:H2'	1.78	0.48
20:LL:80:ARG:NH2	20:LL:106:TYR:OH	2.47	0.48
21:LM:46:GLU:O	21:LM:50:MET:HG3	2.14	0.48
25:LQ:105:LEU:HD23	25:LQ:138:LEU:HD23	1.96	0.48
51:S3:14:A:H61	51:S3:21:A:H8	1.59	0.48
69:SP:61:GLN:HG3	69:SP:62:PRO:HA	1.96	0.48
88:S1:1510:C:H5	88:S1:1515:A:H61	1.60	0.48
88:S1:1911:U:H5	88:S1:1928:G:H1	1.62	0.48
8:L8:87:G:O2'	8:L8:89:C:OP1	2.31	0.48
13:LE:86:GLY:HA3	13:LE:186:ILE:HD12	1.95	0.48
88:S1:814:G:H1'	88:S1:815:U:H5'	1.94	0.48
1:L1:107:C:OP1	17:LI:47:LYS:NZ	2.40	0.48
1:L1:1272:U:H2'	1:L1:1273:U:C6	2.49	0.48
2:L2:1108:U:H5'	12:LD:67:ILE:HD11	1.95	0.48
67:SN:68:TRP:CE2	72:SS:24:ILE:HG12	2.48	0.48
72:SS:49:GLU:CD	72:SS:49:GLU:H	2.21	0.48
73:ST:2:VAL:HG12	88:S1:1202:A:OP1	2.13	0.48
87:Sh:216:GLN:O	87:Sh:220:ASN:N	2.44	0.48
88:S1:2010:G:H1	88:S1:2026:U:H3	1.60	0.48
1:L1:695:OMC:HM23	1:L1:695:OMC:H1'	1.68	0.48
1:L1:1536:C:OP1	28:LT:66:LYS:NZ	2.28	0.48
2:L2:1253:OMG:HM21	2:L2:1255:A:H2'	1.94	0.48
3:L3:145:U:H2'	3:L3:146:G:O4'	2.13	0.48
5:L5:4:A:H62	5:L5:134:C:H5	1.61	0.48
8:L8:16:C:OP2	8:L8:71:C:O2'	2.30	0.48
14:LF:64:VAL:HG11	14:LF:101:ILE:HG21	1.94	0.48
65:SL:107:GLU:O	65:SL:108:LYS:HB3	2.14	0.48
85:Sf:73:LYS:HD2	88:S1:1622:G:H4'	1.94	0.48
1:L1:1638:C:H2'	1:L1:1639:U:C6	2.47	0.48
2:L2:1508:A:H2'	2:L2:1509:C:C6	2.48	0.48
11:LC:91:PHE:O	11:LC:99:ARG:NH2	2.47	0.48
22:LN:206:ILE:HG13	23:LO:295:LYS:HD2	1.95	0.48
57:SD:179:ALA:O	57:SD:182:HIS:ND1	2.35	0.48
79:SZ:61:GLN:HA	79:SZ:89:LEU:HD13	1.94	0.48
86:Sg:139:GLU:N	86:Sg:139:GLU:OE1	2.46	0.48
1:L1:845:OMU:HM23	1:L1:845:OMU:H1'	1.71	0.48
1:L1:1609:A:H5''	28:LT:125:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:816:G:OP2	42:Lh:113:LYS:NZ	2.31	0.48
2:L2:1490:U:H2'	2:L2:1491:G:H8	1.79	0.48
5:L5:39:G:H4'	10:LB:372:ILE:O	2.14	0.48
5:L5:128:G:H2'	5:L5:129:G:C8	2.48	0.48
15:LG:104:LYS:O	15:LG:108:GLU:HG3	2.14	0.48
29:LU:42:ASP:OD1	29:LU:42:ASP:N	2.42	0.48
33:LY:32:VAL:HB	33:LY:37:PRO:HA	1.96	0.48
37:Lc:146:TYR:CZ	37:Lc:239:ASN:HB2	2.49	0.48
52:S4:22:G:H2'	52:S4:23:A:C8	2.48	0.48
77:SX:19:LEU:HD11	77:SX:75:ARG:HG3	1.96	0.48
86:Sg:234:VAL:HG11	86:Sg:254:THR:HG21	1.95	0.48
88:S1:227:U:N3	88:S1:261:A:O2'	2.47	0.48
1:L1:480:U:H2'	1:L1:481:U:H6	1.79	0.48
1:L1:1093:U:H5''	22:LN:196:HIS:NE2	2.28	0.48
3:L3:106:U:H2'	3:L3:107:U:C6	2.48	0.48
12:LD:28:SER:OG	12:LD:29:GLY:N	2.47	0.48
33:LY:59:LYS:HE2	33:LY:59:LYS:HB3	1.59	0.48
62:SI:75:ARG:NH1	62:SI:131:ASP:OD1	2.47	0.48
68:SO:75:VAL:HG22	68:SO:117:MET:HG3	1.96	0.48
86:Sg:229:LEU:HB3	86:Sg:230:PHE:CD1	2.48	0.48
1:L1:52:C:HO2'	1:L1:1653:U:HO2'	1.62	0.48
1:L1:69:A2M:OP1	20:LL:67:PRO:HG3	2.14	0.48
1:L1:480:U:H2'	1:L1:481:U:C6	2.49	0.48
1:L1:967:G:H5'	1:L1:968:A:OP1	2.14	0.48
4:L4:124:A:H2'	4:L4:125:C:C6	2.49	0.48
5:L5:51:A:H4'	5:L5:52:U:OP1	2.12	0.48
5:L5:119:U:OP1	39:Le:62:ASN:ND2	2.46	0.48
11:LC:288:THR:OG1	34:LZ:6:ASP:OD2	2.27	0.48
19:LK:27:ILE:O	19:LK:29:ASP:N	2.44	0.48
33:LY:123:GLY:HA2	33:LY:126:MET:HE3	1.95	0.48
43:Li:95:GLU:OE2	43:Li:98:ARG:NH2	2.45	0.48
60:SG:139:LYS:HG2	60:SG:177:PRO:HB2	1.96	0.48
75:SV:45:LYS:HE3	88:S1:1683:A:H5''	1.95	0.48
1:L1:5:A:O2'	1:L1:6:C:H5'	2.14	0.47
1:L1:682:C:H2'	1:L1:683:G:C8	2.49	0.47
1:L1:720:A:C8	1:L1:721:U:H2'	2.49	0.47
1:L1:731:U:C2	1:L1:732:A:C8	3.02	0.47
2:L2:1369:C:N3	2:L2:1373:C:H5	2.12	0.47
6:L6:70:G:O2'	6:L6:71:A:H5'	2.14	0.47
16:LH:22:PRO:HG2	16:LH:24:ILE:HD11	1.96	0.47
36:Lb:57:LYS:O	36:Lb:61:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Lh:2:SER:O	42:Lh:2:SER:OG	2.29	0.47
54:SA:166:LEU:HD11	54:SA:209:LEU:HD11	1.95	0.47
86:Sg:123:VAL:HG23	86:Sg:133:VAL:HG22	1.95	0.47
88:S1:175:U:OP1	88:S1:317:G:O2'	2.29	0.47
1:L1:516:G:H2'	1:L1:517:U:C6	2.49	0.47
1:L1:586:U:OP1	37:Lc:55:TYR:OH	2.24	0.47
1:L1:848:U:H2'	1:L1:849:U:C6	2.48	0.47
2:L2:14:OMC:HM22	2:L2:15:C:O4'	2.15	0.47
2:L2:412:A:H2'	2:L2:413:A:C8	2.49	0.47
2:L2:1219:A:H2'	2:L2:1220:A:C8	2.48	0.47
3:L3:99:U:H2'	3:L3:100:U:H6	1.77	0.47
51:S3:24:U:H2'	51:S3:25:C:C6	2.49	0.47
51:S3:52:G:C4	51:S3:53:G:C8	3.02	0.47
82:Sc:57:CYS:HB3	82:Sc:60:CYS:HB2	1.70	0.47
88:S1:756:C:O2'	88:S1:768:A:N6	2.42	0.47
1:L1:622:C:O2'	1:L1:623:U:H6	1.98	0.47
1:L1:693:G:H4'	1:L1:694:U:H6	1.80	0.47
1:L1:1451:C:H2'	1:L1:1452:C:C6	2.48	0.47
2:L2:14:OMC:H2'	2:L2:15:C:C6	2.49	0.47
2:L2:1454:A:O2'	2:L2:1455:U:H2'	2.15	0.47
4:L4:126:G:O2'	4:L4:127:G:N2	2.47	0.47
5:L5:112:U:H2'	5:L5:112:U:O2	2.13	0.47
6:L6:34:C:H2'	6:L6:35:U:H6	1.78	0.47
8:L8:35:U:H2'	8:L8:36:A:C8	2.50	0.47
17:LI:93:GLN:HE22	35:La:114:GLN:HE22	1.62	0.47
58:SE:121:MET:HB3	58:SE:138:THR:HB	1.95	0.47
65:SL:23:ALA:HB2	65:SL:75:VAL:HG13	1.97	0.47
67:SN:3:THR:OG1	88:S1:1569:G:OP1	2.30	0.47
73:ST:1:MET:HG2	88:S1:1114:G:OP2	2.15	0.47
1:L1:208:C:HO2'	1:L1:209:C:P	2.36	0.47
1:L1:1085:C:H2'	1:L1:1086:G:O4'	2.14	0.47
2:L2:1066:G:H2'	2:L2:1067:A2M:H8	1.96	0.47
10:LB:57:VAL:HB	10:LB:365:PHE:HB3	1.97	0.47
13:LE:160:LEU:HG	13:LE:178:ILE:HG21	1.95	0.47
15:LG:141:THR:O	15:LG:145:GLU:HG3	2.15	0.47
18:LJ:59:MET:HE3	18:LJ:128:TRP:CH2	2.50	0.47
23:LO:248:MET:HE3	23:LO:248:MET:HB3	1.76	0.47
62:SI:9:ARG:NH2	88:S1:967:A:OP1	2.46	0.47
82:Sc:35:ASP:O	82:Sc:80:TYR:HA	2.15	0.47
87:Sh:177:LEU:HD12	87:Sh:183:ALA:HA	1.97	0.47
1:L1:51:G:H4'	1:L1:863:G:H4'	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:52:C:O2'	1:L1:1653:U:O2'	2.31	0.47
1:L1:338:G:H2'	1:L1:339:C:C6	2.50	0.47
1:L1:482:U:H2'	1:L1:483:C:C6	2.50	0.47
1:L1:553:A:N3	11:LC:323:ARG:HD3	2.30	0.47
1:L1:597:C:H2'	1:L1:598:G:H8	1.79	0.47
2:L2:1123:A:H2'	2:L2:1124:A:C8	2.48	0.47
59:SF:51:LEU:HD21	59:SF:66:ILE:HD13	1.96	0.47
70:SQ:63:ILE:HB	70:SQ:121:VAL:HG22	1.97	0.47
71:SR:26:LYS:HE3	71:SR:54:GLU:HA	1.95	0.47
74:SU:138:VAL:HG12	74:SU:157:VAL:HG22	1.96	0.47
1:L1:553:A:OP2	11:LC:341:LYS:NZ	2.48	0.47
2:L2:1087:C:H2'	2:L2:1088:G:C8	2.50	0.47
12:LD:119:ASP:OD2	12:LD:121:SER:OG	2.33	0.47
14:LF:80:ASP:HB3	14:LF:83:TYR:HD2	1.80	0.47
70:SQ:66:ASP:HB2	70:SQ:92:GLU:HA	1.97	0.47
77:SX:12:GLY:C	77:SX:14:ARG:H	2.23	0.47
88:S1:1718:A:O2'	88:S1:1949:A:N6	2.47	0.47
1:L1:302:G:H5'	43:Li:40:LEU:HB2	1.95	0.47
1:L1:879:A:H2'	1:L1:880:C:C6	2.49	0.47
1:L1:1373:A2M:O5'	1:L1:1373:A2M:H8	2.15	0.47
2:L2:612:C:H2'	2:L2:613:A:C8	2.50	0.47
2:L2:955:C:H2'	2:L2:956:C:C6	2.49	0.47
4:L4:75:C:O2'	4:L4:76:C:H5'	2.15	0.47
6:L6:48:C:C2	14:LF:185:LYS:HD3	2.50	0.47
6:L6:66:A:OP1	14:LF:47:ARG:NH2	2.39	0.47
8:L8:72:U:H2'	8:L8:73:C:C6	2.50	0.47
10:LB:95:THR:OG1	10:LB:98:GLY:O	2.30	0.47
30:LV:58:LYS:HB2	30:LV:58:LYS:HE3	1.69	0.47
33:LY:22:LYS:NZ	33:LY:130:GLN:O	2.42	0.47
40:Lf:35:LYS:HD2	40:Lf:36:PRO:HD2	1.97	0.47
44:Lj:39:TYR:CD1	44:Lj:40:PRO:HA	2.50	0.47
54:SA:148:GLN:NE2	88:S1:1403:A:N3	2.61	0.47
56:SC:6:LYS:HG3	66:SM:22:THR:HG21	1.95	0.47
63:SJ:87:GLU:OE1	63:SJ:97:ARG:NH2	2.47	0.47
63:SJ:107:SER:OG	88:S1:903:G:N2	2.46	0.47
64:SK:117:TYR:O	64:SK:166:ARG:NH1	2.48	0.47
70:SQ:105:ARG:NH2	88:S1:1578:G:O6	2.48	0.47
88:S1:697:G:H1	88:S1:748:C:H5	1.61	0.47
1:L1:1564:C:N3	39:Le:162:LYS:NZ	2.53	0.47
2:L2:1171:G:H2'	2:L2:1172:C:C6	2.50	0.47
11:LC:178:ASP:HB3	11:LC:206:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LD:110:GLU:HG3	12:LD:124:ILE:HG21	1.97	0.47
45:Lk:15:CYS:HB2	45:Lk:61:HIS:CE1	2.50	0.47
52:S4:62:C:H2'	52:S4:63:G:H8	1.79	0.47
52:S4:64:A:H2'	52:S4:65:G:H8	1.79	0.47
55:SB:40:TYR:HD1	55:SB:56:MET:HE2	1.79	0.47
82:Sc:71:LYS:NZ	88:S1:1297:A:OP1	2.44	0.47
88:S1:2170:G:OP1	88:S1:2173:A:H4'	2.15	0.47
1:L1:911:G:O2'	1:L1:946:G:H4'	2.14	0.47
2:L2:2:C:H2'	2:L2:3:C:H6	1.80	0.47
2:L2:105:A:H2'	2:L2:106:A:H8	1.80	0.47
2:L2:422:U:OP1	9:LA:54:ARG:NH2	2.40	0.47
8:L8:53:A:H5''	23:LO:233:SER:HB2	1.95	0.47
8:L8:61:C:H2'	8:L8:62:A:C8	2.50	0.47
23:LO:123:LYS:HE2	23:LO:123:LYS:HB3	1.70	0.47
55:SB:30:THR:HG22	55:SB:169:ARG:NE	2.30	0.47
57:SD:171:VAL:HG13	88:S1:557:A:OP2	2.15	0.47
4:L4:17:A:H2'	4:L4:18:U:C6	2.50	0.47
59:SF:152:ARG:HB3	59:SF:233:THR:HB	1.97	0.47
67:SN:5:VAL:HG22	67:SN:48:GLN:HG2	1.96	0.47
76:SW:22:PHE:HE2	76:SW:29:ILE:HB	1.80	0.47
1:L1:581:G:H2'	1:L1:582:U:C6	2.49	0.46
1:L1:1263:A:N1	2:L2:1295:C:H5''	2.30	0.46
1:L1:1450:U:H2'	1:L1:1451:C:C6	2.50	0.46
2:L2:459:A:H2'	2:L2:460:A:C8	2.50	0.46
3:L3:212:G:H5'	33:LY:131:ARG:HH12	1.81	0.46
5:L5:48:G:H2'	5:L5:49:G:N3	2.30	0.46
7:L7:93:C:C2'	7:L7:94:G:H5''	2.45	0.46
8:L8:8:U:H2'	8:L8:9:A:C8	2.50	0.46
9:LA:32:LEU:HD13	9:LA:163:ARG:HD3	1.96	0.46
18:LJ:110:GLU:OE1	18:LJ:111:MET:N	2.47	0.46
27:LS:68:THR:HG22	27:LS:71:GLY:N	2.27	0.46
28:LT:109:PRO:HA	28:LT:112:MET:HG2	1.97	0.46
62:SI:61:VAL:HG11	62:SI:175:VAL:HG21	1.96	0.46
1:L1:120:G:O2'	1:L1:122:A:N6	2.48	0.46
1:L1:661:G:H2'	1:L1:662:C:H6	1.80	0.46
2:L2:66:A:H2'	2:L2:67:G:O4'	2.15	0.46
2:L2:72:G:OP1	10:LB:251:LEU:N	2.47	0.46
2:L2:742:U:H2'	2:L2:743:C:C6	2.50	0.46
12:LD:122:THR:OG1	12:LD:123:GLY:N	2.47	0.46
30:LV:90:ASP:HB3	30:LV:93:ALA:HB2	1.98	0.46
88:S1:1437:A:H2'	88:S1:1438:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:129:A:C6	49:Lo:42:CYS:HA	2.50	0.46
4:L4:117:C:H2'	4:L4:118:C:O4'	2.15	0.46
8:L8:89:C:H2'	8:L8:90:A:H8	1.80	0.46
13:LE:173:LYS:HB2	47:Lm:127:LEU:HD11	1.97	0.46
52:S4:24:G:H2'	52:S4:25:C:C6	2.50	0.46
54:SA:45:LYS:HE2	54:SA:45:LYS:HB2	1.70	0.46
60:SG:155:ASP:OD2	60:SG:156:VAL:N	2.48	0.46
61:SH:37:HIS:CD2	61:SH:72:LYS:HG2	2.50	0.46
79:SZ:13:ARG:HD2	79:SZ:13:ARG:HA	1.67	0.46
1:L1:113:C:C2	1:L1:114:G:C8	3.04	0.46
1:L1:663:C:O2	41:Lg:128:ALA:HB3	2.14	0.46
1:L1:959:OMG:N1	2:L2:660:G:OP1	2.41	0.46
1:L1:1132:A:OP2	23:LO:135:LYS:NZ	2.48	0.46
1:L1:1750:G:H1	3:L3:170:C:H2'	1.80	0.46
2:L2:955:C:H2'	2:L2:956:C:H6	1.81	0.46
2:L2:1402:G:N2	2:L2:1405:A:OP2	2.38	0.46
2:L2:1483:U:H4'	2:L2:1484:U:H5'	1.96	0.46
6:L6:68:A:H2'	6:L6:70:G:C5	2.50	0.46
11:LC:287:VAL:O	11:LC:291:MET:HG3	2.15	0.46
19:LK:154:MET:HE3	19:LK:154:MET:HB3	1.89	0.46
37:Lc:230:HIS:CE1	37:Lc:238:GLY:HA3	2.50	0.46
52:S4:24:G:H2'	52:S4:25:C:H6	1.81	0.46
55:SB:13:MET:HB2	55:SB:58:TRP:CG	2.51	0.46
62:SI:164:ARG:HH12	88:S1:1018:G:H4'	1.79	0.46
71:SR:117:LYS:HA	71:SR:117:LYS:HD2	1.63	0.46
1:L1:262:C:H5'	31:LW:31:PRO:HD3	1.97	0.46
1:L1:708:A:OP1	24:LP:114:LYS:NZ	2.41	0.46
1:L1:717:G:H2'	1:L1:718:A:C8	2.51	0.46
1:L1:1684:G:H2'	1:L1:1685:G:H8	1.76	0.46
2:L2:564:U:H2'	2:L2:565:OMU:O4'	2.16	0.46
2:L2:565:OMU:HM22	2:L2:565:OMU:H1'	1.63	0.46
2:L2:1150:U:O2'	27:LS:88:ARG:O	2.25	0.46
7:L7:29:C:OP1	17:LI:36:GLN:NE2	2.44	0.46
62:SI:35:LYS:H	62:SI:35:LYS:HD2	1.80	0.46
86:Sg:154:SER:OG	86:Sg:197:VAL:O	2.32	0.46
86:Sg:220:LEU:HD13	86:Sg:230:PHE:CZ	2.51	0.46
88:S1:1662:OMU:HM23	88:S1:1662:OMU:H1'	1.53	0.46
88:S1:1889:G:H5'	88:S1:1890:A:OP2	2.15	0.46
1:L1:24:A:H2'	1:L1:25:C:H6	1.81	0.46
1:L1:522:G:H2'	1:L1:523:A:C8	2.49	0.46
1:L1:766:A:H2'	1:L1:767:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:998:A:H2'	1:L1:999:U:C6	2.51	0.46
2:L2:771:G:N7	9:LA:67:TYR:OH	2.39	0.46
2:L2:1471:G:N7	41:Lg:2:THR:N	2.63	0.46
5:L5:53:G:H2'	5:L5:54:C:H6	1.81	0.46
37:Lc:240:ARG:HB3	37:Lc:243:LEU:HB2	1.96	0.46
70:SQ:94:ARG:HG2	70:SQ:94:ARG:NH1	2.31	0.46
75:SV:104:LYS:HA	75:SV:104:LYS:HD2	1.71	0.46
86:Sg:172:TRP:HA	86:Sg:196:TYR:HB2	1.98	0.46
88:S1:1608:A:H4'	88:S1:1609:U:O5'	2.16	0.46
1:L1:254:U:H5	1:L1:258:A:N7	2.14	0.46
1:L1:1037:A:O2'	37:Lc:132:PRO:O	2.34	0.46
1:L1:1746:C:C2	1:L1:1747:U:C5	3.03	0.46
2:L2:1396:A:H2'	2:L2:1397:OMC:H6	1.80	0.46
3:L3:107:U:H2'	3:L3:108:U:C6	2.51	0.46
3:L3:123:G:N2	3:L3:124:U:O4	2.41	0.46
47:Lm:83:VAL:HG12	47:Lm:87:LYS:HD2	1.98	0.46
69:SP:66:ILE:O	69:SP:68:LYS:NZ	2.47	0.46
73:ST:49:GLN:O	73:ST:53:GLU:HG2	2.15	0.46
82:Sc:14:ARG:NE	88:S1:1362:A:OP1	2.30	0.46
88:S1:1239:A:OP2	88:S1:1258:G:N1	2.33	0.46
88:S1:1889:G:H3'	88:S1:1932:A:N6	2.31	0.46
1:L1:6:C:HO2'	1:L1:7:C:H5	1.58	0.46
1:L1:574:G:H2'	1:L1:577:C:C5	2.50	0.46
1:L1:1231:G:H2'	1:L1:1232:U:C6	2.51	0.46
1:L1:1576:U:H2'	1:L1:1577:U:C6	2.51	0.46
1:L1:1609:A:C5	1:L1:1610:C:C5	3.04	0.46
2:L2:1046:OMG:H1'	2:L2:1046:OMG:HM23	1.68	0.46
2:L2:1195:U:H2'	2:L2:1196:G:C8	2.51	0.46
22:LN:75:TYR:CZ	22:LN:79:ARG:HG3	2.51	0.46
62:SI:82:THR:O	62:SI:86:GLU:HG2	2.15	0.46
73:ST:137:PRO:O	73:ST:138:THR:OG1	2.25	0.46
86:Sg:219:LEU:HD12	86:Sg:231:LYS:HB2	1.95	0.46
87:Sh:147:SER:O	88:S1:198:C:O2'	2.24	0.46
1:L1:33:A:H2'	1:L1:34:C:H6	1.81	0.46
1:L1:963:G:H1	9:LA:208:GLU:CD	2.23	0.46
1:L1:1603:G:H2'	1:L1:1604:U:H6	1.81	0.46
2:L2:93:A:H2'	2:L2:94:A:C8	2.51	0.46
2:L2:1337:C:O2'	13:LE:170:ASP:OD2	2.24	0.46
2:L2:1399:G:H2'	2:L2:1400:U:C6	2.51	0.46
2:L2:1505:A:C6	2:L2:1517:G:C6	3.04	0.46
3:L3:155:A:H61	3:L3:175:A:N6	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L6:36:C:H2'	6:L6:37:C:C6	2.50	0.46
23:LO:107:ARG:NH2	23:LO:119:PHE:O	2.49	0.46
24:LP:153:ARG:O	24:LP:157:ARG:HG2	2.16	0.46
27:LS:119:LYS:HB3	27:LS:119:LYS:HE3	1.71	0.46
31:LW:29:SER:HA	31:LW:46:PRO:HA	1.97	0.46
37:Lc:98:ARG:HA	37:Lc:144:ILE:HG22	1.98	0.46
57:SD:59:LEU:HD21	57:SD:92:LEU:HB3	1.98	0.46
66:SM:88:LEU:HD12	66:SM:95:VAL:HG22	1.97	0.46
82:Sc:12:THR:HG22	88:S1:1359:C:H5'	1.98	0.46
87:Sh:219:ALA:O	87:Sh:223:ILE:HG13	2.16	0.46
88:S1:230:G:OP1	88:S1:281:A:O2'	2.33	0.46
88:S1:1442:U:H5''	88:S1:1443:U:H2'	1.98	0.46
1:L1:574:G:O2'	1:L1:576:G:H2'	2.16	0.46
1:L1:947:A:H5'	9:LA:183:GLY:HA2	1.98	0.46
2:L2:772:A:H2'	2:L2:773:G:C8	2.50	0.46
8:L8:46:A:OP2	8:L8:46:A:H8	1.99	0.46
58:SE:29:ARG:HG2	58:SE:30:PRO:HD2	1.97	0.46
59:SF:100:LYS:HB2	88:S1:1653:U:OP1	2.16	0.46
79:SZ:32:VAL:HG12	79:SZ:34:HIS:HD2	1.81	0.46
79:SZ:93:GLU:OE2	79:SZ:97:ARG:NE	2.42	0.46
88:S1:1560:A:H5''	88:S1:1561:C:OP2	2.16	0.46
88:S1:2185:MA6:H8	88:S1:2185:MA6:H5''	1.97	0.46
1:L1:99:A:H2'	1:L1:100:G:N3	2.31	0.45
1:L1:1017:PSU:H2'	1:L1:1018:A:C8	2.51	0.45
2:L2:749:G:O2'	2:L2:750:U:H6	1.99	0.45
6:L6:20:A:H2'	6:L6:21:A:H8	1.80	0.45
10:LB:291:GLY:HA3	10:LB:328:TYR:CZ	2.51	0.45
21:LM:96:LYS:HD3	21:LM:104:GLN:HE22	1.82	0.45
52:S4:33:U:H1'	61:SH:120:VAL:HG21	1.98	0.45
80:Sa:64:ILE:O	80:Sa:68:ARG:HG2	2.16	0.45
81:Sb:95:ASN:OD1	81:Sb:95:ASN:N	2.48	0.45
86:Sg:298:HIS:CD2	86:Sg:304:ARG:HH11	2.34	0.45
1:L1:92:C:C2	20:LL:55:LYS:HE3	2.52	0.45
1:L1:177:A:H2'	1:L1:178:G:C8	2.50	0.45
1:L1:235:A2M:O5'	1:L1:235:A2M:H8	2.17	0.45
1:L1:1426:A:C2	34:LZ:86:GLY:HA2	2.51	0.45
2:L2:979:A:H2'	2:L2:980:A:H8	1.82	0.45
3:L3:49:A:H2'	3:L3:50:C:C6	2.50	0.45
8:L8:8:U:H2'	8:L8:9:A:H8	1.80	0.45
11:LC:8:SER:OG	11:LC:148:GLU:OE1	2.33	0.45
20:LL:29:GLU:H	20:LL:29:GLU:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:162:GLY:HA2	23:LO:187:PRO:HD3	1.98	0.45
24:LP:71:MET:HE2	24:LP:87:ALA:HB2	1.97	0.45
28:LT:60:PHE:HB3	28:LT:64:ASN:HB3	1.98	0.45
59:SF:162:GLU:HG3	59:SF:163:PRO:HD2	1.96	0.45
68:SO:77:ARG:HH11	68:SO:80:GLU:HB2	1.81	0.45
70:SQ:62:CYS:SG	70:SQ:63:ILE:N	2.89	0.45
86:Sg:27:ILE:HD13	86:Sg:94:LEU:HD13	1.99	0.45
88:S1:1572:C:H5	88:S1:1615:G:H22	1.65	0.45
1:L1:163:U:H2'	1:L1:164:G:C8	2.51	0.45
1:L1:663:C:OP1	16:LH:111:LYS:NZ	2.44	0.45
1:L1:1086:G:H2'	1:L1:1087:A:H8	1.81	0.45
2:L2:21:C:H5''	2:L2:22:A:H5'	1.98	0.45
2:L2:94:A:H2'	2:L2:95:A2M:H8	1.98	0.45
2:L2:386:U:H1'	2:L2:1416:U:H5''	1.98	0.45
2:L2:473:C:H2'	2:L2:474:A:C8	2.51	0.45
2:L2:1101:A:HO2'	2:L2:1102:C:P	2.37	0.45
2:L2:1486:G:H4'	41:Lg:12:LYS:HE2	1.98	0.45
2:L2:1488:C:H2'	2:L2:1489:C:C6	2.51	0.45
11:LC:75:ILE:HG13	11:LC:76:PRO:HD2	1.99	0.45
23:LO:203:ASP:HB3	23:LO:208:LYS:HB3	1.98	0.45
55:SB:148:ILE:HG12	55:SB:162:ILE:HB	1.99	0.45
58:SE:146:TYR:OH	60:SG:209:ARG:NH1	2.46	0.45
61:SH:77:ARG:NH2	88:S1:1945:A:OP1	2.50	0.45
64:SK:68:ALA:HB2	64:SK:201:ILE:HD11	1.98	0.45
70:SQ:46:GLY:HA2	88:S1:1579:A:O2'	2.17	0.45
79:SZ:129:LYS:HD2	88:S1:83:A:H5''	1.97	0.45
1:L1:758:C:H2'	1:L1:759:A:O4'	2.16	0.45
1:L1:850:G:OP2	20:LL:32:ARG:NH1	2.33	0.45
1:L1:1222:A:OP1	41:Lg:120:LYS:NZ	2.49	0.45
2:L2:426:G:H2'	2:L2:427:C:C6	2.50	0.45
2:L2:665:A2M:HM'3	2:L2:665:A2M:H1'	1.79	0.45
4:L4:161:C:H2'	4:L4:162:A:C8	2.52	0.45
10:LB:17:LEU:HD21	10:LB:238:TRP:HH2	1.81	0.45
12:LD:89:LYS:NZ	12:LD:107:GLY:O	2.49	0.45
23:LO:236:MET:HE3	23:LO:236:MET:HB2	1.83	0.45
34:LZ:51:ALA:HB3	34:LZ:96:VAL:HG13	1.98	0.45
37:Lc:69:GLU:HA	37:Lc:69:GLU:OE2	2.17	0.45
52:S4:18:G:H3'	52:S4:18:G:N3	2.31	0.45
60:SG:194:LYS:NZ	88:S1:315:A:OP1	2.34	0.45
64:SK:26:LYS:HG2	64:SK:29:LEU:HD23	1.98	0.45
73:ST:124:ARG:NH2	88:S1:1214:A:OP2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:SW:58:ARG:HH22	88:S1:1974:A:P	2.39	0.45
1:L1:1685:G:H2'	1:L1:1686:C:C6	2.51	0.45
2:L2:84:A:O2'	2:L2:90:G:N7	2.42	0.45
2:L2:340:A:H4'	2:L2:341:A:H5''	1.99	0.45
2:L2:351:C:OP1	25:LQ:88:ARG:NH1	2.50	0.45
2:L2:443:OMC:N4	2:L2:487:U:H2'	2.31	0.45
2:L2:625:U:H2'	2:L2:626:PSU:C6	2.51	0.45
2:L2:653:C:H2'	2:L2:654:U:C6	2.49	0.45
2:L2:1385:G:C2	10:LB:255:ALA:HB1	2.52	0.45
13:LE:13:PRO:O	13:LE:52:ARG:NH2	2.38	0.45
37:Lc:159:TYR:OH	37:Lc:192:GLU:OE2	2.31	0.45
55:SB:92:LYS:HB3	55:SB:92:LYS:HE2	1.71	0.45
88:S1:1590:A:HO2'	88:S1:1591:U:H6	1.65	0.45
88:S1:2012:A:H2'	88:S1:2013:G:C8	2.51	0.45
88:S1:2015:U:H5''	88:S1:2016:C:H5	1.81	0.45
1:L1:479:A:H2'	1:L1:480:U:C6	2.51	0.45
1:L1:626:U:O2'	1:L1:627:C:H6	2.00	0.45
1:L1:1197:G:H2'	1:L1:1198:C:C6	2.51	0.45
2:L2:404:A:O4'	2:L2:406:G:C8	2.70	0.45
4:L4:183:C:H2'	4:L4:184:U:O4'	2.16	0.45
8:L8:93:G:H2'	8:L8:94:A:C8	2.52	0.45
10:LB:400:ARG:HA	10:LB:404:GLU:HG2	1.99	0.45
20:LL:110:LEU:HD23	20:LL:110:LEU:HA	1.75	0.45
41:Lg:56:VAL:C	41:Lg:116:MET:HE3	2.42	0.45
41:Lg:111:HIS:HB3	41:Lg:116:MET:HB3	1.99	0.45
52:S4:19:G:H4'	52:S4:57:G:H22	1.80	0.45
52:S4:21:A:H2'	52:S4:46:G:H1	1.82	0.45
54:SA:139:LEU:HG	54:SA:217:VAL:HG22	1.97	0.45
57:SD:48:LEU:HD23	57:SD:52:ARG:HH21	1.81	0.45
85:Sf:114:GLU:OE1	85:Sf:114:GLU:N	2.50	0.45
88:S1:2086:A:N1	88:S1:2137:U:H5	2.14	0.45
1:L1:1253:OMU:C2	1:L1:1253:OMU:H5'	2.47	0.45
1:L1:1597:G:OP1	46:Ll:50:ASN:HA	2.17	0.45
2:L2:959:A:H2'	2:L2:960:C:C6	2.52	0.45
2:L2:1115:U:H5	23:LO:17:GLN:O	2.00	0.45
2:L2:1116:A:H2'	2:L2:1116:A:N3	2.32	0.45
2:L2:1512:G:C2	39:Le:67:GLY:HA2	2.52	0.45
3:L3:150:A:OP1	45:Lk:35:LYS:NZ	2.41	0.45
4:L4:101:G:H2'	4:L4:102:G:O4'	2.16	0.45
11:LC:63:ALA:HB3	11:LC:91:PHE:CZ	2.52	0.45
60:SG:125:GLU:H	60:SG:125:GLU:CD	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1003:A:H4'	1:L1:1019:G:N2	2.31	0.45
1:L1:1186:A:H2'	1:L1:1187:A:C8	2.52	0.45
1:L1:1761:A:OP2	30:LV:128:ARG:NH2	2.50	0.45
2:L2:29:C:OP1	2:L2:32:C:N4	2.41	0.45
6:L6:68:A:H5'	14:LF:47:ARG:CZ	2.47	0.45
11:LC:55:ARG:HG3	11:LC:56:LEU:HG	1.98	0.45
22:LN:47:PRO:HB3	22:LN:171:TRP:CZ2	2.52	0.45
51:S3:9:G:O2'	51:S3:10:G:N7	2.49	0.45
56:SC:140:LYS:HE2	56:SC:178:ALA:HB1	1.99	0.45
61:SH:157:GLU:CD	80:Sa:61:THR:HG21	2.42	0.45
70:SQ:53:THR:O	70:SQ:59:ALA:HB2	2.17	0.45
77:SX:26:ARG:NH1	88:S1:1948:U:OP2	2.50	0.45
85:Sf:78:ARG:NH1	88:S1:1564:G:OP2	2.50	0.45
88:S1:1209:C:O2'	88:S1:1210:C:OP1	2.31	0.45
88:S1:1961:G:N2	88:S1:1987:G:H1'	2.32	0.45
88:S1:2079:U:H2'	88:S1:2080:G:C8	2.51	0.45
1:L1:205:A:H1'	40:Lf:84:TYR:CE2	2.52	0.45
1:L1:1629:G:O6	42:Lh:11:ARG:NH2	2.44	0.45
1:L1:1686:C:H2'	1:L1:1687:G:C8	2.52	0.45
2:L2:790:U:H2'	2:L2:791:A:H8	1.82	0.45
18:LJ:9:LYS:HD2	18:LJ:9:LYS:HA	1.76	0.45
19:LK:8:CYS:HB3	26:LR:150:SER:HB3	1.99	0.45
35:La:38:THR:O	35:La:38:THR:OG1	2.33	0.45
55:SB:209:ASP:CG	55:SB:211:ASN:H	2.24	0.45
74:SU:20:GLU:C	74:SU:22:ALA:H	2.24	0.45
88:S1:294:G:HO2'	88:S1:295:A:P	2.38	0.45
88:S1:328:C:H2'	88:S1:329:C:C6	2.52	0.45
88:S1:1518:C:H2'	88:S1:1519:G:O4'	2.17	0.45
1:L1:555:U:H2'	1:L1:556:C:O4'	2.17	0.45
1:L1:1006:U:H2'	1:L1:1007:U:C6	2.51	0.45
2:L2:449:U:H2'	2:L2:450:C:C6	2.52	0.45
7:L7:40:A:H2'	7:L7:41:A:C8	2.51	0.45
52:S4:43:C:H2'	52:S4:44:G:H4'	1.99	0.45
58:SE:94:ASP:OD1	58:SE:94:ASP:N	2.49	0.45
60:SG:157:ARG:HG3	60:SG:179:ILE:HD13	1.99	0.45
75:SV:77:GLU:O	75:SV:81:ARG:HG2	2.17	0.45
86:Sg:250:MET:HE2	86:Sg:250:MET:HB3	1.83	0.45
88:S1:263:G:H1	88:S1:274:C:H5	1.63	0.45
1:L1:223:A:N7	4:L4:10:U:H5	2.15	0.44
1:L1:454:U:H2'	1:L1:455:G:H8	1.81	0.44
2:L2:601:G:H4'	28:LT:139:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:30:G:H2'	5:L5:31:C:C6	2.52	0.44
7:L7:7:U:H2'	7:L7:8:C:C6	2.52	0.44
11:LC:118:GLN:HE21	11:LC:118:GLN:HB2	1.59	0.44
13:LE:96:ALA:O	47:Lm:77:VAL:N	2.50	0.44
56:SC:177:ARG:CZ	84:Se:64:LYS:H	2.28	0.44
70:SQ:106:ARG:HA	70:SQ:111:GLU:HA	1.98	0.44
79:SZ:111:ARG:NH1	88:S1:507:G:OP2	2.36	0.44
87:Sh:148:THR:HG22	87:Sh:196:ARG:HE	1.82	0.44
1:L1:61:A:N3	1:L1:76:U:O2'	2.49	0.44
1:L1:196:C:O2'	1:L1:198:A:OP2	2.35	0.44
1:L1:824:U:O2'	1:L1:1128:A:N6	2.50	0.44
1:L1:1019:G:H2'	1:L1:1020:C:C6	2.52	0.44
1:L1:1357:G:H4'	26:LR:117:ARG:HG2	1.99	0.44
1:L1:1770:U:H2'	1:L1:1771:U:C6	2.52	0.44
2:L2:69:A:O4'	5:L5:18:A:H5'	2.18	0.44
2:L2:79:C:O2'	4:L4:81:G:H4'	2.17	0.44
12:LD:77:LYS:HA	12:LD:77:LYS:HD2	1.66	0.44
28:LT:36:ILE:HD12	28:LT:114:ILE:HD13	1.99	0.44
52:S4:44:G:H2'	52:S4:44:G:N3	2.31	0.44
79:SZ:105:LYS:HD2	88:S1:503:C:C4	2.53	0.44
81:Sb:88:VAL:HG22	88:S1:2200:A:C6	2.52	0.44
86:Sg:188:ARG:NH1	86:Sg:224:SER:O	2.51	0.44
88:S1:328:C:O2'	88:S1:329:C:OP1	2.31	0.44
1:L1:545:A:H3'	1:L1:546:G:H4'	1.99	0.44
1:L1:1659:OMU:O5'	1:L1:1659:OMU:H6	2.17	0.44
2:L2:615:G:H2'	2:L2:616:G:C8	2.52	0.44
2:L2:1024:U:O2'	21:LM:126:THR:HB	2.18	0.44
2:L2:1424:U:C2	2:L2:1425:A:C8	3.06	0.44
3:L3:176:U:H2'	3:L3:177:U:O4'	2.17	0.44
6:L6:59:C:H5''	14:LF:69:MET:HE3	1.98	0.44
7:L7:62:A:H4'	7:L7:63:G:O5'	2.18	0.44
8:L8:30:C:H2'	8:L8:31:A:O4'	2.17	0.44
11:LC:146:VAL:HG22	34:LZ:74:PRO:HG2	1.98	0.44
19:LK:89:LYS:HB2	19:LK:89:LYS:HE2	1.81	0.44
58:SE:244:MET:HE3	58:SE:244:MET:HB2	1.76	0.44
66:SM:18:ARG:HB3	66:SM:112:THR:HG23	1.99	0.44
67:SN:53:MET:HG3	67:SN:73:TRP:CE3	2.52	0.44
77:SX:50:MET:HE2	77:SX:112:PRO:HG3	1.98	0.44
80:Sa:29:LYS:H	80:Sa:29:LYS:HD2	1.82	0.44
86:Sg:238:ILE:HA	86:Sg:254:THR:HG22	1.98	0.44
1:L1:398:G:N2	1:L1:401:A:OP2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:578:G:H2'	1:L1:579:G:H8	1.83	0.44
1:L1:701:G:H2'	1:L1:702:A:H8	1.83	0.44
1:L1:925:U:OP2	2:L2:91:C:O2'	2.35	0.44
2:L2:469:G:H2'	2:L2:470:A:C8	2.53	0.44
2:L2:1110:U:H2'	2:L2:1111:C:C6	2.52	0.44
2:L2:1370:U:O2	2:L2:1372:A2M:H8	2.17	0.44
2:L2:1485:G:O6	41:Lg:7:HIS:HB3	2.18	0.44
17:LI:140:LYS:HE3	17:LI:140:LYS:HB2	1.69	0.44
38:Ld:18:LEU:HD13	38:Ld:100:SER:HA	1.99	0.44
61:SH:72:LYS:NZ	88:S1:2031:A:OP1	2.40	0.44
79:SZ:124:LEU:HB3	79:SZ:128:ALA:HB3	1.98	0.44
86:Sg:122:ILE:HB	86:Sg:134:TRP:HB2	1.98	0.44
87:Sh:226:HIS:HA	87:Sh:229:TYR:CE2	2.52	0.44
88:S1:293:U:O2'	88:S1:295:A:N7	2.47	0.44
88:S1:756:C:N4	88:S1:772:A:H62	2.15	0.44
88:S1:783:A:H61	88:S1:835:C:H42	1.66	0.44
1:L1:839:U:H2'	1:L1:840:G:C8	2.52	0.44
1:L1:1092:U:O2'	1:L1:1093:U:H5'	2.18	0.44
2:L2:382:A2M:HM'3	2:L2:382:A2M:H1'	1.85	0.44
2:L2:1003:G:O2'	2:L2:1004:G:H8	2.00	0.44
2:L2:1319:C:H2'	2:L2:1320:U:C6	2.53	0.44
2:L2:1333:G:O2'	47:Lm:100:TYR:O	2.35	0.44
14:LF:194:ASN:OD1	14:LF:195:TRP:N	2.51	0.44
15:LG:64:ARG:HD2	15:LG:64:ARG:HA	1.85	0.44
23:LO:83:LEU:HB3	23:LO:88:ILE:HB	1.99	0.44
55:SB:114:GLN:HG2	55:SB:115:ILE:HG23	2.00	0.44
57:SD:118:ALA:HB1	57:SD:123:HIS:HB3	1.99	0.44
57:SD:181:ARG:HB3	57:SD:181:ARG:NH1	2.33	0.44
64:SK:25:MET:HA	88:S1:443:A:H5'	1.98	0.44
81:Sb:86:ARG:HG3	81:Sb:86:ARG:NH1	2.29	0.44
1:L1:32:A:H2'	1:L1:33:A:C8	2.53	0.44
1:L1:1403:A:H2'	1:L1:1404:U:C6	2.53	0.44
1:L1:1409:U:H2'	1:L1:1410:U:C6	2.52	0.44
2:L2:667:OMU:HM23	2:L2:667:OMU:H1'	1.68	0.44
2:L2:795:U:O2'	2:L2:798:G:O6	2.31	0.44
8:L8:27:A:H2'	8:L8:28:A:C8	2.53	0.44
12:LD:100:ASP:OD1	12:LD:100:ASP:N	2.50	0.44
32:LX:82:VAL:HG21	60:SG:9:ARG:HG2	2.00	0.44
57:SD:132:HIS:ND1	57:SD:161:SER:HB2	2.32	0.44
70:SQ:61:MET:SD	70:SQ:123:ILE:HD13	2.57	0.44
88:S1:679:A:H5'	88:S1:680:G:OP2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:S1:1171:A:H2'	88:S1:1172:G:C8	2.53	0.44
88:S1:2129:C:H2'	88:S1:2130:A:C8	2.53	0.44
1:L1:307:U:H2'	1:L1:308:A:H8	1.83	0.44
1:L1:369:A:O2'	44:Lj:58:ARG:NH2	2.51	0.44
1:L1:419:A:H3'	1:L1:420:C:H6	1.83	0.44
1:L1:495:C:O2'	14:LF:21:ARG:HD3	2.18	0.44
1:L1:1052:A:N1	8:L8:106:C:O2'	2.46	0.44
2:L2:613:A:H2'	2:L2:614:A:C8	2.53	0.44
2:L2:1240:A:H5'	50:Lp:56:PRO:HB3	1.99	0.44
2:L2:1485:G:C2	19:LK:164:MET:HE1	2.52	0.44
4:L4:1:G:H1'	6:L6:3:A:H5'	1.99	0.44
12:LD:55:THR:OG1	12:LD:63:ARG:N	2.51	0.44
25:LQ:181:ARG:HA	25:LQ:181:ARG:HD2	1.86	0.44
40:Lf:98:SER:HB2	40:Lf:101:VAL:HG23	1.99	0.44
57:SD:81:GLU:HG3	57:SD:148:ARG:HG2	2.00	0.44
58:SE:36:ARG:HA	58:SE:36:ARG:HD3	1.86	0.44
60:SG:139:LYS:HE3	60:SG:139:LYS:HB3	1.66	0.44
65:SL:128:ARG:HB3	88:S1:2004:G:C8	2.53	0.44
87:Sh:194:GLU:OE2	87:Sh:197:GLY:N	2.44	0.44
88:S1:640:A:H2'	88:S1:641:A:C8	2.52	0.44
88:S1:1708:A:N1	88:S1:1764:U:H5	2.15	0.44
88:S1:1781:U:O2'	88:S1:1782:G:N7	2.46	0.44
1:L1:422:PSU:H2'	1:L1:423:U:C6	2.53	0.44
1:L1:514:C:H5''	26:LR:70:LYS:HG3	2.00	0.44
2:L2:1082:U:H4'	2:L2:1083:A:O4'	2.18	0.44
10:LB:291:GLY:HA3	10:LB:328:TYR:CE1	2.53	0.44
11:LC:261:ILE:O	11:LC:269:SER:OG	2.35	0.44
17:LI:136:LYS:HE2	17:LI:136:LYS:HB2	1.67	0.44
24:LP:80:LYS:H	24:LP:80:LYS:HG2	1.50	0.44
39:Le:37:ARG:O	39:Le:41:VAL:HG13	2.17	0.44
51:S3:33:U:OP2	65:SL:149:ARG:NH1	2.40	0.44
51:S3:48:C:C4	51:S3:59:A:C8	3.06	0.44
56:SC:31:GLU:HG2	56:SC:57:VAL:HG12	1.99	0.44
56:SC:53:LYS:HB3	56:SC:56:GLU:OE1	2.17	0.44
58:SE:63:ARG:NH1	88:S1:497:A:OP2	2.50	0.44
58:SE:95:ARG:HH21	58:SE:112:SER:HA	1.83	0.44
59:SF:167:PRO:HB2	59:SF:168:MET:HE3	2.00	0.44
67:SN:94:MET:HE3	67:SN:98:GLN:HG2	2.00	0.44
77:SX:95:LYS:HE2	88:S1:1942:A:O3'	2.17	0.44
1:L1:160:C:C2	1:L1:161:A:C8	3.06	0.44
1:L1:1292:G:N2	1:L1:1343:A:N1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:382:A2M:H2	2:L2:389:A:N7	2.33	0.44
3:L3:204:A:H2'	3:L3:205:A:H8	1.80	0.44
7:L7:18:G:H2'	7:L7:19:A:C8	2.52	0.44
16:LH:214:GLU:H	16:LH:214:GLU:HG2	1.65	0.44
59:SF:242:TRP:CD2	63:SJ:68:ARG:HD2	2.53	0.44
62:SI:90:PRO:HB3	88:S1:995:U:H5''	2.00	0.44
73:ST:73:ARG:NH1	88:S1:914:G:H5'	2.32	0.44
88:S1:1170:A:H2'	88:S1:1171:A:C8	2.52	0.44
88:S1:1859:A:H2'	88:S1:1859:A:N3	2.32	0.44
1:L1:464:A:N3	2:L2:609:A:H4'	2.33	0.43
1:L1:1007:U:H2'	1:L1:1008:C:C6	2.53	0.43
1:L1:1558:U:O2'	39:Le:161:ASN:OD1	2.33	0.43
1:L1:1582:A:H2'	1:L1:1583:C:H6	1.82	0.43
2:L2:1183:C:H2'	2:L2:1184:C:O4'	2.18	0.43
2:L2:1195:U:H2'	2:L2:1196:G:H8	1.82	0.43
6:L6:44:G:H2'	6:L6:45:G:C8	2.53	0.43
11:LC:343:MET:HE3	11:LC:343:MET:HB3	1.88	0.43
15:LG:166:TRP:HE1	21:LM:7:LEU:HD12	1.83	0.43
23:LO:132:VAL:HG13	23:LO:178:ALA:HB1	1.99	0.43
37:Lc:129:MET:HE1	37:Lc:137:LEU:HD12	1.99	0.43
47:Lm:94:LYS:HD2	47:Lm:105:VAL:O	2.18	0.43
53:S5:8:U:O2	88:S1:2159:A:H8	1.99	0.43
61:SH:140:MET:HG2	61:SH:162:GLU:HG3	2.00	0.43
1:L1:36:U:H2'	1:L1:37:A:O4'	2.18	0.43
1:L1:595:C:C2	1:L1:596:A:C8	3.06	0.43
1:L1:1099:A:H2'	22:LN:22:PHE:CZ	2.54	0.43
2:L2:451:U:O2	88:S1:1160:A:H2	2.01	0.43
2:L2:659:A:H2'	2:L2:660:G:H8	1.83	0.43
2:L2:949:U:H2'	2:L2:950:G:H8	1.83	0.43
2:L2:959:A:H2'	2:L2:960:C:H6	1.84	0.43
2:L2:1069:A:H2'	2:L2:1070:A:C8	2.51	0.43
2:L2:1175:A:OP1	23:LO:182:ARG:HD3	2.18	0.43
2:L2:1262:G:H2'	2:L2:1263:C:C6	2.52	0.43
3:L3:117:C:H2'	3:L3:118:G:C8	2.53	0.43
50:Lp:23:PHE:HB3	50:Lp:72:LEU:HB3	2.00	0.43
52:S4:64:A:H2'	52:S4:65:G:C8	2.53	0.43
60:SG:177:PRO:HA	88:S1:66:U:H5'	1.99	0.43
71:SR:85:LEU:HD12	71:SR:96:THR:HG22	1.98	0.43
73:ST:140:LYS:HA	73:ST:140:LYS:HD3	1.80	0.43
1:L1:25:C:H42	1:L1:55:A:N6	2.15	0.43
1:L1:301:A:O3'	43:Li:39:HIS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:371:U:H2'	1:L1:372:A:C8	2.53	0.43
1:L1:606:C:H2'	1:L1:607:C:C6	2.53	0.43
1:L1:632:A:C6	11:LC:308:LYS:HG2	2.53	0.43
1:L1:687:C:OP1	40:Lf:28:GLN:HB2	2.18	0.43
1:L1:794:U:O2'	1:L1:795:U:H5'	2.18	0.43
1:L1:823:G:H2'	1:L1:823:G:N3	2.32	0.43
1:L1:1345:C:H3'	1:L1:1346:C:C6	2.54	0.43
2:L2:93:A:H2'	2:L2:94:A:H8	1.83	0.43
2:L2:426:G:H2'	2:L2:427:C:H6	1.82	0.43
2:L2:762:U:H2'	2:L2:763:C:C6	2.52	0.43
8:L8:124:U:H1'	23:LO:267:LYS:NZ	2.32	0.43
19:LK:151:ALA:O	19:LK:155:ASP:HB2	2.18	0.43
22:LN:115:MET:HA	22:LN:115:MET:HE3	2.00	0.43
25:LQ:177:GLU:OE2	88:S1:968:G:N2	2.50	0.43
38:Ld:34:THR:O	38:Ld:38:GLN:HG2	2.18	0.43
41:Lg:75:VAL:HG11	41:Lg:119:VAL:HG11	2.00	0.43
46:Ll:38:ASN:HB3	46:Ll:41:ARG:HG2	2.00	0.43
50:Lp:68:ILE:HB	50:Lp:85:LEU:HB2	2.00	0.43
51:S3:10:G:N2	51:S3:26:G:H1'	2.33	0.43
56:SC:27:GLU:HG2	56:SC:68:LEU:HD21	2.01	0.43
56:SC:58:LEU:HG	56:SC:87:VAL:HG11	2.00	0.43
57:SD:77:ARG:NH2	88:S1:865:U:OP2	2.48	0.43
57:SD:122:HIS:CE1	84:Se:37:ARG:HB2	2.53	0.43
60:SG:227:ASP:OD2	60:SG:228:HIS:N	2.51	0.43
65:SL:107:GLU:C	65:SL:109:ALA:H	2.25	0.43
71:SR:31:LEU:O	71:SR:34:VAL:HG13	2.18	0.43
75:SV:35:ILE:HA	75:SV:38:VAL:HG22	1.99	0.43
76:SW:63:LEU:HD13	76:SW:85:THR:HB	1.99	0.43
76:SW:103:ILE:HD11	76:SW:123:LEU:HD22	2.00	0.43
86:Sg:102:LYS:HB3	86:Sg:102:LYS:HE2	1.73	0.43
88:S1:836:C:H2'	88:S1:837:G:H8	1.84	0.43
88:S1:2121:C:H2'	88:S1:2122:G:H8	1.83	0.43
1:L1:1662:G:H4'	1:L1:1663:U:OP1	2.19	0.43
2:L2:110:C:H5''	49:Lo:8:MET:SD	2.58	0.43
2:L2:1003:G:O2'	2:L2:1004:G:O5'	2.36	0.43
2:L2:1028:A:H2'	2:L2:1029:G:C8	2.53	0.43
5:L5:53:G:H2'	5:L5:54:C:C6	2.54	0.43
23:LO:250:LYS:HE2	23:LO:250:LYS:HB2	1.69	0.43
36:Lb:22:LYS:HA	36:Lb:22:LYS:HD2	1.94	0.43
55:SB:30:THR:O	55:SB:31:ARG:HB3	2.16	0.43
75:SV:71:LEU:HB2	75:SV:74:GLN:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:Sh:163:GLN:HE21	87:Sh:178:ASP:HA	1.84	0.43
88:S1:1409:U:H2'	88:S1:1410:C:C6	2.53	0.43
88:S1:1572:C:H41	88:S1:1615:G:H1	1.64	0.43
1:L1:700:A:H4'	24:LP:172:TYR:CE1	2.54	0.43
1:L1:790:C:H5	11:LC:305:LEU:H	1.67	0.43
1:L1:1369:G:C2	16:LH:78:LYS:HD3	2.53	0.43
1:L1:1582:A:H2'	1:L1:1583:C:C6	2.53	0.43
2:L2:1397:OMC:HM22	2:L2:1398:C:O4'	2.18	0.43
5:L5:51:A:C8	5:L5:53:G:C8	3.06	0.43
5:L5:68:G:H5'	64:SK:92:ARG:HG2	1.99	0.43
11:LC:66:TRP:HB3	11:LC:70:ARG:HD3	2.00	0.43
38:Ld:38:GLN:HG2	38:Ld:38:GLN:H	1.63	0.43
44:Lj:4:GLY:O	44:Lj:8:MET:HG2	2.18	0.43
54:SA:11:LYS:HE2	88:S1:1160:A:C2	2.54	0.43
55:SB:31:ARG:O	55:SB:31:ARG:HG2	2.16	0.43
55:SB:191:THR:HG22	55:SB:192:ILE:HG23	2.01	0.43
64:SK:8:LEU:HB3	64:SK:20:ILE:HG12	1.99	0.43
71:SR:88:GLN:O	71:SR:96:THR:OG1	2.25	0.43
1:L1:128:U:H2'	1:L1:129:C:H6	1.83	0.43
2:L2:447:G:H1'	9:LA:222:PRO:HG2	2.01	0.43
4:L4:44:G:H2'	4:L4:45:G:H8	1.82	0.43
4:L4:144:G:H3'	4:L4:145:C:H6	1.83	0.43
6:L6:51:A:H5'	6:L6:52:G:C8	2.54	0.43
7:L7:17:U:H2'	7:L7:18:G:C8	2.53	0.43
11:LC:63:ALA:HA	11:LC:77:ARG:O	2.18	0.43
21:LM:124:ASP:OD1	21:LM:125:SER:N	2.52	0.43
46:Ll:13:TYR:CE2	46:Ll:51:TYR:HB2	2.54	0.43
46:Ll:30:ARG:HE	46:Ll:30:ARG:HB2	1.64	0.43
51:S3:22:G:H2'	51:S3:23:C:H6	1.83	0.43
60:SG:91:TYR:HE2	88:S1:447:G:H4'	1.84	0.43
84:Se:23:LYS:HE3	84:Se:23:LYS:HB2	1.79	0.43
86:Sg:180:ASN:HD21	86:Sg:183:GLY:HA3	1.83	0.43
88:S1:12:PSU:H2'	88:S1:13:U:C6	2.53	0.43
1:L1:64:A:N1	1:L1:75:A:H5''	2.34	0.43
1:L1:1202:G:C5	1:L1:1203:C:C5	3.07	0.43
1:L1:1350:U:C2'	1:L1:1351:C:H5'	2.48	0.43
2:L2:1488:C:H2'	2:L2:1489:C:H6	1.83	0.43
4:L4:161:C:H2'	4:L4:162:A:H8	1.83	0.43
14:LF:66:SER:O	14:LF:66:SER:OG	2.27	0.43
19:LK:141:LYS:HA	19:LK:141:LYS:HD3	1.71	0.43
33:LY:76:ASN:OD1	33:LY:77:HIS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Lf:3:LYS:HB3	40:Lf:3:LYS:HE3	1.73	0.43
55:SB:57:MET:HG3	55:SB:165:PRO:O	2.19	0.43
62:SI:25:LYS:HE3	62:SI:25:LYS:HB2	1.81	0.43
82:Sc:39:PRO:HD2	82:Sc:62:LYS:NZ	2.34	0.43
88:S1:431:G:OP2	88:S1:466:G:O2'	2.32	0.43
1:L1:661:G:H2'	1:L1:662:C:C6	2.54	0.43
9:LA:107:ILE:O	9:LA:139:HIS:NE2	2.45	0.43
10:LB:286:LYS:NZ	10:LB:359:GLU:O	2.50	0.43
27:LS:151:ALA:HA	27:LS:154:GLU:OE2	2.19	0.43
29:LU:96:LYS:HE3	29:LU:96:LYS:HB3	1.72	0.43
30:LV:60:ILE:HD12	35:La:26:LYS:HE3	2.00	0.43
50:Lp:46:LYS:HE3	50:Lp:54:THR:HB	2.00	0.43
55:SB:6:SER:HB3	78:SY:46:PRO:HD3	2.01	0.43
61:SH:129:PRO:HA	61:SH:132:ARG:HG3	2.01	0.43
70:SQ:30:VAL:HA	70:SQ:33:VAL:HG12	2.00	0.43
72:SS:30:ALA:HB2	88:S1:1551:G:H5''	2.00	0.43
86:Sg:219:LEU:HD23	86:Sg:221:TRP:HZ2	1.82	0.43
88:S1:2014:C:N4	88:S1:2015:U:O4	2.51	0.43
88:S1:2015:U:H5''	88:S1:2016:C:C5	2.54	0.43
1:L1:890:C:O4'	3:L3:124:U:H5''	2.18	0.43
1:L1:1050:G:H2'	1:L1:1051:C:C6	2.53	0.43
1:L1:1153:A:H2'	1:L1:1155:A:H62	1.84	0.43
1:L1:1177:PSU:C4	1:L1:1178:U:C5	3.07	0.43
2:L2:354:A:H2'	2:L2:355:A:C8	2.54	0.43
2:L2:530:C:N4	2:L2:554:C:OP2	2.49	0.43
2:L2:1101:A:H5''	12:LD:107:GLY:HA3	2.01	0.43
16:LH:127:PRO:HG2	16:LH:130:VAL:HG23	2.00	0.43
59:SF:90:ASP:OD2	59:SF:90:ASP:C	2.62	0.43
60:SG:25:ARG:HD2	60:SG:25:ARG:H	1.84	0.43
74:SU:64:LEU:HD23	74:SU:64:LEU:HA	1.90	0.43
1:L1:599:G:P	27:LS:139:ARG:HH21	2.42	0.43
2:L2:6:A:H2'	2:L2:7:C:O4'	2.19	0.43
2:L2:1006:G:H2'	2:L2:1007:U:H6	1.81	0.43
2:L2:1251:A:H2'	2:L2:1252:G:O4'	2.19	0.43
3:L3:66:C:H2'	3:L3:67:A:H8	1.83	0.43
13:LE:16:VAL:O	13:LE:52:ARG:NH2	2.52	0.43
18:LJ:5:GLN:HA	18:LJ:128:TRP:CZ3	2.54	0.43
23:LO:83:LEU:N	23:LO:84:PRO:HD2	2.34	0.43
25:LQ:126:ARG:HH12	25:LQ:141:HIS:CE1	2.37	0.43
33:LY:91:LYS:HB3	33:LY:91:LYS:HE3	1.64	0.43
50:Lp:56:PRO:O	52:S4:75:C:O2'	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S4:37:A:C5	52:S4:38:A:H1'	2.54	0.43
62:SI:2:GLN:HB2	62:SI:5:LEU:HD23	2.01	0.43
86:Sg:193:HIS:ND1	86:Sg:215:ASP:OD2	2.42	0.43
1:L1:1214:G:H2'	1:L1:1215:C:O4'	2.19	0.42
1:L1:1728:A:O2'	1:L1:1729:A:H8	2.02	0.42
2:L2:1042:G:H2'	2:L2:1043:C:H6	1.84	0.42
2:L2:1104:G:H2'	2:L2:1104:G:N3	2.34	0.42
7:L7:91:A:H2'	7:L7:92:C:C6	2.54	0.42
8:L8:97:A:H2'	8:L8:98:C:H6	1.84	0.42
25:LQ:190:ARG:HD3	25:LQ:190:ARG:HA	1.75	0.42
52:S4:39:U:C2	52:S4:40:C:C5	3.07	0.42
56:SC:199:PRO:O	56:SC:201:GLU:N	2.50	0.42
57:SD:112:VAL:HG13	57:SD:117:LEU:HB2	2.01	0.42
69:SP:54:LYS:NZ	69:SP:94:ILE:O	2.30	0.42
77:SX:155:LYS:HD2	77:SX:155:LYS:HA	1.55	0.42
79:SZ:15:SER:HA	88:S1:879:A:H61	1.84	0.42
86:Sg:188:ARG:HD3	86:Sg:226:GLY:HA3	2.01	0.42
2:L2:381:U:H2'	2:L2:382:A2M:C8	2.49	0.42
2:L2:1007:U:H2'	2:L2:1008:C:C6	2.54	0.42
20:LL:64:LYS:O	20:LL:67:PRO:HD2	2.20	0.42
23:LO:41:LYS:HA	23:LO:41:LYS:HD2	1.86	0.42
29:LU:47:PHE:HE1	29:LU:77:LEU:HD22	1.84	0.42
50:Lp:28:TYR:HB3	50:Lp:69:VAL:HB	2.00	0.42
65:SL:88:ARG:NH2	65:SL:119:ASP:OD2	2.52	0.42
77:SX:80:ARG:HD3	88:S1:1938:C:C4	2.54	0.42
81:Sb:83:ILE:HD13	88:S1:2197:G:H1'	2.01	0.42
86:Sg:158:PHE:HE1	86:Sg:181:VAL:HG21	1.84	0.42
88:S1:1166:C:H2'	88:S1:1167:A:C8	2.54	0.42
1:L1:1683:C:H42	1:L1:1709:U:H3	1.67	0.42
1:L1:1683:C:N4	1:L1:1710:U:O4	2.52	0.42
2:L2:603:A:H5'	28:LT:137:THR:CG2	2.48	0.42
4:L4:55:A:H2'	4:L4:56:G:O4'	2.20	0.42
5:L5:63:G:H2'	5:L5:64:G:N3	2.34	0.42
7:L7:4:G:OP1	28:LT:62:ARG:HD3	2.19	0.42
7:L7:58:G:N7	44:Lj:63:ARG:NH2	2.54	0.42
8:L8:52:G:H5'	23:LO:232:PHE:CE1	2.54	0.42
18:LJ:125:ALA:HB1	18:LJ:132:SER:HB2	2.00	0.42
26:LR:12:VAL:O	26:LR:61:LEU:N	2.46	0.42
31:LW:56:LYS:HB3	31:LW:56:LYS:HE2	1.74	0.42
54:SA:29:TRP:CZ2	68:SO:12:PRO:HD3	2.54	0.42
58:SE:261:LYS:HE2	58:SE:261:LYS:HB3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SG:45:GLU:CD	60:SG:46:PHE:H	2.25	0.42
64:SK:187:ARG:HB2	64:SK:203:LEU:HD21	2.01	0.42
67:SN:5:VAL:O	88:S1:1609:U:H1'	2.20	0.42
68:SO:15:LYS:N	68:SO:15:LYS:HD3	2.34	0.42
70:SQ:68:CYS:C	70:SQ:69:GLU:HG2	2.44	0.42
74:SU:52:LYS:NZ	74:SU:59:THR:HG22	2.34	0.42
86:Sg:103:PHE:HB3	86:Sg:134:TRP:CZ3	2.55	0.42
88:S1:558:U:H5	88:S1:587:A:N7	2.17	0.42
88:S1:1905:C:O2'	88:S1:1906:G:O5'	2.34	0.42
1:L1:1185:U:H2'	1:L1:1186:A:O4'	2.19	0.42
2:L2:464:G:H2'	2:L2:465:A:C8	2.55	0.42
2:L2:1477:U:H2'	2:L2:1478:C:C6	2.54	0.42
4:L4:79:U:C2	4:L4:80:A:C8	3.08	0.42
12:LD:34:ARG:NE	12:LD:122:THR:O	2.51	0.42
14:LF:93:ILE:O	14:LF:93:ILE:HG22	2.18	0.42
18:LJ:70:GLU:H	18:LJ:70:GLU:CD	2.27	0.42
21:LM:143:ARG:O	35:La:103:GLU:HB3	2.20	0.42
39:Le:75:LYS:HD3	39:Le:75:LYS:HA	1.80	0.42
41:Lg:4:SER:OG	41:Lg:6:VAL:HG22	2.19	0.42
52:S4:25:C:C2	52:S4:26:A:C8	3.08	0.42
57:SD:47:THR:O	57:SD:51:MET:HG3	2.20	0.42
61:SH:111:SER:OG	61:SH:122:ARG:NH2	2.52	0.42
72:SS:10:ARG:NH2	88:S1:1853:U:OP1	2.52	0.42
86:Sg:16:SER:OG	86:Sg:71:VAL:HG12	2.19	0.42
88:S1:1117:A:H2'	88:S1:1118:G:C8	2.54	0.42
1:L1:1086:G:C4	1:L1:1087:A:C8	3.07	0.42
2:L2:696:A:C6	2:L2:697:G:C6	3.08	0.42
2:L2:1127:G:O2'	2:L2:1132:A:N1	2.48	0.42
4:L4:149:U:H1'	4:L4:150:A:H2'	2.01	0.42
6:L6:11:G:C8	14:LF:186:PRO:HG2	2.55	0.42
7:L7:76:C:H2'	7:L7:77:A:O4'	2.18	0.42
23:LO:126:ASP:HA	23:LO:202:ARG:HG3	2.01	0.42
33:LY:54:VAL:O	33:LY:57:MET:HG3	2.19	0.42
43:Li:57:GLU:HG2	43:Li:93:MET:SD	2.59	0.42
55:SB:15:GLU:CD	55:SB:15:GLU:H	2.27	0.42
59:SF:213:ARG:HD3	88:S1:1449:U:C4	2.54	0.42
60:SG:172:ASP:O	88:S1:73:A:N6	2.53	0.42
67:SN:66:TYR:OH	67:SN:69:ARG:HA	2.19	0.42
88:S1:961:U:H2'	88:S1:962:A:C8	2.54	0.42
1:L1:6:C:C2	1:L1:7:C:C5	3.08	0.42
1:L1:65:A:O2'	1:L1:353:C:O2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:107:C:H4'	1:L1:361:A:H2	1.85	0.42
1:L1:141:U:C1'	1:L1:142:G:H5''	2.48	0.42
1:L1:273:A:H2'	1:L1:274:A:O4'	2.18	0.42
1:L1:774:PSU:H2'	1:L1:775:G:C8	2.55	0.42
1:L1:951:G:H1'	1:L1:1739:A:N6	2.35	0.42
2:L2:14:OMC:H2'	2:L2:15:C:H6	1.84	0.42
2:L2:750:U:H1'	2:L2:751:U:H5'	2.01	0.42
2:L2:968:U:O4	2:L2:969:A:N6	2.53	0.42
3:L3:168:U:H2'	3:L3:169:A:C5	2.55	0.42
30:LV:134:ASP:O	30:LV:138:THR:HG23	2.20	0.42
35:La:53:LYS:HA	35:La:53:LYS:HD3	1.76	0.42
68:SO:50:THR:OG1	88:S1:1147:A:OP1	2.33	0.42
69:SP:48:LYS:HE3	69:SP:48:LYS:HB2	1.87	0.42
1:L1:7:C:H2'	1:L1:8:U:C6	2.55	0.42
1:L1:1090:U:H2'	1:L1:1091:A:H8	1.82	0.42
1:L1:1105:A:H5''	2:L2:1064:A:H61	1.84	0.42
1:L1:1402:U:H2'	1:L1:1403:A:C8	2.53	0.42
1:L1:1772:G:O2'	7:L7:140:U:O2'	2.33	0.42
2:L2:348:A:H2'	2:L2:349:C:O4'	2.19	0.42
2:L2:460:A:H2'	2:L2:461:C:O4'	2.19	0.42
3:L3:100:U:H2'	3:L3:101:G:C8	2.54	0.42
4:L4:1:G:H2'	4:L4:2:U:C6	2.55	0.42
4:L4:139:U:O2'	13:LE:151:GLU:OE2	2.33	0.42
7:L7:77:A:O2'	35:La:42:GLU:HG2	2.20	0.42
7:L7:89:U:H2'	7:L7:90:U:C6	2.54	0.42
9:LA:159:PRO:O	9:LA:162:SER:OG	2.35	0.42
14:LF:172:LYS:HE2	14:LF:172:LYS:HB2	1.71	0.42
19:LK:3:LYS:HA	19:LK:3:LYS:HD2	1.88	0.42
55:SB:40:TYR:CD1	55:SB:56:MET:HE2	2.54	0.42
60:SG:140:ARG:HB3	60:SG:143:LYS:HG3	2.01	0.42
67:SN:63:LYS:HB3	67:SN:63:LYS:HE3	1.69	0.42
86:Sg:255:GLU:HB3	86:Sg:281:GLU:CD	2.45	0.42
88:S1:1576:A:H61	88:S1:1611:C:H41	1.67	0.42
88:S1:1619:G:O2'	88:S1:1849:G:O2'	2.36	0.42
88:S1:1891:A:O2'	88:S1:1908:A:N6	2.53	0.42
1:L1:221:C:H2'	1:L1:222:A:C8	2.55	0.42
1:L1:495:C:OP1	14:LF:28:THR:OG1	2.24	0.42
1:L1:808:A:H5''	36:Lb:30:HIS:CE1	2.55	0.42
2:L2:555:A:N3	2:L2:1399:G:O2'	2.50	0.42
2:L2:780:G:H2'	2:L2:781:G:C8	2.54	0.42
2:L2:783:U:N3	2:L2:800:G:OP1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1320:U:H2'	2:L2:1321:U:H6	1.85	0.42
3:L3:100:U:H2'	3:L3:101:G:H8	1.84	0.42
3:L3:138:U:H2'	3:L3:139:C:C6	2.55	0.42
17:LI:65:CYS:HB2	17:LI:70:HIS:O	2.20	0.42
33:LY:35:GLU:OE1	33:LY:35:GLU:N	2.53	0.42
48:Ln:3:THR:HG23	88:S1:2195:G:O2'	2.19	0.42
55:SB:125:LEU:HD23	55:SB:147:VAL:HG22	2.01	0.42
57:SD:119:LYS:H	57:SD:119:LYS:HG2	1.66	0.42
75:SV:78:ARG:HA	75:SV:81:ARG:HE	1.85	0.42
86:Sg:219:LEU:HD23	86:Sg:221:TRP:CZ2	2.55	0.42
87:Sh:156:LEU:HD22	87:Sh:200:LEU:HD11	2.02	0.42
88:S1:30:G:H2'	88:S1:31:C:C6	2.55	0.42
88:S1:227:U:H3	88:S1:261:A:HO2'	1.67	0.42
1:L1:745:U:O2'	1:L1:815:G:N3	2.53	0.42
1:L1:1092:U:H4'	22:LN:193:ARG:NH1	2.35	0.42
2:L2:342:U:O2'	2:L2:343:U:H6	2.02	0.42
2:L2:560:OMU:HM23	2:L2:560:OMU:H1'	1.55	0.42
2:L2:599:G:H5''	28:LT:86:LYS:HB2	2.02	0.42
2:L2:1003:G:O2'	2:L2:1004:G:C8	2.73	0.42
2:L2:1267:U:C2	2:L2:1268:G:C8	3.07	0.42
4:L4:149:U:OP2	47:Lm:111:ARG:HD3	2.20	0.42
7:L7:71:A:H4'	7:L7:72:A:H5'	2.01	0.42
16:LH:189:LYS:C	16:LH:191:ALA:H	2.26	0.42
17:LI:90:LEU:HD21	17:LI:125:MET:HE2	2.02	0.42
28:LT:112:MET:SD	28:LT:152:GLU:HG2	2.60	0.42
44:Lj:27:TYR:HA	44:Lj:34:CYS:HA	2.02	0.42
52:S4:40:C:H5''	68:SO:56:LYS:HE3	2.02	0.42
54:SA:85:LYS:HE2	54:SA:85:LYS:HB2	1.86	0.42
78:SY:33:ASP:C	78:SY:35:ALA:H	2.28	0.42
82:Sc:54:SER:OG	82:Sc:63:LYS:HE2	2.19	0.42
86:Sg:283:ILE:HD11	86:Sg:299:LYS:HZ3	1.84	0.42
88:S1:67:C:O2'	88:S1:69:C:OP1	2.35	0.42
1:L1:37:A:H5''	20:LL:35:ALA:HB2	2.01	0.42
1:L1:1524:OMG:H5''	1:L1:1527:OMC:C5	2.54	0.42
3:L3:191:C:H4'	3:L3:192:G:O5'	2.19	0.42
5:L5:5:C:H2'	5:L5:6:G:O4'	2.20	0.42
11:LC:316:PRO:HD3	11:LC:324:ARG:NH2	2.35	0.42
14:LF:37:ALA:HA	14:LF:90:THR:HG22	2.02	0.42
14:LF:97:ASP:C	14:LF:99:ALA:H	2.28	0.42
23:LO:134:THR:OG1	23:LO:137:ASP:OD1	2.26	0.42
51:S3:23:C:H2'	51:S3:24:U:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SA:207:LEU:HD23	54:SA:208:PRO:HD2	2.02	0.42
55:SB:70:ALA:HB2	78:SY:42:ALA:HB2	2.02	0.42
67:SN:94:MET:HB3	67:SN:98:GLN:HB3	2.02	0.42
70:SQ:112:VAL:HG23	70:SQ:113:THR:HG23	2.00	0.42
82:Sc:7:ASP:OD1	82:Sc:9:SER:OG	2.36	0.42
88:S1:659:G:H4'	88:S1:661:OMU:H5	2.02	0.42
88:S1:2090:A:H2'	88:S1:2091:G:O4'	2.19	0.42
1:L1:517:U:H2'	1:L1:518:C:H6	1.83	0.41
1:L1:814:C:H2'	1:L1:815:G:C8	2.54	0.41
1:L1:897:A:H2'	1:L1:898:A:O4'	2.20	0.41
2:L2:528:U:O2	2:L2:556:U:H4'	2.20	0.41
3:L3:34:C:O2	3:L3:34:C:H2'	2.20	0.41
10:LB:140:LYS:HE3	10:LB:140:LYS:HB3	1.82	0.41
11:LC:113:LYS:CG	21:LM:203:LYS:HB3	2.49	0.41
19:LK:78:LEU:HD12	19:LK:78:LEU:HA	1.90	0.41
19:LK:148:LEU:HD23	19:LK:148:LEU:HA	1.89	0.41
20:LL:72:THR:HG22	20:LL:108:LYS:HB3	2.02	0.41
26:LR:94:LYS:HE2	26:LR:94:LYS:HB3	1.98	0.41
52:S4:27:G:N2	52:S4:44:G:O2'	2.52	0.41
74:SU:88:GLY:HA3	74:SU:101:ILE:HD12	2.02	0.41
76:SW:107:HIS:CE1	76:SW:131:ARG:HH22	2.38	0.41
81:Sb:68:MET:HE3	81:Sb:68:MET:HB3	1.78	0.41
88:S1:639:C:H2'	88:S1:640:A:C8	2.55	0.41
88:S1:1193:U:H2'	88:S1:1194:C:C6	2.55	0.41
1:L1:495:C:O2	1:L1:495:C:H2'	2.20	0.41
1:L1:738:C:H2'	1:L1:739:U:C6	2.56	0.41
2:L2:88:C:H2'	2:L2:89:G:O4'	2.20	0.41
2:L2:535:U:C2	2:L2:536:C:C5	3.09	0.41
18:LJ:106:ASN:OD1	18:LJ:110:GLU:N	2.53	0.41
43:Li:59:ARG:HA	43:Li:59:ARG:HD2	1.82	0.41
57:SD:84:PHE:CE1	57:SD:103:ILE:HG13	2.56	0.41
67:SN:62:ILE:HG22	67:SN:75:LEU:HD23	2.02	0.41
74:SU:93:THR:O	74:SU:93:THR:HG22	2.20	0.41
86:Sg:196:TYR:CZ	86:Sg:214:LYS:HB2	2.55	0.41
88:S1:15:U:H2'	88:S1:16:G:O4'	2.20	0.41
88:S1:634:A:H2'	88:S1:635:G:C8	2.54	0.41
88:S1:2178:U:H2'	88:S1:2179:A:C8	2.54	0.41
1:L1:214:C:N4	1:L1:215:U:O4	2.53	0.41
1:L1:636:U:H2'	1:L1:637:C:H6	1.84	0.41
2:L2:474:A:H2'	2:L2:475:C:H6	1.85	0.41
2:L2:490:A:H5''	9:LA:243:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1199:A:C5	50:Lp:16:ARG:HD2	2.54	0.41
4:L4:98:A:H2'	4:L4:99:A:C8	2.54	0.41
6:L6:24:C:OP1	13:LE:23:ARG:NH1	2.52	0.41
7:L7:37:U:OP1	7:L7:38:U:O2'	2.35	0.41
7:L7:71:A:O2'	7:L7:83:A:N6	2.38	0.41
7:L7:101:PSU:H2'	7:L7:102:G:C8	2.55	0.41
13:LE:184:THR:OG1	13:LE:185:ASN:N	2.53	0.41
20:LL:36:GLY:O	20:LL:41:HIS:HB2	2.19	0.41
26:LR:42:ARG:HA	26:LR:42:ARG:HD2	1.90	0.41
55:SB:13:MET:HB2	55:SB:58:TRP:CD1	2.55	0.41
70:SQ:96:LYS:O	70:SQ:99:GLN:NE2	2.53	0.41
77:SX:11:ILE:HG22	88:S1:1725:C:O2	2.20	0.41
88:S1:98:A2M:H8	88:S1:98:A2M:O5'	2.20	0.41
88:S1:1914:U:H2'	88:S1:1915:U:O4'	2.20	0.41
88:S1:2140:OMC:H1'	88:S1:2140:OMC:HM23	1.85	0.41
1:L1:205:A:C5	34:LZ:55:PRO:HG3	2.55	0.41
1:L1:311:A:H2'	1:L1:312:C:C6	2.55	0.41
1:L1:706:G:HO2'	11:LC:117:HIS:HD1	1.66	0.41
1:L1:755:A:H2'	1:L1:756:U:C6	2.56	0.41
1:L1:941:C:O2	2:L2:570:A2M:H2	2.19	0.41
7:L7:26:U:H2'	7:L7:27:U:C6	2.55	0.41
8:L8:92:U:H2'	8:L8:93:G:O4'	2.20	0.41
9:LA:180:LEU:HD22	49:Lo:18:TYR:HB3	2.02	0.41
11:LC:209:VAL:HG22	11:LC:228:ALA:HB3	2.02	0.41
31:LW:71:TYR:C	31:LW:73:LEU:H	2.29	0.41
45:Lk:5:ILE:HD11	45:Lk:43:TYR:HB3	2.02	0.41
54:SA:96:ARG:HG3	54:SA:243:ALA:HB2	2.01	0.41
62:SI:34:HIS:O	62:SI:38:ARG:HB2	2.20	0.41
68:SO:128:ILE:O	88:S1:1133:U:O2'	2.37	0.41
76:SW:107:HIS:HE1	76:SW:131:ARG:HH22	1.68	0.41
80:Sa:71:ILE:HB	80:Sa:75:ILE:HD11	2.03	0.41
81:Sb:74:LYS:NZ	88:S1:1180:A:OP1	2.52	0.41
83:Sd:68:LYS:HB3	83:Sd:68:LYS:HE2	1.79	0.41
85:Sf:98:LEU:HD23	85:Sf:98:LEU:HA	1.85	0.41
1:L1:207:C:N3	34:LZ:80:LYS:NZ	2.59	0.41
1:L1:1263:A:O2'	1:L1:1264:A:O5'	2.33	0.41
1:L1:1550:A:H2'	1:L1:1551:A:C8	2.56	0.41
2:L2:113:A:OP2	2:L2:114:A:O2'	2.35	0.41
2:L2:432:U:H5'	2:L2:560:OMU:OP2	2.20	0.41
2:L2:679:C:O2	2:L2:1023:C:H5	2.04	0.41
2:L2:772:A:OP1	9:LA:37:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:775:C:OP1	2:L2:776:C:O2'	2.34	0.41
2:L2:1287:C:O2'	2:L2:1288:G:H8	2.03	0.41
4:L4:102:G:H2'	4:L4:103:C:H6	1.86	0.41
7:L7:26:U:H2'	7:L7:27:U:H6	1.85	0.41
31:LW:3:SER:O	31:LW:5:LYS:N	2.54	0.41
32:LX:6:CYS:HB2	32:LX:36:SER:HB2	2.03	0.41
51:S3:4:G:H2'	51:S3:5:G:C8	2.56	0.41
55:SB:154:ASP:OD1	55:SB:154:ASP:N	2.52	0.41
58:SE:16:MET:HG2	88:S1:889:A:C2	2.55	0.41
62:SI:164:ARG:HD3	62:SI:164:ARG:HA	1.84	0.41
75:SV:3:LYS:HE2	88:S1:1814:U:O2	2.19	0.41
75:SV:43:SER:HB3	75:SV:46:LEU:HB2	2.02	0.41
77:SX:131:GLN:HG2	77:SX:131:GLN:O	2.20	0.41
85:Sf:112:LYS:HD2	85:Sf:112:LYS:HA	1.92	0.41
86:Sg:209:CYS:HB2	86:Sg:223:LEU:HD11	2.03	0.41
88:S1:280:C:H2'	88:S1:281:A:H5''	2.02	0.41
88:S1:1291:U:H2'	88:S1:1292:PSU:C6	2.56	0.41
1:L1:289:U:H2'	1:L1:290:G:C8	2.56	0.41
1:L1:1102:U:H5''	27:LS:19:PHE:HB2	2.03	0.41
1:L1:1165:A:H2'	1:L1:1166:C:C6	2.56	0.41
1:L1:1542:A:N3	2:L2:592:C:O2'	2.51	0.41
1:L1:1571:C:H2'	1:L1:1572:A:O4'	2.20	0.41
2:L2:1337:C:H2'	2:L2:1337:C:H6	1.74	0.41
2:L2:1404:G:C5'	9:LA:220:GLY:HA3	2.51	0.41
3:L3:121:U:O2'	3:L3:123:G:N7	2.47	0.41
3:L3:122:U:O4'	25:LQ:96:MET:HG2	2.21	0.41
13:LE:66:ILE:O	13:LE:69:LEU:HG	2.21	0.41
25:LQ:179:LYS:HE3	25:LQ:179:LYS:HB2	1.83	0.41
37:Lc:129:MET:HE3	37:Lc:129:MET:HA	2.03	0.41
55:SB:59:GLU:OE1	78:SY:83:MET:HG3	2.21	0.41
88:S1:934:U:O2'	88:S1:936:U:OP2	2.38	0.41
88:S1:2118:G:O2'	88:S1:2119:C:O5'	2.38	0.41
1:L1:248:A:OP2	11:LC:221:ASN:HB2	2.21	0.41
1:L1:273:A:C6	44:Lj:79:LYS:HA	2.55	0.41
1:L1:568:U:OP1	1:L1:640:U:H5	2.03	0.41
1:L1:659:G:H2'	1:L1:660:U:C6	2.55	0.41
2:L2:502[A]:A:H61	88:S1:2159:A:H2'	1.86	0.41
2:L2:692:U:H2'	2:L2:693:C:O4'	2.21	0.41
2:L2:974:G:N2	33:LY:133:ARG:O	2.52	0.41
11:LC:264:THR:HG22	11:LC:265:PHE:N	2.36	0.41
13:LE:63:LYS:HE3	13:LE:63:LYS:HB3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LF:53:ILE:HA	14:LF:65:VAL:HG12	2.03	0.41
14:LF:104:GLU:CD	14:LF:104:GLU:N	2.78	0.41
14:LF:104:GLU:HA	14:LF:107:GLN:HG2	2.01	0.41
24:LP:29:LEU:HD23	24:LP:29:LEU:HA	1.90	0.41
47:Lm:123:MET:HE3	47:Lm:123:MET:HB3	1.88	0.41
52:S4:19:G:H4'	52:S4:57:G:N2	2.35	0.41
54:SA:245:GLN:H	54:SA:245:GLN:HG3	1.61	0.41
62:SI:41:LEU:N	62:SI:42:PRO:HD2	2.35	0.41
76:SW:89:ASP:OD1	76:SW:89:ASP:N	2.53	0.41
88:S1:17:C:H2'	88:S1:18:OMC:C6	2.55	0.41
88:S1:761:A:H62	88:S1:768:A:N6	2.18	0.41
88:S1:1496:U:H2'	88:S1:1497:U:C6	2.55	0.41
88:S1:2121:C:H2'	88:S1:2122:G:C8	2.56	0.41
1:L1:114:G:H4'	21:LM:49:ARG:HG2	2.03	0.41
1:L1:662:C:C2	1:L1:663:C:C5	3.08	0.41
1:L1:1397:C:O2'	1:L1:1398:C:H5'	2.21	0.41
1:L1:1685:G:H1	1:L1:1707:U:H3	1.67	0.41
2:L2:390:A:H1'	2:L2:527:A2M:N6	2.36	0.41
7:L7:156:A:OP1	7:L7:158:U:H5	2.04	0.41
25:LQ:137:ASN:HD22	25:LQ:137:ASN:HA	1.69	0.41
31:LW:24:ARG:O	31:LW:28:MET:HG3	2.21	0.41
40:Lf:77:ILE:HD11	40:Lf:97:ILE:HG12	2.03	0.41
52:S4:38:A:OP1	52:S4:38:A:H4'	2.21	0.41
55:SB:36:ALA:HB1	55:SB:157:LEU:HD12	2.03	0.41
57:SD:114:LYS:HA	57:SD:114:LYS:HD3	1.84	0.41
58:SE:171:LYS:HB3	58:SE:171:LYS:HE3	1.79	0.41
58:SE:174:GLN:HA	58:SE:192:ILE:HB	2.01	0.41
64:SK:64:ASN:OD1	88:S1:305:U:O2'	2.31	0.41
69:SP:48:LYS:HE3	88:S1:478:C:H5''	2.03	0.41
80:Sa:97:LYS:HA	80:Sa:97:LYS:HD3	1.78	0.41
88:S1:836:C:H2'	88:S1:837:G:C8	2.56	0.41
1:L1:119:C:H2'	1:L1:120:G:O4'	2.20	0.41
1:L1:458:A:H2'	1:L1:459:A:O4'	2.20	0.41
1:L1:599:G:H2'	1:L1:600:C:C6	2.56	0.41
1:L1:678:A2M:HM'3	1:L1:678:A2M:H1'	1.71	0.41
1:L1:1371:OMU:HM23	1:L1:1371:OMU:H1'	1.69	0.41
1:L1:1538:U:H2'	1:L1:1539:A2M:H8	2.03	0.41
1:L1:1608:A:C4	1:L1:1609:A:C8	3.09	0.41
2:L2:787:G:H2'	2:L2:788:C:C6	2.56	0.41
2:L2:1086:G:H4'	2:L2:1179:A:O2'	2.21	0.41
2:L2:1151:U:H2'	2:L2:1152:PSU:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1388:G:OP1	10:LB:246:LYS:NZ	2.50	0.41
2:L2:1521:A:H2'	2:L2:1522:U:H6	1.85	0.41
4:L4:164:U:H4'	10:LB:349:MET:HE1	2.03	0.41
5:L5:30:G:H2'	5:L5:31:C:H6	1.85	0.41
7:L7:46:G:H2'	7:L7:47:C:C6	2.55	0.41
10:LB:353:THR:HA	10:LB:358:LYS:HE2	2.02	0.41
12:LD:165:PHE:CE2	12:LD:171:GLY:HA3	2.56	0.41
13:LE:44:ASP:HB3	13:LE:57:ILE:HB	2.03	0.41
19:LK:85:GLU:OE2	19:LK:85:GLU:N	2.49	0.41
22:LN:77:VAL:HG22	22:LN:82:LYS:HB3	2.02	0.41
22:LN:99:ILE:HG22	22:LN:123:ASN:HB2	2.02	0.41
25:LQ:174:ARG:NE	88:S1:1101:A:O5'	2.53	0.41
30:LV:81:GLU:H	30:LV:81:GLU:HG2	1.65	0.41
31:LW:24:ARG:HD3	31:LW:72:ARG:O	2.20	0.41
39:Le:131:LEU:HA	39:Le:172:ASN:HB2	2.03	0.41
40:Lf:112:LYS:HA	40:Lf:112:LYS:HD3	1.84	0.41
55:SB:71:VAL:HG13	55:SB:123:ARG:HH21	1.85	0.41
60:SG:108:ASP:OD1	60:SG:108:ASP:N	2.51	0.41
62:SI:9:ARG:HH21	88:S1:967:A:H5'	1.86	0.41
86:Sg:93:ASP:OD1	86:Sg:95:ARG:HG3	2.21	0.41
86:Sg:193:HIS:CE1	86:Sg:219:LEU:HD22	2.56	0.41
88:S1:98:A2M:HM'3	88:S1:98:A2M:H1'	1.93	0.41
88:S1:811:C:O2'	88:S1:812:A:H8	2.04	0.41
88:S1:1582:A:N6	88:S1:1607:G:H1'	2.36	0.41
88:S1:1870:A:H4'	88:S1:1960:G:H4'	2.02	0.41
1:L1:24:A:N3	1:L1:366:C:O2'	2.46	0.41
1:L1:254:U:H4'	31:LW:97:HIS:CD2	2.56	0.41
1:L1:371:U:H2'	1:L1:372:A:H8	1.86	0.41
1:L1:697:A2M:H2'	1:L1:698:A:C8	2.56	0.41
1:L1:786:A:H2'	1:L1:787:A:C8	2.56	0.41
1:L1:1105:A:H5''	2:L2:1064:A:N6	2.36	0.41
1:L1:1390:G:O4'	26:LR:3:LYS:HE3	2.21	0.41
1:L1:1561:A:C8	1:L1:1562:C:C6	3.09	0.41
2:L2:1135:U:H2'	2:L2:1136:U:O4'	2.21	0.41
2:L2:1523:C:H2'	2:L2:1524:A:C8	2.56	0.41
4:L4:147:U:H2'	4:L4:149:U:OP1	2.20	0.41
5:L5:48:G:H2'	5:L5:49:G:C2	2.56	0.41
7:L7:12:A:H2'	7:L7:13:U:C6	2.56	0.41
19:LK:161:LYS:O	19:LK:164:MET:HB2	2.20	0.41
23:LO:10:LYS:HB2	23:LO:10:LYS:HE2	1.95	0.41
57:SD:1:MET:HE2	57:SD:1:MET:HB2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SD:88:GLU:OE2	57:SD:88:GLU:N	2.47	0.41
62:SI:3:PRO:O	62:SI:6:ARG:HG2	2.21	0.41
87:Sh:222:VAL:HG23	88:S1:275:A:H5'	2.03	0.41
88:S1:826:A:H2'	88:S1:827:G:C8	2.56	0.41
1:L1:38:A:H5''	20:LL:35:ALA:HB1	2.04	0.40
1:L1:67:C:O2'	1:L1:100:G:O2'	2.33	0.40
1:L1:456:A:H2'	1:L1:457:C:O4'	2.21	0.40
1:L1:481:U:H2'	1:L1:482:U:C6	2.56	0.40
1:L1:754:G:C2	20:LL:114:HIS:HB2	2.56	0.40
1:L1:1775:U:H2'	1:L1:1776:G:H8	1.84	0.40
2:L2:459:A:O2'	2:L2:1029:G:H5'	2.21	0.40
10:LB:57:VAL:HG22	10:LB:73:VAL:HG22	2.03	0.40
14:LF:191:HIS:CD2	14:LF:192:ARG:HG2	2.56	0.40
15:LG:165:LEU:HD21	21:LM:18:VAL:HG21	2.03	0.40
15:LG:166:TRP:CD1	15:LG:166:TRP:H	2.39	0.40
28:LT:67:ILE:HD11	28:LT:80:LYS:HB3	2.03	0.40
29:LU:68:VAL:HA	29:LU:81:THR:HB	2.03	0.40
31:LW:86:LYS:HE3	31:LW:86:LYS:HB3	1.91	0.40
44:Lj:17:ILE:HG12	44:Lj:29:VAL:HG22	2.02	0.40
52:S4:9:A:O2'	52:S4:10:G:N7	2.46	0.40
52:S4:40:C:C2	52:S4:41:C:C5	3.09	0.40
55:SB:25:ARG:HB3	55:SB:28:ILE:HG13	2.02	0.40
69:SP:67:ARG:NH2	88:S1:618:C:H41	2.19	0.40
79:SZ:13:ARG:N	79:SZ:31:GLU:O	2.47	0.40
86:Sg:269:ILE:H	86:Sg:269:ILE:HG12	1.68	0.40
88:S1:1702:A:N1	88:S1:1773:U:H5	2.19	0.40
1:L1:812:A:H2'	1:L1:813:C:H6	1.86	0.40
1:L1:819:C:H2'	1:L1:820:U:O4'	2.21	0.40
1:L1:1038:U:H2'	1:L1:1039:U:C6	2.57	0.40
1:L1:1062:A:H2'	1:L1:1063:G:C8	2.56	0.40
2:L2:535:U:H2'	2:L2:536:C:H6	1.85	0.40
2:L2:610:G:H22	2:L2:642:G:H1'	1.86	0.40
3:L3:151:A:H5'	45:Lk:26:LYS:HE2	2.03	0.40
4:L4:134:U:H2'	4:L4:135:C:O4'	2.21	0.40
5:L5:38:U:H2'	5:L5:39:G:O4'	2.22	0.40
6:L6:11:G:C4	6:L6:12:C:C5	3.08	0.40
11:LC:264:THR:HG22	11:LC:265:PHE:H	1.87	0.40
19:LK:23:ARG:NH1	19:LK:43:ASP:OD1	2.54	0.40
24:LP:16:ARG:HD3	24:LP:20:TYR:CZ	2.55	0.40
26:LR:14:ARG:HG3	26:LR:15:GLU:O	2.22	0.40
29:LU:97:PHE:HD2	29:LU:98:LEU:HD23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Lg:34:TYR:CD1	41:Lg:136:ARG:HG2	2.56	0.40
62:SI:113:GLN:HE21	62:SI:113:GLN:HB2	1.72	0.40
68:SO:92:ALA:H	68:SO:126:THR:HG22	1.87	0.40
86:Sg:135:ASN:HB3	86:Sg:139:GLU:OE1	2.20	0.40
88:S1:676:C:H2'	88:S1:677:G:O4'	2.21	0.40
88:S1:1186:A:H2'	88:S1:1187:A:C8	2.56	0.40
1:L1:246:A:H4'	1:L1:248:A:N7	2.36	0.40
1:L1:419:A:O2'	31:LW:88:ASN:HA	2.21	0.40
1:L1:1747:U:OP1	42:Lh:34:GLN:NE2	2.52	0.40
2:L2:120:A:H2'	2:L2:121:U:C6	2.56	0.40
2:L2:406:G:H2'	2:L2:407:C:H6	1.83	0.40
2:L2:597:PSU:H2'	2:L2:598:A:H8	1.86	0.40
2:L2:766:A:H2'	2:L2:767:U:C6	2.56	0.40
2:L2:1431:C:H2'	2:L2:1432:U:O4'	2.22	0.40
4:L4:181:C:C2	4:L4:182:A:C8	3.09	0.40
7:L7:102:G:OP2	7:L7:104:A:O2'	2.39	0.40
10:LB:261:HIS:HA	10:LB:262:PRO:C	2.46	0.40
11:LC:356:LYS:HE3	11:LC:356:LYS:HB3	1.93	0.40
12:LD:34:ARG:HB2	12:LD:125:TYR:OH	2.21	0.40
18:LJ:90:LYS:HA	18:LJ:90:LYS:HD2	1.99	0.40
55:SB:37:MET:HG3	55:SB:152:ASP:O	2.21	0.40
56:SC:177:ARG:NH1	84:Se:63:GLY:HA2	2.37	0.40
60:SG:45:GLU:OE2	60:SG:46:PHE:N	2.39	0.40
73:ST:21:THR:HG1	82:Sc:86:HIS:HE2	1.61	0.40
82:Sc:38:CYS:HB3	82:Sc:41:CYS:HB2	1.75	0.40
85:Sf:97:ALA:HA	85:Sf:100:TYR:CD2	2.56	0.40
87:Sh:196:ARG:NH2	88:S1:198:C:O2'	2.55	0.40
88:S1:139:C:H2'	88:S1:140:G:C8	2.55	0.40
88:S1:433:G:H2'	88:S1:434:A:O4'	2.21	0.40
88:S1:1701:A:H2'	88:S1:1702:A:C8	2.56	0.40
88:S1:1932:A:O2'	88:S1:1934:A:OP2	2.31	0.40
88:S1:2146:U:H2'	88:S1:2147:A:H8	1.85	0.40
1:L1:124:C:H2'	1:L1:125:G:H8	1.86	0.40
1:L1:225:C:O2'	1:L1:226:C:O5'	2.39	0.40
1:L1:688:A:OP2	40:Lf:28:GLN:HG3	2.21	0.40
1:L1:719:U:O2'	1:L1:720:A:H5''	2.22	0.40
1:L1:731:U:H2'	1:L1:732:A:H8	1.86	0.40
1:L1:843:C:H2'	1:L1:844:C:H6	1.81	0.40
1:L1:927:A2M:HM'3	1:L1:927:A2M:H1'	1.80	0.40
1:L1:1473:G:OP1	11:LC:204:ARG:NH1	2.54	0.40
1:L1:1772:G:H2'	1:L1:1773:C:H6	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:598:A:H5''	28:LT:83:TRP:O	2.22	0.40
6:L6:7:A:H1'	41:Lg:99:THR:OG1	2.22	0.40
12:LD:39:LEU:HD12	12:LD:39:LEU:HA	1.95	0.40
25:LQ:136:ARG:HE	25:LQ:136:ARG:HB3	1.48	0.40
44:Lj:55:LYS:HA	44:Lj:58:ARG:HD2	2.03	0.40
52:S4:19:G:H4'	52:S4:57:G:H1	1.86	0.40
69:SP:36:ARG:HE	69:SP:36:ARG:HB3	1.65	0.40
71:SR:79:LYS:HA	71:SR:79:LYS:HD3	1.93	0.40
82:Sc:60:CYS:CB	82:Sc:62:LYS:HE3	2.49	0.40
86:Sg:190:LEU:HB3	86:Sg:221:TRP:CZ3	2.56	0.40
87:Sh:190:LYS:HA	87:Sh:190:LYS:HD3	1.81	0.40
87:Sh:227:ARG:CZ	87:Sh:227:ARG:HB2	2.51	0.40
88:S1:157:G:H1	88:S1:167:C:H42	1.69	0.40
88:S1:699:A:H2'	88:S1:700:G:O4'	2.21	0.40
88:S1:1956:C:O2	88:S1:1956:C:H2'	2.22	0.40
88:S1:2021:A2M:H8	88:S1:2021:A2M:H5''	2.04	0.40
1:L1:130:U:H2'	1:L1:132:A:H62	1.86	0.40
1:L1:325:C:H2'	1:L1:326:A:H8	1.86	0.40
1:L1:728:C:H4'	1:L1:729:A:H5''	2.04	0.40
1:L1:1010:OMC:HM22	1:L1:1010:OMC:H1'	1.66	0.40
1:L1:1107:OMU:H6	1:L1:1107:OMU:O5'	2.22	0.40
1:L1:1148:A:C6	1:L1:1151:A:C8	3.10	0.40
1:L1:1479:A:H4'	1:L1:1480:C:O5'	2.21	0.40
2:L2:132:G:H2'	2:L2:133:G:H8	1.86	0.40
14:LF:89:THR:HG21	19:LK:108:PHE:HB2	2.04	0.40
26:LR:91:ARG:HD2	27:LS:150:VAL:HG13	2.04	0.40
30:LV:77:LYS:HE3	30:LV:81:GLU:OE2	2.22	0.40
37:Lc:208:VAL:O	37:Lc:212:MET:HG3	2.22	0.40
53:S5:8:U:O2'	88:S1:2159:A:H1'	2.22	0.40
60:SG:111:LEU:HD13	88:S1:159:C:H5'	2.04	0.40
64:SK:197:ARG:NH2	88:S1:306:U:O2'	2.54	0.40
81:Sb:31:LEU:HD23	81:Sb:31:LEU:HA	1.92	0.40
88:S1:281:A:H2'	88:S1:281:A:N3	2.37	0.40
88:S1:1416:G:C2	88:S1:1430:C:H5''	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LA	256/260 (98%)	249 (97%)	7 (3%)	0	100	100
10	LB	402/419 (96%)	396 (98%)	6 (2%)	0	100	100
11	LC	364/373 (98%)	352 (97%)	12 (3%)	0	100	100
12	LD	173/188 (92%)	171 (99%)	2 (1%)	0	100	100
13	LE	184/190 (97%)	176 (96%)	8 (4%)	0	100	100
14	LF	144/195 (74%)	139 (96%)	5 (4%)	0	100	100
15	LG	238/264 (90%)	235 (99%)	3 (1%)	0	100	100
16	LH	219/222 (99%)	216 (99%)	3 (1%)	0	100	100
17	LI	212/220 (96%)	206 (97%)	6 (3%)	0	100	100
18	LJ	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
19	LK	167/175 (95%)	162 (97%)	5 (3%)	0	100	100
20	LL	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
21	LM	201/204 (98%)	200 (100%)	1 (0%)	0	100	100
22	LN	197/213 (92%)	191 (97%)	6 (3%)	0	100	100
23	LO	294/305 (96%)	286 (97%)	8 (3%)	0	100	100
24	LP	195/198 (98%)	191 (98%)	3 (2%)	1 (0%)	24	43
25	LQ	199/254 (78%)	199 (100%)	0	0	100	100
26	LR	176/179 (98%)	175 (99%)	1 (1%)	0	100	100
27	LS	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
28	LT	149/166 (90%)	145 (97%)	4 (3%)	0	100	100
29	LU	120/129 (93%)	118 (98%)	2 (2%)	0	100	100
30	LV	117/145 (81%)	115 (98%)	2 (2%)	0	100	100
31	LW	119/143 (83%)	116 (98%)	2 (2%)	1 (1%)	16	31
32	LX	81/124 (65%)	79 (98%)	2 (2%)	0	100	100
33	LY	131/134 (98%)	130 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	LZ	143/147 (97%)	143 (100%)	0	0	100	100
35	La	122/127 (96%)	120 (98%)	2 (2%)	0	100	100
36	Lb	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
37	Lc	227/252 (90%)	221 (97%)	6 (3%)	0	100	100
38	Ld	92/104 (88%)	92 (100%)	0	0	100	100
39	Le	184/188 (98%)	184 (100%)	0	0	100	100
40	Lf	126/133 (95%)	121 (96%)	5 (4%)	0	100	100
41	Lg	141/144 (98%)	141 (100%)	0	0	100	100
42	Lh	125/168 (74%)	122 (98%)	3 (2%)	0	100	100
43	Li	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
44	Lj	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
45	Lk	74/83 (89%)	74 (100%)	0	0	100	100
46	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
47	Lm	50/128 (39%)	50 (100%)	0	0	100	100
48	Ln	31/34 (91%)	28 (90%)	3 (10%)	0	100	100
49	Lo	87/92 (95%)	81 (93%)	6 (7%)	0	100	100
50	Lp	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
54	SA	232/264 (88%)	228 (98%)	4 (2%)	0	100	100
55	SB	209/246 (85%)	202 (97%)	7 (3%)	0	100	100
56	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
57	SD	181/190 (95%)	181 (100%)	0	0	100	100
58	SE	258/273 (94%)	251 (97%)	7 (3%)	0	100	100
59	SF	220/265 (83%)	213 (97%)	7 (3%)	0	100	100
60	SG	225/249 (90%)	222 (99%)	3 (1%)	0	100	100
61	SH	179/190 (94%)	172 (96%)	7 (4%)	0	100	100
62	SI	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
63	SJ	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
64	SK	188/220 (86%)	187 (100%)	1 (0%)	0	100	100
65	SL	142/149 (95%)	139 (98%)	3 (2%)	0	100	100
66	SM	99/116 (85%)	98 (99%)	1 (1%)	0	100	100
67	SN	97/168 (58%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	SO	135/144 (94%)	131 (97%)	4 (3%)	0	100	100
69	SP	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
70	SQ	95/141 (67%)	85 (90%)	9 (10%)	1 (1%)	11	22
71	SR	132/153 (86%)	131 (99%)	1 (1%)	0	100	100
72	SS	54/57 (95%)	54 (100%)	0	0	100	100
73	ST	141/151 (93%)	135 (96%)	6 (4%)	0	100	100
74	SU	140/173 (81%)	136 (97%)	4 (3%)	0	100	100
75	SV	120/143 (84%)	119 (99%)	1 (1%)	0	100	100
76	SW	113/152 (74%)	112 (99%)	1 (1%)	0	100	100
77	SX	150/161 (93%)	143 (95%)	7 (5%)	0	100	100
78	SY	86/164 (52%)	83 (96%)	3 (4%)	0	100	100
79	SZ	128/137 (93%)	125 (98%)	3 (2%)	0	100	100
80	Sa	80/120 (67%)	77 (96%)	3 (4%)	0	100	100
81	Sb	102/112 (91%)	101 (99%)	1 (1%)	0	100	100
82	Sc	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
83	Sd	64/87 (74%)	62 (97%)	1 (2%)	1 (2%)	7	14
84	Se	59/66 (89%)	56 (95%)	3 (5%)	0	100	100
85	Sf	42/152 (28%)	41 (98%)	1 (2%)	0	100	100
86	Sg	296/312 (95%)	288 (97%)	8 (3%)	0	100	100
87	Sh	94/235 (40%)	93 (99%)	1 (1%)	0	100	100
All	All	11377/12926 (88%)	11128 (98%)	245 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
70	SQ	112	VAL
24	LP	189	SER
31	LW	4	ILE
83	Sd	76	MET

### 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	
9	LA	200/204 (98%)	196 (98%)	4 (2%)	48	75
10	LB	337/351 (96%)	334 (99%)	3 (1%)	70	87
11	LC	291/301 (97%)	283 (97%)	8 (3%)	39	67
12	LD	147/162 (91%)	143 (97%)	4 (3%)	39	67
13	LE	166/172 (96%)	159 (96%)	7 (4%)	26	52
14	LF	121/153 (79%)	115 (95%)	6 (5%)	22	44
15	LG	199/221 (90%)	198 (100%)	1 (0%)	81	92
16	LH	182/188 (97%)	179 (98%)	3 (2%)	55	79
17	LI	178/183 (97%)	174 (98%)	4 (2%)	45	73
18	LJ	106/111 (96%)	104 (98%)	2 (2%)	50	76
19	LK	138/145 (95%)	134 (97%)	4 (3%)	37	65
20	LL	113/114 (99%)	113 (100%)	0	100	100
21	LM	178/180 (99%)	174 (98%)	4 (2%)	45	73
22	LN	171/179 (96%)	167 (98%)	4 (2%)	44	72
23	LO	232/242 (96%)	226 (97%)	6 (3%)	40	68
24	LP	163/164 (99%)	162 (99%)	1 (1%)	78	91
25	LQ	170/198 (86%)	168 (99%)	2 (1%)	63	83
26	LR	157/159 (99%)	155 (99%)	2 (1%)	61	82
27	LS	132/134 (98%)	129 (98%)	3 (2%)	44	72
28	LT	127/143 (89%)	125 (98%)	2 (2%)	55	79
29	LU	93/114 (82%)	86 (92%)	7 (8%)	12	26
30	LV	102/124 (82%)	100 (98%)	2 (2%)	48	75
31	LW	104/122 (85%)	100 (96%)	4 (4%)	29	56
32	LX	74/104 (71%)	73 (99%)	1 (1%)	59	81
33	LY	111/116 (96%)	108 (97%)	3 (3%)	39	67
34	LZ	114/118 (97%)	111 (97%)	3 (3%)	40	68
35	La	112/118 (95%)	109 (97%)	3 (3%)	39	67
36	Lb	56/58 (97%)	56 (100%)	0	100	100
37	Lc	191/209 (91%)	190 (100%)	1 (0%)	81	92
38	Ld	82/89 (92%)	79 (96%)	3 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Le	154/158 (98%)	153 (99%)	1 (1%)	78	91
40	Lf	111/115 (96%)	107 (96%)	4 (4%)	31	58
41	Lg	120/121 (99%)	116 (97%)	4 (3%)	33	61
42	Lh	107/146 (73%)	105 (98%)	2 (2%)	50	76
43	Li	83/88 (94%)	81 (98%)	2 (2%)	43	70
44	Lj	68/70 (97%)	68 (100%)	0	100	100
45	Lk	64/74 (86%)	64 (100%)	0	100	100
46	Ll	45/47 (96%)	45 (100%)	0	100	100
47	Lm	44/113 (39%)	42 (96%)	2 (4%)	24	49
48	Ln	31/32 (97%)	30 (97%)	1 (3%)	34	62
49	Lo	69/74 (93%)	67 (97%)	2 (3%)	37	65
50	Lp	83/92 (90%)	80 (96%)	3 (4%)	31	58
54	SA	205/222 (92%)	195 (95%)	10 (5%)	22	45
55	SB	177/202 (88%)	172 (97%)	5 (3%)	38	66
56	SC	176/184 (96%)	169 (96%)	7 (4%)	28	54
57	SD	159/164 (97%)	154 (97%)	5 (3%)	35	62
58	SE	216/225 (96%)	214 (99%)	2 (1%)	70	87
59	SF	182/208 (88%)	181 (100%)	1 (0%)	81	92
60	SG	190/208 (91%)	180 (95%)	10 (5%)	20	42
61	SH	153/159 (96%)	149 (97%)	4 (3%)	40	68
62	SI	181/186 (97%)	179 (99%)	2 (1%)	65	84
63	SJ	110/111 (99%)	110 (100%)	0	100	100
64	SK	156/176 (89%)	155 (99%)	1 (1%)	78	91
65	SL	116/120 (97%)	114 (98%)	2 (2%)	53	78
66	SM	92/104 (88%)	87 (95%)	5 (5%)	20	41
67	SN	88/128 (69%)	86 (98%)	2 (2%)	44	72
68	SO	104/113 (92%)	102 (98%)	2 (2%)	50	76
69	SP	114/117 (97%)	112 (98%)	2 (2%)	51	77
70	SQ	56/120 (47%)	50 (89%)	6 (11%)	6	13
71	SR	113/130 (87%)	109 (96%)	4 (4%)	32	58
72	SS	45/49 (92%)	44 (98%)	1 (2%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	ST	126/132 (96%)	124 (98%)	2 (2%)	55	79
74	SU	125/152 (82%)	120 (96%)	5 (4%)	28	54
75	SV	109/126 (86%)	107 (98%)	2 (2%)	51	77
76	SW	98/130 (75%)	95 (97%)	3 (3%)	35	62
77	SX	122/131 (93%)	119 (98%)	3 (2%)	42	69
78	SY	72/116 (62%)	69 (96%)	3 (4%)	26	52
79	SZ	111/118 (94%)	109 (98%)	2 (2%)	51	77
80	Sa	71/95 (75%)	68 (96%)	3 (4%)	26	52
81	Sb	85/93 (91%)	79 (93%)	6 (7%)	13	29
82	Sc	75/76 (99%)	74 (99%)	1 (1%)	61	82
83	Sd	51/75 (68%)	50 (98%)	1 (2%)	48	75
84	Se	52/54 (96%)	49 (94%)	3 (6%)	18	38
85	Sf	37/126 (29%)	37 (100%)	0	100	100
86	Sg	255/265 (96%)	241 (94%)	14 (6%)	19	40
87	Sh	79/177 (45%)	77 (98%)	2 (2%)	42	69
All	All	9627/10798 (89%)	9388 (98%)	239 (2%)	42	69

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	LA	36	GLU
9	LA	148	LEU
9	LA	157	SER
9	LA	245	ARG
10	LB	112	VAL
10	LB	176	VAL
10	LB	217	SER
11	LC	62	SER
11	LC	118	GLN
11	LC	142	GLN
11	LC	146	VAL
11	LC	271	VAL
11	LC	273	LYS
11	LC	285	THR
11	LC	317	THR
12	LD	54	LEU
12	LD	71	CYS

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Mol	Chain	Res	Type
12	LD	109	ASP
12	LD	153	SER
13	LE	16	VAL
13	LE	33	THR
13	LE	42	GLN
13	LE	50	LYS
13	LE	91	VAL
13	LE	137	SER
13	LE	139	VAL
14	LF	66	SER
14	LF	77	ARG
14	LF	89	THR
14	LF	94	SER
14	LF	102	THR
14	LF	147	SER
15	LG	48	SER
16	LH	85	THR
16	LH	86	LYS
16	LH	155	THR
17	LI	67	THR
17	LI	68	VAL
17	LI	104	SER
17	LI	133	MET
18	LJ	53	SER
18	LJ	103	VAL
19	LK	115	VAL
19	LK	135	THR
19	LK	137	VAL
19	LK	168	ILE
21	LM	46	GLU
21	LM	121	VAL
21	LM	123	MET
21	LM	126	THR
22	LN	43	VAL
22	LN	78	LYS
22	LN	81	ASN
22	LN	211	VAL
23	LO	7	VAL
23	LO	132	VAL
23	LO	223	SER
23	LO	224	ASN
23	LO	241	LEU

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Mol	Chain	Res	Type
23	LO	303	LEU
24	LP	129	THR
25	LQ	40	SER
25	LQ	51	ILE
26	LR	61	LEU
26	LR	65	VAL
27	LS	4	SER
27	LS	46	SER
27	LS	68	THR
28	LT	3	HIS
28	LT	152	GLU
29	LU	25	VAL
29	LU	30	CYS
29	LU	31	SER
29	LU	32	ILE
29	LU	70	LEU
29	LU	81	THR
29	LU	110	LEU
30	LV	34	GLN
30	LV	136	LEU
31	LW	59	THR
31	LW	78	LEU
31	LW	90	SER
31	LW	113	LYS
32	LX	27	LEU
33	LY	3	LYS
33	LY	29	SER
33	LY	52	LYS
34	LZ	70	SER
34	LZ	81	THR
34	LZ	93	SER
35	La	43	THR
35	La	81	CYS
35	La	92	THR
37	Lc	96	VAL
38	Ld	26	VAL
38	Ld	38	GLN
38	Ld	90	CYS
39	Le	6	MET
40	Lf	5	THR
40	Lf	8	LYS
40	Lf	10	ILE

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Mol	Chain	Res	Type
40	Lf	96	VAL
41	Lg	22	SER
41	Lg	38	THR
41	Lg	75	VAL
41	Lg	91	SER
42	Lh	3	CYS
42	Lh	123	ASN
43	Li	5	THR
43	Li	28	SER
47	Lm	81	THR
47	Lm	110	CYS
48	Ln	3	THR
49	Lo	42	CYS
49	Lo	47	PHE
50	Lp	2	VAL
50	Lp	22	SER
50	Lp	75	SER
54	SA	8	ARG
54	SA	22	GLU
54	SA	24	MET
54	SA	47	ILE
54	SA	51	THR
54	SA	54	THR
54	SA	166	LEU
54	SA	194	VAL
54	SA	196	SER
54	SA	245	GLN
55	SB	17	ASP
55	SB	21	LEU
55	SB	24	MET
55	SB	79	VAL
55	SB	203	ASP
56	SC	5	SER
56	SC	40	VAL
56	SC	42	THR
56	SC	57	VAL
56	SC	171[A]	CYS
56	SC	171[B]	CYS
56	SC	194	THR
57	SD	19	GLU
57	SD	60	THR
57	SD	121	VAL

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Mol	Chain	Res	Type
57	SD	170	ARG
57	SD	171	VAL
58	SE	158	VAL
58	SE	167	VAL
59	SF	166	ILE
60	SG	22	VAL
60	SG	27	GLN
60	SG	41	ILE
60	SG	69	LEU
60	SG	108	ASP
60	SG	117	SER
60	SG	146	LYS
60	SG	173	ARG
60	SG	232	HIS
60	SG	233	THR
61	SH	13	SER
61	SH	20	SER
61	SH	170	SER
61	SH	173	SER
62	SI	139	VAL
62	SI	165	ILE
64	SK	81	VAL
65	SL	63	SER
65	SL	75	VAL
66	SM	29	VAL
66	SM	34	SER
66	SM	97	LYS
66	SM	99	THR
66	SM	112	THR
67	SN	22	VAL
67	SN	100	PRO
68	SO	45	THR
68	SO	126	THR
69	SP	34	SER
69	SP	105	PHE
70	SQ	53	THR
70	SQ	61	MET
70	SQ	87	ASP
70	SQ	95	GLU
70	SQ	118	CYS
70	SQ	121	VAL
71	SR	15	ARG

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Mol	Chain	Res	Type
71	SR	32	ARG
71	SR	34	VAL
71	SR	102	SER
72	SS	56	LEU
73	ST	48	SER
73	ST	104	ARG
74	SU	31	GLU
74	SU	50	SER
74	SU	67	LYS
74	SU	89	VAL
74	SU	153	ASN
75	SV	73	LEU
75	SV	88	THR
76	SW	22	PHE
76	SW	44	VAL
76	SW	112	VAL
77	SX	95	LYS
77	SX	100	SER
77	SX	103	GLU
78	SY	4	ILE
78	SY	8	ASN
78	SY	69	SER
79	SZ	21	LYS
79	SZ	60	SER
80	Sa	28	SER
80	Sa	36	LEU
80	Sa	63	SER
81	Sb	2	THR
81	Sb	10	ARG
81	Sb	61	VAL
81	Sb	87	THR
81	Sb	88	VAL
81	Sb	95	ASN
82	Sc	45	THR
83	Sd	44	VAL
84	Se	46	SER
84	Se	48	THR
84	Se	49	VAL
86	Sg	52	SER
86	Sg	77	THR
86	Sg	101	ARG
86	Sg	130	VAL

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Mol	Chain	Res	Type
86	Sg	141	MET
86	Sg	166	ILE
86	Sg	168	VAL
86	Sg	229	LEU
86	Sg	259	SER
86	Sg	260	VAL
86	Sg	269	ILE
86	Sg	285	ILE
86	Sg	293	THR
86	Sg	301	ASN
87	Sh	150	LYS
87	Sh	160	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
9	LA	21	HIS
9	LA	38	HIS
10	LB	109	HIS
10	LB	138	ASN
10	LB	184	GLN
11	LC	118	GLN
11	LC	158	GLN
11	LC	257	GLN
12	LD	41	GLN
12	LD	70	HIS
13	LE	133	GLN
14	LF	72	ASN
15	LG	169	ASN
15	LG	220	ASN
15	LG	238	GLN
17	LI	119	GLN
18	LJ	26	ASN
18	LJ	134	HIS
19	LK	21	GLN
19	LK	52	ASN
21	LM	156	HIS
22	LN	73	ASN
23	LO	31	HIS
23	LO	35	GLN
23	LO	190	ASN
23	LO	216	GLN

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Mol	Chain	Res	Type
25	LQ	134	ASN
25	LQ	154	GLN
25	LQ	198	GLN
26	LR	8	HIS
26	LR	85	GLN
27	LS	102	GLN
29	LU	49	GLN
31	LW	110	HIS
32	LX	10	HIS
33	LY	86	ASN
34	LZ	35	ASN
35	La	114	GLN
39	Le	32	ASN
39	Le	172	ASN
40	Lf	21	HIS
40	Lf	79	ASN
42	Lh	111	HIS
43	Li	26	GLN
44	Lj	12	HIS
46	Ll	19	GLN
48	Ln	15	HIS
50	Lp	18	ASN
54	SA	103	HIS
54	SA	182	GLN
55	SB	116	GLN
55	SB	135	GLN
56	SC	144	GLN
57	SD	130	GLN
57	SD	165	ASN
58	SE	64	GLN
58	SE	71	ASN
58	SE	172	ASN
58	SE	245	ASN
60	SG	92	GLN
60	SG	225	GLN
60	SG	232	HIS
61	SH	74	GLN
62	SI	99	GLN
62	SI	178	GLN
63	SJ	120	ASN
64	SK	35	ASN
65	SL	44	GLN

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Mol	Chain	Res	Type
65	SL	104	ASN
67	SN	65	GLN
68	SO	13	ASN
69	SP	61	GLN
69	SP	73	GLN
71	SR	12	HIS
72	SS	50	HIS
73	ST	49	GLN
73	ST	78	ASN
74	SU	11	HIS
74	SU	24	GLN
74	SU	91	HIS
74	SU	153	ASN
75	SV	30	GLN
76	SW	51	ASN
78	SY	71	HIS
79	SZ	36	HIS
79	SZ	61	GLN
79	SZ	119	ASN
80	Sa	106	GLN
81	Sb	75	GLN
83	Sd	41	GLN
83	Sd	62	ASN
84	Se	16	ASN
84	Se	56	HIS
86	Sg	129	ASN
86	Sg	292	ASN
86	Sg	301	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1664/1782 (93%)	342 (20%)	9 (0%)
2	L2	1144/1526 (74%)	217 (18%)	5 (0%)
3	L3	176/216 (81%)	32 (18%)	0
4	L4	183/184 (99%)	31 (16%)	1 (0%)
5	L5	115/135 (85%)	22 (19%)	1 (0%)
51	S3	71/78 (91%)	13 (18%)	0
52	S4	72/76 (94%)	24 (33%)	0
53	S5	8/13 (61%)	3 (37%)	0
6	L6	70/73 (95%)	21 (30%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	L7	163/171 (95%)	26 (15%)	1 (0%)
8	L8	119/124 (95%)	11 (9%)	0
88	S1	1811/2204 (82%)	347 (19%)	13 (0%)
All	All	5596/6582 (85%)	1089 (19%)	31 (0%)

All (1089) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	6	C
1	L1	7	C
1	L1	16	G
1	L1	24	A
1	L1	29	C
1	L1	32	A
1	L1	38	A
1	L1	41	A
1	L1	47	C
1	L1	56	G
1	L1	58	A
1	L1	63	A
1	L1	64	A
1	L1	65	A
1	L1	84	G
1	L1	87	A
1	L1	91	G
1	L1	98	A
1	L1	110	A
1	L1	121	A
1	L1	122	A
1	L1	134	A
1	L1	136	G
1	L1	141	U
1	L1	142	G
1	L1	144	G
1	L1	147	G
1	L1	154	A
1	L1	156	A
1	L1	158	A
1	L1	160	C
1	L1	161	A
1	L1	162	U
1	L1	167	U

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Mol	Chain	Res	Type
1	L1	170	U
1	L1	176	C
1	L1	191	U
1	L1	192	C
1	L1	199	A
1	L1	201	A
1	L1	205	A
1	L1	209	C
1	L1	210	G
1	L1	216	G
1	L1	218	A
1	L1	219	U
1	L1	223	A
1	L1	224	C
1	L1	225	C
1	L1	226	C
1	L1	233	U
1	L1	234	G
1	L1	237	U
1	L1	251	A
1	L1	256	U
1	L1	273	A
1	L1	280	A
1	L1	281	G
1	L1	300	A
1	L1	302	G
1	L1	305	A2M
1	L1	306	G
1	L1	322	A
1	L1	323	U
1	L1	324	G
1	L1	332	A
1	L1	335	U
1	L1	342	G
1	L1	343	U
1	L1	344	A
1	L1	349	U
1	L1	357	A
1	L1	367	A
1	L1	368	G
1	L1	369	A
1	L1	374	G

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Mol	Chain	Res	Type
1	L1	376	A
1	L1	383	U
1	L1	392	A
1	L1	409	U
1	L1	410	U
1	L1	411	U
1	L1	414	A
1	L1	416	A
1	L1	417	G
1	L1	419	A
1	L1	431	G
1	L1	439	U
1	L1	443	A
1	L1	444	C
1	L1	461	G
1	L1	463	C
1	L1	464	A
1	L1	471	G
1	L1	477	C
1	L1	484	A
1	L1	485	A
1	L1	486	C
1	L1	488	G
1	L1	489	C
1	L1	494	A
1	L1	495	C
1	L1	496	C
1	L1	501	C
1	L1	502	U
1	L1	511	A
1	L1	522	G
1	L1	525	C
1	L1	527	A
1	L1	539	C
1	L1	542	C
1	L1	546	G
1	L1	547	U
1	L1	551	A
1	L1	554	A
1	L1	555	U
1	L1	557	U
1	L1	569	G

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Mol	Chain	Res	Type
1	L1	571	A
1	L1	572	A
1	L1	575	A
1	L1	580	A
1	L1	585	U
1	L1	586	U
1	L1	605	G
1	L1	606	C
1	L1	611	C
1	L1	612	G
1	L1	616	U
1	L1	617	G
1	L1	623	U
1	L1	626	U
1	L1	627	C
1	L1	631	G
1	L1	632	A
1	L1	634	G
1	L1	635	C
1	L1	641	G
1	L1	651	G
1	L1	652	A
1	L1	653	A
1	L1	666	C
1	L1	668	C
1	L1	669	C
1	L1	681	A2M
1	L1	692	A
1	L1	709	A
1	L1	710	G
1	L1	718	A
1	L1	721	U
1	L1	729	A
1	L1	736	C
1	L1	743	A
1	L1	748	A
1	L1	750	G
1	L1	753	A
1	L1	763	U
1	L1	769	U
1	L1	771	U
1	L1	778	C

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Mol	Chain	Res	Type
1	L1	779	A
1	L1	783	G
1	L1	790	C
1	L1	795	U
1	L1	803	C
1	L1	810	C
1	L1	818	C
1	L1	823	G
1	L1	828	U
1	L1	832	G
1	L1	835	G
1	L1	836	G
1	L1	838	G
1	L1	850	G
1	L1	867	A
1	L1	868	A
1	L1	895	G
1	L1	900	C
1	L1	904	G
1	L1	912	C
1	L1	925	U
1	L1	930	U
1	L1	957	C
1	L1	959	OMG
1	L1	965	A
1	L1	967	G
1	L1	968	A
1	L1	972	A
1	L1	974	C
1	L1	975	G
1	L1	976	A
1	L1	988	G
1	L1	995	C
1	L1	1010	OMC
1	L1	1011	PSU
1	L1	1013	A
1	L1	1016	A
1	L1	1017	PSU
1	L1	1025	G
1	L1	1031	A
1	L1	1036	U
1	L1	1045	G

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Mol	Chain	Res	Type
1	L1	1053	A
1	L1	1061	G
1	L1	1085	C
1	L1	1093	U
1	L1	1094	C
1	L1	1098	A
1	L1	1100	C
1	L1	1114	A
1	L1	1116	A
1	L1	1122	U
1	L1	1123	G
1	L1	1129	G
1	L1	1135	U
1	L1	1136	G
1	L1	1137	C
1	L1	1141	G
1	L1	1144	G
1	L1	1148	A
1	L1	1150	A
1	L1	1153	A
1	L1	1156	A
1	L1	1159	A
1	L1	1161	A
1	L1	1162	G
1	L1	1165	A
1	L1	1169	A
1	L1	1170	G
1	L1	1174	G
1	L1	1177	PSU
1	L1	1188	G
1	L1	1201	U
1	L1	1202	G
1	L1	1207	A
1	L1	1210	A
1	L1	1217	U
1	L1	1225	U
1	L1	1239	U
1	L1	1240	U
1	L1	1242	U
1	L1	1243	G
1	L1	1248	C
1	L1	1251	U

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Mol	Chain	Res	Type
1	L1	1253	OMU
1	L1	1254	C
1	L1	1258	A
1	L1	1261	U
1	L1	1263	A
1	L1	1264	A
1	L1	1270	U
1	L1	1271	G
1	L1	1274	G
1	L1	1287	A
1	L1	1342	C
1	L1	1346	C
1	L1	1348	A
1	L1	1349	A
1	L1	1351	C
1	L1	1352	C
1	L1	1362	G
1	L1	1364	A
1	L1	1369	G
1	L1	1371	OMU
1	L1	1375	G
1	L1	1378	U
1	L1	1379	A
1	L1	1388	U
1	L1	1389	A
1	L1	1390	G
1	L1	1391	U
1	L1	1395	U
1	L1	1401	U
1	L1	1413	U
1	L1	1416	G
1	L1	1420	G
1	L1	1421	G
1	L1	1422	A
1	L1	1424	A
1	L1	1426	A
1	L1	1438	A
1	L1	1441	U
1	L1	1444	A
1	L1	1445	G
1	L1	1446	C
1	L1	1455	U

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Mol	Chain	Res	Type
1	L1	1464	G
1	L1	1465	G
1	L1	1480	C
1	L1	1489	U
1	L1	1490	G
1	L1	1495	G
1	L1	1504	A
1	L1	1505	U
1	L1	1509	C
1	L1	1519	G
1	L1	1524	OMG
1	L1	1527	OMC
1	L1	1536	C
1	L1	1540	OMG
1	L1	1545	G
1	L1	1547	U
1	L1	1557	A
1	L1	1560	U
1	L1	1566	A
1	L1	1569	U
1	L1	1574	C
1	L1	1586	G
1	L1	1590	G
1	L1	1612	G
1	L1	1613	C
1	L1	1627	U
1	L1	1628	U
1	L1	1639	U
1	L1	1654	A
1	L1	1655	U
1	L1	1661	U
1	L1	1662	G
1	L1	1663	U
1	L1	1666	G
1	L1	1667	G
1	L1	1668	A
1	L1	1671	G
1	L1	1676	G
1	L1	1683	C
1	L1	1727	A
1	L1	1729	A
1	L1	1734	G

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Mol	Chain	Res	Type
1	L1	1737	A
1	L1	1739	A
1	L1	1744	A
1	L1	1746	C
1	L1	1747	U
1	L1	1751	A
1	L1	1757	U
1	L1	1758	U
1	L1	1762	A
1	L1	1763	A
1	L1	1766	G
1	L1	1771	U
1	L1	1772	G
1	L1	1774	A
2	L2	13	A
2	L2	22	A
2	L2	25	A
2	L2	29	C
2	L2	30	A
2	L2	61	C
2	L2	62	A
2	L2	63	U
2	L2	68	A
2	L2	69	A
2	L2	75	C
2	L2	90	G
2	L2	91	C
2	L2	119	C
2	L2	125	C
2	L2	340	A
2	L2	341	A
2	L2	343	U
2	L2	348	A
2	L2	349	C
2	L2	358	G
2	L2	368	G
2	L2	377	A
2	L2	386	U
2	L2	388	A
2	L2	390	A
2	L2	404	A
2	L2	415	U

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Mol	Chain	Res	Type
2	L2	426	G
2	L2	453	A
2	L2	454	A
2	L2	455	U
2	L2	456	G
2	L2	459	A
2	L2	490	A
2	L2	495	G
2	L2	503	C
2	L2	505	A
2	L2	518	G
2	L2	519	G
2	L2	527	A2M
2	L2	528	U
2	L2	529	G
2	L2	534	OMG
2	L2	544	U
2	L2	552	C
2	L2	553	G
2	L2	554	C
2	L2	556	U
2	L2	559	A
2	L2	561	G
2	L2	571	G
2	L2	580	U
2	L2	582	U
2	L2	616	G
2	L2	619	A
2	L2	620	C
2	L2	621	G
2	L2	623	A
2	L2	637	G
2	L2	639	G
2	L2	640	G
2	L2	643	A
2	L2	648	A
2	L2	649	G
2	L2	650	A
2	L2	657	U
2	L2	658	G
2	L2	665	A2M
2	L2	685	G

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Mol	Chain	Res	Type
2	L2	697	G
2	L2	698	G
2	L2	746	A
2	L2	747	A
2	L2	749	G
2	L2	750	U
2	L2	751	U
2	L2	752	G
2	L2	760	U
2	L2	761	A
2	L2	768	G
2	L2	769	A
2	L2	778	A
2	L2	779	U
2	L2	783	U
2	L2	784	U
2	L2	799	G
2	L2	802	PSU
2	L2	803	A
2	L2	805	G
2	L2	810	G
2	L2	811	U
2	L2	819	U
2	L2	823	A
2	L2	851	C
2	L2	955	C
2	L2	970	A
2	L2	971	A
2	L2	972	C
2	L2	975	A
2	L2	976	A
2	L2	979	A
2	L2	985	A
2	L2	1001	C
2	L2	1004	G
2	L2	1010	U
2	L2	1011	G
2	L2	1012	U
2	L2	1019	A
2	L2	1021	A
2	L2	1022	U
2	L2	1023	C

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Mol	Chain	Res	Type
2	L2	1025	G
2	L2	1030	A
2	L2	1033	G
2	L2	1034	G
2	L2	1041	G
2	L2	1046	OMG
2	L2	1053	A
2	L2	1055	A
2	L2	1064	A
2	L2	1075	G
2	L2	1079	U
2	L2	1083	A
2	L2	1096	U
2	L2	1101	A
2	L2	1102	C
2	L2	1104	G
2	L2	1108	U
2	L2	1115	U
2	L2	1116	A
2	L2	1118	A
2	L2	1121	A
2	L2	1123	A
2	L2	1129	A
2	L2	1132	A
2	L2	1141	G
2	L2	1147	C
2	L2	1148	G
2	L2	1155	A
2	L2	1156	G
2	L2	1162	A
2	L2	1171	G
2	L2	1176	A
2	L2	1180	A
2	L2	1181	G
2	L2	1185	A2M
2	L2	1189	A
2	L2	1199	A
2	L2	1200	A
2	L2	1203	A
2	L2	1204	U
2	L2	1206	G
2	L2	1207	G

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Mol	Chain	Res	Type
2	L2	1209	A
2	L2	1215	A
2	L2	1216	A
2	L2	1221	U
2	L2	1229	OMG
2	L2	1233	U
2	L2	1234	G
2	L2	1237	A
2	L2	1238	G
2	L2	1239	A
2	L2	1240	A
2	L2	1241	U
2	L2	1246	A
2	L2	1248	OMC
2	L2	1252	G
2	L2	1255	A
2	L2	1264	PSU
2	L2	1271	G
2	L2	1283	A
2	L2	1285	A
2	L2	1288	G
2	L2	1289	A
2	L2	1305	C
2	L2	1309	G
2	L2	1313	U
2	L2	1325	A
2	L2	1337	C
2	L2	1342	G
2	L2	1348	A
2	L2	1361	PSU
2	L2	1373	C
2	L2	1374	A
2	L2	1379	A
2	L2	1380	C
2	L2	1385	G
2	L2	1389	G
2	L2	1409	A
2	L2	1416	U
2	L2	1421	C
2	L2	1428	U
2	L2	1430	G
2	L2	1433	G

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Mol	Chain	Res	Type
2	L2	1434	G
2	L2	1437	A
2	L2	1441	C
2	L2	1443	A
2	L2	1444	G
2	L2	1445	A
2	L2	1448	A
2	L2	1450	G
2	L2	1454	A
2	L2	1456	C
2	L2	1463	A
2	L2	1465	G
2	L2	1484	U
2	L2	1485	G
2	L2	1486	G
2	L2	1494	G
2	L2	1506	G
2	L2	1510	A
2	L2	1511	U
2	L2	1512	G
2	L2	1513	G
3	L3	6	G
3	L3	16	G
3	L3	21	A
3	L3	22	C
3	L3	34	C
3	L3	35	A
3	L3	41	A
3	L3	48	C
3	L3	52	G
3	L3	70	A
3	L3	99	U
3	L3	110	U
3	L3	111	A
3	L3	112	C
3	L3	113	U
3	L3	114	U
3	L3	124	U
3	L3	125	U
3	L3	132	G
3	L3	149	A
3	L3	150	A

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Mol	Chain	Res	Type
3	L3	151	A
3	L3	169	A
3	L3	178	G
3	L3	179	U
3	L3	181	G
3	L3	182	U
3	L3	187	U
3	L3	192	G
3	L3	196	U
3	L3	199	A
3	L3	202	A
4	L4	9	G
4	L4	10	U
4	L4	24	A
4	L4	31	G
4	L4	39	A
4	L4	40	G
4	L4	50	G
4	L4	60	A
4	L4	61	A
4	L4	67	A
4	L4	83	U
4	L4	85	C
4	L4	86	U
4	L4	87	G
4	L4	102	G
4	L4	106	G
4	L4	114	A
4	L4	120	U
4	L4	121	C
4	L4	128	U
4	L4	133	C
4	L4	144	G
4	L4	149	U
4	L4	150	A
4	L4	151	A
4	L4	153	C
4	L4	158	A
4	L4	159	G
4	L4	168	A
4	L4	171	A
4	L4	180	C

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Mol	Chain	Res	Type
5	L5	3	U
5	L5	4	A
5	L5	6	G
5	L5	15	C
5	L5	24	G
5	L5	29	U
5	L5	50	C
5	L5	51	A
5	L5	52	U
5	L5	65	U
5	L5	68	G
5	L5	71	U
5	L5	88	C
5	L5	89	C
5	L5	92	A
5	L5	99	G
5	L5	105	U
5	L5	106	G
5	L5	109	G
5	L5	113	G
5	L5	120	C
5	L5	135	U
6	L6	7	A
6	L6	15	C
6	L6	25	U
6	L6	31	U
6	L6	33	G
6	L6	41	G
6	L6	42	A
6	L6	43	A
6	L6	44	G
6	L6	45	G
6	L6	52	G
6	L6	54	A
6	L6	55	U
6	L6	56	A
6	L6	64	U
6	L6	67	C
6	L6	68	A
6	L6	70	G
6	L6	71	A
6	L6	72	C

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Mol	Chain	Res	Type
6	L6	73	A
7	L7	16	A
7	L7	22	U
7	L7	33	U
7	L7	48	A
7	L7	59	A
7	L7	62	A
7	L7	63	G
7	L7	68	A
7	L7	72	A
7	L7	80	A
7	L7	81	U
7	L7	82	C
7	L7	84	U
7	L7	87	A
7	L7	88	A
7	L7	94	G
7	L7	103	A
7	L7	105	C
7	L7	110	A
7	L7	120	G
7	L7	124	A
7	L7	125	A
7	L7	127	C
7	L7	157	U
7	L7	158	U
7	L7	167	C
8	L8	11	G
8	L8	26	A
8	L8	46	A
8	L8	52	G
8	L8	57	U
8	L8	67	C
8	L8	68	A
8	L8	76	U
8	L8	95	U
8	L8	104	A
8	L8	114	G
51	S3	8	U
51	S3	13	C
51	S3	16	C
51	S3	17	C

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Mol	Chain	Res	Type
51	S3	18	U
51	S3	46	A
51	S3	47	U
51	S3	48	C
51	S3	49	G
51	S3	52	G
51	S3	70	G
51	S3	74	C
51	S3	76	A
52	S4	4	C
52	S4	7	A
52	S4	8	U
52	S4	13	C
52	S4	15	G
52	S4	16	U
52	S4	17	C
52	S4	18	G
52	S4	19	G
52	S4	20	U
52	S4	21	A
52	S4	30	G
52	S4	32	U
52	S4	33	U
52	S4	38	A
52	S4	44	G
52	S4	47	U
52	S4	48	C
52	S4	49	C
52	S4	54	U
52	S4	59	U
52	S4	61	C
52	S4	70	C
52	S4	76	A
53	S5	4	C
53	S5	5	A
53	S5	8	U
88	S1	3	U
88	S1	17	C
88	S1	25	C
88	S1	26	A
88	S1	34	G
88	S1	42	G

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Mol	Chain	Res	Type
88	S1	47	A
88	S1	66	U
88	S1	68	A
88	S1	85	C
88	S1	109	C
88	S1	112	A
88	S1	114	U
88	S1	117	G
88	S1	122	A
88	S1	129	U
88	S1	144	A
88	S1	145	A
88	S1	146	U
88	S1	147	U
88	S1	158	G
88	S1	164	C
88	S1	165	G
88	S1	167	C
88	S1	171	C
88	S1	174	A
88	S1	175	U
88	S1	176	A
88	S1	181	A
88	S1	182	A
88	S1	195	U
88	S1	227	U
88	S1	228	G
88	S1	236	C
88	S1	249	A
88	S1	252	G
88	S1	257	A
88	S1	264	C
88	S1	275	A
88	S1	276	G
88	S1	277	U
88	S1	287	C
88	S1	288	A
88	S1	295	A
88	S1	298	C
88	S1	309	G
88	S1	310	U
88	S1	313	G

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Mol	Chain	Res	Type
88	S1	316	A
88	S1	321	G
88	S1	322	C
88	S1	324	U
88	S1	325	G
88	S1	326	U
88	S1	329	C
88	S1	353	C
88	S1	356	A
88	S1	358	C
88	S1	360	G
88	S1	364	G
88	S1	381	G
88	S1	382	A
88	S1	396	G
88	S1	404	C
88	S1	423	U
88	S1	433	G
88	S1	443	A
88	S1	444	A
88	S1	445	U
88	S1	446	A
88	S1	447	G
88	S1	454	C
88	S1	462	G
88	S1	464	G
88	S1	467	C
88	S1	469	G
88	S1	477	G
88	S1	481	A
88	S1	482	U
88	S1	487	C
88	S1	488	A
88	S1	497	A
88	S1	507	G
88	S1	516	A
88	S1	523	A
88	S1	525	A
88	S1	548	G
88	S1	551	A
88	S1	552	U
88	S1	556	A

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Mol	Chain	Res	Type
88	S1	559	G
88	S1	565	U
88	S1	566	A
88	S1	580	A
88	S1	581	A
88	S1	585	C
88	S1	589	U
88	S1	590	A
88	S1	591	A
88	S1	593	A
88	S1	600	OMG
88	S1	606	G
88	S1	607	U
88	S1	608	C
88	S1	614	C
88	S1	616	A
88	S1	617	G
88	S1	628	A
88	S1	631	U
88	S1	643	A
88	S1	660	U
88	S1	666	U
88	S1	668	A2M
88	S1	669	A
88	S1	670	A
88	S1	671	G
88	S1	672	G
88	S1	673	G
88	S1	678	U
88	S1	679	A
88	S1	688	G
88	S1	690	G
88	S1	698	C
88	S1	699	A
88	S1	749	U
88	S1	757	C
88	S1	775	C
88	S1	777	A
88	S1	778	G
88	S1	782	C
88	S1	786	G
88	S1	788	A

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Mol	Chain	Res	Type
88	S1	789	G
88	S1	792	G
88	S1	811	C
88	S1	812	A
88	S1	814	G
88	S1	815	U
88	S1	817	A
88	S1	819	G
88	S1	825	C
88	S1	826	A
88	S1	841	U
88	S1	844	U
88	S1	856	A
88	S1	866	G
88	S1	867	A
88	S1	868	C
88	S1	881	U
88	S1	882	U
88	S1	883	G
88	S1	886	U
88	S1	887	U
88	S1	892	U
88	S1	895	A
88	S1	914	G
88	S1	925	A
88	S1	926	G
88	S1	930	A
88	S1	935	U
88	S1	936	U
88	S1	937	C
88	S1	939	G
88	S1	945	G
88	S1	951	U
88	S1	952	U
88	S1	954	A
88	S1	955	A
88	S1	957	G
88	S1	959	U
88	S1	969	A
88	S1	970	U
88	S1	971	U
88	S1	972	A

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Mol	Chain	Res	Type
88	S1	973	U
88	S1	1101	A
88	S1	1103	G
88	S1	1105	A
88	S1	1109	A
88	S1	1119	U
88	S1	1123	G
88	S1	1133	U
88	S1	1139	G
88	S1	1180	A
88	S1	1181	C
88	S1	1182	A
88	S1	1191	A
88	S1	1192	U
88	S1	1199	A
88	S1	1207	U
88	S1	1210	C
88	S1	1211	U
88	S1	1213	A
88	S1	1217	A
88	S1	1232	G
88	S1	1235	A
88	S1	1239	A
88	S1	1251	A
88	S1	1252	A
88	S1	1273	A
88	S1	1275	C
88	S1	1359	C
88	S1	1361	U
88	S1	1362	A
88	S1	1365	U
88	S1	1366	A
88	S1	1371	U
88	S1	1398	C
88	S1	1399	G
88	S1	1443	U
88	S1	1444	G
88	S1	1448	U
88	S1	1449	U
88	S1	1452	A
88	S1	1466	G
88	S1	1467	U

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Mol	Chain	Res	Type
88	S1	1490	A
88	S1	1502	G
88	S1	1510	C
88	S1	1537	U
88	S1	1538	U
88	S1	1543	B8N
88	S1	1546	A
88	S1	1548	A
88	S1	1551	G
88	S1	1552	G
88	S1	1554	A
88	S1	1560	A
88	S1	1565	A
88	S1	1566	PSU
88	S1	1569	G
88	S1	1570	G
88	S1	1579	A
88	S1	1591	U
88	S1	1594	A
88	S1	1595	G
88	S1	1597	G
88	S1	1598	U
88	S1	1609	U
88	S1	1611	C
88	S1	1612	C
88	S1	1613	C
88	S1	1614	U
88	S1	1637	A
88	S1	1638	U
88	S1	1652	A
88	S1	1653	U
88	S1	1658	U
88	S1	1666	U
88	S1	1667	U
88	S1	1673	A
88	S1	1677	G
88	S1	1699	A
88	S1	1703	U
88	S1	1706	A
88	S1	1712	G
88	S1	1713	C
88	S1	1715	C

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Mol	Chain	Res	Type
88	S1	1720	G
88	S1	1724	G
88	S1	1725	C
88	S1	1766	G
88	S1	1768	U
88	S1	1769	C
88	S1	1784	G
88	S1	1788	U
88	S1	1789	U
88	S1	1790	C
88	S1	1794	U
88	S1	1795	G
88	S1	1799	U
88	S1	1800	U
88	S1	1814	U
88	S1	1816	U
88	S1	1823	A
88	S1	1826	G
88	S1	1828	A
88	S1	1829	OMG
88	S1	1833	OMU
88	S1	1836	G
88	S1	1847	A
88	S1	1860	C
88	S1	1861	A
88	S1	1872	A
88	S1	1884	A
88	S1	1887	A
88	S1	1889	G
88	S1	1890	A
88	S1	1891	A
88	S1	1892	A
88	S1	1906	G
88	S1	1907	A
88	S1	1916	G
88	S1	1917	A
88	S1	1918	U
88	S1	1919	C
88	S1	1923	A
88	S1	1933	A
88	S1	1938	C
88	S1	1944	C

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Mol	Chain	Res	Type
88	S1	1948	U
88	S1	1949	A
88	S1	1950	G
88	S1	1956	C
88	S1	1961	G
88	S1	1962	A
88	S1	1976	U
88	S1	1978	A
88	S1	1988	C
88	S1	1989	A
88	S1	1990	A
88	S1	2004	G
88	S1	2010	G
88	S1	2016	C
88	S1	2021	A2M
88	S1	2031	A
88	S1	2036	G
88	S1	2054	C
88	S1	2055	A
88	S1	2061	5MC
88	S1	2063	U
88	S1	2097	C
88	S1	2101	C
88	S1	2119	C
88	S1	2120	C
88	S1	2121	C
88	S1	2125	A
88	S1	2134	A
88	S1	2136	A
88	S1	2137	U
88	S1	2151	OMG
88	S1	2159	A
88	S1	2160	G
88	S1	2165	A
88	S1	2169	A
88	S1	2170	G
88	S1	2172	U
88	S1	2183	G
88	S1	2185	MA6
88	S1	2186	C
88	S1	2195	G
88	S1	2196	G

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Mol	Chain	Res	Type
88	S1	2197	G
88	S1	2198	A
88	S1	2199	C
88	S1	2202	PSU
88	S1	2203	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	141	U
1	L1	208	C
1	L1	443	A
1	L1	574	G
1	L1	967	G
1	L1	1011	PSU
1	L1	1390	G
1	L1	1479	A
1	L1	1662	G
2	L2	696	A
2	L2	1052	C
2	L2	1101	A
2	L2	1170	U
2	L2	1512	G
4	L4	149	U
5	L5	51	A
6	L6	51	A
7	L7	93	C
88	S1	128	C
88	S1	276	G
88	S1	294	G
88	S1	328	C
88	S1	550	C
88	S1	777	A
88	S1	958	G
88	S1	1209	C
88	S1	1360	U
88	S1	1608	A
88	S1	1889	G
88	S1	1989	A
88	S1	2119	C

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

159 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	OMU	L3	13	3	19,22,23	3.02	8 (42%)	25,31,34	1.76	4 (16%)
2	PSU	L2	437	91,2	18,21,22	4.59	7 (38%)	21,30,33	2.06	5 (23%)
88	A2M	S1	512	88,91	22,25,26	3.49	9 (40%)	30,36,39	2.39	12 (40%)
88	OMU	S1	2048	88,91	19,22,23	3.04	8 (42%)	25,31,34	1.82	4 (16%)
2	PSU	L2	597	2	18,21,22	4.60	7 (38%)	21,30,33	1.99	5 (23%)
88	PSU	S1	1657	88	18,21,22	4.65	7 (38%)	21,30,33	1.86	5 (23%)
1	OMG	L1	856	1	23,26,27	2.39	9 (39%)	32,38,41	2.44	12 (37%)
1	OMC	L1	1527	91,1	19,22,23	2.97	8 (42%)	25,31,34	1.01	2 (8%)
2	PSU	L2	802	2	18,21,22	4.67	7 (38%)	21,30,33	1.91	5 (23%)
2	PSU	L2	1265	91,2	18,21,22	4.63	7 (38%)	21,30,33	1.92	5 (23%)
1	OMU	L1	1371	1	19,22,23	3.09	8 (42%)	25,31,34	2.00	6 (24%)
88	OMU	S1	8	88	19,22,23	3.02	8 (42%)	25,31,34	1.91	5 (20%)
2	A2M	L2	572	2	22,25,26	3.48	9 (40%)	30,36,39	2.39	12 (40%)
2	OMG	L2	1078	2	23,26,27	2.37	9 (39%)	32,38,41	2.46	11 (34%)
88	PSU	S1	1566	88,91	18,21,22	4.67	7 (38%)	21,30,33	1.86	5 (23%)
88	OMG	S1	1647	88	23,26,27	2.41	9 (39%)	32,38,41	2.51	11 (34%)
1	PSU	L1	1526	91,1	18,21,22	4.64	7 (38%)	21,30,33	2.06	6 (28%)
2	PSU	L2	1152	2	18,21,22	4.61	7 (38%)	21,30,33	2.02	6 (28%)
2	PSU	L2	512	2	18,21,22	4.70	7 (38%)	21,30,33	1.93	5 (23%)
7	A2M	L7	43	7	22,25,26	3.50	9 (40%)	30,36,39	2.41	11 (36%)
1	A2M	L1	305	1	22,25,26	3.48	9 (40%)	30,36,39	2.37	10 (33%)
2	A2M	L2	382	2,89	22,25,26	3.50	9 (40%)	30,36,39	2.30	9 (30%)
88	OMG	S1	1623	88	23,26,27	2.43	9 (39%)	32,38,41	2.56	10 (31%)
2	OMG	L2	641	91,2	23,26,27	2.39	9 (39%)	32,38,41	2.45	12 (37%)
1	OMU	L1	1659	91,1	19,22,23	3.02	8 (42%)	25,31,34	1.82	5 (20%)
1	OMG	L1	1190	91,1	23,26,27	2.39	9 (39%)	32,38,41	2.42	13 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PSU	L2	1382	91,2	18,21,22	4.63	7 (38%)	21,30,33	1.98	6 (28%)
2	OMU	L2	565	2	19,22,23	3.08	8 (42%)	25,31,34	2.12	7 (28%)
88	OMU	S1	1621	88	19,22,23	3.06	8 (42%)	25,31,34	1.80	5 (20%)
1	A2M	L1	858	1	22,25,26	3.49	9 (40%)	30,36,39	2.46	12 (40%)
88	OMG	S1	1865	88,91	23,26,27	2.43	9 (39%)	32,38,41	2.51	10 (31%)
2	PSU	L2	626	2	18,21,22	4.60	7 (38%)	21,30,33	1.95	5 (23%)
88	OMC	S1	2140	88	19,22,23	3.02	8 (42%)	25,31,34	0.75	0
88	OMC	S1	18	88	19,22,23	3.02	8 (42%)	25,31,34	0.72	0
1	PSU	L1	422	1	18,21,22	4.58	7 (38%)	21,30,33	1.97	5 (23%)
2	OMC	L2	443	91,2	19,22,23	2.95	8 (42%)	25,31,34	0.87	0
88	OMU	S1	661	88	19,22,23	3.06	8 (42%)	25,31,34	1.80	5 (20%)
1	A2M	L1	235	91,1	22,25,26	3.50	9 (40%)	30,36,39	2.36	11 (36%)
1	PSU	L1	940	1	18,21,22	4.66	7 (38%)	21,30,33	1.97	5 (23%)
1	OMG	L1	1540	91,1,2	23,26,27	2.35	9 (39%)	32,38,41	2.46	11 (34%)
2	PSU	L2	1264	2	18,21,22	4.58	7 (38%)	21,30,33	2.01	5 (23%)
2	A2M	L2	570	1,2	22,25,26	3.46	9 (40%)	30,36,39	2.40	12 (40%)
2	PSU	L2	1194	2	18,21,22	4.65	7 (38%)	21,30,33	1.90	5 (23%)
2	OMG	L2	534	2	23,26,27	2.42	9 (39%)	32,38,41	2.55	10 (31%)
2	OMU	L2	56	1,2	19,22,23	3.01	8 (42%)	25,31,34	1.83	4 (16%)
2	5MC	L2	1308	2,89	19,22,23	5.04	13 (68%)	26,32,35	1.45	3 (11%)
2	A2M	L2	1372	2	22,25,26	3.53	9 (40%)	30,36,39	2.30	10 (33%)
1	A2M	L1	697	1	22,25,26	3.53	9 (40%)	30,36,39	2.32	10 (33%)
88	A2M	S1	897	88	22,25,26	3.49	9 (40%)	30,36,39	2.37	11 (36%)
88	OMU	S1	29	88	19,22,23	3.03	8 (42%)	25,31,34	1.83	5 (20%)
88	OMG	S1	2151	88	23,26,27	2.40	9 (39%)	32,38,41	2.54	10 (31%)
7	PSU	L7	74	7	18,21,22	4.63	7 (38%)	21,30,33	2.05	5 (23%)
88	PSU	S1	1539	88	18,21,22	0.92	1 (5%)	21,30,33	0.66	0
2	OMC	L2	583	2	19,22,23	2.97	8 (42%)	25,31,34	0.78	0
1	A2M	L1	1539	91,1,2	22,25,26	3.50	9 (40%)	30,36,39	2.35	9 (30%)
88	5MC	S1	2061	88	19,22,23	3.90	8 (42%)	26,32,35	0.98	2 (7%)
2	PSU	L2	472	2	18,21,22	4.64	7 (38%)	21,30,33	1.99	5 (23%)
2	PSU	L2	1318	91,2	18,21,22	4.57	7 (38%)	21,30,33	1.99	6 (28%)
2	OMU	L2	73	2	19,22,23	3.00	8 (42%)	25,31,34	1.75	5 (20%)
88	PSU	S1	1246	88,91	18,21,22	4.71	7 (38%)	21,30,33	1.92	5 (23%)
88	PSU	S1	1292	88,91	18,21,22	4.70	7 (38%)	21,30,33	1.93	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	L1	672	91,1	18,21,22	4.58	7 (38%)	21,30,33	2.07	5 (23%)
88	G7M	S1	1995	88,51	23,26,27	3.87	12 (52%)	34,39,42	1.72	7 (20%)
88	PSU	S1	33	88	18,21,22	4.73	7 (38%)	21,30,33	1.98	5 (23%)
2	PSU	L2	662	91,2	18,21,22	4.61	7 (38%)	21,30,33	1.99	5 (23%)
2	PSU	L2	593	91,2	18,21,22	4.60	7 (38%)	21,30,33	1.91	6 (28%)
2	OMG	L2	686	2	23,26,27	2.41	9 (39%)	32,38,41	2.52	11 (34%)
88	A2M	S1	28	88,91	22,25,26	3.50	9 (40%)	30,36,39	2.33	11 (36%)
1	PSU	L1	774	1	18,21,22	4.64	7 (38%)	21,30,33	1.99	5 (23%)
1	A2M	L1	1373	1	22,25,26	3.53	9 (40%)	30,36,39	2.33	10 (33%)
1	OMU	L1	1107	1	19,22,23	3.01	8 (42%)	25,31,34	1.88	5 (20%)
2	A2M	L2	604	1,2	22,25,26	3.52	9 (40%)	30,36,39	2.35	11 (36%)
2	PSU	L2	1058	2	18,21,22	4.60	7 (38%)	21,30,33	2.05	5 (23%)
2	OMC	L2	1248	2	19,22,23	3.01	8 (42%)	25,31,34	0.83	0
1	OMC	L1	695	1	19,22,23	2.93	8 (42%)	25,31,34	0.68	0
88	A2M	S1	98	88,91	22,25,26	3.49	9 (40%)	30,36,39	2.31	11 (36%)
88	A2M	S1	479	88	22,25,26	3.48	9 (40%)	30,36,39	2.34	10 (33%)
88	OMU	S1	1833	88,91	19,22,23	3.04	8 (42%)	25,31,34	1.89	5 (20%)
1	A2M	L1	681	1	22,25,26	3.49	9 (40%)	30,36,39	2.36	11 (36%)
1	A2M	L1	69	1	22,25,26	3.48	9 (40%)	30,36,39	2.50	12 (40%)
2	OMG	L2	1231	2	23,26,27	2.39	9 (39%)	32,38,41	2.48	11 (34%)
88	A2M	S1	2021	88	22,25,26	3.47	9 (40%)	30,36,39	2.39	11 (36%)
2	PSU	L2	500	2	18,21,22	4.64	7 (38%)	21,30,33	1.90	5 (23%)
2	OMU	L2	667	2	19,22,23	3.03	8 (42%)	25,31,34	1.88	5 (20%)
88	OMG	S1	1550	88	23,26,27	2.46	9 (39%)	32,38,41	2.58	10 (31%)
2	OMC	L2	14	91,1,2	19,22,23	2.97	8 (42%)	25,31,34	0.81	0
1	OMU	L1	847	1	19,22,23	3.00	8 (42%)	25,31,34	1.86	5 (20%)
1	PSU	L1	1177	1	18,21,22	4.55	7 (38%)	21,30,33	1.80	4 (19%)
1	PSU	L1	239	1	18,21,22	4.63	7 (38%)	21,30,33	1.94	5 (23%)
2	A2M	L2	1185	2	22,25,26	3.48	9 (40%)	30,36,39	2.41	12 (40%)
88	OMG	S1	600	88	23,26,27	2.44	9 (39%)	32,38,41	2.57	10 (31%)
88	OMU	S1	1662	88	19,22,23	3.08	8 (42%)	25,31,34	1.78	4 (16%)
2	PSU	L2	1303	2	18,21,22	4.62	7 (38%)	21,30,33	2.06	6 (28%)
2	PSU	L2	504	2	18,21,22	4.60	7 (38%)	21,30,33	1.95	4 (19%)
88	OMG	S1	1829	88,91	23,26,27	2.43	9 (39%)	32,38,41	2.57	10 (31%)
2	A2M	L2	628	2	22,25,26	3.49	9 (40%)	30,36,39	2.34	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMU	L2	1359	2	19,22,23	3.02	8 (42%)	25,31,34	1.88	5 (20%)
2	A2M	L2	1067	2	22,25,26	3.51	9 (40%)	30,36,39	2.37	11 (36%)
7	A2M	L7	162	7,1	22,25,26	3.54	9 (40%)	30,36,39	2.29	10 (33%)
88	OMC	S1	1866	88	19,22,23	3.02	8 (42%)	25,31,34	0.76	0
1	A2M	L1	955	1	22,25,26	3.52	9 (40%)	30,36,39	2.36	11 (36%)
88	B8N	S1	1543	88,91	25,29,30	0.43	0	28,42,45	0.45	0
1	OMC	L1	1010	91,1	19,22,23	2.98	8 (42%)	25,31,34	0.80	0
2	OMG	L2	71	91,2	23,26,27	2.43	9 (39%)	32,38,41	2.48	12 (37%)
2	PSU	L2	510	2	18,21,22	4.65	7 (38%)	21,30,33	1.91	5 (23%)
1	OMG	L1	1524	1	23,26,27	2.43	9 (39%)	32,38,41	2.58	11 (34%)
1	OMG	L1	959	1	23,26,27	2.43	9 (39%)	32,38,41	2.66	10 (31%)
2	PSU	L2	1403	2	18,21,22	4.63	7 (38%)	21,30,33	2.07	6 (28%)
2	PSU	L2	1213	2	18,21,22	4.66	7 (38%)	21,30,33	1.97	5 (23%)
88	PSU	S1	12	88	18,21,22	4.63	7 (38%)	21,30,33	1.91	5 (23%)
1	PSU	L1	1528	1	18,21,22	4.64	7 (38%)	21,30,33	1.89	5 (23%)
1	OMU	L1	1253	1	19,22,23	3.17	8 (42%)	25,31,34	1.87	5 (20%)
1	OMU	L1	845	1	19,22,23	3.01	8 (42%)	25,31,34	2.31	8 (32%)
1	PSU	L1	1664	1	18,21,22	4.67	7 (38%)	21,30,33	2.02	6 (28%)
2	OMG	L2	1253	2	23,26,27	2.30	8 (34%)	32,38,41	2.37	9 (28%)
4	OMG	L4	74	4	23,26,27	2.39	9 (39%)	32,38,41	2.52	11 (34%)
88	OMC	S1	2059	88	19,22,23	3.00	8 (42%)	25,31,34	1.26	3 (12%)
1	OMG	L1	1626	1	23,26,27	2.42	9 (39%)	32,38,41	2.49	10 (31%)
2	OMG	L2	1360	2	23,26,27	2.43	9 (39%)	32,38,41	2.59	10 (31%)
2	A2M	L2	95	2	22,25,26	3.52	9 (40%)	30,36,39	2.37	10 (33%)
2	A2M	L2	1384	91,2	22,25,26	3.49	9 (40%)	30,36,39	2.36	11 (36%)
2	A2M	L2	527	2	22,25,26	3.41	9 (40%)	30,36,39	2.54	12 (40%)
2	OMU	L2	560	91,2	19,22,23	2.97	8 (42%)	25,31,34	2.10	7 (28%)
7	OMG	L7	75	7	23,26,27	2.42	9 (39%)	32,38,41	2.46	10 (31%)
88	PSU	S1	1533	88	18,21,22	0.94	1 (5%)	21,30,33	0.76	0
1	PSU	L1	1017	91,1	18,21,22	4.61	7 (38%)	21,30,33	2.10	5 (23%)
2	PSU	L2	78	2	18,21,22	4.60	7 (38%)	21,30,33	2.05	5 (23%)
2	OMC	L2	359	2	19,22,23	3.02	8 (42%)	25,31,34	0.69	0
88	MA6	S1	2185	88	23,26,27	1.41	4 (17%)	33,38,41	3.62	11 (33%)
2	OMC	L2	1159	2	19,22,23	3.00	8 (42%)	25,31,34	0.82	0
1	PSU	L1	1533	1,2	18,21,22	4.61	7 (38%)	21,30,33	2.00	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PSU	L7	166	7,1	18,21,22	4.64	7 (38%)	21,30,33	2.01	5 (23%)
2	OMU	L2	1419	2	19,22,23	3.02	8 (42%)	25,31,34	1.78	4 (16%)
2	PSU	L2	1060	2	18,21,22	4.62	7 (38%)	21,30,33	2.03	5 (23%)
7	PSU	L7	69	7	18,21,22	4.65	7 (38%)	21,30,33	2.05	6 (28%)
88	OMU	S1	1979	88	19,22,23	3.07	8 (42%)	25,31,34	1.80	5 (20%)
88	OMC	S1	38	88	19,22,23	3.06	8 (42%)	25,31,34	0.72	0
88	A2M	S1	668	88,91	22,25,26	3.47	9 (40%)	30,36,39	2.41	11 (36%)
2	PSU	L2	1361	91,2	18,21,22	4.65	7 (38%)	21,30,33	2.02	5 (23%)
2	OMC	L2	1397	2	19,22,23	2.96	8 (42%)	25,31,34	0.74	0
2	OMC	L2	1317	2	19,22,23	2.96	8 (42%)	25,31,34	0.77	0
1	A2M	L1	927	91,1	22,25,26	3.46	9 (40%)	30,36,39	2.42	10 (33%)
1	PSU	L1	1529	1	18,21,22	4.63	7 (38%)	21,30,33	2.03	5 (23%)
88	PSU	S1	2202	88	18,21,22	4.68	7 (38%)	21,30,33	1.84	5 (23%)
1	PSU	L1	1011	1,2	18,21,22	4.64	8 (44%)	21,30,33	1.94	6 (28%)
2	A2M	L2	591	2	22,25,26	3.54	9 (40%)	30,36,39	2.32	11 (36%)
2	OMG	L2	1229	2	23,26,27	2.41	9 (39%)	32,38,41	2.52	10 (31%)
7	PSU	L7	101	7	18,21,22	4.62	7 (38%)	21,30,33	1.99	6 (28%)
1	OMU	L1	48	1	19,22,23	3.00	7 (36%)	25,31,34	2.21	8 (32%)
88	5MC	S1	1544	88	19,22,23	0.85	1 (5%)	26,32,35	0.48	0
2	5MC	L2	524	91,2	19,22,23	3.75	8 (42%)	26,32,35	0.97	2 (7%)
88	MA6	S1	2184	88	23,26,27	1.43	4 (17%)	33,38,41	3.54	11 (33%)
1	A2M	L1	678	1,2	22,25,26	3.51	9 (40%)	30,36,39	2.37	11 (36%)
2	OMG	L2	655	91,2	23,26,27	2.43	9 (39%)	32,38,41	2.57	11 (34%)
88	OMG	S1	1478	88	23,26,27	2.39	9 (39%)	32,38,41	2.49	11 (34%)
2	OMU	L2	1077	2	19,22,23	3.01	8 (42%)	25,31,34	1.85	5 (20%)
2	PSU	L2	1144	2	18,21,22	4.61	7 (38%)	21,30,33	2.02	5 (23%)
2	A2M	L2	665	2	22,25,26	3.50	9 (40%)	30,36,39	2.38	11 (36%)
2	OMG	L2	1046	51,2	23,26,27	2.39	9 (39%)	32,38,41	2.55	10 (31%)

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	OMU	L3	13	3	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L2	437	91,2	-	0/7/25/26	0/2/2/2
88	A2M	S1	512	88,91	-	2/9/27/28	0/3/3/3
88	OMU	S1	2048	88,91	-	0/9/27/28	0/2/2/2
2	PSU	L2	597	2	-	0/7/25/26	0/2/2/2
88	PSU	S1	1657	88	-	2/7/25/26	0/2/2/2
1	OMG	L1	856	1	-	0/9/27/28	0/3/3/3
1	OMC	L1	1527	91,1	-	3/9/27/28	0/2/2/2
2	PSU	L2	802	2	-	2/7/25/26	0/2/2/2
2	PSU	L2	1265	91,2	-	0/7/25/26	0/2/2/2
1	OMU	L1	1371	1	-	5/9/27/28	0/2/2/2
88	OMU	S1	8	88	-	4/9/27/28	0/2/2/2
2	A2M	L2	572	2	-	0/9/27/28	0/3/3/3
2	OMG	L2	1078	2	-	0/9/27/28	0/3/3/3
88	PSU	S1	1566	88,91	-	2/7/25/26	0/2/2/2
88	OMG	S1	1647	88	-	0/9/27/28	0/3/3/3
1	PSU	L1	1526	91,1	-	2/7/25/26	0/2/2/2
2	PSU	L2	1152	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	512	2	-	0/7/25/26	0/2/2/2
7	A2M	L7	43	7	-	0/9/27/28	0/3/3/3
1	A2M	L1	305	1	-	2/9/27/28	0/3/3/3
2	A2M	L2	382	2,89	-	0/9/27/28	0/3/3/3
88	OMG	S1	1623	88	-	0/9/27/28	0/3/3/3
2	OMG	L2	641	91,2	-	0/9/27/28	0/3/3/3
1	OMU	L1	1659	91,1	-	0/9/27/28	0/2/2/2
1	OMG	L1	1190	91,1	-	0/9/27/28	0/3/3/3
2	PSU	L2	1382	91,2	-	2/7/25/26	0/2/2/2
2	OMU	L2	565	2	-	3/9/27/28	0/2/2/2
88	OMU	S1	1621	88	-	0/9/27/28	0/2/2/2
1	A2M	L1	858	1	-	1/9/27/28	0/3/3/3
88	OMG	S1	1865	88,91	-	0/9/27/28	0/3/3/3
2	PSU	L2	626	2	-	0/7/25/26	0/2/2/2
88	OMC	S1	2140	88	-	0/9/27/28	0/2/2/2
88	OMC	S1	18	88	-	0/9/27/28	0/2/2/2
1	PSU	L1	422	1	-	0/7/25/26	0/2/2/2
2	OMC	L2	443	91,2	-	4/9/27/28	0/2/2/2
88	OMU	S1	661	88	-	0/9/27/28	0/2/2/2
1	A2M	L1	235	91,1	-	0/9/27/28	0/3/3/3
1	PSU	L1	940	1	-	0/7/25/26	0/2/2/2
1	OMG	L1	1540	91,1,2	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L2	1264	2	-	2/7/25/26	0/2/2/2
2	A2M	L2	570	1,2	-	3/9/27/28	0/3/3/3
2	PSU	L2	1194	2	-	0/7/25/26	0/2/2/2
2	OMG	L2	534	2	-	2/9/27/28	0/3/3/3
2	OMU	L2	56	1,2	-	0/9/27/28	0/2/2/2
2	5MC	L2	1308	2,89	-	4/7/25/26	0/2/2/2
2	A2M	L2	1372	2	-	0/9/27/28	0/3/3/3
1	A2M	L1	697	1	-	0/9/27/28	0/3/3/3
88	A2M	S1	897	88	-	0/9/27/28	0/3/3/3
88	OMU	S1	29	88	-	0/9/27/28	0/2/2/2
88	OMG	S1	2151	88	-	3/9/27/28	0/3/3/3
7	PSU	L7	74	7	-	0/7/25/26	0/2/2/2
88	PSU	S1	1539	88	-	0/7/25/26	0/2/2/2
2	OMC	L2	583	2	-	0/9/27/28	0/2/2/2
1	A2M	L1	1539	91,1,2	-	0/9/27/28	0/3/3/3
88	5MC	S1	2061	88	-	2/7/25/26	0/2/2/2
2	PSU	L2	472	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1318	91,2	-	0/7/25/26	0/2/2/2
2	OMU	L2	73	2	-	0/9/27/28	0/2/2/2
88	PSU	S1	1246	88,91	-	0/7/25/26	0/2/2/2
88	PSU	S1	1292	88,91	-	0/7/25/26	0/2/2/2
1	PSU	L1	672	91,1	-	0/7/25/26	0/2/2/2
88	G7M	S1	1995	88,51	-	2/7/25/26	0/3/3/3
88	PSU	S1	33	88	-	0/7/25/26	0/2/2/2
2	PSU	L2	662	91,2	-	0/7/25/26	0/2/2/2
2	PSU	L2	593	91,2	-	0/7/25/26	0/2/2/2
2	OMG	L2	686	2	-	0/9/27/28	0/3/3/3
88	A2M	S1	28	88,91	-	0/9/27/28	0/3/3/3
1	PSU	L1	774	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1373	1	-	0/9/27/28	0/3/3/3
1	OMU	L1	1107	1	-	1/9/27/28	0/2/2/2
2	A2M	L2	604	1,2	-	0/9/27/28	0/3/3/3
2	PSU	L2	1058	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	1248	2	-	1/9/27/28	0/2/2/2
1	OMC	L1	695	1	-	1/9/27/28	0/2/2/2
88	A2M	S1	98	88,91	-	1/9/27/28	0/3/3/3
88	A2M	S1	479	88	-	0/9/27/28	0/3/3/3
88	OMU	S1	1833	88,91	-	0/9/27/28	0/2/2/2
1	A2M	L1	681	1	-	3/9/27/28	0/3/3/3
1	A2M	L1	69	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L2	1231	2	-	0/9/27/28	0/3/3/3
88	A2M	S1	2021	88	-	1/9/27/28	0/3/3/3
2	PSU	L2	500	2	-	0/7/25/26	0/2/2/2
2	OMU	L2	667	2	-	1/9/27/28	0/2/2/2
88	OMG	S1	1550	88	-	0/9/27/28	0/3/3/3
2	OMC	L2	14	91,1,2	-	0/9/27/28	0/2/2/2
1	OMU	L1	847	1	-	0/9/27/28	0/2/2/2
1	PSU	L1	1177	1	-	2/7/25/26	0/2/2/2
1	PSU	L1	239	1	-	0/7/25/26	0/2/2/2
2	A2M	L2	1185	2	-	2/9/27/28	0/3/3/3
88	OMG	S1	600	88	-	2/9/27/28	0/3/3/3
88	OMU	S1	1662	88	-	1/9/27/28	0/2/2/2
2	PSU	L2	1303	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	504	2	-	3/7/25/26	0/2/2/2
88	OMG	S1	1829	88,91	-	2/9/27/28	0/3/3/3
2	A2M	L2	628	2	-	0/9/27/28	0/3/3/3
2	OMU	L2	1359	2	-	0/9/27/28	0/2/2/2
2	A2M	L2	1067	2	-	1/9/27/28	0/3/3/3
7	A2M	L7	162	7,1	-	1/9/27/28	0/3/3/3
88	OMC	S1	1866	88	-	0/9/27/28	0/2/2/2
1	A2M	L1	955	1	-	0/9/27/28	0/3/3/3
88	B8N	S1	1543	88,91	-	5/16/34/35	0/2/2/2
1	OMC	L1	1010	91,1	-	3/9/27/28	0/2/2/2
2	OMG	L2	71	91,2	-	0/9/27/28	0/3/3/3
2	PSU	L2	510	2	-	0/7/25/26	0/2/2/2
1	OMG	L1	1524	1	-	1/9/27/28	0/3/3/3
1	OMG	L1	959	1	-	1/9/27/28	0/3/3/3
2	PSU	L2	1403	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1213	2	-	0/7/25/26	0/2/2/2
88	PSU	S1	12	88	-	0/7/25/26	0/2/2/2
1	PSU	L1	1528	1	-	0/7/25/26	0/2/2/2
1	OMU	L1	1253	1	-	7/9/27/28	0/2/2/2
1	OMU	L1	845	1	-	3/9/27/28	0/2/2/2
1	PSU	L1	1664	1	-	0/7/25/26	0/2/2/2
2	OMG	L2	1253	2	-	0/9/27/28	0/3/3/3
4	OMG	L4	74	4	-	1/9/27/28	0/3/3/3
88	OMC	S1	2059	88	-	3/9/27/28	0/2/2/2
1	OMG	L1	1626	1	-	0/9/27/28	0/3/3/3
2	OMG	L2	1360	2	-	0/9/27/28	0/3/3/3
2	A2M	L2	95	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	L2	1384	91,2	-	1/9/27/28	0/3/3/3
2	A2M	L2	527	2	-	0/9/27/28	0/3/3/3
2	OMU	L2	560	91,2	-	3/9/27/28	0/2/2/2
7	OMG	L7	75	7	-	0/9/27/28	0/3/3/3
88	PSU	S1	1533	88	-	0/7/25/26	0/2/2/2
1	PSU	L1	1017	91,1	-	2/7/25/26	0/2/2/2
2	PSU	L2	78	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	359	2	-	0/9/27/28	0/2/2/2
88	MA6	S1	2185	88	-	1/11/29/30	0/3/3/3
2	OMC	L2	1159	2	-	0/9/27/28	0/2/2/2
1	PSU	L1	1533	1,2	-	0/7/25/26	0/2/2/2
7	PSU	L7	166	7,1	-	0/7/25/26	0/2/2/2
2	OMU	L2	1419	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	1060	2	-	0/7/25/26	0/2/2/2
7	PSU	L7	69	7	-	0/7/25/26	0/2/2/2
88	OMU	S1	1979	88	-	0/9/27/28	0/2/2/2
88	OMC	S1	38	88	-	0/9/27/28	0/2/2/2
88	A2M	S1	668	88,91	-	5/9/27/28	0/3/3/3
2	PSU	L2	1361	91,2	-	3/7/25/26	0/2/2/2
2	OMC	L2	1397	2	-	0/9/27/28	0/2/2/2
2	OMC	L2	1317	2	-	0/9/27/28	0/2/2/2
1	A2M	L1	927	91,1	-	1/9/27/28	0/3/3/3
1	PSU	L1	1529	1	-	0/7/25/26	0/2/2/2
88	PSU	S1	2202	88	-	1/7/25/26	0/2/2/2
1	PSU	L1	1011	1,2	-	0/7/25/26	0/2/2/2
2	A2M	L2	591	2	-	0/9/27/28	0/3/3/3
2	OMG	L2	1229	2	-	2/9/27/28	0/3/3/3
7	PSU	L7	101	7	-	0/7/25/26	0/2/2/2
1	OMU	L1	48	1	-	2/9/27/28	0/2/2/2
88	5MC	S1	1544	88	-	0/7/25/26	0/2/2/2
2	5MC	L2	524	91,2	-	0/7/25/26	0/2/2/2
88	MA6	S1	2184	88	-	0/11/29/30	0/3/3/3
1	A2M	L1	678	1,2	-	2/9/27/28	0/3/3/3
2	OMG	L2	655	91,2	-	1/9/27/28	0/3/3/3
88	OMG	S1	1478	88	-	1/9/27/28	0/3/3/3
2	OMU	L2	1077	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	1144	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	665	2	-	3/9/27/28	0/3/3/3
2	OMG	L2	1046	51,2	-	3/9/27/28	0/3/3/3

All (1254) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1292	PSU	C6-C5	12.50	1.49	1.35
88	S1	33	PSU	C6-C5	12.48	1.49	1.35
88	S1	1246	PSU	C6-C5	12.43	1.49	1.35
2	L2	512	PSU	C6-C5	12.38	1.49	1.35
2	L2	1194	PSU	C6-C5	12.33	1.48	1.35
1	L1	1664	PSU	C6-C5	12.32	1.48	1.35
88	S1	1566	PSU	C6-C5	12.29	1.48	1.35
2	L2	1265	PSU	C6-C5	12.29	1.48	1.35
2	L2	1213	PSU	C6-C5	12.26	1.48	1.35
88	S1	2202	PSU	C6-C5	12.26	1.48	1.35
1	L1	940	PSU	C6-C5	12.25	1.48	1.35
2	L2	510	PSU	C6-C5	12.25	1.48	1.35
88	S1	12	PSU	C6-C5	12.24	1.48	1.35
2	L2	802	PSU	C6-C5	12.23	1.48	1.35
1	L1	1528	PSU	C6-C5	12.23	1.48	1.35
2	L2	662	PSU	C6-C5	12.22	1.48	1.35
1	L1	1529	PSU	C6-C5	12.22	1.48	1.35
2	L2	1361	PSU	C6-C5	12.22	1.48	1.35
7	L7	74	PSU	C6-C5	12.22	1.48	1.35
1	L1	1017	PSU	C6-C5	12.21	1.48	1.35
2	L2	1060	PSU	C6-C5	12.20	1.48	1.35
7	L7	166	PSU	C6-C5	12.20	1.48	1.35
1	L1	239	PSU	C6-C5	12.20	1.48	1.35
88	S1	1657	PSU	C6-C5	12.19	1.48	1.35
7	L7	69	PSU	C6-C5	12.19	1.48	1.35
2	L2	504	PSU	C6-C5	12.18	1.48	1.35
1	L1	1011	PSU	C6-C5	12.17	1.48	1.35
2	L2	593	PSU	C6-C5	12.16	1.48	1.35
2	L2	472	PSU	C6-C5	12.15	1.48	1.35
2	L2	1382	PSU	C6-C5	12.14	1.48	1.35
1	L1	774	PSU	C6-C5	12.14	1.48	1.35
2	L2	437	PSU	C6-C5	12.14	1.48	1.35
2	L2	626	PSU	C6-C5	12.13	1.48	1.35
7	L7	101	PSU	C6-C5	12.12	1.48	1.35
2	L2	1058	PSU	C6-C5	12.12	1.48	1.35
2	L2	500	PSU	C6-C5	12.12	1.48	1.35
2	L2	597	PSU	C6-C5	12.12	1.48	1.35
1	L1	1533	PSU	C6-C5	12.11	1.48	1.35
2	L2	1144	PSU	C6-C5	12.11	1.48	1.35
2	L2	78	PSU	C6-C5	12.09	1.48	1.35
1	L1	672	PSU	C6-C5	12.08	1.48	1.35
1	L1	1526	PSU	C6-C5	12.08	1.48	1.35
2	L2	1303	PSU	C6-C5	12.03	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1152	PSU	C6-C5	12.02	1.48	1.35
2	L2	1403	PSU	C6-C5	12.01	1.48	1.35
2	L2	1264	PSU	C6-C5	12.00	1.48	1.35
1	L1	422	PSU	C6-C5	11.97	1.48	1.35
2	L2	1318	PSU	C6-C5	11.97	1.48	1.35
1	L1	1177	PSU	C6-C5	11.84	1.48	1.35
88	S1	1995	G7M	C8-N7	11.16	1.52	1.33
88	S1	33	PSU	C2-N1	10.26	1.50	1.36
88	S1	1246	PSU	C2-N1	10.21	1.50	1.36
2	L2	512	PSU	C2-N1	10.16	1.49	1.36
88	S1	2202	PSU	C2-N1	10.15	1.49	1.36
1	L1	940	PSU	C2-N1	10.11	1.49	1.36
2	L2	1213	PSU	C2-N1	10.11	1.49	1.36
88	S1	1566	PSU	C2-N1	10.10	1.49	1.36
1	L1	774	PSU	C2-N1	10.10	1.49	1.36
2	L2	1303	PSU	C2-N1	10.09	1.49	1.36
2	L2	802	PSU	C2-N1	10.08	1.49	1.36
2	L2	472	PSU	C2-N1	10.05	1.49	1.36
88	S1	1292	PSU	C2-N1	10.05	1.49	1.36
88	S1	1657	PSU	C2-N1	10.04	1.49	1.36
1	L1	1528	PSU	C2-N1	10.04	1.49	1.36
2	L2	1194	PSU	C2-N1	10.03	1.49	1.36
2	L2	78	PSU	C2-N1	10.02	1.49	1.36
2	L2	510	PSU	C2-N1	10.02	1.49	1.36
2	L2	500	PSU	C2-N1	10.02	1.49	1.36
2	L2	1144	PSU	C2-N1	10.02	1.49	1.36
7	L7	101	PSU	C2-N1	10.01	1.49	1.36
2	L2	1403	PSU	C2-N1	10.00	1.49	1.36
1	L1	1526	PSU	C2-N1	10.00	1.49	1.36
2	L2	1361	PSU	C2-N1	9.99	1.49	1.36
2	L2	1152	PSU	C2-N1	9.98	1.49	1.36
7	L7	69	PSU	C2-N1	9.98	1.49	1.36
7	L7	166	PSU	C2-N1	9.98	1.49	1.36
1	L1	1529	PSU	C2-N1	9.98	1.49	1.36
2	L2	504	PSU	C2-N1	9.98	1.49	1.36
7	L7	74	PSU	C2-N1	9.98	1.49	1.36
2	L2	1382	PSU	C2-N1	9.97	1.49	1.36
1	L1	1664	PSU	C2-N1	9.96	1.49	1.36
2	L2	1264	PSU	C2-N1	9.96	1.49	1.36
1	L1	1011	PSU	C2-N1	9.94	1.49	1.36
2	L2	662	PSU	C2-N1	9.94	1.49	1.36
88	S1	12	PSU	C2-N1	9.93	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1017	PSU	C2-N1	9.92	1.49	1.36
1	L1	239	PSU	C2-N1	9.91	1.49	1.36
2	L2	597	PSU	C2-N1	9.90	1.49	1.36
2	L2	1058	PSU	C2-N1	9.88	1.49	1.36
2	L2	626	PSU	C2-N1	9.88	1.49	1.36
2	L2	1265	PSU	C2-N1	9.87	1.49	1.36
2	L2	593	PSU	C2-N1	9.87	1.49	1.36
2	L2	1060	PSU	C2-N1	9.86	1.49	1.36
1	L1	1177	PSU	C2-N1	9.85	1.49	1.36
1	L1	1533	PSU	C2-N1	9.81	1.49	1.36
2	L2	437	PSU	C2-N1	9.80	1.49	1.36
2	L2	1318	PSU	C2-N1	9.78	1.49	1.36
1	L1	422	PSU	C2-N1	9.78	1.49	1.36
1	L1	672	PSU	C2-N1	9.73	1.49	1.36
2	L2	1308	5MC	C3'-C4'	-9.59	1.28	1.53
2	L2	1308	5MC	C6-C5	9.45	1.50	1.34
1	L1	1373	A2M	C2'-C1'	-9.29	1.30	1.53
88	S1	2061	5MC	C6-C5	9.26	1.49	1.34
7	L7	162	A2M	C2'-C1'	-9.20	1.30	1.53
1	L1	305	A2M	C2'-C1'	-9.18	1.30	1.53
2	L2	591	A2M	C2'-C1'	-9.16	1.30	1.53
1	L1	1539	A2M	C2'-C1'	-9.15	1.30	1.53
2	L2	1372	A2M	C2'-C1'	-9.13	1.30	1.53
2	L2	604	A2M	C2'-C1'	-9.11	1.30	1.53
2	L2	1067	A2M	C2'-C1'	-9.10	1.30	1.53
1	L1	955	A2M	C2'-C1'	-9.07	1.30	1.53
1	L1	678	A2M	C2'-C1'	-9.07	1.30	1.53
1	L1	697	A2M	C2'-C1'	-9.05	1.30	1.53
2	L2	572	A2M	C2'-C1'	-9.05	1.30	1.53
1	L1	681	A2M	C2'-C1'	-9.04	1.30	1.53
2	L2	524	5MC	C6-C5	9.04	1.49	1.34
2	L2	665	A2M	C2'-C1'	-9.04	1.30	1.53
2	L2	95	A2M	C2'-C1'	-9.02	1.30	1.53
7	L7	43	A2M	C2'-C1'	-9.01	1.30	1.53
88	S1	512	A2M	C2'-C1'	-9.01	1.30	1.53
88	S1	897	A2M	C2'-C1'	-9.00	1.30	1.53
88	S1	28	A2M	C2'-C1'	-8.97	1.31	1.53
2	L2	527	A2M	C2'-C1'	-8.97	1.31	1.53
2	L2	1384	A2M	C2'-C1'	-8.94	1.31	1.53
88	S1	28	A2M	O4'-C1'	8.94	1.62	1.42
1	L1	69	A2M	C2'-C1'	-8.93	1.31	1.53
88	S1	98	A2M	C2'-C1'	-8.93	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	235	A2M	C2'-C1'	-8.92	1.31	1.53
2	L2	382	A2M	C2'-C1'	-8.92	1.31	1.53
88	S1	479	A2M	C2'-C1'	-8.92	1.31	1.53
88	S1	897	A2M	O4'-C1'	8.89	1.62	1.42
2	L2	628	A2M	C2'-C1'	-8.89	1.31	1.53
1	L1	927	A2M	C2'-C1'	-8.88	1.31	1.53
88	S1	512	A2M	O4'-C1'	8.86	1.62	1.42
2	L2	591	A2M	O4'-C1'	8.86	1.62	1.42
88	S1	98	A2M	O4'-C1'	8.85	1.62	1.42
1	L1	955	A2M	O4'-C1'	8.84	1.62	1.42
2	L2	382	A2M	O4'-C1'	8.84	1.62	1.42
1	L1	235	A2M	O4'-C1'	8.82	1.62	1.42
2	L2	1067	A2M	O4'-C1'	8.81	1.62	1.42
1	L1	1373	A2M	O4'-C1'	8.81	1.62	1.42
1	L1	697	A2M	O4'-C1'	8.81	1.62	1.42
2	L2	572	A2M	O4'-C1'	8.80	1.62	1.42
2	L2	1384	A2M	O4'-C1'	8.80	1.62	1.42
1	L1	858	A2M	C2'-C1'	-8.80	1.31	1.53
2	L2	604	A2M	O4'-C1'	8.80	1.62	1.42
88	S1	479	A2M	O4'-C1'	8.80	1.62	1.42
2	L2	95	A2M	O4'-C1'	8.79	1.62	1.42
1	L1	1539	A2M	O4'-C1'	8.79	1.62	1.42
2	L2	570	A2M	C2'-C1'	-8.79	1.31	1.53
2	L2	1185	A2M	C2'-C1'	-8.79	1.31	1.53
2	L2	628	A2M	O4'-C1'	8.78	1.62	1.42
7	L7	162	A2M	O4'-C1'	8.78	1.62	1.42
88	S1	668	A2M	C2'-C1'	-8.77	1.31	1.53
2	L2	1372	A2M	O4'-C1'	8.77	1.62	1.42
88	S1	2021	A2M	C2'-C1'	-8.76	1.31	1.53
7	L7	43	A2M	O4'-C1'	8.75	1.62	1.42
1	L1	678	A2M	O4'-C1'	8.74	1.62	1.42
2	L2	570	A2M	O4'-C1'	8.73	1.62	1.42
1	L1	927	A2M	O4'-C1'	8.71	1.62	1.42
88	S1	2021	A2M	O4'-C1'	8.69	1.62	1.42
1	L1	858	A2M	O4'-C1'	8.68	1.62	1.42
2	L2	665	A2M	O4'-C1'	8.67	1.62	1.42
2	L2	1185	A2M	O4'-C1'	8.67	1.62	1.42
1	L1	69	A2M	O4'-C1'	8.61	1.61	1.42
1	L1	681	A2M	O4'-C1'	8.60	1.61	1.42
1	L1	305	A2M	O4'-C1'	8.59	1.61	1.42
88	S1	668	A2M	O4'-C1'	8.38	1.61	1.42
2	L2	527	A2M	O4'-C1'	8.17	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1308	5MC	O4'-C4'	8.14	1.63	1.45
1	L1	1253	OMU	C2-N1	7.98	1.51	1.38
88	S1	33	PSU	C2-N3	7.97	1.50	1.37
88	S1	2202	PSU	C2-N3	7.95	1.50	1.37
2	L2	472	PSU	C2-N3	7.89	1.50	1.37
88	S1	1292	PSU	C2-N3	7.88	1.50	1.37
2	L2	1403	PSU	C2-N3	7.88	1.50	1.37
2	L2	1361	PSU	C2-N3	7.87	1.50	1.37
88	S1	1246	PSU	C2-N3	7.86	1.50	1.37
1	L1	1664	PSU	C2-N3	7.86	1.50	1.37
2	L2	802	PSU	C2-N3	7.85	1.50	1.37
1	L1	1011	PSU	C2-N3	7.84	1.50	1.37
2	L2	512	PSU	C2-N3	7.84	1.50	1.37
2	L2	500	PSU	C2-N3	7.83	1.50	1.37
7	L7	69	PSU	C2-N3	7.82	1.50	1.37
2	L2	1265	PSU	C2-N3	7.82	1.50	1.37
1	L1	1533	PSU	C2-N3	7.80	1.50	1.37
1	L1	239	PSU	C2-N3	7.77	1.50	1.37
88	S1	1657	PSU	C2-N3	7.77	1.50	1.37
88	S1	1566	PSU	C2-N3	7.77	1.50	1.37
7	L7	166	PSU	C2-N3	7.77	1.50	1.37
1	L1	1526	PSU	C2-N3	7.76	1.50	1.37
2	L2	1152	PSU	C2-N3	7.75	1.50	1.37
2	L2	1213	PSU	C2-N3	7.74	1.50	1.37
7	L7	74	PSU	C2-N3	7.73	1.50	1.37
1	L1	422	PSU	C2-N3	7.73	1.50	1.37
2	L2	626	PSU	C2-N3	7.73	1.50	1.37
1	L1	774	PSU	C2-N3	7.73	1.50	1.37
2	L2	437	PSU	C2-N3	7.73	1.50	1.37
2	L2	1060	PSU	C2-N3	7.73	1.50	1.37
88	S1	12	PSU	C2-N3	7.72	1.50	1.37
1	L1	940	PSU	C2-N3	7.72	1.50	1.37
2	L2	1194	PSU	C2-N3	7.71	1.50	1.37
1	L1	1529	PSU	C2-N3	7.69	1.50	1.37
2	L2	1058	PSU	C2-N3	7.68	1.50	1.37
2	L2	510	PSU	C2-N3	7.67	1.50	1.37
2	L2	1303	PSU	C2-N3	7.67	1.50	1.37
2	L2	1382	PSU	C2-N3	7.66	1.50	1.37
7	L7	101	PSU	C2-N3	7.65	1.50	1.37
1	L1	1371	OMU	C2-N1	7.64	1.50	1.38
1	L1	672	PSU	C2-N3	7.64	1.50	1.37
1	L1	1528	PSU	C2-N3	7.64	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	593	PSU	C2-N3	7.63	1.50	1.37
2	L2	1144	PSU	C2-N3	7.62	1.50	1.37
2	L2	1318	PSU	C2-N3	7.60	1.50	1.37
1	L1	1177	PSU	C2-N3	7.59	1.50	1.37
1	L1	1017	PSU	C2-N3	7.59	1.50	1.37
1	L1	845	OMU	C2-N1	7.58	1.50	1.38
2	L2	662	PSU	C2-N3	7.57	1.49	1.37
2	L2	565	OMU	C2-N1	7.56	1.50	1.38
2	L2	597	PSU	C2-N3	7.55	1.49	1.37
2	L2	1264	PSU	C2-N3	7.54	1.49	1.37
2	L2	78	PSU	C2-N3	7.51	1.49	1.37
2	L2	504	PSU	C2-N3	7.51	1.49	1.37
1	L1	48	OMU	C2-N1	7.47	1.50	1.38
2	L2	1308	5MC	C5-C4	7.20	1.49	1.44
88	S1	1979	OMU	C2-N1	7.16	1.49	1.38
88	S1	1662	OMU	C2-N1	7.14	1.49	1.38
2	L2	56	OMU	C2-N1	7.12	1.49	1.38
1	L1	1253	OMU	C2-N3	7.09	1.50	1.38
88	S1	2048	OMU	C2-N1	7.09	1.49	1.38
88	S1	661	OMU	C2-N1	7.09	1.49	1.38
88	S1	1833	OMU	C2-N1	7.08	1.49	1.38
3	L3	13	OMU	C2-N1	7.07	1.49	1.38
88	S1	1621	OMU	C2-N1	7.03	1.49	1.38
2	L2	667	OMU	C2-N1	7.01	1.49	1.38
2	L2	560	OMU	C2-N1	6.99	1.49	1.38
2	L2	1419	OMU	C2-N1	6.99	1.49	1.38
88	S1	1621	OMU	C2-N3	6.99	1.50	1.38
88	S1	2061	5MC	C4-N3	6.98	1.45	1.34
88	S1	1662	OMU	C2-N3	6.96	1.50	1.38
88	S1	1979	OMU	C2-N3	6.95	1.50	1.38
1	L1	1659	OMU	C2-N1	6.95	1.49	1.38
2	L2	1077	OMU	C2-N1	6.94	1.49	1.38
88	S1	29	OMU	C2-N1	6.93	1.49	1.38
88	S1	8	OMU	C2-N1	6.92	1.49	1.38
2	L2	73	OMU	C2-N1	6.92	1.49	1.38
88	S1	661	OMU	C2-N3	6.91	1.50	1.38
88	S1	29	OMU	C2-N3	6.91	1.50	1.38
1	L1	847	OMU	C2-N3	6.90	1.50	1.38
88	S1	1833	OMU	C2-N3	6.90	1.50	1.38
1	L1	1107	OMU	C2-N1	6.90	1.49	1.38
2	L2	1359	OMU	C2-N3	6.88	1.50	1.38
88	S1	668	A2M	O4'-C4'	-6.88	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1659	OMU	C2-N3	6.88	1.49	1.38
2	L2	1359	OMU	C2-N1	6.88	1.49	1.38
88	S1	2048	OMU	C2-N3	6.87	1.49	1.38
1	L1	847	OMU	C2-N1	6.85	1.49	1.38
1	L1	1371	OMU	C2-N3	6.84	1.49	1.38
1	L1	1107	OMU	C2-N3	6.83	1.49	1.38
2	L2	1077	OMU	C2-N3	6.81	1.49	1.38
2	L2	1419	OMU	C2-N3	6.79	1.49	1.38
2	L2	73	OMU	C2-N3	6.79	1.49	1.38
88	S1	8	OMU	C2-N3	6.77	1.49	1.38
2	L2	565	OMU	C2-N3	6.75	1.49	1.38
2	L2	667	OMU	C2-N3	6.74	1.49	1.38
2	L2	560	OMU	C2-N3	6.73	1.49	1.38
3	L3	13	OMU	C2-N3	6.72	1.49	1.38
2	L2	56	OMU	C2-N3	6.72	1.49	1.38
1	L1	858	A2M	O4'-C4'	-6.62	1.30	1.45
88	S1	1550	OMG	C4-N3	6.62	1.49	1.34
1	L1	48	OMU	C2-N3	6.57	1.49	1.38
1	L1	845	OMU	C2-N3	6.53	1.49	1.38
2	L2	1185	A2M	O4'-C4'	-6.52	1.30	1.45
1	L1	1524	OMG	C4-N3	6.52	1.49	1.34
88	S1	1829	OMG	C4-N3	6.52	1.49	1.34
1	L1	959	OMG	C4-N3	6.50	1.49	1.34
7	L7	162	A2M	O4'-C4'	-6.49	1.30	1.45
88	S1	600	OMG	C4-N3	6.49	1.49	1.34
2	L2	524	5MC	C4-N3	6.48	1.44	1.34
88	S1	1865	OMG	C4-N3	6.48	1.49	1.34
2	L2	359	OMC	C2-N3	6.48	1.49	1.36
1	L1	678	A2M	O4'-C4'	-6.48	1.30	1.45
2	L2	628	A2M	O4'-C4'	-6.46	1.30	1.45
88	S1	1623	OMG	C4-N3	6.46	1.49	1.34
2	L2	1229	OMG	C4-N3	6.46	1.49	1.34
1	L1	697	A2M	O4'-C4'	-6.46	1.30	1.45
1	L1	235	A2M	O4'-C4'	-6.45	1.30	1.45
2	L2	1372	A2M	O4'-C4'	-6.45	1.30	1.45
2	L2	1360	OMG	C4-N3	6.45	1.49	1.34
88	S1	2140	OMC	C2-N3	6.45	1.49	1.36
88	S1	38	OMC	C2-N3	6.45	1.49	1.36
2	L2	655	OMG	C4-N3	6.44	1.49	1.34
7	L7	75	OMG	C4-N3	6.43	1.49	1.34
2	L2	71	OMG	C4-N3	6.42	1.49	1.34
2	L2	534	OMG	C4-N3	6.42	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1647	OMG	C4-N3	6.42	1.48	1.34
2	L2	524	5MC	C5-C4	6.42	1.49	1.44
2	L2	95	A2M	O4'-C4'	-6.41	1.30	1.45
88	S1	1866	OMC	C2-N3	6.41	1.49	1.36
88	S1	2151	OMG	C4-N3	6.40	1.48	1.34
1	L1	1626	OMG	C4-N3	6.40	1.48	1.34
2	L2	382	A2M	O4'-C4'	-6.40	1.30	1.45
88	S1	18	OMC	C2-N3	6.39	1.49	1.36
1	L1	1010	OMC	C2-N3	6.39	1.49	1.36
88	S1	2021	A2M	O4'-C4'	-6.38	1.30	1.45
2	L2	591	A2M	O4'-C4'	-6.38	1.30	1.45
2	L2	1384	A2M	O4'-C4'	-6.37	1.30	1.45
1	L1	955	A2M	O4'-C4'	-6.37	1.30	1.45
2	L2	14	OMC	C2-N3	6.37	1.49	1.36
1	L1	1539	A2M	O4'-C4'	-6.36	1.30	1.45
2	L2	665	A2M	O4'-C4'	-6.36	1.30	1.45
2	L2	527	A2M	O4'-C4'	-6.36	1.30	1.45
1	L1	681	A2M	O4'-C4'	-6.36	1.30	1.45
88	S1	2061	5MC	C5-C4	6.36	1.48	1.44
1	L1	695	OMC	C2-N3	6.35	1.49	1.36
2	L2	686	OMG	C4-N3	6.34	1.48	1.34
4	L4	74	OMG	C4-N3	6.34	1.48	1.34
2	L2	604	A2M	O4'-C4'	-6.34	1.30	1.45
2	L2	1046	OMG	C4-N3	6.34	1.48	1.34
7	L7	43	A2M	O4'-C4'	-6.34	1.30	1.45
88	S1	2059	OMC	C2-N3	6.33	1.48	1.36
1	L1	856	OMG	C4-N3	6.33	1.48	1.34
88	S1	479	A2M	O4'-C4'	-6.33	1.30	1.45
2	L2	1159	OMC	C2-N3	6.31	1.48	1.36
1	L1	1373	A2M	O4'-C4'	-6.31	1.31	1.45
88	S1	1478	OMG	C4-N3	6.30	1.48	1.34
2	L2	1317	OMC	C2-N3	6.30	1.48	1.36
88	S1	2061	5MC	C2-N3	6.29	1.48	1.36
2	L2	1067	A2M	O4'-C4'	-6.29	1.31	1.45
88	S1	98	A2M	O4'-C4'	-6.29	1.31	1.45
2	L2	1248	OMC	C2-N3	6.28	1.48	1.36
1	L1	927	A2M	O4'-C4'	-6.28	1.31	1.45
2	L2	583	OMC	C2-N3	6.28	1.48	1.36
1	L1	69	A2M	O4'-C4'	-6.27	1.31	1.45
2	L2	570	A2M	O4'-C4'	-6.27	1.31	1.45
2	L2	641	OMG	C4-N3	6.26	1.48	1.34
2	L2	1397	OMC	C2-N3	6.26	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1527	OMC	C2-N3	6.26	1.48	1.36
1	L1	305	A2M	O4'-C4'	-6.26	1.31	1.45
88	S1	897	A2M	O4'-C4'	-6.25	1.31	1.45
88	S1	1995	G7M	C5-N7	6.25	1.46	1.39
2	L2	1231	OMG	C4-N3	6.24	1.48	1.34
88	S1	1995	G7M	C2-N3	6.23	1.48	1.33
2	L2	1253	OMG	C4-N3	6.22	1.48	1.34
88	S1	512	A2M	O4'-C4'	-6.20	1.31	1.45
1	L1	1190	OMG	C4-N3	6.20	1.48	1.34
2	L2	572	A2M	O4'-C4'	-6.20	1.31	1.45
2	L2	443	OMC	C6-C5	6.18	1.49	1.35
88	S1	28	A2M	O4'-C4'	-6.18	1.31	1.45
88	S1	38	OMC	C6-C5	6.16	1.49	1.35
2	L2	1078	OMG	C4-N3	6.16	1.48	1.34
2	L2	443	OMC	C2-N3	6.14	1.48	1.36
2	L2	1308	5MC	C4-N3	6.13	1.43	1.34
2	L2	1248	OMC	C6-C5	6.09	1.49	1.35
88	S1	1995	G7M	C8-N9	6.08	1.52	1.35
1	L1	1540	OMG	C4-N3	6.06	1.48	1.34
2	L2	1308	5MC	C2-N3	6.06	1.48	1.36
2	L2	524	5MC	C2-N3	6.05	1.48	1.36
88	S1	18	OMC	C6-C5	6.01	1.49	1.35
88	S1	2140	OMC	C6-C5	6.00	1.49	1.35
88	S1	1866	OMC	C6-C5	6.00	1.49	1.35
2	L2	1397	OMC	C6-C5	5.98	1.48	1.35
2	L2	1159	OMC	C6-C5	5.97	1.48	1.35
1	L1	1010	OMC	C6-C5	5.94	1.48	1.35
2	L2	583	OMC	C6-C5	5.92	1.48	1.35
2	L2	359	OMC	C6-C5	5.92	1.48	1.35
1	L1	695	OMC	C6-C5	5.89	1.48	1.35
2	L2	1317	OMC	C6-C5	5.87	1.48	1.35
2	L2	14	OMC	C6-C5	5.86	1.48	1.35
88	S1	2059	OMC	C6-C5	5.85	1.48	1.35
1	L1	1527	OMC	C6-C5	5.81	1.48	1.35
88	S1	1662	OMU	C6-C5	5.72	1.48	1.35
88	S1	8	OMU	C6-C5	5.69	1.48	1.35
88	S1	1979	OMU	C6-C5	5.68	1.48	1.35
88	S1	661	OMU	C6-C5	5.67	1.48	1.35
88	S1	1621	OMU	C6-C5	5.67	1.48	1.35
88	S1	1995	G7M	C4-N3	5.64	1.47	1.34
88	S1	29	OMU	C6-C5	5.63	1.48	1.35
2	L2	667	OMU	C6-C5	5.63	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	847	OMU	C6-C5	5.63	1.48	1.35
2	L2	1359	OMU	C6-C5	5.60	1.48	1.35
1	L1	1253	OMU	C6-C5	5.60	1.48	1.35
2	L2	1077	OMU	C6-C5	5.59	1.48	1.35
2	L2	1419	OMU	C6-C5	5.58	1.48	1.35
3	L3	13	OMU	C6-C5	5.56	1.48	1.35
1	L1	1107	OMU	C6-C5	5.56	1.48	1.35
88	S1	1833	OMU	C6-C5	5.56	1.48	1.35
88	S1	2048	OMU	C6-C5	5.56	1.48	1.35
2	L2	73	OMU	C6-C5	5.56	1.47	1.35
1	L1	1659	OMU	C6-C5	5.54	1.47	1.35
1	L1	1371	OMU	C6-C5	5.53	1.47	1.35
2	L2	56	OMU	C6-C5	5.52	1.47	1.35
2	L2	565	OMU	C6-C5	5.51	1.47	1.35
88	S1	1566	PSU	C6-N1	5.48	1.45	1.36
88	S1	1657	PSU	C6-N1	5.44	1.45	1.36
2	L2	560	OMU	C6-C5	5.41	1.47	1.35
2	L2	802	PSU	C6-N1	5.40	1.45	1.36
1	L1	48	OMU	C6-C5	5.39	1.47	1.35
88	S1	33	PSU	C6-N1	5.39	1.45	1.36
88	S1	1292	PSU	C6-N1	5.39	1.45	1.36
88	S1	1550	OMG	C2-N3	5.37	1.46	1.33
1	L1	959	OMG	C2-N3	5.36	1.46	1.33
2	L2	500	PSU	C6-N1	5.36	1.45	1.36
88	S1	12	PSU	C6-N1	5.35	1.45	1.36
2	L2	512	PSU	C6-N1	5.34	1.45	1.36
1	L1	239	PSU	C6-N1	5.33	1.45	1.36
88	S1	1246	PSU	C6-N1	5.33	1.45	1.36
88	S1	38	OMC	C4-N3	5.33	1.45	1.34
1	L1	1011	PSU	C6-N1	5.33	1.45	1.36
2	L2	510	PSU	C6-N1	5.32	1.45	1.36
1	L1	774	PSU	C6-N1	5.32	1.45	1.36
2	L2	504	PSU	C6-N1	5.32	1.45	1.36
88	S1	600	OMG	C2-N3	5.31	1.46	1.33
2	L2	1194	PSU	C6-N1	5.31	1.45	1.36
1	L1	1524	OMG	C2-N3	5.31	1.46	1.33
2	L2	1382	PSU	C6-N1	5.30	1.45	1.36
2	L2	1360	OMG	C2-N3	5.30	1.46	1.33
88	S1	2202	PSU	C6-N1	5.29	1.45	1.36
1	L1	1177	PSU	C6-N1	5.29	1.45	1.36
2	L2	472	PSU	C6-N1	5.29	1.45	1.36
7	L7	101	PSU	C6-N1	5.28	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1403	PSU	C6-N1	5.28	1.44	1.36
7	L7	166	PSU	C6-N1	5.28	1.44	1.36
1	L1	940	PSU	C6-N1	5.28	1.44	1.36
88	S1	1829	OMG	C2-N3	5.28	1.46	1.33
1	L1	1664	PSU	C6-N1	5.27	1.44	1.36
88	S1	1866	OMC	C4-N3	5.26	1.44	1.34
2	L2	1303	PSU	C6-N1	5.26	1.44	1.36
2	L2	1213	PSU	C6-N1	5.25	1.44	1.36
1	L1	1526	PSU	C6-N1	5.25	1.44	1.36
1	L1	1533	PSU	C6-N1	5.25	1.44	1.36
2	L2	626	PSU	C6-N1	5.25	1.44	1.36
88	S1	1865	OMG	C2-N3	5.25	1.45	1.33
7	L7	69	PSU	C6-N1	5.25	1.44	1.36
88	S1	1623	OMG	C2-N3	5.24	1.45	1.33
2	L2	1361	PSU	C6-N1	5.24	1.44	1.36
2	L2	662	PSU	C6-N1	5.23	1.44	1.36
88	S1	2140	OMC	C4-N3	5.23	1.44	1.34
2	L2	1264	PSU	C6-N1	5.23	1.44	1.36
1	L1	1528	PSU	C6-N1	5.23	1.44	1.36
2	L2	359	OMC	C4-N3	5.23	1.44	1.34
2	L2	593	PSU	C6-N1	5.22	1.44	1.36
2	L2	1318	PSU	C6-N1	5.22	1.44	1.36
2	L2	71	OMG	C2-N3	5.22	1.45	1.33
1	L1	422	PSU	C6-N1	5.21	1.44	1.36
1	L1	1626	OMG	C2-N3	5.21	1.45	1.33
7	L7	74	PSU	C6-N1	5.21	1.44	1.36
2	L2	597	PSU	C6-N1	5.21	1.44	1.36
2	L2	1144	PSU	C6-N1	5.20	1.44	1.36
1	L1	845	OMU	C6-C5	5.20	1.47	1.35
2	L2	1060	PSU	C6-N1	5.19	1.44	1.36
2	L2	78	PSU	C6-N1	5.19	1.44	1.36
2	L2	1265	PSU	C6-N1	5.17	1.44	1.36
88	S1	18	OMC	C4-N3	5.17	1.44	1.34
2	L2	1152	PSU	C6-N1	5.17	1.44	1.36
88	S1	1647	OMG	C2-N3	5.15	1.45	1.33
7	L7	75	OMG	C2-N3	5.15	1.45	1.33
2	L2	686	OMG	C2-N3	5.14	1.45	1.33
2	L2	534	OMG	C2-N3	5.13	1.45	1.33
88	S1	2151	OMG	C2-N3	5.13	1.45	1.33
2	L2	1058	PSU	C6-N1	5.13	1.44	1.36
2	L2	1229	OMG	C2-N3	5.13	1.45	1.33
1	L1	1017	PSU	C6-N1	5.12	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	655	OMG	C2-N3	5.11	1.45	1.33
1	L1	1010	OMC	C4-N3	5.10	1.44	1.34
2	L2	583	OMC	C4-N3	5.10	1.44	1.34
4	L4	74	OMG	C2-N3	5.06	1.45	1.33
1	L1	1527	OMC	C4-N3	5.06	1.44	1.34
2	L2	1159	OMC	C4-N3	5.05	1.44	1.34
88	S1	1478	OMG	C2-N3	5.05	1.45	1.33
2	L2	1046	OMG	C2-N3	5.05	1.45	1.33
2	L2	1248	OMC	C4-N3	5.04	1.44	1.34
1	L1	695	OMC	C4-N3	5.04	1.44	1.34
2	L2	1397	OMC	C4-N3	5.03	1.44	1.34
2	L2	14	OMC	C4-N3	5.03	1.44	1.34
1	L1	1529	PSU	C6-N1	5.03	1.44	1.36
1	L1	672	PSU	C6-N1	5.02	1.44	1.36
2	L2	1317	OMC	C4-N3	5.01	1.44	1.34
2	L2	641	OMG	C2-N3	4.99	1.45	1.33
2	L2	437	PSU	C6-N1	4.98	1.44	1.36
88	S1	2059	OMC	C4-N3	4.97	1.44	1.34
2	L2	1231	OMG	C2-N3	4.93	1.45	1.33
1	L1	856	OMG	C2-N3	4.93	1.45	1.33
88	S1	2061	5MC	C6-N1	4.93	1.46	1.38
2	L2	443	OMC	C4-N3	4.88	1.44	1.34
1	L1	1190	OMG	C2-N3	4.86	1.45	1.33
2	L2	1078	OMG	C2-N3	4.85	1.44	1.33
88	S1	2059	OMC	C2-N1	4.85	1.50	1.40
88	S1	38	OMC	C4-N4	4.84	1.45	1.33
2	L2	1159	OMC	C4-N4	4.83	1.45	1.33
2	L2	1248	OMC	C4-N4	4.83	1.45	1.33
88	S1	2059	OMC	C4-N4	4.82	1.45	1.33
2	L2	359	OMC	C4-N4	4.82	1.45	1.33
88	S1	2140	OMC	C4-N4	4.82	1.45	1.33
88	S1	18	OMC	C4-N4	4.82	1.45	1.33
88	S1	1550	OMG	C2-N2	4.79	1.45	1.34
88	S1	1866	OMC	C4-N4	4.79	1.45	1.33
88	S1	600	OMG	C2-N2	4.78	1.45	1.34
1	L1	1527	OMC	C2-N1	4.78	1.50	1.40
2	L2	14	OMC	C4-N4	4.75	1.45	1.33
2	L2	443	OMC	C4-N4	4.75	1.45	1.33
7	L7	75	OMG	C2-N2	4.75	1.45	1.34
88	S1	1865	OMG	C2-N2	4.74	1.45	1.34
2	L2	1360	OMG	C2-N2	4.74	1.45	1.34
1	L1	1540	OMG	C2-N3	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1308	5MC	C4-N4	4.73	1.46	1.34
1	L1	1010	OMC	C4-N4	4.73	1.45	1.33
88	S1	1623	OMG	C2-N2	4.73	1.45	1.34
2	L2	655	OMG	C2-N2	4.72	1.45	1.34
1	L1	959	OMG	C2-N2	4.71	1.45	1.34
88	S1	1647	OMG	C2-N2	4.71	1.45	1.34
2	L2	534	OMG	C2-N2	4.71	1.45	1.34
2	L2	1231	OMG	C2-N2	4.70	1.45	1.34
2	L2	1317	OMC	C4-N4	4.70	1.45	1.33
2	L2	686	OMG	C2-N2	4.70	1.45	1.34
2	L2	583	OMC	C4-N4	4.69	1.45	1.33
1	L1	1524	OMG	C2-N2	4.69	1.45	1.34
1	L1	1626	OMG	C2-N2	4.69	1.45	1.34
88	S1	1829	OMG	C2-N2	4.69	1.45	1.34
2	L2	1253	OMG	C2-N3	4.68	1.44	1.33
1	L1	1527	OMC	C4-N4	4.68	1.45	1.33
1	L1	672	PSU	C1'-C5	-4.68	1.39	1.50
88	S1	2151	OMG	C2-N2	4.68	1.45	1.34
2	L2	71	OMG	C2-N2	4.68	1.45	1.34
1	L1	856	OMG	C2-N2	4.67	1.45	1.34
2	L2	1046	OMG	C2-N2	4.67	1.45	1.34
1	L1	695	OMC	C4-N4	4.66	1.45	1.33
2	L2	524	5MC	C6-N1	4.66	1.45	1.38
2	L2	1308	5MC	C6-N1	4.64	1.45	1.38
2	L2	1397	OMC	C4-N4	4.64	1.45	1.33
88	S1	1478	OMG	C2-N2	4.64	1.45	1.34
2	L2	1248	OMC	C2-N1	4.64	1.49	1.40
2	L2	1229	OMG	C2-N2	4.63	1.45	1.34
2	L2	1159	OMC	C2-N1	4.63	1.49	1.40
2	L2	14	OMC	C2-N1	4.62	1.49	1.40
1	L1	1190	OMG	C2-N2	4.62	1.45	1.34
2	L2	641	OMG	C2-N2	4.61	1.45	1.34
4	L4	74	OMG	C2-N2	4.60	1.44	1.34
1	L1	1526	PSU	C1'-C5	-4.60	1.39	1.50
88	S1	18	OMC	C2-N1	4.58	1.49	1.40
88	S1	38	OMC	C2-N1	4.58	1.49	1.40
88	S1	1866	OMC	C2-N1	4.58	1.49	1.40
88	S1	2140	OMC	C2-N1	4.56	1.49	1.40
2	L2	1058	PSU	C1'-C5	-4.56	1.40	1.50
1	L1	1529	PSU	C1'-C5	-4.56	1.40	1.50
2	L2	1213	PSU	C1'-C5	-4.55	1.40	1.50
2	L2	78	PSU	C1'-C5	-4.55	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	359	OMC	C2-N1	4.55	1.49	1.40
7	L7	74	PSU	C1'-C5	-4.54	1.40	1.50
2	L2	583	OMC	C2-N1	4.54	1.49	1.40
1	L1	1540	OMG	C2-N2	4.54	1.44	1.34
1	L1	1017	PSU	C1'-C5	-4.53	1.40	1.50
2	L2	1317	OMC	C2-N1	4.53	1.49	1.40
1	L1	422	PSU	C1'-C5	-4.53	1.40	1.50
88	S1	2061	5MC	C4-N4	4.52	1.45	1.34
2	L2	1303	PSU	C1'-C5	-4.52	1.40	1.50
1	L1	940	PSU	C1'-C5	-4.52	1.40	1.50
2	L2	1152	PSU	C1'-C5	-4.50	1.40	1.50
2	L2	1060	PSU	C1'-C5	-4.50	1.40	1.50
2	L2	1078	OMG	C2-N2	4.50	1.44	1.34
2	L2	1361	PSU	C1'-C5	-4.48	1.40	1.50
1	L1	1533	PSU	C1'-C5	-4.47	1.40	1.50
2	L2	1403	PSU	C1'-C5	-4.47	1.40	1.50
2	L2	437	PSU	C1'-C5	-4.46	1.40	1.50
1	L1	774	PSU	C1'-C5	-4.46	1.40	1.50
7	L7	69	PSU	C1'-C5	-4.46	1.40	1.50
2	L2	1318	PSU	C1'-C5	-4.44	1.40	1.50
2	L2	1144	PSU	C1'-C5	-4.44	1.40	1.50
2	L2	597	PSU	C1'-C5	-4.43	1.40	1.50
2	L2	1397	OMC	C2-N1	4.42	1.49	1.40
2	L2	472	PSU	C1'-C5	-4.42	1.40	1.50
88	S1	1246	PSU	C1'-C5	-4.40	1.40	1.50
88	S1	897	A2M	C6-N6	4.40	1.45	1.34
88	S1	33	PSU	C1'-C5	-4.40	1.40	1.50
1	L1	239	PSU	C1'-C5	-4.39	1.40	1.50
7	L7	166	PSU	C1'-C5	-4.39	1.40	1.50
88	S1	2021	A2M	C6-N6	4.39	1.45	1.34
2	L2	662	PSU	C1'-C5	-4.39	1.40	1.50
88	S1	512	A2M	C6-N6	4.38	1.45	1.34
1	L1	1664	PSU	C1'-C5	-4.38	1.40	1.50
88	S1	479	A2M	C6-N6	4.38	1.45	1.34
88	S1	98	A2M	C6-N6	4.38	1.45	1.34
2	L2	510	PSU	C1'-C5	-4.37	1.40	1.50
2	L2	1382	PSU	C1'-C5	-4.37	1.40	1.50
88	S1	2202	PSU	C1'-C5	-4.37	1.40	1.50
88	S1	1292	PSU	C1'-C5	-4.37	1.40	1.50
88	S1	1657	PSU	C1'-C5	-4.36	1.40	1.50
1	L1	305	A2M	C6-N6	4.36	1.45	1.34
88	S1	1621	OMU	C4-N3	4.35	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1010	OMC	C2-N1	4.35	1.49	1.40
2	L2	802	PSU	C1'-C5	-4.34	1.40	1.50
2	L2	1308	5MC	C2-N1	4.33	1.49	1.40
1	L1	695	OMC	C2-N1	4.33	1.49	1.40
88	S1	668	A2M	C6-N6	4.33	1.45	1.34
2	L2	512	PSU	C1'-C5	-4.32	1.40	1.50
1	L1	678	A2M	C6-N6	4.32	1.45	1.34
2	L2	1194	PSU	C1'-C5	-4.32	1.40	1.50
1	L1	235	A2M	C6-N6	4.32	1.45	1.34
2	L2	95	A2M	C6-N6	4.32	1.45	1.34
1	L1	858	A2M	C6-N6	4.32	1.45	1.34
2	L2	1372	A2M	C6-N6	4.32	1.45	1.34
1	L1	69	A2M	C6-N6	4.31	1.45	1.34
2	L2	591	A2M	C6-N6	4.31	1.45	1.34
1	L1	1528	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	500	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	570	A2M	C6-N6	4.31	1.45	1.34
7	L7	101	PSU	C1'-C5	-4.30	1.40	1.50
7	L7	162	A2M	C6-N6	4.30	1.45	1.34
2	L2	604	A2M	C6-N6	4.30	1.45	1.34
1	L1	1177	PSU	C1'-C5	-4.30	1.40	1.50
1	L1	697	A2M	C6-N6	4.29	1.45	1.34
88	S1	12	PSU	C1'-C5	-4.29	1.40	1.50
2	L2	628	A2M	C6-N6	4.29	1.45	1.34
88	S1	28	A2M	C6-N6	4.28	1.45	1.34
2	L2	1308	5MC	O4'-C1'	-4.28	1.32	1.42
2	L2	1265	PSU	C1'-C5	-4.28	1.40	1.50
2	L2	665	A2M	C6-N6	4.28	1.45	1.34
88	S1	2061	5MC	C2-N1	4.28	1.49	1.40
7	L7	43	A2M	C6-N6	4.28	1.45	1.34
2	L2	1185	A2M	C6-N6	4.27	1.45	1.34
88	S1	1662	OMU	C4-N3	4.27	1.45	1.38
2	L2	593	PSU	C1'-C5	-4.26	1.40	1.50
88	S1	1833	OMU	C4-N3	4.26	1.45	1.38
1	L1	681	A2M	C6-N6	4.25	1.45	1.34
2	L2	1384	A2M	C6-N6	4.24	1.45	1.34
2	L2	1264	PSU	C1'-C5	-4.24	1.40	1.50
1	L1	1539	A2M	C6-N6	4.24	1.45	1.34
2	L2	1067	A2M	C6-N6	4.24	1.45	1.34
88	S1	1566	PSU	C1'-C5	-4.23	1.40	1.50
2	L2	382	A2M	C6-N6	4.23	1.45	1.34
2	L2	626	PSU	C1'-C5	-4.22	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1979	OMU	C4-N3	4.20	1.45	1.38
1	L1	1253	OMU	C4-N3	4.19	1.45	1.38
1	L1	1373	A2M	C6-N6	4.19	1.44	1.34
2	L2	443	OMC	C2-N1	4.19	1.48	1.40
1	L1	927	A2M	C6-N6	4.18	1.44	1.34
1	L1	955	A2M	C6-N6	4.18	1.44	1.34
2	L2	572	A2M	C6-N6	4.18	1.44	1.34
88	S1	661	OMU	C4-N3	4.15	1.45	1.38
1	L1	1011	PSU	C1'-C5	-4.15	1.40	1.50
2	L2	1359	OMU	C4-N3	4.13	1.45	1.38
2	L2	1253	OMG	C2-N2	4.12	1.43	1.34
88	S1	2048	OMU	C4-N3	4.12	1.45	1.38
2	L2	1077	OMU	C4-N3	4.12	1.45	1.38
2	L2	524	5MC	C4-N4	4.12	1.44	1.34
88	S1	29	OMU	C4-N3	4.12	1.45	1.38
88	S1	8	OMU	C4-N3	4.11	1.45	1.38
3	L3	13	OMU	C4-N3	4.10	1.45	1.38
1	L1	1107	OMU	C4-N3	4.09	1.45	1.38
2	L2	73	OMU	C4-N3	4.08	1.45	1.38
2	L2	667	OMU	C4-N3	4.08	1.45	1.38
1	L1	1659	OMU	C4-N3	4.05	1.45	1.38
2	L2	504	PSU	C1'-C5	-4.01	1.41	1.50
2	L2	524	5MC	C2-N1	4.00	1.48	1.40
2	L2	527	A2M	C6-N6	3.99	1.44	1.34
2	L2	1419	OMU	C4-N3	3.98	1.45	1.38
88	S1	33	PSU	C4-N3	3.98	1.46	1.38
2	L2	560	OMU	C4-N3	3.96	1.45	1.38
2	L2	56	OMU	C4-N3	3.93	1.45	1.38
2	L2	500	PSU	C4-N3	3.90	1.46	1.38
2	L2	802	PSU	C4-N3	3.90	1.46	1.38
2	L2	510	PSU	C4-N3	3.90	1.46	1.38
88	S1	1566	PSU	C4-N3	3.90	1.46	1.38
1	L1	1011	PSU	C4-N3	3.89	1.46	1.38
88	S1	1246	PSU	C4-N3	3.87	1.46	1.38
1	L1	1371	OMU	C4-N3	3.85	1.45	1.38
88	S1	2202	PSU	C4-N3	3.84	1.46	1.38
2	L2	1361	PSU	C4-N3	3.84	1.46	1.38
1	L1	1533	PSU	C4-N3	3.84	1.46	1.38
88	S1	2185	MA6	C6-N6	3.83	1.47	1.36
88	S1	2184	MA6	C6-N6	3.83	1.47	1.36
1	L1	847	OMU	C4-N3	3.83	1.45	1.38
88	S1	1292	PSU	C4-N3	3.81	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1403	PSU	C4-N3	3.80	1.46	1.38
2	L2	512	PSU	C4-N3	3.80	1.46	1.38
2	L2	565	OMU	C4-N3	3.79	1.45	1.38
1	L1	1177	PSU	C4-N3	3.79	1.45	1.38
1	L1	239	PSU	C4-N3	3.78	1.45	1.38
1	L1	1664	PSU	C4-N3	3.78	1.45	1.38
2	L2	472	PSU	C4-N3	3.78	1.45	1.38
88	S1	12	PSU	C4-N3	3.77	1.45	1.38
7	L7	69	PSU	C4-N3	3.76	1.45	1.38
7	L7	74	PSU	C4-N3	3.75	1.45	1.38
88	S1	1657	PSU	C4-N3	3.74	1.45	1.38
7	L7	166	PSU	C4-N3	3.73	1.45	1.38
1	L1	422	PSU	C4-N3	3.73	1.45	1.38
2	L2	1264	PSU	C4-N3	3.72	1.45	1.38
7	L7	101	PSU	C4-N3	3.72	1.45	1.38
1	L1	1528	PSU	C4-N3	3.72	1.45	1.38
1	L1	1526	PSU	C4-N3	3.71	1.45	1.38
2	L2	1382	PSU	C4-N3	3.71	1.45	1.38
2	L2	1060	PSU	C4-N3	3.70	1.45	1.38
2	L2	1265	PSU	C4-N3	3.70	1.45	1.38
2	L2	593	PSU	C4-N3	3.70	1.45	1.38
2	L2	626	PSU	C4-N3	3.69	1.45	1.38
2	L2	1303	PSU	C4-N3	3.69	1.45	1.38
2	L2	1213	PSU	C4-N3	3.69	1.45	1.38
2	L2	597	PSU	C4-N3	3.68	1.45	1.38
2	L2	1152	PSU	C4-N3	3.67	1.45	1.38
2	L2	1144	PSU	C4-N3	3.67	1.45	1.38
1	L1	1529	PSU	C4-N3	3.67	1.45	1.38
2	L2	437	PSU	C4-N3	3.66	1.45	1.38
1	L1	774	PSU	C4-N3	3.65	1.45	1.38
1	L1	940	PSU	C4-N3	3.64	1.45	1.38
1	L1	672	PSU	C4-N3	3.63	1.45	1.38
2	L2	1058	PSU	C4-N3	3.63	1.45	1.38
2	L2	504	PSU	C4-N3	3.63	1.45	1.38
2	L2	1194	PSU	C4-N3	3.62	1.45	1.38
2	L2	662	PSU	C4-N3	3.61	1.45	1.38
88	S1	1533	PSU	C6-C5	3.60	1.39	1.35
1	L1	1017	PSU	C4-N3	3.60	1.45	1.38
2	L2	1318	PSU	C4-N3	3.60	1.45	1.38
88	S1	1539	PSU	C6-C5	3.54	1.39	1.35
1	L1	845	OMU	O2-C2	-3.54	1.16	1.23
88	S1	1995	G7M	C2-N1	3.53	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1995	G7M	C6-N1	3.51	1.45	1.38
2	L2	78	PSU	C4-N3	3.47	1.45	1.38
88	S1	1544	5MC	C5-C4	-3.45	1.41	1.44
1	L1	845	OMU	C4-N3	3.44	1.44	1.38
1	L1	48	OMU	C4-N3	3.42	1.44	1.38
88	S1	1995	G7M	C2-N2	3.39	1.42	1.34
88	S1	38	OMC	C6-N1	3.28	1.45	1.38
2	L2	527	A2M	C5-C4	-3.27	1.33	1.39
1	L1	69	A2M	O2'-C2'	3.25	1.50	1.42
2	L2	359	OMC	C6-N1	3.25	1.45	1.38
88	S1	18	OMC	C6-N1	3.24	1.45	1.38
88	S1	1995	G7M	C4-N9	3.24	1.46	1.38
88	S1	1866	OMC	C6-N1	3.23	1.45	1.38
1	L1	48	OMU	O2-C2	-3.23	1.17	1.23
1	L1	1373	A2M	C5-C4	-3.22	1.33	1.39
2	L2	1248	OMC	C6-N1	3.22	1.45	1.38
88	S1	2140	OMC	C6-N1	3.21	1.45	1.38
2	L2	565	OMU	O2-C2	-3.21	1.17	1.23
88	S1	2021	A2M	O2'-C2'	3.20	1.50	1.42
88	S1	1995	G7M	C5-C6	3.19	1.52	1.43
7	L7	43	A2M	C5-C4	-3.19	1.33	1.39
2	L2	1253	OMG	C5-N7	-3.19	1.32	1.39
1	L1	1527	OMC	C6-N1	3.18	1.45	1.38
1	L1	927	A2M	C5-C4	-3.17	1.33	1.39
2	L2	560	OMU	O4-C4	-3.16	1.18	1.24
1	L1	48	OMU	O4-C4	-3.16	1.18	1.24
2	L2	1159	OMC	C6-N1	3.15	1.45	1.38
88	S1	1833	OMU	O4-C4	-3.15	1.18	1.24
2	L2	1419	OMU	O4-C4	-3.15	1.18	1.24
1	L1	1371	OMU	O4-C4	-3.15	1.18	1.24
1	L1	1107	OMU	O4-C4	-3.14	1.18	1.24
2	L2	73	OMU	O4-C4	-3.14	1.18	1.24
88	S1	2059	OMC	O2-C2	-3.14	1.17	1.23
88	S1	2048	OMU	O4-C4	-3.14	1.18	1.24
2	L2	583	OMC	C6-N1	3.14	1.45	1.38
2	L2	14	OMC	C6-N1	3.13	1.45	1.38
1	L1	955	A2M	C5-C4	-3.13	1.33	1.39
2	L2	665	A2M	C5-C4	-3.13	1.33	1.39
1	L1	1010	OMC	C6-N1	3.13	1.45	1.38
2	L2	1397	OMC	C6-N1	3.13	1.45	1.38
88	S1	1995	G7M	O6-C6	-3.13	1.17	1.23
3	L3	13	OMU	O4-C4	-3.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	443	OMC	C6-N1	3.12	1.45	1.38
2	L2	604	A2M	C5-C4	-3.12	1.33	1.39
2	L2	591	A2M	O3'-C3'	-3.11	1.35	1.43
1	L1	1659	OMU	O4-C4	-3.10	1.18	1.24
2	L2	1067	A2M	C5-C4	-3.10	1.33	1.39
88	S1	2184	MA6	C5-C4	-3.10	1.33	1.39
88	S1	28	A2M	C5-C4	-3.10	1.33	1.39
7	L7	162	A2M	C5-C4	-3.09	1.33	1.39
88	S1	8	OMU	O4-C4	-3.09	1.18	1.24
2	L2	56	OMU	O4-C4	-3.08	1.18	1.24
1	L1	681	A2M	C5-C4	-3.08	1.33	1.39
1	L1	69	A2M	C5-C4	-3.08	1.33	1.39
2	L2	591	A2M	C5-C4	-3.07	1.33	1.39
1	L1	858	A2M	C5-C4	-3.07	1.33	1.39
2	L2	1359	OMU	O4-C4	-3.07	1.18	1.24
2	L2	572	A2M	C5-C4	-3.07	1.33	1.39
2	L2	570	A2M	C5-C4	-3.07	1.33	1.39
2	L2	1372	A2M	C5-C4	-3.07	1.33	1.39
2	L2	1185	A2M	C5-C4	-3.07	1.33	1.39
1	L1	678	A2M	C5-C4	-3.06	1.33	1.39
1	L1	697	A2M	C5-C4	-3.06	1.33	1.39
2	L2	565	OMU	O4-C4	-3.06	1.18	1.24
1	L1	1539	A2M	C5-C4	-3.06	1.33	1.39
2	L2	1372	A2M	C5-N7	-3.06	1.33	1.39
88	S1	29	OMU	O4-C4	-3.05	1.18	1.24
2	L2	667	OMU	O4-C4	-3.05	1.18	1.24
88	S1	2059	OMC	C6-N1	3.05	1.45	1.38
2	L2	1384	A2M	C5-C4	-3.04	1.33	1.39
2	L2	504	PSU	O4-C4	-3.03	1.17	1.23
2	L2	382	A2M	C5-C4	-3.03	1.33	1.39
88	S1	668	A2M	C5-C4	-3.02	1.33	1.39
1	L1	845	OMU	O4-C4	-3.02	1.18	1.24
2	L2	1308	5MC	O3'-C3'	3.02	1.50	1.43
2	L2	570	A2M	C5-N7	-3.02	1.33	1.39
1	L1	305	A2M	C5-C4	-3.02	1.33	1.39
2	L2	1077	OMU	O4-C4	-3.02	1.18	1.24
1	L1	681	A2M	O3'-C3'	-3.01	1.35	1.43
2	L2	1317	OMC	C6-N1	3.01	1.45	1.38
1	L1	235	A2M	C5-C4	-3.01	1.33	1.39
88	S1	512	A2M	C5-C4	-3.01	1.33	1.39
7	L7	162	A2M	O3'-C3'	-3.00	1.35	1.43
2	L2	1384	A2M	O2'-C2'	3.00	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	95	A2M	C5-C4	-3.00	1.33	1.39
88	S1	1662	OMU	O4-C4	-2.99	1.18	1.24
1	L1	235	A2M	O3'-C3'	-2.99	1.35	1.43
1	L1	927	A2M	O2'-C2'	2.99	1.50	1.42
1	L1	847	OMU	O4-C4	-2.99	1.18	1.24
2	L2	382	A2M	O2'-C2'	2.99	1.50	1.42
88	S1	897	A2M	C5-C4	-2.99	1.33	1.39
1	L1	678	A2M	O2'-C2'	2.98	1.50	1.42
88	S1	479	A2M	O2'-C2'	2.98	1.50	1.42
88	S1	98	A2M	O2'-C2'	2.98	1.50	1.42
2	L2	524	5MC	O2-C2	-2.98	1.18	1.23
88	S1	2021	A2M	C5-C4	-2.97	1.33	1.39
2	L2	604	A2M	O3'-C3'	-2.97	1.35	1.43
2	L2	628	A2M	C5-C4	-2.97	1.33	1.39
7	L7	162	A2M	O2'-C2'	2.96	1.49	1.42
88	S1	661	OMU	O4-C4	-2.96	1.18	1.24
1	L1	697	A2M	C5-N7	-2.96	1.33	1.39
2	L2	628	A2M	O2'-C2'	2.95	1.49	1.42
2	L2	382	A2M	C5-N7	-2.95	1.33	1.39
2	L2	95	A2M	O2'-C2'	2.95	1.49	1.42
88	S1	1979	OMU	O4-C4	-2.95	1.18	1.24
88	S1	2185	MA6	C5-C4	-2.95	1.33	1.39
1	L1	1373	A2M	O3'-C3'	-2.95	1.35	1.43
7	L7	43	A2M	O3'-C3'	-2.94	1.35	1.43
2	L2	570	A2M	O2'-C2'	2.94	1.49	1.42
1	L1	697	A2M	O3'-C3'	-2.94	1.35	1.43
2	L2	665	A2M	O2'-C2'	2.94	1.49	1.42
1	L1	697	A2M	O2'-C2'	2.94	1.49	1.42
2	L2	604	A2M	O2'-C2'	2.93	1.49	1.42
2	L2	1067	A2M	O2'-C2'	2.93	1.49	1.42
2	L2	71	OMG	C5-N7	-2.93	1.33	1.39
2	L2	78	PSU	O4-C4	-2.93	1.18	1.23
2	L2	1067	A2M	O3'-C3'	-2.93	1.35	1.43
88	S1	479	A2M	C5-C4	-2.92	1.33	1.39
1	L1	955	A2M	O2'-C2'	2.92	1.49	1.42
2	L2	95	A2M	O3'-C3'	-2.92	1.35	1.43
88	S1	98	A2M	C5-C4	-2.92	1.33	1.39
1	L1	235	A2M	O2'-C2'	2.92	1.49	1.42
2	L2	591	A2M	O2'-C2'	2.92	1.49	1.42
88	S1	668	A2M	O2'-C2'	2.92	1.49	1.42
88	S1	668	A2M	O3'-C3'	-2.91	1.35	1.43
88	S1	28	A2M	O2'-C2'	2.91	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	955	A2M	O3'-C3'	-2.91	1.35	1.43
1	L1	858	A2M	O2'-C2'	2.91	1.49	1.42
1	L1	1253	OMU	O4-C4	-2.91	1.18	1.24
1	L1	695	OMC	C6-N1	2.91	1.45	1.38
88	S1	1621	OMU	O4-C4	-2.90	1.18	1.24
2	L2	1382	PSU	O4-C4	-2.90	1.18	1.23
2	L2	1318	PSU	O4-C4	-2.90	1.18	1.23
2	L2	382	A2M	O3'-C3'	-2.90	1.35	1.43
2	L2	1185	A2M	O2'-C2'	2.89	1.49	1.42
88	S1	512	A2M	O3'-C3'	-2.89	1.35	1.43
88	S1	2151	OMG	C5-N7	-2.89	1.33	1.39
1	L1	1539	A2M	O2'-C2'	2.89	1.49	1.42
2	L2	1384	A2M	C5-N7	-2.89	1.33	1.39
88	S1	512	A2M	O2'-C2'	2.89	1.49	1.42
2	L2	1308	5MC	O2-C2	-2.88	1.18	1.23
7	L7	43	A2M	O2'-C2'	2.88	1.49	1.42
88	S1	897	A2M	O2'-C2'	2.88	1.49	1.42
2	L2	583	OMC	O2-C2	-2.88	1.18	1.23
2	L2	1067	A2M	C5-N7	-2.88	1.33	1.39
88	S1	661	OMU	C6-N1	2.88	1.45	1.38
2	L2	437	PSU	O4-C4	-2.88	1.18	1.23
88	S1	1623	OMG	C2-N1	2.88	1.44	1.37
2	L2	686	OMG	C2-N1	2.88	1.44	1.37
88	S1	897	A2M	O3'-C3'	-2.87	1.35	1.43
2	L2	667	OMU	C6-N1	2.87	1.44	1.38
2	L2	1317	OMC	O2-C2	-2.87	1.18	1.23
88	S1	1662	OMU	C6-N1	2.87	1.44	1.38
1	L1	1528	PSU	O4-C4	-2.87	1.18	1.23
2	L2	604	A2M	C5-N7	-2.87	1.33	1.39
1	L1	681	A2M	O2'-C2'	2.86	1.49	1.42
2	L2	1308	5MC	O2'-C2'	-2.86	1.35	1.43
2	L2	527	A2M	O2'-C2'	2.86	1.49	1.42
2	L2	665	A2M	O3'-C3'	-2.86	1.35	1.43
1	L1	678	A2M	O3'-C3'	-2.86	1.35	1.43
2	L2	443	OMC	O2-C2	-2.86	1.18	1.23
1	L1	955	A2M	C5-N7	-2.85	1.33	1.39
1	L1	1626	OMG	C5-N7	-2.85	1.33	1.39
1	L1	1373	A2M	O2'-C2'	2.85	1.49	1.42
88	S1	28	A2M	O3'-C3'	-2.85	1.35	1.43
88	S1	2021	A2M	O3'-C3'	-2.85	1.35	1.43
88	S1	1979	OMU	C6-N1	2.85	1.44	1.38
2	L2	1372	A2M	O2'-C2'	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1529	PSU	O4-C4	-2.84	1.18	1.23
7	L7	75	OMG	C2-N1	2.84	1.44	1.37
2	L2	95	A2M	C5-N7	-2.84	1.33	1.39
1	L1	69	A2M	O3'-C3'	-2.84	1.35	1.43
1	L1	1190	OMG	C4-N9	-2.84	1.30	1.38
88	S1	1829	OMG	C2-N1	2.84	1.44	1.37
1	L1	235	A2M	C5-N7	-2.84	1.33	1.39
88	S1	1865	OMG	C2-N1	2.83	1.44	1.37
3	L3	13	OMU	C6-N1	2.83	1.44	1.38
88	S1	1621	OMU	C6-N1	2.83	1.44	1.38
1	L1	959	OMG	C5-N7	-2.83	1.33	1.39
2	L2	534	OMG	C5-N7	-2.83	1.33	1.39
1	L1	1540	OMG	C2-N1	2.83	1.44	1.37
1	L1	858	A2M	O3'-C3'	-2.83	1.36	1.43
1	L1	927	A2M	O3'-C3'	-2.83	1.36	1.43
2	L2	628	A2M	O3'-C3'	-2.83	1.36	1.43
2	L2	1060	PSU	O4-C4	-2.83	1.18	1.23
1	L1	1527	OMC	O2-C2	-2.83	1.18	1.23
2	L2	591	A2M	C5-N7	-2.82	1.33	1.39
2	L2	1360	OMG	C5-N7	-2.82	1.33	1.39
2	L2	71	OMG	O6-C6	-2.82	1.18	1.23
88	S1	600	OMG	C2-N1	2.82	1.44	1.37
1	L1	1626	OMG	C2-N1	2.82	1.44	1.37
2	L2	1185	A2M	O3'-C3'	-2.82	1.36	1.43
1	L1	1526	PSU	O4-C4	-2.81	1.18	1.23
88	S1	1550	OMG	C2-N1	2.81	1.44	1.37
2	L2	572	A2M	O2'-C2'	2.81	1.49	1.42
2	L2	662	PSU	O4-C4	-2.81	1.18	1.23
88	S1	2048	OMU	C6-N1	2.81	1.44	1.38
2	L2	1194	PSU	O4-C4	-2.81	1.18	1.23
2	L2	1159	OMC	O2-C2	-2.81	1.18	1.23
2	L2	665	A2M	C5-N7	-2.80	1.34	1.39
1	L1	1373	A2M	C5-N7	-2.80	1.34	1.39
2	L2	1229	OMG	O6-C6	-2.80	1.18	1.23
1	L1	1540	OMG	C5-N7	-2.80	1.33	1.39
2	L2	572	A2M	C5-N7	-2.80	1.34	1.39
1	L1	1659	OMU	C6-N1	2.80	1.44	1.38
1	L1	1010	OMC	O2-C2	-2.80	1.18	1.23
2	L2	1078	OMG	O6-C6	-2.80	1.18	1.23
4	L4	74	OMG	C5-N7	-2.80	1.33	1.39
1	L1	1371	OMU	C6-N1	2.80	1.44	1.38
2	L2	641	OMG	C5-N7	-2.80	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1397	OMC	O2-C2	-2.80	1.18	1.23
88	S1	29	OMU	C6-N1	2.80	1.44	1.38
2	L2	1248	OMC	O2-C2	-2.80	1.18	1.23
2	L2	1046	OMG	C5-N7	-2.80	1.33	1.39
88	S1	98	A2M	O3'-C3'	-2.80	1.36	1.43
2	L2	1185	A2M	C5-N7	-2.80	1.34	1.39
2	L2	1231	OMG	C2-N1	2.79	1.44	1.37
1	L1	1664	PSU	O4-C4	-2.79	1.18	1.23
1	L1	681	A2M	C5-N7	-2.79	1.34	1.39
88	S1	1647	OMG	C2-N1	2.79	1.44	1.37
7	L7	101	PSU	O4-C4	-2.79	1.18	1.23
1	L1	858	A2M	C5-N7	-2.79	1.34	1.39
1	L1	672	PSU	O4-C4	-2.79	1.18	1.23
2	L2	14	OMC	O2-C2	-2.79	1.18	1.23
2	L2	1360	OMG	C2-N1	2.79	1.44	1.37
2	L2	686	OMG	C5-N7	-2.79	1.33	1.39
2	L2	1078	OMG	C2-N1	2.79	1.44	1.37
1	L1	1190	OMG	C2-N1	2.79	1.44	1.37
2	L2	597	PSU	O4-C4	-2.78	1.18	1.23
7	L7	162	A2M	C5-N7	-2.78	1.34	1.39
2	L2	655	OMG	C5-N7	-2.78	1.33	1.39
1	L1	1539	A2M	C5-N7	-2.78	1.34	1.39
2	L2	1419	OMU	C6-N1	2.78	1.44	1.38
2	L2	534	OMG	C2-N1	2.78	1.44	1.37
1	L1	959	OMG	C2-N1	2.78	1.44	1.37
88	S1	1478	OMG	C2-N1	2.78	1.44	1.37
1	L1	678	A2M	C5-N7	-2.78	1.34	1.39
2	L2	655	OMG	C2-N1	2.78	1.44	1.37
88	S1	479	A2M	O3'-C3'	-2.77	1.36	1.43
2	L2	1144	PSU	O4-C4	-2.77	1.18	1.23
2	L2	1078	OMG	C4-N9	-2.77	1.31	1.38
2	L2	1264	PSU	O4-C4	-2.77	1.18	1.23
1	L1	1539	A2M	O3'-C3'	-2.77	1.36	1.43
88	S1	2061	5MC	O2-C2	-2.77	1.18	1.23
1	L1	695	OMC	O2-C2	-2.77	1.18	1.23
2	L2	626	PSU	O4-C4	-2.77	1.18	1.23
2	L2	655	OMG	O6-C6	-2.77	1.18	1.23
2	L2	534	OMG	O6-C6	-2.76	1.18	1.23
2	L2	1384	A2M	O3'-C3'	-2.76	1.36	1.43
88	S1	98	A2M	C5-N7	-2.76	1.34	1.39
7	L7	75	OMG	C5-N7	-2.76	1.33	1.39
2	L2	565	OMU	C6-N1	2.76	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1524	OMG	C2-N1	2.76	1.44	1.37
1	L1	305	A2M	C5-N7	-2.76	1.34	1.39
2	L2	1231	OMG	O6-C6	-2.75	1.18	1.23
88	S1	1623	OMG	C5-N7	-2.75	1.33	1.39
2	L2	56	OMU	C6-N1	2.75	1.44	1.38
2	L2	1359	OMU	C6-N1	2.75	1.44	1.38
88	S1	512	A2M	C5-N7	-2.75	1.34	1.39
2	L2	572	A2M	O3'-C3'	-2.75	1.36	1.43
1	L1	856	OMG	C2-N1	2.75	1.44	1.37
88	S1	1833	OMU	C6-N1	2.75	1.44	1.38
88	S1	2151	OMG	C2-N1	2.75	1.44	1.37
2	L2	1058	PSU	O4-C4	-2.75	1.18	1.23
1	L1	1017	PSU	O4-C4	-2.75	1.18	1.23
2	L2	1231	OMG	C5-N7	-2.75	1.33	1.39
88	S1	38	OMC	O2-C2	-2.74	1.18	1.23
1	L1	239	PSU	O4-C4	-2.74	1.18	1.23
88	S1	479	A2M	C5-N7	-2.74	1.34	1.39
2	L2	1372	A2M	O3'-C3'	-2.74	1.36	1.43
2	L2	641	OMG	O6-C6	-2.74	1.18	1.23
88	S1	1865	OMG	C5-N7	-2.74	1.33	1.39
2	L2	1152	PSU	O4-C4	-2.74	1.18	1.23
88	S1	1647	OMG	C5-N7	-2.74	1.33	1.39
2	L2	1077	OMU	C6-N1	2.73	1.44	1.38
2	L2	570	A2M	O3'-C3'	-2.73	1.36	1.43
2	L2	1046	OMG	O6-C6	-2.73	1.18	1.23
88	S1	8	OMU	C6-N1	2.73	1.44	1.38
1	L1	1107	OMU	C6-N1	2.73	1.44	1.38
1	L1	940	PSU	O4-C4	-2.73	1.18	1.23
1	L1	305	A2M	O3'-C3'	-2.73	1.36	1.43
2	L2	73	OMU	C6-N1	2.73	1.44	1.38
1	L1	1524	OMG	C5-N7	-2.73	1.33	1.39
2	L2	593	PSU	O4-C4	-2.73	1.18	1.23
2	L2	1213	PSU	O4-C4	-2.73	1.18	1.23
1	L1	1253	OMU	C6-N1	2.72	1.44	1.38
1	L1	422	PSU	O4-C4	-2.72	1.18	1.23
1	L1	856	OMG	O6-C6	-2.72	1.18	1.23
88	S1	28	A2M	C5-N7	-2.72	1.34	1.39
88	S1	600	OMG	C5-N7	-2.72	1.33	1.39
2	L2	1046	OMG	C2-N1	2.72	1.44	1.37
1	L1	69	A2M	C5-N7	-2.72	1.34	1.39
88	S1	1478	OMG	C5-N7	-2.72	1.33	1.39
2	L2	641	OMG	C2-N1	2.72	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1657	PSU	O4-C4	-2.72	1.18	1.23
88	S1	18	OMC	O2-C2	-2.72	1.18	1.23
1	L1	856	OMG	C5-N7	-2.72	1.33	1.39
7	L7	69	PSU	O4-C4	-2.71	1.18	1.23
4	L4	74	OMG	C2-N1	2.71	1.44	1.37
2	L2	628	A2M	C5-N7	-2.71	1.34	1.39
7	L7	166	PSU	O4-C4	-2.71	1.18	1.23
1	L1	1540	OMG	C4-N9	-2.71	1.31	1.38
2	L2	1303	PSU	O4-C4	-2.71	1.18	1.23
88	S1	1550	OMG	C5-N7	-2.71	1.33	1.39
1	L1	847	OMU	C6-N1	2.70	1.44	1.38
2	L2	512	PSU	O4-C4	-2.70	1.18	1.23
2	L2	641	OMG	C4-N9	-2.70	1.31	1.38
1	L1	927	A2M	C5-N7	-2.70	1.34	1.39
7	L7	43	A2M	C5-N7	-2.70	1.34	1.39
88	S1	1829	OMG	C5-N7	-2.70	1.33	1.39
1	L1	1659	OMU	O2-C2	-2.70	1.18	1.23
1	L1	1540	OMG	O6-C6	-2.69	1.18	1.23
2	L2	1229	OMG	C2-N1	2.69	1.44	1.37
2	L2	56	OMU	O2-C2	-2.69	1.18	1.23
2	L2	71	OMG	C2-N1	2.69	1.44	1.37
2	L2	667	OMU	O2-C2	-2.68	1.18	1.23
2	L2	560	OMU	C6-N1	2.68	1.44	1.38
7	L7	74	PSU	O4-C4	-2.68	1.18	1.23
1	L1	305	A2M	O2'-C2'	2.68	1.49	1.42
88	S1	2021	A2M	C5-N7	-2.68	1.34	1.39
2	L2	1265	PSU	O4-C4	-2.68	1.18	1.23
2	L2	527	A2M	C5-N7	-2.68	1.34	1.39
1	L1	1190	OMG	O6-C6	-2.67	1.18	1.23
1	L1	1626	OMG	O6-C6	-2.67	1.18	1.23
2	L2	1229	OMG	C5-N7	-2.67	1.33	1.39
88	S1	668	A2M	C5-N7	-2.67	1.34	1.39
1	L1	847	OMU	O2-C2	-2.66	1.18	1.23
2	L2	1078	OMG	C5-N7	-2.66	1.33	1.39
88	S1	1292	PSU	O4-C4	-2.66	1.18	1.23
88	S1	1866	OMC	O2-C2	-2.66	1.18	1.23
2	L2	1403	PSU	O4-C4	-2.66	1.18	1.23
2	L2	1419	OMU	O2-C2	-2.66	1.18	1.23
2	L2	1361	PSU	O4-C4	-2.65	1.18	1.23
2	L2	1253	OMG	O6-C6	-2.65	1.18	1.23
1	L1	774	PSU	O4-C4	-2.65	1.18	1.23
2	L2	359	OMC	O2-C2	-2.65	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1478	OMG	O6-C6	-2.65	1.18	1.23
88	S1	12	PSU	O4-C4	-2.65	1.18	1.23
2	L2	510	PSU	O4-C4	-2.64	1.18	1.23
88	S1	2140	OMC	O2-C2	-2.64	1.18	1.23
4	L4	74	OMG	O6-C6	-2.64	1.18	1.23
1	L1	1533	PSU	O4-C4	-2.63	1.18	1.23
88	S1	2048	OMU	O2-C2	-2.62	1.18	1.23
88	S1	897	A2M	C5-N7	-2.62	1.34	1.39
2	L2	1360	OMG	O6-C6	-2.62	1.18	1.23
1	L1	856	OMG	C4-N9	-2.61	1.31	1.38
2	L2	1231	OMG	C4-N9	-2.61	1.31	1.38
1	L1	1190	OMG	C5-N7	-2.61	1.33	1.39
7	L7	75	OMG	O6-C6	-2.61	1.18	1.23
2	L2	1359	OMU	O2-C2	-2.60	1.18	1.23
4	L4	74	OMG	C4-N9	-2.60	1.31	1.38
2	L2	472	PSU	O4-C4	-2.59	1.18	1.23
88	S1	1865	OMG	O6-C6	-2.59	1.18	1.23
2	L2	73	OMU	O2-C2	-2.59	1.18	1.23
2	L2	527	A2M	O3'-C3'	-2.58	1.36	1.43
1	L1	1011	PSU	O4-C4	-2.58	1.18	1.23
88	S1	2184	MA6	C5-N7	-2.58	1.34	1.39
88	S1	1246	PSU	O4-C4	-2.58	1.18	1.23
88	S1	2151	OMG	O6-C6	-2.57	1.18	1.23
2	L2	1253	OMG	C4-N9	-2.57	1.31	1.38
2	L2	71	OMG	C4-N9	-2.57	1.31	1.38
88	S1	1566	PSU	O4-C4	-2.57	1.18	1.23
2	L2	500	PSU	O4-C4	-2.57	1.18	1.23
88	S1	1829	OMG	O6-C6	-2.57	1.18	1.23
88	S1	600	OMG	O6-C6	-2.56	1.18	1.23
1	L1	959	OMG	O6-C6	-2.56	1.18	1.23
88	S1	1647	OMG	O6-C6	-2.56	1.18	1.23
1	L1	1177	PSU	O4-C4	-2.55	1.18	1.23
3	L3	13	OMU	O2-C2	-2.55	1.18	1.23
2	L2	443	OMC	C5-C4	2.55	1.48	1.42
1	L1	1371	OMU	O2-C2	-2.55	1.18	1.23
1	L1	697	A2M	C8-N9	-2.55	1.33	1.37
88	S1	2185	MA6	C5-N7	-2.54	1.34	1.39
2	L2	802	PSU	O4-C4	-2.54	1.18	1.23
1	L1	1524	OMG	C5-C6	2.54	1.53	1.44
88	S1	1550	OMG	O6-C6	-2.53	1.18	1.23
88	S1	1623	OMG	O6-C6	-2.53	1.18	1.23
88	S1	38	OMC	C5-C4	2.53	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1623	OMG	C5-C6	2.53	1.53	1.44
88	S1	1478	OMG	C4-N9	-2.53	1.31	1.38
2	L2	686	OMG	O6-C6	-2.53	1.18	1.23
2	L2	560	OMU	O2-C2	-2.53	1.18	1.23
1	L1	1190	OMG	C5-C6	2.52	1.53	1.44
1	L1	1524	OMG	O6-C6	-2.52	1.18	1.23
88	S1	29	OMU	O2-C2	-2.52	1.18	1.23
1	L1	1190	OMG	C6-N1	2.52	1.43	1.38
2	L2	1077	OMU	O2-C2	-2.52	1.18	1.23
2	L2	95	A2M	C8-N9	-2.52	1.33	1.37
88	S1	661	OMU	O2-C2	-2.52	1.18	1.23
88	S1	1550	OMG	C5-C6	2.52	1.53	1.44
2	L2	655	OMG	C5-C6	2.51	1.53	1.44
88	S1	8	OMU	O2-C2	-2.51	1.18	1.23
88	S1	2202	PSU	O4-C4	-2.51	1.18	1.23
1	L1	1540	OMG	C5-C6	2.51	1.53	1.44
2	L2	686	OMG	C5-C6	2.51	1.53	1.44
7	L7	75	OMG	C5-C6	2.51	1.53	1.44
2	L2	1248	OMC	C5-C4	2.50	1.48	1.42
88	S1	1865	OMG	C5-C6	2.50	1.53	1.44
88	S1	600	OMG	C5-C6	2.50	1.53	1.44
88	S1	1662	OMU	O2-C2	-2.50	1.18	1.23
2	L2	1078	OMG	C5-C6	2.50	1.53	1.44
2	L2	1360	OMG	C5-C6	2.49	1.53	1.44
88	S1	33	PSU	O4-C4	-2.49	1.18	1.23
88	S1	600	OMG	C6-N1	2.49	1.43	1.38
1	L1	1107	OMU	O2-C2	-2.49	1.18	1.23
2	L2	1078	OMG	C6-N1	2.48	1.43	1.38
1	L1	48	OMU	C6-N1	2.48	1.44	1.38
88	S1	1829	OMG	C5-C6	2.48	1.53	1.44
88	S1	1621	OMU	O2-C2	-2.47	1.18	1.23
2	L2	1253	OMG	C5-C6	2.46	1.53	1.44
88	S1	1829	OMG	C6-N1	2.46	1.43	1.38
2	L2	686	OMG	C4-N9	-2.46	1.31	1.38
2	L2	1372	A2M	C8-N9	-2.46	1.33	1.37
2	L2	1229	OMG	C5-C6	2.46	1.53	1.44
2	L2	655	OMG	C6-N1	2.46	1.43	1.38
1	L1	959	OMG	C5-C6	2.45	1.53	1.44
1	L1	681	A2M	C8-N9	-2.45	1.33	1.37
2	L2	1046	OMG	C5-C6	2.45	1.53	1.44
88	S1	1866	OMC	C5-C4	2.45	1.48	1.42
2	L2	686	OMG	C6-N1	2.45	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S1	1550	OMG	C6-N1	2.45	1.43	1.38
88	S1	1623	OMG	C6-N1	2.45	1.43	1.38
88	S1	1647	OMG	C4-N9	-2.45	1.31	1.38
1	L1	1626	OMG	C4-N9	-2.44	1.31	1.38
88	S1	1979	OMU	O2-C2	-2.44	1.18	1.23
1	L1	955	A2M	C8-N9	-2.44	1.33	1.37
88	S1	2151	OMG	C6-N1	2.44	1.43	1.38
88	S1	1647	OMG	C5-C6	2.43	1.53	1.44
88	S1	1478	OMG	C5-C6	2.43	1.53	1.44
7	L7	75	OMG	C4-N9	-2.43	1.31	1.38
1	L1	856	OMG	C5-C6	2.42	1.53	1.44
88	S1	1865	OMG	C6-N1	2.42	1.43	1.38
2	L2	641	OMG	C5-C6	2.42	1.53	1.44
2	L2	591	A2M	C8-N9	-2.42	1.33	1.37
2	L2	1185	A2M	C8-N9	-2.42	1.33	1.37
2	L2	655	OMG	C4-N9	-2.42	1.31	1.38
2	L2	1159	OMC	C5-C4	2.42	1.48	1.42
1	L1	1626	OMG	C5-C6	2.41	1.53	1.44
4	L4	74	OMG	C5-C6	2.41	1.53	1.44
2	L2	359	OMC	C5-C4	2.41	1.48	1.42
88	S1	1833	OMU	O2-C2	-2.41	1.18	1.23
2	L2	534	OMG	C4-N9	-2.41	1.31	1.38
2	L2	71	OMG	C5-C6	2.41	1.53	1.44
88	S1	2140	OMC	C5-C4	2.41	1.48	1.42
2	L2	534	OMG	C5-C6	2.41	1.53	1.44
2	L2	1046	OMG	C4-N9	-2.40	1.31	1.38
1	L1	1524	OMG	C6-N1	2.40	1.43	1.38
88	S1	18	OMC	C5-C4	2.40	1.48	1.42
1	L1	959	OMG	C6-N1	2.40	1.43	1.38
2	L2	1231	OMG	C5-C6	2.40	1.53	1.44
2	L2	570	A2M	C8-N9	-2.39	1.33	1.37
2	L2	1229	OMG	C4-N9	-2.39	1.32	1.38
1	L1	69	A2M	C8-N9	-2.38	1.33	1.37
2	L2	1231	OMG	C6-N1	2.38	1.43	1.38
7	L7	75	OMG	C6-N1	2.38	1.43	1.38
2	L2	1397	OMC	C5-C4	2.38	1.48	1.42
88	S1	1647	OMG	C6-N1	2.37	1.43	1.38
88	S1	1979	OMU	C5-C4	2.37	1.48	1.43
88	S1	1865	OMG	C4-N9	-2.37	1.32	1.38
1	L1	1010	OMC	C5-C4	2.37	1.48	1.42
1	L1	856	OMG	C6-N1	2.36	1.43	1.38
2	L2	665	A2M	C8-N9	-2.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1540	OMG	C6-N1	2.36	1.43	1.38
88	S1	1478	OMG	C6-N1	2.36	1.43	1.38
2	L2	1067	A2M	C8-N9	-2.35	1.33	1.37
1	L1	845	OMU	C6-N1	2.35	1.43	1.38
2	L2	1253	OMG	C2-N1	2.35	1.43	1.37
88	S1	1662	OMU	C5-C4	2.35	1.48	1.43
2	L2	527	A2M	C8-N9	-2.35	1.33	1.37
88	S1	2151	OMG	C4-N9	-2.35	1.32	1.38
4	L4	74	OMG	C6-N1	2.35	1.43	1.38
1	L1	678	A2M	C8-N9	-2.34	1.33	1.37
2	L2	1360	OMG	C6-N1	2.34	1.43	1.38
2	L2	1317	OMC	C5-C4	2.34	1.48	1.42
88	S1	8	OMU	C5-C4	2.34	1.48	1.43
88	S1	1621	OMU	C5-C4	2.33	1.48	1.43
88	S1	2151	OMG	C5-C6	2.33	1.53	1.44
2	L2	583	OMC	C5-C4	2.32	1.48	1.42
1	L1	305	A2M	C8-N9	-2.31	1.33	1.37
88	S1	661	OMU	C5-C4	2.31	1.48	1.43
1	L1	1107	OMU	C5-C4	2.31	1.48	1.43
2	L2	1077	OMU	C5-C4	2.31	1.48	1.43
1	L1	1626	OMG	C6-N1	2.30	1.43	1.38
88	S1	668	A2M	C8-N9	-2.30	1.33	1.37
2	L2	534	OMG	C6-N1	2.30	1.43	1.38
2	L2	641	OMG	C6-N1	2.29	1.43	1.38
2	L2	667	OMU	C5-C4	2.29	1.48	1.43
1	L1	858	A2M	C8-N9	-2.29	1.33	1.37
1	L1	1253	OMU	O2-C2	-2.29	1.19	1.23
1	L1	235	A2M	C8-N9	-2.28	1.33	1.37
88	S1	1829	OMG	C4-N9	-2.28	1.32	1.38
88	S1	2059	OMC	C5-C4	2.27	1.48	1.42
7	L7	162	A2M	C8-N9	-2.27	1.33	1.37
88	S1	29	OMU	C5-C4	2.27	1.48	1.43
2	L2	604	A2M	C8-N9	-2.27	1.33	1.37
88	S1	1623	OMG	C4-N9	-2.26	1.32	1.38
2	L2	1229	OMG	C6-N1	2.26	1.43	1.38
1	L1	1524	OMG	C4-N9	-2.26	1.32	1.38
2	L2	382	A2M	C8-N9	-2.25	1.33	1.37
88	S1	1833	OMU	C5-C4	2.25	1.48	1.43
3	L3	13	OMU	C5-C4	2.25	1.48	1.43
1	L1	1373	A2M	C8-N9	-2.25	1.33	1.37
1	L1	695	OMC	C5-C4	2.25	1.48	1.42
1	L1	1539	A2M	C8-N9	-2.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	14	OMC	C5-C4	2.24	1.48	1.42
2	L2	628	A2M	C8-N9	-2.24	1.33	1.37
88	S1	28	A2M	C8-N9	-2.24	1.33	1.37
88	S1	2021	A2M	C8-N9	-2.24	1.33	1.37
2	L2	1419	OMU	C5-C4	2.23	1.48	1.43
2	L2	572	A2M	C8-N9	-2.23	1.33	1.37
1	L1	927	A2M	C8-N9	-2.23	1.33	1.37
1	L1	847	OMU	C5-C4	2.23	1.48	1.43
88	S1	600	OMG	C4-N9	-2.23	1.32	1.38
88	S1	2048	OMU	C5-C4	2.22	1.48	1.43
1	L1	1371	OMU	C5-C4	2.22	1.48	1.43
1	L1	1253	OMU	C5-C4	2.22	1.48	1.43
88	S1	2184	MA6	C8-N9	-2.21	1.33	1.37
1	L1	1659	OMU	C5-C4	2.21	1.48	1.43
2	L2	1360	OMG	C4-N9	-2.21	1.32	1.38
7	L7	43	A2M	C8-N9	-2.21	1.33	1.37
88	S1	479	A2M	C8-N9	-2.21	1.33	1.37
88	S1	98	A2M	C8-N9	-2.20	1.33	1.37
88	S1	1550	OMG	C4-N9	-2.20	1.32	1.38
2	L2	1359	OMU	C5-C4	2.19	1.48	1.43
1	L1	959	OMG	C4-N9	-2.19	1.32	1.38
1	L1	1527	OMC	C5-C4	2.19	1.48	1.42
2	L2	71	OMG	C6-N1	2.17	1.42	1.38
2	L2	1046	OMG	C6-N1	2.17	1.42	1.38
2	L2	1384	A2M	C8-N9	-2.16	1.33	1.37
2	L2	73	OMU	C5-C4	2.15	1.48	1.43
1	L1	1011	PSU	O4'-C1'	-2.14	1.40	1.43
2	L2	56	OMU	C5-C4	2.14	1.48	1.43
88	S1	512	A2M	C8-N9	-2.14	1.33	1.37
2	L2	565	OMU	C5-C4	2.14	1.48	1.43
88	S1	897	A2M	C8-N9	-2.13	1.33	1.37
1	L1	845	OMU	C5-C4	2.11	1.48	1.43
2	L2	560	OMU	C5-C4	2.09	1.48	1.43
88	S1	2185	MA6	C8-N9	-2.02	1.34	1.37
88	S1	1995	G7M	C5-C4	2.01	1.43	1.38

All (1066) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S1	2185	MA6	N1-C6-N6	-14.03	99.76	116.86
88	S1	2184	MA6	N1-C6-N6	-13.30	100.65	116.86
88	S1	2185	MA6	C5-C6-N6	9.57	140.47	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S1	2184	MA6	C5-C6-N6	9.00	139.58	125.33
1	L1	959	OMG	C1'-N9-C8	-8.27	103.25	126.73
2	L2	1360	OMG	C1'-N9-C8	-7.78	104.61	126.73
88	S1	1829	OMG	C1'-N9-C8	-7.73	104.77	126.73
88	S1	1623	OMG	C1'-N9-C8	-7.71	104.84	126.73
88	S1	600	OMG	C1'-N9-C8	-7.66	104.98	126.73
88	S1	1550	OMG	C1'-N9-C8	-7.64	105.01	126.73
2	L2	1046	OMG	C1'-N9-C8	-7.64	105.03	126.73
2	L2	534	OMG	C1'-N9-C8	-7.63	105.05	126.73
88	S1	2151	OMG	C1'-N9-C8	-7.61	105.11	126.73
2	L2	655	OMG	C1'-N9-C8	-7.57	105.22	126.73
4	L4	74	OMG	C1'-N9-C8	-7.49	105.45	126.73
2	L2	686	OMG	C1'-N9-C8	-7.42	105.64	126.73
2	L2	1253	OMG	C1'-N9-C8	-7.38	105.77	126.73
1	L1	1626	OMG	C1'-N9-C8	-7.37	105.79	126.73
88	S1	1865	OMG	C1'-N9-C8	-7.36	105.82	126.73
2	L2	1229	OMG	C1'-N9-C8	-7.30	106.00	126.73
7	L7	75	OMG	C1'-N9-C8	-7.29	106.03	126.73
88	S1	1647	OMG	C1'-N9-C8	-7.25	106.12	126.73
1	L1	1540	OMG	C1'-N9-C8	-7.23	106.20	126.73
2	L2	1231	OMG	C1'-N9-C8	-7.22	106.22	126.73
88	S1	1478	OMG	C1'-N9-C8	-7.21	106.25	126.73
1	L1	1524	OMG	C1'-N9-C8	-7.18	106.33	126.73
1	L1	856	OMG	C1'-N9-C8	-7.12	106.50	126.73
1	L1	959	OMG	C1'-N9-C4	7.09	147.42	126.49
2	L2	641	OMG	C1'-N9-C8	-7.01	106.81	126.73
2	L2	71	OMG	C1'-N9-C8	-6.94	107.00	126.73
2	L2	1078	OMG	C1'-N9-C8	-6.92	107.06	126.73
2	L2	1360	OMG	C1'-N9-C4	6.76	146.47	126.49
88	S1	2151	OMG	C1'-N9-C4	6.70	146.29	126.49
88	S1	1623	OMG	C1'-N9-C4	6.59	145.96	126.49
88	S1	1829	OMG	C1'-N9-C4	6.59	145.95	126.49
88	S1	600	OMG	C1'-N9-C4	6.54	145.80	126.49
2	L2	1046	OMG	C1'-N9-C4	6.53	145.76	126.49
88	S1	1550	OMG	C1'-N9-C4	6.49	145.65	126.49
2	L2	1253	OMG	C1'-N9-C4	6.49	145.65	126.49
1	L1	845	OMU	C4-N3-C2	-6.44	118.62	126.61
1	L1	1190	OMG	C1'-N9-C8	-6.41	108.53	126.73
2	L2	534	OMG	C1'-N9-C4	6.39	145.36	126.49
2	L2	655	OMG	C1'-N9-C4	6.33	145.20	126.49
2	L2	686	OMG	C1'-N9-C4	6.30	145.10	126.49
4	L4	74	OMG	C1'-N9-C4	6.29	145.07	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1626	OMG	C1'-N9-C4	6.22	144.85	126.49
88	S1	1865	OMG	C1'-N9-C4	6.18	144.75	126.49
7	L7	75	OMG	C1'-N9-C4	6.18	144.75	126.49
2	L2	1229	OMG	C1'-N9-C4	6.09	144.47	126.49
88	S1	1478	OMG	C1'-N9-C4	6.08	144.46	126.49
1	L1	1540	OMG	C1'-N9-C4	6.08	144.44	126.49
2	L2	1231	OMG	C1'-N9-C4	6.06	144.40	126.49
1	L1	48	OMU	C4-N3-C2	-6.06	119.09	126.61
2	L2	560	OMU	C4-N3-C2	-6.05	119.10	126.61
1	L1	1524	OMG	C1'-N9-C4	6.04	144.32	126.49
88	S1	1647	OMG	C1'-N9-C4	5.98	144.15	126.49
7	L7	43	A2M	N3-C2-N1	-5.97	119.54	128.58
1	L1	856	OMG	C1'-N9-C4	5.93	144.01	126.49
88	S1	8	OMU	C4-N3-C2	-5.93	119.25	126.61
88	S1	1833	OMU	C4-N3-C2	-5.93	119.25	126.61
2	L2	667	OMU	C4-N3-C2	-5.87	119.33	126.61
2	L2	527	A2M	N3-C2-N1	-5.87	119.70	128.58
1	L1	1373	A2M	N3-C2-N1	-5.86	119.71	128.58
2	L2	1077	OMU	C4-N3-C2	-5.85	119.35	126.61
88	S1	668	A2M	N3-C2-N1	-5.84	119.74	128.58
2	L2	1359	OMU	C4-N3-C2	-5.82	119.39	126.61
1	L1	69	A2M	N3-C2-N1	-5.80	119.80	128.58
2	L2	71	OMG	C1'-N9-C4	5.79	143.59	126.49
2	L2	382	A2M	N3-C2-N1	-5.78	119.83	128.58
1	L1	1107	OMU	C4-N3-C2	-5.77	119.45	126.61
1	L1	927	A2M	N3-C2-N1	-5.76	119.86	128.58
2	L2	1185	A2M	N3-C2-N1	-5.76	119.86	128.58
1	L1	681	A2M	N3-C2-N1	-5.76	119.86	128.58
2	L2	572	A2M	N3-C2-N1	-5.76	119.86	128.58
2	L2	641	OMG	C1'-N9-C4	5.75	143.47	126.49
88	S1	512	A2M	N3-C2-N1	-5.75	119.88	128.58
7	L7	162	A2M	N3-C2-N1	-5.74	119.89	128.58
2	L2	591	A2M	N3-C2-N1	-5.72	119.92	128.58
2	L2	565	OMU	C4-N3-C2	-5.72	119.51	126.61
2	L2	1078	OMG	C1'-N9-C4	5.72	143.37	126.49
88	S1	2184	MA6	N1-C2-N3	-5.71	119.94	128.58
2	L2	604	A2M	N3-C2-N1	-5.71	119.94	128.58
1	L1	847	OMU	C4-N3-C2	-5.70	119.53	126.61
1	L1	678	A2M	N3-C2-N1	-5.70	119.95	128.58
88	S1	2021	A2M	N3-C2-N1	-5.70	119.95	128.58
2	L2	628	A2M	N3-C2-N1	-5.69	119.97	128.58
1	L1	955	A2M	N3-C2-N1	-5.69	119.97	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	56	OMU	C4-N3-C2	-5.68	119.56	126.61
1	L1	1539	A2M	N3-C2-N1	-5.68	119.98	128.58
88	S1	29	OMU	C4-N3-C2	-5.68	119.56	126.61
88	S1	897	A2M	N3-C2-N1	-5.67	119.99	128.58
2	L2	570	A2M	N3-C2-N1	-5.67	120.00	128.58
2	L2	665	A2M	N3-C2-N1	-5.66	120.01	128.58
1	L1	1659	OMU	C4-N3-C2	-5.65	119.59	126.61
88	S1	479	A2M	N3-C2-N1	-5.64	120.04	128.58
88	S1	1621	OMU	C4-N3-C2	-5.64	119.61	126.61
1	L1	305	A2M	N3-C2-N1	-5.63	120.06	128.58
88	S1	2185	MA6	N1-C2-N3	-5.63	120.06	128.58
2	L2	1372	A2M	N3-C2-N1	-5.62	120.07	128.58
88	S1	28	A2M	N3-C2-N1	-5.62	120.08	128.58
2	L2	1384	A2M	N3-C2-N1	-5.62	120.08	128.58
1	L1	235	A2M	N3-C2-N1	-5.61	120.09	128.58
2	L2	1067	A2M	N3-C2-N1	-5.60	120.10	128.58
88	S1	2048	OMU	C4-N3-C2	-5.59	119.67	126.61
88	S1	98	A2M	N3-C2-N1	-5.59	120.12	128.58
88	S1	1979	OMU	C4-N3-C2	-5.57	119.69	126.61
88	S1	661	OMU	C4-N3-C2	-5.56	119.71	126.61
2	L2	1419	OMU	C4-N3-C2	-5.55	119.72	126.61
1	L1	858	A2M	N3-C2-N1	-5.54	120.19	128.58
2	L2	570	A2M	C5-C4-N3	-5.53	119.10	126.72
1	L1	697	A2M	N3-C2-N1	-5.52	120.22	128.58
88	S1	1662	OMU	C4-N3-C2	-5.51	119.77	126.61
2	L2	95	A2M	N3-C2-N1	-5.51	120.25	128.58
1	L1	1371	OMU	C4-N3-C2	-5.50	119.78	126.61
1	L1	845	OMU	N3-C2-N1	5.40	121.92	114.89
1	L1	1253	OMU	C4-N3-C2	-5.39	119.92	126.61
3	L3	13	OMU	C4-N3-C2	-5.36	119.96	126.61
2	L2	95	A2M	C5-C4-N3	-5.30	119.42	126.72
2	L2	73	OMU	C4-N3-C2	-5.28	120.05	126.61
1	L1	927	A2M	C5-C4-N3	-5.25	119.49	126.72
1	L1	678	A2M	C5-C4-N3	-5.21	119.55	126.72
2	L2	1067	A2M	C5-C4-N3	-5.19	119.57	126.72
1	L1	681	A2M	C5-C4-N3	-5.18	119.58	126.72
1	L1	697	A2M	C5-C4-N3	-5.17	119.59	126.72
1	L1	1190	OMG	C1'-N9-C4	5.14	141.68	126.49
1	L1	235	A2M	C5-C4-N3	-5.14	119.64	126.72
88	S1	512	A2M	C5-C4-N3	-5.14	119.64	126.72
2	L2	382	A2M	C5-C4-N3	-5.11	119.68	126.72
1	L1	1539	A2M	C5-C4-N3	-5.10	119.70	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	604	A2M	C5-C4-N3	-5.08	119.72	126.72
2	L2	572	A2M	C5-C4-N3	-5.07	119.73	126.72
1	L1	48	OMU	N3-C2-N1	5.07	121.50	114.89
2	L2	437	PSU	C4-N3-C2	-5.06	119.40	126.37
1	L1	955	A2M	C5-C4-N3	-5.06	119.75	126.72
7	L7	43	A2M	N6-C6-N1	-5.04	107.15	118.38
2	L2	78	PSU	C4-N3-C2	-5.04	119.43	126.37
2	L2	665	A2M	C5-C4-N3	-5.04	119.78	126.72
2	L2	591	A2M	C5-C4-N3	-5.01	119.82	126.72
2	L2	628	A2M	N6-C6-N1	-5.00	107.23	118.38
1	L1	858	A2M	C5-C4-N3	-4.98	119.85	126.72
7	L7	166	PSU	C4-N3-C2	-4.97	119.52	126.37
88	S1	2021	A2M	C5-C4-N3	-4.97	119.87	126.72
88	S1	98	A2M	C5-C4-N3	-4.97	119.88	126.72
1	L1	305	A2M	C5-C4-N3	-4.96	119.89	126.72
2	L2	1185	A2M	C5-C4-N3	-4.96	119.89	126.72
88	S1	28	A2M	C5-C4-N3	-4.95	119.89	126.72
2	L2	1264	PSU	C4-N3-C2	-4.95	119.56	126.37
1	L1	927	A2M	N6-C6-N1	-4.95	107.36	118.38
1	L1	1017	PSU	C4-N3-C2	-4.94	119.56	126.37
2	L2	1303	PSU	C4-N3-C2	-4.94	119.56	126.37
88	S1	479	A2M	C5-C4-N3	-4.94	119.92	126.72
2	L2	1318	PSU	C4-N3-C2	-4.94	119.57	126.37
2	L2	1382	PSU	C4-N3-C2	-4.94	119.57	126.37
2	L2	504	PSU	C4-N3-C2	-4.93	119.57	126.37
2	L2	1144	PSU	C4-N3-C2	-4.93	119.58	126.37
1	L1	774	PSU	C4-N3-C2	-4.93	119.58	126.37
1	L1	1017	PSU	N1-C2-N3	4.92	120.36	115.17
88	S1	668	A2M	N6-C6-N1	-4.92	107.42	118.38
88	S1	897	A2M	C5-C4-N3	-4.91	119.95	126.72
88	S1	479	A2M	N6-C6-N1	-4.90	107.47	118.38
2	L2	1058	PSU	C4-N3-C2	-4.89	119.63	126.37
2	L2	572	A2M	N6-C6-N1	-4.89	107.50	118.38
1	L1	235	A2M	N6-C6-N1	-4.88	107.50	118.38
1	L1	1526	PSU	C4-N3-C2	-4.88	119.65	126.37
7	L7	74	PSU	C4-N3-C2	-4.88	119.65	126.37
1	L1	1539	A2M	N6-C6-N1	-4.88	107.51	118.38
1	L1	1373	A2M	C5-C4-N3	-4.88	120.00	126.72
1	L1	69	A2M	C5-C4-N3	-4.86	120.02	126.72
1	L1	697	A2M	N6-C6-N1	-4.85	107.57	118.38
1	L1	672	PSU	C4-N3-C2	-4.85	119.69	126.37
1	L1	69	A2M	N6-C6-N1	-4.85	107.58	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1403	PSU	C4-N3-C2	-4.85	119.69	126.37
1	L1	1529	PSU	C4-N3-C2	-4.85	119.69	126.37
1	L1	681	A2M	N6-C6-N1	-4.84	107.59	118.38
2	L2	570	A2M	N6-C6-N1	-4.84	107.60	118.38
2	L2	1384	A2M	C5-C4-N3	-4.84	120.06	126.72
2	L2	597	PSU	C4-N3-C2	-4.84	119.71	126.37
2	L2	1060	PSU	C4-N3-C2	-4.84	119.71	126.37
1	L1	1664	PSU	C4-N3-C2	-4.83	119.72	126.37
1	L1	955	A2M	N6-C6-N1	-4.82	107.64	118.38
2	L2	1372	A2M	C5-C4-N3	-4.82	120.08	126.72
2	L2	665	A2M	N6-C6-N1	-4.81	107.66	118.38
88	S1	897	A2M	N6-C6-N1	-4.81	107.66	118.38
88	S1	1657	PSU	C4-N3-C2	-4.81	119.74	126.37
7	L7	101	PSU	C4-N3-C2	-4.81	119.75	126.37
2	L2	1152	PSU	C4-N3-C2	-4.81	119.75	126.37
2	L2	527	A2M	C5-C4-N3	-4.81	120.09	126.72
1	L1	858	A2M	N6-C6-N1	-4.81	107.67	118.38
1	L1	678	A2M	N6-C6-N1	-4.81	107.67	118.38
1	L1	672	PSU	N1-C2-N3	4.80	120.23	115.17
88	S1	668	A2M	C5-C4-N3	-4.80	120.11	126.72
88	S1	512	A2M	N6-C6-N1	-4.79	107.70	118.38
88	S1	2021	A2M	N6-C6-N1	-4.79	107.70	118.38
7	L7	69	PSU	C4-N3-C2	-4.79	119.78	126.37
1	L1	1373	A2M	N6-C6-N1	-4.78	107.72	118.38
2	L2	628	A2M	C5-C4-N3	-4.78	120.14	126.72
2	L2	626	PSU	C4-N3-C2	-4.78	119.79	126.37
88	S1	33	PSU	C4-N3-C2	-4.78	119.79	126.37
88	S1	2184	MA6	C5-C4-N3	-4.77	120.14	126.72
88	S1	1246	PSU	C4-N3-C2	-4.77	119.80	126.37
1	L1	305	A2M	N6-C6-N1	-4.77	107.75	118.38
2	L2	604	A2M	N6-C6-N1	-4.77	107.75	118.38
2	L2	591	A2M	N6-C6-N1	-4.77	107.75	118.38
2	L2	472	PSU	C4-N3-C2	-4.77	119.80	126.37
2	L2	565	OMU	N3-C2-N1	4.76	121.08	114.89
2	L2	1185	A2M	N6-C6-N1	-4.74	107.81	118.38
1	L1	422	PSU	C4-N3-C2	-4.74	119.84	126.37
1	L1	239	PSU	C4-N3-C2	-4.74	119.85	126.37
1	L1	940	PSU	C4-N3-C2	-4.74	119.85	126.37
1	L1	1533	PSU	C4-N3-C2	-4.73	119.86	126.37
2	L2	1058	PSU	N1-C2-N3	4.73	120.15	115.17
2	L2	95	A2M	N6-C6-N1	-4.72	107.86	118.38
2	L2	1360	OMG	C5-C4-N3	-4.72	120.89	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1144	PSU	N1-C2-N3	4.71	120.14	115.17
2	L2	1361	PSU	C4-N3-C2	-4.71	119.88	126.37
88	S1	28	A2M	N6-C6-N1	-4.71	107.88	118.38
1	L1	959	OMG	C5-C4-N3	-4.71	120.89	128.39
2	L2	1213	PSU	C4-N3-C2	-4.71	119.89	126.37
88	S1	98	A2M	N6-C6-N1	-4.70	107.90	118.38
2	L2	437	PSU	N1-C2-N3	4.70	120.13	115.17
2	L2	1067	A2M	N6-C6-N1	-4.70	107.91	118.38
2	L2	78	PSU	N1-C2-N3	4.70	120.12	115.17
2	L2	1264	PSU	N1-C2-N3	4.70	120.12	115.17
2	L2	500	PSU	C4-N3-C2	-4.69	119.91	126.37
88	S1	1550	OMG	C5-C4-N3	-4.69	120.93	128.39
7	L7	43	A2M	C5-C4-N3	-4.68	120.27	126.72
88	S1	12	PSU	C4-N3-C2	-4.68	119.92	126.37
1	L1	1529	PSU	N1-C2-N3	4.68	120.11	115.17
88	S1	2185	MA6	C5-C4-N3	-4.68	120.27	126.72
2	L2	593	PSU	C4-N3-C2	-4.68	119.92	126.37
1	L1	1528	PSU	C4-N3-C2	-4.68	119.92	126.37
2	L2	1372	A2M	N6-C6-N1	-4.68	107.96	118.38
2	L2	510	PSU	C4-N3-C2	-4.68	119.93	126.37
2	L2	1384	A2M	N6-C6-N1	-4.67	107.97	118.38
2	L2	504	PSU	N1-C2-N3	4.67	120.10	115.17
1	L1	1526	PSU	N1-C2-N3	4.67	120.10	115.17
2	L2	1303	PSU	N1-C2-N3	4.67	120.10	115.17
7	L7	74	PSU	N1-C2-N3	4.67	120.09	115.17
7	L7	162	A2M	C5-C4-N3	-4.67	120.29	126.72
2	L2	662	PSU	C4-N3-C2	-4.67	119.94	126.37
2	L2	1060	PSU	N1-C2-N3	4.66	120.08	115.17
7	L7	69	PSU	N1-C2-N3	4.65	120.08	115.17
2	L2	512	PSU	C4-N3-C2	-4.65	119.96	126.37
88	S1	1292	PSU	C4-N3-C2	-4.65	119.97	126.37
2	L2	1403	PSU	N1-C2-N3	4.64	120.06	115.17
1	L1	1011	PSU	C4-N3-C2	-4.63	119.99	126.37
2	L2	597	PSU	N1-C2-N3	4.63	120.05	115.17
2	L2	802	PSU	C4-N3-C2	-4.63	120.00	126.37
1	L1	1533	PSU	N1-C2-N3	4.61	120.03	115.17
2	L2	662	PSU	N1-C2-N3	4.60	120.02	115.17
88	S1	600	OMG	C5-C4-N3	-4.60	121.07	128.39
7	L7	162	A2M	N6-C6-N1	-4.60	108.14	118.38
2	L2	1194	PSU	C4-N3-C2	-4.59	120.04	126.37
7	L7	101	PSU	N1-C2-N3	4.59	120.01	115.17
2	L2	527	A2M	N6-C6-N1	-4.59	108.16	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S1	1995	G7M	C2-N3-C4	4.59	120.20	112.30
1	L1	1524	OMG	C5-C4-N3	-4.58	121.10	128.39
2	L2	382	A2M	N6-C6-N1	-4.58	108.18	118.38
2	L2	1265	PSU	N1-C2-N3	4.58	120.00	115.17
88	S1	2151	OMG	C5-C4-N3	-4.57	121.12	128.39
88	S1	1566	PSU	C4-N3-C2	-4.56	120.09	126.37
2	L2	1361	PSU	N1-C2-N3	4.56	119.97	115.17
88	S1	2202	PSU	C4-N3-C2	-4.56	120.09	126.37
88	S1	1829	OMG	C5-C4-N3	-4.55	121.14	128.39
7	L7	166	PSU	N1-C2-N3	4.55	119.97	115.17
88	S1	2184	MA6	N9-C8-N7	-4.54	107.49	113.94
88	S1	1623	OMG	C5-C4-N3	-4.54	121.16	128.39
1	L1	1664	PSU	N1-C2-N3	4.54	119.95	115.17
2	L2	1152	PSU	N1-C2-N3	4.53	119.95	115.17
1	L1	774	PSU	N1-C2-N3	4.53	119.94	115.17
2	L2	1318	PSU	N1-C2-N3	4.51	119.92	115.17
1	L1	1177	PSU	C4-N3-C2	-4.50	120.17	126.37
2	L2	655	OMG	C2-N3-C4	4.49	120.03	112.30
2	L2	1046	OMG	C5-C4-N3	-4.49	121.25	128.39
1	L1	422	PSU	N1-C2-N3	4.48	119.90	115.17
88	S1	33	PSU	N1-C2-N3	4.48	119.89	115.17
2	L2	1265	PSU	C4-N3-C2	-4.47	120.21	126.37
1	L1	1011	PSU	N1-C2-N3	4.47	119.88	115.17
2	L2	1382	PSU	N1-C2-N3	4.47	119.88	115.17
2	L2	655	OMG	C5-C4-N3	-4.46	121.29	128.39
2	L2	626	PSU	N1-C2-N3	4.46	119.87	115.17
2	L2	512	PSU	N1-C2-N3	4.45	119.86	115.17
88	S1	1550	OMG	C2-N3-C4	4.44	119.95	112.30
2	L2	1253	OMG	C5-C4-N3	-4.44	121.33	128.39
1	L1	239	PSU	N1-C2-N3	4.44	119.85	115.17
1	L1	940	PSU	N1-C2-N3	4.44	119.85	115.17
2	L2	1229	OMG	C5-C4-N3	-4.43	121.34	128.39
2	L2	1360	OMG	C2-N3-C4	4.43	119.93	112.30
2	L2	472	PSU	N1-C2-N3	4.41	119.82	115.17
2	L2	1213	PSU	N1-C2-N3	4.41	119.82	115.17
88	S1	1292	PSU	N1-C2-N3	4.41	119.82	115.17
2	L2	1229	OMG	C2-N3-C4	4.40	119.88	112.30
2	L2	534	OMG	C5-C4-N3	-4.39	121.40	128.39
2	L2	510	PSU	N1-C2-N3	4.39	119.80	115.17
2	L2	686	OMG	C5-C4-N3	-4.39	121.41	128.39
88	S1	12	PSU	N1-C2-N3	4.39	119.79	115.17
2	L2	802	PSU	N1-C2-N3	4.38	119.79	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1194	PSU	N1-C2-N3	4.38	119.79	115.17
2	L2	593	PSU	N1-C2-N3	4.38	119.78	115.17
2	L2	1046	OMG	C2-N3-C4	4.37	119.82	112.30
88	S1	1865	OMG	C5-C4-N3	-4.37	121.44	128.39
88	S1	1246	PSU	N1-C2-N3	4.37	119.77	115.17
88	S1	600	OMG	C2-N3-C4	4.37	119.82	112.30
88	S1	1623	OMG	C2-N3-C4	4.36	119.81	112.30
88	S1	2151	OMG	C2-N3-C4	4.35	119.80	112.30
2	L2	71	OMG	C5-C4-N3	-4.35	121.46	128.39
2	L2	1078	OMG	C2-N3-C4	4.34	119.78	112.30
1	L1	959	OMG	C2-N3-C4	4.34	119.78	112.30
1	L1	1524	OMG	C2-N3-C4	4.34	119.78	112.30
88	S1	1829	OMG	C2-N3-C4	4.33	119.76	112.30
2	L2	686	OMG	C2-N3-C4	4.33	119.75	112.30
2	L2	1308	5MC	C5-C6-N1	-4.31	118.63	123.31
2	L2	527	A2M	N9-C8-N7	-4.31	107.82	113.94
2	L2	1231	OMG	C2-N3-C4	4.31	119.72	112.30
88	S1	2202	PSU	N1-C2-N3	4.31	119.71	115.17
2	L2	534	OMG	C2-N3-C4	4.30	119.71	112.30
88	S1	1657	PSU	N1-C2-N3	4.30	119.70	115.17
2	L2	71	OMG	C2-N3-C4	4.30	119.70	112.30
88	S1	1478	OMG	C2-N3-C4	4.29	119.69	112.30
88	S1	1647	OMG	C5-C4-N3	-4.29	121.57	128.39
4	L4	74	OMG	C5-C4-N3	-4.28	121.57	128.39
1	L1	1626	OMG	C5-C4-N3	-4.28	121.57	128.39
88	S1	1647	OMG	C2-N3-C4	4.28	119.67	112.30
2	L2	500	PSU	N1-C2-N3	4.28	119.68	115.17
88	S1	1566	PSU	N1-C2-N3	4.27	119.68	115.17
4	L4	74	OMG	C2-N3-C4	4.27	119.66	112.30
88	S1	1865	OMG	C2-N3-C4	4.27	119.65	112.30
1	L1	1528	PSU	N1-C2-N3	4.27	119.67	115.17
1	L1	1190	OMG	C2-N3-C4	4.25	119.61	112.30
1	L1	927	A2M	N9-C8-N7	-4.25	107.91	113.94
1	L1	856	OMG	C2-N3-C4	4.24	119.59	112.30
88	S1	1478	OMG	C5-C4-N3	-4.23	121.66	128.39
88	S1	1995	G7M	C5-C4-N3	-4.22	120.17	128.15
1	L1	69	A2M	N9-C8-N7	-4.22	107.95	113.94
1	L1	1540	OMG	C2-N3-C4	4.21	119.54	112.30
1	L1	845	OMU	C1'-N1-C2	4.20	125.14	117.59
2	L2	1067	A2M	N9-C8-N7	-4.20	107.97	113.94
1	L1	1626	OMG	C2-N3-C4	4.20	119.53	112.30
7	L7	75	OMG	C5-C4-N3	-4.20	121.71	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	847	OMU	N3-C2-N1	4.19	120.34	114.89
7	L7	43	A2M	N9-C8-N7	-4.18	108.01	113.94
88	S1	668	A2M	N9-C8-N7	-4.17	108.02	113.94
2	L2	665	A2M	N9-C8-N7	-4.17	108.02	113.94
2	L2	641	OMG	C2-N3-C4	4.16	119.47	112.30
88	S1	2021	A2M	N9-C8-N7	-4.16	108.04	113.94
1	L1	305	A2M	N9-C8-N7	-4.16	108.04	113.94
1	L1	1177	PSU	N1-C2-N3	4.16	119.55	115.17
7	L7	162	A2M	N9-C8-N7	-4.15	108.05	113.94
1	L1	858	A2M	N9-C8-N7	-4.14	108.07	113.94
88	S1	2185	MA6	N9-C8-N7	-4.13	108.08	113.94
7	L7	75	OMG	C2-N3-C4	4.13	119.41	112.30
88	S1	897	A2M	N9-C8-N7	-4.12	108.09	113.94
2	L2	1231	OMG	C5-C4-N3	-4.11	121.84	128.39
88	S1	512	A2M	N9-C8-N7	-4.11	108.10	113.94
88	S1	2184	MA6	C4-C5-C6	4.10	120.15	115.91
1	L1	1373	A2M	N9-C8-N7	-4.10	108.12	113.94
2	L2	560	OMU	N3-C2-N1	4.10	120.22	114.89
2	L2	1185	A2M	N9-C8-N7	-4.09	108.14	113.94
88	S1	28	A2M	N9-C8-N7	-4.08	108.14	113.94
1	L1	955	A2M	N9-C8-N7	-4.08	108.15	113.94
2	L2	1384	A2M	N9-C8-N7	-4.07	108.16	113.94
2	L2	604	A2M	N9-C8-N7	-4.07	108.16	113.94
2	L2	572	A2M	N9-C8-N7	-4.07	108.17	113.94
2	L2	641	OMG	C5-C4-N3	-4.07	121.92	128.39
1	L1	856	OMG	C5-C4-N3	-4.05	121.94	128.39
88	S1	8	OMU	N3-C2-N1	4.05	120.16	114.89
2	L2	1078	OMG	C5-C4-N3	-4.05	121.95	128.39
2	L2	667	OMU	N3-C2-N1	4.04	120.16	114.89
1	L1	1371	OMU	N3-C2-N1	4.03	120.13	114.89
88	S1	1833	OMU	C5-C4-N3	4.01	120.42	114.80
2	L2	1359	OMU	N3-C2-N1	4.01	120.11	114.89
1	L1	1539	A2M	N9-C8-N7	-4.00	108.25	113.94
88	S1	479	A2M	N9-C8-N7	-4.00	108.26	113.94
2	L2	628	A2M	N9-C8-N7	-3.99	108.28	113.94
7	L7	43	A2M	C5-C6-N6	3.98	133.13	123.29
1	L1	1540	OMG	C5-C4-N3	-3.96	122.08	128.39
1	L1	235	A2M	N9-C8-N7	-3.96	108.32	113.94
1	L1	681	A2M	N9-C8-N7	-3.95	108.33	113.94
2	L2	56	OMU	N3-C2-N1	3.95	120.03	114.89
1	L1	1190	OMG	N9-C8-N7	-3.95	106.08	113.40
88	S1	98	A2M	N9-C8-N7	-3.94	108.34	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	591	A2M	N9-C8-N7	-3.94	108.35	113.94
2	L2	95	A2M	N9-C8-N7	-3.94	108.35	113.94
88	S1	2048	OMU	N3-C2-N1	3.92	120.00	114.89
1	L1	678	A2M	N9-C8-N7	-3.91	108.38	113.94
1	L1	48	OMU	C1'-N1-C2	3.91	124.62	117.59
2	L2	565	OMU	C1'-N1-C2	3.91	124.61	117.59
1	L1	1659	OMU	N3-C2-N1	3.90	119.97	114.89
1	L1	1253	OMU	N3-C2-N1	3.90	119.97	114.89
88	S1	2185	MA6	C4-C5-C6	3.90	119.94	115.91
2	L2	628	A2M	C5-C6-N6	3.87	132.88	123.29
88	S1	1995	G7M	C5-C6-N1	3.87	119.83	111.84
88	S1	29	OMU	N3-C2-N1	3.86	119.92	114.89
88	S1	661	OMU	N3-C2-N1	3.85	119.90	114.89
1	L1	1107	OMU	C5-C4-N3	3.84	120.19	114.80
2	L2	1419	OMU	N3-C2-N1	3.84	119.89	114.89
2	L2	1077	OMU	C5-C4-N3	3.84	120.17	114.80
88	S1	1621	OMU	N3-C2-N1	3.82	119.87	114.89
88	S1	1979	OMU	N3-C2-N1	3.82	119.87	114.89
2	L2	1077	OMU	N3-C2-N1	3.82	119.87	114.89
1	L1	1371	OMU	C1'-N1-C2	3.82	124.45	117.59
2	L2	667	OMU	C5-C4-N3	3.81	120.14	114.80
2	L2	1372	A2M	N9-C8-N7	-3.80	108.54	113.94
88	S1	668	A2M	C5-C6-N6	3.79	132.67	123.29
2	L2	572	A2M	C5-C6-N6	3.79	132.67	123.29
88	S1	1662	OMU	N3-C2-N1	3.79	119.82	114.89
2	L2	1265	PSU	C6-N1-C2	-3.77	119.19	122.69
1	L1	1190	OMG	C5-C4-N3	-3.77	122.39	128.39
2	L2	1078	OMG	N9-C8-N7	-3.77	106.42	113.40
2	L2	641	OMG	N9-C8-N7	-3.76	106.42	113.40
3	L3	13	OMU	C5-C4-N3	3.75	120.06	114.80
1	L1	1107	OMU	N3-C2-N1	3.75	119.77	114.89
2	L2	73	OMU	N3-C2-N1	3.74	119.76	114.89
1	L1	697	A2M	C5-C6-N6	3.73	132.53	123.29
88	S1	1647	OMG	N9-C8-N7	-3.72	106.50	113.40
1	L1	697	A2M	N9-C8-N7	-3.71	108.67	113.94
2	L2	1359	OMU	C5-C4-N3	3.71	120.00	114.80
2	L2	570	A2M	N9-C8-N7	-3.71	108.68	113.94
2	L2	591	A2M	C5-C6-N6	3.70	132.46	123.29
88	S1	479	A2M	C5-C6-N6	3.70	132.45	123.29
88	S1	29	OMU	C5-C4-N3	3.70	119.98	114.80
1	L1	69	A2M	C5-C6-N6	3.70	132.44	123.29
88	S1	8	OMU	C5-C4-N3	3.69	119.97	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	235	A2M	C5-C6-N6	3.69	132.42	123.29
2	L2	1229	OMG	N9-C8-N7	-3.68	106.57	113.40
2	L2	382	A2M	N9-C8-N7	-3.68	108.71	113.94
1	L1	1539	A2M	C5-C6-N6	3.68	132.39	123.29
2	L2	534	OMG	N9-C8-N7	-3.67	106.59	113.40
1	L1	678	A2M	C5-C6-N6	3.67	132.37	123.29
1	L1	1540	OMG	N9-C8-N7	-3.67	106.59	113.40
1	L1	1659	OMU	C5-C4-N3	3.67	119.94	114.80
88	S1	897	A2M	C5-C6-N6	3.67	132.36	123.29
2	L2	56	OMU	C5-C4-N3	3.67	119.93	114.80
2	L2	1185	A2M	C5-C6-N6	3.66	132.35	123.29
1	L1	1524	OMG	N9-C8-N7	-3.66	106.61	113.40
1	L1	681	A2M	C5-C6-N6	3.66	132.35	123.29
2	L2	560	OMU	C5-C4-N3	3.65	119.92	114.80
1	L1	858	A2M	C5-C6-N6	3.65	132.33	123.29
2	L2	570	A2M	C5-C6-N6	3.65	132.33	123.29
1	L1	955	A2M	C5-C6-N6	3.65	132.32	123.29
2	L2	665	A2M	C5-C6-N6	3.65	132.32	123.29
2	L2	1372	A2M	C5-C6-N6	3.65	132.32	123.29
1	L1	927	A2M	C5-C6-N6	3.65	132.32	123.29
4	L4	74	OMG	N9-C8-N7	-3.65	106.64	113.40
2	L2	570	A2M	C2-N3-C4	3.64	120.72	111.83
88	S1	2021	A2M	C5-C6-N6	3.63	132.28	123.29
2	L2	1419	OMU	C5-C4-N3	3.63	119.89	114.80
2	L2	71	OMG	N9-C8-N7	-3.63	106.67	113.40
88	S1	2048	OMU	C5-C4-N3	3.63	119.88	114.80
2	L2	655	OMG	N9-C8-N7	-3.63	106.67	113.40
1	L1	927	A2M	C2-N3-C4	3.62	120.66	111.83
88	S1	1979	OMU	C5-C4-N3	3.62	119.86	114.80
88	S1	1833	OMU	N3-C2-N1	3.62	119.60	114.89
88	S1	512	A2M	C5-C6-N6	3.61	132.24	123.29
2	L2	1253	OMG	C2-N3-C4	3.61	118.52	112.30
2	L2	95	A2M	C5-C6-N6	3.61	132.21	123.29
1	L1	1373	A2M	C5-C6-N6	3.60	132.20	123.29
1	L1	856	OMG	N9-C8-N7	-3.60	106.73	113.40
88	S1	661	OMU	C5-C4-N3	3.60	119.84	114.80
2	L2	604	A2M	C5-C6-N6	3.60	132.19	123.29
2	L2	1384	A2M	C5-C6-N6	3.60	132.19	123.29
2	L2	686	OMG	N9-C8-N7	-3.60	106.73	113.40
88	S1	1550	OMG	N9-C8-N7	-3.59	106.74	113.40
88	S1	98	A2M	C5-C6-N6	3.59	132.18	123.29
2	L2	1231	OMG	N9-C8-N7	-3.59	106.74	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S1	1621	OMU	C5-C4-N3	3.59	119.83	114.80
1	L1	1626	OMG	N9-C8-N7	-3.58	106.75	113.40
88	S1	1865	OMG	N9-C8-N7	-3.58	106.76	113.40
1	L1	305	A2M	C5-C6-N6	3.58	132.15	123.29
88	S1	1478	OMG	N9-C8-N7	-3.58	106.76	113.40
88	S1	28	A2M	C5-C6-N6	3.56	132.10	123.29
1	L1	1371	OMU	C5-C4-N3	3.56	119.78	114.80
88	S1	1662	OMU	C5-C4-N3	3.55	119.77	114.80
7	L7	75	OMG	N9-C8-N7	-3.54	106.83	113.40
1	L1	678	A2M	C2-N3-C4	3.53	120.45	111.83
2	L2	1067	A2M	C5-C6-N6	3.52	132.01	123.29
7	L7	162	A2M	C5-C6-N6	3.51	131.98	123.29
88	S1	1623	OMG	N9-C8-N7	-3.50	106.92	113.40
88	S1	600	OMG	N9-C8-N7	-3.49	106.92	113.40
2	L2	1361	PSU	C6-N1-C2	-3.49	119.45	122.69
1	L1	681	A2M	C2-N3-C4	3.49	120.35	111.83
1	L1	959	OMG	N9-C8-N7	-3.49	106.94	113.40
88	S1	1829	OMG	N9-C8-N7	-3.48	106.94	113.40
1	L1	1539	A2M	C2-N3-C4	3.48	120.33	111.83
2	L2	73	OMU	C5-C4-N3	3.47	119.66	114.80
88	S1	512	A2M	C2-N3-C4	3.47	120.31	111.83
1	L1	1017	PSU	C6-N1-C2	-3.47	119.47	122.69
1	L1	235	A2M	C2-N3-C4	3.47	120.30	111.83
3	L3	13	OMU	N3-C2-N1	3.47	119.41	114.89
2	L2	382	A2M	C2-N3-C4	3.47	120.30	111.83
2	L2	604	A2M	C2-N3-C4	3.47	120.30	111.83
1	L1	1011	PSU	C6-N1-C2	-3.47	119.47	122.69
2	L2	1046	OMG	N9-C8-N7	-3.46	106.98	113.40
1	L1	955	A2M	C2-N3-C4	3.45	120.27	111.83
7	L7	69	PSU	C6-N1-C2	-3.45	119.49	122.69
1	L1	69	A2M	C2-N3-C4	3.45	120.25	111.83
1	L1	1529	PSU	C6-N1-C2	-3.45	119.49	122.69
88	S1	2185	MA6	C2-N1-C6	3.44	120.23	111.83
2	L2	527	A2M	O4'-C1'-N9	3.44	114.70	108.09
1	L1	1373	A2M	C2-N3-C4	3.43	120.21	111.83
2	L2	572	A2M	C2-N3-C4	3.43	120.20	111.83
88	S1	2184	MA6	C2-N1-C6	3.43	120.20	111.83
1	L1	672	PSU	C6-C5-C4	3.43	120.49	118.17
2	L2	1067	A2M	C2-N3-C4	3.43	120.20	111.83
88	S1	668	A2M	C2-N3-C4	3.42	120.19	111.83
2	L2	665	A2M	C2-N3-C4	3.42	120.19	111.83
2	L2	662	PSU	C6-N1-C2	-3.41	119.53	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	591	A2M	C2-N3-C4	3.41	120.15	111.83
2	L2	1060	PSU	C6-N1-C2	-3.40	119.53	122.69
2	L2	1403	PSU	C6-N1-C2	-3.40	119.53	122.69
2	L2	527	A2M	C2-N3-C4	3.40	120.14	111.83
88	S1	2021	A2M	C2-N3-C4	3.40	120.14	111.83
88	S1	479	A2M	C2-N3-C4	3.40	120.14	111.83
2	L2	504	PSU	C6-N1-C2	-3.40	119.54	122.69
1	L1	305	A2M	C2-N3-C4	3.39	120.11	111.83
1	L1	858	A2M	C2-N3-C4	3.39	120.10	111.83
2	L2	95	A2M	C2-N3-C4	3.39	120.10	111.83
2	L2	382	A2M	C5-C6-N6	3.39	131.67	123.29
1	L1	1533	PSU	C6-N1-C2	-3.38	119.55	122.69
88	S1	897	A2M	C2-N3-C4	3.38	120.09	111.83
2	L2	1194	PSU	C6-N1-C2	-3.38	119.55	122.69
7	L7	101	PSU	C6-N1-C2	-3.38	119.56	122.69
7	L7	43	A2M	C2-N3-C4	3.38	120.07	111.83
88	S1	98	A2M	C2-N3-C4	3.37	120.07	111.83
2	L2	512	PSU	C6-N1-C2	-3.37	119.56	122.69
1	L1	847	OMU	C5-C4-N3	3.37	119.52	114.80
1	L1	1526	PSU	C6-N1-C2	-3.37	119.56	122.69
2	L2	628	A2M	C2-N3-C4	3.37	120.06	111.83
1	L1	697	A2M	C2-N3-C4	3.37	120.06	111.83
2	L2	1058	PSU	C6-N1-C2	-3.37	119.57	122.69
2	L2	1185	A2M	C2-N3-C4	3.36	120.05	111.83
88	S1	1833	OMU	O4-C4-C5	-3.36	119.37	125.16
1	L1	1177	PSU	C6-N1-C2	-3.36	119.58	122.69
88	S1	28	A2M	C2-N3-C4	3.35	120.00	111.83
1	L1	672	PSU	C6-N1-C2	-3.34	119.59	122.69
2	L2	1360	OMG	N9-C8-N7	-3.34	107.21	113.40
2	L2	1384	A2M	C2-N3-C4	3.34	119.98	111.83
1	L1	1253	OMU	C5-C4-N3	3.33	119.47	114.80
2	L2	527	A2M	C5-C6-N6	3.33	131.54	123.29
7	L7	74	PSU	C6-N1-C2	-3.33	119.60	122.69
1	L1	422	PSU	C6-N1-C2	-3.33	119.60	122.69
2	L2	802	PSU	C6-N1-C2	-3.32	119.61	122.69
2	L2	1152	PSU	C6-N1-C2	-3.32	119.61	122.69
88	S1	1995	G7M	O6-C6-C5	-3.32	120.61	128.01
88	S1	1292	PSU	C6-N1-C2	-3.31	119.62	122.69
2	L2	626	PSU	C6-N1-C2	-3.31	119.62	122.69
7	L7	162	A2M	C2-N3-C4	3.31	119.91	111.83
1	L1	681	A2M	N3-C4-N9	3.29	132.77	127.17
88	S1	2184	MA6	N3-C4-N9	3.29	132.76	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1372	A2M	C2-N3-C4	3.28	119.85	111.83
2	L2	1067	A2M	N3-C4-N9	3.28	132.74	127.17
88	S1	2184	MA6	C2-N3-C4	3.27	119.81	111.83
1	L1	927	A2M	N3-C4-N9	3.26	132.72	127.17
2	L2	1213	PSU	C6-N1-C2	-3.25	119.68	122.69
88	S1	2185	MA6	C2-N3-C4	3.24	119.74	111.83
88	S1	33	PSU	C6-N1-C2	-3.23	119.69	122.69
2	L2	1144	PSU	C6-N1-C2	-3.23	119.69	122.69
2	L2	570	A2M	N3-C4-N9	3.23	132.65	127.17
88	S1	2202	PSU	C6-N1-C2	-3.23	119.70	122.69
2	L2	382	A2M	N3-C4-N9	3.22	132.64	127.17
2	L2	1264	PSU	C6-N1-C2	-3.21	119.71	122.69
2	L2	1303	PSU	C6-C5-C4	3.21	120.34	118.17
2	L2	1303	PSU	C6-N1-C2	-3.21	119.72	122.69
2	L2	95	A2M	N3-C4-N9	3.21	132.62	127.17
2	L2	597	PSU	C6-N1-C2	-3.20	119.72	122.69
1	L1	239	PSU	C6-N1-C2	-3.20	119.72	122.69
1	L1	1664	PSU	C6-N1-C2	-3.19	119.73	122.69
2	L2	472	PSU	C6-N1-C2	-3.19	119.73	122.69
2	L2	1253	OMG	N9-C8-N7	-3.19	107.48	113.40
1	L1	1528	PSU	C6-N1-C2	-3.19	119.73	122.69
2	L2	510	PSU	C6-N1-C2	-3.19	119.73	122.69
2	L2	437	PSU	C6-C5-C4	3.19	120.33	118.17
1	L1	940	PSU	C6-C5-C4	3.19	120.33	118.17
2	L2	1403	PSU	C6-C5-C4	3.18	120.32	118.17
2	L2	565	OMU	C5-C4-N3	3.18	119.26	114.80
88	S1	512	A2M	N3-C4-N9	3.16	132.54	127.17
7	L7	74	PSU	C6-C5-C4	3.15	120.30	118.17
88	S1	2151	OMG	N9-C8-N7	-3.14	107.57	113.40
1	L1	1017	PSU	C6-C5-C4	3.14	120.29	118.17
88	S1	1566	PSU	C6-N1-C2	-3.12	119.79	122.69
1	L1	1526	PSU	C6-C5-C4	3.11	120.28	118.17
2	L2	593	PSU	C6-N1-C2	-3.11	119.80	122.69
2	L2	78	PSU	C6-C5-C4	3.10	120.27	118.17
2	L2	524	5MC	C5-C6-N1	-3.10	119.95	123.31
2	L2	1152	PSU	C6-C5-C4	3.10	120.27	118.17
2	L2	1361	PSU	O2-C2-N1	-3.10	119.59	122.79
1	L1	697	A2M	N3-C4-N9	3.10	132.44	127.17
2	L2	527	A2M	N3-C4-N9	3.10	132.43	127.17
1	L1	1539	A2M	N3-C4-N9	3.09	132.43	127.17
88	S1	12	PSU	C6-N1-C2	-3.09	119.83	122.69
2	L2	604	A2M	N3-C4-N9	3.08	132.41	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	678	A2M	N3-C4-N9	3.08	132.40	127.17
1	L1	305	A2M	N3-C4-N9	3.07	132.39	127.17
2	L2	572	A2M	N3-C4-N9	3.06	132.38	127.17
2	L2	591	A2M	N3-C4-N9	3.06	132.37	127.17
2	L2	527	A2M	C2'-C1'-N9	-3.05	108.72	113.75
1	L1	774	PSU	C6-N1-C2	-3.05	119.86	122.69
7	L7	69	PSU	C6-C5-C4	3.05	120.23	118.17
2	L2	472	PSU	C6-C5-C4	3.05	120.23	118.17
2	L2	1213	PSU	C6-C5-C4	3.04	120.23	118.17
2	L2	500	PSU	C6-N1-C2	-3.04	119.87	122.69
2	L2	1308	5MC	C4'-O4'-C1'	-3.03	102.77	109.47
2	L2	1382	PSU	C6-N1-C2	-3.03	119.88	122.69
88	S1	1657	PSU	C6-N1-C2	-3.03	119.88	122.69
2	L2	78	PSU	C6-N1-C2	-3.02	119.88	122.69
2	L2	665	A2M	N3-C4-N9	3.02	132.31	127.17
2	L2	1185	A2M	N3-C4-N9	3.02	132.31	127.17
1	L1	927	A2M	C5-N7-C8	3.02	108.20	103.45
2	L2	1359	OMU	O4-C4-C5	-3.02	119.95	125.16
2	L2	1067	A2M	C5-N7-C8	3.02	108.19	103.45
88	S1	98	A2M	N3-C4-N9	3.02	132.30	127.17
88	S1	28	A2M	N3-C4-N9	3.02	132.30	127.17
88	S1	1246	PSU	C6-N1-C2	-3.01	119.89	122.69
1	L1	940	PSU	C6-N1-C2	-3.01	119.90	122.69
7	L7	166	PSU	C6-N1-C2	-3.01	119.90	122.69
88	S1	2184	MA6	C4-N9-C8	3.00	108.89	105.74
2	L2	662	PSU	C6-C5-C4	3.00	120.20	118.17
1	L1	1107	OMU	O4-C4-C5	-2.99	120.00	125.16
2	L2	1318	PSU	C6-C5-C4	2.99	120.19	118.17
1	L1	955	A2M	N3-C4-N9	2.99	132.26	127.17
1	L1	1664	PSU	C6-C5-C4	2.99	120.19	118.17
2	L2	1058	PSU	C6-C5-C4	2.99	120.19	118.17
1	L1	1253	OMU	C1'-N1-C2	2.99	122.96	117.59
1	L1	1524	OMG	C2-N1-C6	-2.98	119.70	125.11
88	S1	2059	OMC	O2-C2-N3	-2.98	117.63	122.33
1	L1	235	A2M	N3-C4-N9	2.98	132.23	127.17
88	S1	2059	OMC	C1'-N1-C2	2.97	125.01	118.44
1	L1	858	A2M	N3-C4-N9	2.97	132.23	127.17
1	L1	1659	OMU	O4-C4-C5	-2.97	120.04	125.16
1	L1	1373	A2M	N3-C4-N9	2.97	132.22	127.17
1	L1	845	OMU	C5-C4-N3	2.97	118.95	114.80
88	S1	2021	A2M	N3-C4-N9	2.96	132.21	127.17
88	S1	29	OMU	O4-C4-C5	-2.96	120.05	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	69	A2M	O2'-C2'-C1'	2.96	114.61	108.99
1	L1	1533	PSU	O2-C2-N1	-2.96	119.73	122.79
2	L2	1077	OMU	O4-C4-C5	-2.96	120.06	125.16
88	S1	2048	OMU	O4-C4-C5	-2.96	120.06	125.16
1	L1	69	A2M	C5-N7-C8	2.96	108.10	103.45
2	L2	560	OMU	O4-C4-C5	-2.96	120.06	125.16
88	S1	2061	5MC	C5-C6-N1	-2.95	120.11	123.31
1	L1	955	A2M	C5-N7-C8	2.95	108.08	103.45
2	L2	1360	OMG	C2-N1-C6	-2.95	119.77	125.11
2	L2	686	OMG	C2-N1-C6	-2.94	119.77	125.11
88	S1	1979	OMU	O4-C4-C5	-2.94	120.09	125.16
1	L1	69	A2M	N3-C4-N9	2.94	132.17	127.17
88	S1	1995	G7M	C2-N1-C6	-2.94	119.78	125.11
88	S1	2185	MA6	N3-C4-N9	2.93	132.16	127.17
4	L4	74	OMG	C2-N1-C6	-2.93	119.79	125.11
1	L1	1529	PSU	C6-C5-C4	2.93	120.15	118.17
2	L2	560	OMU	C2'-C1'-N1	-2.93	108.68	114.24
1	L1	845	OMU	O2-C2-N3	-2.93	116.09	121.49
2	L2	665	A2M	C5-N7-C8	2.93	108.05	103.45
88	S1	479	A2M	N3-C4-N9	2.93	132.15	127.17
88	S1	2021	A2M	C5-N7-C8	2.92	108.04	103.45
2	L2	1361	PSU	C6-C5-C4	2.92	120.14	118.17
88	S1	600	OMG	C2-N1-C6	-2.91	119.83	125.11
1	L1	959	OMG	N9-C4-N3	2.91	131.78	125.95
88	S1	2184	MA6	C5-N7-C8	2.91	108.02	103.45
1	L1	1253	OMU	O4-C4-C5	-2.91	120.15	125.16
2	L2	1046	OMG	C2-N1-C6	-2.90	119.85	125.11
1	L1	48	OMU	C5-C4-N3	2.90	118.86	114.80
2	L2	572	A2M	C5-N7-C8	2.90	108.01	103.45
2	L2	437	PSU	C6-N1-C2	-2.90	120.00	122.69
2	L2	570	A2M	C5-N7-C8	2.90	108.01	103.45
1	L1	305	A2M	C5-N7-C8	2.90	108.00	103.45
88	S1	2151	OMG	C2-N1-C6	-2.90	119.86	125.11
1	L1	1190	OMG	C2-N1-C6	-2.90	119.86	125.11
2	L2	1384	A2M	C5-N7-C8	2.90	108.00	103.45
1	L1	1539	A2M	C5-N7-C8	2.89	108.00	103.45
2	L2	1060	PSU	C6-C5-C4	2.89	120.13	118.17
88	S1	1829	OMG	C2-N1-C6	-2.89	119.86	125.11
88	S1	897	A2M	N3-C4-N9	2.89	132.08	127.17
88	S1	1623	OMG	C2-N1-C6	-2.89	119.87	125.11
2	L2	56	OMU	O4-C4-C5	-2.89	120.18	125.16
88	S1	512	A2M	C5-N7-C8	2.89	107.99	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S1	1621	OMU	O4-C4-C5	-2.88	120.19	125.16
2	L2	1078	OMG	C2-N1-C6	-2.88	119.89	125.11
88	S1	1865	OMG	C2-N1-C6	-2.88	119.89	125.11
1	L1	959	OMG	C2-N1-C6	-2.88	119.89	125.11
2	L2	1185	A2M	C5-N7-C8	2.88	107.98	103.45
2	L2	655	OMG	C2-N1-C6	-2.88	119.89	125.11
88	S1	1662	OMU	O4-C4-C5	-2.88	120.20	125.16
88	S1	1550	OMG	C2-N1-C6	-2.88	119.89	125.11
3	L3	13	OMU	O4-C4-C5	-2.87	120.20	125.16
1	L1	678	A2M	C5-N7-C8	2.87	107.97	103.45
1	L1	235	A2M	C5-N7-C8	2.87	107.97	103.45
2	L2	95	A2M	C5-N7-C8	2.87	107.97	103.45
88	S1	661	OMU	O4-C4-C5	-2.87	120.21	125.16
88	S1	897	A2M	C5-N7-C8	2.86	107.95	103.45
2	L2	73	OMU	O4-C4-C5	-2.86	120.22	125.16
88	S1	1478	OMG	C2-N1-C6	-2.86	119.92	125.11
2	L2	641	OMG	C2-N1-C6	-2.86	119.93	125.11
1	L1	858	A2M	C5-N7-C8	2.85	107.94	103.45
7	L7	166	PSU	O2-C2-N1	-2.85	119.85	122.79
1	L1	774	PSU	C6-C5-C4	2.85	120.09	118.17
1	L1	1371	OMU	O4-C4-C5	-2.84	120.26	125.16
2	L2	667	OMU	O4-C4-C5	-2.84	120.26	125.16
88	S1	668	A2M	C5-N7-C8	2.84	107.91	103.45
88	S1	28	A2M	C5-N7-C8	2.84	107.91	103.45
2	L2	1318	PSU	C6-N1-C2	-2.83	120.06	122.69
2	L2	437	PSU	O2-C2-N1	-2.83	119.87	122.79
1	L1	672	PSU	O2-C2-N1	-2.83	119.87	122.79
2	L2	1144	PSU	C6-C5-C4	2.83	120.08	118.17
1	L1	1373	A2M	C5-N7-C8	2.83	107.89	103.45
88	S1	668	A2M	N3-C4-N9	2.83	131.97	127.17
2	L2	1372	A2M	N3-C4-N9	2.82	131.97	127.17
2	L2	604	A2M	C5-N7-C8	2.82	107.89	103.45
1	L1	1626	OMG	C2-N1-C6	-2.82	119.99	125.11
88	S1	1647	OMG	C2-N1-C6	-2.82	119.99	125.11
88	S1	33	PSU	C6-C5-C4	2.82	120.08	118.17
1	L1	1017	PSU	O2-C2-N1	-2.82	119.88	122.79
2	L2	1231	OMG	C2-N1-C6	-2.82	120.00	125.11
2	L2	1229	OMG	C2-N1-C6	-2.82	120.00	125.11
7	L7	162	A2M	N3-C4-N9	2.82	131.96	127.17
2	L2	591	A2M	C5-N7-C8	2.82	107.88	103.45
7	L7	43	A2M	C5-N7-C8	2.81	107.86	103.45
1	L1	681	A2M	C5-N7-C8	2.81	107.86	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	71	OMG	C2-N1-C6	-2.81	120.02	125.11
1	L1	1011	PSU	O2-C2-N1	-2.81	119.89	122.79
1	L1	1533	PSU	C6-C5-C4	2.81	120.07	118.17
88	S1	479	A2M	C5-N7-C8	2.80	107.86	103.45
2	L2	1419	OMU	O4-C4-C5	-2.80	120.33	125.16
2	L2	527	A2M	C5-N7-C8	2.80	107.86	103.45
2	L2	1403	PSU	O2-C2-N1	-2.80	119.90	122.79
2	L2	534	OMG	C2-N1-C6	-2.80	120.04	125.11
88	S1	8	OMU	O4-C4-C5	-2.80	120.34	125.16
1	L1	422	PSU	C6-C5-C4	2.79	120.06	118.17
88	S1	33	PSU	O2-C2-N1	-2.79	119.91	122.79
2	L2	472	PSU	O2-C2-N1	-2.79	119.91	122.79
1	L1	69	A2M	C2'-C1'-N9	-2.79	109.16	113.75
7	L7	162	A2M	C5-N7-C8	2.79	107.84	103.45
7	L7	75	OMG	C2-N1-C6	-2.79	120.05	125.11
1	L1	1540	OMG	C2-N1-C6	-2.79	120.05	125.11
2	L2	628	A2M	C5-N7-C8	2.78	107.83	103.45
88	S1	98	A2M	C5-N7-C8	2.78	107.82	103.45
7	L7	166	PSU	C6-C5-C4	2.78	120.05	118.17
7	L7	43	A2M	C2'-C1'-N9	-2.78	109.18	113.75
2	L2	1384	A2M	N3-C4-N9	2.77	131.88	127.17
2	L2	1265	PSU	O2-C2-N1	-2.75	119.95	122.79
2	L2	597	PSU	C6-C5-C4	2.75	120.03	118.17
2	L2	527	A2M	C4'-O4'-C1'	-2.75	103.40	109.47
1	L1	847	OMU	O4-C4-C5	-2.75	120.43	125.16
7	L7	43	A2M	N3-C4-N9	2.74	131.83	127.17
1	L1	697	A2M	C5-N7-C8	2.74	107.76	103.45
2	L2	1372	A2M	C5-N7-C8	2.74	107.76	103.45
2	L2	628	A2M	N3-C4-N9	2.72	131.80	127.17
88	S1	2185	MA6	C5-N7-C8	2.72	107.73	103.45
7	L7	69	PSU	O2-C2-N1	-2.72	119.99	122.79
88	S1	1550	OMG	N9-C4-N3	2.71	131.38	125.95
1	L1	1529	PSU	O2-C2-N1	-2.71	119.99	122.79
88	S1	2202	PSU	C6-C5-C4	2.71	120.00	118.17
2	L2	1229	OMG	C5-C6-N1	2.71	120.14	113.25
1	L1	1190	OMG	C5-C6-N1	2.70	120.14	113.25
2	L2	71	OMG	C5-C6-N1	2.70	120.12	113.25
4	L4	74	OMG	C5-C6-N1	2.70	120.12	113.25
2	L2	1152	PSU	O2-C2-N1	-2.69	120.01	122.79
2	L2	655	OMG	C5-C6-N1	2.69	120.11	113.25
2	L2	1360	OMG	N9-C4-N3	2.69	131.33	125.95
1	L1	1524	OMG	C5-C6-N1	2.68	120.09	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1046	OMG	C5-C6-N1	2.68	120.08	113.25
7	L7	74	PSU	O2-C2-N1	-2.68	120.02	122.79
2	L2	1058	PSU	O2-C2-N1	-2.68	120.03	122.79
88	S1	1550	OMG	C5-C6-N1	2.67	120.05	113.25
1	L1	239	PSU	O2-C2-N1	-2.67	120.04	122.79
88	S1	1246	PSU	C6-C5-C4	2.66	119.97	118.17
88	S1	1478	OMG	C5-C6-N1	2.66	120.03	113.25
88	S1	1865	OMG	C5-C6-N1	2.66	120.03	113.25
2	L2	1231	OMG	C5-C6-N1	2.66	120.02	113.25
2	L2	1360	OMG	C5-C6-N1	2.66	120.01	113.25
88	S1	1647	OMG	C5-C6-N1	2.65	120.01	113.25
88	S1	600	OMG	N9-C4-N3	2.65	131.26	125.95
2	L2	382	A2M	C5-N7-C8	2.65	107.62	103.45
2	L2	641	OMG	C5-C6-N1	2.65	120.00	113.25
1	L1	1664	PSU	O2-C2-N1	-2.65	120.05	122.79
1	L1	1626	OMG	C5-C6-N1	2.65	120.00	113.25
88	S1	1829	OMG	N9-C4-N3	2.65	131.25	125.95
1	L1	422	PSU	O2-C2-N1	-2.64	120.06	122.79
2	L2	597	PSU	O2-C2-N1	-2.64	120.06	122.79
2	L2	1060	PSU	O2-C2-N1	-2.64	120.06	122.79
2	L2	560	OMU	O3'-C3'-C4'	2.64	118.67	111.08
2	L2	1144	PSU	O2-C2-N1	-2.64	120.07	122.79
88	S1	1829	OMG	C5-C6-N1	2.63	119.96	113.25
2	L2	565	OMU	O4-C4-C5	-2.63	120.62	125.16
88	S1	600	OMG	C5-C6-N1	2.63	119.95	113.25
2	L2	534	OMG	C5-C6-N1	2.63	119.94	113.25
2	L2	1078	OMG	C5-C6-N1	2.63	119.94	113.25
2	L2	527	A2M	C4-N9-C8	2.63	108.50	105.74
88	S1	2151	OMG	C5-C6-N1	2.62	119.93	113.25
2	L2	686	OMG	C5-C6-N1	2.62	119.93	113.25
1	L1	48	OMU	O4-C4-C5	-2.62	120.64	125.16
88	S1	1623	OMG	C5-C6-N1	2.62	119.92	113.25
2	L2	1078	OMG	N2-C2-N1	2.61	122.27	116.76
1	L1	856	OMG	C2-N1-C6	-2.61	120.38	125.11
2	L2	1382	PSU	O2-C2-N1	-2.61	120.10	122.79
88	S1	1623	OMG	N9-C4-N3	2.60	131.15	125.95
2	L2	500	PSU	O2-C2-N1	-2.60	120.11	122.79
2	L2	1382	PSU	C6-C5-C4	2.60	119.93	118.17
1	L1	959	OMG	C5-C6-N1	2.59	119.85	113.25
2	L2	1264	PSU	O2-C2-N1	-2.59	120.11	122.79
1	L1	1190	OMG	C2'-C1'-N9	-2.59	109.33	114.24
7	L7	101	PSU	C6-C5-C4	2.58	119.92	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	802	PSU	O2-C2-N1	-2.58	120.12	122.79
1	L1	1540	OMG	N2-C2-N1	2.58	122.21	116.76
2	L2	500	PSU	C6-C5-C4	2.58	119.92	118.17
2	L2	655	OMG	N9-C4-N3	2.58	131.10	125.95
88	S1	12	PSU	O2-C2-N1	-2.57	120.13	122.79
88	S1	1292	PSU	O2-C2-N1	-2.57	120.13	122.79
2	L2	1265	PSU	C6-C5-C4	2.57	119.91	118.17
2	L2	1303	PSU	O2-C2-N1	-2.57	120.14	122.79
2	L2	512	PSU	C6-C5-C4	2.57	119.91	118.17
2	L2	626	PSU	O2-C2-N1	-2.57	120.14	122.79
7	L7	75	OMG	C5-C6-N1	2.57	119.79	113.25
1	L1	847	OMU	O2-C2-N1	-2.56	119.46	122.80
2	L2	534	OMG	N9-C4-N3	2.56	131.07	125.95
88	S1	2151	OMG	N9-C4-N3	2.56	131.07	125.95
88	S1	8	OMU	O2-C2-N1	-2.56	119.47	122.80
88	S1	2151	OMG	O6-C6-C5	-2.55	119.79	126.53
2	L2	1046	OMG	N9-C4-N3	2.55	131.05	125.95
88	S1	1292	PSU	C6-C5-C4	2.55	119.89	118.17
1	L1	856	OMG	C5-C6-N1	2.55	119.74	113.25
2	L2	510	PSU	O2-C2-N1	-2.55	120.16	122.79
2	L2	1253	OMG	C2-N1-C6	-2.55	120.49	125.11
1	L1	858	A2M	C4'-O4'-C1'	-2.55	103.84	109.47
2	L2	71	OMG	C2'-C1'-N9	-2.55	109.41	114.24
2	L2	593	PSU	O2-C2-N1	-2.55	120.16	122.79
1	L1	1528	PSU	O2-C2-N1	-2.53	120.18	122.79
1	L1	1107	OMU	O2-C2-N1	-2.52	119.51	122.80
1	L1	1526	PSU	O2-C2-N1	-2.52	120.19	122.79
1	L1	239	PSU	C6-C5-C4	2.51	119.87	118.17
1	L1	1524	OMG	N9-C4-N3	2.51	130.98	125.95
1	L1	1190	OMG	N2-C2-N1	2.51	122.06	116.76
1	L1	48	OMU	O2-C2-N3	-2.51	116.87	121.49
88	S1	1657	PSU	O2-C2-N1	-2.50	120.21	122.79
1	L1	1540	OMG	C5-C6-N1	2.50	119.62	113.25
88	S1	2202	PSU	O2-C2-N1	-2.49	120.22	122.79
2	L2	1229	OMG	N9-C4-N3	2.48	130.92	125.95
2	L2	1264	PSU	C6-C5-C4	2.48	119.85	118.17
88	S1	1865	OMG	N9-C4-N3	2.48	130.91	125.95
1	L1	940	PSU	O2-C2-N1	-2.48	120.23	122.79
1	L1	1527	OMC	O2-C2-N3	-2.47	118.43	122.33
2	L2	802	PSU	C6-C5-C4	2.47	119.84	118.17
88	S1	1647	OMG	N9-C4-N3	2.47	130.88	125.95
1	L1	774	PSU	O2-C2-N1	-2.46	120.25	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1524	OMG	C8-N7-C5	2.46	108.64	104.26
88	S1	1829	OMG	O6-C6-C5	-2.46	120.04	126.53
2	L2	71	OMG	O6-C6-C5	-2.45	120.06	126.53
7	L7	101	PSU	O2-C2-N1	-2.45	120.26	122.79
1	L1	858	A2M	C2'-C1'-N9	-2.45	109.72	113.75
88	S1	12	PSU	C6-C5-C4	2.45	119.83	118.17
1	L1	1524	OMG	O2'-C2'-C1'	2.45	113.64	108.99
1	L1	1190	OMG	C8-N7-C5	2.44	108.61	104.26
1	L1	1527	OMC	C1'-N1-C2	2.44	123.82	118.44
88	S1	600	OMG	O6-C6-C5	-2.44	120.10	126.53
88	S1	1566	PSU	C6-C5-C4	2.43	119.82	118.17
1	L1	845	OMU	O4-C4-C5	-2.43	120.97	125.16
2	L2	662	PSU	O2-C2-N1	-2.43	120.28	122.79
2	L2	78	PSU	O2-C2-N1	-2.42	120.29	122.79
2	L2	512	PSU	O2-C2-N1	-2.42	120.29	122.79
2	L2	1359	OMU	O2-C2-N1	-2.42	119.65	122.80
2	L2	1194	PSU	O2-C2-N1	-2.42	120.29	122.79
2	L2	534	OMG	C8-N7-C5	2.41	108.56	104.26
2	L2	1229	OMG	C8-N7-C5	2.41	108.56	104.26
2	L2	565	OMU	O2-C2-N3	-2.41	117.04	121.49
88	S1	1550	OMG	C8-N7-C5	2.41	108.55	104.26
4	L4	74	OMG	O6-C6-C5	-2.41	120.18	126.53
2	L2	1046	OMG	O6-C6-C5	-2.40	120.19	126.53
2	L2	95	A2M	C6-C5-C4	2.40	120.46	117.18
2	L2	510	PSU	C6-C5-C4	2.40	119.79	118.17
1	L1	959	OMG	O6-C6-C5	-2.40	120.21	126.53
88	S1	1647	OMG	O6-C6-C5	-2.40	120.21	126.53
88	S1	1865	OMG	O6-C6-C5	-2.39	120.21	126.53
2	L2	71	OMG	N9-C4-N3	2.39	130.74	125.95
2	L2	686	OMG	O6-C6-C5	-2.39	120.22	126.53
2	L2	1078	OMG	O6-C6-C5	-2.39	120.22	126.53
2	L2	1360	OMG	O6-C6-C5	-2.39	120.23	126.53
1	L1	1626	OMG	N9-C4-N3	2.39	130.73	125.95
4	L4	74	OMG	N9-C4-N3	2.39	130.73	125.95
88	S1	1623	OMG	O6-C6-C5	-2.39	120.23	126.53
2	L2	1318	PSU	O2-C2-N1	-2.39	120.33	122.79
2	L2	1194	PSU	C6-C5-C4	2.39	119.78	118.17
88	S1	897	A2M	C2'-C1'-N9	-2.38	109.83	113.75
1	L1	1524	OMG	O6-C6-C5	-2.38	120.25	126.53
1	L1	1626	OMG	O6-C6-C5	-2.38	120.25	126.53
88	S1	1550	OMG	O6-C6-C5	-2.38	120.25	126.53
2	L2	570	A2M	C4-C5-N7	-2.38	107.86	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S1	2185	MA6	C4-N9-C8	2.38	108.23	105.74
2	L2	1231	OMG	O6-C6-C5	-2.37	120.26	126.53
88	S1	1246	PSU	O2-C2-N1	-2.37	120.34	122.79
88	S1	1647	OMG	C8-N7-C5	2.37	108.49	104.26
2	L2	593	PSU	C6-C5-C4	2.37	119.77	118.17
2	L2	655	OMG	O6-C6-C5	-2.37	120.28	126.53
88	S1	1478	OMG	O6-C6-C5	-2.37	120.28	126.53
2	L2	686	OMG	C8-N7-C5	2.37	108.48	104.26
7	L7	75	OMG	O6-C6-C5	-2.37	120.28	126.53
2	L2	1213	PSU	O2-C2-N1	-2.37	120.35	122.79
2	L2	534	OMG	O6-C6-C5	-2.36	120.30	126.53
2	L2	641	OMG	O6-C6-C5	-2.36	120.31	126.53
1	L1	959	OMG	C8-N7-C5	2.35	108.45	104.26
2	L2	565	OMU	C6-N1-C2	-2.35	118.13	121.00
2	L2	626	PSU	C6-C5-C4	2.35	119.76	118.17
2	L2	1229	OMG	O6-C6-C5	-2.35	120.32	126.53
1	L1	955	A2M	C4-C5-N7	-2.35	107.89	110.58
1	L1	1190	OMG	C6-C5-N7	2.35	134.57	130.29
1	L1	1540	OMG	C8-N7-C5	2.35	108.44	104.26
1	L1	845	OMU	C6-C5-C4	2.34	122.53	119.53
2	L2	95	A2M	C4-C5-N7	-2.34	107.91	110.58
2	L2	655	OMG	C8-N7-C5	2.34	108.42	104.26
88	S1	1623	OMG	C8-N7-C5	2.34	108.42	104.26
2	L2	641	OMG	C8-N7-C5	2.33	108.42	104.26
88	S1	1995	G7M	N9-C8-N7	-2.33	106.82	112.48
1	L1	69	A2M	C4-N9-C8	2.33	108.18	105.74
2	L2	686	OMG	N9-C4-N3	2.33	130.61	125.95
2	L2	71	OMG	C8-N7-C5	2.33	108.41	104.26
2	L2	1253	OMG	N9-C4-N3	2.32	130.60	125.95
2	L2	1078	OMG	C8-N7-C5	2.32	108.40	104.26
1	L1	235	A2M	C4-C5-N7	-2.32	107.93	110.58
1	L1	1626	OMG	C8-N7-C5	2.31	108.38	104.26
1	L1	678	A2M	C4-C5-N7	-2.31	107.94	110.58
88	S1	600	OMG	C8-N7-C5	2.31	108.37	104.26
1	L1	856	OMG	O6-C6-C5	-2.31	120.44	126.53
1	L1	48	OMU	C6-C5-C4	2.30	122.48	119.53
2	L2	1384	A2M	C2'-C1'-N9	-2.30	109.97	113.75
2	L2	1231	OMG	C8-N7-C5	2.30	108.36	104.26
88	S1	1865	OMG	C8-N7-C5	2.30	108.36	104.26
1	L1	69	A2M	C4-C5-N7	-2.30	107.95	110.58
88	S1	1657	PSU	C6-C5-C4	2.30	119.72	118.17
2	L2	1185	A2M	C2'-C1'-N9	-2.30	109.97	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	697	A2M	C6-C5-C4	2.29	120.30	117.18
7	L7	75	OMG	C8-N7-C5	2.29	108.34	104.26
7	L7	162	A2M	C4-N9-C8	2.29	108.14	105.74
88	S1	1566	PSU	O2-C2-N1	-2.28	120.43	122.79
2	L2	665	A2M	C4-C5-N7	-2.28	107.97	110.58
2	L2	628	A2M	C4-C5-N7	-2.28	107.98	110.58
4	L4	74	OMG	C8-N7-C5	2.28	108.32	104.26
88	S1	1829	OMG	C8-N7-C5	2.28	108.32	104.26
88	S1	2021	A2M	C4-C5-N7	-2.28	107.98	110.58
2	L2	667	OMU	O2-C2-N1	-2.27	119.84	122.80
7	L7	69	PSU	O4'-C1'-C2'	2.27	108.30	105.15
88	S1	1478	OMG	C8-N7-C5	2.27	108.31	104.26
2	L2	570	A2M	C6-C5-C4	2.27	120.28	117.18
2	L2	1403	PSU	O4'-C1'-C2'	2.27	108.29	105.15
1	L1	305	A2M	C4-N9-C8	2.27	108.12	105.74
88	S1	668	A2M	C4-N9-C8	2.26	108.12	105.74
1	L1	1190	OMG	O6-C6-C5	-2.26	120.56	126.53
2	L2	1046	OMG	C8-N7-C5	2.26	108.29	104.26
88	S1	29	OMU	O2-C2-N1	-2.26	119.86	122.80
2	L2	1303	PSU	O4'-C1'-C2'	2.26	108.28	105.15
1	L1	927	A2M	C4-C5-N7	-2.26	108.00	110.58
2	L2	1231	OMG	N2-C2-N1	2.25	121.52	116.76
2	L2	1384	A2M	C4-C5-N7	-2.25	108.01	110.58
2	L2	1360	OMG	C8-N7-C5	2.25	108.27	104.26
1	L1	927	A2M	C4-N9-C8	2.25	108.10	105.74
2	L2	73	OMU	O2-C2-N1	-2.24	119.88	122.80
7	L7	75	OMG	N9-C4-N3	2.24	130.43	125.95
2	L2	1067	A2M	C4-N9-C8	2.24	108.09	105.74
1	L1	845	OMU	C6-N1-C2	-2.24	118.28	121.00
1	L1	856	OMG	C8-N7-C5	2.24	108.24	104.26
88	S1	512	A2M	C2'-C1'-N9	-2.23	110.08	113.75
2	L2	570	A2M	C5-C4-N9	2.23	108.25	105.81
2	L2	1308	5MC	C5-C4-N3	-2.23	119.47	121.75
2	L2	1067	A2M	C6-C5-C4	2.23	120.22	117.18
88	S1	1647	OMG	C2'-C1'-N9	-2.23	110.00	114.24
88	S1	668	A2M	C4-C5-N7	-2.23	108.03	110.58
88	S1	1478	OMG	N9-C4-N3	2.23	130.41	125.95
88	S1	897	A2M	C4-C5-N7	-2.23	108.03	110.58
1	L1	1659	OMU	O2-C2-N1	-2.23	119.89	122.80
88	S1	2021	A2M	O2'-C2'-C1'	2.23	113.22	108.99
1	L1	1177	PSU	O2-C2-N1	-2.23	120.49	122.79
1	L1	1539	A2M	C4-C5-N7	-2.22	108.04	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L7	43	A2M	C4-N9-C8	2.22	108.07	105.74
1	L1	858	A2M	C4-C5-N7	-2.21	108.05	110.58
2	L2	572	A2M	C4-C5-N7	-2.21	108.05	110.58
1	L1	697	A2M	C4-C5-N7	-2.21	108.05	110.58
2	L2	1185	A2M	C4-C5-N7	-2.21	108.05	110.58
1	L1	1540	OMG	O6-C6-C5	-2.21	120.70	126.53
1	L1	1526	PSU	O4'-C1'-C2'	2.21	108.21	105.15
2	L2	1067	A2M	C4-C5-N7	-2.20	108.06	110.58
2	L2	641	OMG	N9-C4-N3	2.20	130.36	125.95
4	L4	74	OMG	N2-C2-N1	2.20	121.41	116.76
88	S1	661	OMU	O2-C2-N1	-2.20	119.93	122.80
2	L2	665	A2M	C4-N9-C8	2.20	108.05	105.74
2	L2	504	PSU	O2-C2-N1	-2.20	120.52	122.79
1	L1	1528	PSU	C6-C5-C4	2.19	119.65	118.17
2	L2	572	A2M	C2'-C1'-N9	-2.19	110.14	113.75
1	L1	1190	OMG	C4-C5-N7	-2.19	107.20	110.67
2	L2	641	OMG	N2-C2-N1	2.19	121.39	116.76
2	L2	1185	A2M	C4-N9-C8	2.19	108.03	105.74
7	L7	101	PSU	O4'-C1'-C2'	2.18	108.17	105.15
1	L1	858	A2M	C4-N9-C8	2.18	108.03	105.74
88	S1	479	A2M	C4-C5-N7	-2.18	108.09	110.58
88	S1	2021	A2M	C4-N9-C8	2.18	108.03	105.74
1	L1	1664	PSU	O4'-C1'-C2'	2.17	108.16	105.15
1	L1	856	OMG	N2-C2-N1	2.17	121.34	116.76
2	L2	591	A2M	C4-C5-N7	-2.17	108.11	110.58
2	L2	1077	OMU	O2-C2-N1	-2.16	119.98	122.80
1	L1	305	A2M	C4-C5-N7	-2.16	108.11	110.58
1	L1	1011	PSU	O4'-C1'-C2'	2.16	108.13	105.15
2	L2	1372	A2M	C4-C5-N7	-2.16	108.12	110.58
88	S1	2061	5MC	CM5-C5-C6	-2.15	119.94	122.85
88	S1	1621	OMU	O2-C2-N1	-2.14	120.01	122.80
2	L2	1231	OMG	N9-C4-N3	2.14	130.23	125.95
88	S1	1833	OMU	O2-C2-N1	-2.14	120.01	122.80
88	S1	668	A2M	C3'-C2'-C1'	2.14	106.90	102.81
88	S1	1478	OMG	N2-C2-N1	2.14	121.27	116.76
2	L2	1318	PSU	O4'-C1'-C2'	2.14	108.11	105.15
1	L1	1373	A2M	C4-N9-C8	2.13	107.98	105.74
2	L2	641	OMG	C2'-C1'-N9	-2.13	110.20	114.24
1	L1	681	A2M	C4-N9-C8	2.13	107.97	105.74
88	S1	28	A2M	C4-N9-C8	2.13	107.97	105.74
2	L2	686	OMG	N2-C2-N1	2.13	121.25	116.76
7	L7	43	A2M	C4-C5-N7	-2.13	108.15	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	235	A2M	C5-C4-N9	2.12	108.13	105.81
1	L1	856	OMG	N9-C4-N3	2.12	130.20	125.95
88	S1	98	A2M	C4-C5-N7	-2.12	108.16	110.58
88	S1	512	A2M	C4-C5-N7	-2.12	108.16	110.58
2	L2	1152	PSU	O4'-C1'-C2'	2.11	108.07	105.15
88	S1	28	A2M	C4-C5-N7	-2.11	108.17	110.58
2	L2	1253	OMG	O6-C6-C5	-2.11	120.96	126.53
2	L2	604	A2M	C4-C5-N7	-2.11	108.17	110.58
88	S1	897	A2M	C4-N9-C8	2.11	107.95	105.74
2	L2	1372	A2M	C6-C5-C4	2.11	120.05	117.18
1	L1	681	A2M	C4-C5-N7	-2.10	108.18	110.58
88	S1	28	A2M	C6-C5-C4	2.10	120.04	117.18
1	L1	678	A2M	C6-C5-C4	2.09	120.04	117.18
2	L2	591	A2M	C6-C5-C4	2.09	120.03	117.18
1	L1	48	OMU	C6-N1-C2	-2.09	118.45	121.00
88	S1	512	A2M	C4-N9-C8	2.09	107.93	105.74
1	L1	681	A2M	C6-C5-C4	2.08	120.02	117.18
1	L1	235	A2M	C6-C5-C4	2.08	120.02	117.18
2	L2	560	OMU	O2-C2-N1	-2.07	120.10	122.80
88	S1	2059	OMC	C1'-N1-C6	-2.07	116.35	120.78
1	L1	1540	OMG	C4-C5-N7	-2.07	107.39	110.67
2	L2	604	A2M	C4-N9-C8	2.07	107.91	105.74
7	L7	162	A2M	C4-C5-N7	-2.07	108.22	110.58
2	L2	1384	A2M	C5-C4-N9	2.07	108.06	105.81
1	L1	1371	OMU	O2-C2-N3	-2.07	117.68	121.49
2	L2	572	A2M	C6-C5-C4	2.07	120.00	117.18
88	S1	98	A2M	C6-C5-C4	2.06	120.00	117.18
2	L2	628	A2M	C5-C4-N9	2.06	108.06	105.81
2	L2	604	A2M	C6-C5-C4	2.06	119.99	117.18
88	S1	512	A2M	C6-C5-C4	2.06	119.99	117.18
2	L2	1185	A2M	C6-C5-C4	2.06	119.99	117.18
1	L1	678	A2M	C5-C4-N9	2.06	108.05	105.81
1	L1	1373	A2M	C4-C5-N7	-2.06	108.23	110.58
88	S1	1995	G7M	C5-C4-N9	2.05	110.27	105.88
2	L2	1382	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	L2	665	A2M	C6-C5-C4	2.05	119.98	117.18
1	L1	955	A2M	C4-N9-C8	2.05	107.89	105.74
2	L2	382	A2M	C6-C5-C4	2.05	119.97	117.18
2	L2	570	A2M	C3'-C2'-C1'	2.04	106.72	102.81
2	L2	593	PSU	O4'-C1'-C2'	2.04	107.97	105.15
2	L2	1078	OMG	C4-C5-N7	-2.04	107.44	110.67
2	L2	572	A2M	C4-N9-C8	2.04	107.88	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1253	OMG	C5-C6-N1	2.03	118.42	113.25
1	L1	955	A2M	C6-C5-C4	2.03	119.94	117.18
1	L1	856	OMG	N1-C2-N3	-2.03	119.61	123.32
2	L2	524	5MC	CM5-C5-C6	-2.02	120.12	122.85
88	S1	479	A2M	C4-N9-C8	2.02	107.86	105.74
2	L2	655	OMG	N2-C2-N1	2.02	121.02	116.76
88	S1	2151	OMG	C8-N7-C5	2.02	107.85	104.26
2	L2	628	A2M	C4-N9-C8	2.02	107.85	105.74
2	L2	591	A2M	C4-N9-C8	2.01	107.85	105.74
1	L1	1011	PSU	C6-C5-C4	2.01	119.53	118.17
2	L2	71	OMG	N1-C2-N3	-2.01	119.65	123.32
88	S1	98	A2M	C4-N9-C8	2.01	107.84	105.74
88	S1	1979	OMU	O2-C2-N1	-2.00	120.19	122.80

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L7	162	A2M	C1'-C2'-O2'-CM'
1	L1	48	OMU	O4'-C1'-N1-C2
1	L1	48	OMU	O4'-C1'-N1-C6
1	L1	69	A2M	C1'-C2'-O2'-CM'
1	L1	305	A2M	O4'-C4'-C5'-O5'
1	L1	678	A2M	C1'-C2'-O2'-CM'
1	L1	681	A2M	O4'-C4'-C5'-O5'
1	L1	695	OMC	C1'-C2'-O2'-CM2
1	L1	845	OMU	O4'-C1'-N1-C2
1	L1	845	OMU	O4'-C1'-N1-C6
1	L1	845	OMU	C1'-C2'-O2'-CM2
1	L1	1010	OMC	C1'-C2'-O2'-CM2
1	L1	1177	PSU	O4'-C4'-C5'-O5'
1	L1	1253	OMU	O4'-C1'-N1-C2
1	L1	1253	OMU	O4'-C1'-N1-C6
1	L1	1253	OMU	C4'-C5'-O5'-P
1	L1	1371	OMU	O4'-C1'-N1-C2
1	L1	1371	OMU	O4'-C1'-N1-C6
1	L1	1371	OMU	C1'-C2'-O2'-CM2
1	L1	1524	OMG	C1'-C2'-O2'-CM2
1	L1	1540	OMG	O4'-C4'-C5'-O5'
2	L2	443	OMC	C2'-C1'-N1-C6
2	L2	504	PSU	C2'-C1'-C5-C4
2	L2	504	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
2	L2	504	PSU	O4'-C1'-C5-C6
2	L2	534	OMG	O4'-C4'-C5'-O5'
2	L2	560	OMU	C1'-C2'-O2'-CM2
2	L2	565	OMU	O4'-C1'-N1-C2
2	L2	565	OMU	O4'-C1'-N1-C6
2	L2	565	OMU	C1'-C2'-O2'-CM2
2	L2	667	OMU	C1'-C2'-O2'-CM2
2	L2	802	PSU	O4'-C4'-C5'-O5'
2	L2	1046	OMG	O4'-C4'-C5'-O5'
2	L2	1046	OMG	C1'-C2'-O2'-CM2
2	L2	1067	A2M	C1'-C2'-O2'-CM'
2	L2	1229	OMG	O4'-C4'-C5'-O5'
2	L2	1264	PSU	C3'-C4'-C5'-O5'
2	L2	1264	PSU	O4'-C4'-C5'-O5'
88	S1	1543	B8N	O4'-C4'-C5'-O5'
88	S1	1566	PSU	C3'-C4'-C5'-O5'
88	S1	1566	PSU	O4'-C4'-C5'-O5'
88	S1	1657	PSU	C2'-C1'-C5-C4
88	S1	1662	OMU	C1'-C2'-O2'-CM2
88	S1	2021	A2M	C1'-C2'-O2'-CM'
88	S1	2059	OMC	O4'-C1'-N1-C2
88	S1	2059	OMC	O4'-C1'-N1-C6
88	S1	2151	OMG	O4'-C4'-C5'-O5'
88	S1	2202	PSU	O4'-C1'-C5-C6
1	L1	1010	OMC	O4'-C4'-C5'-O5'
1	L1	1177	PSU	C3'-C4'-C5'-O5'
1	L1	1253	OMU	C3'-C4'-C5'-O5'
1	L1	1540	OMG	C3'-C4'-C5'-O5'
2	L2	534	OMG	C3'-C4'-C5'-O5'
2	L2	802	PSU	C3'-C4'-C5'-O5'
2	L2	1229	OMG	C3'-C4'-C5'-O5'
2	L2	1361	PSU	C3'-C4'-C5'-O5'
2	L2	1361	PSU	O4'-C4'-C5'-O5'
88	S1	600	OMG	O4'-C4'-C5'-O5'
88	S1	2151	OMG	C3'-C4'-C5'-O5'
88	S1	1543	B8N	N34-C33-C34-O36
2	L2	443	OMC	C2'-C1'-N1-C2
1	L1	305	A2M	C3'-C4'-C5'-O5'
2	L2	665	A2M	O4'-C4'-C5'-O5'
2	L2	665	A2M	C3'-C4'-C5'-O5'
1	L1	681	A2M	C3'-C4'-C5'-O5'
2	L2	1046	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
88	S1	1543	B8N	C3'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C6
1	L1	1010	OMC	C3'-C4'-C5'-O5'
88	S1	512	A2M	C3'-C4'-C5'-O5'
88	S1	668	A2M	O4'-C4'-C5'-O5'
88	S1	668	A2M	C3'-C4'-C5'-O5'
88	S1	600	OMG	C3'-C4'-C5'-O5'
88	S1	1995	G7M	O4'-C4'-C5'-O5'
88	S1	2061	5MC	O4'-C4'-C5'-O5'
1	L1	1253	OMU	O4'-C4'-C5'-O5'
88	S1	98	A2M	O4'-C4'-C5'-O5'
88	S1	1995	G7M	C3'-C4'-C5'-O5'
88	S1	2061	5MC	C3'-C4'-C5'-O5'
88	S1	512	A2M	O4'-C4'-C5'-O5'
1	L1	681	A2M	C4'-C5'-O5'-P
2	L2	1384	A2M	C1'-C2'-O2'-CM'
1	L1	1526	PSU	C3'-C4'-C5'-O5'
1	L1	1526	PSU	O4'-C4'-C5'-O5'
88	S1	8	OMU	C2'-C1'-N1-C6
1	L1	1017	PSU	C3'-C4'-C5'-O5'
1	L1	1017	PSU	O4'-C4'-C5'-O5'
2	L2	1185	A2M	C3'-C4'-C5'-O5'
2	L2	570	A2M	C2'-C1'-N9-C8
88	S1	668	A2M	C2'-C1'-N9-C8
1	L1	1253	OMU	C2'-C1'-N1-C6
2	L2	1308	5MC	O4'-C1'-N1-C6
1	L1	1371	OMU	C3'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C2
88	S1	1829	OMG	O4'-C4'-C5'-O5'
88	S1	2059	OMC	O4'-C4'-C5'-O5'
2	L2	1248	OMC	C4'-C5'-O5'-P
88	S1	8	OMU	O4'-C1'-N1-C6
1	L1	1527	OMC	C3'-C2'-O2'-CM2
2	L2	560	OMU	C4'-C5'-O5'-P
2	L2	1185	A2M	C4'-C5'-O5'-P
2	L2	1361	PSU	C4'-C5'-O5'-P
2	L2	1382	PSU	O4'-C1'-C5-C4
88	S1	1657	PSU	O4'-C1'-C5-C4
2	L2	443	OMC	O4'-C1'-N1-C2
2	L2	443	OMC	O4'-C1'-N1-C6
1	L1	1107	OMU	C3'-C2'-O2'-CM2
2	L2	655	OMG	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
88	S1	1829	OMG	C4'-C5'-O5'-P
4	L4	74	OMG	C3'-C4'-C5'-O5'
2	L2	1308	5MC	O4'-C1'-N1-C2
2	L2	570	A2M	O4'-C1'-N9-C8
88	S1	1478	OMG	C4'-C5'-O5'-P
1	L1	927	A2M	C1'-C2'-O2'-CM'
2	L2	665	A2M	C1'-C2'-O2'-CM'
88	S1	2185	MA6	C4'-C5'-O5'-P
2	L2	1382	PSU	O4'-C1'-C5-C6
1	L1	959	OMG	O4'-C4'-C5'-O5'
1	L1	1371	OMU	O4'-C4'-C5'-O5'
1	L1	1527	OMC	C2'-C1'-N1-C6
2	L2	570	A2M	C2'-C1'-N9-C4
2	L2	560	OMU	C3'-C4'-C5'-O5'
88	S1	668	A2M	O4'-C1'-N9-C8
88	S1	8	OMU	O4'-C4'-C5'-O5'
3	L3	13	OMU	C4'-C5'-O5'-P
88	S1	2151	OMG	C3'-C2'-O2'-CM2
88	S1	668	A2M	C2'-C1'-N9-C4
88	S1	8	OMU	O4'-C1'-N1-C2
1	L1	858	A2M	O4'-C1'-N9-C8
1	L1	1253	OMU	C2'-C1'-N1-C2
88	S1	1543	B8N	N3-C31-C32-C33
1	L1	1527	OMC	C2'-C1'-N1-C2
88	S1	1543	B8N	N34-C33-C34-O35
1	L1	678	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

67 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L2	597	PSU	1	0
1	L1	1527	OMC	3	0
1	L1	1371	OMU	1	0
2	L2	1078	OMG	1	0
2	L2	1152	PSU	1	0
7	L7	43	A2M	1	0
2	L2	382	A2M	4	0
1	L1	1659	OMU	1	0
1	L1	1190	OMG	2	0
2	L2	565	OMU	3	0
2	L2	626	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	S1	2140	OMC	1	0
88	S1	18	OMC	1	0
1	L1	422	PSU	1	0
2	L2	443	OMC	1	0
88	S1	661	OMU	2	0
1	L1	235	A2M	1	0
1	L1	1540	OMG	1	0
2	L2	570	A2M	2	0
2	L2	1372	A2M	1	0
1	L1	697	A2M	3	0
1	L1	1539	A2M	1	0
2	L2	1318	PSU	1	0
88	S1	1292	PSU	1	0
88	S1	1995	G7M	1	0
1	L1	774	PSU	1	0
1	L1	1373	A2M	1	0
1	L1	1107	OMU	1	0
2	L2	604	A2M	1	0
1	L1	695	OMC	2	0
88	S1	98	A2M	2	0
88	S1	479	A2M	1	0
1	L1	69	A2M	1	0
88	S1	2021	A2M	1	0
2	L2	667	OMU	1	0
2	L2	14	OMC	3	0
1	L1	847	OMU	1	0
1	L1	1177	PSU	3	0
88	S1	1662	OMU	1	0
2	L2	1067	A2M	1	0
7	L7	162	A2M	1	0
1	L1	955	A2M	1	0
1	L1	1010	OMC	1	0
1	L1	1524	OMG	2	0
1	L1	959	OMG	1	0
88	S1	12	PSU	1	0
1	L1	1528	PSU	1	0
1	L1	1253	OMU	3	0
1	L1	845	OMU	4	0
2	L2	1253	OMG	1	0
4	L4	74	OMG	1	0
88	S1	2059	OMC	1	0
2	L2	95	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L2	527	A2M	1	0
2	L2	560	OMU	4	0
1	L1	1017	PSU	2	0
88	S1	2185	MA6	1	0
1	L1	1533	PSU	1	0
2	L2	1397	OMC	2	0
1	L1	927	A2M	1	0
88	S1	2202	PSU	1	0
2	L2	591	A2M	2	0
7	L7	101	PSU	1	0
1	L1	48	OMU	1	0
1	L1	678	A2M	1	0
2	L2	665	A2M	2	0
2	L2	1046	OMG	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 496 ligands modelled in this entry, 495 are monoatomic - leaving 1 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	$\# Z  > 2$
92	A1IWA	L2	1708	89	22,22,22	4.10	9 (40%)	26,29,29	1.26	2 (7%)

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
92	A1IWA	L2	1708	89	-	0/12/25/25	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	L2	1708	A1IWA	C02-C17	-12.64	1.31	1.53
92	L2	1708	A1IWA	C17-C05	8.02	1.69	1.53
92	L2	1708	A1IWA	C05-N04	-7.49	1.33	1.47
92	L2	1708	A1IWA	C03-C02	5.89	1.61	1.53
92	L2	1708	A1IWA	C03-N04	3.36	1.58	1.47
92	L2	1708	A1IWA	O18-C19	2.47	1.40	1.35
92	L2	1708	A1IWA	C06-C07	2.45	1.57	1.51
92	L2	1708	A1IWA	C20-C19	2.33	1.57	1.49
92	L2	1708	A1IWA	C16-C07	2.05	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	L2	1708	A1IWA	O18-C19-C20	4.77	119.60	111.09
92	L2	1708	A1IWA	C07-C06-C05	-2.42	109.30	113.40

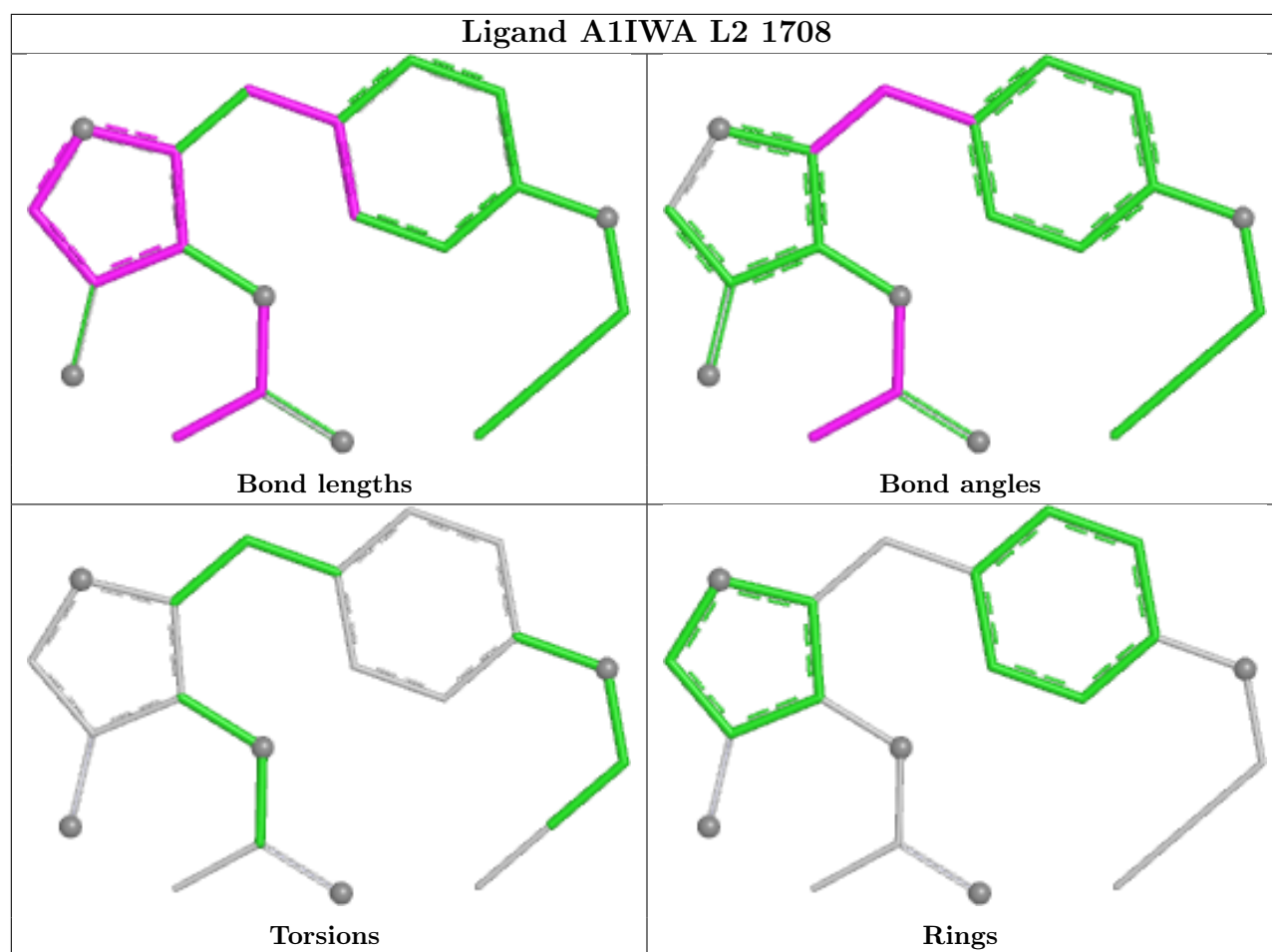
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

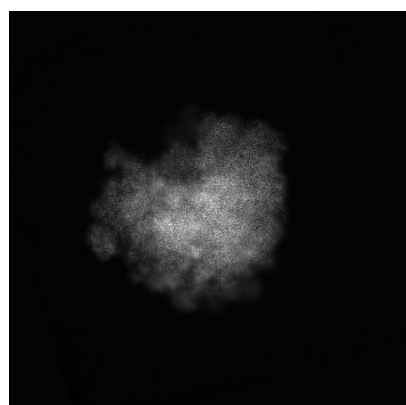
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52247. These allow visual inspection of the internal detail of the map and identification of artifacts.

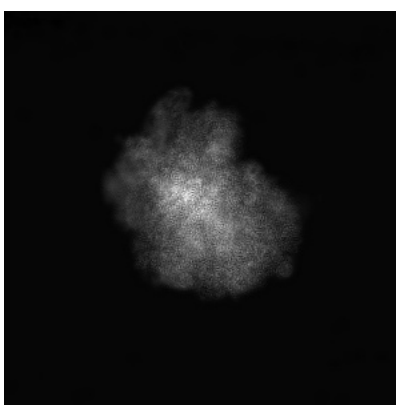
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

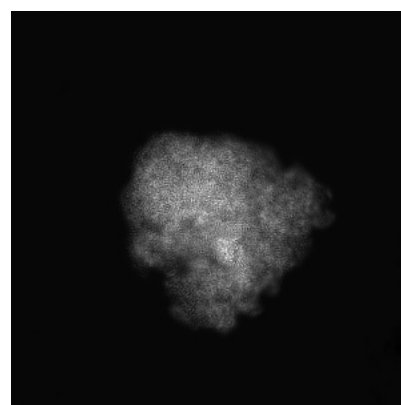
#### 6.1.1 Primary map



X



Y

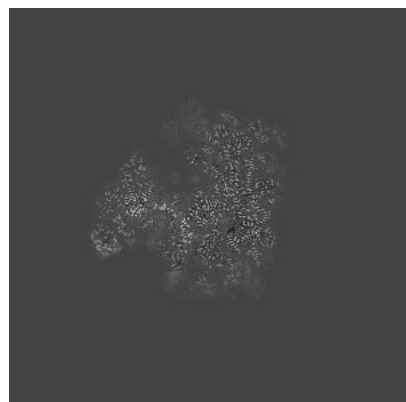


Z

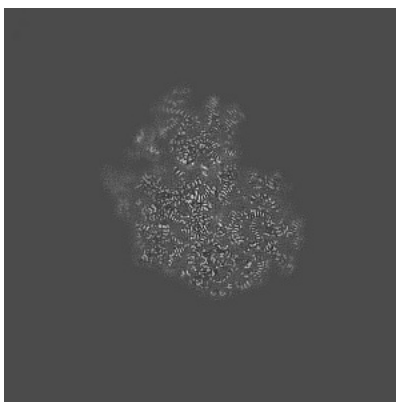
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

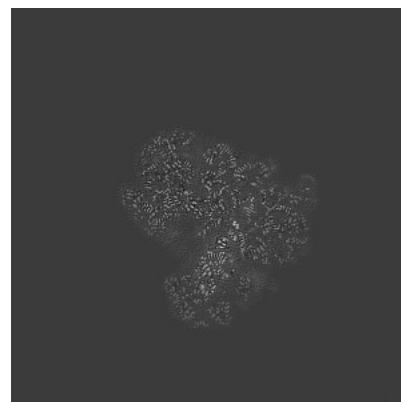
#### 6.2.1 Primary map



X Index: 320



Y Index: 320

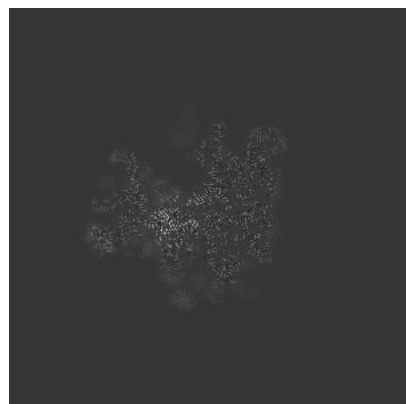


Z Index: 320

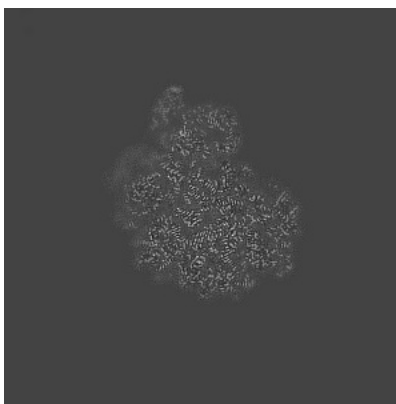
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

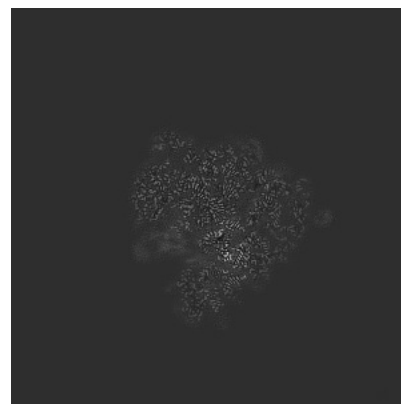
### 6.3.1 Primary map



X Index: 345



Y Index: 345

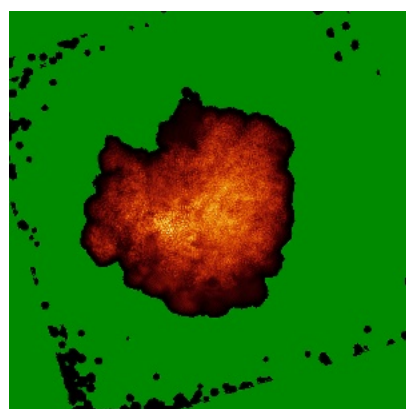


Z Index: 299

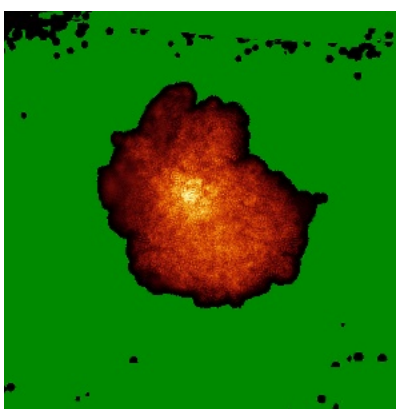
The images above show the largest variance slices of the map in three orthogonal directions.

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

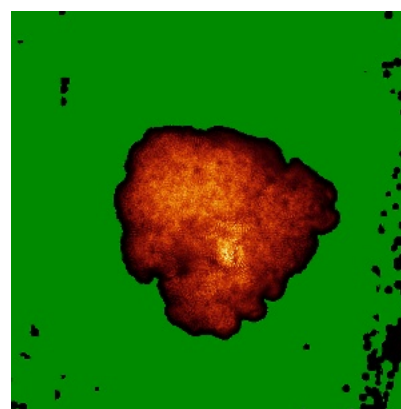
### 6.4.1 Primary map



X



Y

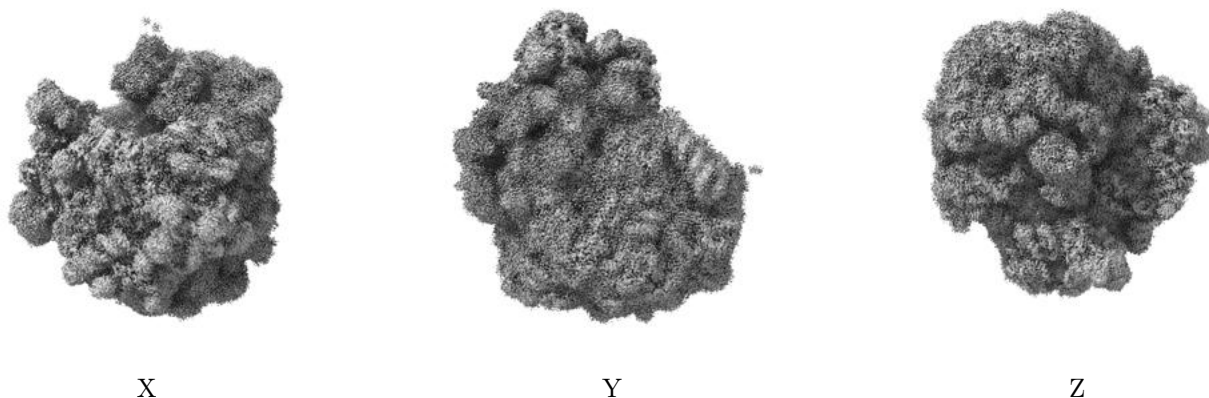


Z

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.

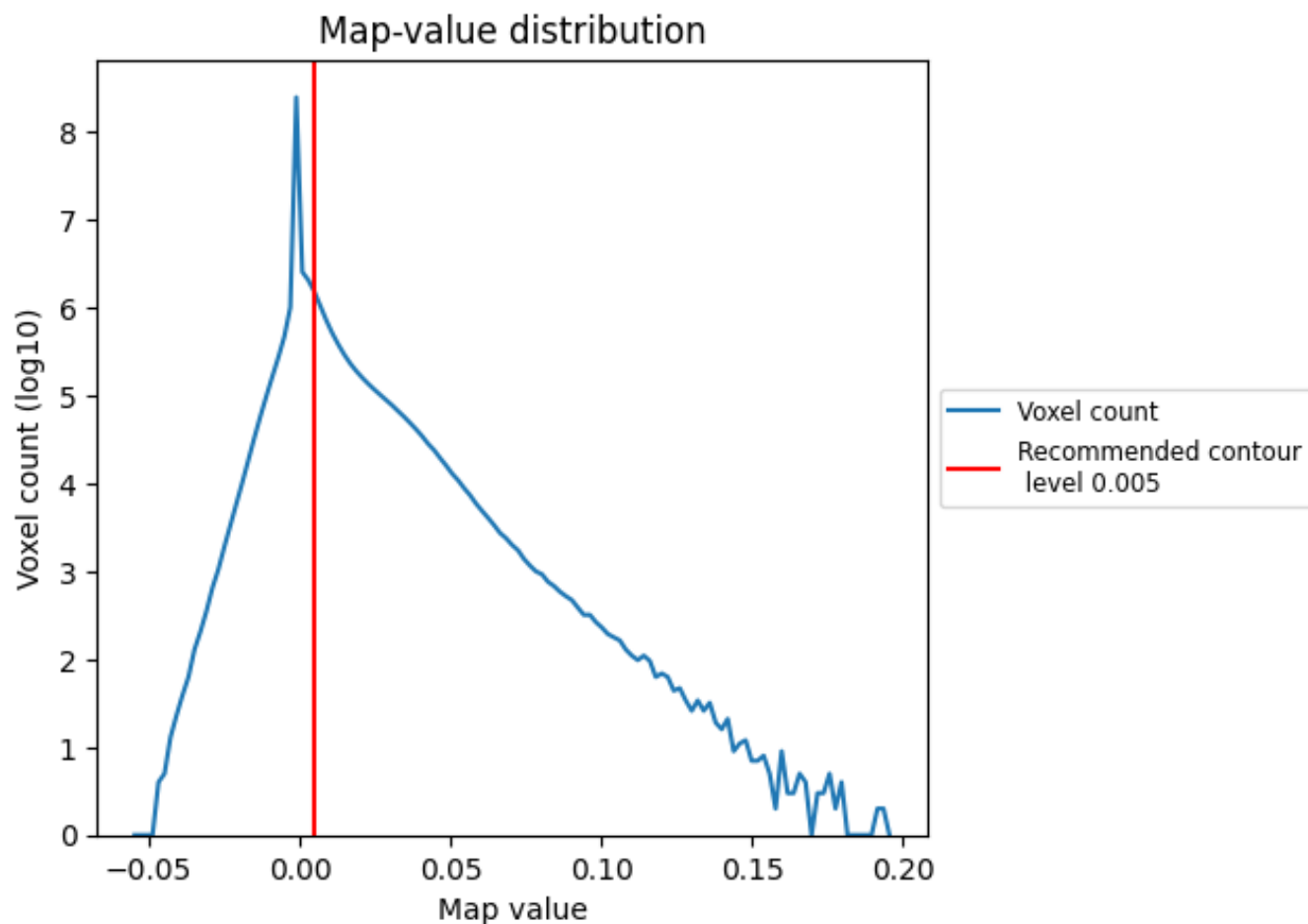
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

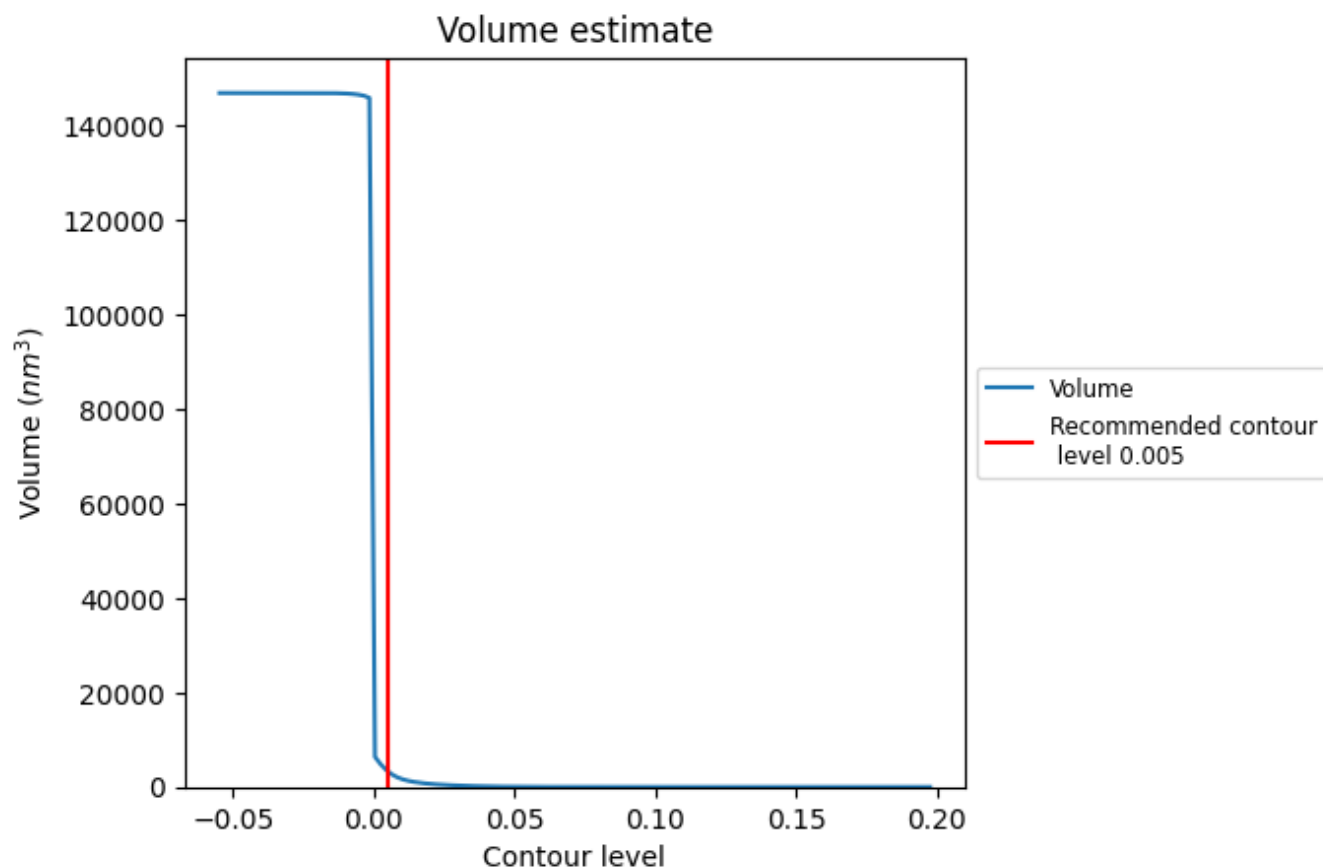
This section contains the results of statistical analysis of the map.

### 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.

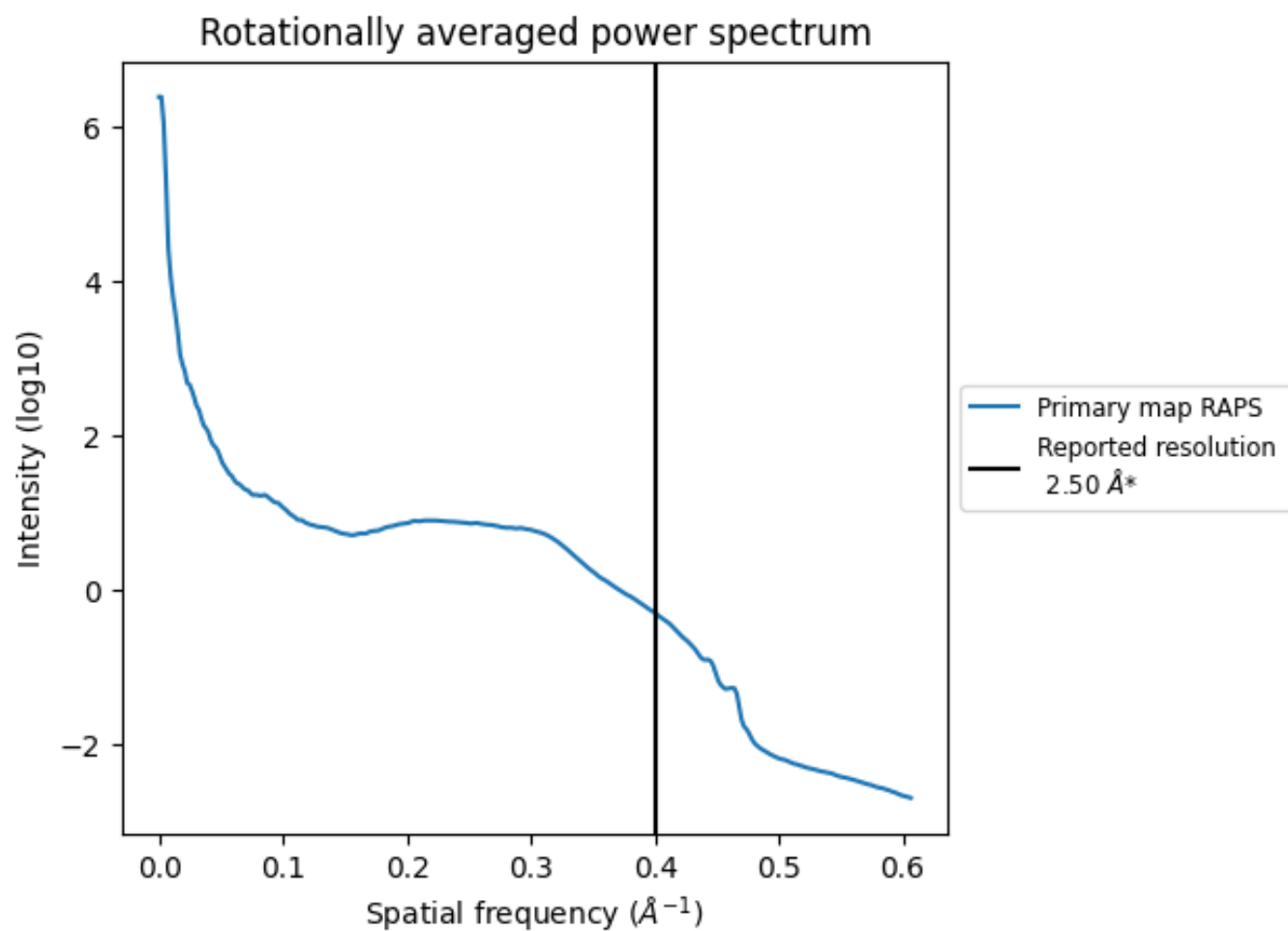
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $3337 \text{ nm}^3$ ; this corresponds to an approximate mass of 3014 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 0.400 Å<sup>-1</sup>

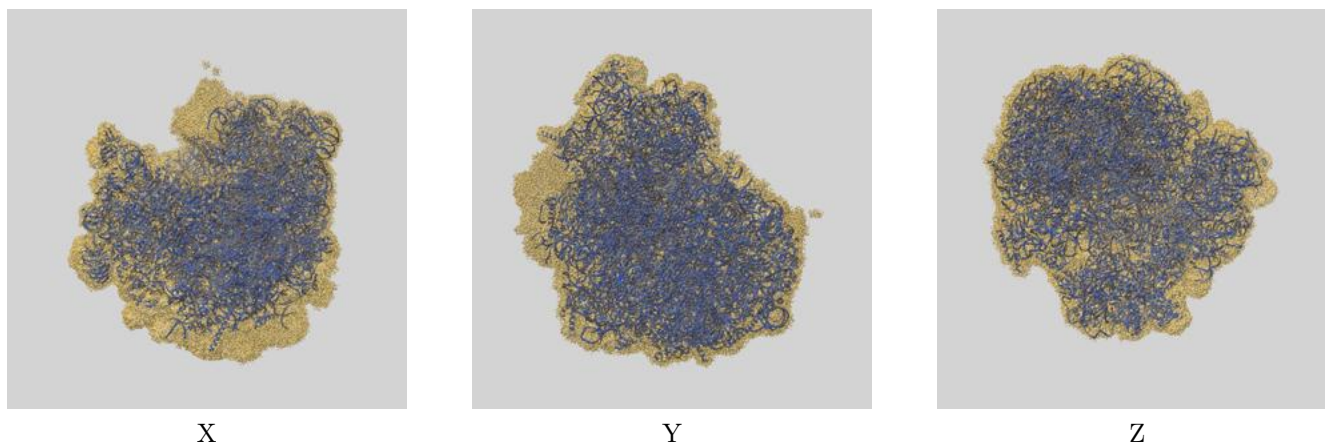
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

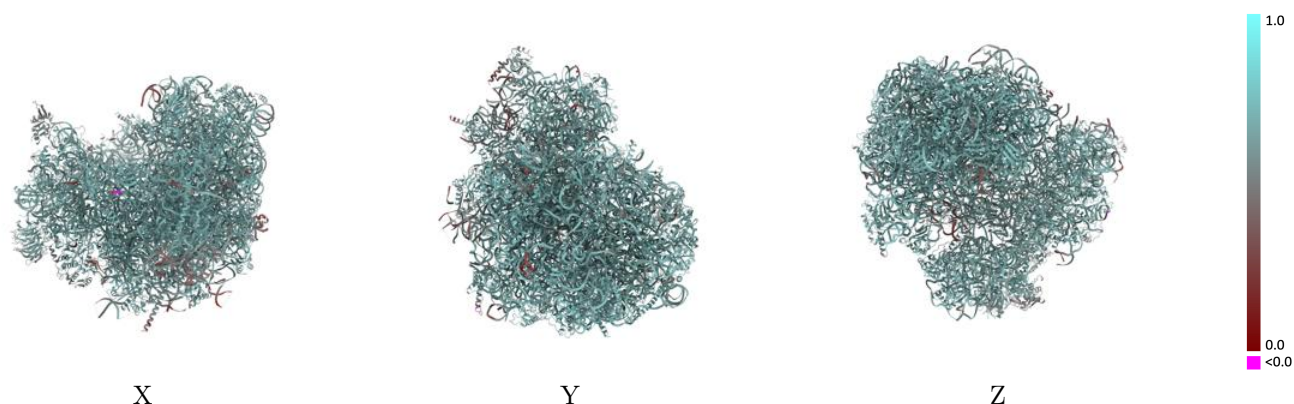
This section contains information regarding the fit between EMDB map EMD-52247 and PDB model 9HL9. Per-residue inclusion information can be found in section [3](#) on page [26](#).

### 9.1 Map-model overlay [i](#)



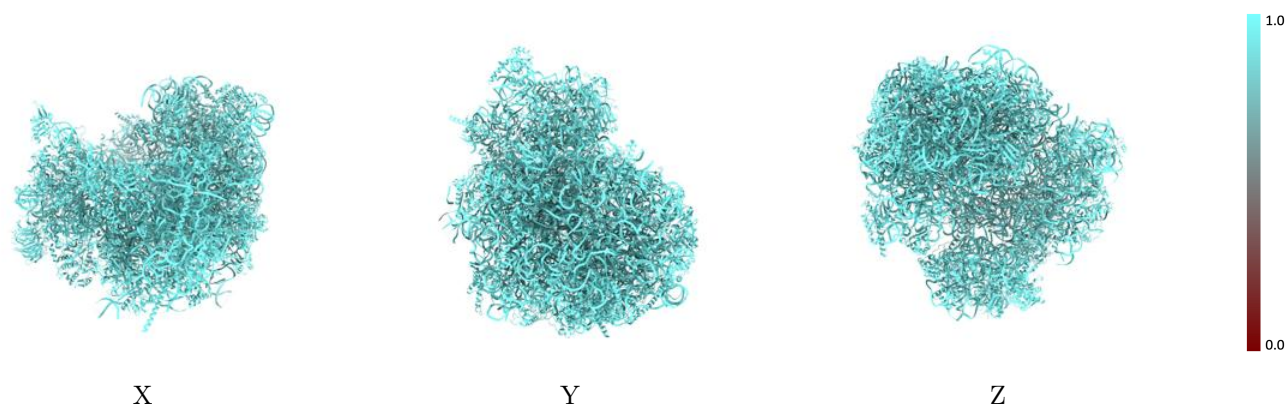
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



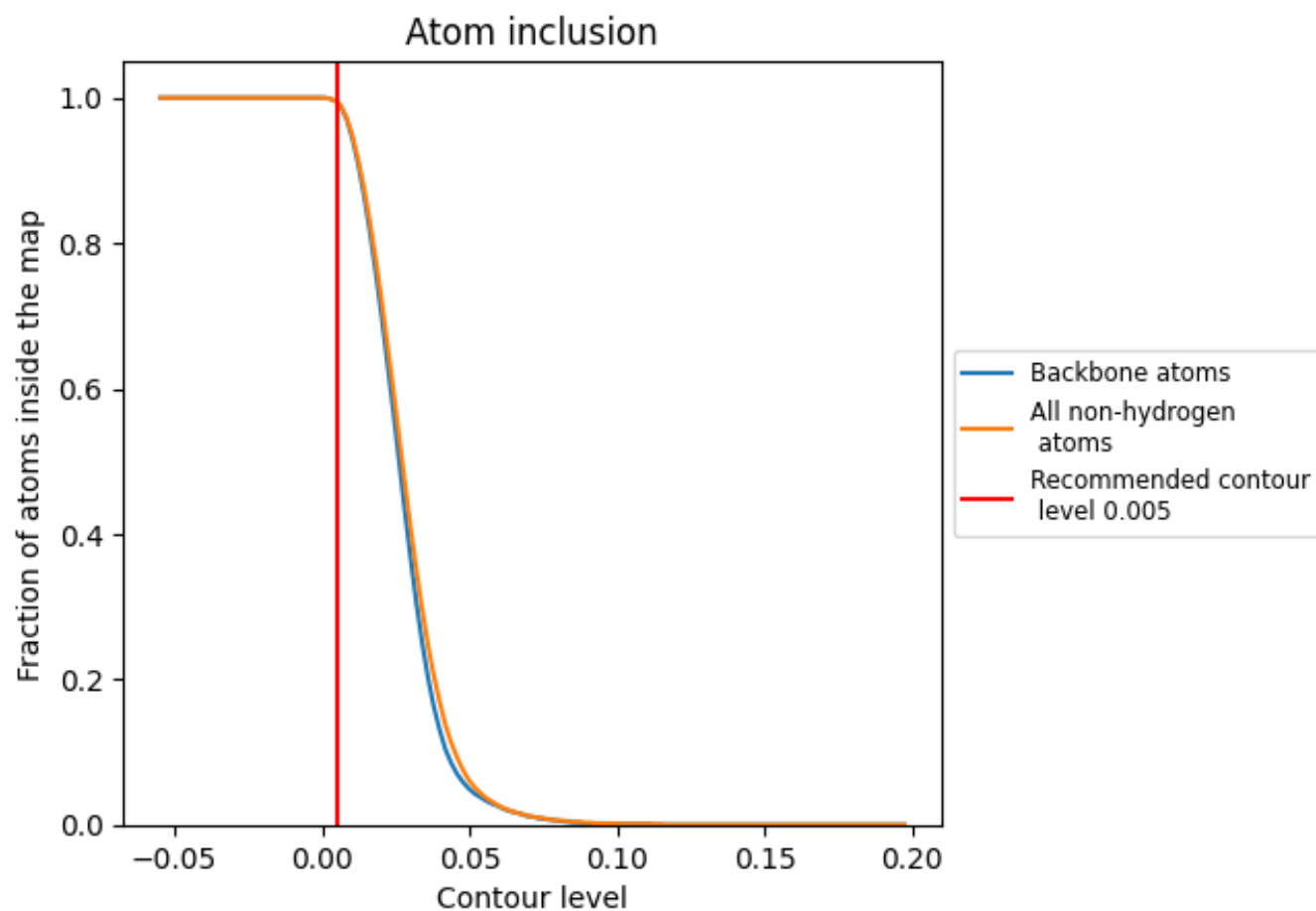
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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	 0.9950	 0.6530
L1	 0.9960	 0.6550
L2	 0.9970	 0.6570
L3	 0.9910	 0.6350
L4	 0.9990	 0.6730
L5	 0.9960	 0.6540
L6	 0.9910	 0.6350
L7	 0.9890	 0.6480
L8	 0.9990	 0.6680
LA	 1.0000	 0.7040
LB	 0.9940	 0.6960
LC	 0.9990	 0.6860
LD	 0.9940	 0.6310
LE	 0.9940	 0.6750
LF	 0.9930	 0.6560
LG	 0.9870	 0.6580
LH	 0.9970	 0.6960
LI	 0.9900	 0.6680
LJ	 0.9970	 0.6950
LK	 0.9950	 0.6650
LL	 0.9970	 0.6970
LM	 0.9990	 0.7050
LN	 0.9970	 0.6800
LO	 0.9880	 0.6470
LP	 0.9990	 0.6900
LQ	 0.9960	 0.6530
LR	 0.9970	 0.6920
LS	 0.9950	 0.6750
LT	 0.9980	 0.7050
LU	 0.9850	 0.5680
LV	 0.9970	 0.6880
LW	 0.9970	 0.6750
LX	 0.9970	 0.6700
LY	 1.0000	 0.6660
LZ	 0.9990	 0.6750



























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Chain	Atom inclusion	Q-score
La	 0.9960	 0.6660
Lb	 0.9980	 0.6890
Lc	 0.9980	 0.6940
Ld	 0.9970	 0.6780
Le	 0.9910	 0.6540
Lf	 0.9990	 0.6850
Lg	 1.0000	 0.6910
Lh	 0.9980	 0.6760
Li	 0.9950	 0.6580
Lj	 0.9980	 0.7070
Lk	 0.9930	 0.6500
Ll	 0.9980	 0.6970
Lm	 0.9980	 0.6770
Ln	 0.9960	 0.6750
Lo	 0.9940	 0.6990
Lp	 0.9990	 0.6850
S1	 0.9960	 0.6430
S3	 0.9930	 0.4950
S4	 0.9870	 0.3730
S5	 1.0000	 0.5600
SA	 0.9940	 0.6650
SB	 0.9960	 0.6220
SC	 0.9930	 0.6480
SD	 0.9920	 0.6490
SE	 0.9940	 0.6620
SF	 0.9900	 0.6660
SG	 0.9950	 0.6420
SH	 0.9940	 0.6670
SI	 0.9930	 0.6410
SJ	 0.9960	 0.6860
SK	 0.9910	 0.6590
SL	 0.9980	 0.6880
SM	 0.9880	 0.6530
SN	 0.9860	 0.6400
SO	 0.9920	 0.6750
SP	 0.9980	 0.6820
SQ	 0.9950	 0.5050
SR	 0.9970	 0.6540
SS	 1.0000	 0.6840
ST	 0.9960	 0.6820
SU	 0.9940	 0.6790
SV	 0.9840	 0.5930

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Chain	Atom inclusion	Q-score
SW	 0.9860	 0.6420
SX	 0.9950	 0.6740
SY	 0.9860	 0.6290
SZ	 0.9920	 0.6410
Sa	 0.9790	 0.6360
Sb	 1.0000	 0.6780
Sc	 0.9920	 0.6130
Sd	 0.9960	 0.6400
Se	 0.9830	 0.5910
Sf	 0.9860	 0.5350
Sg	 1.0000	 0.6050
Sh	 0.9920	 0.5030