



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:37 PM UTC

PDB ID : 8RXH / pdb_00008rxh
EMDB ID : EMD-19576
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME
WITH A/P/E-site tRNA AND mRNA : PARENTAL STRAIN
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2024-02-07
Resolution : 2.93 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

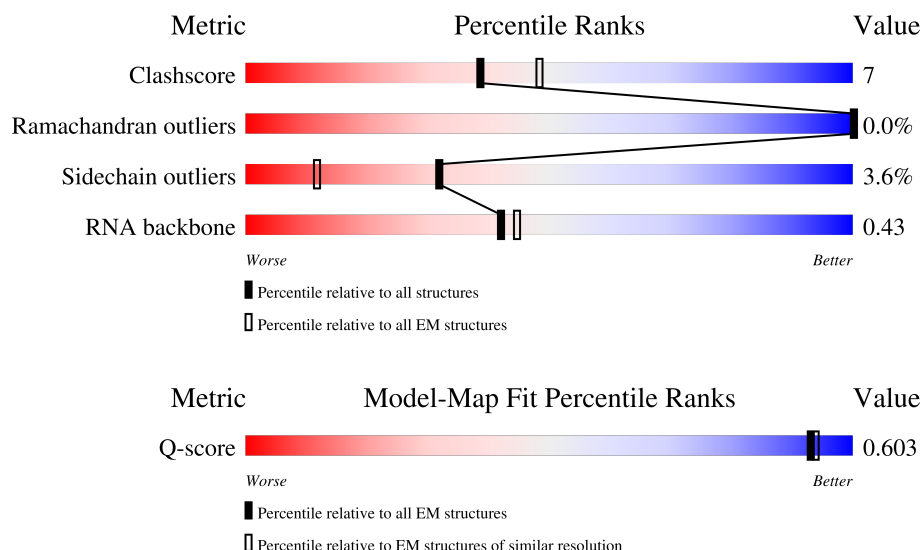
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.93 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.



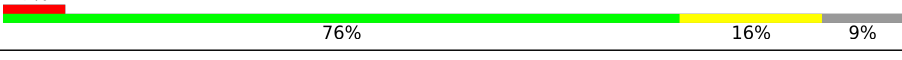
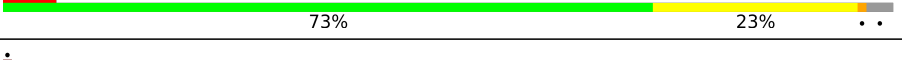
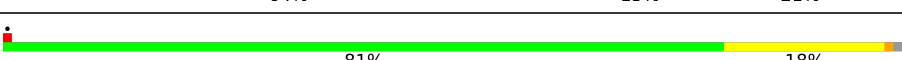
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13037 (2.43 - 3.43)

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

Mol	Chain	Length	Quality of chain
1	L1	1782	
2	L2	1526	
3	L3	216	

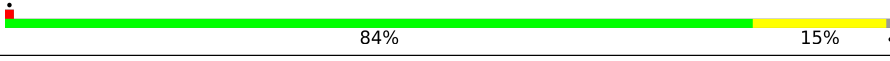
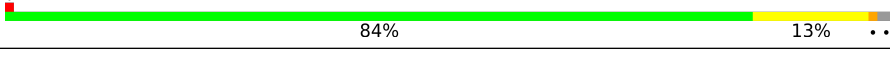
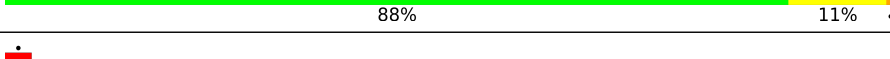
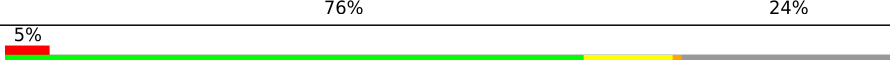
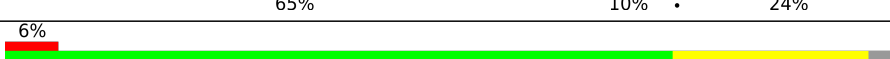
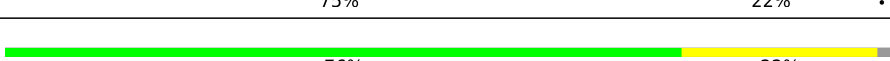
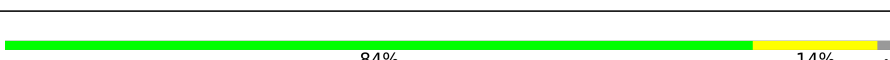
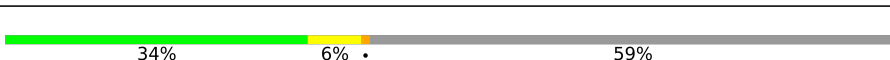
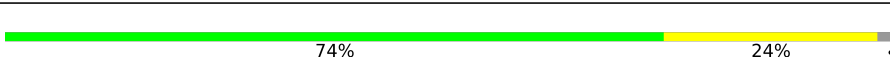
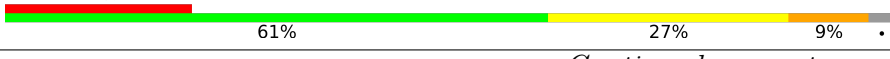
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Mol	Chain	Length	Quality of chain
4	L4	184	
5	L5	135	
6	L6	73	
7	L7	171	
8	L8	124	
9	LA	260	
10	LB	419	
11	LC	373	
12	LD	188	
13	LE	190	
14	LF	195	
15	LG	264	
16	LH	222	
17	LI	220	
18	LJ	139	
19	LK	175	
20	LL	145	
21	LM	204	
22	LN	213	
23	LO	305	
24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

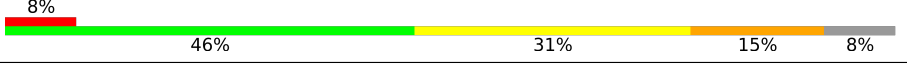
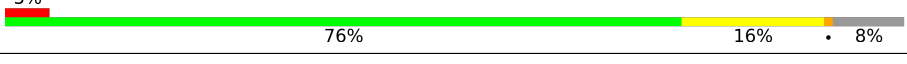
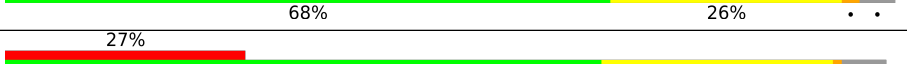
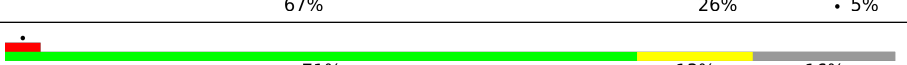
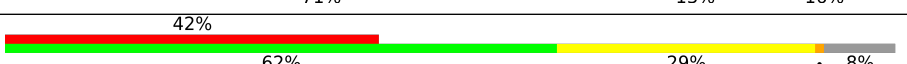
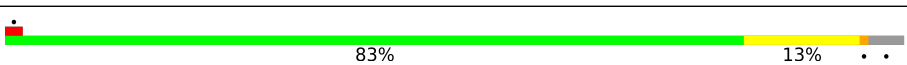
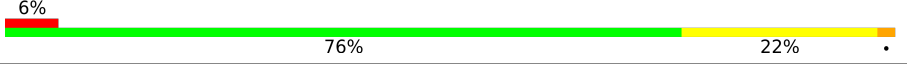
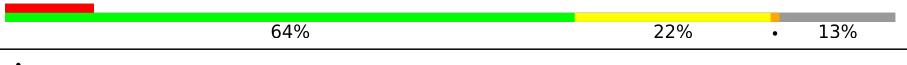
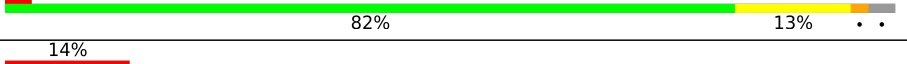
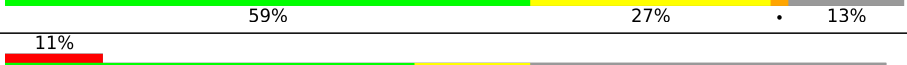
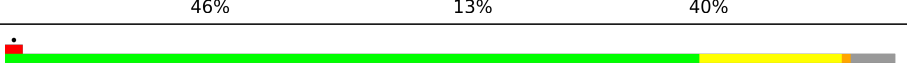
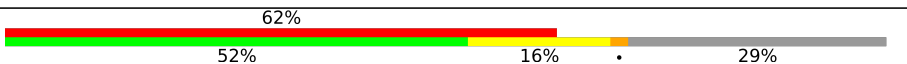
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Mol	Chain	Length	Quality of chain
29	LU	129	
30	LV	145	
31	LW	143	
32	LX	124	
33	LY	134	
34	LZ	147	
35	La	127	
36	Lb	70	
37	Lc	252	
38	Ld	104	
39	Le	188	
40	Lf	133	
41	Lg	144	
42	Lh	168	
43	Li	105	
44	Lj	83	
45	Lk	83	
46	Ll	51	
47	Lm	128	
48	Ln	34	
49	Lo	92	
50	Lp	106	
51	S1	2204	
52	S2	76	
53	S3	77	

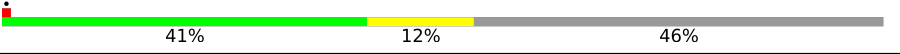
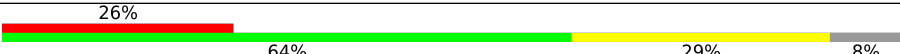
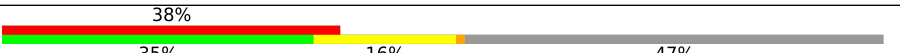
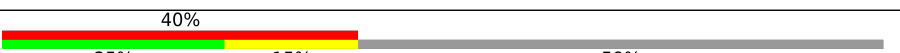
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Mol	Chain	Length	Quality of chain
54	S4	76	
55	S5	13	
56	SA	264	
57	SB	246	
58	SC	219	
59	SD	190	
60	SE	273	
61	SF	265	
62	SG	249	
63	SH	190	
64	SI	200	
65	SJ	130	
66	SK	220	
67	SL	149	
68	SM	116	
69	SN	168	
70	SO	144	
71	SP	143	
72	SQ	141	
73	SR	153	
74	SS	57	
75	ST	151	
76	SU	173	
77	SV	143	
78	SW	152	

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Mol	Chain	Length	Quality of chain
79	SX	161	
80	SY	164	
81	SZ	137	
82	Sa	120	
83	Sb	112	
84	Sc	86	
85	Sd	87	
86	Se	66	
87	Sf	152	
88	Sg	312	
89	Sh	235	

2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 216694 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_chain_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1677	Total	C	N	O	P	1	0
			35987	16086	6578	11645	1678		

- Molecule 2 is a RNA chain called LSUb_rRNA_chain_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	1155	Total	C	N	O	P	0	0
			24715	11065	4453	8042	1155		

- Molecule 3 is a RNA chain called SR1_chain_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L3	183	Total	C	N	O	P	0	0
			3877	1735	669	1290	183		

- Molecule 4 is a RNA chain called SR2_chain_4.

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_chain_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	120	Total	C	N	O	P	0	0
			2555	1140	455	840	120		

- Molecule 6 is a RNA chain called SR6_chain_6.

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_chain_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	166	Total	C	N	O	P	0	0
			3533	1583	626	1159	165		

- Molecule 8 is a RNA chain called 5S_rRNA_chain_8.

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	149	Total	C	N	O	S	0	0
			1151	731	216	202	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	241	Total	C	N	O	S	0	0
			1905	1199	376	323	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	205	Total	C	N	O	S	0	0
			1665	1050	329	271	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	152	Total	C	N	O	S	0	0
			1217	761	241	205	10		

- 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	125	Total	C	N	O	S	0	0
			1043	650	217	172	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	97	Total	C	N	O	S	0	0
			744	464	136	139	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	102	Total	C	N	O	S	0	0
			807	508	163	133	3		

- 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	78	Total	C	N	O	S	0	0
			608	383	119	103	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
			450	291	95	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
			417	263	85	64	5		

- Molecule 48 is a protein called 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 SSU_rRNA_chain_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S1	1844	Total	C	N	O	P	0	0
			39438	17643	7112	12839	1844		

- Molecule 52 is a RNA chain called A-site_tRNA_chain_S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S2	76	Total	C	N	O	P	0	0
			1626	729	290	531	75		

- Molecule 53 is a RNA chain called P-site_tRNA_chain_S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	75	Total	C	N	O	P	0	0
			1602	714	292	521	75		

- Molecule 54 is a RNA chain called E-site_tRNA_chain_S4.

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

- Molecule 55 is a RNA chain called mRNA_chain_S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S5	12	Total	C	N	O	P	0	0
			251	113	43	83	12		

- Molecule 56 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SA	244	Total	C	N	O	S	0	0
			1943	1213	375	344	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SB	211	Total	C	N	O	S	0	0
			1661	1055	303	292	11		

- Molecule 58 is a protein called Putative 40S ribosomal protein S3.

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

- Molecule 59 is a protein called Putative 40S ribosomal protein S9.

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

- Molecule 60 is a protein called 40S ribosomal protein S4.

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

- Molecule 61 is a protein called 40S ribosomal protein S2.

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

- Molecule 62 is a protein called 40S ribosomal protein S6.

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

- Molecule 63 is a protein called 40S ribosomal protein S5.

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

- Molecule 64 is a protein called 40S ribosomal protein S7.

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

- Molecule 65 is a protein called Putative 40S ribosomal protein S15A.

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

- Molecule 66 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SK	192	Total	C	N	O	S	0	0
			1550	967	320	261	2		

- Molecule 67 is a protein called Putative 40S ribosomal protein S16.

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

- Molecule 68 is a protein called Putative ribosomal protein S20.

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

- Molecule 69 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SN	100	Total	C	N	O	S	0	0
			818	525	143	143	7		

- Molecule 70 is a protein called 40S ribosomal protein S14.

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

- Molecule 71 is a protein called Putative 40S ribosomal protein S23.

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

- Molecule 72 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SQ	100	Total	C	N	O	S	0	0
			670	411	121	133	5		

- Molecule 73 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SR	142	Total	C	N	O	S	0	0
			1138	715	226	192	5		

- Molecule 74 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SS	56	Total	C	N	O	S	0	0
			452	279	94	73	6		

- Molecule 75 is a protein called Putative 40S ribosomal protein S13.

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

- Molecule 76 is a protein called Ribosomal protein S17 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SU	153	Total	C	N	O	S	0	0
			1257	795	251	206	5		

- Molecule 77 is a protein called Putative 40S ribosomal protein S17.

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

- Molecule 78 is a protein called Putative 40S ribosomal protein S15.

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

- Molecule 79 is a protein called 40S ribosomal protein S19-like protein.

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

- Molecule 80 is a protein called Putative 40S ribosomal protein S21.

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

- Molecule 81 is a protein called 40S ribosomal protein S24.

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

- Molecule 82 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sa	105	Total	C	N	O	S	0	0
			798	502	147	145	4		

- Molecule 83 is a protein called 40S ribosomal protein S26.

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

- Molecule 84 is a protein called Putative 40S ribosomal protein S27-1.

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

- Molecule 85 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sd	66	Total	C	N	O	S	0	0
			496	301	100	91	4		

- Molecule 86 is a protein called 40S ribosomal protein S30.

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

- Molecule 87 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Sf	80	Total	C	N	O	S	0	0
			659	413	130	110	6		

- Molecule 88 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Sg	303	Total	C	N	O	S	0	0
			2354	1475	420	446	13		

- Molecule 89 is a protein called Putative RNA binding protein.

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

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	L1	116	Total 116	Mg 116	0
90	L2	74	Total 74	Mg 74	0
90	L3	4	Total 4	Mg 4	0
90	L4	4	Total 4	Mg 4	0
90	L5	1	Total 1	Mg 1	0
90	L6	1	Total 1	Mg 1	0
90	L7	9	Total 9	Mg 9	0
90	L8	5	Total 5	Mg 5	0
90	LA	1	Total 1	Mg 1	0
90	LB	1	Total 1	Mg 1	0
90	LJ	1	Total 1	Mg 1	0
90	LS	1	Total 1	Mg 1	0
90	LT	1	Total 1	Mg 1	0
90	Lf	1	Total 1	Mg 1	0
90	Lh	1	Total 1	Mg 1	0
90	Lj	1	Total 1	Mg 1	0
90	S1	64	Total 64	Mg 64	0
90	S5	2	Total 2	Mg 2	0
90	SX	1	Total 1	Mg 1	0

- Molecule 91 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
91	L1	29	Total 29	Na 29	0

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Mol	Chain	Residues	Atoms		AltConf
91	L2	21	Total 21	Na 21	0
91	L4	4	Total 4	Na 4	0
91	L5	3	Total 3	Na 3	0
91	L8	1	Total 1	Na 1	0
91	LA	2	Total 2	Na 2	0
91	LE	1	Total 1	Na 1	0
91	LH	1	Total 1	Na 1	0
91	LM	2	Total 2	Na 2	0
91	LN	2	Total 2	Na 2	0
91	LR	1	Total 1	Na 1	0
91	Lf	1	Total 1	Na 1	0
91	S1	16	Total 16	Na 16	0
91	SH	1	Total 1	Na 1	0
91	SP	1	Total 1	Na 1	0

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

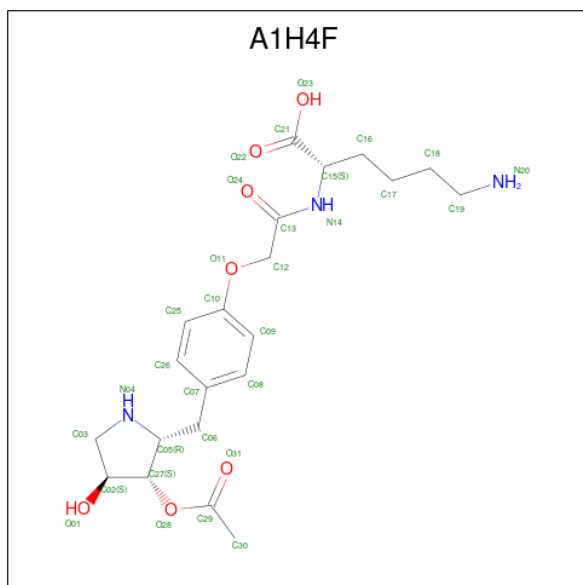
Mol	Chain	Residues	Atoms		AltConf
92	L1	55	Total 55	K 55	0
92	L2	33	Total 33	K 33	0
92	L3	2	Total 2	K 2	0
92	L4	6	Total 6	K 6	0
92	L5	2	Total 2	K 2	0

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Mol	Chain	Residues	Atoms		AltConf
92	L7	5	Total	K	0
			5	5	
92	L8	1	Total	K	0
			1	1	
92	LB	2	Total	K	0
			2	2	
92	LC	2	Total	K	0
			2	2	
92	LZ	1	Total	K	0
			1	1	
92	Lh	1	Total	K	0
			1	1	
92	S1	30	Total	K	0
			30	30	
92	SS	1	Total	K	0
			1	1	
92	ST	1	Total	K	0
			1	1	
92	Sb	1	Total	K	0
			1	1	

- Molecule 93 is (2S)-2-[2-[4-[(2R,3S,4S)-3-acetyloxy-4-oxidanyl-pyrrolidin-2-yl]methyl]phenoxy]ethanoylamino]-6-azanyl-hexanoic acid (CCD ID: A1H4F) (formula: C₂₁H₃₁N₃O₇).



Mol	Chain	Residues	Atoms				AltConf
93	L2	1	Total	C	N	O	0
			31	21	3	7	

- Molecule 94 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
94	Lp	1	Total 1	Zn 1	0

- Molecule 95 is water.

Mol	Chain	Residues	Atoms		AltConf
95	L1	152	Total 152	O 152	0
95	L2	119	Total 119	O 119	0
95	L3	10	Total 10	O 10	0
95	L4	11	Total 11	O 11	0
95	L5	3	Total 3	O 3	0
95	L7	11	Total 11	O 11	0
95	L8	1	Total 1	O 1	0
95	LA	7	Total 7	O 7	0
95	LB	5	Total 5	O 5	0
95	LC	4	Total 4	O 4	0
95	LG	1	Total 1	O 1	0
95	LH	2	Total 2	O 2	0
95	LI	2	Total 2	O 2	0
95	LL	5	Total 5	O 5	0
95	LM	7	Total 7	O 7	0
95	LP	2	Total 2	O 2	0
95	LQ	2	Total 2	O 2	0
95	LS	2	Total 2	O 2	0

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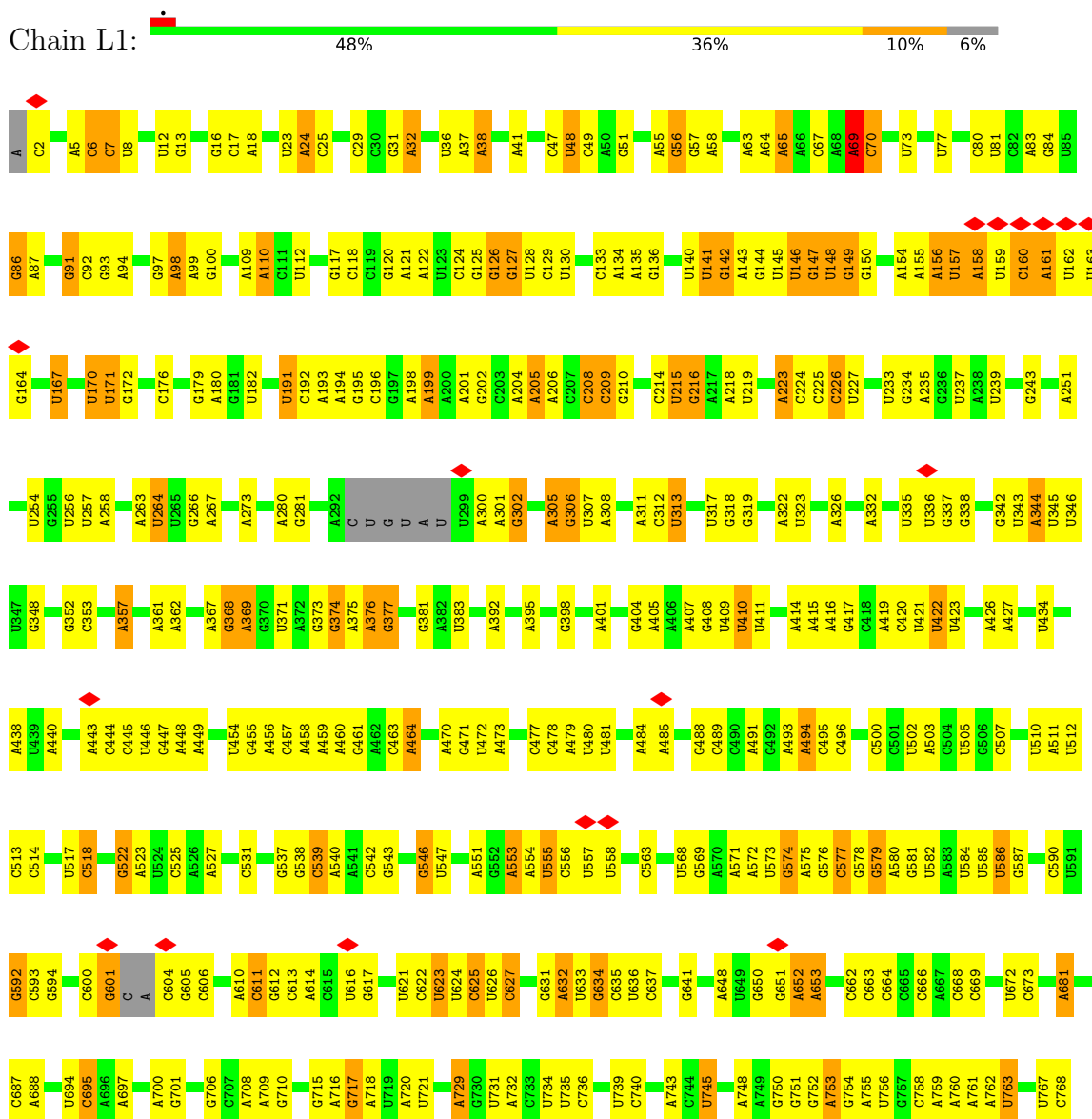
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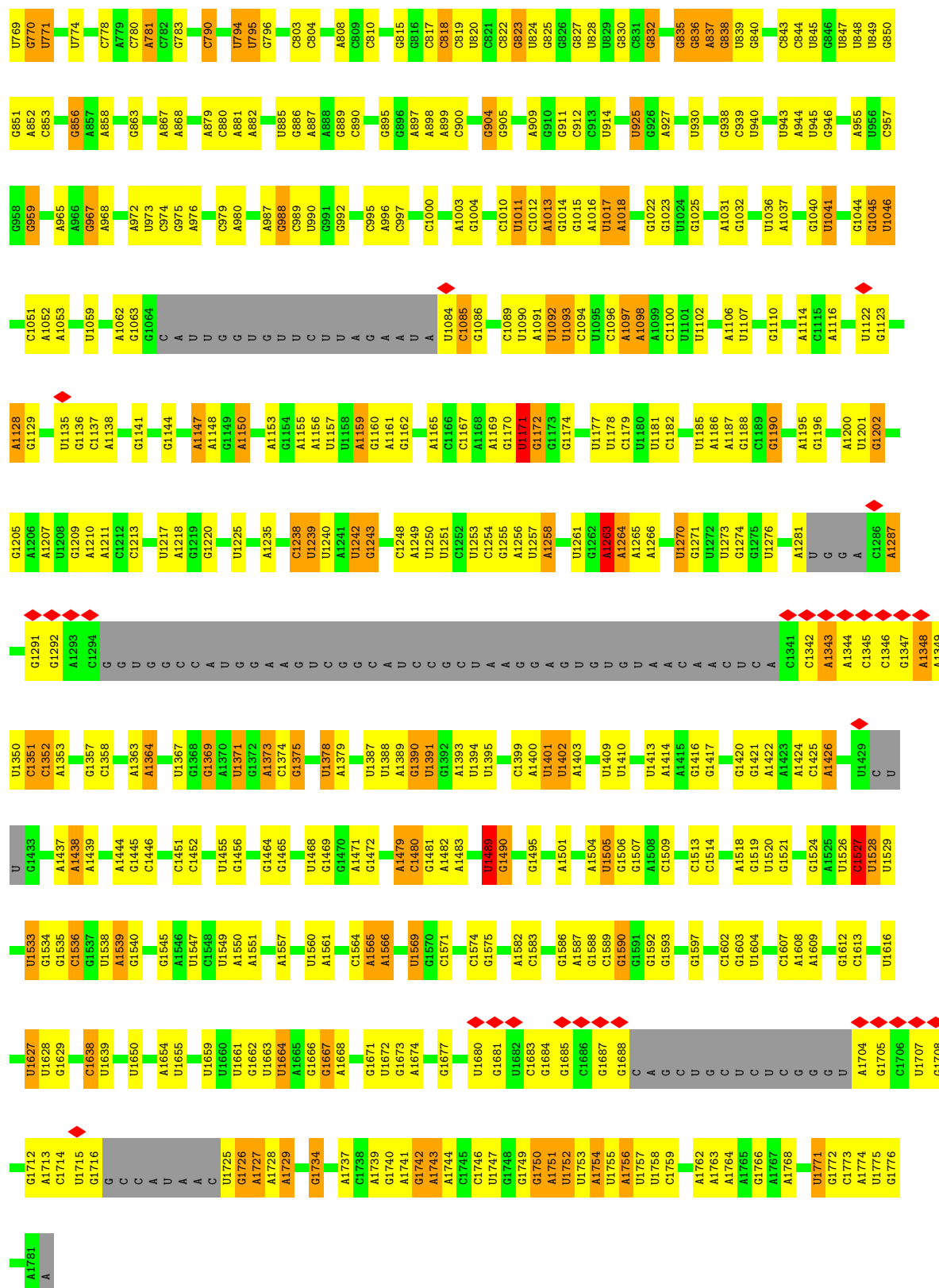
Mol	Chain	Residues	Atoms		AltConf
95	LT	2	Total 2	O 2	0
95	LV	1	Total 1	O 1	0
95	LW	1	Total 1	O 1	0
95	La	2	Total 2	O 2	0
95	Lb	2	Total 2	O 2	0
95	Le	1	Total 1	O 1	0
95	Lf	2	Total 2	O 2	0
95	Lh	1	Total 1	O 1	0
95	Lj	4	Total 4	O 4	0
95	Lo	1	Total 1	O 1	0
95	Lp	2	Total 2	O 2	0
95	S1	47	Total 47	O 47	0
95	SA	1	Total 1	O 1	0

3 Residue-property plots

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

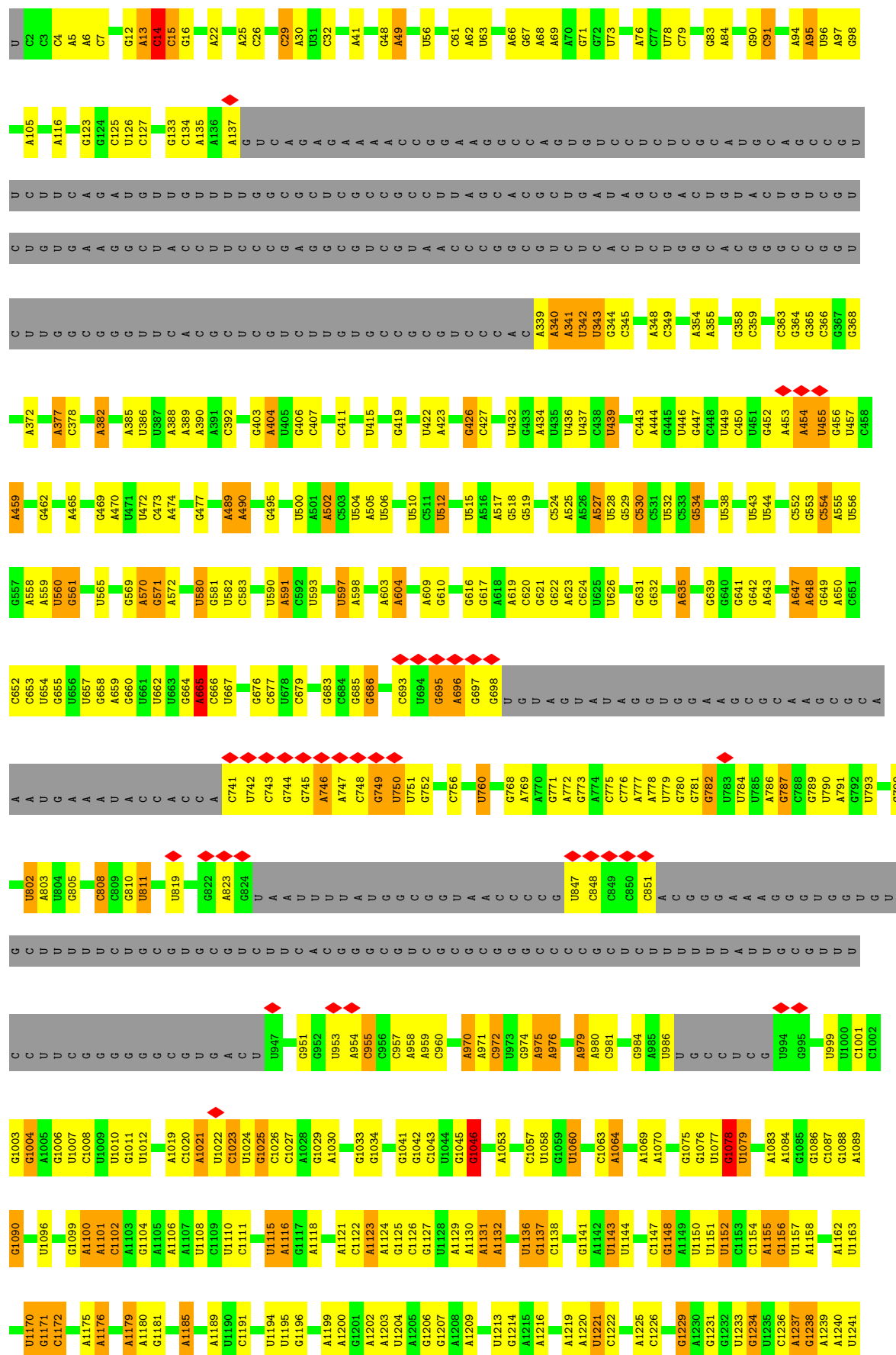
• Molecule 1: LSUa_rRNA_chain_1

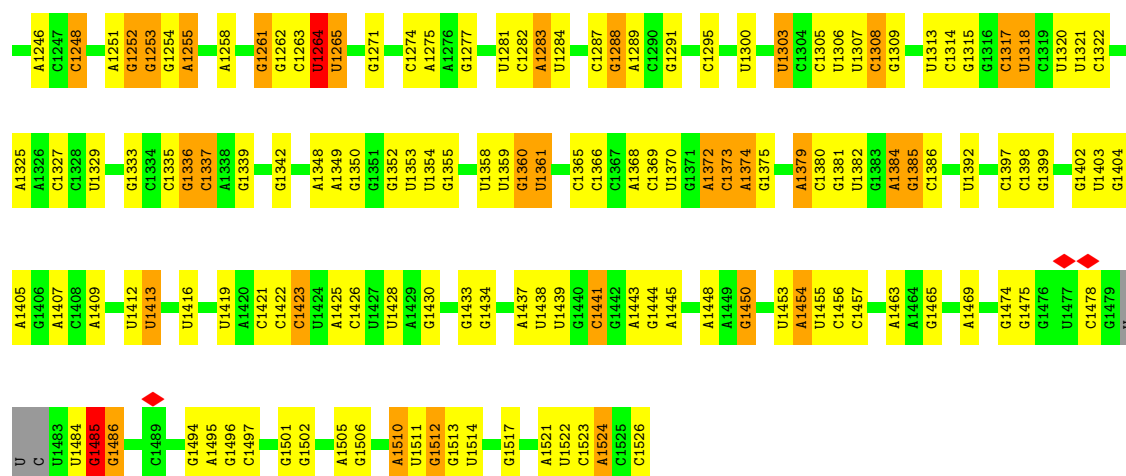




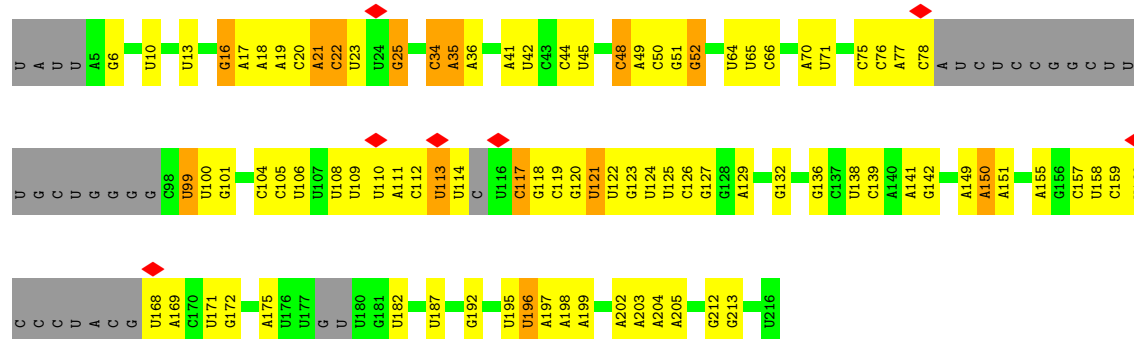
• Molecule 2: LSub_rRNA_chain_2

Chain L2: 40% 28% 8% 24%

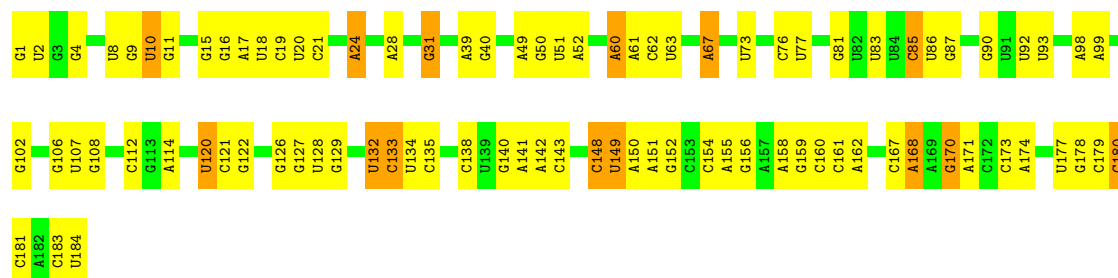




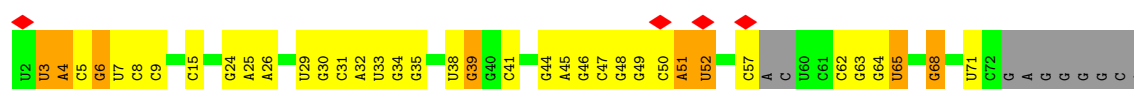
Chain L3: 43% 36% 6% 15%

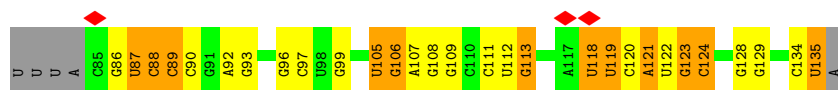


Chain L4: 52% 41% 8%



Chain L5: 5% 40% 34% 15% 11%

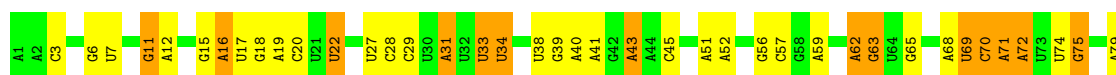




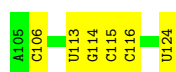
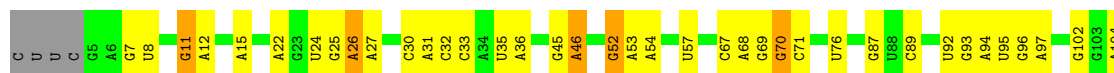
• Molecule 6: SR6_chain_6



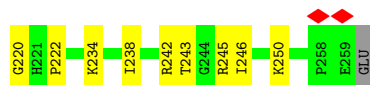
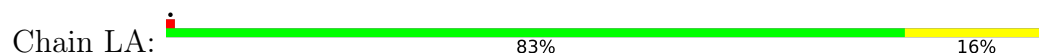
• Molecule 7: 5.8S_rRNA_chain_7



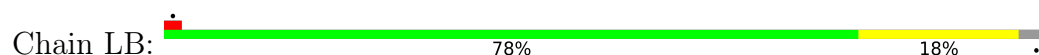
• Molecule 8: 5S_rRNA_chain_8

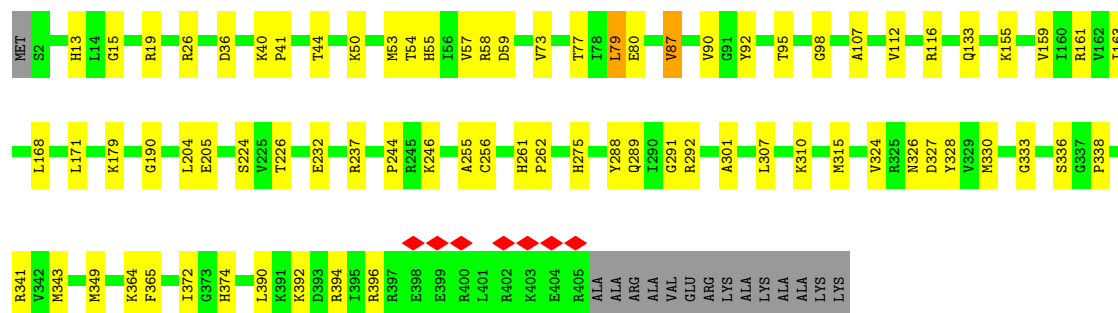


• Molecule 9: Putative 60S ribosomal protein L2



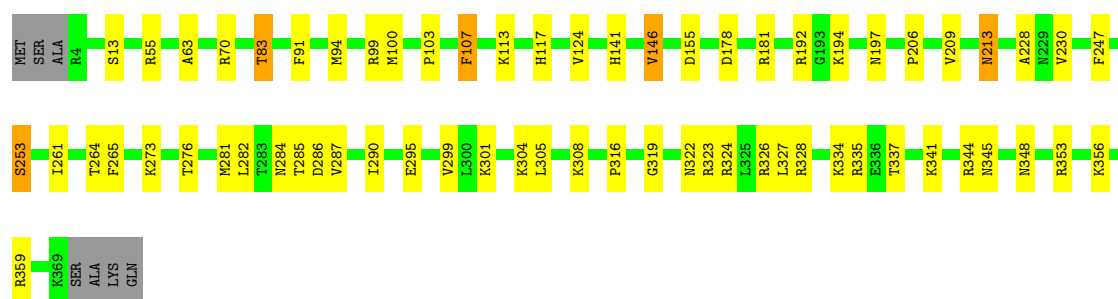
• Molecule 10: Putative ribosomal protein L3





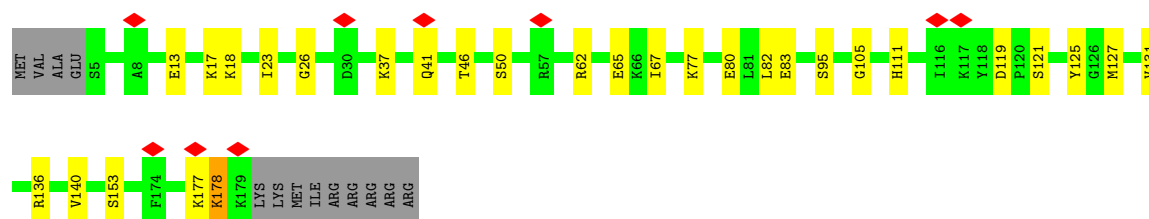
- Molecule 11: Putative ribosomal protein L1a

Chain LC: 81% 16% ..



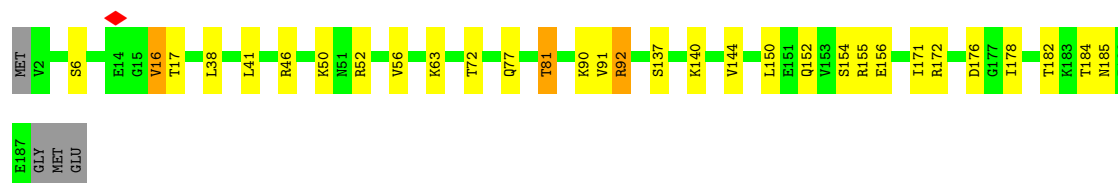
- Molecule 12: 60S ribosomal protein L11

Chain LD: 5% 78% 15% • 7%



- Molecule 13: Putative 60S ribosomal protein L9

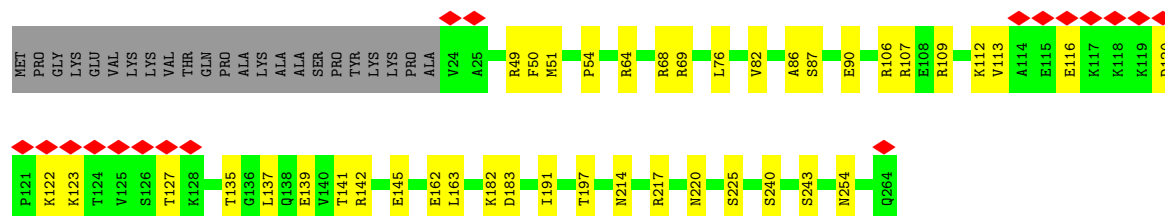
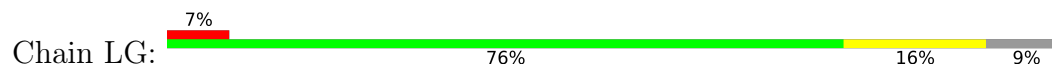
Chain LE: 82% 15% ..



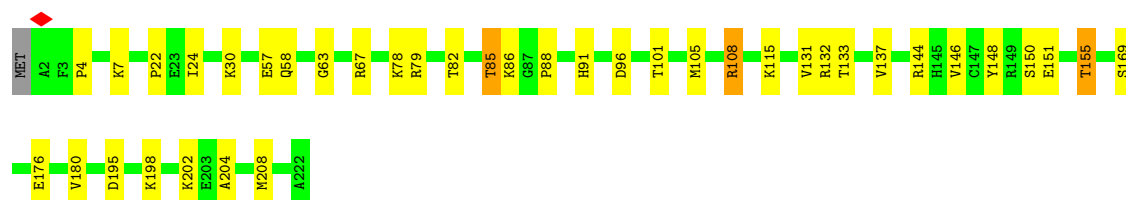
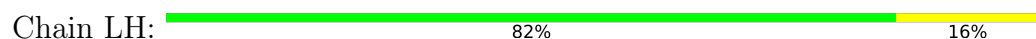
- Molecule 14: Putative 60S ribosomal protein L6

Chain LF: 60% 16% • 24%

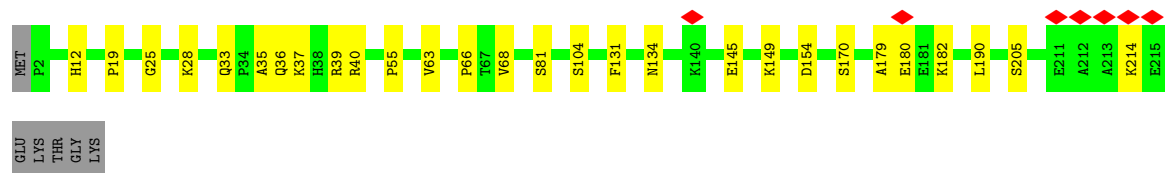
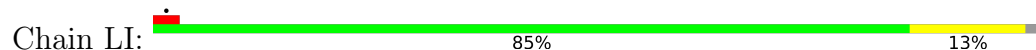
- Molecule 15: 60S ribosomal protein L7a



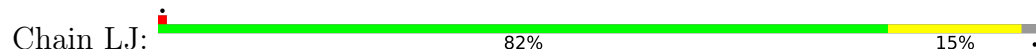
- Molecule 16: Putative 60S ribosomal protein L13a



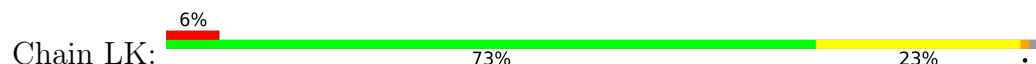
- Molecule 17: Putative 60S ribosomal protein L13

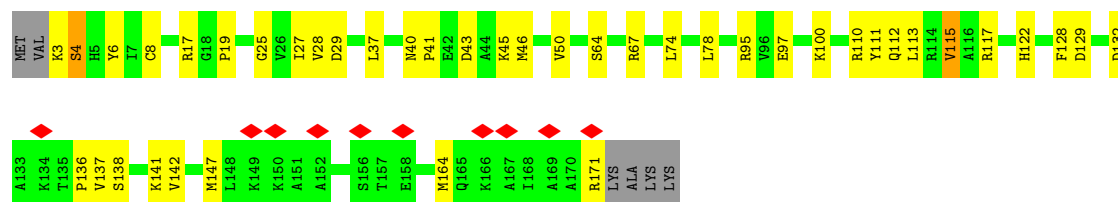


- Molecule 18: Putative 60S ribosomal protein L23

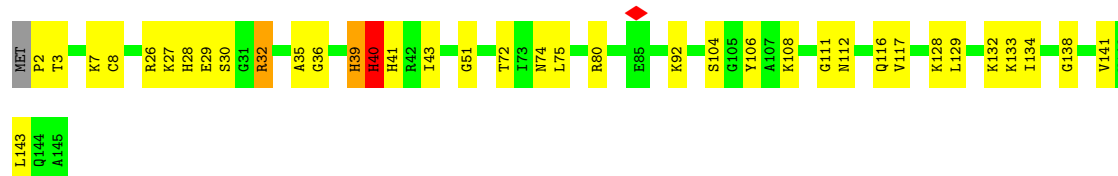
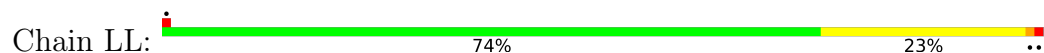


- Molecule 19: Putative 40S ribosomal protein L14

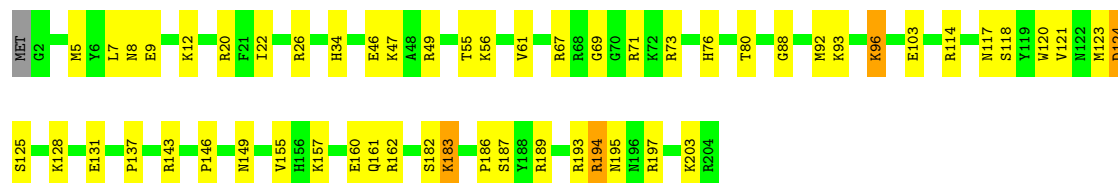




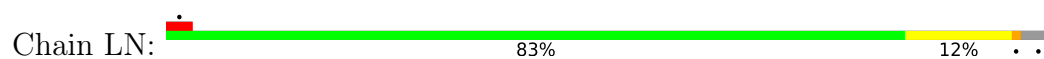
- Molecule 20: Putative 60S ribosomal protein L27A/L29



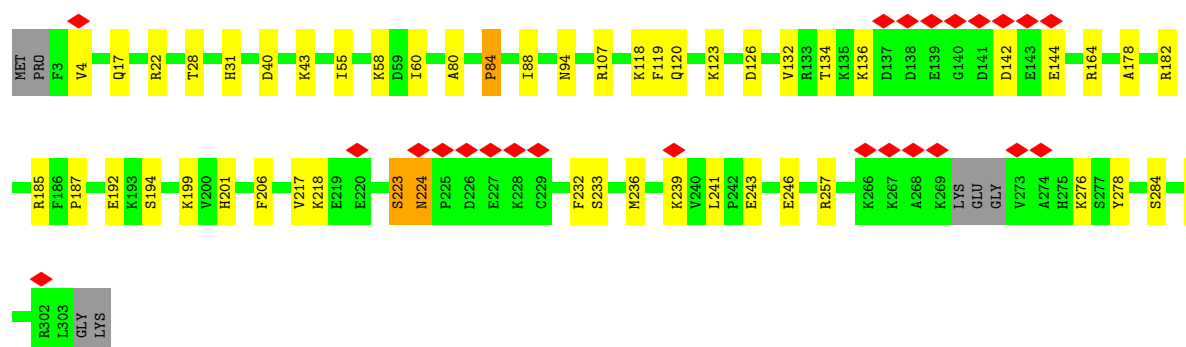
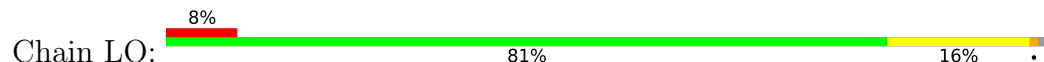
- Molecule 21: Ribosomal protein L15



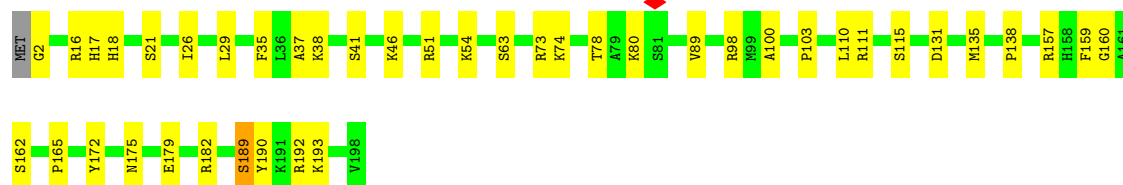
- Molecule 22: Putative 60S ribosomal protein L10

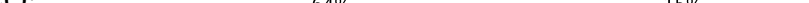


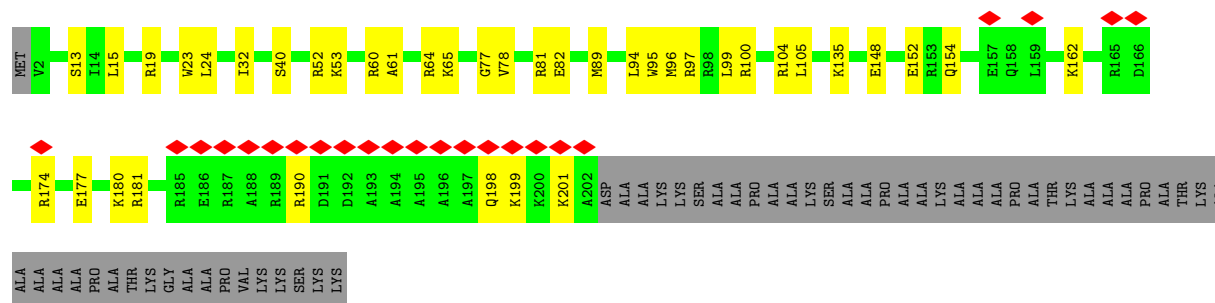
- Molecule 23: Putative 60S ribosomal protein L5



- Molecule 24: 60S ribosomal protein L18

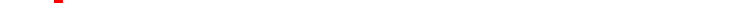


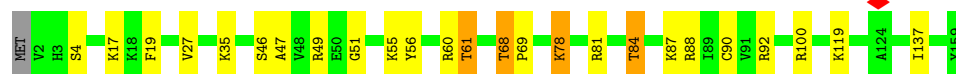
- Chain LQ: 



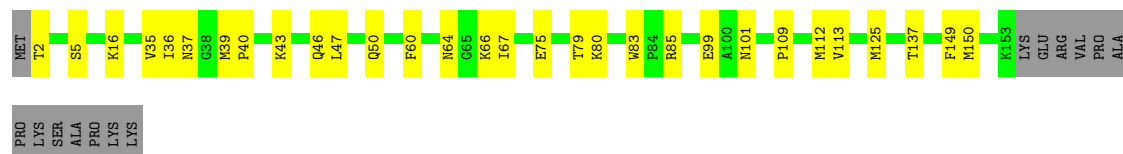
- Chain LR: 81% 18%



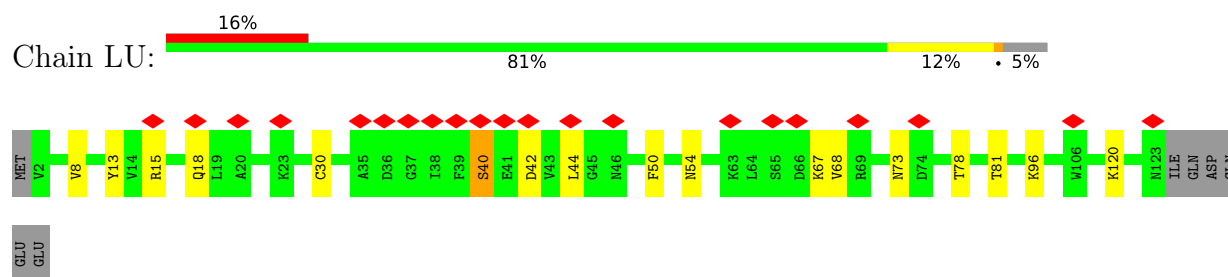
- Chain LS:  84% 13% ..



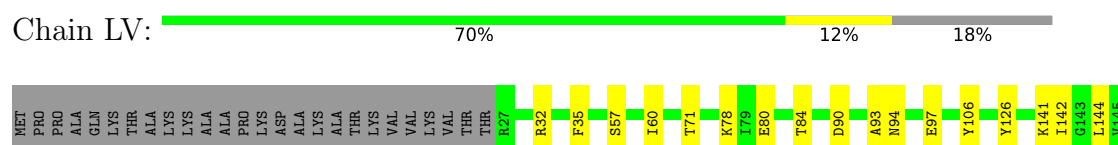
- Chain LT: 73% 18% 8%



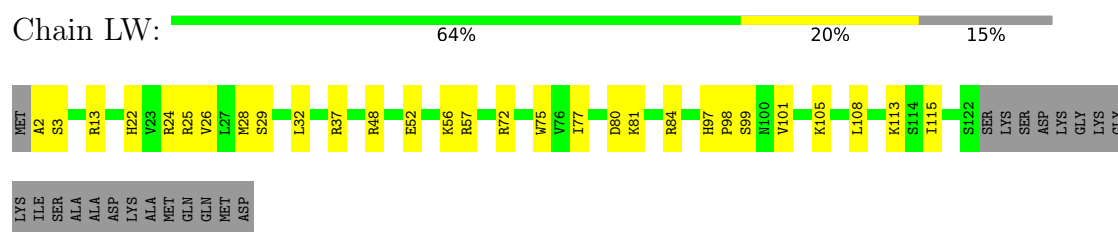
- Molecule 29: Putative 60S ribosomal protein L22



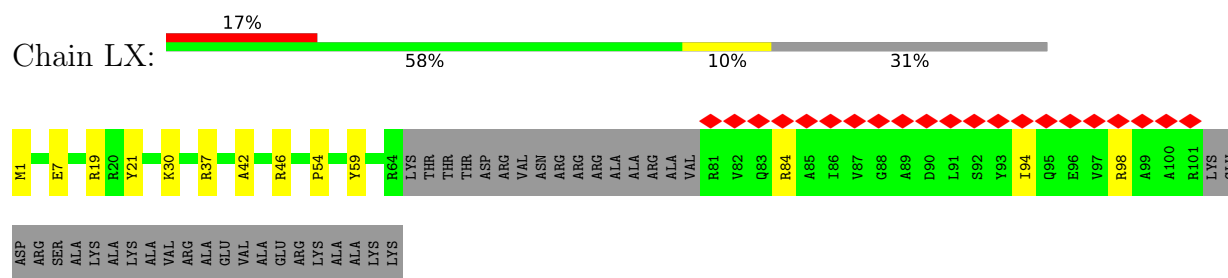
- Molecule 30: Putative 60S ribosomal protein L23a



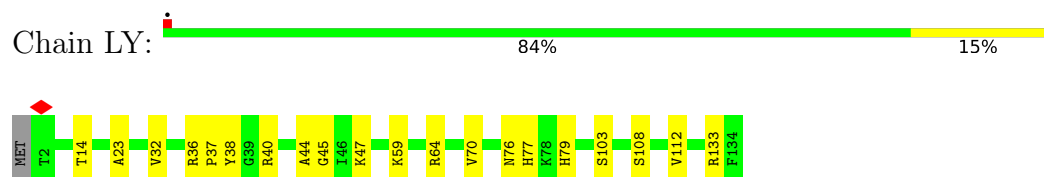
- Molecule 31: Putative 60S ribosomal protein L26



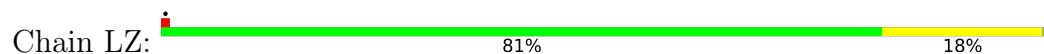
- Molecule 32: Putative ribosomal protein L24



- Molecule 33: 60S ribosomal protein L27

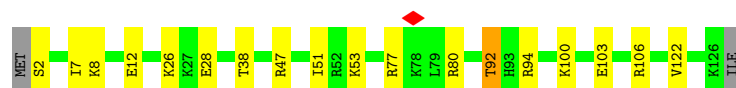
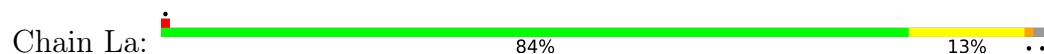


- Molecule 34: Putative 60S ribosomal protein L28





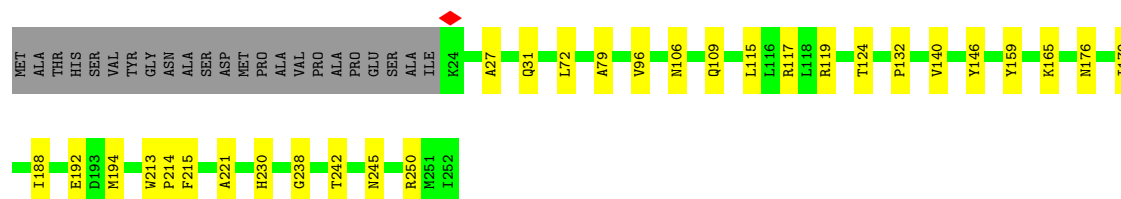
- Molecule 35: Putative 60S ribosomal protein L35



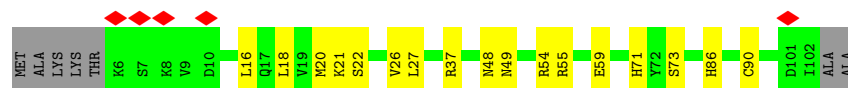
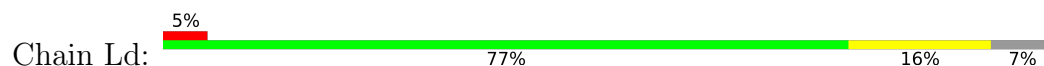
- Molecule 36: 60S ribosomal protein L29



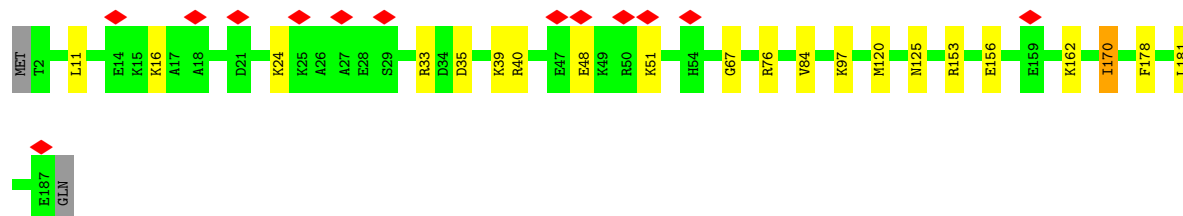
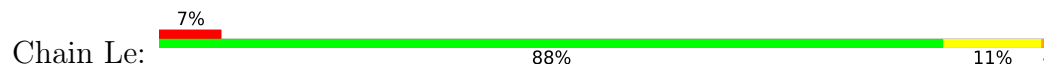
- Molecule 37: Putative 60S ribosomal protein L7



- Molecule 38: 60S ribosomal protein L30

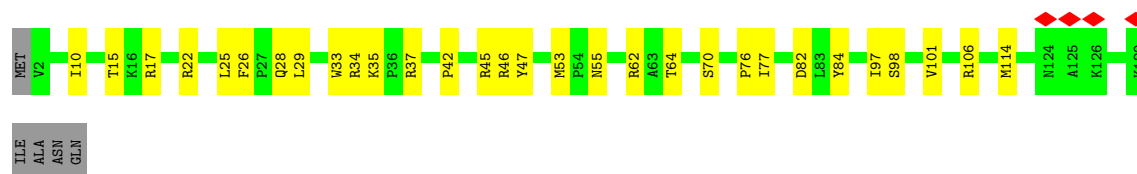


- Molecule 39: Putative 60S ribosomal subunit protein L31



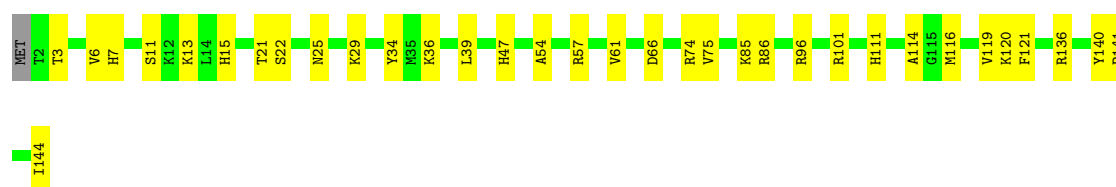
- Molecule 40: 60S ribosomal protein L32

Chain Lf:  74% 23%



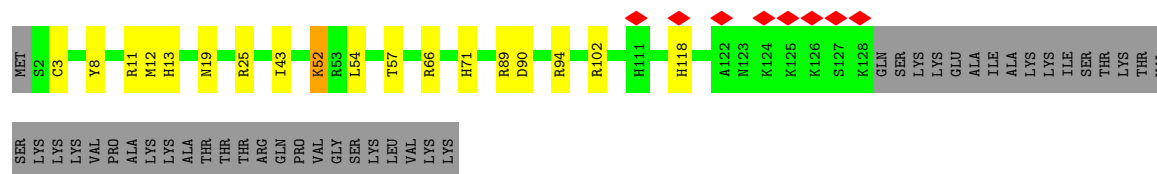
- Molecule 41: Putative ribosomal protein l35a

Chain Lg:  76% 24%



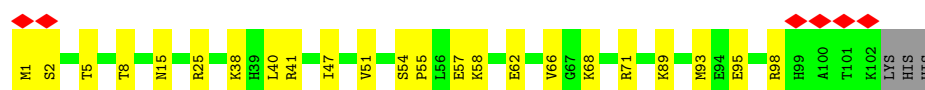
- Molecule 42: Putative 60S ribosomal protein L34

Chain Lh:  5% 65% 10% 24%



- Molecule 43: Putative 60S Ribosomal protein L36

Chain Li:  6% 75% 22%



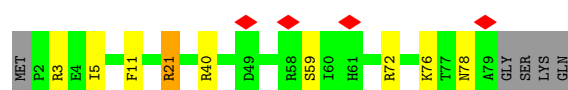
- Molecule 44: Ribosomal protein L37

Chain Lj:  76% 22%



- Molecule 45: Putative ribosomal protein L38

Chain Lk:  5% 83% 10% 6%



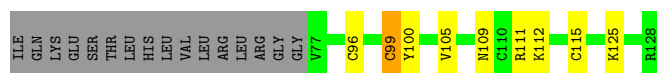
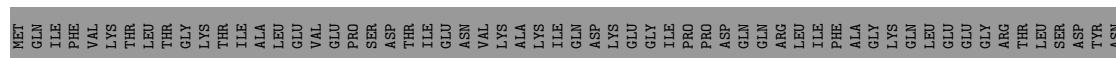
- Molecule 46: Putative 60S ribosomal protein L39

Chain Ll:  84% 14%



- Molecule 47: Ubiquitin-60S ribosomal protein L40

Chain Lm:  34% 6% 59%



- Molecule 48: 60S ribosomal protein L41

Chain Ln:  74% 24%



- Molecule 49: 60S ribosomal protein L37a

Chain Lo:  75% 22%



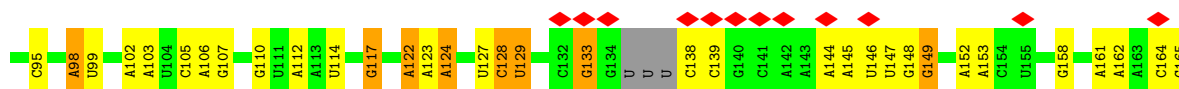
- Molecule 50: Putative 60S ribosomal protein L44

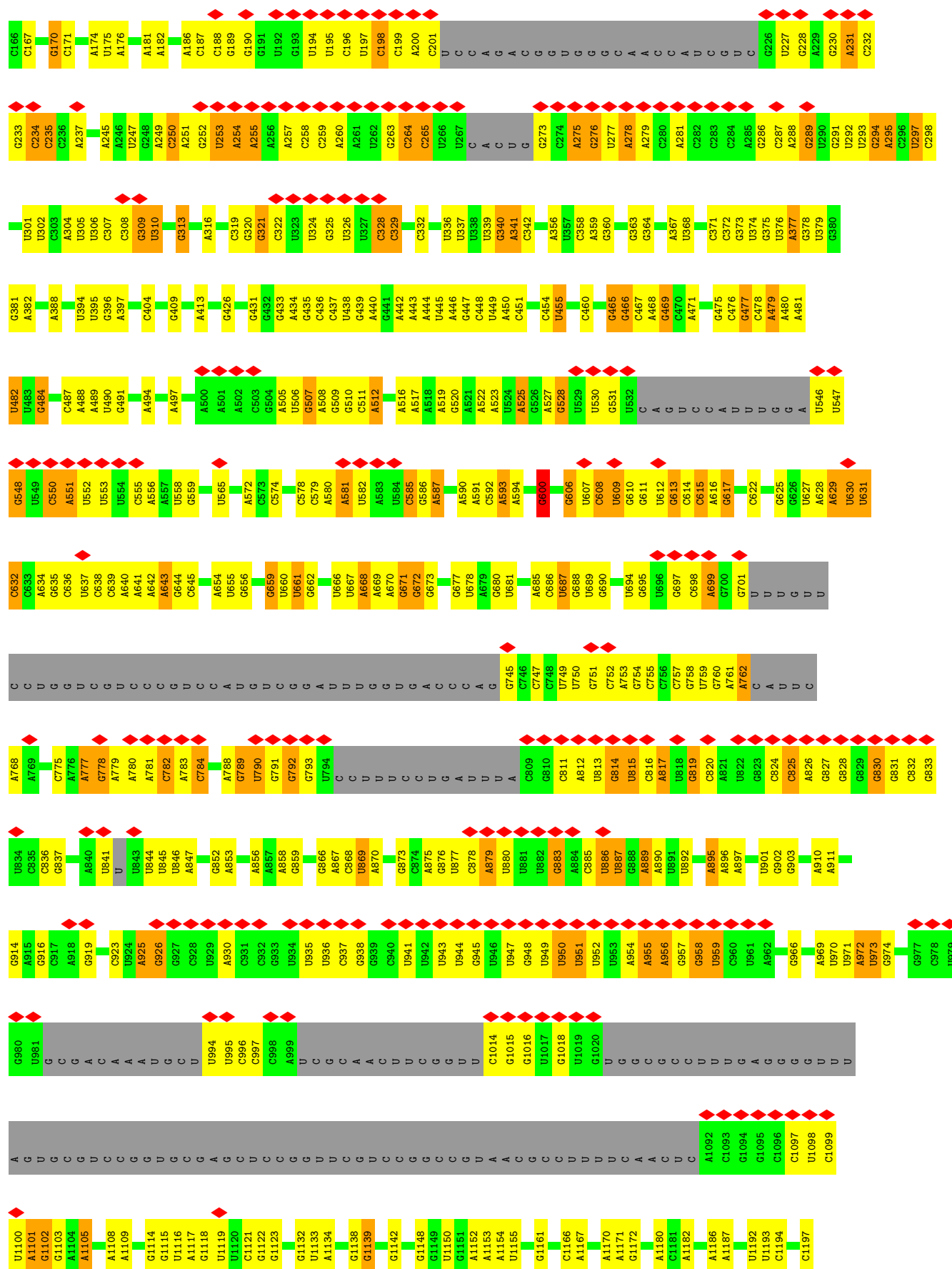
Chain Lp:  83% 8% 8%



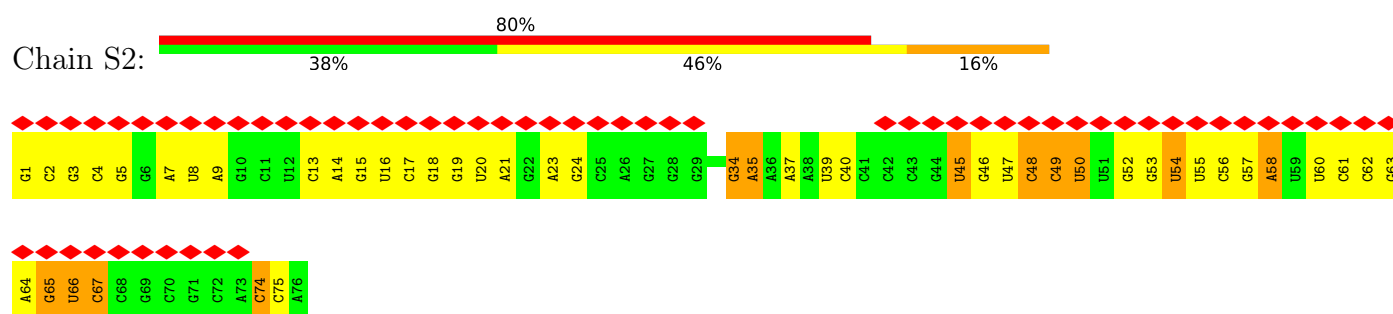
- Molecule 51: SSU_rRNA_chain_S1

Chain S1:  11% 41% 33% 9% 16%

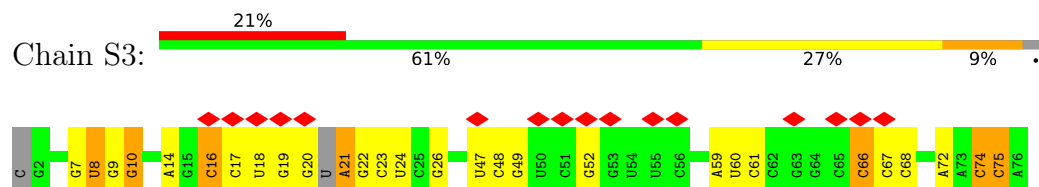




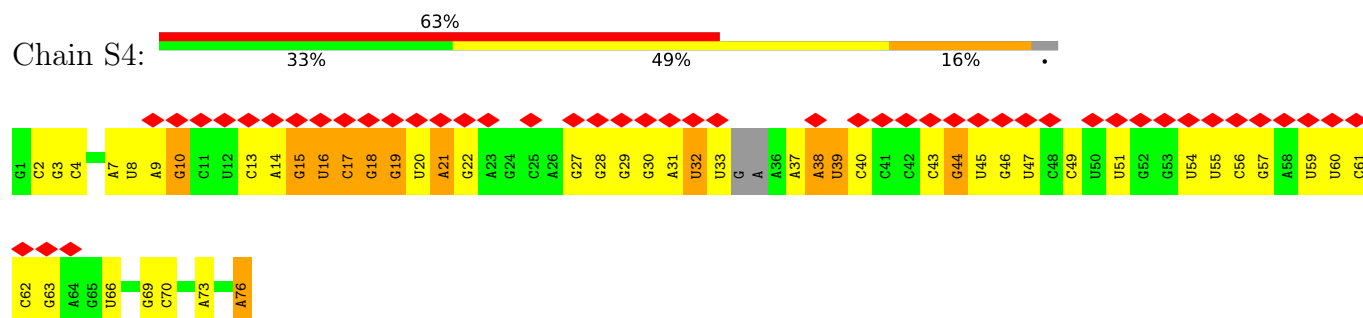
- Molecule 52: A-site tRNA chain S2



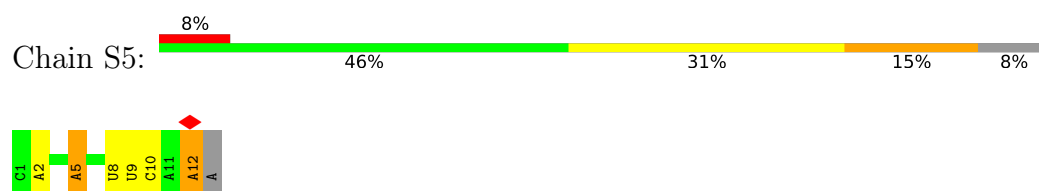
- Molecule 53: P-site_tRNA_chain_S3



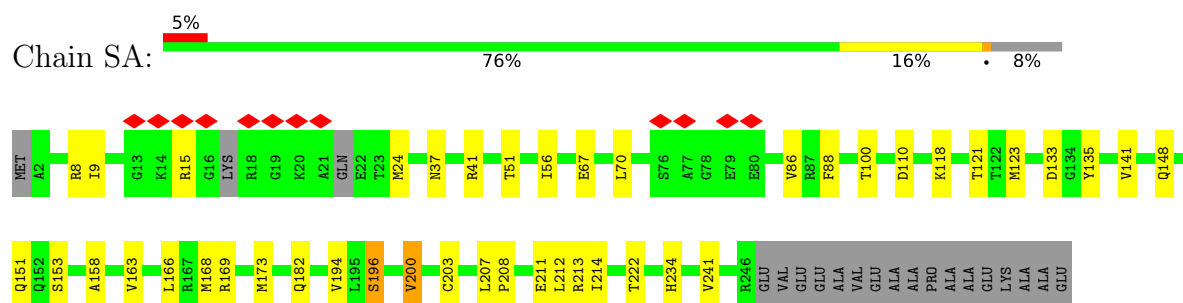
- Molecule 54: E-site_tRNA_chain_S4



- Molecule 55: mRNA_chain_S5

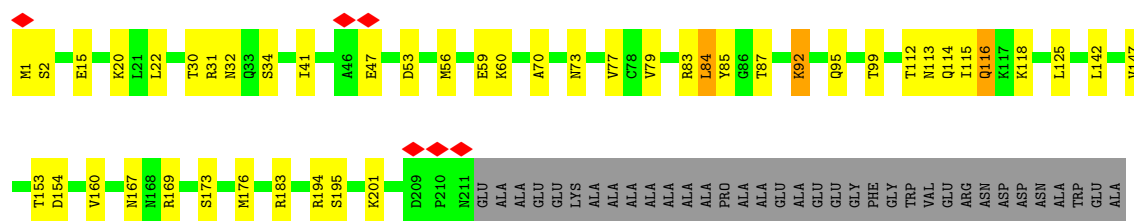


- Molecule 56: 40S ribosomal protein S3a

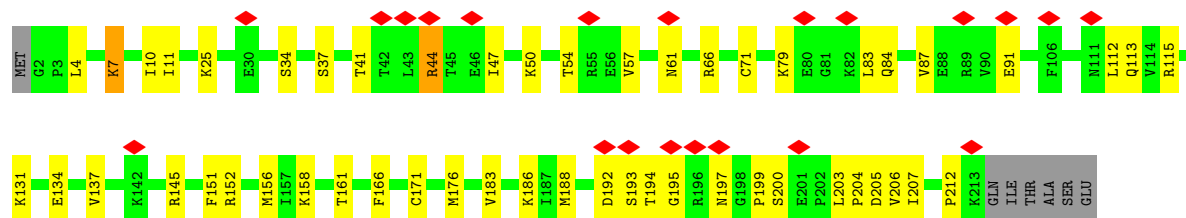
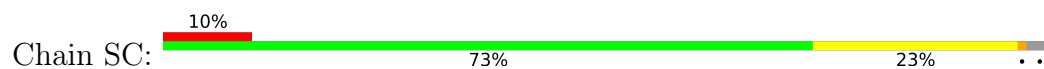


- Molecule 57: 40S ribosomal protein SA

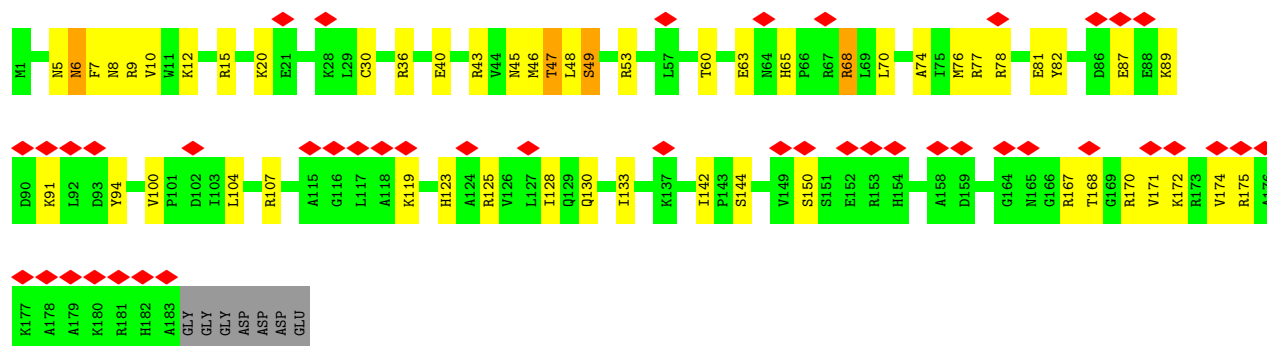




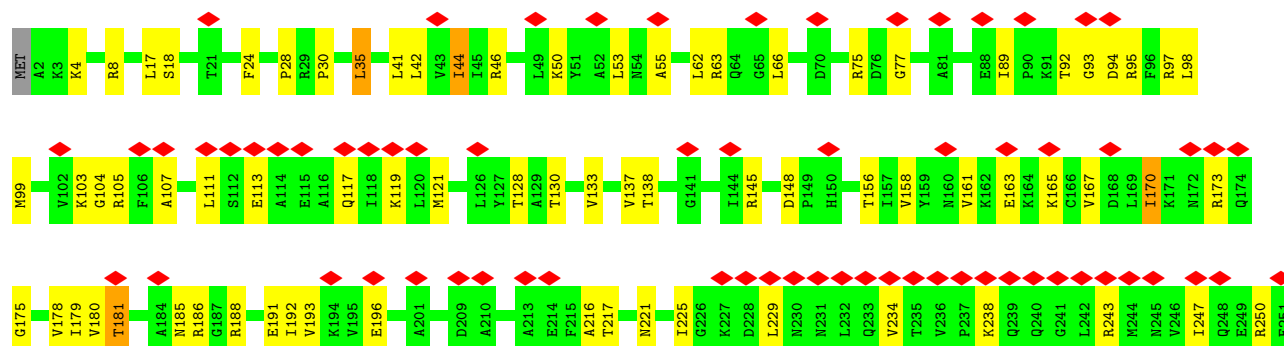
• Molecule 58: Putative 40S ribosomal protein S3

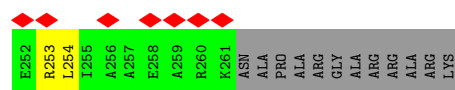


• Molecule 59: Putative 40S ribosomal protein S9

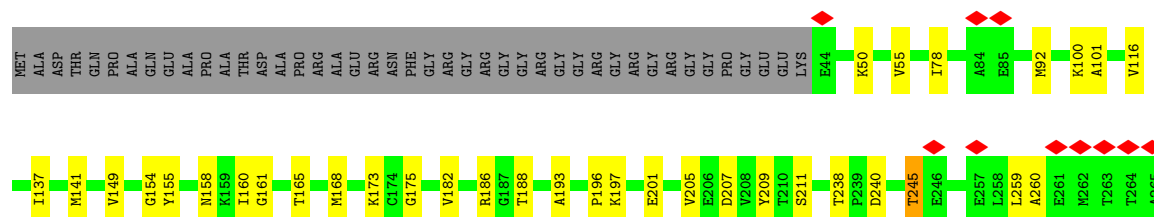


• Molecule 60: 40S ribosomal protein S4

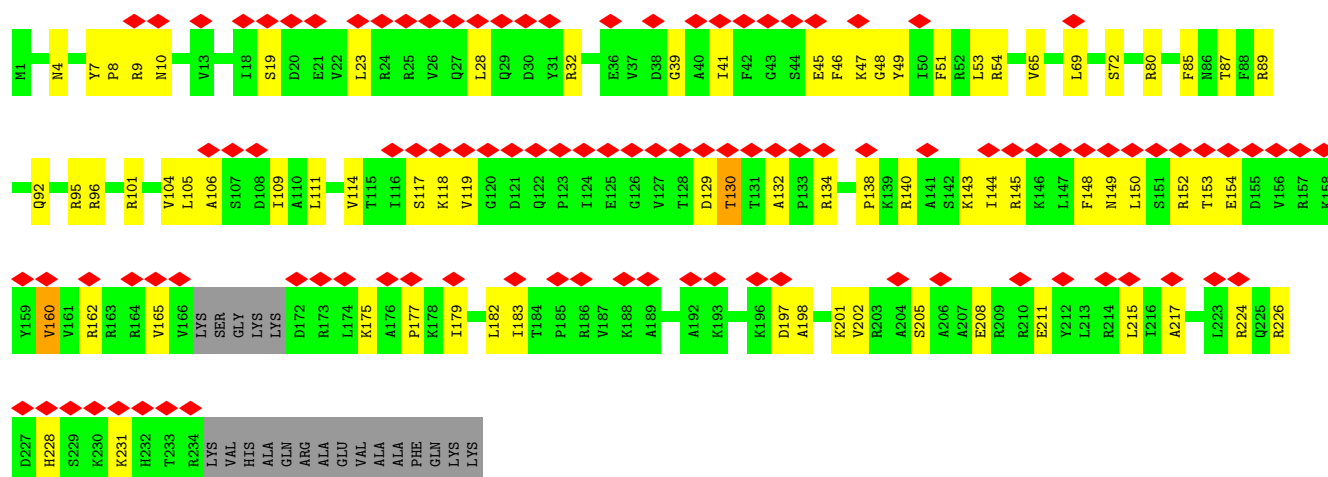
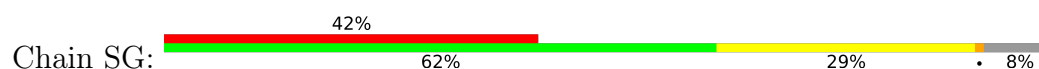




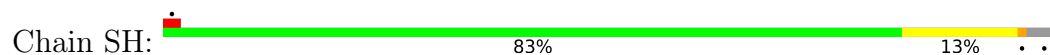
- Molecule 61: 40S ribosomal protein S2



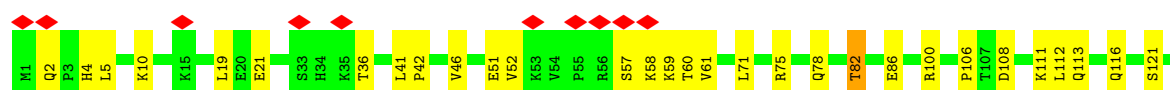
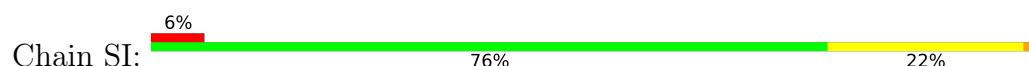
- Molecule 62: 40S ribosomal protein S6

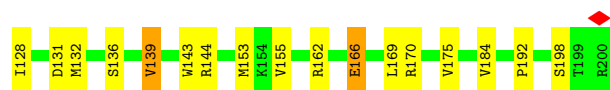


- Molecule 63: 40S ribosomal protein S5

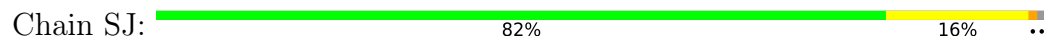


- Molecule 64: 40S ribosomal protein S7

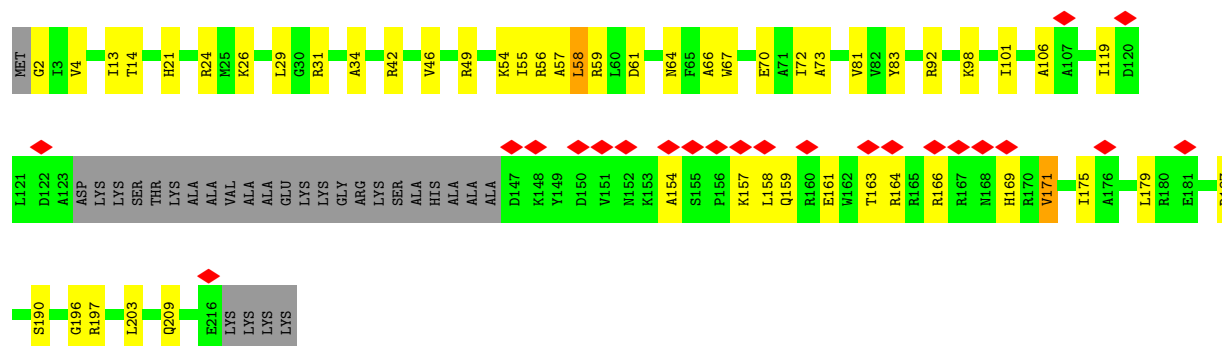




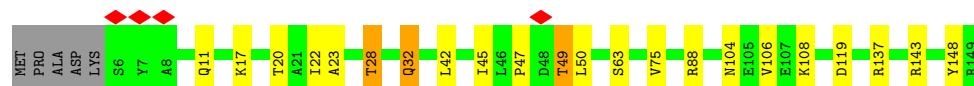
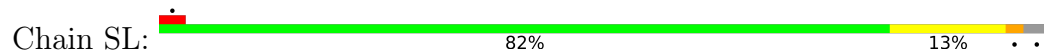
- Molecule 65: Putative 40S ribosomal protein S15A



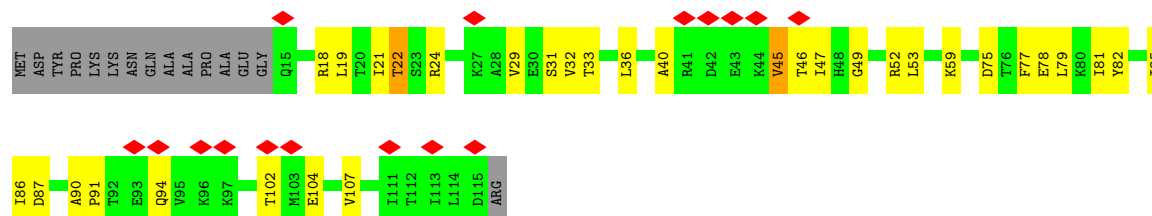
- Molecule 66: 40S ribosomal protein S8



- Molecule 67: Putative 40S ribosomal protein S16



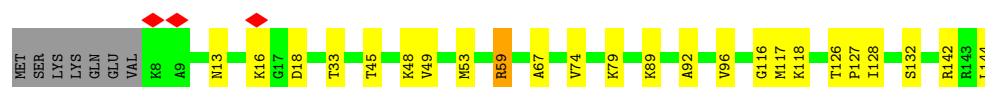
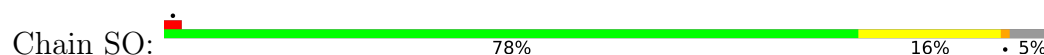
- Molecule 68: Putative ribosomal protein S20



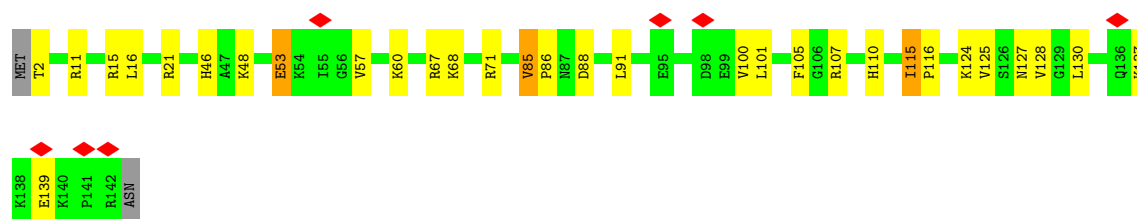
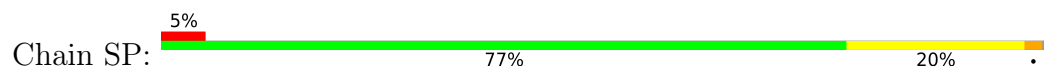
- Molecule 69: Putative 40S ribosomal protein S10



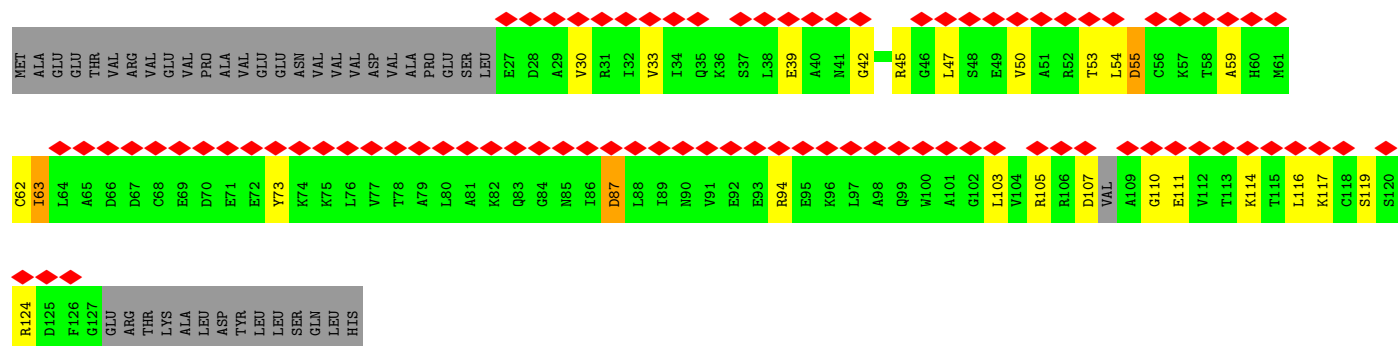
- Molecule 70: 40S ribosomal protein S14



- Molecule 71: Putative 40S ribosomal protein S23

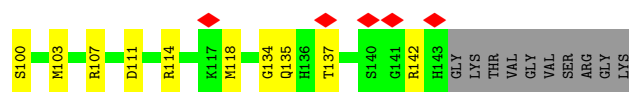


- Molecule 72: 40S ribosomal protein S12



- Molecule 73: Putative 40S ribosomal protein S18

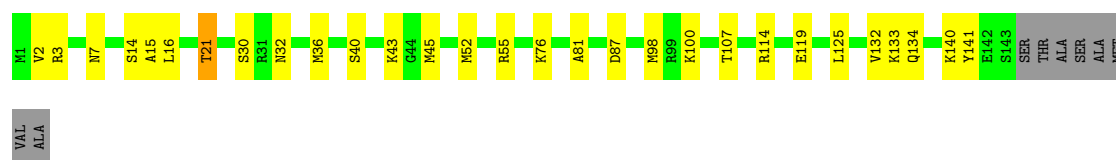
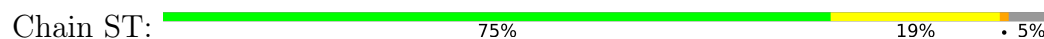




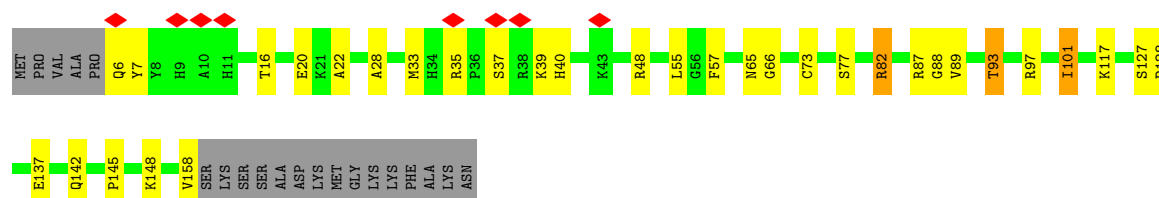
- Molecule 74: Putative ribosomal protein S29



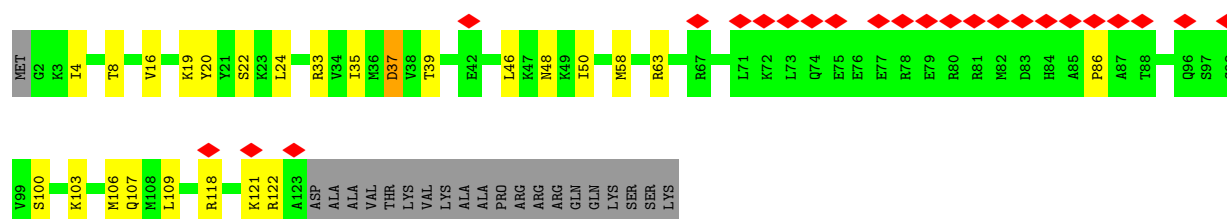
- Molecule 75: Putative 40S ribosomal protein S13



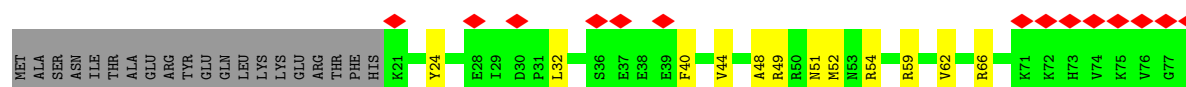
- Molecule 76: Ribosomal protein S17 family protein



- Molecule 77: Putative 40S ribosomal protein S17

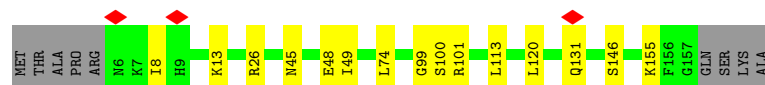
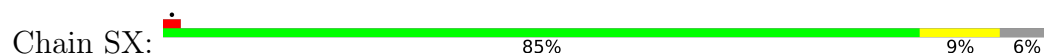


- Molecule 78: Putative 40S ribosomal protein S15

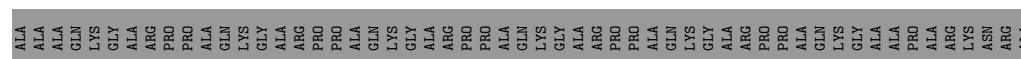
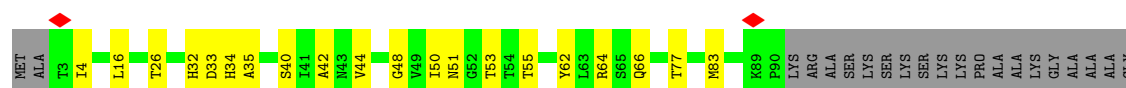




- Molecule 79: 40S ribosomal protein S19-like protein



- Molecule 80: Putative 40S ribosomal protein S21





- Molecule 84: Putative 40S ribosomal protein S27-1



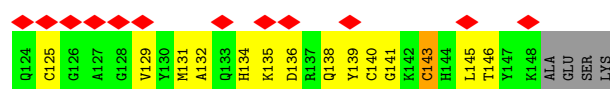
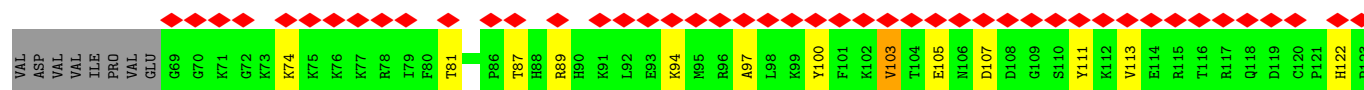
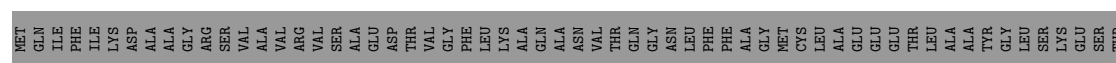
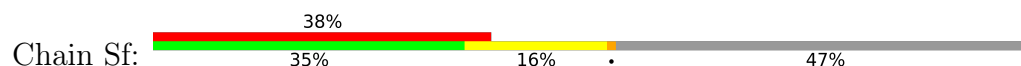
- Molecule 85: Putative 40S ribosomal protein S33



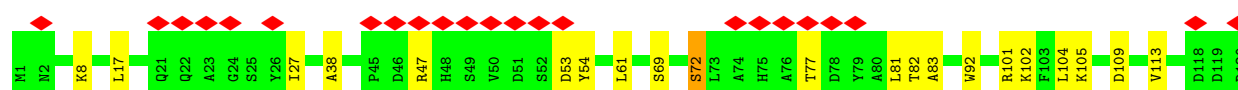
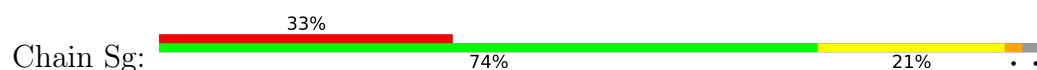
- Molecule 86: 40S ribosomal protein S30



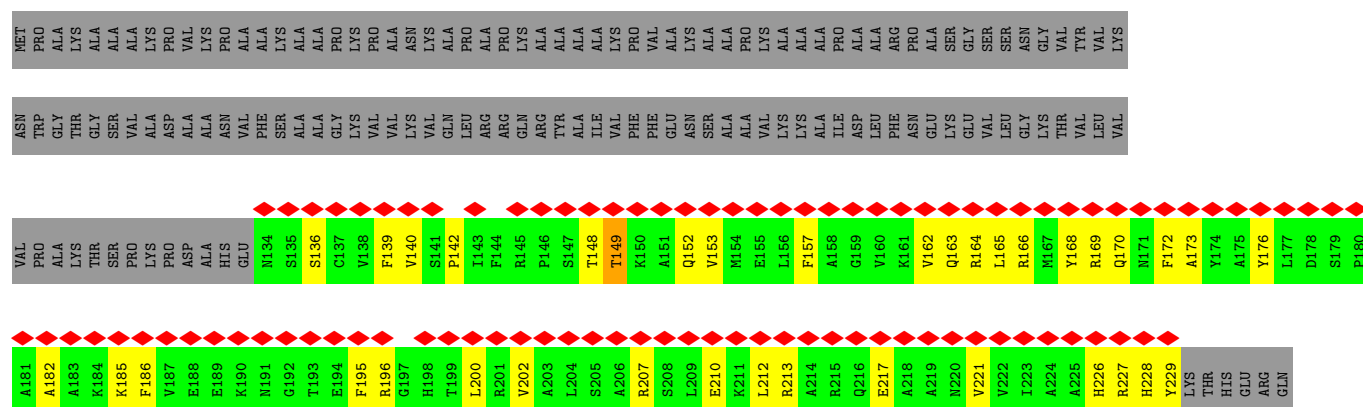
- Molecule 87: Ubiquitin-60S ribosomal protein L40



- Molecule 88: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 89: Putative RNA binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	419524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.9340390798620625	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, OMG, 5MC, B8N, MA6, A2M, A1H4F, MG, K, OMU, OMC, NA, PSU, ZN, MIA

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	0.29	2/39236 (0.0%)	0.48	4/61175 (0.0%)
2	L2	0.31	2/25973 (0.0%)	0.47	3/40481 (0.0%)
3	L3	0.22	0/4302	0.37	0/6687
4	L4	0.25	0/4376	0.43	0/6822
5	L5	0.31	0/2852	0.54	1/4438 (0.0%)
6	L6	0.18	0/1683	0.37	0/2618
7	L7	0.27	0/3782	0.62	3/5889 (0.1%)
8	L8	0.32	0/2851	0.49	0/4439
9	LA	0.25	0/2007	0.47	0/2696
10	LB	0.17	0/3283	0.33	0/4412
11	LC	0.16	0/2870	0.30	0/3861
12	LD	0.11	0/1410	0.25	0/1884
13	LE	0.15	0/1497	0.33	0/2017
14	LF	0.15	0/1173	0.31	0/1586
15	LG	0.14	0/1932	0.32	0/2599
16	LH	0.19	0/1803	0.38	0/2422
17	LI	0.20	0/1728	0.40	1/2313 (0.0%)
18	LJ	0.16	0/1029	0.33	0/1388
19	LK	0.24	0/1355	0.42	0/1816
20	LL	0.24	0/1151	0.52	4/1538 (0.3%)
21	LM	0.32	0/1751	0.55	1/2338 (0.0%)
22	LN	0.14	0/1697	0.31	0/2269
23	LO	0.16	0/2370	0.32	1/3172 (0.0%)
24	LP	0.31	0/1564	0.45	1/2092 (0.0%)
25	LQ	0.12	0/1701	0.24	0/2250
26	LR	0.19	0/1489	0.31	0/2008
27	LS	0.20	0/1290	0.46	2/1736 (0.1%)
28	LT	0.17	0/1241	0.35	0/1665
29	LU	0.10	0/976	0.26	0/1303
30	LV	0.14	0/968	0.29	0/1302
31	LW	0.14	0/981	0.30	0/1310
32	LX	0.14	0/735	0.27	0/989

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LY	0.13	0/1088	0.25	0/1455
34	LZ	0.15	0/1133	0.28	0/1516
35	La	0.13	0/1054	0.25	0/1399
36	Lb	0.33	0/557	0.45	0/743
37	Lc	0.15	0/1896	0.30	0/2540
38	Ld	0.13	0/754	0.26	0/1019
39	Le	0.16	0/1488	0.31	0/1979
40	Lf	0.26	0/1066	0.48	1/1424 (0.1%)
41	Lg	0.20	0/1172	0.33	0/1573
42	Lh	0.20	0/1045	0.31	0/1390
43	Li	0.13	0/822	0.30	0/1099
44	Lj	0.28	0/686	0.53	0/915
45	Lk	0.13	0/617	0.27	0/828
46	Ll	0.15	0/463	0.31	0/617
47	Lm	0.14	0/423	0.33	0/563
48	Ln	0.22	0/300	0.54	0/390
49	Lo	0.17	0/705	0.40	0/940
50	Lp	0.16	0/797	0.27	0/1053
51	S1	0.23	0/42995	0.38	0/66976
52	S2	0.44	0/1783	0.60	0/2776
53	S3	0.32	0/1790	0.51	0/2789
54	S4	0.13	0/1757	0.31	0/2735
55	S5	0.15	0/279	0.30	0/431
56	SA	0.13	0/1967	0.30	0/2641
57	SB	0.13	0/1695	0.31	0/2292
58	SC	0.17	0/1674	0.29	0/2240
59	SD	0.12	0/1536	0.32	0/2059
60	SE	0.12	0/2092	0.32	0/2819
61	SF	0.13	0/1744	0.29	0/2362
62	SG	0.12	0/1851	0.29	0/2474
63	SH	0.12	0/1469	0.26	0/1970
64	SI	0.13	0/1679	0.29	0/2255
65	SJ	0.14	0/1038	0.29	0/1391
66	SK	0.12	0/1573	0.26	0/2107
67	SL	0.20	0/1161	0.37	0/1559
68	SM	0.12	0/802	0.29	0/1088
69	SN	0.13	0/842	0.36	0/1141
70	SO	0.26	0/1039	0.43	0/1395
71	SP	0.13	0/1120	0.29	0/1500
72	SQ	0.13	0/671	0.36	0/911
73	SR	0.11	0/1158	0.26	0/1553
74	SS	0.13	0/458	0.34	0/607
75	ST	0.15	0/1190	0.31	0/1594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SU	0.13	0/1286	0.29	0/1727
77	SV	0.11	0/1002	0.24	0/1334
78	SW	0.11	0/948	0.25	0/1275
79	SX	0.25	0/1237	0.39	0/1661
80	SY	0.12	0/673	0.29	0/913
81	SZ	0.09	0/1071	0.28	0/1425
82	Sa	0.14	0/807	0.34	0/1082
83	Sb	0.14	0/842	0.30	0/1127
84	Sc	0.13	0/688	0.31	0/921
85	Sd	0.11	0/498	0.35	0/668
86	Se	0.43	0/496	0.63	0/658
87	Sf	0.13	0/674	0.34	0/892
88	Sg	0.12	0/2412	0.32	0/3276
89	Sh	0.13	0/783	0.38	0/1053
All	All	0.24	4/227902 (0.0%)	0.41	22/334635 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	LH	0	1
21	LM	0	4
24	LP	0	1
40	Lf	0	1
44	Lj	0	2
70	SO	0	1
79	SX	0	1
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	69	A2M	O3'-P	5.57	1.61	1.56
1	L1	847	OMU	O3'-P	5.36	1.61	1.56
2	L2	527	A2M	O3'-P	5.25	1.61	1.56
2	L2	1384	A2M	O3'-P	5.06	1.61	1.56

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L7	6	G	O3'-P-O5'	-31.06	57.42	104.00
7	L7	6	G	OP1-P-O3'	10.03	138.08	108.00
27	LS	78	LYS	CB-CG-CD	9.02	132.05	111.30
27	LS	78	LYS	CA-CB-CG	8.21	130.51	114.10
20	LL	40	HIS	CA-CB-CG	8.03	121.83	113.80
20	LL	39	HIS	CB-CA-C	-7.93	99.23	110.34
24	LP	160	GLY	CA-C-O	-6.77	117.82	122.22
1	L1	1489	U	C4'-C3'-O3'	6.46	119.10	109.40
7	L7	7	U	O5'-P-OP1	-6.37	88.89	108.00
17	LI	25	GLY	CA-C-O	-6.23	117.96	122.45
2	L2	1485	G	P-O3'-C3'	6.11	129.37	120.20
1	L1	1734	G	O3'-P-O5'	-6.00	95.00	104.00
20	LL	39	HIS	CA-C-O	-5.80	112.90	119.98
2	L2	382	A2M	OP2-P-O3'	5.66	117.66	105.20
40	Lf	42	PRO	N-CA-CB	-5.63	97.55	103.52
5	L5	33	U	O3'-P-O5'	5.58	112.37	104.00
2	L2	527	A2M	OP2-P-O3'	5.48	117.26	105.20
1	L1	1263	A	O3'-P-O5'	-5.44	95.84	104.00
23	LO	84	PRO	CA-N-CD	-5.36	104.49	112.00
21	LM	69	GLY	CA-C-O	-5.30	117.42	122.13
1	L1	967	G	P-O3'-C3'	5.14	127.91	120.20
20	LL	39	HIS	CA-CB-CG	5.09	118.89	113.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	LH	108	ARG	Sidechain
21	LM	189	ARG	Sidechain
21	LM	193	ARG	Sidechain
21	LM	194	ARG	Sidechain
21	LM	71	ARG	Sidechain
24	LP	157	ARG	Sidechain
40	Lf	37	ARG	Sidechain
44	Lj	63	ARG	Sidechain
44	Lj	72	ARG	Sidechain
70	SO	59	ARG	Sidechain
79	SX	101	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	35987	0	18149	449	0
2	L2	24715	0	12526	299	0
3	L3	3877	0	1966	52	0
4	L4	3937	0	1989	48	0
5	L5	2555	0	1298	44	0
6	L6	1506	0	768	30	0
7	L7	3533	0	1791	50	0
8	L8	2551	0	1293	21	0
9	LA	1962	0	2011	27	0
10	LB	3216	0	3334	55	0
11	LC	2820	0	2926	51	0
12	LD	1387	0	1425	17	0
13	LE	1477	0	1558	16	0
14	LF	1151	0	1216	21	0
15	LG	1905	0	2033	29	0
16	LH	1767	0	1872	25	0
17	LI	1695	0	1764	20	0
18	LJ	1012	0	1057	18	0
19	LK	1336	0	1403	32	0
20	LL	1124	0	1151	27	0
21	LM	1711	0	1790	36	0
22	LN	1665	0	1740	17	0
23	LO	2329	0	2418	35	0
24	LP	1539	0	1648	32	0
25	LQ	1682	0	1801	27	0
26	LR	1455	0	1492	26	0
27	LS	1261	0	1311	24	0
28	LT	1217	0	1251	22	0
29	LU	960	0	987	10	0
30	LV	953	0	1016	12	0
31	LW	967	0	1040	22	0
32	LX	714	0	727	11	0
33	LY	1067	0	1140	14	0
34	LZ	1117	0	1164	19	0
35	La	1043	0	1142	16	0
36	Lb	546	0	575	5	0
37	Lc	1862	0	1959	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Ld	744	0	770	10	0
39	Le	1469	0	1599	17	0
40	Lf	1046	0	1106	18	0
41	Lg	1149	0	1203	25	0
42	Lh	1029	0	1084	14	0
43	Li	807	0	865	14	0
44	Lj	672	0	688	11	0
45	Lk	608	0	641	7	0
46	Ll	450	0	483	7	0
47	Lm	417	0	447	7	0
48	Ln	296	0	342	7	0
49	Lo	693	0	716	16	0
50	Lp	784	0	841	4	0
51	S1	39438	0	19929	566	0
52	S2	1626	0	833	37	0
53	S3	1602	0	815	12	0
54	S4	1574	0	801	22	0
55	S5	251	0	130	2	0
56	SA	1943	0	2027	30	0
57	SB	1661	0	1689	30	0
58	SC	1646	0	1716	34	0
59	SD	1508	0	1582	38	0
60	SE	2054	0	2148	51	0
61	SF	1708	0	1754	22	0
62	SG	1829	0	1942	55	0
63	SH	1447	0	1480	18	0
64	SI	1649	0	1752	35	0
65	SJ	1021	0	1050	16	0
66	SK	1550	0	1629	33	0
67	SL	1140	0	1197	14	0
68	SM	792	0	835	19	0
69	SN	818	0	807	10	0
70	SO	1024	0	1052	24	0
71	SP	1100	0	1146	21	0
72	SQ	670	0	601	21	0
73	SR	1138	0	1186	31	0
74	SS	452	0	461	10	0
75	ST	1167	0	1243	21	0
76	SU	1257	0	1299	22	0
77	SV	992	0	1065	18	0
78	SW	928	0	955	13	0
79	SX	1206	0	1231	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	SY	663	0	658	13	0
81	SZ	1051	0	1130	35	0
82	Sa	798	0	836	24	0
83	Sb	825	0	861	12	0
84	Sc	674	0	674	12	0
85	Sd	496	0	511	12	0
86	Se	487	0	542	20	0
87	Sf	659	0	678	23	0
88	Sg	2354	0	2273	37	0
89	Sh	768	0	780	28	0
90	L1	116	0	0	0	0
90	L2	74	0	0	0	0
90	L3	4	0	0	0	0
90	L4	4	0	0	0	0
90	L5	1	0	0	0	0
90	L6	1	0	0	0	0
90	L7	9	0	0	0	0
90	L8	5	0	0	0	0
90	LA	1	0	0	0	0
90	LB	1	0	0	0	0
90	LJ	1	0	0	0	0
90	LS	1	0	0	0	0
90	LT	1	0	0	0	0
90	Lf	1	0	0	0	0
90	Lh	1	0	0	0	0
90	Lj	1	0	0	0	0
90	S1	64	0	0	0	0
90	S5	2	0	0	0	0
90	SX	1	0	0	0	0
91	L1	29	0	0	0	0
91	L2	21	0	0	0	0
91	L4	4	0	0	0	0
91	L5	3	0	0	0	0
91	L8	1	0	0	0	0
91	LA	2	0	0	0	0
91	LE	1	0	0	0	0
91	LH	1	0	0	0	0
91	LM	2	0	0	0	0
91	LN	2	0	0	0	0
91	LR	1	0	0	0	0
91	Lf	1	0	0	0	0
91	S1	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	SH	1	0	0	0	0
91	SP	1	0	0	0	0
92	L1	55	0	0	0	0
92	L2	33	0	0	0	0
92	L3	2	0	0	0	0
92	L4	6	0	0	0	0
92	L5	2	0	0	0	0
92	L7	5	0	0	0	0
92	L8	1	0	0	0	0
92	LB	2	0	0	0	0
92	LC	2	0	0	0	0
92	LZ	1	0	0	0	0
92	Lh	1	0	0	0	0
92	S1	30	0	0	0	0
92	SS	1	0	0	0	0
92	ST	1	0	0	0	0
92	Sb	1	0	0	0	0
93	L2	31	0	0	1	0
94	Lp	1	0	0	0	0
95	L1	152	0	0	0	0
95	L2	119	0	0	0	0
95	L3	10	0	0	0	0
95	L4	11	0	0	0	0
95	L5	3	0	0	0	0
95	L7	11	0	0	0	0
95	L8	1	0	0	0	0
95	LA	7	0	0	0	0
95	LB	5	0	0	0	0
95	LC	4	0	0	0	0
95	LG	1	0	0	0	0
95	LH	2	0	0	0	0
95	LI	2	0	0	0	0
95	LL	5	0	0	0	0
95	LM	7	0	0	0	0
95	LP	2	0	0	0	0
95	LQ	2	0	0	0	0
95	LS	2	0	0	0	0
95	LT	2	0	0	0	0
95	LV	1	0	0	0	0
95	LW	1	0	0	0	0
95	La	2	0	0	0	0
95	Lb	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	Le	1	0	0	0	0
95	Lf	2	0	0	0	0
95	Lh	1	0	0	0	0
95	Lj	4	0	0	0	0
95	Lo	1	0	0	0	0
95	Lp	2	0	0	0	0
95	S1	47	0	0	0	0
95	SA	1	0	0	0	0
All	All	216694	0	158814	2678	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2678) 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)
62:SG:150:LEU:HD12	62:SG:154:GLU:CD	1.53	1.34
62:SG:150:LEU:HD12	62:SG:154:GLU:OE1	1.24	1.29
62:SG:150:LEU:CD1	62:SG:154:GLU:OE1	1.92	1.18
51:S1:1152:A:O3'	70:SO:59:ARG:NH1	1.80	1.12
51:S1:146:U:H4'	62:SG:183:ILE:HD13	1.26	1.10
1:L1:1741:A:H2'	1:L1:1742:G:H5'	1.40	1.02
11:LC:295:GLU:OE1	24:LP:135:MET:HE1	1.62	0.99
51:S1:1114:G:H1	51:S1:1207:U:H3	1.05	0.99
2:L2:1152:PSU:OP1	27:LS:78:LYS:NZ	1.98	0.97
2:L2:1191:C:H42	54:S4:76:A:H8	1.14	0.96
1:L1:1680:U:H3	1:L1:1712:G:H1	1.02	0.95
33:LY:59:LYS:H	33:LY:59:LYS:HD2	1.31	0.95
1:L1:1677:G:H1	1:L1:1715:U:H3	1.03	0.95
77:SV:106:MET:HE3	77:SV:122:ARG:HG2	1.49	0.94
89:Sh:140:VAL:HG12	89:Sh:202:VAL:HG12	1.47	0.94
51:S1:1788:U:H5'	77:SV:48:ASN:HB3	1.50	0.93
1:L1:1741:A:C2'	1:L1:1742:G:H5'	1.99	0.93
5:L5:68:G:H1	5:L5:90:C:H5	1.16	0.90
3:L3:101:G:H1	3:L3:139:C:H5	1.18	0.89
51:S1:528:G:H1	51:S1:553:U:H3	0.90	0.89
5:L5:35:G:H1	5:L5:111:C:H5	1.21	0.88
51:S1:1369:U:H3	51:S1:1401:G:H1	1.16	0.88
4:L4:129:G:H1	4:L4:161:C:H5	1.23	0.86
1:L1:374:G:H1	7:L7:28:C:H5	1.24	0.86
2:L2:1441:C:H5	6:L6:6:G:H1	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SP:127:ASN:O	71:SP:127:ASN:ND2	2.09	0.85
1:L1:118:C:H5	1:L1:150:G:H1	1.24	0.85
28:LT:40:PRO:HD2	28:LT:43:LYS:HD3	1.60	0.84
51:S1:124:A:OP2	62:SG:201:LYS:NZ	2.09	0.84
1:L1:32:A:N7	1:L1:48:OMU:H5	1.93	0.84
49:Lo:30:GLU:HA	49:Lo:33:GLN:HG2	1.60	0.83
2:L2:133:G:H1	2:L2:345:C:H5	1.26	0.83
2:L2:1510:A:H61	10:LB:327:ASP:H	1.23	0.82
72:SQ:111:GLU:OE1	72:SQ:111:GLU:N	2.13	0.82
10:LB:13:HIS:HD2	10:LB:15:GLY:H	1.28	0.81
21:LM:121:VAL:HG11	21:LM:131:GLU:HG3	1.61	0.81
86:Se:58:ASN:OD1	86:Se:60:GLN:NE2	2.12	0.81
1:L1:1182:C:O2	1:L1:1190:OMG:N2	2.13	0.81
2:L2:683:G:H1	2:L2:756:C:H5	1.28	0.81
1:L1:1238:C:H5''	1:L1:1239:U:H5'	1.63	0.80
27:LS:78:LYS:HG2	27:LS:87:LYS:HG3	1.62	0.80
33:LY:59:LYS:HD2	33:LY:59:LYS:N	1.97	0.80
2:L2:569:G:O2'	2:L2:571:G:OP2	2.00	0.80
5:L5:30:G:H1	5:L5:124:C:H5	1.29	0.80
51:S1:559:G:H1	51:S1:592:C:H5	1.28	0.80
1:L1:373:G:H1	7:L7:29:C:H5	1.27	0.79
1:L1:1472:G:H1	1:L1:1514:C:H5	1.28	0.79
4:L4:138:C:H5	4:L4:152:G:H1	1.30	0.79
52:S2:58:A:H1'	52:S2:60:U:H3	1.47	0.79
2:L2:1261:G:H1	2:L2:1305:C:H5	1.28	0.79
1:L1:77:U:H5''	21:LM:186:PRO:HG3	1.64	0.78
2:L2:1078:OMG:N2	2:L2:1236:C:O2	2.13	0.78
51:S1:1945:A:H4'	67:SL:47:PRO:HG3	1.65	0.78
3:L3:22:C:H5	3:L3:213:G:H1	1.32	0.78
1:L1:853:C:H5	1:L1:992:G:H1	1.30	0.78
18:LJ:35:ASN:HD21	18:LJ:65:LYS:HB2	1.49	0.77
1:L1:593:C:H42	1:L1:614:A:H61	1.33	0.77
71:SP:101:LEU:HB3	71:SP:124:LYS:HB2	1.65	0.76
14:LF:154:GLN:NE2	14:LF:158:ASP:OD2	2.19	0.76
3:L3:104:C:H5	3:L3:136:G:H1	1.32	0.76
51:S1:1431:A:O2'	80:SY:66:GLN:NE2	2.18	0.76
71:SP:11:ARG:NH2	76:SU:117:LYS:O	2.18	0.76
2:L2:781:G:H1	2:L2:808:C:H5	1.32	0.75
51:S1:1908:A:H5''	51:S1:1909:C:H5	1.51	0.75
3:L3:21:A:O2'	3:L3:22:C:O2	2.03	0.75
59:SD:107:ARG:HH22	59:SD:125:ARG:HH21	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1363:A:H4'	1:L1:1364:A:H5''	1.69	0.75
1:L1:1674:A:H2	1:L1:1726:G:H21	1.33	0.75
48:Ln:3:THR:CG2	51:S1:2195:G:O2'	2.34	0.75
51:S1:2102:A:H61	51:S1:2121:C:H42	1.35	0.75
64:SI:144:ARG:HG3	65:SJ:51:GLU:HG3	1.68	0.75
1:L1:514:C:H5	1:L1:537:G:H1	1.35	0.75
51:S1:1860:C:OP2	73:SR:137:THR:OG1	2.05	0.74
2:L2:652:C:O2	2:L2:1253:OMG:N2	2.16	0.74
60:SE:103:LYS:HD2	60:SE:105:ARG:HH12	1.52	0.74
11:LC:295:GLU:OE1	24:LP:135:MET:CE	2.35	0.74
1:L1:352:G:OP2	43:Li:25:ARG:NH2	2.20	0.74
23:LO:134:THR:HG22	23:LO:136:LYS:H	1.50	0.74
32:LX:7:GLU:OE1	32:LX:30:LYS:NZ	2.19	0.73
1:L1:148:U:HO2'	1:L1:149:G:H8	1.32	0.73
51:S1:695:G:H22	51:S1:750:U:H3	1.36	0.73
51:S1:1142:G:H21	70:SO:45:THR:HG21	1.52	0.73
84:Sc:22:ARG:NH1	84:Sc:27:GLN:OE1	2.21	0.73
2:L2:1214:G:H1	2:L2:1222:C:H5	1.37	0.73
59:SD:76:MET:HA	59:SD:76:MET:HE3	1.69	0.73
1:L1:263:A:HO2'	31:LW:2:ALA:N	1.87	0.73
2:L2:134:C:H5	2:L2:344:G:H1	1.34	0.73
2:L2:1156:G:O6	27:LS:78:LYS:HE2	1.88	0.73
5:L5:123:G:O2'	5:L5:124:C:O2	2.06	0.73
76:SU:35:ARG:O	76:SU:35:ARG:NH1	2.21	0.73
23:LO:120:GLN:HE21	23:LO:123:LYS:HE2	1.52	0.73
83:Sb:78:CYS:SG	83:Sb:81:CYS:N	2.62	0.73
1:L1:1257[B]:U:N3	1:L1:1263:A:OP1	2.16	0.72
41:Lg:61:VAL:HG13	41:Lg:66:ASP:HB3	1.70	0.72
51:S1:1963:C:OP1	73:SR:135:GLN:NE2	2.21	0.72
11:LC:155:ASP:OD1	11:LC:253:SER:OG	2.06	0.72
51:S1:232:C:H2'	51:S1:233:G:H8	1.52	0.72
51:S1:587:A:OP2	59:SD:170:ARG:NH2	2.21	0.72
51:S1:84:U:H4'	51:S1:153:A:H4'	1.71	0.72
1:L1:1051:C:H5	1:L1:1097:A:H62	1.34	0.72
2:L2:590:U:H2'	2:L2:591:A2M:H8	1.70	0.72
2:L2:1170:U:H2'	2:L2:1171:G:H8	1.55	0.72
2:L2:847:U:H3	2:L2:951:G:H1	1.37	0.72
54:S4:31:A:H3'	54:S4:32:U:H5''	1.72	0.72
1:L1:889:G:H21	3:L3:124:U:H5'	1.55	0.72
51:S1:506:U:OP1	81:SZ:115:LYS:NZ	2.22	0.72
51:S1:617:G:H4'	71:SP:88:ASP:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:2035:C:H2'	63:SH:46:ARG:HD3	1.72	0.71
2:L2:695:G:H2'	2:L2:696:A:C8	2.25	0.71
2:L2:1360:OMG:HN1	52:S2:75:C:H42	1.36	0.71
89:Sh:148:THR:HG23	89:Sh:152:GLN:HG2	1.72	0.71
62:SG:45:GLU:N	62:SG:45:GLU:OE2	2.22	0.71
5:L5:65:U:H3	5:L5:93:G:H1	1.39	0.71
51:S1:846:U:H2'	51:S1:847:A:H8	1.56	0.71
62:SG:150:LEU:HD12	62:SG:154:GLU:OE2	1.89	0.71
83:Sb:46:MET:HE3	83:Sb:69:PRO:HB2	1.71	0.71
1:L1:1250:U:OP2	16:LH:67:ARG:NH1	2.23	0.70
51:S1:1623:OMG:N2	51:S1:1840:C:O2	2.20	0.70
1:L1:836:G:OP2	24:LP:98:ARG:NH2	2.24	0.70
2:L2:1282:C:H5	2:L2:1336:G:H22	1.40	0.70
11:LC:327:LEU:HD21	11:LC:334:LYS:HE2	1.72	0.70
48:Ln:3:THR:HG23	51:S1:2195:G:O2'	1.91	0.70
51:S1:996:C:H5''	64:SI:59:LYS:NZ	2.07	0.70
52:S2:53:G:N2	52:S2:58:A:H62	1.90	0.70
51:S1:1117:A:H2'	51:S1:1118:G:C8	2.27	0.70
68:SM:21:ILE:HD13	68:SM:33:THR:HG22	1.74	0.70
2:L2:1510:A:N6	10:LB:327:ASP:H	1.88	0.70
51:S1:639:C:OP1	86:Se:43:ARG:NH2	2.20	0.70
23:LO:55:ILE:HG21	23:LO:164:ARG:HH21	1.56	0.70
39:Le:120:MET:HE3	39:Le:153:ARG:HB2	1.74	0.70
31:LW:28:MET:HB3	31:LW:98:PRO:HG2	1.72	0.70
1:L1:1536:C:OP1	28:LT:66:LYS:NZ	2.25	0.69
18:LJ:72:ARG:NH2	51:S1:2078:A:OP1	2.24	0.69
51:S1:889:A:OP2	60:SE:105:ARG:NH2	2.25	0.69
51:S1:1281:C:HO2'	65:SJ:2:THR:N	1.89	0.69
1:L1:381:G:N7	11:LC:192:ARG:HD3	2.07	0.69
1:L1:408:G:O2'	1:L1:410:U:OP1	2.10	0.69
3:L3:45:U:OP1	42:Lh:25:ARG:NH2	2.22	0.69
1:L1:763:U:O2'	20:LL:132:LYS:NZ	2.25	0.69
1:L1:890:C:H5	1:L1:905:G:H1	1.39	0.69
1:L1:1771:U:OP1	42:Lh:66:ARG:NH2	2.25	0.69
76:SU:73:CYS:O	76:SU:77:SER:OG	2.11	0.69
1:L1:897:A:N6	51:S1:1218:A:N1	2.40	0.69
2:L2:1151:U:H5''	27:LS:87:LYS:HE3	1.73	0.69
51:S1:701:G:H1	51:S1:745:G:H1	1.41	0.69
81:SZ:32:VAL:HG11	81:SZ:41:VAL:HG21	1.75	0.69
89:Sh:148:THR:CG2	89:Sh:152:GLN:HG2	2.21	0.69
51:S1:148:G:H2'	51:S1:149:G:C8	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:275:A:HO2'	51:S1:276:G:H8	1.38	0.69
1:L1:55:A:C2'	1:L1:56:G:H5'	2.23	0.69
2:L2:525:A:N7	2:L2:532:U:H5	1.90	0.68
88:Sg:121:LEU:HD21	88:Sg:181:VAL:HG11	1.75	0.68
51:S1:198:C:O2'	89:Sh:196:ARG:NH1	2.26	0.68
54:S4:32:U:OP1	63:SH:122:ARG:NH2	2.26	0.68
59:SD:125:ARG:HD2	86:Se:33:ARG:HE	1.58	0.68
2:L2:1136:U:H2'	2:L2:1137:G:C8	2.28	0.68
52:S2:52:G:H2'	52:S2:53:G:C8	2.27	0.68
2:L2:1170:U:H2'	2:L2:1171:G:C8	2.29	0.68
51:S1:278:A:OP2	62:SG:224:ARG:NH1	2.27	0.68
73:SR:40:ARG:NH2	79:SX:49:ILE:O	2.26	0.68
34:LZ:30:ASP:HB3	34:LZ:33:ASN:HB2	1.75	0.68
51:S1:878:C:H2'	51:S1:879:A:C8	2.28	0.68
73:SR:27:VAL:HG11	73:SR:51:ILE:HD11	1.74	0.68
70:SO:79:LYS:HE2	70:SO:117:MET:HE2	1.74	0.68
62:SG:7:TYR:CE2	62:SG:9:ARG:HB3	2.29	0.68
73:SR:87:ARG:HD2	73:SR:99:LEU:HD11	1.76	0.68
2:L2:1506:G:H22	39:Le:40:ARG:HH11	1.40	0.67
51:S1:2059:OMC:H5	51:S1:2166:A:H61	1.41	0.67
73:SR:88:GLN:HA	73:SR:96:THR:HG23	1.76	0.67
1:L1:594:G:H1	1:L1:613:C:H5	1.41	0.67
51:S1:2119:C:H4'	51:S1:2120:C:OP1	1.92	0.67
53:S3:16:C:H1'	53:S3:59:A:H2	1.58	0.67
20:LL:129:LEU:HG	20:LL:133:LYS:HD2	1.76	0.67
54:S4:38:A:H2	70:SO:59:ARG:HH21	1.40	0.67
43:Li:66:VAL:HG23	43:Li:68:LYS:HG3	1.76	0.67
89:Sh:195:PHE:HB3	89:Sh:200:LEU:HD13	1.77	0.67
2:L2:4:C:O2	3:L3:18:A:O2'	2.12	0.67
51:S1:255:A:H5''	51:S1:943:U:H1'	1.76	0.67
51:S1:1980:U:H4'	51:S1:2019:C:H4'	1.77	0.67
1:L1:120:G:O6	15:LG:142:ARG:NH2	2.24	0.67
51:S1:1207:U:H5'	75:ST:55:ARG:HD3	1.76	0.67
1:L1:148:U:O2'	1:L1:149:G:H8	1.77	0.67
5:L5:88:C:O2'	5:L5:89:C:O5'	2.12	0.67
88:Sg:281:GLU:HB3	88:Sg:299:LYS:HD3	1.77	0.66
2:L2:1379:A:H5''	2:L2:1381:G:H4'	1.78	0.66
11:LC:316:PRO:HB3	11:LC:322:ASN:OD1	1.96	0.66
1:L1:1147:A:O2'	1:L1:1150:A:N1	2.28	0.66
9:LA:234:LYS:HG2	9:LA:238:ILE:HG12	1.77	0.66
51:S1:793:G:O6	51:S1:830:G:O6	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SI:100:ARG:NH2	64:SI:131:ASP:OD2	2.28	0.66
1:L1:824:U:O2'	1:L1:1128:A:N6	2.28	0.66
7:L7:93:C:O2'	7:L7:94:G:OP1	2.12	0.66
12:LD:111:HIS:HD2	12:LD:125:TYR:H	1.43	0.66
51:S1:340:G:H5''	60:SE:137:VAL:HG21	1.78	0.66
2:L2:83:G:O2'	2:L2:580:U:O4	2.12	0.66
1:L1:1773:C:O2'	7:L7:139:A:N3	2.29	0.66
3:L3:23:U:O2'	3:L3:25:G:OP1	2.14	0.66
51:S1:701:G:H22	51:S1:745:G:H22	1.42	0.66
11:LC:113:LYS:HG2	21:LM:203:LYS:HB3	1.78	0.66
24:LP:35:PHE:HA	24:LP:38:LYS:HE2	1.78	0.66
56:SA:200:VAL:HG22	56:SA:212:LEU:HB3	1.76	0.66
51:S1:1767:G:N2	51:S1:1767:G:OP1	2.29	0.66
60:SE:97:ARG:HB3	60:SE:111:LEU:HD11	1.78	0.66
15:LG:82:VAL:HG21	15:LG:182:LYS:HD3	1.78	0.66
1:L1:611:C:OP2	11:LC:359:ARG:NH1	2.28	0.65
1:L1:716:A:OP2	17:LI:33:GLN:NE2	2.27	0.65
1:L1:830:G:OP1	24:LP:192:ARG:NH2	2.29	0.65
2:L2:786:A:H4'	2:L2:787:G:C8	2.31	0.65
4:L4:4:G:H1	4:L4:20:U:H3	1.44	0.65
71:SP:11:ARG:HD2	71:SP:15:ARG:HH21	1.62	0.65
51:S1:286:G:N2	51:S1:289:G:OP1	2.29	0.65
58:SC:10:ILE:HD13	68:SM:81:ILE:HG12	1.78	0.65
14:LF:54:LEU:HD11	14:LF:66:SER:HB3	1.77	0.65
51:S1:1695:C:H5	51:S1:1780:C:H42	1.43	0.65
58:SC:207:ILE:HD13	77:SV:50:ILE:HD11	1.77	0.65
1:L1:140:U:OP2	15:LG:107:ARG:NH2	2.26	0.65
51:S1:31:C:O3'	71:SP:137:LYS:NZ	2.29	0.65
51:S1:877:U:O4	81:SZ:16:GLN:NE2	2.29	0.65
10:LB:13:HIS:CD2	10:LB:15:GLY:H	2.13	0.65
13:LE:16:VAL:O	13:LE:52:ARG:NH2	2.29	0.65
17:LI:131:PHE:HB2	35:La:122:VAL:HG13	1.79	0.65
4:L4:24:A:H5''	16:LH:7:LYS:HB2	1.78	0.65
23:LO:224:ASN:N	23:LO:224:ASN:OD1	2.28	0.65
10:LB:224:SER:HB3	10:LB:343:MET:HG2	1.79	0.65
51:S1:105:C:OP1	51:S1:426:G:O2'	2.15	0.65
51:S1:2072:C:O2	51:S1:2151:OMG:N2	2.20	0.65
61:SF:173:LYS:NZ	61:SF:175:GLY:O	2.30	0.65
22:LN:208:MET:HA	22:LN:208:MET:HE3	1.77	0.65
88:Sg:234:VAL:HG11	88:Sg:254:THR:HG21	1.79	0.65
51:S1:792:G:O6	51:S1:831:G:O6	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Se:56:HIS:ND1	86:Se:59:LYS:HD2	2.12	0.65
48:Ln:6:ARG:HD2	48:Ln:8:ARG:HD2	1.78	0.64
52:S2:49:C:H1'	52:S2:65:G:N1	2.12	0.64
67:SL:47:PRO:HD2	67:SL:50:LEU:HB2	1.79	0.64
1:L1:790:C:H5	11:LC:305:LEU:H	1.43	0.64
51:S1:1403:A:N3	56:SA:148:GLN:NE2	2.45	0.64
1:L1:1092:U:HO2'	1:L1:1093:U:H6	1.42	0.64
51:S1:17:C:O2'	51:S1:1489:A:N1	2.28	0.64
51:S1:286:G:H1'	62:SG:217:ALA:HB1	1.78	0.64
51:S1:685:A:H5'	65:SJ:31:SER:HB3	1.78	0.64
1:L1:1110:G:H21	27:LS:61:THR:HG21	1.61	0.64
1:L1:1729:A:N7	30:LV:32:ARG:NH2	2.44	0.64
31:LW:32:LEU:HB2	31:LW:37:ARG:HD2	1.78	0.64
16:LH:151:GLU:OE2	26:LR:155:GLN:NE2	2.30	0.64
51:S1:1801:G:OP1	77:SV:63:ARG:NH2	2.31	0.64
54:S4:38:A:C2	70:SO:59:ARG:NH2	2.66	0.64
1:L1:706:G:HO2'	11:LC:117:HIS:HD1	1.45	0.64
14:LF:194:ASN:O	19:LK:110:ARG:NH2	2.31	0.64
51:S1:1523:A:H2'	51:S1:1524:G:C8	2.33	0.64
60:SE:95:ARG:HH21	60:SE:113:GLU:HA	1.62	0.64
86:Se:56:HIS:HB2	86:Se:59:LYS:HG3	1.80	0.64
3:L3:204:A:H2'	3:L3:205:A:C8	2.33	0.64
24:LP:37:ALA:O	24:LP:46:LYS:NZ	2.31	0.64
29:LU:18:GLN:OE1	29:LU:67:LYS:NZ	2.30	0.63
69:SN:5:VAL:HG11	69:SN:52:LEU:HD21	1.80	0.63
1:L1:700:A:C2	1:L1:845:OMU:H5	2.34	0.63
2:L2:454:A:N6	2:L2:477:G:OP1	2.31	0.63
51:S1:1152:A:H4'	70:SO:59:ARG:NH1	2.13	0.63
51:S1:2004:G:N2	51:S1:2031:A:OP2	2.28	0.63
1:L1:1273:U:O2'	1:L1:1274:G:H5''	1.98	0.63
56:SA:123:MET:HE2	56:SA:166:LEU:HD22	1.79	0.63
8:L8:33:C:O2'	8:L8:54:A:N1	2.28	0.63
51:S1:1133:U:O2'	70:SO:128:ILE:O	2.15	0.63
73:SR:111:ASP:OD1	73:SR:114:ARG:NH1	2.30	0.63
1:L1:368:G:OP2	11:LC:55:ARG:NH1	2.31	0.63
7:L7:90:U:O2'	31:LW:22:HIS:ND1	2.29	0.63
21:LM:124:ASP:OD1	21:LM:125:SER:N	2.31	0.63
51:S1:790:U:O2	62:SG:226:ARG:NH1	2.31	0.63
51:S1:2136:A:O2'	51:S1:2137:U:O2	2.12	0.63
51:S1:1577:U:OP2	72:SQ:114:LYS:NZ	2.31	0.63
81:SZ:11:CYS:HB3	81:SZ:33:ASN:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1171:PSU:H5'	1:L1:1171:PSU:H6	1.63	0.63
51:S1:1769:C:H41	79:SX:131:GLN:HG2	1.62	0.63
40:Lf:45:ARG:NH1	40:Lf:47:TYR:OH	2.32	0.63
1:L1:1609:A:H5''	28:LT:125:MET:HE1	1.81	0.62
5:L5:26:A:OP2	10:LB:116:ARG:NH2	2.31	0.62
51:S1:824:C:H5''	51:S1:825:C:H4'	1.81	0.62
16:LH:85:THR:O	16:LH:86:LYS:HG2	1.98	0.62
20:LL:72:THR:HG22	20:LL:108:LYS:HB3	1.80	0.62
49:Lo:8:MET:HB2	49:Lo:11:MET:HB2	1.79	0.62
49:Lo:11:MET:HE3	49:Lo:27:LYS:HA	1.81	0.62
60:SE:188:ARG:HH11	60:SE:243:ARG:HE	1.46	0.62
51:S1:1659:U:H3	51:S1:1670:G:H22	1.47	0.62
2:L2:1127:G:O2'	2:L2:1132:A:N1	2.31	0.62
11:LC:178:ASP:HB3	11:LC:206:PRO:HD3	1.80	0.62
27:LS:78:LYS:HG2	27:LS:87:LYS:CG	2.30	0.62
35:La:77:ARG:HA	35:La:80:ARG:HE	1.65	0.62
51:S1:1576:A:OP2	72:SQ:105:ARG:NH1	2.28	0.62
64:SI:153:MET:CE	64:SI:155:VAL:HG23	2.30	0.62
75:ST:40:SER:HB3	75:ST:45:MET:HE2	1.81	0.62
49:Lo:11:MET:HE1	49:Lo:30:GLU:OE1	1.99	0.62
51:S1:1397:A:O2'	51:S1:1399:G:OP2	2.17	0.62
54:S4:16:U:H2'	54:S4:17:C:H4'	1.82	0.62
64:SI:153:MET:HE2	64:SI:184:VAL:HG23	1.81	0.62
2:L2:780:G:H2'	2:L2:781:G:C8	2.34	0.62
51:S1:1569:G:O6	74:SS:8:ARG:NH1	2.33	0.62
4:L4:154:C:H4'	13:LE:155:ARG:HE	1.64	0.62
37:Lc:176:ASN:HA	37:Lc:179:ILE:HD12	1.82	0.62
51:S1:92:U:H1'	60:SE:4:LYS:HD2	1.82	0.62
51:S1:639:C:H2'	51:S1:640:A:C8	2.35	0.61
18:LJ:86:SER:OG	32:LX:19:ARG:NH1	2.33	0.61
51:S1:528:G:N2	51:S1:553:U:O2	2.29	0.61
52:S2:58:A:O2'	52:S2:60:U:OP2	2.16	0.61
61:SF:238:THR:HG22	61:SF:240:ASP:H	1.65	0.61
1:L1:989:C:OP2	20:LL:26:ARG:NH1	2.32	0.61
2:L2:1510:A:N6	10:LB:327:ASP:OD1	2.33	0.61
51:S1:1911:U:H5	51:S1:1928:G:H1	1.49	0.61
10:LB:374:HIS:O	32:LX:37:ARG:NH2	2.32	0.61
31:LW:52:GLU:HG3	31:LW:105:LYS:HB3	1.82	0.61
72:SQ:47:LEU:HD13	87:Sf:97:ALA:HB3	1.82	0.61
67:SL:32:GLN:HG3	79:SX:13:LYS:HB3	1.82	0.61
1:L1:73:U:H5''	17:LI:63:VAL:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1333:G:O2'	47:Lm:100:TYR:O	2.16	0.61
2:L2:1335:C:H2'	2:L2:1337:C:H5'	1.82	0.61
51:S1:2124:A:H2'	51:S1:2125:A:H5''	1.83	0.61
68:SM:19:LEU:HD13	68:SM:36:LEU:HD13	1.82	0.61
84:Sc:11:PRO:HB2	84:Sc:16:GLU:HG2	1.81	0.61
1:L1:1292:G:H1	1:L1:1343:A:H61	1.47	0.61
56:SA:8:ARG:HG2	56:SA:8:ARG:HH11	1.65	0.61
88:Sg:168:VAL:HG13	88:Sg:178:VAL:HG22	1.82	0.61
2:L2:1339:G:O2'	4:L4:52:A:N1	2.33	0.61
2:L2:1402:G:N2	2:L2:1405:A:OP2	2.31	0.61
12:LD:13:GLU:OE1	12:LD:136:ARG:NH2	2.34	0.61
68:SM:77:PHE:HB3	74:SS:53:PHE:HB3	1.83	0.61
77:SV:37:ASP:OD1	77:SV:37:ASP:N	2.31	0.61
1:L1:1092:U:O2'	1:L1:1093:U:O5'	2.19	0.61
6:L6:67:C:OP1	41:Lg:96:ARG:NH2	2.34	0.61
1:L1:745:U:H5'	1:L1:830:G:H1'	1.83	0.60
20:LL:80:ARG:NH2	20:LL:106:TYR:OH	2.34	0.60
51:S1:490:U:OP1	60:SE:46:ARG:NH1	2.34	0.60
51:S1:2182:G:OP2	51:S1:2182:G:N2	2.30	0.60
64:SI:170:ARG:NH1	64:SI:170:ARG:HB3	2.15	0.60
68:SM:53:LEU:HD21	68:SM:85:ILE:HG12	1.82	0.60
1:L1:1238:C:H5''	1:L1:1239:U:C5'	2.30	0.60
2:L2:97:A:O2'	2:L2:366:C:O2	2.18	0.60
14:LF:50:ARG:NH1	14:LF:180:SER:OG	2.34	0.60
15:LG:214:ASN:OD1	15:LG:217:ARG:NH2	2.34	0.60
34:LZ:41:ARG:HH11	34:LZ:102:ASP:HB2	1.65	0.60
1:L1:1265:A:H2'	1:L1:1266:A:C8	2.36	0.60
59:SD:63:GLU:OE1	59:SD:68:ARG:NH1	2.33	0.60
1:L1:1687:G:H22	1:L1:1705:G:H22	1.49	0.60
51:S1:640:A:H2'	51:S1:641:A:C8	2.36	0.60
51:S1:1186:A:H2'	51:S1:1187:A:C8	2.37	0.60
9:LA:79:PRO:HD2	9:LA:82:MET:SD	2.41	0.60
16:LH:115:LYS:HB3	16:LH:115:LYS:NZ	2.15	0.60
18:LJ:106:ASN:HD21	18:LJ:110:GLU:HB2	1.65	0.60
1:L1:1045:G:N2	1:L1:1046:U:O4	2.25	0.60
3:L3:16:G:N2	3:L3:21:A:OP1	2.31	0.60
6:L6:51:A:H5'	6:L6:52:G:C8	2.36	0.60
30:LV:71:THR:HG21	35:La:38:THR:HG22	1.82	0.60
51:S1:165:G:H5'	62:SG:89:ARG:HE	1.67	0.60
73:SR:47:LYS:NZ	79:SX:48:GLU:O	2.33	0.60
1:L1:1403:A:OP1	24:LP:2:GLY:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1725:U:H2'	1:L1:1726:G:H5'	1.82	0.60
2:L2:590:U:H2'	2:L2:591:A2M:C8	2.32	0.60
15:LG:163:LEU:HD13	21:LM:7:LEU:HD21	1.83	0.60
34:LZ:35:ASN:ND2	34:LZ:37:ASN:OD1	2.34	0.60
51:S1:582:U:OP2	81:SZ:5:LYS:NZ	2.33	0.60
60:SE:44:ILE:HD11	60:SE:98:LEU:HD11	1.83	0.60
1:L1:69:A2M:HM'3	2:L2:1216:A:H4'	1.84	0.60
1:L1:1242:U:OP1	19:LK:17:ARG:NH2	2.35	0.60
8:L8:53:A:H5''	23:LO:233:SER:HB2	1.83	0.60
71:SP:85:VAL:HG12	71:SP:130:LEU:HD21	1.83	0.60
1:L1:1764:A:OP2	45:Lk:21:ARG:NH2	2.34	0.60
7:L7:70:C:H5'	31:LW:25:ARG:CZ	2.32	0.60
51:S1:1203:U:OP1	51:S1:1410:C:O2'	2.20	0.60
51:S1:2030:G:OP1	63:SH:37:HIS:NE2	2.21	0.60
54:S4:27:G:N2	54:S4:44:G:O2'	2.34	0.60
5:L5:118:U:H3'	5:L5:119:U:H5''	1.84	0.60
51:S1:1138:G:H2'	51:S1:1139:G:C8	2.37	0.60
68:SM:59:LYS:HE2	68:SM:78:GLU:HG2	1.82	0.60
1:L1:1776:G:H22	2:L2:6:A:H2	1.51	0.59
51:S1:442:A:OP1	66:SK:49:ARG:NH2	2.34	0.59
51:S1:1171:A:H2'	51:S1:1172:G:C8	2.36	0.59
81:SZ:19:VAL:HG22	81:SZ:26:LYS:HG2	1.85	0.59
51:S1:304:A:H2'	51:S1:305:U:C6	2.37	0.59
51:S1:304:A:H2'	51:S1:305:U:H6	1.66	0.59
51:S1:873:G:H21	51:S1:875:A:H1'	1.67	0.59
51:S1:1152:A:C3'	70:SO:59:ARG:NH1	2.66	0.59
51:S1:1409:U:H2'	51:S1:1410:C:C6	2.37	0.59
64:SI:52:VAL:O	64:SI:60:THR:OG1	2.20	0.59
73:SR:103:MET:HE2	73:SR:107:ARG:HH21	1.67	0.59
1:L1:1715:U:H3'	1:L1:1716:G:H21	1.67	0.59
2:L2:343:U:H2'	2:L2:344:G:H8	1.67	0.59
51:S1:520:G:O2'	51:S1:870:A:N3	2.29	0.59
1:L1:1059:U:H3	1:L1:1093:U:H3	1.48	0.59
2:L2:1485:G:H1'	19:LK:164:MET:HA	1.84	0.59
35:La:77:ARG:HG2	35:La:80:ARG:HH21	1.67	0.59
51:S1:1186:A:OP1	75:ST:114:ARG:NH2	2.36	0.59
51:S1:1921:A:N3	51:S1:1982:G:O2'	2.32	0.59
64:SI:153:MET:HE3	64:SI:155:VAL:HG23	1.84	0.59
85:Sd:75:LEU:O	85:Sd:76:MET:HG2	2.03	0.59
1:L1:1090:U:H2'	1:L1:1091:A:C8	2.37	0.59
1:L1:1352:C:H2'	1:L1:1353:A:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:382:A2M:H2	2:L2:389:A:N7	2.18	0.59
2:L2:743:C:H2'	2:L2:744:G:H8	1.68	0.59
2:L2:1131:A:O2'	2:L2:1132:A:O5'	2.19	0.59
2:L2:1143:U:OP2	2:L2:1180:A:O2'	2.19	0.59
19:LK:8:CYS:HB3	26:LR:150:SER:HB3	1.85	0.59
25:LQ:94:LEU:HD23	25:LQ:97:ARG:HH21	1.68	0.59
51:S1:450:A:H2'	51:S1:451:C:H6	1.68	0.59
51:S1:1961:G:H5'	79:SX:99:GLY:HA2	1.83	0.59
51:S1:2028:C:OP1	67:SL:20:THR:OG1	2.19	0.59
57:SB:194:ARG:HE	80:SY:48:GLY:HA3	1.66	0.59
1:L1:1255:G:H2'	1:L1:1256:A:C8	2.38	0.59
7:L7:63:G:H22	7:L7:96:A:H2	1.49	0.59
22:LN:162:ARG:NH2	26:LR:86:ARG:O	2.36	0.59
59:SD:70:LEU:HD12	60:SE:247:ILE:HG13	1.84	0.59
1:L1:1391:U:C5	19:LK:19:PRO:HB2	2.37	0.59
7:L7:34:U:H5''	7:L7:34:U:H6	1.67	0.59
88:Sg:128:ASP:OD1	88:Sg:128:ASP:N	2.30	0.59
36:Lb:46:ARG:HG2	36:Lb:46:ARG:HH11	1.67	0.59
51:S1:117:G:H1'	51:S1:440:A:C5	2.38	0.59
52:S2:2:C:H2'	52:S2:3:G:H8	1.67	0.59
58:SC:134:GLU:HG3	58:SC:152:ARG:HG2	1.83	0.59
1:L1:636:U:H2'	1:L1:637:C:C6	2.38	0.58
2:L2:13:A:H2'	2:L2:14:OMC:H5''	1.84	0.58
2:L2:749:G:HO2'	2:L2:750:U:H6	1.49	0.58
6:L6:47:G:N2	14:LF:185:LYS:HD2	2.18	0.58
7:L7:29:C:OP1	17:LI:36:GLN:NE2	2.33	0.58
51:S1:1724:G:O2'	67:SL:32:GLN:OE1	2.13	0.58
51:S1:1881:G:H2'	51:S1:1882:A:C8	2.37	0.58
85:Sd:21:ALA:HA	85:Sd:76:MET:HA	1.84	0.58
2:L2:66:A:H2'	2:L2:67:G:O4'	2.02	0.58
2:L2:422:U:OP1	9:LA:54:ARG:NH2	2.28	0.58
59:SD:30:CYS:SG	86:Se:36:LYS:NZ	2.69	0.58
76:SU:87:ARG:HB2	76:SU:87:ARG:HH11	1.67	0.58
81:SZ:121:ASN:HB3	81:SZ:129:LYS:HE3	1.85	0.58
2:L2:1407:A:N7	9:LA:215:ASN:ND2	2.50	0.58
4:L4:126:G:O2'	4:L4:127:G:N2	2.37	0.58
12:LD:111:HIS:HB3	12:LD:127:MET:HE1	1.84	0.58
51:S1:1905:C:O2'	51:S1:1906:G:O5'	2.18	0.58
33:LY:77:HIS:HB3	38:Ld:37:ARG:HD3	1.86	0.58
51:S1:482:U:H3	51:S1:512:A2M:H62	1.52	0.58
87:Sf:97:ALA:HA	87:Sf:100:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:472:U:H2'	1:L1:473:A:C8	2.38	0.58
1:L1:1707:U:H2'	1:L1:1708:G:C8	2.38	0.58
2:L2:1450:G:O2'	6:L6:14:A:N6	2.30	0.58
5:L5:64:G:OP2	5:L5:64:G:N2	2.31	0.58
51:S1:450:A:H2'	51:S1:451:C:C6	2.39	0.58
54:S4:16:U:H3	54:S4:60:U:H6	1.51	0.58
54:S4:38:A:H2	70:SO:59:ARG:NH2	2.01	0.58
2:L2:515:U:O2'	2:L2:517:A:N7	2.31	0.58
51:S1:1101:A:H2'	51:S1:1102:G:C4	2.39	0.58
51:S1:1781:U:O2'	51:S1:1782:G:N7	2.31	0.58
62:SG:197:ASP:OD1	62:SG:197:ASP:N	2.34	0.58
78:SW:24:TYR:HB3	78:SW:32:LEU:HD11	1.86	0.58
2:L2:1469:A:C2	41:Lg:6:VAL:HG11	2.39	0.58
51:S1:1551:G:H5''	74:SS:30:ALA:HB2	1.86	0.58
51:S1:1572:C:H5	51:S1:1615:G:H22	1.51	0.58
51:S1:1603:U:H2'	51:S1:1604:C:C6	2.39	0.58
88:Sg:171:SER:OG	88:Sg:172:TRP:N	2.35	0.58
1:L1:31:G:H21	1:L1:49:C:H5	1.51	0.58
1:L1:494:A:OP1	14:LF:82:ARG:NE	2.34	0.58
1:L1:600:C:H2'	1:L1:601:G:H4'	1.85	0.58
2:L2:780:G:H2'	2:L2:781:G:H8	1.69	0.58
47:Lm:96:CYS:SG	47:Lm:99:CYS:N	2.62	0.58
51:S1:2121:C:H2'	51:S1:2122:G:H8	1.68	0.58
52:S2:66:U:H3'	52:S2:67:C:H5''	1.86	0.58
1:L1:415:A:H4'	1:L1:416:A:H5'	1.86	0.58
1:L1:700:A:N1	1:L1:845:OMU:H5	2.18	0.58
1:L1:1629:G:O6	42:Lh:11:ARG:NH2	2.35	0.58
2:L2:958:A:H2'	2:L2:959:A:H8	1.69	0.58
30:LV:94:ASN:HB3	30:LV:97:GLU:HG2	1.86	0.58
51:S1:21:U:O2	59:SD:15:ARG:NH2	2.37	0.58
51:S1:2016:C:OP1	74:SS:20:ARG:NH2	2.37	0.58
61:SF:154:GLY:N	61:SF:165:THR:O	2.31	0.58
38:Ld:48:ASN:ND2	38:Ld:73:SER:O	2.36	0.58
42:Lh:90:ASP:OD2	42:Lh:94:ARG:NH1	2.37	0.58
51:S1:1695:C:H5''	68:SM:49:GLY:HA3	1.86	0.58
51:S1:1701:A:H2'	51:S1:1702:A:C8	2.39	0.58
59:SD:6:ASN:OD1	59:SD:6:ASN:N	2.37	0.58
1:L1:592:G:H2'	1:L1:593:C:C6	2.39	0.57
21:LM:123:MET:HB3	21:LM:128:LYS:HG3	1.86	0.57
31:LW:24:ARG:NH1	31:LW:72:ARG:O	2.33	0.57
51:S1:672:G:N1	51:S1:1217:A:OP1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1696:A:N1	51:S1:1779:U:H5	2.02	0.57
78:SW:44:VAL:O	78:SW:49:ARG:NH1	2.38	0.57
1:L1:155:A:N7	17:LI:104:SER:OG	2.37	0.57
1:L1:157:U:H5'	1:L1:158:A:H5'	1.86	0.57
21:LM:5:MET:O	21:LM:9:GLU:HG2	2.05	0.57
51:S1:1132:G:H2'	51:S1:1133:U:C6	2.39	0.57
53:S3:9:G:O2'	53:S3:10:G:N7	2.38	0.57
67:SL:23:ALA:HB2	67:SL:75:VAL:HG13	1.86	0.57
88:Sg:102:LYS:HD2	88:Sg:104:LEU:HD11	1.85	0.57
2:L2:1124:A:H2'	2:L2:1125:G:C8	2.39	0.57
42:Lh:12:MET:SD	42:Lh:19:ASN:CG	2.86	0.57
51:S1:340:G:HO2'	51:S1:341:A:H8	1.51	0.57
88:Sg:178:VAL:O	88:Sg:187:GLU:N	2.35	0.57
1:L1:1276:U:H5	1:L1:1353:A:N1	2.01	0.57
51:S1:1166:C:H2'	51:S1:1167:A:C8	2.39	0.57
51:S1:1863:G:OP2	73:SR:142:ARG:NH1	2.38	0.57
51:S1:1959:G:H2'	51:S1:1960:G:H5'	1.86	0.57
1:L1:1092:U:O2'	1:L1:1093:U:H6	1.87	0.57
21:LM:121:VAL:CG1	21:LM:131:GLU:HG3	2.33	0.57
51:S1:522:A:OP1	59:SD:144:SER:OG	2.20	0.57
51:S1:955:A:C8	51:S1:956:A:C8	2.93	0.57
69:SN:84:ARG:NH1	69:SN:93:ALA:O	2.37	0.57
71:SP:67:ARG:HD3	71:SP:115:ILE:HG12	1.87	0.57
19:LK:136:PRO:HB3	19:LK:141:LYS:HB3	1.85	0.57
51:S1:484:G:H1	51:S1:511:C:H5	1.52	0.57
51:S1:615:C:H2'	51:S1:616:A:C8	2.39	0.57
77:SV:22:SER:O	88:Sg:214:LYS:NZ	2.37	0.57
1:L1:55:A:O2'	1:L1:56:G:H5'	2.05	0.57
1:L1:882:A:N1	1:L1:914:U:H5	2.03	0.57
2:L2:558:A:OP1	2:L2:560:OMU:H5	2.04	0.57
5:L5:25:A:H5''	10:LB:179:LYS:HG3	1.87	0.57
60:SE:163:GLU:HG2	60:SE:165:LYS:HB3	1.86	0.57
88:Sg:239:ASN:ND2	88:Sg:282:CYS:O	2.31	0.57
1:L1:1687:G:H22	1:L1:1705:G:H1	1.51	0.57
2:L2:603:A:H5'	28:LT:137:THR:HG23	1.87	0.57
38:Ld:59:GLU:OE2	38:Ld:71:HIS:NE2	2.33	0.57
51:S1:146:U:C4'	62:SG:183:ILE:HD13	2.19	0.57
51:S1:527:A:H4'	59:SD:119:LYS:HZ3	1.69	0.57
51:S1:2101:C:OP2	62:SG:32:ARG:NH1	2.26	0.57
68:SM:31:SER:OG	68:SM:104:GLU:OE1	2.23	0.57
1:L1:93:G:H2'	1:L1:94:A:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:112:U:H3	1:L1:357:A:H62	1.53	0.57
34:LZ:22:ARG:HB3	40:Lf:76:PRO:HG2	1.86	0.57
51:S1:581:A:OP1	59:SD:167:ARG:NH1	2.37	0.57
51:S1:2198:A:N6	83:Sb:9:GLY:HA3	2.20	0.57
1:L1:1685:G:H22	1:L1:1707:U:H3	1.51	0.56
2:L2:1502:G:OP2	39:Le:33:ARG:NH1	2.38	0.56
4:L4:92:U:H2'	4:L4:93:U:C6	2.39	0.56
51:S1:1589:G:H1	51:S1:1600:C:H5	1.52	0.56
56:SA:123:MET:HE3	56:SA:163:VAL:HG22	1.85	0.56
58:SC:91:GLU:OE1	58:SC:197:ASN:ND2	2.38	0.56
58:SC:212:PRO:HD3	77:SV:19:LYS:HD3	1.86	0.56
7:L7:102:G:OP2	7:L7:104:A:O2'	2.23	0.56
25:LQ:105:LEU:HD13	25:LQ:135:LYS:HE2	1.86	0.56
51:S1:1853:U:OP1	74:SS:10:ARG:NH1	2.38	0.56
73:SR:16:LEU:HG	73:SR:17:LEU:HD12	1.87	0.56
88:Sg:81:LEU:HD11	88:Sg:122:ILE:HG12	1.86	0.56
2:L2:447:G:H1'	9:LA:222:PRO:HG2	1.88	0.56
4:L4:170:G:H4'	4:L4:171:A:H3'	1.86	0.56
26:LR:70:LYS:O	26:LR:74:ARG:NH2	2.38	0.56
43:Li:95:GLU:OE1	43:Li:98:ARG:NH2	2.38	0.56
44:Lj:4:GLY:O	44:Lj:8:MET:HG2	2.05	0.56
51:S1:128:C:H4'	51:S1:129:U:O5'	2.05	0.56
51:S1:449:U:H2'	51:S1:450:A:H8	1.69	0.56
51:S1:846:U:H2'	51:S1:847:A:C8	2.39	0.56
51:S1:1905:C:O2'	51:S1:1906:G:H8	1.88	0.56
85:Sd:26:ILE:HD11	85:Sd:73:LEU:HD21	1.87	0.56
87:Sf:97:ALA:HA	87:Sf:100:TYR:HD2	1.70	0.56
3:L3:118:G:H2'	3:L3:119:C:O2	2.05	0.56
51:S1:608:C:H2'	51:S1:609:U:H4'	1.86	0.56
62:SG:47:LYS:HE3	62:SG:48:GLY:H	1.71	0.56
73:SR:24:LYS:NZ	82:Sa:38:ASN:O	2.37	0.56
1:L1:1549:U:H2'	1:L1:1550:A:C8	2.40	0.56
2:L2:1412:U:H2'	2:L2:1413:PSU:C6	2.40	0.56
5:L5:65:U:O2	5:L5:93:G:N2	2.36	0.56
21:LM:114:ARG:HG3	21:LM:137:PRO:HG3	1.87	0.56
40:Lf:33:TRP:O	40:Lf:34:ARG:NH1	2.38	0.56
42:Lh:43:ILE:HG22	42:Lh:54:LEU:HD12	1.87	0.56
51:S1:528:G:O6	51:S1:553:U:O4	2.24	0.56
51:S1:2132:C:H2'	51:S1:2133:G:O4'	2.05	0.56
62:SG:80:ARG:HG2	62:SG:87:THR:HA	1.86	0.56
1:L1:237:U:OP1	31:LW:57:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:398:G:N2	1:L1:401:A:OP2	2.34	0.56
1:L1:694:U:H2'	1:L1:695:OMC:C6	2.40	0.56
51:S1:259:C:H2'	51:S1:260:A:C8	2.40	0.56
60:SE:66:LEU:HD13	81:SZ:22:LEU:HD12	1.88	0.56
64:SI:52:VAL:HG22	64:SI:61:VAL:HB	1.88	0.56
68:SM:40:ALA:HB3	68:SM:47:ILE:HD11	1.86	0.56
6:L6:68:A:H5'	14:LF:47:ARG:NH2	2.21	0.56
8:L8:11:G:OP2	23:LO:22:ARG:NH1	2.39	0.56
11:LC:299:VAL:HG21	24:LP:138:PRO:HB2	1.86	0.56
31:LW:26:VAL:O	31:LW:29:SER:OG	2.23	0.56
51:S1:1586:A:OP2	51:S1:1597:G:O2'	2.15	0.56
51:S1:2121:C:H2'	51:S1:2122:G:C8	2.41	0.56
57:SB:73:ASN:HD21	61:SF:260:ALA:HB2	1.71	0.56
87:Sf:122:HIS:CE1	87:Sf:145:LEU:HD13	2.39	0.56
2:L2:1522:U:H2'	2:L2:1523:C:C6	2.41	0.56
5:L5:68:G:H5'	66:SK:92:ARG:HG3	1.88	0.56
20:LL:74:ASN:OD1	20:LL:112:ASN:HB3	2.05	0.56
62:SG:51:PHE:HB3	62:SG:114:VAL:HB	1.87	0.56
2:L2:1314:C:O2'	52:S2:75:C:O2	2.23	0.56
6:L6:42:A:O2'	19:LK:95:ARG:HG2	2.06	0.56
20:LL:92:LYS:HG3	20:LL:138:GLY:HA3	1.88	0.56
24:LP:165:PRO:HB3	24:LP:193:LYS:HB2	1.88	0.56
37:Lc:159:TYR:OH	37:Lc:192:GLU:OE2	2.17	0.56
51:S1:294:G:O2'	51:S1:295:A:OP1	2.23	0.56
59:SD:65:HIS:HB3	59:SD:68:ARG:HB3	1.87	0.56
62:SG:41:ILE:H	62:SG:41:ILE:HD12	1.70	0.56
66:SK:119:ILE:HD11	66:SK:166:ARG:HD3	1.87	0.56
88:Sg:82:THR:HB	88:Sg:92:TRP:HE1	1.70	0.56
1:L1:576:G:O2'	1:L1:577:C:OP1	2.18	0.56
2:L2:972:C:N4	38:Ld:49:ASN:O	2.38	0.56
3:L3:138:U:H2'	3:L3:139:C:O2	2.05	0.56
9:LA:179:VAL:HG13	9:LA:184:ASN:HB2	1.86	0.56
40:Lf:77:ILE:HD11	40:Lf:97:ILE:HG12	1.88	0.56
49:Lo:10:VAL:HG13	49:Lo:11:MET:HE2	1.87	0.56
62:SG:101:ARG:HH22	62:SG:106:ALA:HB3	1.70	0.56
1:L1:226:C:H2'	1:L1:227:U:H6	1.71	0.55
1:L1:344:A:N1	2:L2:1221:U:H5	2.04	0.55
1:L1:1627:U:OP1	30:LV:126:TYR:OH	2.22	0.55
2:L2:133:G:OP1	25:LQ:104:ARG:NH1	2.39	0.55
2:L2:1020:C:O2'	2:L2:1021:A:O5'	2.23	0.55
13:LE:152:GLN:O	13:LE:156:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1362:A:OP1	84:Sc:17:ARG:NH2	2.35	0.55
56:SA:88:PHE:HB3	56:SA:100:THR:HB	1.88	0.55
66:SK:34:ALA:HB2	66:SK:56:ARG:HD3	1.88	0.55
69:SN:15:ARG:HB3	69:SN:37:LEU:HD11	1.88	0.55
1:L1:1257[A]:U:H4'	1:L1:1258:A:O5'	2.04	0.55
23:LO:40:ASP:HB2	23:LO:43:LYS:HG3	1.89	0.55
34:LZ:67:ASP:N	34:LZ:67:ASP:OD1	2.39	0.55
51:S1:448:C:O2'	62:SG:95:ARG:O	2.21	0.55
51:S1:635:G:H5''	86:Se:23:LYS:HB2	1.87	0.55
51:S1:1714:C:H5''	79:SX:8:ILE:HD11	1.88	0.55
60:SE:191:GLU:HB2	60:SE:229:LEU:HD22	1.87	0.55
61:SF:197:LYS:NZ	61:SF:201:GLU:OE2	2.39	0.55
62:SG:23:LEU:HD12	62:SG:28:LEU:HD21	1.87	0.55
72:SQ:55:ASP:OD1	72:SQ:55:ASP:N	2.39	0.55
1:L1:179:G:H2'	1:L1:180:A:C8	2.41	0.55
1:L1:739:U:H2'	1:L1:740:C:C6	2.41	0.55
2:L2:419:G:H5''	9:LA:18:VAL:HG23	1.88	0.55
4:L4:51:U:H2'	4:L4:52:A:H8	1.70	0.55
18:LJ:12:ARG:HD2	18:LJ:13:PHE:O	2.07	0.55
51:S1:2012:A:H2'	51:S1:2013:G:C8	2.40	0.55
56:SA:169:ARG:O	56:SA:173:MET:HG3	2.07	0.55
78:SW:48:ALA:O	78:SW:52:MET:HG3	2.07	0.55
1:L1:1602:C:H2'	1:L1:1603:G:C8	2.41	0.55
2:L2:953:U:N3	2:L2:954:A:N7	2.54	0.55
51:S1:374:U:H2'	51:S1:375:G:C8	2.42	0.55
51:S1:639:C:H2'	51:S1:640:A:H8	1.71	0.55
51:S1:1836:G:O6	69:SN:71:TYR:OH	2.17	0.55
51:S1:2085:A:H2'	51:S1:2086:A:C8	2.41	0.55
1:L1:1041:U:H4'	27:LS:100:ARG:HB2	1.89	0.55
18:LJ:8:VAL:HB	18:LJ:127:LEU:HD13	1.88	0.55
51:S1:1716:A:H61	79:SX:26:ARG:HH22	1.53	0.55
64:SI:82:THR:O	64:SI:86:GLU:HG3	2.06	0.55
72:SQ:54:LEU:HA	72:SQ:59:ALA:HB2	1.88	0.55
88:Sg:109:ASP:OD2	88:Sg:127:ARG:NH1	2.40	0.55
2:L2:1132:A:H8	2:L2:1132:A:OP1	1.89	0.55
22:LN:182:GLU:OE1	22:LN:185:ARG:NH2	2.40	0.55
51:S1:307:C:OP1	51:S1:308:C:N4	2.39	0.55
51:S1:2164:U:OP2	55:S5:5:A:O2'	2.24	0.55
80:SY:62:TYR:O	80:SY:66:GLN:HG2	2.06	0.55
4:L4:180:C:H1'	5:L5:5:C:H1'	1.87	0.55
5:L5:4:A:H62	5:L5:134:C:H5	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Lh:12:MET:HE1	42:Lh:19:ASN:HB2	1.89	0.55
1:L1:318:G:N7	21:LM:183:LYS:HE3	2.22	0.55
1:L1:472:U:H2'	1:L1:473:A:H8	1.72	0.55
1:L1:715:G:H2'	1:L1:716:A:O4'	2.07	0.55
2:L2:1485:G:C4	19:LK:164:MET:HG2	2.42	0.55
51:S1:478:C:H5''	71:SP:48:LYS:HG3	1.88	0.55
51:S1:525:A:H5'	86:Se:34:ALA:HB2	1.89	0.55
1:L1:214:C:C2'	1:L1:215:U:H5'	2.36	0.55
1:L1:904:G:N7	49:Lo:2:ALA:N	2.55	0.55
2:L2:772:A:OP1	9:LA:37:ARG:NH2	2.40	0.55
11:LC:91:PHE:O	11:LC:99:ARG:NH2	2.39	0.55
50:Lp:25:VAL:HG22	50:Lp:72:LEU:HD23	1.89	0.55
51:S1:1896:G:H1	51:S1:1905:C:H5	1.55	0.55
51:S1:2012:A:H2'	51:S1:2013:G:H8	1.71	0.55
1:L1:12:U:H2'	1:L1:13:G:H8	1.71	0.55
1:L1:540:A:N6	26:LR:68:ASP:O	2.37	0.55
1:L1:1688:G:H1	1:L1:1704:A:H61	1.54	0.55
40:Lf:10:ILE:HG12	40:Lf:64:THR:HB	1.89	0.55
51:S1:263:G:H5'	89:Sh:169:ARG:HG3	1.89	0.55
51:S1:1572:C:H41	51:S1:1615:G:H1	1.54	0.55
52:S2:49:C:H1'	52:S2:65:G:H1	1.69	0.55
72:SQ:30:VAL:HG21	72:SQ:63:ILE:HD11	1.89	0.55
88:Sg:105:LYS:HG3	88:Sg:132:ARG:HD3	1.88	0.55
1:L1:1160:G:OP1	37:Lc:119:ARG:NH2	2.40	0.54
1:L1:1728:A:HO2'	1:L1:1729:A:H8	1.55	0.54
14:LF:30:ARG:NH2	41:Lg:144:ILE:OXT	2.38	0.54
15:LG:220:ASN:O	15:LG:225:SER:OG	2.20	0.54
51:S1:641:A:O2'	51:S1:645:C:OP1	2.25	0.54
51:S1:1974:A:OP2	78:SW:54:ARG:NH1	2.40	0.54
71:SP:139:GLU:OE1	71:SP:139:GLU:N	2.40	0.54
28:LT:39:MET:HE1	28:LT:47:LEU:HD22	1.88	0.54
73:SR:88:GLN:O	73:SR:96:THR:OG1	2.19	0.54
1:L1:1352:C:H2'	1:L1:1353:A:H8	1.73	0.54
2:L2:1086:G:H4'	2:L2:1179:A:O2'	2.07	0.54
3:L3:105:C:H2'	3:L3:106:U:C6	2.42	0.54
10:LB:59:ASP:OD2	10:LB:364:LYS:HD2	2.06	0.54
16:LH:131:VAL:HG12	16:LH:132:ARG:HG3	1.89	0.54
51:S1:38:OMC:O3'	59:SD:5:ASN:ND2	2.39	0.54
51:S1:1360:U:H4'	51:S1:1361:U:O5'	2.08	0.54
64:SI:78:GLN:O	64:SI:82:THR:OG1	2.19	0.54
82:Sa:55:PRO:O	82:Sa:56:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:29:C:OP1	2:L2:32:C:N4	2.36	0.54
2:L2:652:C:H2'	2:L2:653:C:C6	2.42	0.54
1:L1:460:A:H5''	1:L1:662:C:H5''	1.90	0.54
2:L2:653:C:H2'	2:L2:654:U:H6	1.71	0.54
2:L2:659:A:H2'	2:L2:660:G:H8	1.73	0.54
51:S1:1014:C:H2'	51:S1:1015:G:C8	2.42	0.54
51:S1:1287:U:H2'	51:S1:1288:G:C8	2.42	0.54
60:SE:156:THR:HG23	60:SE:170:ILE:HD12	1.90	0.54
71:SP:107:ARG:HB3	71:SP:110:HIS:HB3	1.90	0.54
72:SQ:103:LEU:HD22	72:SQ:116:LEU:HB2	1.90	0.54
2:L2:343:U:H2'	2:L2:344:G:C8	2.42	0.54
49:Lo:26:ALA:O	49:Lo:30:GLU:HG3	2.08	0.54
51:S1:2118:G:H1'	51:S1:2119:C:H5'	1.90	0.54
57:SB:31:ARG:NH1	57:SB:47:GLU:O	2.40	0.54
66:SK:61:ASP:OD1	66:SK:61:ASP:N	2.41	0.54
88:Sg:154:SER:OG	88:Sg:197:VAL:O	2.21	0.54
89:Sh:182:ALA:O	89:Sh:186:PHE:N	2.40	0.54
1:L1:306:G:OP1	21:LM:47:LYS:HE2	2.08	0.54
59:SD:45:ASN:O	59:SD:49:SER:OG	2.25	0.54
68:SM:24:ARG:HD2	68:SM:79:LEU:HD21	1.90	0.54
72:SQ:87:ASP:OD1	72:SQ:87:ASP:N	2.41	0.54
76:SU:87:ARG:HB2	76:SU:87:ARG:NH1	2.22	0.54
2:L2:749:G:O2'	2:L2:750:U:H5'	2.08	0.54
15:LG:113:VAL:HG11	15:LG:127:THR:HG22	1.89	0.54
27:LS:56:TYR:O	27:LS:60:ARG:NH1	2.41	0.54
51:S1:511:C:O2'	51:S1:572:A:N6	2.41	0.54
51:S1:2039:C:H2'	51:S1:2040:C:O2	2.07	0.54
52:S2:54:U:C5	52:S2:57:G:H5''	2.43	0.54
59:SD:49:SER:O	59:SD:53:ARG:HG3	2.07	0.54
1:L1:980:A:O2'	44:Lj:49:TRP:O	2.26	0.54
2:L2:403:G:N7	9:LA:152:SER:OG	2.35	0.54
6:L6:49:C:N4	41:Lg:29:LYS:O	2.40	0.54
51:S1:16:G:H2'	51:S1:17:C:C6	2.42	0.54
51:S1:1523:A:H2'	51:S1:1524:G:H8	1.73	0.54
81:SZ:18:LYS:HB3	81:SZ:27:GLN:HG3	1.89	0.54
88:Sg:47:ARG:HD2	88:Sg:54:TYR:HA	1.90	0.54
1:L1:1667:G:OP2	21:LM:34:HIS:NE2	2.39	0.54
3:L3:203:A:H2'	3:L3:204:A:C8	2.42	0.54
10:LB:95:THR:OG1	10:LB:98:GLY:O	2.25	0.54
51:S1:1945:A:OP1	63:SH:77:ARG:NH2	2.41	0.54
56:SA:207:LEU:HD23	56:SA:208:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:317:U:O2'	1:L1:319:G:N7	2.35	0.53
2:L2:340:A:H4'	2:L2:341:A:H5''	1.89	0.53
2:L2:743:C:H2'	2:L2:744:G:C8	2.43	0.53
3:L3:20:C:H5	42:Lh:71:HIS:NE2	2.06	0.53
6:L6:11:G:OP1	41:Lg:36:LYS:NZ	2.41	0.53
28:LT:16:LYS:O	28:LT:101:ASN:ND2	2.39	0.53
51:S1:30:G:OP1	71:SP:124:LYS:NZ	2.41	0.53
51:S1:413:A:H2	65:SJ:91:LYS:HZ1	1.56	0.53
51:S1:1984:C:OP1	73:SR:40:ARG:HD3	2.08	0.53
1:L1:70:C:H1'	17:LI:66:PRO:O	2.08	0.53
9:LA:246:ILE:HD12	9:LA:250:LYS:HE2	1.89	0.53
48:Ln:13:LYS:NZ	51:S1:2177:G:N7	2.50	0.53
51:S1:610:G:H2'	51:S1:611:G:C8	2.44	0.53
51:S1:815:U:O2'	51:S1:817:A:OP2	2.25	0.53
62:SG:138:PRO:HG2	62:SG:144:ILE:HD13	1.90	0.53
1:L1:650:G:O2'	1:L1:652:A:H5'	2.09	0.53
16:LH:79:ARG:HA	16:LH:88:PRO:HD2	1.90	0.53
29:LU:13:TYR:HE2	29:LU:15:ARG:HG3	1.73	0.53
49:Lo:32:SER:OG	49:Lo:69:TYR:O	2.18	0.53
51:S1:519:A:O2'	59:SD:8:ASN:O	2.20	0.53
51:S1:1908:A:H5''	51:S1:1909:C:C5	2.40	0.53
60:SE:97:ARG:HH22	60:SE:119:LYS:HA	1.72	0.53
62:SG:160:VAL:HG22	62:SG:162:ARG:NH1	2.22	0.53
64:SI:106:PRO:HD2	64:SI:112:LEU:HD12	1.91	0.53
75:ST:15:ALA:HB1	84:Sc:27:GLN:HG2	1.90	0.53
1:L1:1374:C:H2'	1:L1:1375:G:O4'	2.09	0.53
2:L2:653:C:H2'	2:L2:654:U:C6	2.44	0.53
3:L3:129:A:O4'	38:Ld:54:ARG:NH2	2.36	0.53
4:L4:77:U:C5	10:LB:53:MET:HE2	2.43	0.53
5:L5:122:U:O2'	5:L5:123:G:H5'	2.08	0.53
33:LY:44:ALA:HB1	33:LY:112:VAL:HG11	1.91	0.53
39:Le:125:ASN:HB3	39:Le:170:ILE:HD11	1.90	0.53
51:S1:1579:A:H1'	51:S1:1581:G:N3	2.23	0.53
51:S1:1718:A:O2'	51:S1:1949:A:N6	2.42	0.53
57:SB:167:ASN:OD1	57:SB:169:ARG:NH1	2.41	0.53
67:SL:88:ARG:NH2	67:SL:119:ASP:OD2	2.42	0.53
2:L2:603:A:H2'	2:L2:604:A2M:H8	1.89	0.53
10:LB:80:GLU:HG3	10:LB:324:VAL:HG13	1.90	0.53
51:S1:886:U:H3'	60:SE:238:LYS:NZ	2.23	0.53
51:S1:994:U:H3	51:S1:1018:G:H1	1.56	0.53
80:SY:77:THR:OG1	80:SY:83:MET:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Sg:113:VAL:HG12	88:Sg:124:SER:HB2	1.91	0.53
1:L1:1084:U:H3'	1:L1:1085:C:H5''	1.90	0.53
2:L2:13:A:C2'	2:L2:14:OMC:H5''	2.39	0.53
2:L2:847:U:H2'	2:L2:848:C:C6	2.44	0.53
2:L2:974:G:N2	33:LY:133:ARG:O	2.40	0.53
7:L7:18:G:H2'	7:L7:19:A:C8	2.43	0.53
52:S2:52:G:H2'	52:S2:53:G:H8	1.69	0.53
54:S4:62:C:H2'	54:S4:63:G:H8	1.73	0.53
61:SF:149:VAL:HG12	80:SY:32:HIS:CD2	2.44	0.53
66:SK:159:GLN:OE1	66:SK:159:GLN:N	2.41	0.53
2:L2:974:G:O2'	2:L2:975:A:H8	1.92	0.53
2:L2:1274:C:O2	22:LN:158:LYS:NZ	2.41	0.53
16:LH:57:GLU:HG2	16:LH:58:GLN:HG2	1.91	0.53
51:S1:507:G:OP2	81:SZ:111:ARG:NH1	2.42	0.53
86:Se:41:THR:O	86:Se:46:SER:N	2.41	0.53
1:L1:881:A:O2'	2:L2:49:A:OP1	2.27	0.53
22:LN:54:SER:OG	22:LN:130:ARG:O	2.26	0.53
51:S1:68:A:OP2	62:SG:175:LYS:NZ	2.42	0.53
51:S1:699:A:N6	51:S1:747:C:H42	2.07	0.53
51:S1:1150:U:H1'	51:S1:1153:A:N7	2.23	0.53
1:L1:601:G:N2	1:L1:604:C:O2'	2.42	0.53
1:L1:1741:A:C3'	1:L1:1742:G:H5'	2.38	0.53
41:Lg:3:THR:HG22	41:Lg:7:HIS:HD2	1.74	0.53
44:Lj:39:TYR:CD1	44:Lj:40:PRO:HA	2.43	0.53
51:S1:600:OMG:N2	51:S1:622:C:O2	2.19	0.53
51:S1:1919:C:H5	79:SX:45:ASN:H	1.55	0.53
51:S1:2095:A:H5'	66:SK:58:LEU:HD21	1.90	0.53
53:S3:16:C:H1'	53:S3:59:A:C2	2.41	0.53
1:L1:369:A:O2'	44:Lj:58:ARG:NH2	2.41	0.53
1:L1:1018:A:N3	27:LS:81:ARG:NH2	2.57	0.53
2:L2:741:C:H2'	2:L2:742:U:C6	2.44	0.53
2:L2:1365:C:H2'	2:L2:1366:C:C6	2.44	0.53
4:L4:167:C:H2'	4:L4:168:A:O4'	2.09	0.53
30:LV:57:SER:HB3	30:LV:60:ILE:HG12	1.91	0.53
51:S1:2198:A:H62	83:Sb:9:GLY:HA3	1.75	0.53
70:SO:92:ALA:H	70:SO:126:THR:HB	1.73	0.53
1:L1:179:G:H2'	1:L1:180:A:H8	1.73	0.52
1:L1:505:U:H4'	11:LC:344:ARG:HG2	1.91	0.52
1:L1:836:G:OP1	24:LP:63:SER:OG	2.18	0.52
2:L2:760:U:H5'	15:LG:69:ARG:HG3	1.89	0.52
51:S1:95:C:O2'	51:S1:469:G:H5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:258:C:H2'	51:S1:259:C:C6	2.44	0.52
51:S1:701:G:N2	51:S1:745:G:H22	2.08	0.52
51:S1:1170:A:H2'	51:S1:1171:A:C8	2.43	0.52
55:S5:12:A:O2'	58:SC:145:ARG:NH1	2.39	0.52
61:SF:160:ILE:O	61:SF:186:ARG:NH2	2.42	0.52
1:L1:2:C:N4	7:L7:169:A:O2'	2.39	0.52
56:SA:67:GLU:OE1	70:SO:89:LYS:NZ	2.43	0.52
62:SG:140:ARG:HB3	62:SG:143:LYS:HB2	1.91	0.52
84:Sc:39:PRO:HG2	84:Sc:62:LYS:HE2	1.92	0.52
2:L2:1337:C:O2'	13:LE:172:ARG:NH2	2.42	0.52
5:L5:62:C:H3'	5:L5:63:G:N2	2.24	0.52
7:L7:43:A2M:N1	7:L7:100:U:H5	2.06	0.52
33:LY:108:SER:O	33:LY:112:VAL:HG23	2.08	0.52
60:SE:121:MET:HG3	60:SE:138:THR:HG21	1.92	0.52
82:Sa:50:LEU:HD12	82:Sa:54:VAL:HG21	1.90	0.52
89:Sh:140:VAL:HG21	89:Sh:157:PHE:HZ	1.75	0.52
1:L1:1159:A:N6	37:Lc:117:ARG:O	2.39	0.52
1:L1:1680:U:O4	1:L1:1712:G:O6	2.27	0.52
2:L2:1385:G:C2	10:LB:255:ALA:HB1	2.45	0.52
39:Le:48:GLU:HA	39:Le:51:LYS:HD2	1.92	0.52
51:S1:17:C:H2'	51:S1:18:OMC:C6	2.45	0.52
51:S1:1966:A:N1	51:S1:1983:U:H5	2.07	0.52
64:SI:162:ARG:HG3	64:SI:166:GLU:HG3	1.91	0.52
2:L2:342:U:HO2'	2:L2:343:U:H6	1.57	0.52
2:L2:512:PSU:OP1	53:S3:24:U:O2'	2.28	0.52
5:L5:6:G:H2'	5:L5:7:U:C6	2.44	0.52
51:S1:2015:U:H5''	51:S1:2016:C:H5	1.74	0.52
51:S1:2188:U:H2'	51:S1:2189:G:H8	1.74	0.52
56:SA:211:GLU:OE2	56:SA:213:ARG:NH2	2.39	0.52
10:LB:57:VAL:HB	10:LB:365:PHE:HB3	1.92	0.52
11:LC:316:PRO:HG2	11:LC:328:ARG:HH22	1.74	0.52
16:LH:204:ALA:O	16:LH:208:MET:HG2	2.08	0.52
51:S1:994:U:H2'	51:S1:995:U:H6	1.74	0.52
51:S1:1108:A:H5''	75:ST:16:LEU:HD12	1.92	0.52
62:SG:228:HIS:HA	62:SG:231:LYS:HG2	1.91	0.52
79:SX:74:LEU:HD13	79:SX:120:LEU:HD22	1.91	0.52
1:L1:1527:OMC:HM22	11:LC:94:MET:HG3	1.90	0.52
2:L2:1253:OMG:HM21	2:L2:1255:A:H2'	1.92	0.52
2:L2:1404:G:H5'	9:LA:220:GLY:HA3	1.91	0.52
7:L7:93:C:H2'	7:L7:94:G:H5''	1.92	0.52
51:S1:950:U:H3'	51:S1:951:U:H5''	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1694:C:O2	68:SM:52:ARG:NH1	2.42	0.52
65:SJ:67:GLY:HA3	80:SY:26:THR:HB	1.91	0.52
87:Sf:135:LYS:H	87:Sf:135:LYS:HD2	1.75	0.52
88:Sg:246:ASN:OD1	88:Sg:247:ARG:HG3	2.10	0.52
1:L1:404:G:OP2	44:Lj:52:LYS:NZ	2.43	0.52
1:L1:1479:A:H5''	1:L1:1481:G:O4'	2.09	0.52
2:L2:598:A:H5''	28:LT:83:TRP:O	2.09	0.52
7:L7:70:C:H5''	31:LW:115:ILE:HD11	1.92	0.52
51:S1:1440:C:OP1	83:Sb:6:ARG:NH1	2.43	0.52
70:SO:96:VAL:HG12	70:SO:132:SER:HB2	1.92	0.52
2:L2:538:U:HO2'	51:S1:2076:U:HO2'	1.57	0.52
25:LQ:174:ARG:NH1	25:LQ:174:ARG:HB2	2.24	0.52
32:LX:98:ARG:HH21	62:SG:149:ASN:HD21	1.58	0.52
51:S1:308:C:OP1	51:S1:310:U:N3	2.31	0.52
52:S2:53:G:H2'	52:S2:54:U:H4'	1.92	0.52
54:S4:43:C:H2'	54:S4:44:G:H4'	1.92	0.52
78:SW:105:ASN:HB2	78:SW:129:SER:HA	1.91	0.52
89:Sh:163:GLN:N	89:Sh:176:TYR:O	2.43	0.52
5:L5:118:U:H5	10:LB:396:ARG:HD2	1.75	0.52
21:LM:160:GLU:OE2	21:LM:161:GLN:NE2	2.43	0.52
30:LV:90:ASP:HB3	30:LV:93:ALA:HB2	1.92	0.52
51:S1:694:U:H3	51:S1:751:G:H22	1.58	0.52
51:S1:1911:U:H2'	51:S1:1912:A:C8	2.44	0.52
69:SN:29:ARG:HD2	69:SN:47:ILE:HD13	1.92	0.52
1:L1:848:U:H2'	1:L1:849:U:C6	2.45	0.51
2:L2:1136:U:H2'	2:L2:1137:G:H8	1.71	0.51
38:Ld:18:LEU:HD23	38:Ld:21:LYS:HE3	1.92	0.51
51:S1:490:U:H2'	51:S1:491:G:O4'	2.10	0.51
51:S1:547:U:H3'	51:S1:548:G:H8	1.75	0.51
51:S1:1692:G:H2'	51:S1:1693:C:C6	2.45	0.51
61:SF:158:ASN:HB3	61:SF:160:ILE:HD13	1.92	0.51
82:Sa:64:ILE:O	82:Sa:68:ARG:HG2	2.10	0.51
1:L1:1281:A:O2'	1:L1:1348:A:N6	2.43	0.51
2:L2:406:G:H2'	2:L2:407:C:C6	2.44	0.51
2:L2:1076:G:N3	2:L2:1185:A2M:H2	2.25	0.51
6:L6:67:C:N4	41:Lg:96:ARG:O	2.38	0.51
51:S1:29:OMU:H2'	51:S1:30:G:H8	1.76	0.51
51:S1:814:G:N2	51:S1:819:G:O2'	2.32	0.51
53:S3:23:C:H2'	53:S3:24:U:C6	2.44	0.51
61:SF:55:VAL:HG21	61:SF:78:ILE:HG23	1.91	0.51
66:SK:161:GLU:HG3	66:SK:164:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Se:56:HIS:CB	86:Se:59:LYS:HG3	2.39	0.51
1:L1:822:C:H4'	1:L1:823:G:H5'	1.91	0.51
1:L1:1672:U:H2'	1:L1:1673:G:O4'	2.10	0.51
2:L2:1369:C:H5''	18:LJ:42:LYS:HD3	1.91	0.51
7:L7:39:G:H1'	7:L7:103:A:N6	2.24	0.51
51:S1:161:A:H2'	51:S1:162:A:O4'	2.11	0.51
52:S2:34:G:H2'	52:S2:35:A:C8	2.45	0.51
57:SB:41:ILE:HD11	57:SB:153:THR:HG23	1.91	0.51
1:L1:514:C:H5''	26:LR:70:LYS:HG3	1.91	0.51
1:L1:1243:G:OP2	26:LR:2:VAL:N	2.43	0.51
8:L8:31:A:H2'	8:L8:32:C:C6	2.45	0.51
13:LE:184:THR:OG1	13:LE:185:ASN:N	2.43	0.51
51:S1:99:U:H6	66:SK:21:HIS:HB2	1.75	0.51
51:S1:1215:U:OP1	51:S1:1280:A:O2'	2.27	0.51
51:S1:1595:G:N7	78:SW:59:ARG:NH2	2.59	0.51
67:SL:42:LEU:HA	67:SL:45:ILE:HD12	1.92	0.51
88:Sg:234:VAL:O	88:Sg:235:GLU:HG2	2.10	0.51
2:L2:958:A:H2'	2:L2:959:A:C8	2.45	0.51
2:L2:1469:A:H2	41:Lg:6:VAL:HG11	1.74	0.51
19:LK:129:ASP:OD2	41:Lg:22:SER:OG	2.18	0.51
51:S1:1154:A:H2'	51:S1:1155:U:H6	1.76	0.51
52:S2:2:C:H2'	52:S2:3:G:C8	2.45	0.51
52:S2:53:G:H22	52:S2:58:A:H62	1.57	0.51
59:SD:87:GLU:H	59:SD:87:GLU:CD	2.19	0.51
81:SZ:48:LYS:O	81:SZ:52:THR:OG1	2.25	0.51
89:Sh:140:VAL:HG12	89:Sh:202:VAL:CG1	2.31	0.51
10:LB:57:VAL:HG22	10:LB:73:VAL:HG22	1.93	0.51
22:LN:188:GLY:HA3	22:LN:212:MET:HE3	1.92	0.51
51:S1:667:U:H5''	51:S1:1277:A:C5	2.45	0.51
51:S1:1134:A:H5''	70:SO:127:PRO:HB3	1.92	0.51
51:S1:1652:A:H5'	51:S1:1653:U:OP2	2.11	0.51
1:L1:1032:G:O4'	36:Lb:26:PRO:HG3	2.10	0.51
1:L1:1098:A:N3	2:L2:1060:PSU:O2'	2.38	0.51
2:L2:1078:OMG:H5''	2:L2:1079:U:C6	2.46	0.51
12:LD:119:ASP:OD1	12:LD:121:SER:OG	2.29	0.51
13:LE:92:ARG:NH2	13:LE:140:LYS:O	2.44	0.51
21:LM:20:ARG:HH21	43:Li:55:PRO:HD3	1.76	0.51
22:LN:184:LEU:HB3	22:LN:190:LEU:HD13	1.92	0.51
73:SR:25:ARG:HB2	73:SR:30:ALA:HB2	1.91	0.51
1:L1:447:G:OP1	1:L1:1505:U:O2'	2.28	0.51
1:L1:1538:U:H2'	1:L1:1539:A2M:H8	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1101:A:O2'	2:L2:1102:C:OP1	2.23	0.51
12:LD:26:GLY:HA2	12:LD:67:ILE:HB	1.93	0.51
51:S1:901:U:H2'	51:S1:902:G:H8	1.76	0.51
51:S1:1227:G:H4'	51:S1:2179:A:H4'	1.92	0.51
61:SF:182:VAL:HB	61:SF:209:TYR:HB2	1.91	0.51
87:Sf:103:VAL:HG13	87:Sf:113:VAL:HG22	1.92	0.51
1:L1:1091:A:H2'	1:L1:1092:U:H5''	1.92	0.51
1:L1:1195:A:O2'	37:Lc:106:ASN:ND2	2.43	0.51
1:L1:1684:G:H1	1:L1:1708:G:H22	1.58	0.51
2:L2:473:C:H2'	2:L2:474:A:H8	1.76	0.51
23:LO:120:GLN:HB3	23:LO:123:LYS:HE2	1.92	0.51
51:S1:373:G:H5'	66:SK:98:LYS:HB3	1.92	0.51
51:S1:955:A:O2'	51:S1:956:A:H8	1.93	0.51
52:S2:9:A:H1'	52:S2:45:U:C2	2.46	0.51
54:S4:27:G:H2'	54:S4:28:G:H8	1.76	0.51
58:SC:205:ASP:OD1	58:SC:205:ASP:N	2.36	0.51
62:SG:105:LEU:HD13	62:SG:109:ILE:HD12	1.92	0.51
2:L2:6:A:H2'	2:L2:7:C:O4'	2.11	0.51
2:L2:1175:A:OP1	23:LO:182:ARG:HD3	2.11	0.51
4:L4:28:A:N1	4:L4:177:U:H5	2.09	0.51
10:LB:87:VAL:HG23	10:LB:163:ILE:HG22	1.92	0.51
11:LC:209:VAL:HG22	11:LC:228:ALA:HB3	1.91	0.51
14:LF:64:VAL:HG11	14:LF:101:ILE:HG21	1.92	0.51
30:LV:60:ILE:HD12	35:La:26:LYS:HE3	1.93	0.51
51:S1:625:G:H4'	51:S1:629:A:C4	2.46	0.51
71:SP:86:PRO:HD2	71:SP:130:LEU:HD23	1.93	0.51
6:L6:64:U:OP2	14:LF:78:ARG:NE	2.34	0.50
10:LB:77:THR:OG1	10:LB:333:GLY:O	2.27	0.50
16:LH:22:PRO:HG2	16:LH:24:ILE:HD11	1.93	0.50
18:LJ:106:ASN:ND2	18:LJ:110:GLU:O	2.44	0.50
51:S1:106:A:H2'	51:S1:107:G:C8	2.46	0.50
51:S1:1820:G:H21	58:SC:161:THR:HG23	1.75	0.50
54:S4:32:U:OP1	54:S4:32:U:H4'	2.09	0.50
58:SC:200:SER:O	58:SC:200:SER:OG	2.25	0.50
59:SD:170:ARG:O	59:SD:174:VAL:HG12	2.10	0.50
72:SQ:94:ARG:HD3	72:SQ:117:LYS:CD	2.41	0.50
74:SS:22:CYS:SG	74:SS:40:CYS:N	2.79	0.50
76:SU:137:GLU:HB3	76:SU:158:VAL:HB	1.93	0.50
88:Sg:148:GLY:HA2	88:Sg:179:TRP:HH2	1.76	0.50
2:L2:554:C:H3'	2:L2:555:A:H2'	1.93	0.50
2:L2:1258:A:H2	93:L2:1601:A1H4F:O23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1318:PSU:H1'	10:LB:255:ALA:HB3	1.93	0.50
3:L3:113:U:H2'	38:Ld:86:HIS:NE2	2.27	0.50
4:L4:148:C:O2'	47:Lm:111:ARG:HD3	2.10	0.50
11:LC:178:ASP:OD1	11:LC:181:ARG:NH1	2.44	0.50
74:SS:8:ARG:O	74:SS:12:LYS:HG3	2.11	0.50
1:L1:1015:G:O5'	20:LL:29:GLU:HG3	2.11	0.50
2:L2:1321:U:H2'	2:L2:1322:C:C6	2.46	0.50
3:L3:48:C:OP1	25:LQ:60:ARG:NE	2.45	0.50
3:L3:99:U:H2'	3:L3:100:U:C6	2.46	0.50
5:L5:112:U:H5''	5:L5:113:G:H5''	1.93	0.50
7:L7:17:U:H2'	7:L7:18:G:C8	2.46	0.50
12:LD:23:ILE:HG12	12:LD:127:MET:HB3	1.92	0.50
14:LF:68:PRO:HA	14:LF:158:ASP:OD1	2.11	0.50
22:LN:38:ARG:HH22	22:LN:45:GLU:CD	2.20	0.50
51:S1:67:C:O2'	51:S1:69:C:OP1	2.25	0.50
51:S1:187:C:H2'	51:S1:188:C:O4'	2.12	0.50
52:S2:64:A:H2'	52:S2:65:G:H1'	1.93	0.50
62:SG:4:ASN:ND2	62:SG:111:LEU:HD11	2.26	0.50
64:SI:2:GLN:OE1	64:SI:2:GLN:N	2.40	0.50
3:L3:129:A:C6	49:Lo:42:CYS:HA	2.47	0.50
20:LL:134:ILE:HG21	20:LL:141:VAL:HG23	1.93	0.50
27:LS:68:THR:HG23	27:LS:69:PRO:HD2	1.94	0.50
51:S1:230:G:H2'	51:S1:231:A:C8	2.47	0.50
51:S1:1809:U:H2'	51:S1:1810:G:O4'	2.11	0.50
72:SQ:50:VAL:HA	72:SQ:53:THR:HG22	1.94	0.50
1:L1:767:U:H2'	1:L1:768:C:O4'	2.11	0.50
17:LI:190:LEU:HB2	20:LL:143:LEU:HD11	1.92	0.50
51:S1:1512:A:H2'	51:S1:1513:C:C6	2.46	0.50
89:Sh:210:GLU:HA	89:Sh:213:ARG:HD2	1.94	0.50
1:L1:56:G:H2'	1:L1:57:G:C8	2.47	0.50
1:L1:808:A:H5''	36:Lb:30:HIS:CE1	2.47	0.50
2:L2:1225:A:H2'	2:L2:1226:C:H6	1.77	0.50
2:L2:1454:A:O2'	2:L2:1455:U:H2'	2.12	0.50
51:S1:586:G:H3'	59:SD:170:ARG:HH21	1.76	0.50
59:SD:36:ARG:HG2	59:SD:40:GLU:OE2	2.12	0.50
1:L1:223:A:N7	4:L4:10:U:H5	2.10	0.50
1:L1:263:A:O2'	31:LW:2:ALA:N	2.45	0.50
1:L1:1687:G:N2	1:L1:1705:G:H22	2.09	0.50
2:L2:665:A2M:H2'	2:L2:666:C:C6	2.47	0.50
8:L8:92:U:H2'	8:L8:93:G:O4'	2.11	0.50
9:LA:83:PHE:HB3	49:Lo:64:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:176:GLU:O	16:LH:180:VAL:HG23	2.12	0.50
19:LK:25:GLY:HA2	19:LK:40:ASN:HB2	1.93	0.50
25:LQ:95:TRP:CZ2	25:LQ:99:LEU:HD22	2.47	0.50
48:Ln:22:LEU:HD21	51:S1:2153:A:H4'	1.93	0.50
51:S1:32:U:O2'	51:S1:643:A:N1	2.38	0.50
51:S1:1155:U:O2'	51:S1:1243:U:O2'	2.25	0.50
51:S1:1646:G:O2'	51:S1:1673:A:N1	2.40	0.50
82:Sa:9:LYS:H	82:Sa:12:LYS:HB3	1.77	0.50
1:L1:754:G:H2'	1:L1:755:A:C8	2.46	0.50
2:L2:1130:A:N6	23:LO:28:THR:O	2.40	0.50
2:L2:1486:G:OP2	19:LK:171:ARG:NH1	2.40	0.50
4:L4:148:C:H2'	47:Lm:111:ARG:NH1	2.27	0.50
6:L6:43:A:H1'	26:LR:174:LYS:NZ	2.27	0.50
43:Li:38:LYS:HG2	43:Li:41:ARG:NH2	2.27	0.50
51:S1:958:G:O2'	51:S1:959:U:OP1	2.22	0.50
59:SD:12:LYS:HD3	59:SD:46:MET:HE3	1.94	0.50
1:L1:938:G:H2'	1:L1:939:C:C6	2.47	0.50
1:L1:1085:C:H2'	1:L1:1086:G:O4'	2.12	0.50
1:L1:1571:C:H5	28:LT:85:ARG:HH21	1.60	0.50
1:L1:1775:U:H2'	1:L1:1776:G:C8	2.47	0.50
2:L2:679:C:O2	2:L2:1023:C:H5	1.95	0.50
2:L2:1157:U:H5	2:L2:1237:A:N1	2.10	0.50
51:S1:146:U:H4'	62:SG:183:ILE:CD1	2.20	0.50
51:S1:1518:C:H2'	51:S1:1519:G:O4'	2.12	0.50
76:SU:55:LEU:HB2	76:SU:57:PHE:CE2	2.47	0.50
1:L1:1638:C:H2'	1:L1:1639:U:C6	2.47	0.49
7:L7:167:C:OP1	15:LG:182:LYS:HE2	2.12	0.49
8:L8:31:A:H2'	8:L8:32:C:H6	1.77	0.49
8:L8:52:G:OP2	23:LO:94:ASN:HB3	2.12	0.49
51:S1:363:G:H4'	51:S1:367:A:C8	2.46	0.49
51:S1:949:U:H2'	51:S1:950:U:C6	2.46	0.49
66:SK:2:GLY:O	66:SK:24:ARG:NH1	2.45	0.49
71:SP:125:VAL:O	71:SP:128:VAL:HG12	2.11	0.49
72:SQ:107:ASP:N	72:SQ:110:GLY:O	2.44	0.49
84:Sc:3:PHE:HD1	84:Sc:4:PHE:H	1.60	0.49
89:Sh:140:VAL:CG1	89:Sh:202:VAL:HG12	2.31	0.49
3:L3:35:A:H5'	3:L3:35:A:C8	2.47	0.49
20:LL:75:LEU:HG	20:LL:111:GLY:HA2	1.93	0.49
23:LO:55:ILE:HG12	23:LO:60:ILE:HG12	1.93	0.49
51:S1:878:C:H5	51:S1:883:G:H1	1.61	0.49
51:S1:895:A:H3'	51:S1:896:A:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:SZ:62:VAL:HG13	81:SZ:82:ILE:HG22	1.94	0.49
1:L1:593:C:H2'	1:L1:594:G:C8	2.47	0.49
1:L1:1378:U:O2'	26:LR:157:ARG:NH1	2.37	0.49
1:L1:1533:PSU:H2'	1:L1:1534:G:C8	2.47	0.49
2:L2:1264:PSU:H5'	2:L2:1264:PSU:H6	1.77	0.49
25:LQ:89:MET:O	25:LQ:89:MET:HG2	2.11	0.49
33:LY:14:THR:HB	42:Lh:89:ARG:HG3	1.94	0.49
51:S1:409:G:OP1	51:S1:859:G:O2'	2.22	0.49
51:S1:671:G:O2'	51:S1:1279:G:H5'	2.13	0.49
60:SE:133:VAL:HG11	60:SE:145:ARG:CZ	2.42	0.49
89:Sh:139:PHE:HE1	89:Sh:172:PHE:HB2	1.76	0.49
1:L1:817:C:H2'	1:L1:818:C:O4'	2.12	0.49
2:L2:772:A:H2'	2:L2:773:G:C8	2.47	0.49
12:LD:37:LYS:O	12:LD:41:GLN:HG2	2.13	0.49
18:LJ:82:ARG:NH1	18:LJ:119:PRO:O	2.38	0.49
33:LY:64:ARG:NH1	33:LY:64:ARG:O	2.46	0.49
51:S1:376:U:OP1	66:SK:31:ARG:NH1	2.44	0.49
51:S1:2133:G:OP1	66:SK:24:ARG:NH2	2.42	0.49
78:SW:62:VAL:O	78:SW:66:ARG:HG3	2.12	0.49
1:L1:141:U:H1'	1:L1:142:G:H5''	1.94	0.49
23:LO:118:LYS:NZ	23:LO:144:GLU:OE2	2.46	0.49
51:S1:972:A:H4'	51:S1:973:U:H5''	1.93	0.49
64:SI:58:LYS:O	64:SI:59:LYS:HG2	2.12	0.49
88:Sg:83:ALA:HB2	88:Sg:113:VAL:HG13	1.94	0.49
8:L8:46:A:OP2	8:L8:46:A:H8	1.96	0.49
51:S1:659:G:H4'	51:S1:661:OMU:H5	1.94	0.49
51:S1:836:C:H2'	51:S1:837:G:C8	2.48	0.49
51:S1:1653:U:OP1	61:SF:100:LYS:HB2	2.13	0.49
52:S2:48:C:H3'	52:S2:48:C:OP2	2.12	0.49
70:SO:33:THR:HG21	70:SO:67:ALA:HB2	1.94	0.49
1:L1:171:U:H2'	1:L1:172:G:C8	2.47	0.49
1:L1:1287:A:N6	1:L1:1348:A:H1'	2.28	0.49
2:L2:786:A:H4'	2:L2:787:G:H8	1.75	0.49
51:S1:1684:U:H3	51:S1:1820:G:H22	1.59	0.49
60:SE:92:THR:OG1	60:SE:94:ASP:OD1	2.20	0.49
78:SW:113:GLU:OE1	78:SW:115:LYS:HE2	2.12	0.49
1:L1:434:U:H5	1:L1:438:A:N7	2.11	0.49
1:L1:885:U:H2'	1:L1:886:G:O4'	2.13	0.49
2:L2:1484:U:O2'	19:LK:171:ARG:NH1	2.45	0.49
32:LX:84:ARG:NH1	62:SG:132:ALA:O	2.44	0.49
51:S1:1571:A:H3'	51:S1:1572:C:O2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:2190:C:H2'	51:S1:2191:A:C8	2.48	0.49
88:Sg:174:ASN:ND2	88:Sg:194:SER:O	2.46	0.49
1:L1:586:U:C5'	11:LC:335:ARG:HD2	2.43	0.49
5:L5:62:C:H3'	5:L5:63:G:H21	1.77	0.49
10:LB:390:LEU:O	10:LB:394:ARG:HG3	2.13	0.49
23:LO:218:LYS:HG2	23:LO:236:MET:HE2	1.95	0.49
41:Lg:39:LEU:HD11	41:Lg:54:ALA:HB1	1.95	0.49
51:S1:612:U:O2'	86:Se:13:LYS:HE2	2.13	0.49
51:S1:1200:G:H2'	51:S1:1201:G:C8	2.48	0.49
51:S1:1272:A:H2'	51:S1:1274:A:H5''	1.94	0.49
51:S1:1910:C:H2'	51:S1:1911:U:O4'	2.13	0.49
51:S1:1995:7MG:H82	82:Sa:27:TRP:HB3	1.93	0.49
81:SZ:117:ARG:HG3	81:SZ:120:ARG:HH21	1.77	0.49
1:L1:879:A:H2'	1:L1:880:C:C6	2.47	0.49
3:L3:117:C:H2'	3:L3:118:G:C8	2.48	0.49
27:LS:51:GLY:HA3	27:LS:92:ARG:HG3	1.95	0.49
51:S1:342:C:H1'	60:SE:30:PRO:HG3	1.94	0.49
51:S1:813:U:C2'	51:S1:814:G:H5'	2.42	0.49
51:S1:1108:A:N1	51:S1:1210:C:O2'	2.42	0.49
54:S4:10:G:O6	54:S4:44:G:C6	2.66	0.49
72:SQ:47:LEU:HB2	72:SQ:73:TYR:CE2	2.48	0.49
77:SV:20:TYR:O	77:SV:24:LEU:HG	2.13	0.49
87:Sf:139:TYR:HB3	87:Sf:146:THR:HG23	1.95	0.49
1:L1:824:U:HO2'	1:L1:1128:A:H61	1.59	0.48
4:L4:140:G:N1	4:L4:149:U:OP1	2.38	0.48
58:SC:131:LYS:HB3	58:SC:131:LYS:HE3	1.62	0.48
88:Sg:17:LEU:HD21	88:Sg:303:ILE:HD13	1.95	0.48
1:L1:377:G:OP2	11:LC:197:ASN:ND2	2.42	0.48
1:L1:835:G:H2'	1:L1:835:G:N3	2.29	0.48
2:L2:411:C:OP1	21:LM:76:HIS:NE2	2.37	0.48
4:L4:21:C:O2'	5:L5:135:U:O4	2.30	0.48
4:L4:181:C:H4'	5:L5:3:U:H5	1.78	0.48
21:LM:157:LYS:O	21:LM:162:ARG:NH1	2.46	0.48
30:LV:106:TYR:CE1	30:LV:142:ILE:HG12	2.48	0.48
51:S1:792:G:N7	51:S1:831:G:N1	2.60	0.48
51:S1:1603:U:H1'	87:Sf:134:HIS:HE1	1.79	0.48
68:SM:45:VAL:HG21	68:SM:90:ALA:HB2	1.94	0.48
71:SP:46:HIS:HB3	71:SP:101:LEU:HD11	1.94	0.48
1:L1:167:U:OP1	17:LI:134:ASN:HB2	2.14	0.48
1:L1:653:A:H5''	41:Lg:86:ARG:CZ	2.43	0.48
1:L1:911:G:O2'	1:L1:946:G:H4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:75:C:O2'	45:Lk:3:ARG:NH1	2.45	0.48
6:L6:11:G:C8	14:LF:186:PRO:HG2	2.48	0.48
7:L7:93:C:HO2'	7:L7:94:G:P	2.33	0.48
31:LW:77:ILE:HG23	31:LW:98:PRO:HG3	1.94	0.48
31:LW:80:ASP:OD1	31:LW:81:LYS:N	2.46	0.48
38:Ld:55:ARG:O	38:Ld:59:GLU:HG3	2.12	0.48
45:Lk:40:ARG:HH11	45:Lk:40:ARG:HG3	1.79	0.48
51:S1:368:U:OP1	76:SU:148:LYS:HE3	2.14	0.48
51:S1:519:A:OP1	59:SD:9:ARG:NH2	2.35	0.48
51:S1:887:U:OP1	60:SE:238:LYS:NZ	2.43	0.48
51:S1:2129:C:H2'	51:S1:2130:A:C8	2.48	0.48
57:SB:34:SER:HB2	57:SB:154:ASP:HA	1.94	0.48
64:SI:170:ARG:HB3	64:SI:170:ARG:HH11	1.78	0.48
51:S1:88:C:O2'	51:S1:494:A:OP1	2.30	0.48
51:S1:996:C:H5''	64:SI:59:LYS:HZ1	1.77	0.48
51:S1:1576:A:H61	51:S1:1611:C:N4	2.12	0.48
64:SI:4:HIS:NE2	64:SI:21:GLU:OE2	2.47	0.48
1:L1:1044:G:N3	2:L2:1064:A:H2'	2.29	0.48
1:L1:1052:A:N1	8:L8:106:C:O2'	2.44	0.48
1:L1:1749:G:H2'	1:L1:1751:A:N7	2.28	0.48
2:L2:1089:A:H2'	2:L2:1090:G:C8	2.49	0.48
2:L2:1127:G:H5''	27:LS:17:LYS:HG2	1.94	0.48
3:L3:35:A:H5'	3:L3:35:A:H8	1.78	0.48
25:LQ:94:LEU:HD23	25:LQ:97:ARG:NH2	2.28	0.48
26:LR:82:TYR:HE1	26:LR:92:MET:HE3	1.79	0.48
56:SA:241:VAL:HG23	70:SO:13:ASN:HD22	1.78	0.48
58:SC:7:LYS:HE3	58:SC:7:LYS:HB3	1.68	0.48
72:SQ:42:GLY:O	72:SQ:124:ARG:N	2.42	0.48
76:SU:48:ARG:NH1	76:SU:66:GLY:O	2.46	0.48
82:Sa:51:ARG:HE	82:Sa:51:ARG:HB3	1.45	0.48
1:L1:632:A:C6	11:LC:308:LYS:HG2	2.49	0.48
1:L1:839:U:H2'	1:L1:840:G:C8	2.49	0.48
26:LR:142:ALA:HA	26:LR:145:HIS:CE1	2.48	0.48
45:Lk:5:ILE:HD13	45:Lk:11:PHE:HA	1.96	0.48
51:S1:1398:C:H5	56:SA:168:MET:HG2	1.79	0.48
51:S1:1459:G:O2'	51:S1:1460:G:H5'	2.14	0.48
51:S1:2015:U:H5''	51:S1:2016:C:C5	2.49	0.48
71:SP:127:ASN:HD22	71:SP:127:ASN:C	2.09	0.48
1:L1:65:A:O2'	1:L1:353:C:O2	2.31	0.48
1:L1:126:G:H2'	1:L1:127:G:H8	1.77	0.48
1:L1:226:C:H2'	1:L1:227:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1350:U:C2'	1:L1:1351:C:H5'	2.43	0.48
2:L2:974:G:O6	42:Lh:102:ARG:NH2	2.42	0.48
2:L2:1370:U:O2	2:L2:1372:A2M:H8	2.14	0.48
3:L3:196:U:H5''	3:L3:197:A:OP2	2.14	0.48
9:LA:62:GLU:OE1	9:LA:73:LYS:HG3	2.14	0.48
41:Lg:57:ARG:NH1	41:Lg:114:ALA:O	2.40	0.48
43:Li:47:ILE:O	43:Li:51:VAL:HG22	2.13	0.48
51:S1:616:A:H1'	86:Se:14:VAL:HG23	1.94	0.48
51:S1:1115:G:H2'	51:S1:1116:U:C6	2.49	0.48
51:S1:1152:A:C4'	70:SO:59:ARG:NH1	2.75	0.48
52:S2:3:G:H2'	52:S2:4:C:C6	2.49	0.48
54:S4:37:A:H3'	54:S4:38:A:O4'	2.14	0.48
58:SC:203:LEU:HD13	58:SC:204:PRO:HD2	1.96	0.48
60:SE:50:LYS:HE3	60:SE:50:LYS:HB3	1.65	0.48
73:SR:66:GLU:O	73:SR:70:GLU:HG3	2.13	0.48
74:SS:31:LEU:HD23	74:SS:33:ARG:HG2	1.96	0.48
1:L1:1752:U:H2'	1:L1:1754:A:OP2	2.14	0.48
2:L2:452:G:H2'	2:L2:455:U:C5	2.47	0.48
2:L2:1368:A:O2'	18:LJ:40:SER:OG	2.25	0.48
41:Lg:74:ARG:HG2	41:Lg:141:PRO:HD3	1.95	0.48
51:S1:53:G:H2'	51:S1:54:C:C6	2.49	0.48
51:S1:996:C:H2'	51:S1:997:C:C6	2.49	0.48
51:S1:1121:C:H2'	51:S1:1122:G:C8	2.48	0.48
51:S1:1965:G:H2'	51:S1:1966:A:C8	2.49	0.48
65:SJ:86:TYR:OH	65:SJ:121:THR:O	2.25	0.48
71:SP:68:LYS:HB3	71:SP:91:LEU:HD13	1.95	0.48
1:L1:456:A:H2'	1:L1:457:C:O4'	2.13	0.48
1:L1:1291:G:H2'	1:L1:1292:G:C8	2.49	0.48
1:L1:1357:G:H4'	26:LR:117:ARG:HG2	1.94	0.48
2:L2:465:A:OP2	43:Li:71:ARG:NH1	2.43	0.48
2:L2:1485:G:O2'	2:L2:1486:G:P	2.72	0.48
3:L3:10:U:O2'	33:LY:79:HIS:ND1	2.38	0.48
3:L3:157:C:H2'	3:L3:158:U:C6	2.48	0.48
4:L4:31:G:OP2	10:LB:26:ARG:NH2	2.33	0.48
23:LO:276:LYS:HD3	23:LO:278:TYR:CZ	2.48	0.48
24:LP:16:ARG:HD2	24:LP:18:HIS:O	2.14	0.48
28:LT:60:PHE:HB3	28:LT:64:ASN:HB3	1.95	0.48
38:Ld:16:LEU:O	38:Ld:20:MET:HG2	2.14	0.48
51:S1:328:C:H2'	51:S1:329:C:C6	2.48	0.48
51:S1:789:G:OP2	60:SE:173:ARG:NH2	2.45	0.48
51:S1:1560:A:H5''	51:S1:1561:C:OP2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:2199:C:O2	83:Sb:96:ARG:HB3	2.14	0.48
59:SD:77:ARG:NH2	59:SD:81:GLU:OE1	2.47	0.48
1:L1:146:U:OP2	15:LG:197:THR:OG1	2.31	0.48
1:L1:448:A:C2	7:L7:16:A:H1'	2.49	0.48
1:L1:701:G:H5''	24:LP:159:PHE:HE1	1.79	0.48
1:L1:1037:A:O2'	37:Lc:132:PRO:O	2.28	0.48
1:L1:1714:C:H2'	1:L1:1715:U:C6	2.48	0.48
2:L2:473:C:H2'	2:L2:474:A:C8	2.49	0.48
2:L2:1287:C:HO2'	2:L2:1288:G:H8	1.60	0.48
3:L3:64:U:H2'	3:L3:65:U:C6	2.49	0.48
4:L4:132:U:H2'	4:L4:133:C:H5''	1.96	0.48
51:S1:439:G:N1	51:S1:442:A:OP2	2.44	0.48
51:S1:608:C:H42	51:S1:634:A:H61	1.62	0.48
58:SC:156:MET:CE	58:SC:186:LYS:HB2	2.44	0.48
60:SE:62:LEU:HD13	60:SE:77:GLY:HA2	1.96	0.48
66:SK:26:LYS:HG2	66:SK:29:LEU:HD23	1.94	0.48
66:SK:154:ALA:HB1	66:SK:158:LEU:HD23	1.96	0.48
81:SZ:97:ARG:O	81:SZ:101:MET:HG2	2.13	0.48
88:Sg:109:ASP:HB2	88:Sg:127:ARG:HG3	1.95	0.48
89:Sh:140:VAL:HG23	89:Sh:173:ALA:HB3	1.95	0.48
1:L1:264:U:H5'	31:LW:3:SER:H	1.78	0.47
1:L1:546:G:H5''	26:LR:3:LYS:HD3	1.96	0.47
2:L2:382:A2M:H8	2:L2:382:A2M:O5'	2.14	0.47
19:LK:97:GLU:OE1	19:LK:100:LYS:NZ	2.33	0.47
21:LM:103:GLU:OE1	21:LM:118:SER:OG	2.23	0.47
21:LM:120:TRP:HZ2	21:LM:123:MET:HG2	1.78	0.47
51:S1:310:U:H1'	66:SK:55:ILE:HD11	1.96	0.47
51:S1:520:G:H5''	59:SD:10:VAL:HG22	1.96	0.47
56:SA:41:ARG:NH2	56:SA:234:HIS:O	2.47	0.47
66:SK:46:VAL:N	66:SK:54:LYS:O	2.42	0.47
73:SR:3:LEU:HD21	82:Sa:79:GLY:HA2	1.95	0.47
76:SU:39:LYS:HG2	76:SU:40:HIS:CD2	2.48	0.47
80:SY:51:ASN:OD1	80:SY:53:THR:OG1	2.32	0.47
1:L1:23:U:H4'	1:L1:24:A:N7	2.29	0.47
1:L1:837:A:H4'	1:L1:838:G:O5'	2.13	0.47
1:L1:990:U:O2'	2:L2:648:A:N1	2.42	0.47
2:L2:16:G:O2'	46:Ll:3:ARG:O	2.32	0.47
2:L2:1506:G:H22	39:Le:40:ARG:NH1	2.10	0.47
3:L3:158:U:H2'	3:L3:159:C:C6	2.49	0.47
12:LD:82:LEU:HD13	12:LD:131:VAL:HG21	1.95	0.47
19:LK:113:LEU:O	19:LK:117:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:42:ALA:O	32:LX:46:ARG:HG3	2.13	0.47
48:Ln:24:LEU:O	48:Ln:28:ARG:HG3	2.14	0.47
51:S1:53:G:H2'	51:S1:54:C:H6	1.79	0.47
51:S1:836:C:H2'	51:S1:837:G:H8	1.80	0.47
60:SE:180:VAL:HB	60:SE:186:ARG:HA	1.96	0.47
60:SE:185:ASN:ND2	60:SE:216:ALA:O	2.47	0.47
63:SH:19:THR:O	63:SH:25:ARG:NH2	2.47	0.47
73:SR:85:LEU:HD12	73:SR:96:THR:HG22	1.95	0.47
1:L1:128:U:H2'	1:L1:129:C:C6	2.49	0.47
1:L1:522:G:H2'	1:L1:523:A:C8	2.49	0.47
1:L1:1265:A:H2'	1:L1:1266:A:H8	1.79	0.47
7:L7:40:A:H2'	7:L7:41:A:C8	2.49	0.47
41:Lg:85:LYS:HG3	41:Lg:101:ARG:NH2	2.29	0.47
51:S1:550:C:H2'	51:S1:551:A:C8	2.49	0.47
51:S1:615:C:H2'	51:S1:616:A:H8	1.79	0.47
71:SP:60:LYS:HE3	71:SP:116:PRO:HA	1.95	0.47
75:ST:132:VAL:HG23	75:ST:134:GLN:HG2	1.94	0.47
81:SZ:34:HIS:HB2	81:SZ:37:TRP:HB2	1.96	0.47
84:Sc:38:CYS:HB3	84:Sc:41:CYS:HB2	1.63	0.47
1:L1:771:U:H5'	24:LP:73:ARG:NH1	2.29	0.47
1:L1:823:G:H2'	1:L1:823:G:N3	2.28	0.47
2:L2:1126:C:O2	27:LS:49:ARG:NH1	2.48	0.47
4:L4:112:C:O2'	5:L5:41:C:OP1	2.29	0.47
6:L6:48:C:C2	14:LF:185:LYS:HD3	2.49	0.47
7:L7:142:C:O2'	30:LV:97:GLU:OE2	2.25	0.47
11:LC:107:PHE:HZ	17:LI:19:PRO:HD2	1.80	0.47
37:Lc:242:THR:O	37:Lc:245:ASN:ND2	2.44	0.47
56:SA:9:ILE:HG21	56:SA:15:ARG:HH11	1.79	0.47
58:SC:61:ASN:O	58:SC:66:ARG:NH2	2.47	0.47
58:SC:79:LYS:HA	58:SC:79:LYS:HD3	1.61	0.47
60:SE:28:PRO:HD2	60:SE:35:LEU:HD12	1.95	0.47
62:SG:80:ARG:HA	62:SG:85:PHE:HD2	1.79	0.47
1:L1:578:G:H2'	1:L1:579:G:H8	1.79	0.47
1:L1:708:A:N7	24:LP:111:ARG:NH2	2.62	0.47
1:L1:717:G:OP1	17:LI:40:ARG:HD2	2.15	0.47
51:S1:171:C:H4'	62:SG:134:ARG:HD3	1.96	0.47
51:S1:247:U:OP1	76:SU:37:SER:HB2	2.14	0.47
51:S1:449:U:H2'	51:S1:450:A:C8	2.48	0.47
51:S1:1512:A:O2'	51:S1:2040:C:H5	1.96	0.47
51:S1:1512:A:HO2'	51:S1:2040:C:H5	1.62	0.47
51:S1:1530:G:H5'	51:S1:1542:C:H42	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S3:7:G:OP1	53:S3:16:C:N4	2.36	0.47
60:SE:181:THR:N	60:SE:221:ASN:O	2.46	0.47
1:L1:731:U:H2'	1:L1:732:A:H8	1.79	0.47
1:L1:1373:A2M:O5'	1:L1:1373:A2M:H8	2.15	0.47
2:L2:1441:C:H5	6:L6:6:G:N1	2.02	0.47
7:L7:125:A:C2	7:L7:126:G:H1'	2.49	0.47
25:LQ:199:LYS:HB2	25:LQ:199:LYS:HE3	1.72	0.47
42:Lh:43:ILE:HD13	42:Lh:57:THR:HB	1.96	0.47
43:Li:58:LYS:O	43:Li:62:GLU:HG3	2.13	0.47
51:S1:15:U:H2'	51:S1:16:G:O4'	2.15	0.47
51:S1:41:G:O2'	51:S1:480:A:O2'	2.28	0.47
51:S1:556:A:H5''	59:SD:172:LYS:HE3	1.97	0.47
51:S1:1615:G:H2'	51:S1:1616:A:O4'	2.14	0.47
62:SG:140:ARG:O	62:SG:144:ILE:HG12	2.15	0.47
1:L1:345:U:H2'	1:L1:346:U:C6	2.50	0.47
1:L1:745:U:O2'	1:L1:815:G:N3	2.48	0.47
1:L1:1138:A:H5''	27:LS:35:LYS:HD2	1.96	0.47
1:L1:1410:U:OP1	40:Lf:62:ARG:NH1	2.46	0.47
2:L2:96:U:H2'	2:L2:97:A:O4'	2.15	0.47
2:L2:1163:U:O2'	27:LS:90:CYS:O	2.32	0.47
6:L6:19:C:H2'	6:L6:20:A:C8	2.49	0.47
6:L6:70:G:O2'	6:L6:71:A:H5'	2.14	0.47
7:L7:137:U:H2'	7:L7:138:C:O4'	2.15	0.47
10:LB:58:ARG:HA	10:LB:364:LYS:HG3	1.96	0.47
10:LB:107:ALA:HB2	10:LB:204:LEU:HD22	1.97	0.47
14:LF:80:ASP:HB3	14:LF:83:TYR:HD2	1.80	0.47
33:LY:32:VAL:HB	33:LY:37:PRO:HA	1.97	0.47
51:S1:117:G:H1'	51:S1:440:A:N7	2.30	0.47
51:S1:340:G:O2'	51:S1:341:A:H8	1.96	0.47
51:S1:490:U:O2'	60:SE:24:PHE:O	2.31	0.47
51:S1:779:A:H2'	51:S1:780:A:H8	1.78	0.47
51:S1:813:U:H2'	51:S1:814:G:H5'	1.96	0.47
51:S1:1247:U:O2'	51:S1:1249:G:N7	2.41	0.47
51:S1:1522:G:C2	51:S1:1523:A:C8	3.03	0.47
51:S1:1769:C:N4	79:SX:131:GLN:HG2	2.30	0.47
51:S1:1862:C:H1'	82:Sa:17:ASN:HD22	1.79	0.47
51:S1:1978:A:H5''	73:SR:134:GLY:HA3	1.96	0.47
51:S1:2016:C:C4'	51:S1:2019:C:H41	2.27	0.47
53:S3:74:C:O2'	53:S3:75:C:H5'	2.15	0.47
59:SD:171:VAL:O	59:SD:175:ARG:HG2	2.15	0.47
61:SF:50:LYS:HB3	61:SF:259:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SI:52:VAL:HG21	64:SI:175:VAL:HG22	1.97	0.47
66:SK:190:SER:OG	66:SK:197:ARG:O	2.33	0.47
67:SL:17:LYS:HD2	67:SL:22:ILE:HG23	1.97	0.47
77:SV:35:ILE:O	77:SV:39:THR:OG1	2.29	0.47
1:L1:86:G:H5''	24:LP:175:ASN:OD1	2.15	0.47
2:L2:1150:U:H2'	2:L2:1151:U:O2	2.14	0.47
2:L2:1175:A:H2'	2:L2:1176:A:C8	2.50	0.47
2:L2:1320:U:H2'	2:L2:1321:U:C6	2.49	0.47
7:L7:93:C:C2'	7:L7:94:G:H5''	2.44	0.47
40:Lf:98:SER:HB2	40:Lf:101:VAL:HG23	1.96	0.47
51:S1:1367:U:H2'	51:S1:1368:C:C6	2.50	0.47
86:Se:38:LEU:O	86:Se:41:THR:HG22	2.15	0.47
1:L1:768:C:O2'	1:L1:769:U:H5''	2.14	0.47
1:L1:820:U:H5	1:L1:823:G:H22	1.61	0.47
1:L1:1350:U:H2'	1:L1:1351:C:H5'	1.96	0.47
10:LB:92:TYR:HB2	10:LB:159:VAL:HB	1.97	0.47
17:LI:28:LYS:HB2	21:LM:197:ARG:HD3	1.96	0.47
35:La:2:SER:O	35:La:47:ARG:NH1	2.45	0.47
40:Lf:82:ASP:OD2	40:Lf:82:ASP:N	2.47	0.47
46:LI:28:ARG:HG2	46:LI:28:ARG:HH11	1.80	0.47
51:S1:379:U:O2'	76:SU:145:PRO:O	2.31	0.47
51:S1:558:U:H2'	51:S1:559:G:C8	2.50	0.47
51:S1:777:A:H4'	51:S1:778:G:O5'	2.15	0.47
51:S1:781:A:H2'	51:S1:782:C:O4'	2.15	0.47
51:S1:947:U:H2'	51:S1:948:G:H8	1.80	0.47
51:S1:2037:U:H2'	51:S1:2038:C:C6	2.50	0.47
60:SE:104:GLY:O	60:SE:186:ARG:NE	2.48	0.47
60:SE:158:VAL:HG13	60:SE:167:VAL:HG22	1.97	0.47
73:SR:86:ASN:OD1	73:SR:86:ASN:N	2.48	0.47
75:ST:119:GLU:OE1	75:ST:141:TYR:CE2	2.67	0.47
86:Se:15:LYS:HA	86:Se:15:LYS:HD2	1.75	0.47
1:L1:148:U:H5''	21:LM:55:THR:O	2.15	0.47
2:L2:1108:U:H5'	12:LD:67:ILE:HD11	1.96	0.47
2:L2:1495:A:H2'	2:L2:1496:G:C8	2.50	0.47
3:L3:71:U:H5	3:L3:150:A:N7	2.13	0.47
39:Le:39:LYS:NZ	39:Le:39:LYS:HB3	2.30	0.47
51:S1:431:G:OP2	51:S1:466:G:O2'	2.32	0.47
51:S1:1961:G:C5'	79:SX:99:GLY:HA2	2.44	0.47
54:S4:27:G:H2'	54:S4:28:G:C8	2.50	0.47
57:SB:22:LEU:HD11	77:SV:109:LEU:HD21	1.97	0.47
75:ST:119:GLU:HA	75:ST:119:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:447:G:N2	7:L7:15:G:O2'	2.46	0.46
1:L1:624:U:O2'	1:L1:625:C:H4'	2.15	0.46
2:L2:505:A:N6	51:S1:2065:G:O2'	2.48	0.46
2:L2:970:A:H5''	49:Lo:87:ARG:NE	2.30	0.46
6:L6:51:A:H4'	6:L6:52:G:O5'	2.14	0.46
7:L7:20:C:OP1	11:LC:194:LYS:HE3	2.16	0.46
11:LC:213:ASN:OD1	11:LC:213:ASN:N	2.46	0.46
51:S1:754:G:N3	51:S1:754:G:H5''	2.29	0.46
51:S1:1701:A:H2'	51:S1:1702:A:H8	1.79	0.46
58:SC:71:CYS:SG	69:SN:22:VAL:HG11	2.55	0.46
1:L1:254:U:H5	1:L1:258:A:N7	2.12	0.46
1:L1:843:C:H2'	1:L1:844:C:C6	2.51	0.46
1:L1:1742:G:C2'	1:L1:1743:A:O5'	2.64	0.46
2:L2:79:C:O2'	4:L4:81:G:H4'	2.15	0.46
2:L2:1335:C:H5''	47:Lm:125:LYS:HG3	1.96	0.46
2:L2:1404:G:C5'	9:LA:220:GLY:HA3	2.45	0.46
8:L8:26:A:H2'	8:L8:27:A:C8	2.50	0.46
9:LA:28:LYS:HE3	9:LA:28:LYS:HB2	1.69	0.46
16:LH:202:LYS:NZ	16:LH:202:LYS:HB3	2.31	0.46
19:LK:27:ILE:O	19:LK:29:ASP:N	2.41	0.46
23:LO:192:GLU:C	23:LO:194:SER:H	2.24	0.46
25:LQ:148:GLU:O	25:LQ:152:GLU:HG2	2.14	0.46
51:S1:200:A:H2'	51:S1:201:C:O4'	2.15	0.46
51:S1:585:C:H2'	51:S1:586:G:O4'	2.15	0.46
51:S1:616:A:N1	51:S1:629:A:N6	2.55	0.46
57:SB:70:ALA:HB2	80:SY:42:ALA:HB2	1.96	0.46
1:L1:97:G:N7	17:LI:12:HIS:NE2	2.63	0.46
1:L1:491:A:O2'	6:L6:65:C:H5	1.98	0.46
2:L2:659:A:H2'	2:L2:660:G:C8	2.51	0.46
2:L2:1100:A:H4'	12:LD:105:GLY:C	2.40	0.46
2:L2:1510:A:N1	10:LB:326:ASN:OD1	2.48	0.46
4:L4:49:A:H61	4:L4:60:A:H3'	1.80	0.46
21:LM:7:LEU:HB3	21:LM:46:GLU:HG2	1.96	0.46
27:LS:119:LYS:HE3	27:LS:119:LYS:HB3	1.65	0.46
28:LT:16:LYS:HG2	28:LT:149:PHE:HB3	1.97	0.46
37:Lc:221:ALA:O	37:Lc:250:ARG:HD2	2.15	0.46
51:S1:61:C:O2	51:S1:319:C:O2'	2.33	0.46
51:S1:1098:U:H2'	51:S1:1099:C:C6	2.51	0.46
51:S1:1605:U:H5''	87:Sf:129:VAL:HG22	1.96	0.46
53:S3:10:G:N2	53:S3:26:G:H1'	2.30	0.46
60:SE:175:GLY:HA2	60:SE:191:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sa:69:LEU:HB2	82:Sa:71:ILE:HG12	1.97	0.46
1:L1:36:U:H2'	1:L1:37:A:O4'	2.15	0.46
2:L2:454:A:H1'	2:L2:455:U:H3'	1.96	0.46
2:L2:1045:G:O2'	2:L2:1303:PSU:OP1	2.21	0.46
4:L4:129:G:N1	4:L4:161:C:H5	2.04	0.46
11:LC:319:GLY:O	11:LC:326:ARG:HG2	2.15	0.46
13:LE:77:GLN:O	13:LE:81:THR:HG22	2.16	0.46
19:LK:41:PRO:HD2	19:LK:78:LEU:HD12	1.98	0.46
51:S1:616:A:N3	86:Se:14:VAL:HG21	2.30	0.46
56:SA:166:LEU:HD12	56:SA:203:CYS:HB3	1.98	0.46
57:SB:20:LYS:HE3	57:SB:183:ARG:HH21	1.80	0.46
60:SE:103:LYS:HD2	60:SE:105:ARG:NH1	2.26	0.46
61:SF:137:ILE:O	61:SF:141:MET:HG3	2.15	0.46
85:Sd:22:GLN:HG2	85:Sd:46:LEU:HD12	1.97	0.46
88:Sg:38:ALA:HB3	88:Sg:61:LEU:HB2	1.96	0.46
89:Sh:166:ARG:HD3	89:Sh:166:ARG:HA	1.67	0.46
1:L1:576:G:O6	11:LC:324:ARG:HG3	2.15	0.46
1:L1:1565:A:O2'	1:L1:1566:A:O5'	2.30	0.46
2:L2:1453:U:H4'	2:L2:1454:A:H5''	1.97	0.46
5:L5:38:U:H5''	10:LB:315:MET:HE2	1.97	0.46
5:L5:48:G:H2'	5:L5:49:G:N3	2.30	0.46
5:L5:112:U:H5	5:L5:121:A:N7	2.13	0.46
51:S1:438:U:H2'	51:S1:439:G:O4'	2.16	0.46
51:S1:636:C:C4	51:S1:637:U:C4	3.04	0.46
51:S1:641:A:H2'	51:S1:642:A:O4'	2.16	0.46
51:S1:1100:U:O2'	51:S1:1102:G:OP1	2.28	0.46
51:S1:1193:U:H2'	51:S1:1194:C:C6	2.50	0.46
51:S1:1513:C:C2	51:S1:1514:A:C8	3.04	0.46
51:S1:2026:U:H2'	51:S1:2027:G:C8	2.50	0.46
51:S1:2188:U:H2'	51:S1:2189:G:C8	2.51	0.46
52:S2:34:G:H2'	52:S2:35:A:H8	1.79	0.46
57:SB:32:ASN:O	57:SB:153:THR:HG22	2.15	0.46
82:Sa:58:LYS:O	82:Sa:102:THR:OG1	2.25	0.46
82:Sa:91:LEU:HD21	82:Sa:94:CYS:HB2	1.98	0.46
89:Sh:185:LYS:HE2	89:Sh:185:LYS:HB3	1.86	0.46
1:L1:636:U:H2'	1:L1:637:C:H6	1.81	0.46
1:L1:1218:A:O2'	40:Lf:55:ASN:OD1	2.31	0.46
1:L1:1602:C:H2'	1:L1:1603:G:H8	1.81	0.46
2:L2:1385:G:N3	10:LB:255:ALA:HB1	2.31	0.46
16:LH:208:MET:HE3	16:LH:208:MET:HB2	1.81	0.46
18:LJ:91:ASP:HB2	32:LX:1:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LT:112:MET:HE3	28:LT:150:MET:HG3	1.97	0.46
29:LU:96:LYS:HE3	29:LU:96:LYS:HB3	1.61	0.46
51:S1:199:C:H2'	51:S1:200:A:C8	2.51	0.46
51:S1:484:G:H22	51:S1:511:C:H5	1.63	0.46
1:L1:1270:U:O2	4:L4:143:C:N4	2.34	0.46
2:L2:432:U:C5	9:LA:200:ARG:HD3	2.51	0.46
2:L2:454:A:H4'	2:L2:455:U:OP1	2.16	0.46
2:L2:1254:G:O4'	2:L2:1308:5MC:HM53	2.16	0.46
5:L5:48:G:H3'	5:L5:49:G:H21	1.80	0.46
51:S1:505:A:H5''	81:SZ:118:ARG:NH2	2.31	0.46
51:S1:1717:U:O2'	51:S1:1718:A:OP1	2.32	0.46
59:SD:74:ALA:O	59:SD:78:ARG:HG3	2.15	0.46
64:SI:4:HIS:HE2	64:SI:21:GLU:CD	2.24	0.46
85:Sd:46:LEU:HD23	85:Sd:57:ARG:HG3	1.97	0.46
1:L1:592:G:H2'	1:L1:593:C:H6	1.78	0.46
2:L2:126:U:P	29:LU:8:VAL:HG21	2.56	0.46
2:L2:1123:A:H2'	2:L2:1124:A:C8	2.50	0.46
5:L5:128:G:H2'	5:L5:129:G:C8	2.51	0.46
8:L8:115:C:H2'	8:L8:116:C:C6	2.51	0.46
19:LK:3:LYS:HG2	19:LK:4:SER:H	1.81	0.46
51:S1:789:G:P	60:SE:173:ARG:HH22	2.39	0.46
51:S1:1014:C:H2'	51:S1:1015:G:H8	1.80	0.46
51:S1:1511:C:N4	51:S1:1637:A:H5'	2.31	0.46
51:S1:1961:G:O2'	51:S1:1987:G:N2	2.49	0.46
52:S2:4:C:H2'	52:S2:5:G:C8	2.50	0.46
52:S2:65:G:N3	52:S2:65:G:H2'	2.30	0.46
56:SA:133:ASP:OD2	56:SA:133:ASP:N	2.41	0.46
76:SU:88:GLY:HA3	76:SU:101:ILE:HD12	1.98	0.46
1:L1:454:U:H2'	1:L1:455:G:C8	2.50	0.46
1:L1:464:A:N3	2:L2:609:A:H4'	2.30	0.46
1:L1:610:A:H4'	11:LC:359:ARG:HG3	1.98	0.46
1:L1:790:C:C5	11:LC:304:LYS:HD3	2.51	0.46
1:L1:1479:A:H4'	1:L1:1480:C:O5'	2.16	0.46
2:L2:1089:A:H2'	2:L2:1090:G:H8	1.81	0.46
2:L2:1132:A:N6	27:LS:47:ALA:O	2.49	0.46
7:L7:22:U:OP1	31:LW:13:ARG:NH2	2.45	0.46
12:LD:62:ARG:HE	12:LD:65:GLU:HB2	1.81	0.46
30:LV:78:LYS:HB3	30:LV:84:THR:HB	1.96	0.46
35:La:28:GLU:HG3	35:La:51:ILE:HD13	1.97	0.46
40:Lf:22:ARG:HD2	40:Lf:25:LEU:HD12	1.97	0.46
51:S1:578:C:H2'	51:S1:579:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1105:A:OP2	64:SI:116:GLN:NE2	2.48	0.46
52:S2:40:C:OP1	82:Sa:9:LYS:HE2	2.16	0.46
56:SA:8:ARG:HG2	56:SA:8:ARG:NH1	2.31	0.46
57:SB:114:GLN:HG2	57:SB:115:ILE:HG23	1.98	0.46
57:SB:116:GLN:C	57:SB:118:LYS:H	2.23	0.46
1:L1:820:U:H6	1:L1:823:G:H1	1.63	0.46
1:L1:1202:G:H1'	40:Lf:46:ARG:HH21	1.81	0.46
1:L1:1536:C:H5	2:L2:603:A:H62	1.63	0.46
2:L2:635:A:H5''	28:LT:80:LYS:HD3	1.98	0.46
7:L7:29:C:H5'	17:LI:35:ALA:HB1	1.97	0.46
11:LC:287:VAL:HA	11:LC:290:ILE:HD12	1.96	0.46
23:LO:185:ARG:HA	23:LO:185:ARG:HD2	1.74	0.46
51:S1:479:A2M:O5'	51:S1:479:A2M:H8	2.16	0.46
51:S1:654:A:OP2	51:S1:655:U:O2'	2.31	0.46
51:S1:1905:C:HO2'	51:S1:1906:G:P	2.37	0.46
54:S4:22:G:N7	54:S4:46:G:N2	2.61	0.46
54:S4:39:U:H2'	54:S4:40:C:H6	1.80	0.46
66:SK:187:ARG:HB2	66:SK:203:LEU:HD21	1.98	0.46
70:SO:116:GLY:O	70:SO:117:MET:HG2	2.15	0.46
72:SQ:45:ARG:HH12	72:SQ:103:LEU:HB2	1.81	0.46
88:Sg:255:GLU:HA	88:Sg:281:GLU:HG3	1.97	0.46
1:L1:155:A:H3'	1:L1:156:A:H5'	1.99	0.45
2:L2:1195:U:H2'	2:L2:1196:G:C8	2.51	0.45
2:L2:1219:A:H5''	17:LI:205:SER:OG	2.16	0.45
6:L6:30:C:H3'	13:LE:50:LYS:HD3	1.98	0.45
10:LB:19:ARG:HB2	10:LB:237:ARG:NH2	2.31	0.45
10:LB:90:VAL:HG23	10:LB:161:ARG:HB2	1.98	0.45
51:S1:309:G:O2'	51:S1:310:U:OP2	2.30	0.45
51:S1:1199:A:H4'	75:ST:98:MET:HE3	1.98	0.45
81:SZ:20:ASN:HD21	81:SZ:25:ARG:HE	1.64	0.45
86:Se:58:ASN:OD1	86:Se:58:ASN:C	2.59	0.45
88:Sg:240:GLN:HG2	88:Sg:285:ILE:HG12	1.97	0.45
1:L1:38:A:H5''	20:LL:35:ALA:HB1	1.97	0.45
1:L1:160:C:O2'	1:L1:161:A:O5'	2.35	0.45
1:L1:493:A:H5'	14:LF:82:ARG:HG3	1.97	0.45
1:L1:795:U:OP1	11:LC:301:LYS:NZ	2.35	0.45
1:L1:1439:A:H2	24:LP:38:LYS:HE3	1.80	0.45
7:L7:89:U:H2'	7:L7:90:U:C6	2.50	0.45
7:L7:101:PSU:H2'	7:L7:102:G:C8	2.51	0.45
8:L8:87:G:O2'	8:L8:89:C:OP1	2.33	0.45
15:LG:106:ARG:HG3	15:LG:109:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LU:13:TYR:CE2	29:LU:15:ARG:HG3	2.50	0.45
37:Lc:27:ALA:O	37:Lc:31:GLN:HG3	2.15	0.45
52:S2:62:C:H2'	52:S2:63:G:C8	2.50	0.45
67:SL:104:ASN:ND2	67:SL:106:VAL:HB	2.31	0.45
2:L2:134:C:H2'	2:L2:135:A:C8	2.51	0.45
2:L2:1353:U:O2'	2:L2:1373:C:O2	2.27	0.45
3:L3:105:C:H2'	3:L3:106:U:H6	1.81	0.45
5:L5:7:U:H2'	5:L5:8:C:H6	1.82	0.45
9:LA:80:GLU:HG3	49:Lo:66:GLY:HA2	1.99	0.45
13:LE:150:LEU:O	13:LE:154:SER:OG	2.34	0.45
16:LH:101:THR:O	16:LH:105:MET:HG3	2.16	0.45
20:LL:51:GLY:HA2	24:LP:182:ARG:N	2.30	0.45
23:LO:199:LYS:HD2	23:LO:199:LYS:HA	1.71	0.45
23:LO:217:VAL:HG12	23:LO:236:MET:HE3	1.98	0.45
41:Lg:111:HIS:HB3	41:Lg:116:MET:HB3	1.99	0.45
51:S1:956:A:C4	51:S1:957:G:C8	3.05	0.45
51:S1:1586:A:H2	87:Sf:139:TYR:OH	1.98	0.45
51:S1:1603:U:H1'	87:Sf:134:HIS:CE1	2.52	0.45
51:S1:1662:OMU:HM23	51:S1:1662:OMU:H1'	1.58	0.45
51:S1:2034:A:OP2	63:SH:49:LYS:NZ	2.49	0.45
51:S1:2100:A:H3'	51:S1:2101:C:H5''	1.98	0.45
56:SA:151:GLN:HG3	56:SA:153:SER:H	1.81	0.45
60:SE:253:ARG:HE	60:SE:254:LEU:HD22	1.81	0.45
62:SG:179:ILE:HG22	62:SG:182:LEU:HB2	1.99	0.45
1:L1:147:G:OP2	1:L1:147:G:H8	2.00	0.45
1:L1:681:A2M:HM'3	1:L1:681:A2M:H1'	1.65	0.45
4:L4:174:A:C6	16:LH:4:PRO:HD3	2.51	0.45
5:L5:39:G:H4'	10:LB:372:ILE:O	2.16	0.45
18:LJ:106:ASN:HB2	18:LJ:107:PRO:HD2	1.98	0.45
21:LM:146:PRO:HG3	35:La:106:ARG:HB3	1.99	0.45
25:LQ:180:LYS:NZ	51:S1:966:G:O6	2.43	0.45
35:La:92:THR:HG22	35:La:94:ARG:H	1.82	0.45
51:S1:309:G:N2	51:S1:310:U:O2	2.42	0.45
51:S1:394:U:OP1	51:S1:395:U:O2'	2.27	0.45
51:S1:701:G:H22	51:S1:745:G:N2	2.12	0.45
51:S1:1503:A:OP1	51:S1:2171:G:N2	2.35	0.45
51:S1:1612:C:OP2	87:Sf:89:ARG:NH1	2.49	0.45
51:S1:2016:C:H4'	51:S1:2019:C:H41	1.81	0.45
63:SH:178:LYS:HB3	63:SH:178:LYS:HE3	1.55	0.45
73:SR:32:ARG:HE	73:SR:32:ARG:HB2	1.65	0.45
78:SW:131:ARG:HE	78:SW:131:ARG:HB3	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sa:82:GLN:O	82:Sa:86:GLU:HG3	2.16	0.45
89:Sh:164:ARG:HB3	89:Sh:176:TYR:HD2	1.81	0.45
1:L1:1185:U:H2'	1:L1:1186:A:O4'	2.16	0.45
2:L2:1020:C:O2'	2:L2:1021:A:C8	2.67	0.45
2:L2:1137:G:H2'	2:L2:1138:C:C6	2.51	0.45
4:L4:51:U:H2'	4:L4:52:A:C8	2.51	0.45
13:LE:38:LEU:HD13	13:LE:72:THR:HG23	1.98	0.45
16:LH:91:HIS:HB3	16:LH:96:ASP:HB3	1.97	0.45
51:S1:955:A:O2'	51:S1:956:A:O5'	2.34	0.45
51:S1:1271:C:OP1	51:S1:1479:A:O2'	2.32	0.45
51:S1:1832:C:O2	51:S1:1838:U:H5	1.98	0.45
51:S1:2200:A:C6	83:Sb:88:VAL:HG22	2.52	0.45
60:SE:41:LEU:HD23	60:SE:41:LEU:HA	1.81	0.45
66:SK:42:ARG:HH21	66:SK:59:ARG:NH1	2.14	0.45
1:L1:720:A:C8	1:L1:721:U:H2'	2.52	0.45
1:L1:758:C:H2'	1:L1:759:A:O4'	2.17	0.45
1:L1:1292:G:H1	1:L1:1343:A:N6	2.12	0.45
2:L2:94:A:H2'	2:L2:95:A2M:H8	1.98	0.45
9:LA:117:GLU:HB2	9:LA:162:SER:HB2	1.99	0.45
16:LH:146:VAL:HB	26:LR:157:ARG:HG3	1.98	0.45
22:LN:212:MET:HE2	22:LN:212:MET:HB2	1.80	0.45
51:S1:117:G:H1'	51:S1:440:A:C8	2.52	0.45
51:S1:128:C:H5''	51:S1:181:A:OP1	2.16	0.45
51:S1:297:U:N3	76:SU:28:ALA:HB2	2.31	0.45
51:S1:996:C:H2'	51:S1:997:C:H6	1.82	0.45
57:SB:92:LYS:HD2	57:SB:92:LYS:HA	1.69	0.45
57:SB:125:LEU:HD23	57:SB:147:VAL:HG22	1.98	0.45
58:SC:44:ARG:NH2	58:SC:84:GLN:HB2	2.31	0.45
60:SE:148:ASP:OD1	60:SE:148:ASP:N	2.49	0.45
63:SH:8:LEU:HD21	63:SH:55:VAL:HG11	1.98	0.45
72:SQ:45:ARG:HG2	72:SQ:103:LEU:HD12	1.99	0.45
81:SZ:61:GLN:HA	81:SZ:89:LEU:HD13	1.98	0.45
1:L1:216:G:O6	34:LZ:140:LYS:HD2	2.16	0.45
1:L1:1393:A:H2'	1:L1:1394:U:C6	2.52	0.45
1:L1:1677:G:O6	1:L1:1715:U:O4	2.35	0.45
2:L2:979:A:H2'	2:L2:980:A:H8	1.82	0.45
2:L2:1087:C:H2'	2:L2:1088:G:H8	1.81	0.45
2:L2:1262:G:H2'	2:L2:1263:C:H6	1.82	0.45
2:L2:1291:G:O2'	22:LN:158:LYS:O	2.26	0.45
4:L4:179:C:OP1	10:LB:133:GLN:N	2.48	0.45
5:L5:89:C:H2'	5:L5:90:C:O2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:223:SER:OG	23:LO:224:ASN:OD1	2.31	0.45
43:Li:57:GLU:HB3	43:Li:93:MET:SD	2.56	0.45
51:S1:436:C:H2'	51:S1:437:C:C6	2.51	0.45
51:S1:616:A:C2	51:S1:632:C:H1'	2.52	0.45
51:S1:1291:U:H2'	51:S1:1292:PSU:C6	2.52	0.45
51:S1:1716:A:H61	79:SX:26:ARG:NH2	2.15	0.45
56:SA:37:ASN:OD1	56:SA:37:ASN:N	2.45	0.45
62:SG:129:ASP:OD1	62:SG:129:ASP:N	2.50	0.45
82:Sa:61:THR:HB	82:Sa:64:ILE:HD12	1.99	0.45
1:L1:734:U:H2'	1:L1:735:U:C6	2.51	0.45
1:L1:959:OMG:HM22	1:L1:959:OMG:N3	2.31	0.45
4:L4:98:A:H2'	4:L4:99:A:H8	1.82	0.45
17:LI:179:ALA:HA	17:LI:182:LYS:HD2	1.99	0.45
22:LN:153:ARG:HG3	22:LN:154:ARG:N	2.31	0.45
31:LW:24:ARG:HD3	31:LW:72:ARG:O	2.17	0.45
51:S1:371:C:H2'	51:S1:372:C:C6	2.52	0.45
51:S1:1555:A:C2	51:S1:1975:A:C4	3.05	0.45
51:S1:2197:G:H1'	83:Sb:83:ILE:HD13	1.98	0.45
52:S2:3:G:H2'	52:S2:4:C:H6	1.81	0.45
62:SG:150:LEU:HD13	62:SG:154:GLU:OE1	2.06	0.45
81:SZ:107:ARG:HB3	81:SZ:107:ARG:HH11	1.82	0.45
82:Sa:56:LYS:HA	82:Sa:103:ARG:HD3	1.99	0.45
88:Sg:17:LEU:HB3	88:Sg:286:ALA:HB2	1.98	0.45
1:L1:411:U:H4'	1:L1:445:C:H5'	1.98	0.45
1:L1:578:G:H2'	1:L1:579:G:C8	2.52	0.45
1:L1:755:A:H2'	1:L1:756:U:C6	2.52	0.45
1:L1:759:A:H2	1:L1:761:A:H61	1.65	0.45
1:L1:1090:U:H2'	1:L1:1091:A:H8	1.82	0.45
2:L2:631:G:H5'	4:L4:170:G:C2	2.51	0.45
8:L8:52:G:H5'	23:LO:232:PHE:CE1	2.52	0.45
40:Lf:17:ARG:HE	40:Lf:17:ARG:HB3	1.56	0.45
42:Lh:52:LYS:HE3	42:Lh:52:LYS:HB3	1.33	0.45
51:S1:558:U:H1'	59:SD:130:GLN:HG2	1.98	0.45
51:S1:1494:A:H2'	51:S1:1495:A:C8	2.52	0.45
60:SE:89:ILE:O	60:SE:93:GLY:N	2.48	0.45
61:SF:155:TYR:OH	61:SF:161:GLY:O	2.24	0.45
88:Sg:101:ARG:NH1	88:Sg:137:ALA:HA	2.31	0.45
1:L1:196:C:O2'	1:L1:198:A:OP2	2.35	0.45
7:L7:62:A:H4'	7:L7:63:G:O5'	2.17	0.45
17:LI:214:LYS:HD3	17:LI:214:LYS:HA	1.63	0.45
26:LR:29:PHE:CE1	26:LR:46:MET:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Le:11:LEU:HD12	39:Le:16:LYS:HD3	1.99	0.45
51:S1:250:C:H2'	51:S1:251:A:O4'	2.17	0.45
51:S1:292:U:H2'	51:S1:293:U:C6	2.52	0.45
53:S3:7:G:P	53:S3:16:C:H42	2.39	0.45
61:SF:92:MET:HE2	61:SF:137:ILE:HG12	1.99	0.45
62:SG:152:ARG:HG3	62:SG:153:THR:HG23	1.98	0.45
84:Sc:20:HIS:HB3	84:Sc:23:ARG:HG2	1.99	0.45
2:L2:1317:OMC:HM21	10:LB:244:PRO:HD3	1.99	0.44
11:LC:146:VAL:HG22	34:LZ:74:PRO:HG2	1.99	0.44
15:LG:76:LEU:HD11	21:LM:22:ILE:HG13	2.00	0.44
19:LK:74:LEU:HD12	19:LK:74:LEU:O	2.17	0.44
51:S1:606:G:H22	51:S1:635:G:H1	1.64	0.44
51:S1:1015:G:H2'	51:S1:1016:G:H8	1.80	0.44
51:S1:1150:U:O2'	51:S1:1152:A:N7	2.43	0.44
51:S1:1471:U:H2'	51:S1:1472:U:C6	2.53	0.44
51:S1:1496:U:H2'	51:S1:1497:U:C6	2.51	0.44
51:S1:1619:G:O2'	51:S1:1849:G:O2'	2.33	0.44
51:S1:1658:U:H2'	51:S1:1659:U:C6	2.52	0.44
51:S1:1762:A:H5'	79:SX:13:LYS:NZ	2.31	0.44
57:SB:112:THR:HG21	57:SB:142:LEU:HD12	2.00	0.44
66:SK:106:ALA:HB1	66:SK:179:LEU:HD13	1.98	0.44
72:SQ:73:TYR:CZ	72:SQ:119:SER:HB2	2.52	0.44
81:SZ:75:LYS:HE2	81:SZ:75:LYS:HB2	1.77	0.44
81:SZ:93:GLU:HB3	81:SZ:98:LYS:HG3	1.99	0.44
1:L1:361:A:H2'	1:L1:362:A:C8	2.52	0.44
1:L1:449:A:N3	1:L1:687:C:O2'	2.46	0.44
1:L1:553:A:N7	11:LC:341:LYS:NZ	2.66	0.44
1:L1:1409:U:H2'	1:L1:1410:U:C6	2.52	0.44
1:L1:1755:U:H2'	1:L1:1756:A:O4'	2.17	0.44
2:L2:1069:A:H2'	2:L2:1070:A:C8	2.53	0.44
9:LA:207:VAL:HG13	9:LA:208:GLU:HG3	1.98	0.44
11:LC:264:THR:HG22	11:LC:265:PHE:N	2.32	0.44
15:LG:135:THR:HG21	15:LG:191:ILE:HD13	1.99	0.44
19:LK:43:ASP:HB3	19:LK:46:MET:HB2	1.99	0.44
23:LO:241:LEU:HB3	23:LO:243:GLU:OE2	2.17	0.44
27:LS:78:LYS:CG	27:LS:87:LYS:HG3	2.40	0.44
27:LS:84:THR:HG23	36:Lb:22:LYS:O	2.16	0.44
41:Lg:11:SER:O	41:Lg:15:HIS:ND1	2.47	0.44
51:S1:1572:C:H5	51:S1:1615:G:H1	1.66	0.44
64:SI:108:ASP:HB3	64:SI:111:LYS:HG3	1.98	0.44
76:SU:6:GLN:HB3	76:SU:7:TYR:H	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Sc:57:CYS:HB3	84:Sc:60:CYS:HB2	1.77	0.44
1:L1:422:PSU:H2'	1:L1:423:U:C6	2.52	0.44
1:L1:479:A:H2'	1:L1:480:U:C6	2.53	0.44
1:L1:770:G:O6	24:LP:103:PRO:HD3	2.17	0.44
1:L1:856:OMG:H2'	1:L1:987:A:H61	1.83	0.44
1:L1:1249:A:H5'	1:L1:1250:U:OP1	2.18	0.44
1:L1:1402:U:H2'	1:L1:1403:A:H8	1.82	0.44
2:L2:1046:OMG:HM23	2:L2:1046:OMG:H1'	1.72	0.44
2:L2:1496:G:H2'	2:L2:1497:C:C6	2.52	0.44
4:L4:1:G:H1'	6:L6:3:A:H5'	1.98	0.44
8:L8:96:G:H2'	8:L8:97:A:C8	2.51	0.44
22:LN:207:THR:HG22	22:LN:208:MET:N	2.32	0.44
31:LW:108:LEU:HB3	31:LW:113:LYS:HE3	2.00	0.44
51:S1:1484:A:H2'	51:S1:1485:A:C8	2.53	0.44
52:S2:53:G:C6	52:S2:54:U:H1'	2.52	0.44
58:SC:54:THR:HG23	58:SC:87:VAL:HG22	2.00	0.44
73:SR:31:LEU:O	73:SR:34:VAL:HG13	2.18	0.44
73:SR:36:GLY:O	73:SR:98:HIS:NE2	2.48	0.44
79:SX:155:LYS:HD2	79:SX:155:LYS:HA	1.60	0.44
1:L1:147:G:O6	15:LG:139:GLU:HG3	2.17	0.44
1:L1:543:G:N2	1:L1:1393:A:OP1	2.51	0.44
1:L1:752:G:OP1	20:LL:128:LYS:HG2	2.17	0.44
2:L2:610:G:H22	2:L2:642:G:H1'	1.83	0.44
3:L3:51:G:H2'	3:L3:52:G:H8	1.83	0.44
4:L4:120:U:O2'	18:LJ:14:ARG:NH2	2.51	0.44
7:L7:52:A:H4'	46:L1:19:GLN:HA	1.99	0.44
10:LB:50:LYS:HA	10:LB:79:LEU:HD23	1.99	0.44
19:LK:111:TYR:O	19:LK:115:VAL:HG13	2.18	0.44
23:LO:107:ARG:NH2	23:LO:119:PHE:O	2.51	0.44
25:LQ:23:TRP:HB2	25:LQ:53:LYS:HD2	1.99	0.44
37:Lc:230:HIS:CE1	37:Lc:238:GLY:HA3	2.52	0.44
51:S1:29:OMU:H2'	51:S1:30:G:C8	2.53	0.44
51:S1:680:G:H2'	51:S1:681:U:C6	2.53	0.44
51:S1:903:G:N2	65:SJ:107:SER:OG	2.39	0.44
51:S1:966:G:H5'	64:SI:10:LYS:HB2	1.99	0.44
51:S1:1398:C:C5	56:SA:168:MET:HG2	2.52	0.44
62:SG:118:LYS:HE3	62:SG:118:LYS:HB3	1.71	0.44
75:ST:32:ASN:O	75:ST:36:MET:HG2	2.16	0.44
78:SW:40:PHE:HE2	78:SW:93:THR:HG22	1.81	0.44
85:Sd:47:MET:HE3	85:Sd:47:MET:HB3	1.90	0.44
86:Se:38:LEU:HD11	86:Se:42:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:148:U:OP1	21:LM:49:ARG:NE	2.50	0.44
1:L1:458:A:H2'	1:L1:459:A:O4'	2.18	0.44
1:L1:586:U:H5'	11:LC:335:ARG:HD2	1.98	0.44
1:L1:1004:G:H1'	1:L1:1172:G:H5''	1.99	0.44
1:L1:1550:A:H2'	1:L1:1551:A:C8	2.53	0.44
2:L2:98:G:O2'	25:LQ:82:GLU:O	2.31	0.44
2:L2:1274:C:H2'	2:L2:1275:A:O4'	2.15	0.44
2:L2:1523:C:H2'	2:L2:1524:A:C8	2.53	0.44
4:L4:62:C:H2'	4:L4:63:U:O2	2.18	0.44
5:L5:106:G:N7	39:Le:97:LYS:HE3	2.32	0.44
7:L7:45:C:H5''	46:Ll:15:LYS:HD2	2.00	0.44
9:LA:79:PRO:HD3	9:LA:165:MET:SD	2.57	0.44
18:LJ:35:ASN:ND2	18:LJ:65:LYS:HB2	2.25	0.44
51:S1:1618:U:H2'	51:S1:1619:G:C8	2.53	0.44
51:S1:2010:G:H1	51:S1:2026:U:H3	1.64	0.44
53:S3:66:C:H2'	53:S3:67:C:H6	1.82	0.44
54:S4:15:G:H22	54:S4:21:A:H1'	1.83	0.44
63:SH:108:ARG:N	63:SH:183:GLU:OE2	2.41	0.44
66:SK:57:ALA:HB2	66:SK:196:GLY:HA2	2.00	0.44
77:SV:16:VAL:HG11	77:SV:35:ILE:HD12	1.99	0.44
1:L1:51:G:H4'	1:L1:863:G:H4'	2.00	0.44
1:L1:687:C:H2'	1:L1:688:A:C8	2.53	0.44
1:L1:751:G:O2'	1:L1:815:G:H5''	2.18	0.44
1:L1:795:U:HO2'	1:L1:796:G:H8	1.66	0.44
1:L1:955:A2M:HM'3	1:L1:955:A2M:H1'	1.67	0.44
2:L2:749:G:O2'	2:L2:750:U:H6	1.99	0.44
2:L2:1101:A:HO2'	2:L2:1102:C:P	2.41	0.44
2:L2:1219:A:H2'	2:L2:1220:A:C8	2.53	0.44
2:L2:1236:C:H5'	2:L2:1238:G:H5''	1.99	0.44
2:L2:1329:U:H5	2:L2:1350:G:O6	2.00	0.44
15:LG:240:SER:OG	15:LG:243:SER:OG	2.36	0.44
19:LK:28:VAL:HB	19:LK:37:LEU:O	2.17	0.44
22:LN:113:THR:O	22:LN:113:THR:OG1	2.33	0.44
24:LP:131:ASP:OD2	24:LP:131:ASP:N	2.51	0.44
30:LV:141:LYS:HE2	30:LV:141:LYS:HB2	1.65	0.44
50:Lp:4:TYR:HB3	50:Lp:93:LEU:HD23	1.99	0.44
51:S1:181:A:N6	51:S1:313:G:O2'	2.43	0.44
51:S1:189:G:H2'	51:S1:190:G:H8	1.82	0.44
51:S1:1152:A:C3'	70:SO:59:ARG:HH12	2.30	0.44
52:S2:1:G:H2'	52:S2:2:C:C6	2.53	0.44
53:S3:8:U:HO2'	53:S3:21:A:H62	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SB:60:LYS:HD2	57:SB:60:LYS:HA	1.82	0.44
60:SE:63:ARG:HA	60:SE:75:ARG:HB3	1.99	0.44
66:SK:67:TRP:HB3	66:SK:72:ILE:HG22	1.99	0.44
77:SV:33:ARG:HD3	77:SV:33:ARG:HA	1.83	0.44
85:Sd:28:LYS:HB2	85:Sd:28:LYS:HE2	1.85	0.44
85:Sd:75:LEU:C	85:Sd:77:GLU:H	2.25	0.44
1:L1:120:G:H1'	1:L1:122:A:H62	1.82	0.44
1:L1:148:U:O2'	1:L1:149:G:O5'	2.36	0.44
1:L1:553:A:N3	11:LC:323:ARG:HD3	2.33	0.44
1:L1:1414:A:OP1	24:LP:17:HIS:NE2	2.45	0.44
2:L2:1195:U:H2'	2:L2:1196:G:H8	1.81	0.44
3:L3:171:U:H3'	3:L3:172:G:H21	1.82	0.44
4:L4:155:A:H2'	4:L4:156:G:O4'	2.18	0.44
7:L7:71:A:H4'	7:L7:72:A:O5'	2.17	0.44
31:LW:24:ARG:HG2	31:LW:75:TRP:CH2	2.53	0.44
51:S1:17:C:H2'	51:S1:18:OMC:H6	1.83	0.44
51:S1:869:U:C2	59:SD:142:ILE:HD13	2.53	0.44
51:S1:910:A:H2'	51:S1:911:A:H8	1.83	0.44
51:S1:994:U:H2'	51:S1:995:U:C6	2.52	0.44
58:SC:131:LYS:HB2	58:SC:188:MET:HG2	1.99	0.44
62:SG:138:PRO:HB3	62:SG:143:LYS:HG2	1.99	0.44
73:SR:87:ARG:HH21	73:SR:91:PRO:HD2	1.83	0.44
81:SZ:127:LYS:HA	81:SZ:127:LYS:HD3	1.72	0.44
89:Sh:142:PRO:HD2	89:Sh:200:LEU:HD12	2.00	0.44
2:L2:426:G:H2'	2:L2:427:C:C6	2.52	0.44
2:L2:790:U:H2'	2:L2:791:A:H8	1.83	0.44
2:L2:1024:U:H2'	2:L2:1025:G:C8	2.53	0.44
2:L2:1321:U:H2'	2:L2:1322:C:H6	1.82	0.44
3:L3:51:G:H2'	3:L3:52:G:C8	2.53	0.44
10:LB:112:VAL:O	10:LB:116:ARG:HG3	2.17	0.44
27:LS:78:LYS:HG2	27:LS:87:LYS:CD	2.47	0.44
51:S1:512:A2M:HM'3	51:S1:512:A2M:H1'	1.73	0.44
51:S1:1829:OMG:HM23	51:S1:1829:OMG:H1'	1.76	0.44
51:S1:1859:A:H2'	51:S1:1859:A:N3	2.32	0.44
60:SE:225:ILE:HD11	60:SE:234:VAL:HG22	1.99	0.44
68:SM:91:PRO:HD2	68:SM:94:GLN:HB3	2.00	0.44
1:L1:124:C:H2'	1:L1:125:G:H8	1.83	0.44
1:L1:191:U:H5	1:L1:258:A:N1	2.16	0.44
1:L1:687:C:OP1	40:Lf:28:GLN:HB2	2.17	0.44
1:L1:1714:C:H2'	1:L1:1715:U:H6	1.82	0.44
2:L2:1087:C:H2'	2:L2:1088:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:159:C:H2'	3:L3:160:U:O4'	2.18	0.44
10:LB:232:GLU:OE1	10:LB:275:HIS:ND1	2.45	0.44
40:Lf:26:PHE:HB2	40:Lf:29:LEU:HG	1.99	0.44
51:S1:39:A:O2'	51:S1:517:A:N6	2.51	0.44
51:S1:341:A:N3	60:SE:30:PRO:HB3	2.33	0.44
51:S1:1438:A:C5	51:S1:1439:G:H1'	2.52	0.44
51:S1:1541:A:N3	51:S1:1546:A:O2'	2.50	0.44
87:Sf:94:LYS:HA	87:Sf:94:LYS:HD2	1.75	0.44
87:Sf:135:LYS:HD2	87:Sf:135:LYS:N	2.32	0.44
1:L1:159:U:O2'	1:L1:160:C:H5'	2.18	0.43
1:L1:307:U:H2'	1:L1:308:A:H8	1.83	0.43
1:L1:828:U:O5'	2:L2:1148:G:H4'	2.18	0.43
1:L1:1263:A:N1	2:L2:1295:C:H5''	2.33	0.43
1:L1:1564:C:H2'	1:L1:1565:A:H5''	2.00	0.43
2:L2:14:OMC:HM22	2:L2:15:C:O4'	2.18	0.43
2:L2:439:U:H1'	2:L2:561:G:N2	2.33	0.43
3:L3:77:A:H2'	3:L3:78:C:O4'	2.17	0.43
5:L5:119:U:OP1	5:L5:119:U:H4'	2.18	0.43
16:LH:115:LYS:HB3	16:LH:115:LYS:HZ3	1.81	0.43
24:LP:80:LYS:HD3	24:LP:80:LYS:HA	1.78	0.43
25:LQ:24:LEU:HD23	25:LQ:32:ILE:HG21	2.00	0.43
25:LQ:162:LYS:HB2	25:LQ:162:LYS:HE2	1.72	0.43
26:LR:94:LYS:HE2	26:LR:94:LYS:HB3	1.84	0.43
51:S1:281:A:N3	51:S1:281:A:H2'	2.32	0.43
51:S1:558:U:H2'	51:S1:559:G:H8	1.83	0.43
51:S1:1115:G:O2'	75:ST:52:MET:HE1	2.18	0.43
51:S1:1805:A:H2'	51:S1:1806:A:C8	2.53	0.43
62:SG:39:GLY:HA3	62:SG:46:PHE:O	2.18	0.43
64:SI:128:ILE:HG22	64:SI:132:MET:HE3	2.00	0.43
70:SO:142:ARG:NH1	70:SO:144:LEU:HD13	2.32	0.43
76:SU:93:THR:O	76:SU:93:THR:OG1	2.24	0.43
84:Sc:68:THR:HG22	84:Sc:69:GLY:N	2.33	0.43
87:Sf:125:CYS:HB2	87:Sf:143:CYS:HB3	1.89	0.43
88:Sg:251:CYS:HB3	88:Sg:285:ILE:HD12	1.99	0.43
1:L1:128:U:H2'	1:L1:129:C:H6	1.83	0.43
1:L1:302:G:H5'	43:Li:40:LEU:HB2	1.99	0.43
1:L1:925:U:OP2	2:L2:91:C:O2'	2.35	0.43
1:L1:1489:U:HO2'	1:L1:1490:G:H8	1.61	0.43
1:L1:1684:G:H1	1:L1:1708:G:N2	2.17	0.43
1:L1:1684:G:H22	1:L1:1708:G:N2	2.16	0.43
2:L2:652:C:H2'	2:L2:653:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1003:G:O2'	2:L2:1004:G:C8	2.67	0.43
2:L2:1251:A:H2'	2:L2:1252:G:O4'	2.18	0.43
3:L3:198:A:OP2	49:Lo:49:ARG:NH2	2.45	0.43
4:L4:161:C:H2'	4:L4:162:A:C8	2.53	0.43
5:L5:51:A:H4'	5:L5:52:U:OP1	2.18	0.43
6:L6:44:G:H2'	6:L6:45:G:C8	2.53	0.43
7:L7:154:A:H2'	7:L7:155:U:O4'	2.17	0.43
17:LI:180:GLU:CD	17:LI:180:GLU:H	2.25	0.43
23:LO:132:VAL:HG13	23:LO:178:ALA:HB1	2.01	0.43
25:LQ:61:ALA:O	25:LQ:65:LYS:HG3	2.19	0.43
25:LQ:190:ARG:HD3	25:LQ:190:ARG:HA	1.83	0.43
29:LU:42:ASP:OD1	29:LU:42:ASP:N	2.46	0.43
33:LY:76:ASN:OD1	33:LY:77:HIS:N	2.52	0.43
37:Lc:109:GLN:HG3	37:Lc:140:VAL:HG12	2.00	0.43
51:S1:105:C:H2'	51:S1:106:A:H8	1.83	0.43
51:S1:1538:U:H2'	51:S1:1539:PSU:O4'	2.18	0.43
51:S1:2199:C:OP2	83:Sb:5:ARG:NH1	2.51	0.43
52:S2:23:A:H2'	52:S2:24:G:C8	2.53	0.43
63:SH:88:LEU:O	82:Sa:58:LYS:NZ	2.47	0.43
77:SV:103:LYS:O	77:SV:107:GLN:HG3	2.18	0.43
80:SY:44:VAL:HG22	80:SY:50:ILE:HG22	2.00	0.43
1:L1:426:A:H2'	1:L1:427:A:C8	2.53	0.43
1:L1:626:U:O2'	1:L1:627:C:H6	2.00	0.43
1:L1:1186:A:H2'	1:L1:1187:A:C8	2.53	0.43
2:L2:811:U:H5	2:L2:1007:U:O2	2.01	0.43
3:L3:34:C:H2'	3:L3:34:C:O2	2.18	0.43
10:LB:338:PRO:HD2	10:LB:341:ARG:HD2	2.00	0.43
22:LN:167:MET:HE3	22:LN:178:ARG:HH21	1.83	0.43
32:LX:54:PRO:HA	32:LX:59:TYR:CG	2.53	0.43
35:La:100:LYS:HD3	35:La:100:LYS:HA	1.83	0.43
51:S1:377:A:C8	66:SK:49:ARG:HD2	2.53	0.43
51:S1:505:A:O3'	81:SZ:118:ARG:NH1	2.45	0.43
64:SI:41:LEU:N	64:SI:42:PRO:HD2	2.33	0.43
71:SP:53:GLU:HG2	71:SP:71:ARG:HG3	1.99	0.43
72:SQ:39:GLU:N	72:SQ:39:GLU:OE2	2.51	0.43
78:SW:51:ASN:HD22	78:SW:91:VAL:HG23	1.82	0.43
81:SZ:89:LEU:O	81:SZ:93:GLU:HB2	2.18	0.43
1:L1:852:A:H5''	20:LL:27:LYS:HE2	2.00	0.43
1:L1:889:G:N2	3:L3:124:U:H5'	2.30	0.43
1:L1:943:U:H2'	1:L1:944:A:O4'	2.18	0.43
1:L1:1425:C:H2'	34:LZ:108:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:469:G:H2'	2:L2:470:A:C8	2.53	0.43
2:L2:1115:U:H5	23:LO:17:GLN:O	2.02	0.43
2:L2:1384:A2M:H5''	2:L2:1385:G:H5'	1.99	0.43
4:L4:134:U:H2'	4:L4:135:C:O4'	2.18	0.43
5:L5:5:C:H2'	5:L5:6:G:O4'	2.19	0.43
5:L5:105:U:O2	5:L5:108:G:H5'	2.17	0.43
6:L6:68:A:H2'	6:L6:70:G:C5	2.53	0.43
7:L7:63:G:O2'	35:La:53:LYS:NZ	2.41	0.43
8:L8:15:A:N1	8:L8:70:G:O2'	2.50	0.43
39:Le:84:VAL:HG13	39:Le:120:MET:HE1	2.01	0.43
44:Lj:55:LYS:HA	44:Lj:58:ARG:HD2	1.99	0.43
51:S1:886:U:H3'	60:SE:238:LYS:HZ1	1.83	0.43
51:S1:1608:A:H4'	51:S1:1609:U:O5'	2.18	0.43
54:S4:37:A:H5''	54:S4:38:A:H8	1.83	0.43
57:SB:201:LYS:NZ	77:SV:86:PRO:O	2.45	0.43
66:SK:70:GLU:HB2	66:SK:72:ILE:HG22	2.00	0.43
70:SO:16:LYS:HB2	70:SO:16:LYS:HE3	1.57	0.43
72:SQ:47:LEU:CD1	87:Sf:97:ALA:HB3	2.47	0.43
89:Sh:217:GLU:O	89:Sh:221:VAL:HG22	2.18	0.43
1:L1:1684:G:H1	1:L1:1708:G:H1	1.67	0.43
2:L2:1314:C:H2'	2:L2:1315:G:O4'	2.18	0.43
23:LO:284:SER:OG	23:LO:287:GLU:OE2	2.34	0.43
33:LY:23:ALA:HA	33:LY:45:GLY:HA2	2.00	0.43
51:S1:253:U:O2'	51:S1:254:A:O5'	2.36	0.43
51:S1:1015:G:H2'	51:S1:1016:G:C8	2.53	0.43
51:S1:1437:A:H2'	51:S1:1438:A:C8	2.53	0.43
51:S1:1477:A:C5	51:S1:1478:OMG:H1'	2.54	0.43
51:S1:1501:G:H1'	51:S1:2168:A:C4	2.53	0.43
51:S1:1973:C:C2	74:SS:13:ILE:HD13	2.53	0.43
57:SB:15:GLU:OE1	77:SV:118:ARG:HG3	2.19	0.43
57:SB:113:ASN:HB3	57:SB:116:GLN:HG3	2.00	0.43
60:SE:117:GLN:HA	60:SE:161:VAL:HG22	2.01	0.43
65:SJ:26:LEU:HD23	65:SJ:62:VAL:HG22	2.01	0.43
76:SU:20:GLU:C	76:SU:22:ALA:H	2.27	0.43
76:SU:82:ARG:O	76:SU:142:GLN:HB3	2.19	0.43
1:L1:17:C:H2'	1:L1:18:A:H8	1.83	0.43
1:L1:36:U:H4'	20:LL:32:ARG:HD3	2.00	0.43
1:L1:163:U:H2'	1:L1:164:G:C8	2.53	0.43
1:L1:695:OMC:HM23	1:L1:695:OMC:H1'	1.73	0.43
1:L1:729:A:N1	7:L7:27:U:O2'	2.49	0.43
1:L1:845:OMU:H5'	20:LL:7:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:897:A:C2	51:S1:677:G:H4'	2.54	0.43
2:L2:1003:G:O2'	2:L2:1004:G:H8	2.02	0.43
5:L5:128:G:H2'	5:L5:129:G:H8	1.83	0.43
7:L7:31:A:O2'	7:L7:33:U:OP2	2.34	0.43
10:LB:226:THR:HG22	10:LB:336:SER:HB3	1.99	0.43
10:LB:292:ARG:HA	10:LB:292:ARG:HD2	1.70	0.43
10:LB:301:ALA:HB3	10:LB:310:LYS:HB2	2.00	0.43
20:LL:27:LYS:HD3	20:LL:27:LYS:HA	1.76	0.43
23:LO:276:LYS:HD3	23:LO:278:TYR:OH	2.18	0.43
51:S1:489:A:C6	51:S1:490:U:C4	3.06	0.43
51:S1:1875:G:H2'	51:S1:1876:U:C6	2.54	0.43
51:S1:1917:A:H4'	51:S1:1918:U:H3'	1.99	0.43
51:S1:1959:G:C2'	51:S1:1960:G:H5'	2.49	0.43
52:S2:50:U:H1'	52:S2:63:G:H22	1.83	0.43
57:SB:53:ASP:HB3	57:SB:56:MET:HB2	1.99	0.43
59:SD:128:ILE:HG13	59:SD:133:ILE:HD13	2.01	0.43
89:Sh:149:THR:O	89:Sh:153:VAL:HG13	2.18	0.43
1:L1:593:C:H2'	1:L1:594:G:H8	1.83	0.43
2:L2:1521:A:H2'	2:L2:1522:U:C6	2.53	0.43
15:LG:112:LYS:O	15:LG:116:GLU:HG2	2.18	0.43
21:LM:96:LYS:HB2	21:LM:96:LYS:HE2	1.83	0.43
25:LQ:174:ARG:HB2	25:LQ:174:ARG:HH11	1.81	0.43
29:LU:120:LYS:HE3	29:LU:120:LYS:HB3	1.65	0.43
39:Le:24:LYS:HE3	39:Le:24:LYS:HB3	1.78	0.43
51:S1:189:G:H2'	51:S1:190:G:C8	2.54	0.43
51:S1:275:A:O2'	51:S1:276:G:H8	2.00	0.43
51:S1:509:G:H2'	51:S1:510:G:C8	2.53	0.43
51:S1:1360:U:O4	64:SI:198:SER:OG	2.27	0.43
51:S1:1621:OMU:H4'	51:S1:1622:G:O5'	2.19	0.43
51:S1:1999:G:H2'	51:S1:2000:U:C6	2.54	0.43
87:Sf:105:GLU:HG3	87:Sf:111:TYR:CE1	2.54	0.43
87:Sf:132:ALA:O	87:Sf:138:GLN:HG3	2.18	0.43
88:Sg:179:TRP:HA	88:Sg:186:CYS:HA	1.99	0.43
1:L1:996:A:H2'	1:L1:997:C:C6	2.54	0.43
2:L2:1352:G:N3	2:L2:1372:A2M:H2	2.33	0.43
2:L2:1354:U:H1'	18:LJ:46:GLY:HA3	2.01	0.43
2:L2:1374:A:H2'	2:L2:1375:G:C8	2.54	0.43
5:L5:96:G:H2'	5:L5:97:C:C6	2.54	0.43
9:LA:180:LEU:HD22	49:Lo:18:TYR:HB3	2.01	0.43
10:LB:261:HIS:HA	10:LB:262:PRO:C	2.44	0.43
11:LC:282:LEU:HD11	24:LP:29:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:111:LEU:HB3	22:LN:112:GLN:H	1.66	0.43
41:Lg:47:HIS:CD2	41:Lg:47:HIS:H	2.36	0.43
51:S1:148:G:H2'	51:S1:149:G:H8	1.78	0.43
51:S1:2048:PSU:OP1	83:Sb:93:VAL:HG23	2.19	0.43
58:SC:166:PHE:CD2	58:SC:199:PRO:HG3	2.54	0.43
70:SO:49:VAL:HG13	70:SO:53:MET:HE2	2.01	0.43
89:Sh:152:GLN:HG3	89:Sh:195:PHE:HZ	1.83	0.43
1:L1:98:A:OP1	21:LM:195:ASN:HB3	2.18	0.43
1:L1:622:C:O2'	1:L1:623:U:H6	2.02	0.43
1:L1:1750:G:H5''	1:L1:1751:A:N7	2.34	0.43
2:L2:1214:G:H22	2:L2:1222:C:H5	1.66	0.43
5:L5:44:G:H2'	5:L5:45:A:C8	2.54	0.43
6:L6:52:G:H5''	19:LK:122:HIS:NE2	2.34	0.43
17:LI:55:PRO:HB3	17:LI:154:ASP:HB2	2.01	0.43
19:LK:67:ARG:NH1	26:LR:146:ALA:O	2.52	0.43
21:LM:73:ARG:NH1	21:LM:88:GLY:O	2.52	0.43
21:LM:143:ARG:O	35:La:103:GLU:HB3	2.19	0.43
21:LM:149:ASN:ND2	35:La:103:GLU:O	2.52	0.43
29:LU:68:VAL:HG22	29:LU:81:THR:HG22	2.01	0.43
34:LZ:97:ALA:HB2	34:LZ:104:ALA:HB2	2.01	0.43
37:Lc:124:THR:HB	37:Lc:215:PHE:HB2	2.00	0.43
40:Lf:35:LYS:HD2	40:Lf:53:MET:HE2	2.00	0.43
51:S1:559:G:N1	51:S1:592:C:H5	2.06	0.43
51:S1:630:U:H2'	51:S1:631:U:C6	2.54	0.43
51:S1:916:G:H22	75:ST:133:LYS:HB2	1.82	0.43
51:S1:925:A:H5'	51:S1:926:G:OP2	2.19	0.43
51:S1:1153:A:H2'	51:S1:1154:A:C8	2.54	0.43
52:S2:63:G:H2'	52:S2:64:A:C8	2.54	0.43
61:SF:245:THR:HG23	80:SY:4:ILE:HD13	2.00	0.43
62:SG:211:GLU:O	62:SG:215:LEU:HG	2.18	0.43
70:SO:118:LYS:HA	70:SO:118:LYS:HD3	1.76	0.43
70:SO:144:LEU:HD23	70:SO:144:LEU:H	1.83	0.43
75:ST:100:LYS:HD3	75:ST:100:LYS:HA	1.92	0.43
76:SU:97:ARG:HE	76:SU:128:PRO:HG3	1.84	0.43
1:L1:25:C:H42	1:L1:55:A:N6	2.17	0.43
1:L1:266:G:H2'	1:L1:267:A:C8	2.54	0.43
1:L1:273:A:C6	44:Lj:79:LYS:HA	2.53	0.43
1:L1:574:G:H5''	1:L1:575:A:OP1	2.19	0.43
1:L1:1501:A:OP1	40:Lf:106:ARG:NH2	2.52	0.43
1:L1:1538:U:OP1	28:LT:67:ILE:HG22	2.19	0.43
2:L2:847:U:H2'	2:L2:848:C:H6	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1020:C:O2'	2:L2:1021:A:H8	2.01	0.43
2:L2:1087:C:O2'	2:L2:1172:C:O2	2.37	0.43
2:L2:1110:U:H2'	2:L2:1111:C:C6	2.53	0.43
2:L2:1111:C:OP1	12:LD:18:LYS:NZ	2.42	0.43
2:L2:1116:A:H2'	2:L2:1116:A:N3	2.34	0.43
2:L2:1225:A:H2'	2:L2:1226:C:C6	2.53	0.43
2:L2:1398:C:H2'	2:L2:1399:G:C8	2.54	0.43
3:L3:196:U:H3'	3:L3:197:A:C8	2.54	0.43
6:L6:6:G:H5''	6:L6:7:A:OP2	2.19	0.43
11:LC:281:MET:HE2	24:LP:110:LEU:HB3	2.00	0.43
12:LD:177:LYS:HB2	12:LD:177:LYS:HE2	1.77	0.43
13:LE:46:ARG:NH2	19:LK:6:TYR:OH	2.50	0.43
23:LO:58:LYS:HD2	23:LO:58:LYS:HA	1.80	0.43
51:S1:506:U:H5''	81:SZ:115:LYS:HZ1	1.84	0.43
51:S1:759:U:H2'	51:S1:760:G:O4'	2.19	0.43
51:S1:761:A:H62	51:S1:768:A:H61	1.66	0.43
51:S1:910:A:H61	64:SI:113:GLN:HE22	1.66	0.43
51:S1:1206:C:H5''	75:ST:14:SER:HB3	2.00	0.43
58:SC:207:ILE:HD11	77:SV:46:LEU:HD13	2.01	0.43
61:SF:193:ALA:HB3	61:SF:196:PRO:HD2	2.01	0.43
78:SW:115:LYS:HD3	78:SW:115:LYS:HA	1.69	0.43
81:SZ:32:VAL:HG12	81:SZ:34:HIS:HD2	1.83	0.43
81:SZ:116:GLU:O	81:SZ:120:ARG:HD3	2.19	0.43
1:L1:5:A:O2'	1:L1:6:C:H5'	2.18	0.42
1:L1:478:C:H2'	1:L1:479:A:C8	2.54	0.42
1:L1:581:G:H2'	1:L1:582:U:C6	2.54	0.42
1:L1:1513:C:O3'	34:LZ:21:LYS:HE2	2.19	0.42
1:L1:1520:U:O4	20:LL:3:THR:OG1	2.32	0.42
2:L2:1234:G:N7	50:Lp:63:LYS:NZ	2.61	0.42
2:L2:1384:A2M:HM'3	2:L2:1384:A2M:H1'	1.86	0.42
3:L3:101:G:N1	3:L3:139:C:H5	2.00	0.42
7:L7:11:G:H1'	28:LT:5:SER:HB3	2.01	0.42
7:L7:56:G:H2'	7:L7:57:C:O4'	2.19	0.42
7:L7:75:OMG:HM23	7:L7:75:OMG:H1'	1.87	0.42
10:LB:289:GLN:HG2	10:LB:330:MET:HE3	2.00	0.42
13:LE:176:ASP:OD1	13:LE:176:ASP:N	2.51	0.42
26:LR:46:MET:O	26:LR:50:LYS:HB2	2.18	0.42
51:S1:234:C:C2	51:S1:235:C:C5	3.07	0.42
51:S1:264:C:H2'	51:S1:265:C:C6	2.53	0.42
51:S1:437:C:H2'	51:S1:438:U:C6	2.54	0.42
51:S1:1510:C:H5	51:S1:1515:A:H61	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:2086:A:N1	51:S1:2137:U:H5	2.17	0.42
58:SC:115:ARG:HG2	58:SC:151:PHE:CE1	2.54	0.42
62:SG:10:ASN:ND2	62:SG:130:THR:O	2.45	0.42
63:SH:35:VAL:HG11	67:SL:49:THR:HA	2.00	0.42
66:SK:66:ALA:HA	66:SK:73:ALA:HA	2.00	0.42
68:SM:19:LEU:O	68:SM:85:ILE:HA	2.19	0.42
80:SY:33:ASP:OD1	80:SY:34:HIS:N	2.52	0.42
1:L1:208:C:H2'	1:L1:209:C:O4'	2.19	0.42
1:L1:754:G:H2'	1:L1:755:A:H8	1.84	0.42
1:L1:1270:U:H2'	47:Lm:109:ASN:ND2	2.34	0.42
1:L1:1687:G:H1	1:L1:1705:G:H1	1.68	0.42
2:L2:980:A:H2'	2:L2:981:C:O4'	2.19	0.42
2:L2:1006:G:H2'	2:L2:1007:U:C6	2.54	0.42
4:L4:24:A:N1	4:L4:181:C:O2'	2.47	0.42
7:L7:12:A:H5'	28:LT:2:THR:HB	2.01	0.42
8:L8:24:U:H2'	8:L8:25:G:O4'	2.19	0.42
11:LC:206:PRO:HB3	11:LC:247:PHE:CD2	2.55	0.42
12:LD:178:LYS:H	12:LD:178:LYS:HG2	1.46	0.42
14:LF:36:GLY:HA2	14:LF:93:ILE:HG12	2.01	0.42
19:LK:45:LYS:HA	19:LK:45:LYS:HD2	1.85	0.42
39:Le:162:LYS:HA	39:Le:162:LYS:HD3	1.72	0.42
48:Ln:23:LYS:HD3	51:S1:1467:U:H5''	2.01	0.42
51:S1:476:C:H2'	51:S1:477:G:O4'	2.18	0.42
51:S1:530:U:H2'	51:S1:531:G:C8	2.53	0.42
51:S1:642:A:H4'	51:S1:644:G:H4'	2.00	0.42
51:S1:858:A:C5	51:S1:859:G:C8	3.07	0.42
51:S1:1989:A:H2'	51:S1:1990:A:C8	2.54	0.42
54:S4:18:G:H5''	54:S4:19:G:O5'	2.19	0.42
58:SC:25:LYS:HE2	58:SC:25:LYS:HB3	1.81	0.42
58:SC:137:VAL:HG22	58:SC:183:VAL:HG12	2.01	0.42
78:SW:88:ARG:NH1	78:SW:105:ASN:HA	2.34	0.42
1:L1:198:A:H3'	34:LZ:139:ARG:NH2	2.34	0.42
1:L1:416:A:O4'	31:LW:84:ARG:HD3	2.18	0.42
1:L1:446:U:H4'	1:L1:1506:G:H4'	2.01	0.42
1:L1:531:C:H1'	26:LR:132:PRO:HG3	2.00	0.42
1:L1:653:A:H5''	41:Lg:86:ARG:NH1	2.34	0.42
1:L1:717:G:N7	17:LI:37:LYS:NZ	2.63	0.42
1:L1:845:OMU:HM23	1:L1:845:OMU:H1'	1.80	0.42
1:L1:1680:U:H2'	1:L1:1681:G:H8	1.84	0.42
2:L2:693:C:N3	2:L2:746:A:N6	2.64	0.42
13:LE:63:LYS:HE3	13:LE:63:LYS:HB3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:107:ARG:HD2	23:LO:257:ARG:HG2	2.00	0.42
26:LR:9:TYR:CE1	26:LR:65:VAL:HG23	2.54	0.42
26:LR:97:ARG:HG2	26:LR:141:ILE:HG23	2.01	0.42
37:Lc:165:LYS:HG2	37:Lc:213:TRP:HE3	1.84	0.42
51:S1:783:A:H2'	51:S1:784:C:O2	2.18	0.42
51:S1:1220:A:H2'	51:S1:1221:A:C8	2.54	0.42
51:S1:1644:G:H2'	51:S1:1645:U:C6	2.54	0.42
51:S1:1956:C:O2	51:S1:1956:C:H2'	2.19	0.42
58:SC:192:ASP:HB3	58:SC:195:GLY:H	1.83	0.42
69:SN:66:TYR:OH	69:SN:69:ARG:HA	2.19	0.42
73:SR:82:ASP:OD1	73:SR:96:THR:HG21	2.20	0.42
89:Sh:139:PHE:CE1	89:Sh:172:PHE:HB2	2.53	0.42
1:L1:149:G:H2'	1:L1:150:G:H8	1.83	0.42
1:L1:199:A:N1	34:LZ:140:LYS:NZ	2.62	0.42
1:L1:555:U:H2'	1:L1:556:C:C6	2.55	0.42
1:L1:563:C:O2	1:L1:563:C:H2'	2.20	0.42
1:L1:989:C:OP1	1:L1:1013:A:O2'	2.36	0.42
1:L1:1400:A:HO2'	1:L1:1401:U:P	2.40	0.42
2:L2:597:PSU:H2'	2:L2:598:A:H8	1.83	0.42
2:L2:957:C:H2'	2:L2:958:A:H8	1.84	0.42
2:L2:1287:C:O2'	2:L2:1288:G:H8	2.01	0.42
5:L5:6:G:H2'	5:L5:7:U:H6	1.84	0.42
5:L5:87:U:C2'	5:L5:88:C:H5'	2.49	0.42
7:L7:166:PSU:H5'	15:LG:64:ARG:HH11	1.83	0.42
7:L7:168:G:H2'	7:L7:169:A:C8	2.55	0.42
9:LA:40:TYR:HA	9:LA:91:GLY:HA3	2.02	0.42
10:LB:36:ASP:O	10:LB:190:GLY:HA2	2.19	0.42
10:LB:291:GLY:HA3	10:LB:328:TYR:CE1	2.54	0.42
44:Lj:17:ILE:HG12	44:Lj:29:VAL:HG22	2.02	0.42
49:Lo:67:GLY:HA3	49:Lo:70:THR:O	2.19	0.42
51:S1:273:G:H4'	89:Sh:227:ARG:NH2	2.34	0.42
51:S1:613:G:H22	51:S1:629:A:H5'	1.84	0.42
51:S1:1874:U:O4	63:SH:145:ARG:HG3	2.19	0.42
56:SA:158:ALA:HB1	56:SA:207:LEU:HD11	2.02	0.42
58:SC:156:MET:HE3	58:SC:186:LYS:HB2	2.01	0.42
60:SE:98:LEU:HD23	60:SE:98:LEU:HA	1.84	0.42
60:SE:178:VAL:HG11	60:SE:192:ILE:HD11	2.01	0.42
60:SE:247:ILE:H	60:SE:247:ILE:HD12	1.84	0.42
64:SI:59:LYS:HB3	64:SI:59:LYS:HE2	1.72	0.42
86:Se:39:LYS:O	86:Se:43:ARG:HG2	2.19	0.42
89:Sh:164:ARG:O	89:Sh:176:TYR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:662:C:H2'	1:L1:663:C:C6	2.55	0.42
1:L1:701:G:H5''	24:LP:159:PHE:CE1	2.53	0.42
1:L1:1468:U:H2'	1:L1:1469:G:H8	1.84	0.42
2:L2:389:A:OP2	2:L2:570:A2M:H8	2.18	0.42
2:L2:775:C:OP1	2:L2:776:C:O2'	2.23	0.42
3:L3:76:C:H2'	3:L3:77:A:C8	2.54	0.42
4:L4:160:C:H2'	4:L4:161:C:O2	2.20	0.42
6:L6:31:U:O2'	6:L6:32:U:H5'	2.19	0.42
8:L8:35:U:H2'	8:L8:36:A:C8	2.55	0.42
10:LB:392:LYS:H	10:LB:392:LYS:HG3	1.57	0.42
37:Lc:194:MET:HE2	37:Lc:194:MET:HB3	1.82	0.42
46:Ll:5:LYS:HG3	46:Ll:10:LYS:HB2	2.01	0.42
51:S1:955:A:HO2'	51:S1:956:A:H8	1.68	0.42
51:S1:1209:C:HO2'	51:S1:1210:C:P	2.40	0.42
51:S1:1850:U:H2'	51:S1:1851:U:H6	1.84	0.42
51:S1:1995:7MG:H2'	51:S1:1996:A:C8	2.54	0.42
61:SF:188:THR:HB	61:SF:207:ASP:HB3	2.00	0.42
72:SQ:62:CYS:SG	72:SQ:63:ILE:N	2.92	0.42
82:Sa:71:ILE:HB	82:Sa:75:ILE:HD11	2.02	0.42
1:L1:899:A:O5'	1:L1:899:A:H8	2.02	0.42
1:L1:1096:C:O2'	1:L1:1097:A:OP2	2.34	0.42
1:L1:1471:A:H2'	1:L1:1472:G:C8	2.54	0.42
1:L1:1582:A:H2'	1:L1:1583:C:H6	1.85	0.42
2:L2:449:U:H2'	2:L2:450:C:C6	2.55	0.42
2:L2:1057:C:C5	27:LS:4:SER:HB3	2.54	0.42
2:L2:1214:G:N1	2:L2:1222:C:H5	2.12	0.42
3:L3:121:U:O2'	3:L3:123:G:N7	2.39	0.42
4:L4:141:A:H2'	4:L4:142:A:O4'	2.20	0.42
15:LG:120:ASP:HB3	15:LG:123:LYS:HE2	2.01	0.42
20:LL:28:HIS:CD2	20:LL:32:ARG:HG3	2.55	0.42
22:LN:150:GLU:OE2	22:LN:153:ARG:NE	2.52	0.42
32:LX:59:TYR:CD1	32:LX:59:TYR:C	2.98	0.42
51:S1:438:U:O2'	62:SG:92:GLN:OE1	2.37	0.42
51:S1:555:C:H2'	51:S1:556:A:C8	2.55	0.42
51:S1:1366:A:N1	51:S1:1404:U:H5	2.18	0.42
51:S1:1602:U:O2'	87:Sf:134:HIS:ND1	2.49	0.42
52:S2:39:U:H2'	52:S2:40:C:H6	1.84	0.42
56:SA:196:SER:O	56:SA:200:VAL:HG23	2.20	0.42
59:SD:78:ARG:O	59:SD:82:TYR:HD2	2.03	0.42
64:SI:51:GLU:OE2	64:SI:60:THR:HG21	2.19	0.42
83:Sb:102:LYS:HB2	83:Sb:102:LYS:HE2	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:405:A:H1'	11:LC:83:THR:CG2	2.50	0.42
1:L1:1437:A:N6	34:LZ:105:ASP:OD2	2.51	0.42
2:L2:603:A:H2'	2:L2:604:A2M:C8	2.50	0.42
2:L2:622:G:H2'	2:L2:623:A:C8	2.54	0.42
2:L2:1063:C:H5''	2:L2:1064:A:H5''	2.01	0.42
4:L4:1:G:H2'	4:L4:2:U:C6	2.55	0.42
7:L7:71:A:H3'	31:LW:48:ARG:HB2	2.02	0.42
11:LC:281:MET:SD	24:LP:26:ILE:HG12	2.60	0.42
13:LE:91:VAL:CG1	13:LE:178:ILE:HG22	2.50	0.42
14:LF:173:GLU:OE1	19:LK:112:GLN:NE2	2.40	0.42
15:LG:86:ALA:O	15:LG:90:GLU:HG2	2.19	0.42
17:LI:145:GLU:O	17:LI:149:LYS:HG2	2.20	0.42
19:LK:147:MET:HE1	41:Lg:13:LYS:HG2	2.01	0.42
25:LQ:96:MET:O	25:LQ:100:ARG:HG3	2.20	0.42
28:LT:35:VAL:HG13	28:LT:36:ILE:HG23	2.00	0.42
43:Li:1:MET:SD	43:Li:2:SER:N	2.92	0.42
45:Lk:40:ARG:HG3	45:Lk:40:ARG:NH1	2.34	0.42
50:Lp:70:LEU:HD21	50:Lp:91:PHE:CZ	2.54	0.42
51:S1:1598:U:OP2	74:SS:3:HIS:ND1	2.46	0.42
57:SB:32:ASN:O	57:SB:154:ASP:HB3	2.20	0.42
57:SB:83:ARG:O	57:SB:84:LEU:HB3	2.17	0.42
62:SG:53:LEU:HD23	62:SG:114:VAL:HG12	2.01	0.42
69:SN:7:LYS:HG3	69:SN:10:ARG:HH21	1.83	0.42
69:SN:37:LEU:HD12	69:SN:37:LEU:HA	1.90	0.42
88:Sg:8:LYS:HB2	88:Sg:302:LEU:HD11	2.00	0.42
1:L1:146:U:H5''	15:LG:137:LEU:HB2	2.02	0.42
1:L1:170:U:H1'	1:L1:171:U:OP2	2.19	0.42
1:L1:307:U:H2'	1:L1:308:A:C8	2.54	0.42
1:L1:1062:A:H2'	1:L1:1063:G:C8	2.54	0.42
1:L1:1369:G:C2	16:LH:78:LYS:HD3	2.55	0.42
1:L1:1400:A:O2'	1:L1:1401:U:O5'	2.30	0.42
1:L1:1582:A:H2'	1:L1:1583:C:C6	2.55	0.42
2:L2:363:C:H2'	2:L2:364:G:O4'	2.20	0.42
2:L2:771:G:H4'	15:LG:50:PHE:CE1	2.55	0.42
4:L4:85:C:H4'	39:Le:97:LYS:HE2	2.00	0.42
10:LB:107:ALA:HB1	10:LB:205:GLU:HG3	2.01	0.42
10:LB:237:ARG:HG3	10:LB:275:HIS:HB2	2.01	0.42
12:LD:17:LYS:HA	12:LD:17:LYS:HD2	1.77	0.42
15:LG:162:GLU:OE2	21:LM:26:ARG:NH2	2.41	0.42
29:LU:40:SER:O	29:LU:44:LEU:HD23	2.20	0.42
33:LY:36:ARG:HD3	33:LY:40:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:306:U:O4'	66:SK:64:ASN:ND2	2.47	0.42
51:S1:359:A:C2	51:S1:397:A:C5	3.07	0.42
51:S1:656:G:H5'	51:S1:662:G:N2	2.35	0.42
51:S1:954:A:H2'	51:S1:955:A:H5'	2.02	0.42
54:S4:15:G:N2	54:S4:21:A:H1'	2.35	0.42
56:SA:135:TYR:CE2	56:SA:222:THR:HG22	2.55	0.42
58:SC:4:LEU:HD23	58:SC:4:LEU:HA	1.81	0.42
63:SH:83:LEU:HD22	63:SH:94:PRO:HB2	2.01	0.42
1:L1:91:G:H5'	1:L1:93:G:N7	2.35	0.42
1:L1:109:A:H4'	1:L1:110:A:H5'	2.01	0.42
1:L1:375:A:H2'	1:L1:376:A:O4'	2.20	0.42
1:L1:395:A:N1	11:LC:83:THR:HG23	2.35	0.42
1:L1:979:C:H2'	1:L1:980:A:C8	2.55	0.42
1:L1:1264:A:C2	2:L2:1295:C:H5'	2.55	0.42
1:L1:1750:G:O2'	45:Lk:78:ASN:ND2	2.52	0.42
2:L2:554:C:H2'	2:L2:555:A:C8	2.55	0.42
6:L6:46:C:C2	6:L6:47:G:C8	3.08	0.42
7:L7:162:A2M:HM'3	7:L7:162:A2M:H1'	1.76	0.42
14:LF:97:ASP:C	14:LF:99:ALA:H	2.27	0.42
15:LG:64:ARG:O	15:LG:68:ARG:HG3	2.19	0.42
15:LG:122:LYS:HE3	15:LG:122:LYS:HB3	1.85	0.42
16:LH:108:ARG:HE	16:LH:108:ARG:HB2	1.66	0.42
37:Lc:96:VAL:HG13	37:Lc:146:TYR:HB3	2.02	0.42
51:S1:133:G:C8	51:S1:133:G:OP2	2.72	0.42
51:S1:1367:U:H2'	51:S1:1368:C:H6	1.85	0.42
51:S1:1611:C:H6	51:S1:1611:C:H2'	1.70	0.42
51:S1:1663:U:H4'	77:SV:4:ILE:HD11	2.01	0.42
56:SA:24:MET:HE3	56:SA:24:MET:HB3	1.95	0.42
57:SB:167:ASN:O	57:SB:173:SER:OG	2.21	0.42
60:SE:250:ARG:O	60:SE:254:LEU:HD23	2.20	0.42
61:SF:149:VAL:HG12	80:SY:32:HIS:HD2	1.84	0.42
61:SF:168:MET:HE3	61:SF:168:MET:HB3	1.93	0.42
62:SG:49:TYR:CD1	62:SG:119:VAL:HA	2.54	0.42
65:SJ:18:GLU:HG3	65:SJ:69:LEU:HB3	2.02	0.42
70:SO:48:LYS:HB3	70:SO:48:LYS:HE3	1.89	0.42
1:L1:205:A:C5	34:LZ:55:PRO:HG3	2.55	0.42
1:L1:1022:G:H2'	1:L1:1023:G:C8	2.55	0.42
1:L1:1102:U:H5''	27:LS:19:PHE:HB2	2.01	0.42
1:L1:1603:G:H2'	1:L1:1604:U:C6	2.54	0.42
2:L2:432:U:H5	9:LA:200:ARG:HD3	1.85	0.42
2:L2:490:A:H5''	9:LA:243:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:66:C:OP2	25:LQ:64:ARG:NH2	2.50	0.42
5:L5:8:C:H2'	5:L5:9:C:H6	1.85	0.42
8:L8:11:G:H2'	8:L8:12:A:H8	1.84	0.42
20:LL:36:GLY:O	20:LL:41:HIS:HB2	2.20	0.42
31:LW:97:HIS:ND1	31:LW:99:SER:OG	2.49	0.42
51:S1:1985:G:OP1	73:SR:41:PHE:N	2.52	0.42
57:SB:77:VAL:O	57:SB:99:THR:HB	2.20	0.42
59:SD:100:VAL:O	59:SD:104:LEU:HD12	2.20	0.42
63:SH:127:VAL:HG13	63:SH:131:ARG:HD3	2.02	0.42
64:SI:19:LEU:HD23	64:SI:19:LEU:HA	1.90	0.42
67:SL:137:ARG:HG2	67:SL:143:ARG:HD2	2.01	0.42
1:L1:513:C:H2'	1:L1:514:C:O2	2.20	0.41
1:L1:1650:U:H5''	21:LM:67:ARG:HD2	2.02	0.41
1:L1:1775:U:H2'	1:L1:1776:G:H8	1.84	0.41
2:L2:354:A:H2'	2:L2:355:A:C8	2.54	0.41
2:L2:959:A:H2'	2:L2:960:C:C6	2.56	0.41
3:L3:126:C:H2'	3:L3:127:G:C8	2.55	0.41
4:L4:92:U:H2'	4:L4:93:U:H6	1.83	0.41
9:LA:96:LEU:HD11	9:LA:107:ILE:HG23	2.02	0.41
15:LG:137:LEU:O	15:LG:141:THR:OG1	2.30	0.41
23:LO:84:PRO:HD3	23:LO:88:ILE:O	2.20	0.41
24:LP:51:ARG:HA	24:LP:54:LYS:HG3	2.02	0.41
24:LP:74:LYS:O	24:LP:78:THR:OG1	2.25	0.41
26:LR:146:ALA:HB3	26:LR:149:LEU:HB2	2.02	0.41
28:LT:40:PRO:HA	28:LT:113:VAL:HA	2.02	0.41
34:LZ:51:ALA:HB3	34:LZ:96:VAL:HG13	2.01	0.41
43:Li:54:SER:OG	43:Li:57:GLU:HG3	2.20	0.41
51:S1:506:U:P	81:SZ:118:ARG:HH12	2.43	0.41
51:S1:752:C:H2'	51:S1:753:A:N3	2.35	0.41
51:S1:1578:G:O2'	51:S1:1608:A:N1	2.53	0.41
51:S1:1800:U:H2'	51:S1:1801:G:O4'	2.20	0.41
52:S2:57:G:O2'	52:S2:58:A:O5'	2.32	0.41
52:S2:65:G:H3'	52:S2:66:U:H6	1.85	0.41
61:SF:137:ILE:HG22	61:SF:141:MET:HE3	2.01	0.41
82:Sa:51:ARG:NH1	82:Sa:86:GLU:OE2	2.53	0.41
82:Sa:97:LYS:HD3	82:Sa:97:LYS:HA	1.81	0.41
1:L1:420:C:H2'	1:L1:421:U:H6	1.84	0.41
1:L1:507:C:OP2	11:LC:353:ARG:NH2	2.49	0.41
1:L1:622:C:O2'	1:L1:623:U:H5'	2.19	0.41
1:L1:753:A:N1	1:L1:832:G:O2'	2.44	0.41
1:L1:890:C:H5	1:L1:905:G:N1	2.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:134:C:H2'	2:L2:135:A:H8	1.84	0.41
2:L2:377:A:H2'	2:L2:378:C:H5'	2.02	0.41
2:L2:1026:C:H2'	2:L2:1027:C:C6	2.56	0.41
3:L3:204:A:H2'	3:L3:205:A:H8	1.80	0.41
10:LB:204:LEU:HD23	10:LB:204:LEU:HA	1.86	0.41
11:LC:141:HIS:ND1	11:LC:178:ASP:OD2	2.40	0.41
11:LC:273:LYS:HB3	11:LC:273:LYS:HE3	1.90	0.41
11:LC:356:LYS:HE3	11:LC:356:LYS:HB3	1.91	0.41
16:LH:63:GLY:O	16:LH:155:THR:HG22	2.20	0.41
38:Ld:18:LEU:O	38:Ld:22:SER:OG	2.27	0.41
43:Li:8:THR:HG23	43:Li:15:ASN:HB2	2.02	0.41
51:S1:51:A:H2'	51:S1:52:U:O4'	2.21	0.41
51:S1:123:A:O2'	51:S1:124:A:H5'	2.20	0.41
51:S1:339:U:O2'	51:S1:340:G:H8	2.03	0.41
51:S1:760:G:H3'	51:S1:761:A:C2	2.55	0.41
51:S1:1862:C:H1'	82:Sa:17:ASN:ND2	2.35	0.41
58:SC:50:LYS:HE3	58:SC:50:LYS:HB3	1.78	0.41
62:SG:198:ALA:O	62:SG:202:VAL:HG13	2.19	0.41
66:SK:13:ILE:HG13	66:SK:14:THR:N	2.35	0.41
82:Sa:41:MET:HE2	82:Sa:41:MET:HB3	1.86	0.41
88:Sg:128:ASP:OD2	88:Sg:132:ARG:NH1	2.53	0.41
1:L1:55:A:H2'	1:L1:56:G:H5'	1.98	0.41
1:L1:1588:G:O2'	1:L1:1590:G:OP2	2.37	0.41
2:L2:790:U:H2'	2:L2:791:A:C8	2.56	0.41
2:L2:1360:OMG:HN1	52:S2:75:C:N4	2.11	0.41
3:L3:99:U:H2'	3:L3:100:U:H6	1.85	0.41
3:L3:160:U:H2'	3:L3:168:U:C4	2.55	0.41
14:LF:156:LYS:HE2	14:LF:156:LYS:HB3	1.75	0.41
19:LK:132:ASP:OD1	19:LK:137:VAL:HG12	2.20	0.41
21:LM:56:LYS:HB3	21:LM:56:LYS:HE3	1.83	0.41
25:LQ:19:ARG:HA	25:LQ:19:ARG:HD2	1.84	0.41
31:LW:56:LYS:HB3	31:LW:56:LYS:HE2	1.73	0.41
51:S1:686:C:OP1	65:SJ:32:LYS:HG3	2.20	0.41
63:SH:78:LEU:HD22	63:SH:156:PRO:HD3	2.02	0.41
65:SJ:3:MET:HE3	65:SJ:3:MET:HB2	1.82	0.41
65:SJ:89:TRP:O	65:SJ:93:ILE:HG12	2.19	0.41
66:SK:83:TYR:HB3	66:SK:101:ILE:HB	2.03	0.41
66:SK:166:ARG:HE	66:SK:166:ARG:HB2	1.74	0.41
68:SM:18:ARG:NE	68:SM:87:ASP:OD2	2.38	0.41
75:ST:76:LYS:HG3	75:ST:81:ALA:HB2	2.02	0.41
82:Sa:104:ILE:H	82:Sa:104:ILE:HG13	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sb:91:ARG:NH2	83:Sb:96:ARG:O	2.53	0.41
86:Se:54:LYS:HD2	86:Se:56:HIS:CD2	2.55	0.41
88:Sg:172:TRP:HA	88:Sg:196:TYR:HB2	2.02	0.41
1:L1:517:U:H2'	1:L1:518:C:C6	2.56	0.41
1:L1:898:A:OP1	75:ST:140:LYS:HE2	2.20	0.41
1:L1:1534:G:H2'	1:L1:1535:G:O4'	2.20	0.41
2:L2:1277:G:O6	2:L2:1283:A:O2'	2.23	0.41
2:L2:1287:C:O2'	2:L2:1288:G:H5'	2.21	0.41
3:L3:100:U:H2'	3:L3:101:G:C8	2.56	0.41
10:LB:40:LYS:HE3	10:LB:41:PRO:O	2.20	0.41
10:LB:54:THR:OG1	10:LB:55:HIS:N	2.53	0.41
10:LB:155:LYS:HD3	10:LB:155:LYS:HA	1.79	0.41
11:LC:230:VAL:HG22	11:LC:261:ILE:HD12	2.01	0.41
16:LH:30:LYS:HA	16:LH:58:GLN:HB2	2.01	0.41
28:LT:37:ASN:O	28:LT:37:ASN:ND2	2.34	0.41
47:Lm:112:LYS:HB2	47:Lm:115:CYS:SG	2.61	0.41
51:S1:18:OMC:HM23	51:S1:18:OMC:H1'	1.76	0.41
51:S1:95:C:O2	51:S1:468:A:O2'	2.36	0.41
51:S1:170:G:OP1	62:SG:8:PRO:HB3	2.21	0.41
51:S1:320:G:H2'	51:S1:321:G:C8	2.55	0.41
51:S1:378:G:H2'	51:S1:379:U:C6	2.55	0.41
51:S1:471:A:O4'	51:S1:507:G:N2	2.52	0.41
51:S1:876:G:H1	51:S1:885:C:H5	1.69	0.41
51:S1:1695:C:H2'	51:S1:1696:A:C8	2.55	0.41
58:SC:166:PHE:CE2	58:SC:203:LEU:HD22	2.56	0.41
63:SH:17:LEU:HD12	63:SH:17:LEU:HA	1.93	0.41
63:SH:112:THR:HG21	85:Sd:39:VAL:HG21	2.02	0.41
68:SM:75:ASP:HB3	68:SM:77:PHE:CE2	2.55	0.41
75:ST:21:THR:HG23	84:Sc:86:HIS:NE2	2.35	0.41
87:Sf:74:LYS:HE2	87:Sf:74:LYS:HB3	1.82	0.41
1:L1:205:A:H1'	40:Lf:84:TYR:CE2	2.55	0.41
1:L1:326:A:C2	21:LM:93:LYS:HD3	2.55	0.41
1:L1:574:G:O2'	1:L1:576:G:H2'	2.20	0.41
1:L1:1683:C:H2'	1:L1:1684:G:H8	1.85	0.41
2:L2:339:A:C6	76:SU:16:THR:HG22	2.55	0.41
2:L2:505:A:H3'	2:L2:506:U:H6	1.85	0.41
3:L3:155:A:H61	3:L3:175:A:N6	2.18	0.41
4:L4:183:C:H2'	4:L4:184:U:O4'	2.20	0.41
9:LA:108:THR:HB	49:Lo:86:LEU:HD13	2.01	0.41
24:LP:189:SER:HB3	24:LP:190:TYR:H	1.74	0.41
25:LQ:181:ARG:HD2	25:LQ:181:ARG:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:198:GLN:HG3	25:LQ:201:LYS:NZ	2.35	0.41
28:LT:46:GLN:O	28:LT:50:GLN:HG3	2.21	0.41
41:Lg:34:TYR:CE1	41:Lg:136:ARG:HG2	2.55	0.41
51:S1:550:C:H2'	51:S1:551:A:H8	1.83	0.41
57:SB:84:LEU:O	57:SB:84:LEU:HG	2.21	0.41
58:SC:176:MET:HE3	58:SC:176:MET:HB3	1.91	0.41
59:SD:43:ARG:O	59:SD:47:THR:OG1	2.31	0.41
63:SH:112:THR:HG23	63:SH:113:ARG:HD3	2.02	0.41
75:ST:87:ASP:OD2	75:ST:125:LEU:HD21	2.20	0.41
85:Sd:29:VAL:HG22	85:Sd:42:VAL:HG12	2.02	0.41
1:L1:7:C:H2'	1:L1:8:U:C6	2.55	0.41
1:L1:160:C:O2'	1:L1:161:A:O4'	2.38	0.41
1:L1:1106:A:H5''	8:L8:102:G:O2'	2.21	0.41
1:L1:1680:U:H2'	1:L1:1681:G:C8	2.55	0.41
2:L2:782:G:H3'	2:L2:786:A:N7	2.36	0.41
2:L2:959:A:H2'	2:L2:960:C:H6	1.85	0.41
2:L2:1150:U:O2'	27:LS:88:ARG:O	2.26	0.41
4:L4:67:A:H5'	18:LJ:13:PHE:CE1	2.56	0.41
11:LC:63:ALA:HB3	11:LC:91:PHE:CZ	2.55	0.41
13:LE:41:LEU:HD23	13:LE:41:LEU:HA	1.83	0.41
18:LJ:9:LYS:HD2	18:LJ:9:LYS:HA	1.62	0.41
23:LO:239:LYS:HA	23:LO:239:LYS:HD3	1.85	0.41
28:LT:67:ILE:HD11	28:LT:80:LYS:HB3	2.01	0.41
51:S1:54:C:O2'	81:SZ:115:LYS:HE3	2.19	0.41
51:S1:122:A:N1	51:S1:337:U:H5	2.18	0.41
51:S1:852:G:H2'	51:S1:853:A:H8	1.85	0.41
51:S1:1605:U:H2'	51:S1:1606:C:C6	2.55	0.41
53:S3:14:A:H61	53:S3:21:A:H8	1.68	0.41
56:SA:121:THR:HG22	56:SA:123:MET:HG3	2.03	0.41
60:SE:42:LEU:HD11	60:SE:55:ALA:HA	2.01	0.41
1:L1:538:G:H2'	1:L1:539:C:H5''	2.02	0.41
1:L1:795:U:O2'	1:L1:796:G:H8	2.03	0.41
1:L1:843:C:H5''	20:LL:2:PRO:HD2	2.01	0.41
1:L1:989:C:C5	20:LL:26:ARG:HD2	2.55	0.41
1:L1:1451:C:H2'	1:L1:1452:C:C6	2.56	0.41
1:L1:1569:U:O4'	28:LT:50:GLN:HG2	2.21	0.41
1:L1:1684:G:H22	1:L1:1708:G:H22	1.69	0.41
2:L2:979:A:H2'	2:L2:980:A:C8	2.56	0.41
2:L2:1254:G:C8	2:L2:1307:U:H3'	2.56	0.41
3:L3:172:G:OP2	3:L3:172:G:N2	2.47	0.41
8:L8:30:C:H2'	8:L8:31:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LF:66:SER:HB2	14:LF:76:ILE:HA	2.03	0.41
18:LJ:98:GLU:HG3	32:LX:21:TYR:OH	2.21	0.41
19:LK:128:PHE:O	19:LK:132:ASP:HB2	2.20	0.41
19:LK:138:SER:O	19:LK:142:VAL:HG23	2.20	0.41
20:LL:116:GLN:HB3	24:LP:100:ALA:HB2	2.02	0.41
23:LO:126:ASP:OD1	23:LO:126:ASP:N	2.45	0.41
23:LO:206:PHE:HB3	23:LO:246:GLU:HG2	2.02	0.41
25:LQ:77:GLY:O	25:LQ:81:ARG:HG3	2.20	0.41
28:LT:99:GLU:HG3	28:LT:109:PRO:HB3	2.02	0.41
33:LY:36:ARG:NH1	33:LY:38:TYR:OH	2.54	0.41
35:La:8:LYS:NZ	35:La:12:GLU:OE2	2.52	0.41
39:Le:178:PHE:HA	39:Le:181:LEU:HD12	2.03	0.41
51:S1:253:U:H2'	51:S1:941:U:O2	2.21	0.41
51:S1:762:A:H2	51:S1:768:A:H5'	1.86	0.41
51:S1:827:G:H2'	51:S1:828:G:C8	2.56	0.41
51:S1:1590:A:O2'	51:S1:1591:U:H6	2.04	0.41
51:S1:2117:C:O2'	51:S1:2118:G:N7	2.43	0.41
64:SI:139:VAL:HG13	64:SI:192:PRO:HB3	2.03	0.41
75:ST:3:ARG:NH2	75:ST:7:ASN:HA	2.35	0.41
81:SZ:64:LEU:HB3	81:SZ:67:PHE:HE2	1.86	0.41
1:L1:480:U:H2'	1:L1:481:U:C6	2.55	0.41
1:L1:1668:A:OP2	15:LG:54:PRO:HA	2.21	0.41
2:L2:363:C:C4'	4:L4:108:G:H21	2.34	0.41
2:L2:1007:U:H2'	2:L2:1008:C:C6	2.56	0.41
2:L2:1512:G:N1	39:Le:35:ASP:OD1	2.40	0.41
7:L7:164:U:O4	15:LG:49:ARG:HA	2.21	0.41
10:LB:288:TYR:HB2	10:LB:330:MET:HG2	2.02	0.41
16:LH:86:LYS:HE2	16:LH:86:LYS:HB3	1.69	0.41
41:Lg:120:LYS:NZ	41:Lg:121:PHE:O	2.53	0.41
44:Lj:38:ALA:HB2	44:Lj:45:ARG:HG3	2.02	0.41
51:S1:291:G:H2'	51:S1:292:U:O4'	2.20	0.41
57:SB:1:MET:N	57:SB:59:GLU:O	2.52	0.41
64:SI:5:LEU:HD23	64:SI:5:LEU:HA	1.88	0.41
64:SI:143:TRP:HZ3	65:SJ:54:ASP:HB2	1.85	0.41
65:SJ:78:ARG:HB3	65:SJ:124:LYS:HB3	2.02	0.41
71:SP:100:VAL:HG12	71:SP:125:VAL:HG23	2.02	0.41
73:SR:107:ARG:HA	73:SR:107:ARG:HD3	1.83	0.41
80:SY:35:ALA:O	80:SY:64:ARG:HD3	2.20	0.41
89:Sh:165:LEU:O	89:Sh:166:ARG:NH1	2.47	0.41
89:Sh:168:TYR:HB2	89:Sh:172:PHE:O	2.20	0.41
1:L1:148:U:O2'	1:L1:149:G:P	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:780:C:C2'	1:L1:781:A:H5'	2.51	0.41
1:L1:1157:U:O2'	37:Lc:115:LEU:O	2.38	0.41
1:L1:1565:A:H2'	1:L1:1566:A:C8	2.55	0.41
1:L1:1727:A:H2'	1:L1:1728:A:H5'	2.03	0.41
2:L2:404:A:O4'	2:L2:406:G:C8	2.74	0.41
2:L2:489:A:C8	9:LA:245:ARG:HG3	2.56	0.41
2:L2:543:U:O2	2:L2:1358:U:H5'	2.21	0.41
2:L2:623:A:H5''	2:L2:624:C:H5	1.86	0.41
2:L2:664:G:H5'	2:L2:664:G:N3	2.36	0.41
2:L2:954:A:H2'	42:Lh:118:HIS:NE2	2.35	0.41
2:L2:1131:A:H3'	2:L2:1131:A:OP2	2.20	0.41
2:L2:1512:G:C2	39:Le:67:GLY:HA2	2.56	0.41
3:L3:122:U:O4'	25:LQ:96:MET:HG2	2.21	0.41
4:L4:17:A:H2'	4:L4:18:U:C6	2.56	0.41
5:L5:46:G:H2'	5:L5:47:C:C6	2.56	0.41
8:L8:7:G:H2'	8:L8:8:U:C6	2.56	0.41
11:LC:100:MET:SD	11:LC:103:PRO:HA	2.61	0.41
12:LD:77:LYS:O	12:LD:77:LYS:HD3	2.21	0.41
14:LF:43:ALA:HB2	41:Lg:140:TYR:CE2	2.55	0.41
15:LG:141:THR:O	15:LG:145:GLU:HG3	2.21	0.41
22:LN:48:VAL:HG21	22:LN:145:VAL:HG22	2.01	0.41
25:LQ:177:GLU:O	25:LQ:181:ARG:HG2	2.21	0.41
34:LZ:124:VAL:HG22	40:Lf:114:MET:HE3	2.03	0.41
37:Lc:213:TRP:CD1	37:Lc:214:PRO:HD2	2.56	0.41
41:Lg:75:VAL:HG11	41:Lg:119:VAL:HG11	2.03	0.41
45:Lk:72:ARG:HG2	45:Lk:76:LYS:HE3	2.03	0.41
51:S1:29:OMU:HM23	51:S1:29:OMU:H1'	1.72	0.41
51:S1:105:C:H2'	51:S1:106:A:C8	2.56	0.41
51:S1:124:A:OP2	51:S1:124:A:H8	2.03	0.41
51:S1:138:C:H2'	51:S1:139:C:C6	2.56	0.41
51:S1:245:A:H5''	76:SU:33:MET:HE1	2.02	0.41
51:S1:687:U:OP2	65:SJ:32:LYS:HD3	2.21	0.41
51:S1:853:A:H4'	60:SE:217:THR:HA	2.03	0.41
51:S1:1209:C:O2'	51:S1:1210:C:OP1	2.28	0.41
51:S1:1512:A:H2'	51:S1:1513:C:H6	1.86	0.41
51:S1:1587:C:H2'	51:S1:1588:A:H8	1.86	0.41
51:S1:1857:C:OP1	51:S1:1858:G:H2'	2.21	0.41
51:S1:1976:U:O2'	51:S1:1977:U:H2'	2.21	0.41
52:S2:74:C:H2'	52:S2:75:C:O4'	2.20	0.41
58:SC:11:ILE:HD13	58:SC:11:ILE:HA	1.87	0.41
58:SC:47:ILE:HD12	58:SC:83:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SC:57:VAL:HG21	58:SC:87:VAL:HG21	2.03	0.41
60:SE:99:MET:O	60:SE:107:ALA:N	2.51	0.41
66:SK:169:HIS:HE1	66:SK:171:VAL:HB	1.86	0.41
66:SK:171:VAL:O	76:SU:7:TYR:HA	2.21	0.41
68:SM:32:VAL:HG21	68:SM:107:VAL:HG11	2.03	0.41
71:SP:11:ARG:O	71:SP:15:ARG:HG3	2.20	0.41
72:SQ:45:ARG:NH1	72:SQ:103:LEU:HB2	2.35	0.41
73:SR:26:LYS:NZ	73:SR:54:GLU:O	2.52	0.41
73:SR:27:VAL:HG23	73:SR:55:ARG:O	2.21	0.41
77:SV:24:LEU:HB2	77:SV:58:MET:HE2	2.03	0.41
86:Se:56:HIS:CD2	86:Se:56:HIS:N	2.89	0.41
89:Sh:212:LEU:HD12	89:Sh:212:LEU:HA	1.90	0.41
1:L1:129:C:H2'	1:L1:130:U:H6	1.86	0.41
1:L1:794:U:O2'	1:L1:795:U:H6	2.04	0.41
1:L1:988:G:N2	1:L1:1012:C:OP1	2.53	0.41
1:L1:1357:G:H2'	1:L1:1358:C:C6	2.55	0.41
2:L2:676:G:H2'	2:L2:677:C:C6	2.56	0.41
2:L2:954:A:H5'	2:L2:955:C:O5'	2.21	0.41
2:L2:975:A:O2'	2:L2:976:A:C8	2.70	0.41
2:L2:1042:G:H2'	2:L2:1043:C:H6	1.86	0.41
2:L2:1155:A:C2	20:LL:43:ILE:HG23	2.56	0.41
6:L6:23:A:H5'	6:L6:24:C:C6	2.56	0.41
10:LB:349:MET:HB3	10:LB:349:MET:HE2	1.88	0.41
16:LH:195:ASP:HA	16:LH:198:LYS:HE2	2.02	0.41
19:LK:50:VAL:HG23	26:LR:71:LEU:HD13	2.02	0.41
21:LM:92:MET:HE3	21:LM:92:MET:HB3	1.86	0.41
23:LO:60:ILE:H	23:LO:80:ALA:HB3	1.86	0.41
26:LR:132:PRO:HD2	26:LR:135:GLU:OE2	2.20	0.41
27:LS:137:ILE:HG12	37:Lc:79:ALA:HB2	2.02	0.41
29:LU:50:PHE:O	29:LU:54:ASN:HB2	2.20	0.41
43:Li:89:LYS:HB2	43:Li:89:LYS:HE2	1.93	0.41
44:Lj:67:LEU:HD23	44:Lj:67:LEU:HA	1.85	0.41
46:Ll:28:ARG:HG2	46:Ll:28:ARG:NH1	2.36	0.41
51:S1:146:U:O2	62:SG:145:ARG:NH2	2.54	0.41
51:S1:635:G:H2'	51:S1:636:C:C6	2.55	0.41
51:S1:895:A:H3'	51:S1:896:A:C8	2.53	0.41
51:S1:1097:C:H2'	51:S1:1098:U:C6	2.56	0.41
51:S1:1575:G:H2'	51:S1:1576:A:H8	1.85	0.41
88:Sg:179:TRP:CD1	88:Sg:179:TRP:N	2.88	0.41
1:L1:827:G:H5'	36:Lb:38:LEU:HD21	2.03	0.40
1:L1:882:A:H4'	2:L2:48:G:H4'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1425:C:H2'	34:LZ:108:PHE:HZ	1.86	0.40
1:L1:1438:A:OP2	34:LZ:41:ARG:NH2	2.55	0.40
1:L1:1597:G:OP1	46:L1:50:ASN:HA	2.20	0.40
2:L2:530:C:N4	2:L2:554:C:OP2	2.53	0.40
2:L2:560:OMU:HM23	2:L2:560:OMU:H1'	1.74	0.40
2:L2:1422:C:H2'	2:L2:1423:C:C6	2.56	0.40
11:LC:345:ASN:HB3	11:LC:348:ASN:HB2	2.03	0.40
12:LD:178:LYS:HE2	12:LD:178:LYS:HB3	1.39	0.40
19:LK:141:LYS:HA	19:LK:141:LYS:HD3	1.63	0.40
39:Le:76:ARG:HA	39:Le:76:ARG:HD3	1.93	0.40
51:S1:301:U:H2'	51:S1:302:U:O2	2.20	0.40
51:S1:637:U:H2'	51:S1:638:C:C6	2.56	0.40
51:S1:2122:G:H2'	51:S1:2123:A:O4'	2.22	0.40
56:SA:70:LEU:HD13	56:SA:86:VAL:HG21	2.04	0.40
57:SB:2:SER:OG	57:SB:59:GLU:OE2	2.26	0.40
59:SD:91:LYS:HB2	59:SD:94:TYR:CE2	2.56	0.40
62:SG:80:ARG:HG3	62:SG:85:PHE:CE2	2.55	0.40
81:SZ:26:LYS:HE2	81:SZ:82:ILE:HD11	2.02	0.40
87:Sf:131:MET:HG3	87:Sf:139:TYR:O	2.21	0.40
89:Sh:226:HIS:HA	89:Sh:229:TYR:CD2	2.57	0.40
1:L1:80:C:H2'	1:L1:81:U:O4'	2.21	0.40
1:L1:193:A:H2'	1:L1:194:A:C8	2.56	0.40
1:L1:700:A:H4'	24:LP:172:TYR:CE1	2.56	0.40
2:L2:1382:U:H1'	10:LB:256:CYS:SG	2.61	0.40
5:L5:31:C:H2'	5:L5:32:A:C8	2.56	0.40
7:L7:65:G:H5''	35:La:7:ILE:HD13	2.03	0.40
7:L7:79:A:H4'	35:La:47:ARG:NH2	2.36	0.40
21:LM:46:GLU:H	21:LM:46:GLU:HG3	1.69	0.40
32:LX:94:ILE:HG23	62:SG:148:PHE:CD1	2.56	0.40
51:S1:38:OMC:HM21	59:SD:7:PHE:HB3	2.04	0.40
51:S1:546:U:C2	51:S1:547:U:H1'	2.55	0.40
56:SA:51:THR:HG23	56:SA:56:ILE:HA	2.03	0.40
57:SB:30:THR:C	57:SB:32:ASN:H	2.30	0.40
57:SB:83:ARG:C	57:SB:85:TYR:H	2.29	0.40
75:ST:3:ARG:HH22	75:ST:7:ASN:HA	1.85	0.40
87:Sf:136:ASP:OD2	87:Sf:136:ASP:N	2.45	0.40
87:Sf:140:CYS:SG	87:Sf:141:GLY:N	2.94	0.40
1:L1:91:G:O5'	1:L1:92:C:H5''	2.22	0.40
1:L1:633:U:H5''	1:L1:634:G:H5'	2.02	0.40
1:L1:819:C:H2'	1:L1:820:U:O4'	2.20	0.40
1:L1:886:G:H1'	1:L1:909:A:N6	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1426:A:N1	34:LZ:86:GLY:HA2	2.37	0.40
1:L1:1716:G:O2'	1:L1:1725:U:OP1	2.32	0.40
2:L2:459:A:O2'	2:L2:1029:G:H5'	2.21	0.40
15:LG:51:MET:HE1	30:LV:35:PHE:HD2	1.87	0.40
16:LH:144:ARG:HG2	16:LH:148:TYR:CD2	2.56	0.40
20:LL:51:GLY:HA2	24:LP:182:ARG:H	1.87	0.40
23:LO:187:PRO:HG2	23:LO:201:HIS:HD2	1.86	0.40
42:Lh:8:TYR:HB2	42:Lh:13:HIS:CE1	2.57	0.40
44:Lj:64:CYS:O	44:Lj:68:LYS:HG2	2.21	0.40
51:S1:186:A:H2'	51:S1:187:C:C6	2.55	0.40
51:S1:477:G:N1	51:S1:480:A:OP2	2.50	0.40
51:S1:1099:C:H2'	51:S1:1100:U:O4'	2.21	0.40
51:S1:1409:U:H2'	51:S1:1410:C:H6	1.86	0.40
51:S1:1884:A:H2'	51:S1:1885:A:C8	2.56	0.40
51:S1:2202:PSU:H2'	56:SA:118:LYS:HB2	2.04	0.40
56:SA:123:MET:CE	56:SA:166:LEU:HD22	2.50	0.40
57:SB:20:LYS:HB3	57:SB:176:MET:HE3	2.03	0.40
59:SD:89:LYS:HD2	59:SD:94:TYR:CD1	2.56	0.40
64:SI:71:LEU:O	64:SI:75:ARG:HG2	2.21	0.40
65:SJ:55:ASP:OD1	65:SJ:55:ASP:N	2.54	0.40
68:SM:22:THR:HA	68:SM:82:TYR:O	2.22	0.40
68:SM:40:ALA:CB	68:SM:47:ILE:HD11	2.50	0.40
73:SR:21:VAL:HG13	73:SR:30:ALA:HB1	2.02	0.40
73:SR:118:MET:H	73:SR:118:MET:HG2	1.63	0.40
85:Sd:27:ILE:N	85:Sd:43:ARG:O	2.46	0.40
85:Sd:33:THR:HB	85:Sd:39:VAL:HG12	2.02	0.40
88:Sg:134:TRP:HB2	88:Sg:140:CYS:H	1.85	0.40
1:L1:925:U:OP1	10:LB:246:LYS:HG2	2.22	0.40
1:L1:1687:G:H22	1:L1:1705:G:N2	2.18	0.40
2:L2:597:PSU:H2'	2:L2:598:A:C8	2.56	0.40
13:LE:90:LYS:HG2	13:LE:144:VAL:HG22	2.02	0.40
20:LL:51:GLY:C	24:LP:179:GLU:HA	2.46	0.40
21:LM:8:ASN:O	21:LM:12:LYS:HG3	2.21	0.40
25:LQ:15:LEU:HD13	25:LQ:52:ARG:HB2	2.02	0.40
26:LR:29:PHE:CE2	26:LR:31:VAL:HB	2.57	0.40
51:S1:1207:U:H2'	51:S1:1208:U:H6	1.85	0.40
51:S1:1497:U:O2	61:SF:101:ALA:HB3	2.21	0.40
58:SC:44:ARG:NH2	58:SC:84:GLN:OE1	2.54	0.40
59:SD:119:LYS:HE3	59:SD:123:HIS:CE1	2.56	0.40
60:SE:8:ARG:CZ	60:SE:17:LEU:HB3	2.51	0.40
62:SG:80:ARG:HA	62:SG:85:PHE:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SG:96:ARG:HE	62:SG:96:ARG:HB2	1.56	0.40
69:SN:86:TYR:HD1	69:SN:87:LEU:HD23	1.86	0.40
75:ST:43:LYS:HA	75:ST:43:LYS:HD3	1.85	0.40
81:SZ:93:GLU:HB3	81:SZ:98:LYS:CG	2.51	0.40
81:SZ:113:SER:HB2	81:SZ:117:ARG:HH21	1.86	0.40
82:Sa:29:LYS:HE2	82:Sa:29:LYS:HB2	1.89	0.40
84:Sc:35:ASP:O	84:Sc:80:TYR:HA	2.21	0.40
1:L1:99:A:H2'	1:L1:100:G:N3	2.37	0.40
1:L1:851:G:H2'	1:L1:852:A:N7	2.36	0.40
1:L1:1390:G:H4'	1:L1:1391:U:O5'	2.21	0.40
2:L2:1474:G:O2'	2:L2:1475:G:H5'	2.22	0.40
2:L2:1505:A:C6	2:L2:1517:G:C6	3.10	0.40
6:L6:43:A:H1'	26:LR:174:LYS:HZ2	1.86	0.40
6:L6:73:A:O2'	41:Lg:25:ASN:ND2	2.55	0.40
11:LC:284:ASN:C	11:LC:286:ASP:H	2.30	0.40
51:S1:45:U:O2'	51:S1:46:U:H2'	2.22	0.40
51:S1:66:U:H5	62:SG:177:PRO:HG3	1.87	0.40
51:S1:465:G:H2'	51:S1:466:G:C8	2.56	0.40
51:S1:593:A:H5'	51:S1:594:A:OP2	2.21	0.40
51:S1:1858:G:N2	51:S1:1978:A:OP2	2.55	0.40
51:S1:1999:G:H5''	67:SL:148:TYR:HE2	1.84	0.40
52:S2:49:C:H1'	52:S2:65:G:C2	2.56	0.40
56:SA:141:VAL:HG22	56:SA:214:ILE:HG12	2.02	0.40
64:SI:169:LEU:HD23	64:SI:169:LEU:HA	1.90	0.40
66:SK:157:LYS:HE3	66:SK:157:LYS:HB3	1.78	0.40
67:SL:11:GLN:HG3	67:SL:28:THR:HB	2.03	0.40
81:SZ:4:GLN:OE1	81:SZ:4:GLN:N	2.55	0.40
81:SZ:32:VAL:N	81:SZ:76:THR:O	2.45	0.40
88:Sg:72:SER:O	88:Sg:81:LEU:N	2.50	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%)	390 (97%)	12 (3%)	0	100	100
11	LC	364/373 (98%)	353 (97%)	11 (3%)	0	100	100
12	LD	173/188 (92%)	170 (98%)	3 (2%)	0	100	100
13	LE	184/190 (97%)	175 (95%)	9 (5%)	0	100	100
14	LF	145/195 (74%)	138 (95%)	7 (5%)	0	100	100
15	LG	239/264 (90%)	234 (98%)	5 (2%)	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%)	161 (96%)	6 (4%)	0	100	100
20	LL	142/145 (98%)	135 (95%)	6 (4%)	1 (1%)	18	40
21	LM	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
22	LN	201/213 (94%)	195 (97%)	6 (3%)	0	100	100
23	LO	294/305 (96%)	288 (98%)	6 (2%)	0	100	100
24	LP	195/198 (98%)	190 (97%)	4 (2%)	1 (0%)	24	49
25	LQ	199/254 (78%)	198 (100%)	1 (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	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
29	LU	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
30	LV	117/145 (81%)	116 (99%)	1 (1%)	0	100	100
31	LW	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
32	LX	81/124 (65%)	78 (96%)	3 (4%)	0	100	100
33	LY	131/134 (98%)	131 (100%)	0	0	100	100
34	LZ	143/147 (97%)	141 (99%)	2 (1%)	0	100	100
35	La	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
36	Lb	66/70 (94%)	63 (96%)	2 (3%)	1 (2%)	8	23
37	Lc	227/252 (90%)	221 (97%)	6 (3%)	0	100	100
38	Ld	95/104 (91%)	95 (100%)	0	0	100	100
39	Le	184/188 (98%)	183 (100%)	1 (0%)	0	100	100
40	Lf	126/133 (95%)	122 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
44	Lj	79/83 (95%)	79 (100%)	0	0	100	100
45	Lk	76/83 (92%)	75 (99%)	1 (1%)	0	100	100
46	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
47	Lm	50/128 (39%)	50 (100%)	0	0	100	100
48	Ln	31/34 (91%)	31 (100%)	0	0	100	100
49	Lo	87/92 (95%)	80 (92%)	7 (8%)	0	100	100
50	Lp	95/106 (90%)	93 (98%)	2 (2%)	0	100	100
56	SA	240/264 (91%)	232 (97%)	8 (3%)	0	100	100
57	SB	209/246 (85%)	202 (97%)	7 (3%)	0	100	100
58	SC	211/219 (96%)	207 (98%)	4 (2%)	0	100	100
59	SD	181/190 (95%)	178 (98%)	3 (2%)	0	100	100
60	SE	258/273 (94%)	253 (98%)	5 (2%)	0	100	100
61	SF	220/265 (83%)	220 (100%)	0	0	100	100
62	SG	225/249 (90%)	218 (97%)	7 (3%)	0	100	100
63	SH	179/190 (94%)	177 (99%)	2 (1%)	0	100	100
64	SI	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
65	SJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
66	SK	188/220 (86%)	188 (100%)	0	0	100	100
67	SL	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
68	SM	99/116 (85%)	99 (100%)	0	0	100	100
69	SN	98/168 (58%)	93 (95%)	4 (4%)	1 (1%)	12	31
70	SO	135/144 (94%)	131 (97%)	4 (3%)	0	100	100
71	SP	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
72	SQ	96/141 (68%)	93 (97%)	3 (3%)	0	100	100
73	SR	140/153 (92%)	138 (99%)	2 (1%)	0	100	100
74	SS	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
75	ST	141/151 (93%)	139 (99%)	2 (1%)	0	100	100
76	SU	151/173 (87%)	144 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	SV	120/143 (84%)	119 (99%)	1 (1%)	0	100	100
78	SW	113/152 (74%)	113 (100%)	0	0	100	100
79	SX	150/161 (93%)	144 (96%)	6 (4%)	0	100	100
80	SY	86/164 (52%)	86 (100%)	0	0	100	100
81	SZ	128/137 (93%)	122 (95%)	6 (5%)	0	100	100
82	Sa	103/120 (86%)	94 (91%)	9 (9%)	0	100	100
83	Sb	102/112 (91%)	101 (99%)	1 (1%)	0	100	100
84	Sc	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
85	Sd	64/87 (74%)	61 (95%)	3 (5%)	0	100	100
86	Se	59/66 (89%)	57 (97%)	2 (3%)	0	100	100
87	Sf	78/152 (51%)	73 (94%)	5 (6%)	0	100	100
88	Sg	297/312 (95%)	286 (96%)	11 (4%)	0	100	100
89	Sh	94/235 (40%)	92 (98%)	2 (2%)	0	100	100
All	All	11480/12926 (89%)	11208 (98%)	268 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
69	SN	40	ASN
36	Lb	10	HIS
20	LL	40	HIS
24	LP	189	SER

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%)	193 (96%)	7 (4%)	32	56
10	LB	337/351 (96%)	331 (98%)	6 (2%)	51	72
11	LC	291/301 (97%)	280 (96%)	11 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	LD	147/162 (91%)	139 (95%)	8 (5%)	20	42
13	LE	166/172 (96%)	157 (95%)	9 (5%)	20	42
14	LF	122/153 (80%)	115 (94%)	7 (6%)	18	41
15	LG	198/221 (90%)	195 (98%)	3 (2%)	57	75
16	LH	182/188 (97%)	175 (96%)	7 (4%)	29	54
17	LI	178/183 (97%)	174 (98%)	4 (2%)	45	69
18	LJ	106/111 (96%)	105 (99%)	1 (1%)	70	82
19	LK	138/145 (95%)	135 (98%)	3 (2%)	45	69
20	LL	113/114 (99%)	106 (94%)	7 (6%)	16	37
21	LM	178/180 (99%)	168 (94%)	10 (6%)	19	41
22	LN	175/179 (98%)	169 (97%)	6 (3%)	32	58
23	LO	232/242 (96%)	227 (98%)	5 (2%)	45	69
24	LP	163/164 (99%)	158 (97%)	5 (3%)	35	60
25	LQ	170/198 (86%)	166 (98%)	4 (2%)	43	67
26	LR	157/159 (99%)	152 (97%)	5 (3%)	34	59
27	LS	132/134 (98%)	126 (96%)	6 (4%)	24	49
28	LT	127/143 (89%)	125 (98%)	2 (2%)	55	74
29	LU	93/114 (82%)	89 (96%)	4 (4%)	26	51
30	LV	102/124 (82%)	100 (98%)	2 (2%)	48	70
31	LW	104/122 (85%)	103 (99%)	1 (1%)	68	81
32	LX	74/104 (71%)	74 (100%)	0	100	100
33	LY	111/116 (96%)	108 (97%)	3 (3%)	39	64
34	LZ	114/118 (97%)	109 (96%)	5 (4%)	25	50
35	La	114/118 (97%)	113 (99%)	1 (1%)	70	82
36	Lb	56/58 (97%)	55 (98%)	1 (2%)	51	72
37	Lc	191/209 (91%)	189 (99%)	2 (1%)	68	81
38	Ld	85/89 (96%)	82 (96%)	3 (4%)	32	56
39	Le	154/158 (98%)	152 (99%)	2 (1%)	61	77
40	Lf	111/115 (96%)	109 (98%)	2 (2%)	51	72
41	Lg	120/121 (99%)	119 (99%)	1 (1%)	73	84
42	Lh	107/146 (73%)	105 (98%)	2 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Li	84/88 (96%)	83 (99%)	1 (1%)	63	78
44	Lj	68/70 (97%)	68 (100%)	0	100	100
45	Lk	65/74 (88%)	63 (97%)	2 (3%)	35	60
46	Ll	46/47 (98%)	46 (100%)	0	100	100
47	Lm	43/113 (38%)	41 (95%)	2 (5%)	23	48
48	Ln	31/32 (97%)	31 (100%)	0	100	100
49	Lo	69/74 (93%)	68 (99%)	1 (1%)	59	76
50	Lp	83/92 (90%)	81 (98%)	2 (2%)	43	67
56	SA	206/222 (93%)	201 (98%)	5 (2%)	43	67
57	SB	178/202 (88%)	170 (96%)	8 (4%)	24	49
58	SC	176/184 (96%)	163 (93%)	13 (7%)	13	30
59	SD	159/164 (97%)	150 (94%)	9 (6%)	18	41
60	SE	216/225 (96%)	205 (95%)	11 (5%)	21	45
61	SF	182/208 (88%)	178 (98%)	4 (2%)	45	69
62	SG	190/208 (91%)	178 (94%)	12 (6%)	16	36
63	SH	153/159 (96%)	151 (99%)	2 (1%)	61	77
64	SI	181/186 (97%)	173 (96%)	8 (4%)	25	50
65	SJ	110/111 (99%)	107 (97%)	3 (3%)	39	64
66	SK	157/176 (89%)	150 (96%)	7 (4%)	24	49
67	SL	116/120 (97%)	111 (96%)	5 (4%)	26	51
68	SM	92/104 (88%)	86 (94%)	6 (6%)	15	35
69	SN	88/128 (69%)	83 (94%)	5 (6%)	18	41
70	SO	104/113 (92%)	102 (98%)	2 (2%)	50	71
71	SP	114/117 (97%)	106 (93%)	8 (7%)	14	32
72	SQ	57/120 (48%)	53 (93%)	4 (7%)	14	32
73	SR	120/130 (92%)	115 (96%)	5 (4%)	26	52
74	SS	47/49 (96%)	45 (96%)	2 (4%)	26	51
75	ST	126/132 (96%)	122 (97%)	4 (3%)	34	59
76	SU	135/152 (89%)	129 (96%)	6 (4%)	25	50
77	SV	109/126 (86%)	105 (96%)	4 (4%)	30	55
78	SW	98/130 (75%)	97 (99%)	1 (1%)	68	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	SX	122/131 (93%)	119 (98%)	3 (2%)	42	66
80	SY	72/116 (62%)	69 (96%)	3 (4%)	26	52
81	SZ	111/118 (94%)	104 (94%)	7 (6%)	16	36
82	Sa	83/95 (87%)	80 (96%)	3 (4%)	31	56
83	Sb	85/93 (91%)	78 (92%)	7 (8%)	10	26
84	Sc	75/76 (99%)	73 (97%)	2 (3%)	39	64
85	Sd	52/75 (69%)	49 (94%)	3 (6%)	18	40
86	Se	52/54 (96%)	51 (98%)	1 (2%)	50	71
87	Sf	70/126 (56%)	65 (93%)	5 (7%)	13	31
88	Sg	259/265 (98%)	240 (93%)	19 (7%)	13	31
89	Sh	79/177 (45%)	73 (92%)	6 (8%)	12	29
All	All	9711/10798 (90%)	9365 (96%)	346 (4%)	32	56

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	LA	148	LEU
9	LA	157	SER
9	LA	185	SER
9	LA	190	ARG
9	LA	202	VAL
9	LA	219	ILE
9	LA	242	ARG
10	LB	44	THR
10	LB	79	LEU
10	LB	87	VAL
10	LB	168	LEU
10	LB	171	LEU
10	LB	307	LEU
11	LC	13	SER
11	LC	70	ARG
11	LC	83	THR
11	LC	107	PHE
11	LC	124	VAL
11	LC	146	VAL
11	LC	213	ASN
11	LC	253	SER
11	LC	276	THR

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Mol	Chain	Res	Type
11	LC	285	THR
11	LC	337	THR
12	LD	46	THR
12	LD	50	SER
12	LD	80	GLU
12	LD	83	GLU
12	LD	95	SER
12	LD	140	VAL
12	LD	153	SER
12	LD	178	LYS
13	LE	6	SER
13	LE	16	VAL
13	LE	17	THR
13	LE	56	VAL
13	LE	81	THR
13	LE	92	ARG
13	LE	137	SER
13	LE	171	ILE
13	LE	182	THR
14	LF	19	VAL
14	LF	66	SER
14	LF	70	LYS
14	LF	81	SER
14	LF	84	VAL
14	LF	98	THR
14	LF	152	GLN
15	LG	87	SER
15	LG	183	ASP
15	LG	254	ASN
16	LH	82	THR
16	LH	85	THR
16	LH	133	THR
16	LH	137	VAL
16	LH	150	SER
16	LH	155	THR
16	LH	169	SER
17	LI	39	ARG
17	LI	68	VAL
17	LI	81	SER
17	LI	170	SER
18	LJ	100	ASN
19	LK	4	SER

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Mol	Chain	Res	Type
19	LK	64	SER
19	LK	115	VAL
20	LL	8	CYS
20	LL	30	SER
20	LL	32	ARG
20	LL	39	HIS
20	LL	40	HIS
20	LL	104	SER
20	LL	117	VAL
21	LM	61	VAL
21	LM	80	THR
21	LM	96	LYS
21	LM	117	ASN
21	LM	124	ASP
21	LM	155	VAL
21	LM	182	SER
21	LM	183	LYS
21	LM	187	SER
21	LM	194	ARG
22	LN	43	VAL
22	LN	48	VAL
22	LN	54	SER
22	LN	189	LYS
22	LN	206	ILE
22	LN	211	VAL
23	LO	4	VAL
23	LO	31	HIS
23	LO	142	ASP
23	LO	223	SER
23	LO	224	ASN
24	LP	21	SER
24	LP	41	SER
24	LP	89	VAL
24	LP	115	SER
24	LP	162	SER
25	LQ	13	SER
25	LQ	40	SER
25	LQ	78	VAL
25	LQ	154	GLN
26	LR	41	SER
26	LR	61	LEU
26	LR	65	VAL

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Mol	Chain	Res	Type
26	LR	75	ASN
26	LR	87	CYS
27	LS	27	VAL
27	LS	46	SER
27	LS	55	LYS
27	LS	61	THR
27	LS	68	THR
27	LS	84	THR
28	LT	75	GLU
28	LT	79	THR
29	LU	30	CYS
29	LU	40	SER
29	LU	73	ASN
29	LU	78	THR
30	LV	80	GLU
30	LV	144	LEU
31	LW	101	VAL
33	LY	47	LYS
33	LY	70	VAL
33	LY	103	SER
34	LZ	14	GLN
34	LZ	17	ARG
34	LZ	93	SER
34	LZ	135	ILE
34	LZ	138	SER
35	La	92	THR
36	Lb	14	SER
37	Lc	72	LEU
37	Lc	188	ILE
38	Ld	26	VAL
38	Ld	27	LEU
38	Ld	90	CYS
39	Le	156	GLU
39	Le	170	ILE
40	Lf	15	THR
40	Lf	70	SER
41	Lg	21	THR
42	Lh	3	CYS
42	Lh	52	LYS
43	Li	5	THR
45	Lk	21	ARG
45	Lk	59	SER

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Mol	Chain	Res	Type
47	Lm	99	CYS
47	Lm	105	VAL
49	Lo	41	PHE
50	Lp	2	VAL
50	Lp	26	VAL
56	SA	110	ASP
56	SA	182	GLN
56	SA	194	VAL
56	SA	196	SER
56	SA	200	VAL
57	SB	79	VAL
57	SB	84	LEU
57	SB	87	THR
57	SB	92	LYS
57	SB	95	GLN
57	SB	116	GLN
57	SB	160	VAL
57	SB	195	SER
58	SC	7	LYS
58	SC	34	SER
58	SC	37	SER
58	SC	41	THR
58	SC	44	ARG
58	SC	112	LEU
58	SC	113	GLN
58	SC	158	LYS
58	SC	171[A]	CYS
58	SC	171[B]	CYS
58	SC	193	SER
58	SC	194	THR
58	SC	206	VAL
59	SD	6	ASN
59	SD	20	LYS
59	SD	47	THR
59	SD	48	LEU
59	SD	49	SER
59	SD	60	THR
59	SD	68	ARG
59	SD	150	SER
59	SD	168	THR
60	SE	18	SER
60	SE	35	LEU

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Mol	Chain	Res	Type
60	SE	44	ILE
60	SE	53	LEU
60	SE	128	THR
60	SE	130	THR
60	SE	170	ILE
60	SE	179	ILE
60	SE	181	THR
60	SE	193	VAL
60	SE	196	GLU
61	SF	116	VAL
61	SF	205	VAL
61	SF	211	SER
61	SF	245	THR
62	SG	19	SER
62	SG	54	ARG
62	SG	65	VAL
62	SG	69	LEU
62	SG	72	SER
62	SG	104	VAL
62	SG	117	SER
62	SG	130	THR
62	SG	160	VAL
62	SG	165	VAL
62	SG	205	SER
62	SG	208	GLU
63	SH	55	VAL
63	SH	111	SER
64	SI	36	THR
64	SI	46	VAL
64	SI	57	SER
64	SI	82	THR
64	SI	121	SER
64	SI	136	SER
64	SI	139	VAL
64	SI	166	GLU
65	SJ	2	THR
65	SJ	30	SER
65	SJ	83	THR
66	SK	4	VAL
66	SK	58	LEU
66	SK	81	VAL
66	SK	163	THR

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Mol	Chain	Res	Type
66	SK	171	VAL
66	SK	175	ILE
66	SK	209	GLN
67	SL	28	THR
67	SL	32	GLN
67	SL	49	THR
67	SL	63	SER
67	SL	108	LYS
68	SM	22	THR
68	SM	29	VAL
68	SM	45	VAL
68	SM	46	THR
68	SM	86	ILE
68	SM	102	THR
69	SN	3	THR
69	SN	23	ILE
69	SN	41	THR
69	SN	44	VAL
69	SN	49	VAL
70	SO	18	ASP
70	SO	74	VAL
71	SP	2	THR
71	SP	16	LEU
71	SP	21	ARG
71	SP	53	GLU
71	SP	57	VAL
71	SP	85	VAL
71	SP	105	PHE
71	SP	115	ILE
72	SQ	33	VAL
72	SQ	55	ASP
72	SQ	63	ILE
72	SQ	87	ASP
73	SR	32	ARG
73	SR	34	VAL
73	SR	44	LEU
73	SR	88	GLN
73	SR	100	SER
74	SS	9	SER
74	SS	56	LEU
75	ST	2	VAL
75	ST	21	THR

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Mol	Chain	Res	Type
75	ST	30	SER
75	ST	107	THR
76	SU	65	ASN
76	SU	82	ARG
76	SU	89	VAL
76	SU	93	THR
76	SU	101	ILE
76	SU	127	SER
77	SV	8	THR
77	SV	37	ASP
77	SV	100	SER
77	SV	121	LYS
78	SW	112	VAL
79	SX	100	SER
79	SX	113	LEU
79	SX	146	SER
80	SY	16	LEU
80	SY	40	SER
80	SY	55	THR
81	SZ	30	VAL
81	SZ	45	LEU
81	SZ	50	LEU
81	SZ	52	THR
81	SZ	60	SER
81	SZ	69	THR
81	SZ	81	LEU
82	Sa	32	SER
82	Sa	36	LEU
82	Sa	98	THR
83	Sb	2	THR
83	Sb	32	THR
83	Sb	42	VAL
83	Sb	78	CYS
83	Sb	87	THR
83	Sb	88	VAL
83	Sb	97	LYS
84	Sc	8	LEU
84	Sc	37	SER
85	Sd	33	THR
85	Sd	73	LEU
85	Sd	74	SER
86	Se	49	VAL

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Mol	Chain	Res	Type
87	Sf	81	THR
87	Sf	87	THR
87	Sf	103	VAL
87	Sf	107	ASP
87	Sf	143	CYS
88	Sg	27	ILE
88	Sg	53	ASP
88	Sg	69	SER
88	Sg	72	SER
88	Sg	77	THR
88	Sg	128	ASP
88	Sg	130	VAL
88	Sg	136	VAL
88	Sg	156	ILE
88	Sg	179	TRP
88	Sg	194	SER
88	Sg	199	THR
88	Sg	203	SER
88	Sg	209	CYS
88	Sg	258	LEU
88	Sg	260	VAL
88	Sg	273	THR
88	Sg	285	ILE
88	Sg	294	LEU
89	Sh	136	SER
89	Sh	149	THR
89	Sh	162	VAL
89	Sh	170	GLN
89	Sh	207	ARG
89	Sh	228	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
9	LA	21	HIS
9	LA	216	HIS
10	LB	68	ASN
10	LB	229	HIS
10	LB	248	HIS
10	LB	384	ASN
11	LC	54	ASN
11	LC	118	GLN

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Mol	Chain	Res	Type
11	LC	158	GLN
11	LC	237	HIS
11	LC	257	GLN
11	LC	284	ASN
11	LC	318	ASN
12	LD	111	HIS
12	LD	155	HIS
13	LE	97	HIS
13	LE	161	HIS
16	LH	187	HIS
17	LI	93	GLN
17	LI	108	ASN
18	LJ	35	ASN
18	LJ	77	ASN
18	LJ	106	ASN
19	LK	40	ASN
20	LL	44	ASN
20	LL	144	GLN
21	LM	23	GLN
22	LN	73	ASN
22	LN	92	HIS
23	LO	35	GLN
23	LO	66	GLN
23	LO	90	HIS
23	LO	120	GLN
24	LP	18	HIS
24	LP	58	ASN
26	LR	121	HIS
27	LS	129	GLN
30	LV	64	ASN
33	LY	86	ASN
34	LZ	35	ASN
34	LZ	37	ASN
35	La	105	ASN
36	Lb	50	HIS
38	Ld	31	GLN
38	Ld	96	ASN
39	Le	62	ASN
40	Lf	21	HIS
41	Lg	25	ASN
43	Li	18	HIS
45	Lk	28	ASN

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Mol	Chain	Res	Type
45	Lk	78	ASN
46	Ll	33	ASN
56	SA	49	ASN
56	SA	103	HIS
57	SB	135	GLN
59	SD	3	ASN
59	SD	32	GLN
59	SD	45	ASN
59	SD	64	ASN
60	SE	172	ASN
63	SH	10	ASN
63	SH	27	HIS
64	SI	99	GLN
64	SI	113	GLN
64	SI	196	GLN
65	SJ	42	GLN
65	SJ	56	HIS
65	SJ	64	ASN
66	SK	52	ASN
66	SK	99	ASN
67	SL	138	HIS
68	SM	25	ASN
69	SN	65	GLN
69	SN	70	HIS
70	SO	13	ASN
73	SR	135	GLN
73	SR	136	HIS
74	SS	27	ASN
74	SS	38	ASN
74	SS	50	HIS
75	ST	62	GLN
75	ST	78	ASN
75	ST	134	GLN
76	SU	91	HIS
76	SU	104	ASN
76	SU	107	HIS
76	SU	113	GLN
76	SU	125	HIS
77	SV	15	GLN
77	SV	74	GLN
78	SW	107	HIS
79	SX	45	ASN

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Mol	Chain	Res	Type
80	SY	13	ASN
80	SY	66	GLN
82	Sa	17	ASN
82	Sa	37	GLN
85	Sd	22	GLN
85	Sd	62	ASN
87	Sf	138	GLN
88	Sg	21	GLN
88	Sg	228	GLN
89	Sh	171	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1667/1782 (93%)	447 (26%)	18 (1%)
2	L2	1148/1526 (75%)	280 (24%)	14 (1%)
3	L3	178/216 (82%)	45 (25%)	3 (1%)
4	L4	183/184 (99%)	43 (23%)	2 (1%)
5	L5	117/135 (86%)	33 (28%)	3 (2%)
51	S1	1822/2204 (82%)	441 (24%)	26 (1%)
52	S2	75/76 (98%)	27 (36%)	8 (10%)
53	S3	74/77 (96%)	19 (25%)	2 (2%)
54	S4	72/76 (94%)	37 (51%)	1 (1%)
55	S5	11/13 (84%)	6 (54%)	0
6	L6	70/73 (95%)	32 (45%)	1 (1%)
7	L7	164/171 (95%)	40 (24%)	2 (1%)
8	L8	119/124 (95%)	19 (15%)	1 (0%)
All	All	5700/6657 (85%)	1469 (25%)	81 (1%)

All (1469) 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

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Mol	Chain	Res	Type
1	L1	56	G
1	L1	58	A
1	L1	63	A
1	L1	64	A
1	L1	65	A
1	L1	67	C
1	L1	69	A2M
1	L1	70	C
1	L1	83	A
1	L1	84	G
1	L1	86	G
1	L1	87	A
1	L1	91	G
1	L1	98	A
1	L1	110	A
1	L1	117	G
1	L1	121	A
1	L1	126	G
1	L1	127	G
1	L1	133	C
1	L1	134	A
1	L1	135	A
1	L1	136	G
1	L1	141	U
1	L1	142	G
1	L1	143	A
1	L1	144	G
1	L1	145	U
1	L1	146	U
1	L1	147	G
1	L1	148	U
1	L1	149	G
1	L1	154	A
1	L1	156	A
1	L1	157	U
1	L1	158	A
1	L1	160	C
1	L1	161	A
1	L1	162	U
1	L1	167	U
1	L1	170	U
1	L1	171	U

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Mol	Chain	Res	Type
1	L1	176	C
1	L1	182	U
1	L1	191	U
1	L1	192	C
1	L1	195	G
1	L1	199	A
1	L1	201	A
1	L1	202	G
1	L1	204	A
1	L1	205	A
1	L1	206	A
1	L1	209	C
1	L1	210	G
1	L1	215	U
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	243	G
1	L1	251	A
1	L1	256	U
1	L1	257	U
1	L1	264	U
1	L1	280	A
1	L1	281	G
1	L1	300	A
1	L1	301	A
1	L1	302	G
1	L1	305	A2M
1	L1	306	G
1	L1	311	A
1	L1	312	C
1	L1	313	PSU
1	L1	322	A
1	L1	323	U
1	L1	332	A
1	L1	335	U

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Mol	Chain	Res	Type
1	L1	336	U
1	L1	337	G
1	L1	338	G
1	L1	342	G
1	L1	343	U
1	L1	344	A
1	L1	348	G
1	L1	357	A
1	L1	367	A
1	L1	368	G
1	L1	369	A
1	L1	371	U
1	L1	374	G
1	L1	376	A
1	L1	377	G
1	L1	383	U
1	L1	392	A
1	L1	409	U
1	L1	410	U
1	L1	414	A
1	L1	417	G
1	L1	419	A
1	L1	440	A
1	L1	443	A
1	L1	444	C
1	L1	461	G
1	L1	463	C
1	L1	464	A
1	L1	470	A
1	L1	471	G
1	L1	477	C
1	L1	484	A
1	L1	485	A
1	L1	488	G
1	L1	489	C
1	L1	494	A
1	L1	495	C
1	L1	496	C
1	L1	500	C
1	L1	502	U
1	L1	503	A
1	L1	511	A

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Mol	Chain	Res	Type
1	L1	512	U
1	L1	518	C
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	553	A
1	L1	554	A
1	L1	555	U
1	L1	557	U
1	L1	558	U
1	L1	568	U
1	L1	569	G
1	L1	571	A
1	L1	572	A
1	L1	573	U
1	L1	574	G
1	L1	577	C
1	L1	579	G
1	L1	580	A
1	L1	584	U
1	L1	585	U
1	L1	586	U
1	L1	587	G
1	L1	590	C
1	L1	592	G
1	L1	601	G
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	621	U
1	L1	623	U
1	L1	625	C
1	L1	627	C
1	L1	631	G

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Mol	Chain	Res	Type
1	L1	632	A
1	L1	634	G
1	L1	635	C
1	L1	641	G
1	L1	648	A
1	L1	651	G
1	L1	652	A
1	L1	653	A
1	L1	664	C
1	L1	666	C
1	L1	668	C
1	L1	669	C
1	L1	673	C
1	L1	681	A2M
1	L1	709	A
1	L1	710	G
1	L1	717	G
1	L1	718	A
1	L1	729	A
1	L1	736	C
1	L1	743	A
1	L1	745	U
1	L1	748	A
1	L1	750	G
1	L1	753	A
1	L1	760	A
1	L1	762	A
1	L1	763	U
1	L1	770	G
1	L1	771	U
1	L1	778	C
1	L1	781	A
1	L1	783	G
1	L1	790	C
1	L1	794	U
1	L1	795	U
1	L1	803	C
1	L1	804	C
1	L1	810	C
1	L1	818	C
1	L1	823	G
1	L1	825	G

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Mol	Chain	Res	Type
1	L1	832	G
1	L1	836	G
1	L1	838	G
1	L1	850	G
1	L1	867	A
1	L1	868	A
1	L1	887	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	945	U
1	L1	957	C
1	L1	965	A
1	L1	967	G
1	L1	968	A
1	L1	972	A
1	L1	973	U
1	L1	974	C
1	L1	975	G
1	L1	976	A
1	L1	988	G
1	L1	995	C
1	L1	1000	C
1	L1	1003	A
1	L1	1010	OMC
1	L1	1011	PSU
1	L1	1013	A
1	L1	1014	G
1	L1	1016	A
1	L1	1017	PSU
1	L1	1018	A
1	L1	1025	G
1	L1	1031	A
1	L1	1036	U
1	L1	1040	G
1	L1	1041	U
1	L1	1045	G
1	L1	1046	U
1	L1	1053	A

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Mol	Chain	Res	Type
1	L1	1085	C
1	L1	1089	C
1	L1	1092	U
1	L1	1093	U
1	L1	1094	C
1	L1	1097	A
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	1128	A
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	1147	A
1	L1	1148	A
1	L1	1150	A
1	L1	1153	A
1	L1	1155	A
1	L1	1156	A
1	L1	1159	A
1	L1	1161	A
1	L1	1162	G
1	L1	1165	A
1	L1	1167	C
1	L1	1169	A
1	L1	1170	G
1	L1	1171	PSU
1	L1	1172	G
1	L1	1174	G
1	L1	1178	U
1	L1	1179	C
1	L1	1188	G
1	L1	1196	G
1	L1	1201	U
1	L1	1202	G
1	L1	1205	G

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Mol	Chain	Res	Type
1	L1	1207	A
1	L1	1209	G
1	L1	1210	A
1	L1	1211	A
1	L1	1213	C
1	L1	1217	U
1	L1	1220	G
1	L1	1225	U
1	L1	1235	A
1	L1	1238	C
1	L1	1239	U
1	L1	1240	U
1	L1	1242	U
1	L1	1243	G
1	L1	1248	C
1	L1	1251	U
1	L1	1253	U
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	1287	A
1	L1	1342	C
1	L1	1343	A
1	L1	1344	A
1	L1	1345	C
1	L1	1346	C
1	L1	1348	A
1	L1	1349	A
1	L1	1351	C
1	L1	1352	C
1	L1	1364	A
1	L1	1367	U
1	L1	1369	G
1	L1	1371	OMU
1	L1	1375	G
1	L1	1378	U
1	L1	1379	A
1	L1	1387	U

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Mol	Chain	Res	Type
1	L1	1388	U
1	L1	1389	A
1	L1	1390	G
1	L1	1391	U
1	L1	1395	U
1	L1	1399	C
1	L1	1401	U
1	L1	1402	U
1	L1	1413	U
1	L1	1416	G
1	L1	1417	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	1444	A
1	L1	1445	G
1	L1	1446	C
1	L1	1455	U
1	L1	1456	G
1	L1	1464	G
1	L1	1465	G
1	L1	1480	C
1	L1	1482	A
1	L1	1483	A
1	L1	1489	U
1	L1	1490	G
1	L1	1495	G
1	L1	1504	A
1	L1	1505	U
1	L1	1507	G
1	L1	1509	C
1	L1	1518	A
1	L1	1519	G
1	L1	1521	G
1	L1	1527	OMC
1	L1	1528	PSU
1	L1	1536	C
1	L1	1540	OMG
1	L1	1545	G

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Mol	Chain	Res	Type
1	L1	1547	U
1	L1	1557	A
1	L1	1560	U
1	L1	1561	A
1	L1	1566	A
1	L1	1569	U
1	L1	1574	C
1	L1	1575	G
1	L1	1586	G
1	L1	1587	A
1	L1	1589	C
1	L1	1590	G
1	L1	1592	G
1	L1	1593	G
1	L1	1607	C
1	L1	1608	A
1	L1	1612	G
1	L1	1613	C
1	L1	1616	U
1	L1	1627	U
1	L1	1628	U
1	L1	1638	C
1	L1	1654	A
1	L1	1655	U
1	L1	1661	U
1	L1	1662	G
1	L1	1663	U
1	L1	1664	PSU
1	L1	1666	G
1	L1	1667	G
1	L1	1671	G
1	L1	1713	A
1	L1	1726	G
1	L1	1727	A
1	L1	1729	A
1	L1	1734	G
1	L1	1737	A
1	L1	1739	A
1	L1	1740	G
1	L1	1742	G
1	L1	1743	A
1	L1	1744	A

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Mol	Chain	Res	Type
1	L1	1746	C
1	L1	1747	U
1	L1	1750	G
1	L1	1751	A
1	L1	1752	U
1	L1	1753	U
1	L1	1754	A
1	L1	1756	A
1	L1	1757	U
1	L1	1758	U
1	L1	1759	C
1	L1	1762	A
1	L1	1763	A
1	L1	1766	G
1	L1	1768	A
1	L1	1771	U
1	L1	1772	G
1	L1	1774	A
2	L2	5	A
2	L2	12	G
2	L2	13	A
2	L2	14	OMC
2	L2	15	C
2	L2	22	A
2	L2	25	A
2	L2	26	C
2	L2	29	C
2	L2	30	A
2	L2	41	A
2	L2	49	A
2	L2	61	C
2	L2	62	A
2	L2	63	U
2	L2	68	A
2	L2	69	A
2	L2	76	A
2	L2	84	A
2	L2	90	G
2	L2	91	C
2	L2	105	A
2	L2	116	A
2	L2	123	G

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Mol	Chain	Res	Type
2	L2	125	C
2	L2	127	C
2	L2	137	A
2	L2	340	A
2	L2	341	A
2	L2	342	U
2	L2	343	U
2	L2	348	A
2	L2	349	C
2	L2	358	G
2	L2	365	G
2	L2	368	G
2	L2	372	A
2	L2	377	A
2	L2	385	A
2	L2	386	U
2	L2	388	A
2	L2	390	A
2	L2	392	C
2	L2	404	A
2	L2	415	U
2	L2	423	A
2	L2	426	G
2	L2	434	A
2	L2	436	U
2	L2	439	U
2	L2	443	OMC
2	L2	444	A
2	L2	446	U
2	L2	453	A
2	L2	454	A
2	L2	455	U
2	L2	456	G
2	L2	457	U
2	L2	459	A
2	L2	462	G
2	L2	489	A
2	L2	490	A
2	L2	495	G
2	L2	502	A2M
2	L2	518	G
2	L2	519	G

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Mol	Chain	Res	Type
2	L2	527	A2M
2	L2	528	U
2	L2	529	G
2	L2	530	C
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	581	G
2	L2	582	U
2	L2	616	G
2	L2	617	G
2	L2	619	A
2	L2	620	C
2	L2	621	G
2	L2	632	G
2	L2	635	A
2	L2	639	G
2	L2	643	A
2	L2	647	A2M
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
2	L2	686	OMG
2	L2	695	G
2	L2	696	A
2	L2	697	G
2	L2	698	G
2	L2	745	G
2	L2	746	A
2	L2	747	A
2	L2	749	G

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Mol	Chain	Res	Type
2	L2	750	U
2	L2	751	U
2	L2	752	G
2	L2	760	U
2	L2	768	G
2	L2	769	A
2	L2	777	A
2	L2	778	A
2	L2	779	U
2	L2	782	G
2	L2	784	U
2	L2	787	G
2	L2	789	G
2	L2	793	U
2	L2	799	G
2	L2	802	PSU
2	L2	803	A
2	L2	805	G
2	L2	808	C
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	984	G
2	L2	986	U
2	L2	999	U
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

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Mol	Chain	Res	Type
2	L2	1023	C
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	1064	A
2	L2	1075	G
2	L2	1078	OMG
2	L2	1079	U
2	L2	1083	A
2	L2	1084	A
2	L2	1090	G
2	L2	1096	U
2	L2	1099	G
2	L2	1100	A
2	L2	1102	C
2	L2	1104	G
2	L2	1106	A
2	L2	1115	U
2	L2	1116	A
2	L2	1118	A
2	L2	1121	A
2	L2	1122	C
2	L2	1123	A
2	L2	1129	A
2	L2	1132	A
2	L2	1137	G
2	L2	1141	G
2	L2	1143	U
2	L2	1147	C
2	L2	1148	G
2	L2	1154	C
2	L2	1155	A
2	L2	1156	G
2	L2	1158	A
2	L2	1162	A
2	L2	1171	G
2	L2	1172	C
2	L2	1176	A

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Mol	Chain	Res	Type
2	L2	1179	A
2	L2	1181	G
2	L2	1189	A
2	L2	1199	A
2	L2	1200	A
2	L2	1202	A
2	L2	1203	A
2	L2	1204	U
2	L2	1206	G
2	L2	1207	G
2	L2	1209	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	1261	G
2	L2	1264	PSU
2	L2	1265	PSU
2	L2	1271	G
2	L2	1281	U
2	L2	1283	A
2	L2	1288	G
2	L2	1289	A
2	L2	1300	U
2	L2	1306	U
2	L2	1309	G
2	L2	1313	U
2	L2	1325	A
2	L2	1327	C
2	L2	1336	G
2	L2	1337	C
2	L2	1342	G
2	L2	1348	A

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Mol	Chain	Res	Type
2	L2	1349	A
2	L2	1355	G
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	1386	C
2	L2	1392	U
2	L2	1409	A
2	L2	1416	U
2	L2	1421	C
2	L2	1423	C
2	L2	1425	A
2	L2	1426	C
2	L2	1428	U
2	L2	1430	G
2	L2	1433	G
2	L2	1434	G
2	L2	1437	A
2	L2	1438	U
2	L2	1439	U
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	1457	C
2	L2	1463	A
2	L2	1465	G
2	L2	1478	C
2	L2	1485	G
2	L2	1486	G
2	L2	1494	G
2	L2	1501	G
2	L2	1510	A
2	L2	1511	U
2	L2	1512	G

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Mol	Chain	Res	Type
2	L2	1513	G
2	L2	1514	U
2	L2	1524	A
2	L2	1526	C
3	L3	6	G
3	L3	16	G
3	L3	17	A
3	L3	19	A
3	L3	21	A
3	L3	22	C
3	L3	25	G
3	L3	34	C
3	L3	35	A
3	L3	36	A
3	L3	41	A
3	L3	42	U
3	L3	44	C
3	L3	48	C
3	L3	49	A
3	L3	50	C
3	L3	52	G
3	L3	70	A
3	L3	99	U
3	L3	108	U
3	L3	109	U
3	L3	110	U
3	L3	111	A
3	L3	112	C
3	L3	113	U
3	L3	114	U
3	L3	117	C
3	L3	120	G
3	L3	121	U
3	L3	125	U
3	L3	132	G
3	L3	141	A
3	L3	142	G
3	L3	149	A
3	L3	150	A
3	L3	151	A
3	L3	169	A
3	L3	182	U

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Mol	Chain	Res	Type
3	L3	187	U
3	L3	192	G
3	L3	195	U
3	L3	196	U
3	L3	199	A
3	L3	202	A
3	L3	212	G
4	L4	8	U
4	L4	9	G
4	L4	10	U
4	L4	11	G
4	L4	15	G
4	L4	16	G
4	L4	19	C
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	73	U
4	L4	76	C
4	L4	83	U
4	L4	85	C
4	L4	86	U
4	L4	87	G
4	L4	90	G
4	L4	102	G
4	L4	106	G
4	L4	107	U
4	L4	114	A
4	L4	120	U
4	L4	121	C
4	L4	122	G
4	L4	128	U
4	L4	132	U
4	L4	133	C
4	L4	148	C
4	L4	149	U
4	L4	150	A

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Mol	Chain	Res	Type
4	L4	151	A
4	L4	158	A
4	L4	159	G
4	L4	168	A
4	L4	170	G
4	L4	173	C
4	L4	178	G
4	L4	180	C
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	34	G
5	L5	39	G
5	L5	50	C
5	L5	51	A
5	L5	52	U
5	L5	57	C
5	L5	65	U
5	L5	68	G
5	L5	71	U
5	L5	86	G
5	L5	87	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	107	A
5	L5	109	G
5	L5	113	G
5	L5	118	U
5	L5	119	U
5	L5	120	C
5	L5	121	A
5	L5	123	G
5	L5	124	C
5	L5	135	U
6	L6	7	A

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Mol	Chain	Res	Type
6	L6	12	C
6	L6	14	A
6	L6	15	C
6	L6	22	G
6	L6	23	A
6	L6	24	C
6	L6	25	U
6	L6	31	U
6	L6	32	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	49	C
6	L6	51	A
6	L6	52	G
6	L6	54	A
6	L6	55	U
6	L6	56	A
6	L6	58	U
6	L6	64	U
6	L6	65	C
6	L6	67	C
6	L6	68	A
6	L6	69	A
6	L6	70	G
6	L6	71	A
6	L6	72	C
6	L6	73	A
7	L7	3	C
7	L7	11	G
7	L7	16	A
7	L7	22	U
7	L7	31	A
7	L7	33	U
7	L7	34	U
7	L7	38	U
7	L7	51	A
7	L7	59	A
7	L7	62	A

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Mol	Chain	Res	Type
7	L7	63	G
7	L7	68	A
7	L7	69	PSU
7	L7	70	C
7	L7	71	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	104	A
7	L7	105	C
7	L7	107	C
7	L7	110	A
7	L7	115	G
7	L7	117	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	159	C
7	L7	167	C
7	L7	169	A
8	L8	11	G
8	L8	22	A
8	L8	26	A
8	L8	45	G
8	L8	46	A
8	L8	52	G
8	L8	57	U
8	L8	67	C
8	L8	68	A
8	L8	69	G
8	L8	70	G
8	L8	71	C
8	L8	76	U

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Mol	Chain	Res	Type
8	L8	94	A
8	L8	95	U
8	L8	104	A
8	L8	113	U
8	L8	114	G
8	L8	124	U
51	S1	3	U
51	S1	8	OMU
51	S1	17	C
51	S1	26	A
51	S1	34	G
51	S1	42	G
51	S1	45	U
51	S1	47	A
51	S1	60	U
51	S1	61	C
51	S1	65	A
51	S1	66	U
51	S1	68	A
51	S1	98	A2M
51	S1	102	A
51	S1	103	A
51	S1	110	G
51	S1	112	A
51	S1	114	U
51	S1	117	G
51	S1	122	A
51	S1	124	A
51	S1	127	U
51	S1	129	U
51	S1	133	G
51	S1	144	A
51	S1	145	A
51	S1	147	U
51	S1	149	G
51	S1	152	A
51	S1	158	G
51	S1	164	C
51	S1	167	C
51	S1	170	G
51	S1	174	A
51	S1	175	U

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Mol	Chain	Res	Type
51	S1	176	A
51	S1	182	A
51	S1	194	U
51	S1	195	U
51	S1	196	C
51	S1	197	U
51	S1	198	C
51	S1	227	U
51	S1	228	G
51	S1	231	A
51	S1	234	C
51	S1	235	C
51	S1	237	A
51	S1	249	A
51	S1	250	C
51	S1	252	G
51	S1	253	U
51	S1	254	A
51	S1	255	A
51	S1	257	A
51	S1	264	C
51	S1	265	C
51	S1	275	A
51	S1	276	G
51	S1	277	U
51	S1	278	A
51	S1	279	A
51	S1	287	C
51	S1	288	A
51	S1	289	G
51	S1	295	A
51	S1	297	U
51	S1	298	C
51	S1	309	G
51	S1	310	U
51	S1	313	G
51	S1	316	A
51	S1	321	G
51	S1	322	C
51	S1	324	U
51	S1	325	G
51	S1	326	U

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Mol	Chain	Res	Type
51	S1	329	C
51	S1	332	C
51	S1	336	U
51	S1	340	G
51	S1	341	A
51	S1	356	A
51	S1	358	C
51	S1	360	G
51	S1	364	G
51	S1	377	A
51	S1	381	G
51	S1	382	A
51	S1	388	A
51	S1	396	G
51	S1	404	C
51	S1	433	G
51	S1	434	A
51	S1	435	G
51	S1	443	A
51	S1	444	A
51	S1	445	U
51	S1	446	A
51	S1	447	G
51	S1	454	C
51	S1	455	PSU
51	S1	460	C
51	S1	465	G
51	S1	466	G
51	S1	467	C
51	S1	469	G
51	S1	475	G
51	S1	477	G
51	S1	481	A
51	S1	482	U
51	S1	484	G
51	S1	487	C
51	S1	488	A
51	S1	497	A
51	S1	507	G
51	S1	508	A
51	S1	516	A
51	S1	523	A

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Mol	Chain	Res	Type
51	S1	525	A
51	S1	528	G
51	S1	548	G
51	S1	551	A
51	S1	552	U
51	S1	565	U
51	S1	574	C
51	S1	580	A
51	S1	581	A
51	S1	585	C
51	S1	587	A
51	S1	590	A
51	S1	591	A
51	S1	593	A
51	S1	600	OMG
51	S1	606	G
51	S1	607	U
51	S1	608	C
51	S1	609	U
51	S1	613	G
51	S1	614	C
51	S1	615	C
51	S1	617	G
51	S1	627	U
51	S1	628	A
51	S1	629	A
51	S1	630	U
51	S1	631	U
51	S1	632	C
51	S1	643	A
51	S1	659	G
51	S1	660	U
51	S1	666	U
51	S1	668	A2M
51	S1	669	A
51	S1	670	A
51	S1	671	G
51	S1	672	G
51	S1	673	G
51	S1	678	U
51	S1	687	U
51	S1	688	G

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Mol	Chain	Res	Type
51	S1	689	U
51	S1	690	G
51	S1	697	G
51	S1	698	C
51	S1	699	A
51	S1	749	U
51	S1	755	C
51	S1	757	C
51	S1	758	G
51	S1	762	A
51	S1	775	C
51	S1	778	G
51	S1	782	C
51	S1	784	C
51	S1	788	A
51	S1	789	G
51	S1	790	U
51	S1	791	G
51	S1	792	G
51	S1	811	C
51	S1	812	A
51	S1	814	G
51	S1	815	U
51	S1	816	C
51	S1	817	A
51	S1	819	G
51	S1	820	C
51	S1	825	C
51	S1	826	A
51	S1	830	G
51	S1	832	C
51	S1	833	G
51	S1	841	U
51	S1	844	U
51	S1	845	U
51	S1	856	A
51	S1	866	G
51	S1	867	A
51	S1	868	C
51	S1	869	U
51	S1	879	A
51	S1	880	U

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Mol	Chain	Res	Type
51	S1	883	G
51	S1	886	U
51	S1	887	U
51	S1	890	A
51	S1	892	U
51	S1	895	A
51	S1	914	G
51	S1	919	G
51	S1	923	C
51	S1	925	A
51	S1	926	G
51	S1	930	A
51	S1	935	U
51	S1	936	U
51	S1	937	C
51	S1	938	G
51	S1	944	U
51	S1	945	G
51	S1	950	U
51	S1	951	U
51	S1	952	U
51	S1	955	A
51	S1	956	A
51	S1	959	U
51	S1	969	A
51	S1	970	U
51	S1	971	U
51	S1	972	A
51	S1	973	U
51	S1	974	G
51	S1	1101	A
51	S1	1102	G
51	S1	1103	G
51	S1	1105	A
51	S1	1109	A
51	S1	1119	U
51	S1	1123	G
51	S1	1139	G
51	S1	1148	G
51	S1	1161	G
51	S1	1180	A
51	S1	1182	A

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Mol	Chain	Res	Type
51	S1	1197	C
51	S1	1198	A
51	S1	1199	A
51	S1	1207	U
51	S1	1210	C
51	S1	1211	U
51	S1	1213	A
51	S1	1217	A
51	S1	1232	G
51	S1	1235	A
51	S1	1239	A
51	S1	1240	A
51	S1	1251	A
51	S1	1270	G
51	S1	1271	C
51	S1	1272	A
51	S1	1273	A
51	S1	1275	C
51	S1	1359	C
51	S1	1360	U
51	S1	1361	U
51	S1	1365	U
51	S1	1371	U
51	S1	1398	C
51	S1	1399	G
51	S1	1431	A
51	S1	1443	U
51	S1	1444	G
51	S1	1448	U
51	S1	1449	U
51	S1	1452	A
51	S1	1466	G
51	S1	1467	U
51	S1	1490	A
51	S1	1502	G
51	S1	1503	A
51	S1	1510	C
51	S1	1531	G
51	S1	1537	U
51	S1	1543	B8N
51	S1	1546	A
51	S1	1548	A

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Mol	Chain	Res	Type
51	S1	1551	G
51	S1	1552	G
51	S1	1554	A
51	S1	1565	A
51	S1	1566	PSU
51	S1	1569	G
51	S1	1570	G
51	S1	1579	A
51	S1	1582	A
51	S1	1591	U
51	S1	1594	A
51	S1	1595	G
51	S1	1597	G
51	S1	1598	U
51	S1	1603	U
51	S1	1609	U
51	S1	1611	C
51	S1	1612	C
51	S1	1613	C
51	S1	1614	U
51	S1	1622	G
51	S1	1625	G
51	S1	1637	A
51	S1	1638	U
51	S1	1640	G
51	S1	1652	A
51	S1	1653	U
51	S1	1658	U
51	S1	1666	U
51	S1	1667	U
51	S1	1673	A
51	S1	1675	C
51	S1	1677	G
51	S1	1689	G
51	S1	1690	C
51	S1	1699	A
51	S1	1706	A
51	S1	1712	G
51	S1	1713	C
51	S1	1715	C
51	S1	1718	A
51	S1	1719	G

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Mol	Chain	Res	Type
51	S1	1720	G
51	S1	1724	G
51	S1	1725	C
51	S1	1762	A
51	S1	1764	U
51	S1	1766	G
51	S1	1768	U
51	S1	1769	C
51	S1	1770	G
51	S1	1784	G
51	S1	1788	U
51	S1	1789	U
51	S1	1794	U
51	S1	1795	G
51	S1	1799	U
51	S1	1800	U
51	S1	1801	G
51	S1	1806	A
51	S1	1814	U
51	S1	1816	U
51	S1	1825	A
51	S1	1826	G
51	S1	1828	A
51	S1	1829	OMG
51	S1	1832	C
51	S1	1833	OMU
51	S1	1837	A
51	S1	1846	A
51	S1	1847	A
51	S1	1848	U
51	S1	1858	G
51	S1	1860	C
51	S1	1861	A
51	S1	1867	A
51	S1	1872	A
51	S1	1874	U
51	S1	1878	A
51	S1	1884	A
51	S1	1887	A
51	S1	1888	A
51	S1	1889	G
51	S1	1890	A

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Mol	Chain	Res	Type
51	S1	1891	A
51	S1	1905	C
51	S1	1906	G
51	S1	1907	A
51	S1	1916	G
51	S1	1917	A
51	S1	1918	U
51	S1	1919	C
51	S1	1920	A
51	S1	1923	A
51	S1	1931	G
51	S1	1932	A
51	S1	1933	A
51	S1	1944	C
51	S1	1948	U
51	S1	1949	A
51	S1	1950	G
51	S1	1956	C
51	S1	1961	G
51	S1	1962	A
51	S1	1976	U
51	S1	1978	A
51	S1	1988	C
51	S1	1989	A
51	S1	1995	7MG
51	S1	2003	C
51	S1	2004	G
51	S1	2010	G
51	S1	2015	U
51	S1	2016	C
51	S1	2020	A
51	S1	2021	A2M
51	S1	2031	A
51	S1	2036	G
51	S1	2052	C
51	S1	2054	C
51	S1	2061	5MC
51	S1	2062	G
51	S1	2063	U
51	S1	2070	U
51	S1	2090	A
51	S1	2097	C

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Mol	Chain	Res	Type
51	S1	2099	G
51	S1	2101	C
51	S1	2118	G
51	S1	2119	C
51	S1	2120	C
51	S1	2121	C
51	S1	2125	A
51	S1	2134	A
51	S1	2136	A
51	S1	2137	U
51	S1	2156	A
51	S1	2158	A
51	S1	2163	G
51	S1	2164	U
51	S1	2165	A
51	S1	2169	A
51	S1	2170	G
51	S1	2172	U
51	S1	2183	G
51	S1	2185	MA6
51	S1	2195	G
51	S1	2196	G
51	S1	2197	G
51	S1	2198	A
51	S1	2199	C
51	S1	2202	PSU
51	S1	2203	U
52	S2	7	A
52	S2	8	U
52	S2	14	A
52	S2	15	G
52	S2	16	U
52	S2	17	C
52	S2	18	G
52	S2	19	G
52	S2	20	U
52	S2	21	A
52	S2	34	G
52	S2	35	A
52	S2	45	U
52	S2	46	G
52	S2	47	U

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Mol	Chain	Res	Type
52	S2	48	C
52	S2	49	C
52	S2	50	U
52	S2	54	U
52	S2	55	U
52	S2	56	C
52	S2	58	A
52	S2	61	C
52	S2	65	G
52	S2	66	U
52	S2	67	C
52	S2	74	C
53	S3	8	U
53	S3	10	G
53	S3	16	C
53	S3	17	C
53	S3	18	U
53	S3	19	G
53	S3	20	G
53	S3	21	A
53	S3	22	G
53	S3	47	U
53	S3	48	C
53	S3	49	G
53	S3	52	G
53	S3	61	C
53	S3	66	C
53	S3	68	C
53	S3	72	A
53	S3	74	C
53	S3	75	C
54	S4	2	C
54	S4	3	G
54	S4	4	C
54	S4	7	A
54	S4	8	U
54	S4	9	A
54	S4	10	G
54	S4	14	A
54	S4	15	G
54	S4	16	U
54	S4	17	C

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Mol	Chain	Res	Type
54	S4	18	G
54	S4	19	G
54	S4	20	U
54	S4	21	A
54	S4	29	G
54	S4	30	G
54	S4	32	U
54	S4	33	U
54	S4	38	A
54	S4	39	U
54	S4	44	G
54	S4	45	U
54	S4	47	U
54	S4	49	C
54	S4	51	U
54	S4	54	U
54	S4	55	U
54	S4	56	C
54	S4	57	G
54	S4	59	U
54	S4	61	C
54	S4	66	U
54	S4	69	G
54	S4	70	C
54	S4	73	A
54	S4	76	A
55	S5	2	A
55	S5	5	A
55	S5	8	U
55	S5	9	U
55	S5	10	C
55	S5	12	A

All (81) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	141	U
1	L1	170	U
1	L1	191	U
1	L1	208	C
1	L1	554	A
1	L1	557	U

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Mol	Chain	Res	Type
1	L1	584	U
1	L1	835	G
1	L1	837	A
1	L1	967	G
1	L1	1200	A
1	L1	1347	G
1	L1	1390	G
1	L1	1479	A
1	L1	1565	A
1	L1	1574	C
1	L1	1612	G
1	L1	1662	G
2	L2	443	OMC
2	L2	454	A
2	L2	620	C
2	L2	696	A
2	L2	748	C
2	L2	1083	A
2	L2	1101	A
2	L2	1131	A
2	L2	1136	U
2	L2	1170	U
2	L2	1237	A
2	L2	1437	A
2	L2	1485	G
2	L2	1512	G
3	L3	34	C
3	L3	35	A
3	L3	149	A
4	L4	148	C
4	L4	149	U
5	L5	51	A
5	L5	106	G
5	L5	119	U
6	L6	51	A
7	L7	71	A
7	L7	93	C
8	L8	113	U
51	S1	128	C
51	S1	254	A
51	S1	276	G
51	S1	294	G

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Mol	Chain	Res	Type
51	S1	309	G
51	S1	328	C
51	S1	550	C
51	S1	613	G
51	S1	628	A
51	S1	629	A
51	S1	631	U
51	S1	777	A
51	S1	889	A
51	S1	937	C
51	S1	958	G
51	S1	1209	C
51	S1	1360	U
51	S1	1608	A
51	S1	1672	C
51	S1	1717	U
51	S1	1761	C
51	S1	1858	G
51	S1	1889	G
51	S1	1915	U
51	S1	1931	G
51	S1	2119	C
52	S2	7	A
52	S2	13	C
52	S2	34	G
52	S2	45	U
52	S2	47	U
52	S2	48	C
52	S2	49	C
52	S2	54	U
53	S3	20	G
53	S3	60	U
54	S4	13	C

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

170 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$
51	OMC	S1	2059	51	19,22,23	3.00	8 (42%)	25,31,34	1.25	2 (8%)
2	PSU	L2	1194	2	18,21,22	4.63	7 (38%)	21,30,33	1.92	4 (19%)
51	A2M	S1	897	51	22,25,26	3.52	9 (40%)	30,36,39	2.42	12 (40%)
51	PSU	S1	1292	91,90,51	18,21,22	4.59	7 (38%)	21,30,33	1.92	5 (23%)
51	5MC	S1	2061	51	19,22,23	3.74	8 (42%)	26,32,35	0.93	1 (3%)
2	PSU	L2	500	2	18,21,22	4.64	7 (38%)	21,30,33	1.95	5 (23%)
2	PSU	L2	626	2	18,21,22	4.60	7 (38%)	21,30,33	1.85	5 (23%)
51	OMG	S1	1829	90,51	23,26,27	0.31	0	32,38,41	0.32	0
1	OMG	L1	1626	1	23,26,27	0.31	0	32,38,41	0.52	0
2	OMC	L2	359	2	19,22,23	3.01	8 (42%)	25,31,34	0.71	0
51	PSU	S1	1657	51	18,21,22	4.63	7 (38%)	21,30,33	1.92	5 (23%)
2	A2M	L2	628	2	22,25,26	0.23	0	30,36,39	0.34	0
2	OMG	L2	686	2	23,26,27	2.43	9 (39%)	32,38,41	2.55	11 (34%)
51	PSU	S1	1566	51	18,21,22	4.69	8 (44%)	21,30,33	1.86	5 (23%)
1	PSU	L1	422	1	18,21,22	4.64	7 (38%)	21,30,33	1.87	5 (23%)
2	5MC	L2	524	90,2	19,22,23	0.88	1 (5%)	26,32,35	0.53	0
2	OMC	L2	583	2	19,22,23	2.94	8 (42%)	25,31,34	0.71	0
2	PSU	L2	662	90,2	18,21,22	4.57	7 (38%)	21,30,33	1.89	5 (23%)
2	OMU	L2	1077	2	19,22,23	3.06	8 (42%)	25,31,34	1.81	4 (16%)
2	OMG	L2	641	2	23,26,27	2.39	9 (39%)	32,38,41	2.46	11 (34%)
2	OMG	L2	655	2	23,26,27	2.43	9 (39%)	32,38,41	2.56	12 (37%)
2	PSU	L2	1403	2	18,21,22	4.63	7 (38%)	21,30,33	2.02	6 (28%)
1	PSU	L1	940	1	18,21,22	4.62	7 (38%)	21,30,33	1.94	5 (23%)
2	OMC	L2	14	1,2	19,22,23	0.31	0	25,31,34	0.66	1 (4%)
1	OMC	L1	1010	1,90,91	19,22,23	0.32	0	25,31,34	0.46	0
1	OMG	L1	856	1	23,26,27	2.41	9 (39%)	32,38,41	2.50	11 (34%)
2	OMG	L2	71	92,2	23,26,27	2.44	9 (39%)	32,38,41	2.54	10 (31%)
2	PSU	L2	512	2	18,21,22	4.66	7 (38%)	21,30,33	1.93	5 (23%)
7	PSU	L7	166	1,7	18,21,22	4.66	7 (38%)	21,30,33	1.96	5 (23%)
2	OMU	L2	1359	92,2	19,22,23	3.03	8 (42%)	25,31,34	1.79	4 (16%)
1	PSU	L1	1181	1	18,21,22	4.64	7 (38%)	21,30,33	1.96	5 (23%)
2	OMC	L2	443	90,91,2	19,22,23	0.39	0	25,31,34	0.60	0
52	MIA	S2	37	52	28,31,32	2.53	4 (14%)	38,44,47	4.67	19 (50%)
51	PSU	S1	1246	51	18,21,22	4.66	7 (38%)	21,30,33	1.97	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L2	604	1,2	22,25,26	3.53	9 (40%)	30,36,39	2.33	10 (33%)
2	OMC	L2	1159	2	19,22,23	0.31	0	25,31,34	0.50	0
51	OMU	S1	1979	51	19,22,23	3.10	8 (42%)	25,31,34	1.82	4 (16%)
1	OMC	L1	1527	1,90	19,22,23	2.96	8 (42%)	25,31,34	0.81	0
1	A2M	L1	235	1	22,25,26	3.49	9 (40%)	30,36,39	2.35	11 (36%)
2	OMG	L2	534	2	23,26,27	2.42	9 (39%)	32,38,41	2.56	10 (31%)
2	A2M	L2	527	90,2	22,25,26	3.48	9 (40%)	30,36,39	2.58	13 (43%)
2	OMU	L2	1419	2	19,22,23	3.02	8 (42%)	25,31,34	1.78	4 (16%)
2	OMG	L2	1046	53,90,2	23,26,27	2.42	9 (39%)	32,38,41	2.57	10 (31%)
51	OMG	S1	1478	51	23,26,27	2.40	9 (39%)	32,38,41	2.48	12 (37%)
1	PSU	L1	1664	1	18,21,22	0.94	1 (5%)	21,30,33	0.68	0
51	OMU	S1	1833	51	19,22,23	3.07	8 (42%)	25,31,34	1.92	5 (20%)
3	OMU	L3	13	3	19,22,23	3.06	8 (42%)	25,31,34	1.87	4 (16%)
2	A2M	L2	647	2	22,25,26	3.45	9 (40%)	30,36,39	2.57	12 (40%)
1	PSU	L1	1528	1	18,21,22	4.63	7 (38%)	21,30,33	1.95	5 (23%)
2	PSU	L2	1060	2	18,21,22	4.60	7 (38%)	21,30,33	2.08	5 (23%)
1	A2M	L1	1539	1,90,2	22,25,26	3.54	9 (40%)	30,36,39	2.32	9 (30%)
1	A2M	L1	955	1	22,25,26	0.22	0	30,36,39	0.39	0
2	PSU	L2	1265	2	18,21,22	4.62	7 (38%)	21,30,33	1.85	4 (19%)
2	PSU	L2	1144	2	18,21,22	4.61	7 (38%)	21,30,33	2.04	5 (23%)
2	PSU	L2	565	2	18,21,22	0.92	1 (5%)	21,30,33	0.76	0
1	A2M	L1	69	1	22,25,26	3.44	8 (36%)	30,36,39	2.55	14 (46%)
2	A2M	L2	382	2	22,25,26	3.53	9 (40%)	30,36,39	2.27	11 (36%)
7	PSU	L7	74	7	18,21,22	4.65	7 (38%)	21,30,33	1.97	5 (23%)
7	PSU	L7	69	90,7	18,21,22	4.61	7 (38%)	21,30,33	1.97	6 (28%)
2	A2M	L2	1067	2	22,25,26	0.24	0	30,36,39	0.40	0
4	OMG	L4	74	4	23,26,27	0.32	0	32,38,41	0.32	0
1	OMU	L1	1371	1	19,22,23	3.13	8 (42%)	25,31,34	1.97	6 (24%)
1	OMU	L1	1107	1	19,22,23	3.06	8 (42%)	25,31,34	1.86	5 (20%)
2	PSU	L2	1213	2	18,21,22	4.60	7 (38%)	21,30,33	1.98	5 (23%)
2	A2M	L2	591	92,2	22,25,26	3.54	9 (40%)	30,36,39	2.27	9 (30%)
2	A2M	L2	1372	2	22,25,26	3.54	9 (40%)	30,36,39	2.33	9 (30%)
51	OMU	S1	29	51	19,22,23	3.09	8 (42%)	25,31,34	1.82	5 (20%)
1	PSU	L1	672	1,90	18,21,22	0.90	1 (5%)	21,30,33	0.65	0
51	PSU	S1	1533	51	18,21,22	4.66	7 (38%)	21,30,33	1.96	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	1011	1,2	18,21,22	0.83	1 (5%)	21,30,33	0.77	0
7	A2M	L7	162	1,7	22,25,26	3.54	9 (40%)	30,36,39	2.32	10 (33%)
1	OMC	L1	695	1	19,22,23	2.91	8 (42%)	25,31,34	0.71	0
2	A2M	L2	665	2	22,25,26	3.53	9 (40%)	30,36,39	2.41	10 (33%)
2	PSU	L2	437	2	18,21,22	0.90	1 (5%)	21,30,33	0.71	0
2	OMG	L2	1360	52,2	23,26,27	2.43	9 (39%)	32,38,41	2.56	10 (31%)
1	OMU	L1	48	1	19,22,23	0.37	0	25,31,34	1.06	2 (8%)
1	A2M	L1	305	1	22,25,26	3.49	9 (40%)	30,36,39	2.40	13 (43%)
1	PSU	L1	1529	1	18,21,22	4.61	7 (38%)	21,30,33	1.96	5 (23%)
2	A2M	L2	1384	90,2	22,25,26	3.51	9 (40%)	30,36,39	2.34	9 (30%)
51	OMG	S1	600	51	23,26,27	2.42	9 (39%)	32,38,41	2.59	10 (31%)
1	OMG	L1	1190	1,90	23,26,27	2.39	9 (39%)	32,38,41	2.43	14 (43%)
2	PSU	L2	593	92,2	18,21,22	4.58	7 (38%)	21,30,33	1.84	5 (23%)
2	OMG	L2	1253	2	23,26,27	2.36	9 (39%)	32,38,41	2.53	11 (34%)
1	OMG	L1	1524	1	23,26,27	2.43	9 (39%)	32,38,41	2.56	13 (40%)
2	OMC	L2	1397	2	19,22,23	2.95	8 (42%)	25,31,34	0.79	0
51	A2M	S1	668	90,51	22,25,26	3.47	9 (40%)	30,36,39	2.37	12 (40%)
51	PSU	S1	1192	51	18,21,22	4.62	7 (38%)	21,30,33	1.87	5 (23%)
51	B8N	S1	1543	-	25,29,30	4.43	15 (60%)	28,42,45	2.24	9 (32%)
51	OMU	S1	1662	51	19,22,23	3.07	8 (42%)	25,31,34	1.79	4 (16%)
51	PSU	S1	2048	51	18,21,22	0.92	1 (5%)	21,30,33	0.79	0
2	PSU	L2	472	2	18,21,22	4.62	7 (38%)	21,30,33	1.90	5 (23%)
1	OMU	L1	845	1	19,22,23	0.37	0	25,31,34	0.86	0
1	PSU	L1	1177	1	18,21,22	4.63	7 (38%)	21,30,33	1.87	5 (23%)
51	OMG	S1	1550	51	23,26,27	0.31	0	32,38,41	0.40	0
51	7MG	S1	1995	53,51	23,26,27	3.91	11 (47%)	27,39,42	2.20	9 (33%)
51	MA6	S1	2184	51	23,26,27	1.49	5 (21%)	33,38,41	2.88	12 (36%)
1	A2M	L1	697	1	22,25,26	3.51	9 (40%)	30,36,39	2.38	11 (36%)
51	PSU	S1	455	51	18,21,22	4.70	7 (38%)	21,30,33	1.86	5 (23%)
1	PSU	L1	774	1	18,21,22	0.92	1 (5%)	21,30,33	0.84	1 (4%)
2	OMC	L2	1317	2	19,22,23	2.93	8 (42%)	25,31,34	0.77	0
2	OMU	L2	56	1,2	19,22,23	3.06	8 (42%)	25,31,34	1.83	4 (16%)
51	A2M	S1	479	51	22,25,26	3.49	9 (40%)	30,36,39	2.33	10 (33%)
1	A2M	L1	407	1	22,25,26	3.50	9 (40%)	30,36,39	2.41	11 (36%)
1	A2M	L1	927	1	22,25,26	3.52	9 (40%)	30,36,39	2.32	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L1	313	1	18,21,22	4.60	7 (38%)	21,30,33	1.85	4 (19%)
2	PSU	L2	1413	2	18,21,22	4.53	7 (38%)	21,30,33	1.97	5 (23%)
51	OMU	S1	1621	90,51	19,22,23	3.08	8 (42%)	25,31,34	1.83	5 (20%)
1	PSU	L1	1526	1	18,21,22	4.62	8 (44%)	21,30,33	1.99	6 (28%)
2	OMU	L2	73	92,2	19,22,23	3.07	8 (42%)	25,31,34	1.77	4 (16%)
1	PSU	L1	1017	1,91	18,21,22	4.60	7 (38%)	21,30,33	1.97	5 (23%)
1	PSU	L1	1171	1,91	18,21,22	4.62	8 (44%)	21,30,33	1.91	4 (19%)
2	PSU	L2	1152	2	18,21,22	4.62	7 (38%)	21,30,33	2.09	5 (23%)
2	PSU	L2	597	2	18,21,22	4.59	7 (38%)	21,30,33	1.91	5 (23%)
2	PSU	L2	1264	91,2	18,21,22	4.57	8 (44%)	21,30,33	1.82	4 (19%)
51	A2M	S1	512	51	22,25,26	3.50	9 (40%)	30,36,39	2.37	11 (36%)
2	PSU	L2	1284	2	18,21,22	4.67	7 (38%)	21,30,33	1.94	5 (23%)
2	A2M	L2	502	2	22,25,26	3.50	9 (40%)	30,36,39	2.39	10 (33%)
2	PSU	L2	504	2	18,21,22	4.69	7 (38%)	21,30,33	1.99	5 (23%)
1	OMG	L1	959	1	23,26,27	0.33	0	32,38,41	0.72	1 (3%)
2	PSU	L2	1318	2	18,21,22	4.61	7 (38%)	21,30,33	2.00	5 (23%)
51	PSU	S1	1539	51	18,21,22	4.65	7 (38%)	21,30,33	1.93	5 (23%)
7	A2M	L7	43	90,7	22,25,26	3.55	9 (40%)	30,36,39	2.45	11 (36%)
1	A2M	L1	681	1	22,25,26	0.22	0	30,36,39	0.34	0
51	OMU	S1	8	51	19,22,23	0.26	0	25,31,34	0.61	1 (4%)
1	A2M	L1	1373	1	22,25,26	3.54	9 (40%)	30,36,39	2.29	9 (30%)
51	OMC	S1	18	51	19,22,23	2.94	8 (42%)	25,31,34	0.81	0
1	A2M	L1	678	1,2	22,25,26	0.23	0	30,36,39	0.40	0
2	OMU	L2	560	2	19,22,23	0.28	0	25,31,34	1.24	4 (16%)
51	OMG	S1	1865	51	23,26,27	2.45	9 (39%)	32,38,41	2.54	11 (34%)
2	OMU	L2	667	2	19,22,23	3.03	8 (42%)	25,31,34	1.83	5 (20%)
2	PSU	L2	1361	92,2,52	18,21,22	4.65	7 (38%)	21,30,33	1.94	5 (23%)
51	MA6	S1	2185	90,51	23,26,27	1.47	5 (21%)	33,38,41	3.01	13 (39%)
51	OMG	S1	1623	91,51	23,26,27	2.42	9 (39%)	32,38,41	2.62	10 (31%)
2	A2M	L2	570	1,2	22,25,26	3.50	9 (40%)	30,36,39	2.44	11 (36%)
51	PSU	S1	2046	51	18,21,22	4.64	7 (38%)	21,30,33	1.97	5 (23%)
51	PSU	S1	12	51	18,21,22	0.93	1 (5%)	21,30,33	0.66	0
1	PSU	L1	239	1	18,21,22	0.93	1 (5%)	21,30,33	0.70	0
2	OMG	L2	1078	2	23,26,27	2.38	9 (39%)	32,38,41	2.41	12 (37%)
2	PSU	L2	802	2	18,21,22	4.66	7 (38%)	21,30,33	1.96	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	A2M	S1	98	90,51	22,25,26	3.53	9 (40%)	30,36,39	2.34	12 (40%)
1	PSU	L1	510	1	18,21,22	0.95	1 (5%)	21,30,33	0.68	0
51	OMC	S1	38	51	19,22,23	3.01	8 (42%)	25,31,34	0.85	0
51	A2M	S1	28	51	22,25,26	3.53	9 (40%)	30,36,39	2.32	10 (33%)
2	PSU	L2	78	2	18,21,22	4.60	7 (38%)	21,30,33	1.95	5 (23%)
51	PSU	S1	2202	51	18,21,22	4.60	8 (44%)	21,30,33	1.85	5 (23%)
1	PSU	L1	1533	1,2	18,21,22	4.62	7 (38%)	21,30,33	2.02	5 (23%)
51	OMC	S1	2140	51	19,22,23	3.03	8 (42%)	25,31,34	0.79	0
1	A2M	L1	858	1	22,25,26	3.50	9 (40%)	30,36,39	2.52	14 (46%)
1	OMU	L1	847	1	19,22,23	0.25	0	25,31,34	0.64	0
51	A2M	S1	2021	51	22,25,26	0.22	0	30,36,39	0.46	0
51	PSU	S1	33	51	18,21,22	4.69	7 (38%)	21,30,33	1.94	5 (23%)
51	OMG	S1	1647	51	23,26,27	2.44	9 (39%)	32,38,41	2.58	12 (37%)
2	A2M	L2	95	2	22,25,26	3.53	9 (40%)	30,36,39	2.33	10 (33%)
51	OMG	S1	2151	51	23,26,27	2.41	9 (39%)	32,38,41	2.55	11 (34%)
2	PSU	L2	1058	2	18,21,22	4.63	7 (38%)	21,30,33	2.11	5 (23%)
1	OMU	L1	1659	1,90	19,22,23	3.02	8 (42%)	25,31,34	1.79	4 (16%)
2	A2M	L2	572	2	22,25,26	3.52	9 (40%)	30,36,39	2.34	11 (36%)
2	OMC	L2	1248	2	19,22,23	2.99	8 (42%)	25,31,34	0.88	0
7	PSU	L7	101	7	18,21,22	4.57	8 (44%)	21,30,33	1.95	6 (28%)
51	5MC	S1	1544	51	19,22,23	0.90	1 (5%)	26,32,35	0.52	0
2	OMG	L2	1231	2	23,26,27	2.40	9 (39%)	32,38,41	2.54	11 (34%)
7	OMG	L7	75	7	23,26,27	2.43	9 (39%)	32,38,41	2.50	10 (31%)
1	OMG	L1	1540	1,2	23,26,27	0.33	0	32,38,41	0.36	0
2	5MC	L2	1308	2	19,22,23	4.76	13 (68%)	26,32,35	1.28	2 (7%)
51	OMC	S1	1866	51	19,22,23	2.97	8 (42%)	25,31,34	0.80	0
51	OMU	S1	661	51	19,22,23	3.04	8 (42%)	25,31,34	1.78	5 (20%)
2	PSU	L2	1303	2	18,21,22	4.65	7 (38%)	21,30,33	2.01	6 (28%)
2	PSU	L2	510	2	18,21,22	4.62	7 (38%)	21,30,33	1.91	5 (23%)
2	OMG	L2	1229	2	23,26,27	2.43	9 (39%)	32,38,41	2.49	10 (31%)
2	A2M	L2	1185	2	22,25,26	3.48	9 (40%)	30,36,39	2.45	13 (43%)

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
51	OMC	S1	2059	51	-	3/9/27/28	0/2/2/2
2	PSU	L2	1194	2	-	0/7/25/26	0/2/2/2
51	A2M	S1	897	51	-	0/9/27/28	0/3/3/3
51	PSU	S1	1292	91,90,51	-	0/7/25/26	0/2/2/2
51	5MC	S1	2061	51	-	2/7/25/26	0/2/2/2
2	PSU	L2	500	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	626	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1829	90,51	-	2/9/27/28	0/3/3/3
1	OMG	L1	1626	1	-	0/9/27/28	0/3/3/3
2	OMC	L2	359	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1657	51	-	1/7/25/26	0/2/2/2
2	A2M	L2	628	2	-	0/9/27/28	0/3/3/3
2	OMG	L2	686	2	-	2/9/27/28	0/3/3/3
51	PSU	S1	1566	51	-	2/7/25/26	0/2/2/2
1	PSU	L1	422	1	-	0/7/25/26	0/2/2/2
2	5MC	L2	524	90,2	-	0/7/25/26	0/2/2/2
2	OMC	L2	583	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	662	90,2	-	0/7/25/26	0/2/2/2
2	OMU	L2	1077	2	-	0/9/27/28	0/2/2/2
2	OMG	L2	641	2	-	0/9/27/28	0/3/3/3
2	OMG	L2	655	2	-	0/9/27/28	0/3/3/3
2	PSU	L2	1403	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	940	1	-	0/7/25/26	0/2/2/2
2	OMC	L2	14	1,2	-	2/9/27/28	0/2/2/2
1	OMC	L1	1010	1,90,91	-	2/9/27/28	0/2/2/2
1	OMG	L1	856	1	-	0/9/27/28	0/3/3/3
2	OMG	L2	71	92,2	-	0/9/27/28	0/3/3/3
2	PSU	L2	512	2	-	0/7/25/26	0/2/2/2
7	PSU	L7	166	1,7	-	0/7/25/26	0/2/2/2
2	OMU	L2	1359	92,2	-	0/9/27/28	0/2/2/2
1	PSU	L1	1181	1	-	0/7/25/26	0/2/2/2
2	OMC	L2	443	90,91,2	-	4/9/27/28	0/2/2/2
52	MIA	S2	37	52	-	0/15/33/34	0/3/3/3
51	PSU	S1	1246	51	-	0/7/25/26	0/2/2/2
2	A2M	L2	604	1,2	-	0/9/27/28	0/3/3/3
2	OMC	L2	1159	2	-	0/9/27/28	0/2/2/2
51	OMU	S1	1979	51	-	1/9/27/28	0/2/2/2
1	OMC	L1	1527	1,90	-	0/9/27/28	0/2/2/2
1	A2M	L1	235	1	-	0/9/27/28	0/3/3/3
2	OMG	L2	534	2	-	2/9/27/28	0/3/3/3
2	A2M	L2	527	90,2	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	L2	1419	2	-	0/9/27/28	0/2/2/2
2	OMG	L2	1046	53,90,2	-	3/9/27/28	0/3/3/3
51	OMG	S1	1478	51	-	1/9/27/28	0/3/3/3
1	PSU	L1	1664	1	-	2/7/25/26	0/2/2/2
51	OMU	S1	1833	51	-	1/9/27/28	0/2/2/2
3	OMU	L3	13	3	-	0/9/27/28	0/2/2/2
2	A2M	L2	647	2	-	4/9/27/28	0/3/3/3
1	PSU	L1	1528	1	-	2/7/25/26	0/2/2/2
2	PSU	L2	1060	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	1539	1,90,2	-	1/9/27/28	0/3/3/3
1	A2M	L1	955	1	-	1/9/27/28	0/3/3/3
2	PSU	L2	1265	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1144	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	565	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	69	1	-	2/9/27/28	0/3/3/3
2	A2M	L2	382	2	-	0/9/27/28	0/3/3/3
7	PSU	L7	74	7	-	0/7/25/26	0/2/2/2
7	PSU	L7	69	90,7	-	0/7/25/26	0/2/2/2
2	A2M	L2	1067	2	-	0/9/27/28	0/3/3/3
4	OMG	L4	74	4	-	3/9/27/28	0/3/3/3
1	OMU	L1	1371	1	-	3/9/27/28	0/2/2/2
1	OMU	L1	1107	1	-	0/9/27/28	0/2/2/2
2	PSU	L2	1213	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	591	92,2	-	0/9/27/28	0/3/3/3
2	A2M	L2	1372	2	-	0/9/27/28	0/3/3/3
51	OMU	S1	29	51	-	1/9/27/28	0/2/2/2
1	PSU	L1	672	1,90	-	0/7/25/26	0/2/2/2
51	PSU	S1	1533	51	-	0/7/25/26	0/2/2/2
1	PSU	L1	1011	1,2	-	0/7/25/26	0/2/2/2
7	A2M	L7	162	1,7	-	1/9/27/28	0/3/3/3
1	OMC	L1	695	1	-	1/9/27/28	0/2/2/2
2	A2M	L2	665	2	-	2/9/27/28	0/3/3/3
2	PSU	L2	437	2	-	0/7/25/26	0/2/2/2
2	OMG	L2	1360	52,2	-	0/9/27/28	0/3/3/3
1	OMU	L1	48	1	-	2/9/27/28	0/2/2/2
1	A2M	L1	305	1	-	2/9/27/28	0/3/3/3
1	PSU	L1	1529	1	-	0/7/25/26	0/2/2/2
2	A2M	L2	1384	90,2	-	0/9/27/28	0/3/3/3
51	OMG	S1	600	51	-	2/9/27/28	0/3/3/3
1	OMG	L1	1190	1,90	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L2	593	92,2	-	0/7/25/26	0/2/2/2
2	OMG	L2	1253	2	-	0/9/27/28	0/3/3/3
1	OMG	L1	1524	1	-	1/9/27/28	0/3/3/3
2	OMC	L2	1397	2	-	0/9/27/28	0/2/2/2
51	A2M	S1	668	90,51	-	6/9/27/28	0/3/3/3
51	PSU	S1	1192	51	-	2/7/25/26	0/2/2/2
51	B8N	S1	1543	-	-	10/16/34/35	0/2/2/2
51	OMU	S1	1662	51	-	1/9/27/28	0/2/2/2
51	PSU	S1	2048	51	-	0/7/25/26	0/2/2/2
2	PSU	L2	472	2	-	0/7/25/26	0/2/2/2
1	OMU	L1	845	1	-	3/9/27/28	0/2/2/2
1	PSU	L1	1177	1	-	0/7/25/26	0/2/2/2
51	OMG	S1	1550	51	-	1/9/27/28	0/3/3/3
51	7MG	S1	1995	53,51	-	2/7/37/38	0/3/3/3
51	MA6	S1	2184	51	-	0/11/29/30	0/3/3/3
1	A2M	L1	697	1	-	0/9/27/28	0/3/3/3
51	PSU	S1	455	51	-	2/7/25/26	0/2/2/2
1	PSU	L1	774	1	-	0/7/25/26	0/2/2/2
2	OMC	L2	1317	2	-	0/9/27/28	0/2/2/2
2	OMU	L2	56	1,2	-	1/9/27/28	0/2/2/2
51	A2M	S1	479	51	-	0/9/27/28	0/3/3/3
1	A2M	L1	407	1	-	0/9/27/28	0/3/3/3
1	A2M	L1	927	1	-	0/9/27/28	0/3/3/3
1	PSU	L1	313	1	-	2/7/25/26	0/2/2/2
2	PSU	L2	1413	2	-	0/7/25/26	0/2/2/2
51	OMU	S1	1621	90,51	-	0/9/27/28	0/2/2/2
1	PSU	L1	1526	1	-	4/7/25/26	0/2/2/2
2	OMU	L2	73	92,2	-	0/9/27/28	0/2/2/2
1	PSU	L1	1017	1,91	-	2/7/25/26	0/2/2/2
1	PSU	L1	1171	1,91	-	2/7/25/26	0/2/2/2
2	PSU	L2	1152	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	597	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1264	91,2	-	2/7/25/26	0/2/2/2
51	A2M	S1	512	51	-	2/9/27/28	0/3/3/3
2	PSU	L2	1284	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	502	2	-	2/9/27/28	0/3/3/3
2	PSU	L2	504	2	-	0/7/25/26	0/2/2/2
1	OMG	L1	959	1	-	3/9/27/28	0/3/3/3
2	PSU	L2	1318	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	PSU	S1	1539	51	-	1/7/25/26	0/2/2/2
7	A2M	L7	43	90,7	-	0/9/27/28	0/3/3/3
1	A2M	L1	681	1	-	4/9/27/28	0/3/3/3
51	OMU	S1	8	51	-	7/9/27/28	0/2/2/2
1	A2M	L1	1373	1	-	0/9/27/28	0/3/3/3
51	OMC	S1	18	51	-	1/9/27/28	0/2/2/2
1	A2M	L1	678	1,2	-	0/9/27/28	0/3/3/3
2	OMU	L2	560	2	-	3/9/27/28	0/2/2/2
51	OMG	S1	1865	51	-	0/9/27/28	0/3/3/3
2	OMU	L2	667	2	-	0/9/27/28	0/2/2/2
2	PSU	L2	1361	92,2,52	-	5/7/25/26	0/2/2/2
51	MA6	S1	2185	90,51	-	1/11/29/30	0/3/3/3
51	OMG	S1	1623	91,51	-	0/9/27/28	0/3/3/3
2	A2M	L2	570	1,2	-	3/9/27/28	0/3/3/3
51	PSU	S1	2046	51	-	0/7/25/26	0/2/2/2
51	PSU	S1	12	51	-	0/7/25/26	0/2/2/2
1	PSU	L1	239	1	-	0/7/25/26	0/2/2/2
2	OMG	L2	1078	2	-	2/9/27/28	0/3/3/3
2	PSU	L2	802	2	-	2/7/25/26	0/2/2/2
51	A2M	S1	98	90,51	-	2/9/27/28	0/3/3/3
1	PSU	L1	510	1	-	1/7/25/26	0/2/2/2
51	OMC	S1	38	51	-	0/9/27/28	0/2/2/2
51	A2M	S1	28	51	-	0/9/27/28	0/3/3/3
2	PSU	L2	78	2	-	0/7/25/26	0/2/2/2
51	PSU	S1	2202	51	-	1/7/25/26	0/2/2/2
1	PSU	L1	1533	1,2	-	0/7/25/26	0/2/2/2
51	OMC	S1	2140	51	-	2/9/27/28	0/2/2/2
1	A2M	L1	858	1	-	1/9/27/28	0/3/3/3
1	OMU	L1	847	1	-	0/9/27/28	0/2/2/2
51	A2M	S1	2021	51	-	1/9/27/28	0/3/3/3
51	PSU	S1	33	51	-	1/7/25/26	0/2/2/2
51	OMG	S1	1647	51	-	0/9/27/28	0/3/3/3
2	A2M	L2	95	2	-	1/9/27/28	0/3/3/3
51	OMG	S1	2151	51	-	2/9/27/28	0/3/3/3
2	PSU	L2	1058	2	-	0/7/25/26	0/2/2/2
1	OMU	L1	1659	1,90	-	0/9/27/28	0/2/2/2
2	A2M	L2	572	2	-	0/9/27/28	0/3/3/3
2	OMC	L2	1248	2	-	1/9/27/28	0/2/2/2
7	PSU	L7	101	7	-	0/7/25/26	0/2/2/2
51	5MC	S1	1544	51	-	0/7/25/26	0/2/2/2

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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
7	OMG	L7	75	7	-	0/9/27/28	0/3/3/3
1	OMG	L1	1540	1,2	-	2/9/27/28	0/3/3/3
2	5MC	L2	1308	2	-	4/7/25/26	0/2/2/2
51	OMC	S1	1866	51	-	0/9/27/28	0/2/2/2
51	OMU	S1	661	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	1303	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	510	2	-	0/7/25/26	0/2/2/2
2	OMG	L2	1229	2	-	2/9/27/28	0/3/3/3
2	A2M	L2	1185	2	-	2/9/27/28	0/3/3/3

All (1118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1566	PSU	C6-C5	12.48	1.49	1.35
7	L7	166	PSU	C6-C5	12.42	1.49	1.35
2	L2	504	PSU	C6-C5	12.41	1.49	1.35
1	L1	1171	PSU	C6-C5	12.36	1.49	1.35
1	L1	313	PSU	C6-C5	12.36	1.49	1.35
51	S1	455	PSU	C6-C5	12.34	1.49	1.35
1	L1	1528	PSU	C6-C5	12.32	1.48	1.35
1	L1	1529	PSU	C6-C5	12.31	1.48	1.35
51	S1	33	PSU	C6-C5	12.30	1.48	1.35
1	L1	1177	PSU	C6-C5	12.29	1.48	1.35
2	L2	1265	PSU	C6-C5	12.28	1.48	1.35
2	L2	512	PSU	C6-C5	12.27	1.48	1.35
1	L1	1181	PSU	C6-C5	12.25	1.48	1.35
2	L2	1058	PSU	C6-C5	12.25	1.48	1.35
51	S1	1533	PSU	C6-C5	12.24	1.48	1.35
2	L2	1284	PSU	C6-C5	12.22	1.48	1.35
51	S1	2046	PSU	C6-C5	12.20	1.48	1.35
2	L2	1194	PSU	C6-C5	12.20	1.48	1.35
2	L2	1361	PSU	C6-C5	12.20	1.48	1.35
51	S1	1192	PSU	C6-C5	12.19	1.48	1.35
2	L2	1303	PSU	C6-C5	12.18	1.48	1.35
2	L2	802	PSU	C6-C5	12.18	1.48	1.35
1	L1	1017	PSU	C6-C5	12.16	1.48	1.35
2	L2	626	PSU	C6-C5	12.16	1.48	1.35
51	S1	1539	PSU	C6-C5	12.15	1.48	1.35
1	L1	422	PSU	C6-C5	12.15	1.48	1.35
2	L2	472	PSU	C6-C5	12.15	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	500	PSU	C6-C5	12.14	1.48	1.35
2	L2	1403	PSU	C6-C5	12.13	1.48	1.35
2	L2	1318	PSU	C6-C5	12.13	1.48	1.35
51	S1	1246	PSU	C6-C5	12.13	1.48	1.35
2	L2	510	PSU	C6-C5	12.13	1.48	1.35
1	L1	940	PSU	C6-C5	12.12	1.48	1.35
51	S1	1657	PSU	C6-C5	12.11	1.48	1.35
2	L2	1144	PSU	C6-C5	12.11	1.48	1.35
7	L7	69	PSU	C6-C5	12.10	1.48	1.35
2	L2	593	PSU	C6-C5	12.10	1.48	1.35
2	L2	1060	PSU	C6-C5	12.10	1.48	1.35
7	L7	74	PSU	C6-C5	12.09	1.48	1.35
2	L2	597	PSU	C6-C5	12.09	1.48	1.35
2	L2	1213	PSU	C6-C5	12.08	1.48	1.35
2	L2	1152	PSU	C6-C5	12.08	1.48	1.35
2	L2	78	PSU	C6-C5	12.08	1.48	1.35
2	L2	662	PSU	C6-C5	12.07	1.48	1.35
51	S1	1292	PSU	C6-C5	12.05	1.48	1.35
1	L1	1533	PSU	C6-C5	12.01	1.48	1.35
7	L7	101	PSU	C6-C5	11.99	1.48	1.35
51	S1	2202	PSU	C6-C5	11.97	1.48	1.35
1	L1	1526	PSU	C6-C5	11.96	1.48	1.35
2	L2	1264	PSU	C6-C5	11.95	1.48	1.35
2	L2	1413	PSU	C6-C5	11.79	1.48	1.35
51	S1	1543	B8N	C2'-C3'	-10.49	1.24	1.53
51	S1	33	PSU	C2-N1	10.20	1.50	1.36
51	S1	1246	PSU	C2-N1	10.20	1.50	1.36
51	S1	1539	PSU	C2-N1	10.15	1.49	1.36
51	S1	455	PSU	C2-N1	10.12	1.49	1.36
51	S1	1533	PSU	C2-N1	10.11	1.49	1.36
2	L2	1152	PSU	C2-N1	10.11	1.49	1.36
7	L7	74	PSU	C2-N1	10.09	1.49	1.36
1	L1	1526	PSU	C2-N1	10.07	1.49	1.36
2	L2	1303	PSU	C2-N1	10.06	1.49	1.36
2	L2	802	PSU	C2-N1	10.05	1.49	1.36
1	L1	1533	PSU	C2-N1	10.05	1.49	1.36
1	L1	422	PSU	C2-N1	10.05	1.49	1.36
1	L1	940	PSU	C2-N1	10.04	1.49	1.36
2	L2	500	PSU	C2-N1	10.04	1.49	1.36
51	S1	2046	PSU	C2-N1	10.03	1.49	1.36
2	L2	1403	PSU	C2-N1	10.02	1.49	1.36
2	L2	1284	PSU	C2-N1	10.00	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	512	PSU	C2-N1	10.00	1.49	1.36
1	L1	1181	PSU	C2-N1	9.99	1.49	1.36
2	L2	504	PSU	C2-N1	9.97	1.49	1.36
7	L7	166	PSU	C2-N1	9.96	1.49	1.36
2	L2	1318	PSU	C2-N1	9.94	1.49	1.36
2	L2	1060	PSU	C2-N1	9.94	1.49	1.36
1	L1	1017	PSU	C2-N1	9.93	1.49	1.36
2	L2	1213	PSU	C2-N1	9.93	1.49	1.36
2	L2	1361	PSU	C2-N1	9.93	1.49	1.36
2	L2	78	PSU	C2-N1	9.92	1.49	1.36
51	S1	1657	PSU	C2-N1	9.92	1.49	1.36
2	L2	472	PSU	C2-N1	9.92	1.49	1.36
2	L2	1144	PSU	C2-N1	9.92	1.49	1.36
2	L2	510	PSU	C2-N1	9.92	1.49	1.36
2	L2	1194	PSU	C2-N1	9.92	1.49	1.36
51	S1	1566	PSU	C2-N1	9.91	1.49	1.36
51	S1	2202	PSU	C2-N1	9.90	1.49	1.36
2	L2	626	PSU	C2-N1	9.89	1.49	1.36
1	L1	1177	PSU	C2-N1	9.88	1.49	1.36
7	L7	69	PSU	C2-N1	9.87	1.49	1.36
2	L2	1058	PSU	C2-N1	9.86	1.49	1.36
2	L2	597	PSU	C2-N1	9.85	1.49	1.36
2	L2	593	PSU	C2-N1	9.84	1.49	1.36
1	L1	1529	PSU	C2-N1	9.84	1.49	1.36
1	L1	1528	PSU	C2-N1	9.84	1.49	1.36
51	S1	1292	PSU	C2-N1	9.82	1.49	1.36
51	S1	1192	PSU	C2-N1	9.79	1.49	1.36
2	L2	662	PSU	C2-N1	9.78	1.49	1.36
2	L2	1264	PSU	C2-N1	9.75	1.49	1.36
2	L2	1413	PSU	C2-N1	9.74	1.49	1.36
2	L2	1265	PSU	C2-N1	9.72	1.49	1.36
7	L7	101	PSU	C2-N1	9.70	1.49	1.36
51	S1	1995	7MG	C8-N9	9.69	1.52	1.45
1	L1	1171	PSU	C2-N1	9.63	1.49	1.36
1	L1	313	PSU	C2-N1	9.63	1.49	1.36
1	L1	1539	A2M	C2'-C1'	-9.32	1.30	1.53
1	L1	1373	A2M	C2'-C1'	-9.32	1.30	1.53
2	L2	1308	5MC	C6-C5	9.23	1.49	1.34
7	L7	43	A2M	C2'-C1'	-9.22	1.30	1.53
7	L7	162	A2M	C2'-C1'	-9.22	1.30	1.53
1	L1	305	A2M	C2'-C1'	-9.22	1.30	1.53
1	L1	927	A2M	C2'-C1'	-9.20	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	604	A2M	C2'-C1'	-9.18	1.30	1.53
2	L2	665	A2M	C2'-C1'	-9.18	1.30	1.53
51	S1	897	A2M	C2'-C1'	-9.18	1.30	1.53
2	L2	382	A2M	C2'-C1'	-9.15	1.30	1.53
51	S1	28	A2M	C2'-C1'	-9.14	1.30	1.53
2	L2	1372	A2M	C2'-C1'	-9.14	1.30	1.53
51	S1	98	A2M	C2'-C1'	-9.13	1.30	1.53
2	L2	572	A2M	C2'-C1'	-9.12	1.30	1.53
2	L2	502	A2M	C2'-C1'	-9.10	1.30	1.53
2	L2	591	A2M	C2'-C1'	-9.10	1.30	1.53
2	L2	95	A2M	C2'-C1'	-9.08	1.30	1.53
1	L1	407	A2M	C2'-C1'	-9.07	1.30	1.53
2	L2	527	A2M	C2'-C1'	-9.06	1.30	1.53
2	L2	1384	A2M	C2'-C1'	-9.03	1.30	1.53
1	L1	697	A2M	C2'-C1'	-9.02	1.30	1.53
51	S1	512	A2M	C2'-C1'	-9.01	1.30	1.53
51	S1	479	A2M	C2'-C1'	-8.94	1.31	1.53
2	L2	570	A2M	C2'-C1'	-8.94	1.31	1.53
51	S1	2061	5MC	C6-C5	8.93	1.49	1.34
51	S1	512	A2M	O4'-C1'	8.92	1.62	1.42
1	L1	69	A2M	C2'-C1'	-8.92	1.31	1.53
51	S1	28	A2M	O4'-C1'	8.90	1.62	1.42
52	S2	37	MIA	C2-S10	8.90	1.83	1.75
1	L1	235	A2M	C2'-C1'	-8.89	1.31	1.53
2	L2	572	A2M	O4'-C1'	8.88	1.62	1.42
2	L2	604	A2M	O4'-C1'	8.86	1.62	1.42
1	L1	407	A2M	O4'-C1'	8.86	1.62	1.42
1	L1	858	A2M	C2'-C1'	-8.86	1.31	1.53
2	L2	382	A2M	O4'-C1'	8.85	1.62	1.42
7	L7	162	A2M	O4'-C1'	8.85	1.62	1.42
7	L7	43	A2M	O4'-C1'	8.85	1.62	1.42
51	S1	897	A2M	O4'-C1'	8.85	1.62	1.42
2	L2	591	A2M	O4'-C1'	8.84	1.62	1.42
51	S1	98	A2M	O4'-C1'	8.83	1.62	1.42
2	L2	1372	A2M	O4'-C1'	8.82	1.62	1.42
51	S1	668	A2M	C2'-C1'	-8.82	1.31	1.53
51	S1	479	A2M	O4'-C1'	8.81	1.62	1.42
2	L2	1185	A2M	C2'-C1'	-8.79	1.31	1.53
2	L2	95	A2M	O4'-C1'	8.78	1.62	1.42
1	L1	697	A2M	O4'-C1'	8.78	1.62	1.42
2	L2	570	A2M	O4'-C1'	8.78	1.62	1.42
2	L2	1384	A2M	O4'-C1'	8.77	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1308	5MC	C3'-C4'	-8.76	1.30	1.53
1	L1	235	A2M	O4'-C1'	8.76	1.62	1.42
2	L2	502	A2M	O4'-C1'	8.75	1.62	1.42
1	L1	1373	A2M	O4'-C1'	8.74	1.62	1.42
2	L2	665	A2M	O4'-C1'	8.74	1.62	1.42
1	L1	927	A2M	O4'-C1'	8.73	1.62	1.42
1	L1	1539	A2M	O4'-C1'	8.72	1.62	1.42
2	L2	647	A2M	C2'-C1'	-8.71	1.31	1.53
1	L1	858	A2M	O4'-C1'	8.70	1.62	1.42
1	L1	305	A2M	O4'-C1'	8.60	1.61	1.42
2	L2	1185	A2M	O4'-C1'	8.58	1.61	1.42
1	L1	69	A2M	O4'-C1'	8.55	1.61	1.42
2	L2	647	A2M	O4'-C1'	8.54	1.61	1.42
51	S1	1995	7MG	C5-N7	8.46	1.46	1.35
51	S1	668	A2M	O4'-C1'	8.39	1.61	1.42
2	L2	527	A2M	O4'-C1'	8.28	1.61	1.42
51	S1	1543	B8N	C4-N3	-8.09	1.26	1.40
2	L2	1284	PSU	C2-N3	8.00	1.50	1.37
51	S1	455	PSU	C2-N3	8.00	1.50	1.37
2	L2	504	PSU	C2-N3	7.97	1.50	1.37
52	S2	37	MIA	C6-N6	7.97	1.46	1.34
2	L2	1361	PSU	C2-N3	7.96	1.50	1.37
51	S1	1566	PSU	C2-N3	7.92	1.50	1.37
51	S1	33	PSU	C2-N3	7.90	1.50	1.37
2	L2	512	PSU	C2-N3	7.88	1.50	1.37
51	S1	1192	PSU	C2-N3	7.87	1.50	1.37
51	S1	1246	PSU	C2-N3	7.86	1.50	1.37
2	L2	1265	PSU	C2-N3	7.86	1.50	1.37
1	L1	1533	PSU	C2-N3	7.85	1.50	1.37
2	L2	802	PSU	C2-N3	7.84	1.50	1.37
7	L7	74	PSU	C2-N3	7.84	1.50	1.37
1	L1	1171	PSU	C2-N3	7.82	1.50	1.37
51	S1	1657	PSU	C2-N3	7.82	1.50	1.37
7	L7	166	PSU	C2-N3	7.81	1.50	1.37
2	L2	1303	PSU	C2-N3	7.81	1.50	1.37
2	L2	500	PSU	C2-N3	7.81	1.50	1.37
51	S1	1533	PSU	C2-N3	7.80	1.50	1.37
2	L2	510	PSU	C2-N3	7.80	1.50	1.37
51	S1	2046	PSU	C2-N3	7.80	1.50	1.37
51	S1	2202	PSU	C2-N3	7.79	1.50	1.37
1	L1	1528	PSU	C2-N3	7.79	1.50	1.37
2	L2	1152	PSU	C2-N3	7.79	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	472	PSU	C2-N3	7.78	1.50	1.37
2	L2	1213	PSU	C2-N3	7.77	1.50	1.37
2	L2	1403	PSU	C2-N3	7.77	1.50	1.37
1	L1	1181	PSU	C2-N3	7.77	1.50	1.37
51	S1	1539	PSU	C2-N3	7.76	1.50	1.37
1	L1	1371	OMU	C2-N1	7.75	1.50	1.38
2	L2	1264	PSU	C2-N3	7.75	1.50	1.37
1	L1	1526	PSU	C2-N3	7.75	1.50	1.37
51	S1	1292	PSU	C2-N3	7.74	1.50	1.37
7	L7	69	PSU	C2-N3	7.74	1.50	1.37
1	L1	313	PSU	C2-N3	7.74	1.50	1.37
1	L1	422	PSU	C2-N3	7.73	1.50	1.37
2	L2	1194	PSU	C2-N3	7.73	1.50	1.37
1	L1	1177	PSU	C2-N3	7.72	1.50	1.37
1	L1	940	PSU	C2-N3	7.72	1.50	1.37
2	L2	1318	PSU	C2-N3	7.71	1.50	1.37
51	S1	1543	B8N	C6-N1	7.70	1.55	1.36
2	L2	1413	PSU	C2-N3	7.69	1.50	1.37
2	L2	1058	PSU	C2-N3	7.69	1.50	1.37
7	L7	101	PSU	C2-N3	7.68	1.50	1.37
2	L2	597	PSU	C2-N3	7.67	1.50	1.37
2	L2	1060	PSU	C2-N3	7.67	1.50	1.37
1	L1	1529	PSU	C2-N3	7.66	1.50	1.37
2	L2	626	PSU	C2-N3	7.66	1.50	1.37
1	L1	1017	PSU	C2-N3	7.65	1.50	1.37
2	L2	78	PSU	C2-N3	7.64	1.50	1.37
2	L2	1144	PSU	C2-N3	7.63	1.50	1.37
2	L2	662	PSU	C2-N3	7.57	1.49	1.37
2	L2	593	PSU	C2-N3	7.56	1.49	1.37
2	L2	1308	5MC	O4'-C4'	7.34	1.61	1.45
51	S1	1979	OMU	C2-N1	7.20	1.49	1.38
2	L2	1077	OMU	C2-N1	7.19	1.49	1.38
2	L2	56	OMU	C2-N1	7.19	1.49	1.38
2	L2	73	OMU	C2-N1	7.18	1.49	1.38
51	S1	29	OMU	C2-N1	7.16	1.49	1.38
1	L1	1107	OMU	C2-N1	7.14	1.49	1.38
51	S1	1833	OMU	C2-N1	7.12	1.49	1.38
51	S1	1662	OMU	C2-N1	7.08	1.49	1.38
51	S1	1543	B8N	C4-C5	7.08	1.63	1.47
2	L2	667	OMU	C2-N1	7.08	1.49	1.38
51	S1	1621	OMU	C2-N1	7.08	1.49	1.38
2	L2	1359	OMU	C2-N1	7.07	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1979	OMU	C2-N3	7.07	1.50	1.38
3	L3	13	OMU	C2-N1	7.07	1.49	1.38
2	L2	1419	OMU	C2-N1	7.05	1.49	1.38
1	L1	1659	OMU	C2-N1	7.04	1.49	1.38
51	S1	29	OMU	C2-N3	7.02	1.50	1.38
51	S1	1662	OMU	C2-N3	7.02	1.50	1.38
51	S1	1621	OMU	C2-N3	7.01	1.50	1.38
51	S1	1833	OMU	C2-N3	7.00	1.50	1.38
51	S1	661	OMU	C2-N1	6.98	1.49	1.38
51	S1	1995	7MG	C4-N9	6.98	1.46	1.37
2	L2	73	OMU	C2-N3	6.94	1.50	1.38
3	L3	13	OMU	C2-N3	6.93	1.50	1.38
2	L2	56	OMU	C2-N3	6.91	1.50	1.38
1	L1	1107	OMU	C2-N3	6.90	1.50	1.38
2	L2	1077	OMU	C2-N3	6.90	1.50	1.38
1	L1	1371	OMU	C2-N3	6.89	1.50	1.38
2	L2	1359	OMU	C2-N3	6.84	1.49	1.38
2	L2	1419	OMU	C2-N3	6.84	1.49	1.38
51	S1	661	OMU	C2-N3	6.82	1.49	1.38
2	L2	667	OMU	C2-N3	6.79	1.49	1.38
1	L1	1659	OMU	C2-N3	6.79	1.49	1.38
51	S1	668	A2M	O4'-C4'	-6.77	1.29	1.45
51	S1	2061	5MC	C4-N3	6.75	1.44	1.34
1	L1	858	A2M	O4'-C4'	-6.63	1.30	1.45
51	S1	1865	OMG	C4-N3	6.60	1.49	1.34
2	L2	647	A2M	O4'-C4'	-6.60	1.30	1.45
2	L2	71	OMG	C4-N3	6.58	1.49	1.34
2	L2	1185	A2M	O4'-C4'	-6.58	1.30	1.45
51	S1	1647	OMG	C4-N3	6.56	1.49	1.34
2	L2	1384	A2M	O4'-C4'	-6.55	1.30	1.45
1	L1	69	A2M	O4'-C4'	-6.54	1.30	1.45
1	L1	1539	A2M	O4'-C4'	-6.54	1.30	1.45
2	L2	1046	OMG	C4-N3	6.54	1.49	1.34
1	L1	927	A2M	O4'-C4'	-6.51	1.30	1.45
2	L2	1360	OMG	C4-N3	6.51	1.49	1.34
1	L1	235	A2M	O4'-C4'	-6.50	1.30	1.45
1	L1	856	OMG	C4-N3	6.50	1.49	1.34
7	L7	75	OMG	C4-N3	6.49	1.49	1.34
2	L2	95	A2M	O4'-C4'	-6.49	1.30	1.45
2	L2	527	A2M	O4'-C4'	-6.48	1.30	1.45
2	L2	655	OMG	C4-N3	6.47	1.49	1.34
51	S1	1623	OMG	C4-N3	6.47	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	359	OMC	C2-N3	6.47	1.49	1.36
51	S1	2140	OMC	C2-N3	6.47	1.49	1.36
51	S1	600	OMG	C4-N3	6.47	1.49	1.34
2	L2	534	OMG	C4-N3	6.46	1.49	1.34
1	L1	1524	OMG	C4-N3	6.46	1.49	1.34
2	L2	686	OMG	C4-N3	6.46	1.49	1.34
2	L2	1229	OMG	C4-N3	6.45	1.49	1.34
51	S1	38	OMC	C2-N3	6.45	1.49	1.36
2	L2	665	A2M	O4'-C4'	-6.44	1.30	1.45
51	S1	2151	OMG	C4-N3	6.44	1.49	1.34
51	S1	479	A2M	O4'-C4'	-6.43	1.30	1.45
51	S1	1543	B8N	O4'-C4'	-6.42	1.30	1.45
2	L2	1248	OMC	C2-N3	6.42	1.49	1.36
7	L7	162	A2M	O4'-C4'	-6.41	1.30	1.45
2	L2	591	A2M	O4'-C4'	-6.41	1.30	1.45
2	L2	1372	A2M	O4'-C4'	-6.41	1.30	1.45
2	L2	382	A2M	O4'-C4'	-6.41	1.30	1.45
1	L1	1373	A2M	O4'-C4'	-6.40	1.30	1.45
7	L7	43	A2M	O4'-C4'	-6.39	1.30	1.45
1	L1	305	A2M	O4'-C4'	-6.39	1.30	1.45
2	L2	570	A2M	O4'-C4'	-6.39	1.30	1.45
51	S1	1866	OMC	C2-N3	6.39	1.49	1.36
1	L1	697	A2M	O4'-C4'	-6.38	1.30	1.45
2	L2	604	A2M	O4'-C4'	-6.36	1.30	1.45
51	S1	2059	OMC	C2-N3	6.36	1.49	1.36
2	L2	1231	OMG	C4-N3	6.36	1.48	1.34
51	S1	897	A2M	O4'-C4'	-6.36	1.30	1.45
51	S1	98	A2M	O4'-C4'	-6.35	1.30	1.45
51	S1	28	A2M	O4'-C4'	-6.35	1.30	1.45
51	S1	18	OMC	C2-N3	6.32	1.48	1.36
1	L1	695	OMC	C2-N3	6.31	1.48	1.36
51	S1	1478	OMG	C4-N3	6.30	1.48	1.34
2	L2	1308	5MC	C4-N3	6.29	1.44	1.34
1	L1	1527	OMC	C2-N3	6.29	1.48	1.36
1	L1	407	A2M	O4'-C4'	-6.28	1.31	1.45
2	L2	572	A2M	O4'-C4'	-6.27	1.31	1.45
2	L2	583	OMC	C2-N3	6.26	1.48	1.36
2	L2	1397	OMC	C2-N3	6.26	1.48	1.36
2	L2	641	OMG	C4-N3	6.25	1.48	1.34
2	L2	502	A2M	O4'-C4'	-6.24	1.31	1.45
1	L1	1190	OMG	C4-N3	6.23	1.48	1.34
2	L2	1253	OMG	C4-N3	6.22	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1317	OMC	C2-N3	6.22	1.48	1.36
51	S1	512	A2M	O4'-C4'	-6.20	1.31	1.45
51	S1	1995	7MG	C2-N3	6.19	1.48	1.33
51	S1	2061	5MC	C5-C4	6.18	1.48	1.44
2	L2	1078	OMG	C4-N3	6.16	1.48	1.34
51	S1	2061	5MC	C2-N3	6.05	1.48	1.36
2	L2	1248	OMC	C6-C5	6.00	1.49	1.35
51	S1	2140	OMC	C6-C5	6.00	1.49	1.35
51	S1	38	OMC	C6-C5	6.00	1.49	1.35
2	L2	359	OMC	C6-C5	5.94	1.48	1.35
1	L1	1527	OMC	C6-C5	5.93	1.48	1.35
51	S1	1866	OMC	C6-C5	5.92	1.48	1.35
2	L2	1317	OMC	C6-C5	5.92	1.48	1.35
2	L2	1308	5MC	C2-N3	5.92	1.48	1.36
2	L2	1397	OMC	C6-C5	5.90	1.48	1.35
2	L2	583	OMC	C6-C5	5.89	1.48	1.35
51	S1	2059	OMC	C6-C5	5.88	1.48	1.35
51	S1	18	OMC	C6-C5	5.84	1.48	1.35
1	L1	695	OMC	C6-C5	5.83	1.48	1.35
51	S1	29	OMU	C6-C5	5.75	1.48	1.35
51	S1	1979	OMU	C6-C5	5.71	1.48	1.35
1	L1	1107	OMU	C6-C5	5.68	1.48	1.35
51	S1	1621	OMU	C6-C5	5.68	1.48	1.35
2	L2	1308	5MC	C5-C4	5.66	1.48	1.44
51	S1	1662	OMU	C6-C5	5.65	1.48	1.35
1	L1	1371	OMU	C6-C5	5.64	1.48	1.35
2	L2	73	OMU	C6-C5	5.63	1.48	1.35
51	S1	661	OMU	C6-C5	5.63	1.48	1.35
2	L2	667	OMU	C6-C5	5.62	1.48	1.35
51	S1	1995	7MG	C4-N3	5.62	1.47	1.34
3	L3	13	OMU	C6-C5	5.61	1.48	1.35
2	L2	56	OMU	C6-C5	5.60	1.48	1.35
2	L2	1077	OMU	C6-C5	5.59	1.48	1.35
2	L2	1359	OMU	C6-C5	5.59	1.48	1.35
51	S1	1833	OMU	C6-C5	5.59	1.48	1.35
1	L1	1659	OMU	C6-C5	5.55	1.47	1.35
2	L2	1419	OMU	C6-C5	5.54	1.47	1.35
7	L7	74	PSU	C6-N1	5.44	1.45	1.36
2	L2	802	PSU	C6-N1	5.40	1.45	1.36
51	S1	1533	PSU	C6-N1	5.39	1.45	1.36
51	S1	33	PSU	C6-N1	5.38	1.45	1.36
2	L2	500	PSU	C6-N1	5.37	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1657	PSU	C6-N1	5.37	1.45	1.36
51	S1	1539	PSU	C6-N1	5.36	1.45	1.36
51	S1	455	PSU	C6-N1	5.35	1.45	1.36
51	S1	1543	B8N	C2-N1	5.35	1.54	1.39
2	L2	1403	PSU	C6-N1	5.35	1.45	1.36
51	S1	1865	OMG	C2-N3	5.33	1.46	1.33
1	L1	422	PSU	C6-N1	5.33	1.45	1.36
2	L2	597	PSU	C6-N1	5.32	1.45	1.36
2	L2	1194	PSU	C6-N1	5.32	1.45	1.36
2	L2	472	PSU	C6-N1	5.32	1.45	1.36
2	L2	626	PSU	C6-N1	5.32	1.45	1.36
51	S1	1566	PSU	C6-N1	5.31	1.45	1.36
51	S1	1192	PSU	C6-N1	5.31	1.45	1.36
2	L2	512	PSU	C6-N1	5.30	1.45	1.36
1	L1	1526	PSU	C6-N1	5.30	1.45	1.36
2	L2	1284	PSU	C6-N1	5.30	1.45	1.36
2	L2	1303	PSU	C6-N1	5.30	1.45	1.36
51	S1	2140	OMC	C4-N3	5.30	1.45	1.34
2	L2	1152	PSU	C6-N1	5.29	1.45	1.36
51	S1	1246	PSU	C6-N1	5.29	1.45	1.36
2	L2	510	PSU	C6-N1	5.28	1.44	1.36
1	L1	1524	OMG	C2-N3	5.27	1.46	1.33
51	S1	1623	OMG	C2-N3	5.27	1.46	1.33
7	L7	69	PSU	C6-N1	5.27	1.44	1.36
7	L7	166	PSU	C6-N1	5.27	1.44	1.36
2	L2	504	PSU	C6-N1	5.26	1.44	1.36
2	L2	359	OMC	C4-N3	5.25	1.44	1.34
51	S1	2046	PSU	C6-N1	5.25	1.44	1.36
2	L2	1361	PSU	C6-N1	5.25	1.44	1.36
2	L2	1058	PSU	C6-N1	5.25	1.44	1.36
51	S1	38	OMC	C4-N3	5.25	1.44	1.34
1	L1	1528	PSU	C6-N1	5.25	1.44	1.36
2	L2	78	PSU	C6-N1	5.24	1.44	1.36
1	L1	940	PSU	C6-N1	5.24	1.44	1.36
2	L2	71	OMG	C2-N3	5.24	1.45	1.33
2	L2	686	OMG	C2-N3	5.23	1.45	1.33
2	L2	662	PSU	C6-N1	5.23	1.44	1.36
2	L2	1144	PSU	C6-N1	5.23	1.44	1.36
1	L1	1181	PSU	C6-N1	5.23	1.44	1.36
51	S1	2202	PSU	C6-N1	5.23	1.44	1.36
51	S1	1647	OMG	C2-N3	5.23	1.45	1.33
2	L2	1360	OMG	C2-N3	5.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1177	PSU	C6-N1	5.22	1.44	1.36
51	S1	1292	PSU	C6-N1	5.21	1.44	1.36
51	S1	1543	B8N	C3'-C4'	5.21	1.66	1.53
2	L2	593	PSU	C6-N1	5.19	1.44	1.36
2	L2	1318	PSU	C6-N1	5.19	1.44	1.36
7	L7	75	OMG	C2-N3	5.18	1.45	1.33
1	L1	1527	OMC	C4-N3	5.18	1.44	1.34
2	L2	1213	PSU	C6-N1	5.18	1.44	1.36
51	S1	600	OMG	C2-N3	5.18	1.45	1.33
1	L1	1533	PSU	C6-N1	5.17	1.44	1.36
2	L2	583	OMC	C4-N3	5.16	1.44	1.34
2	L2	1046	OMG	C2-N3	5.16	1.45	1.33
2	L2	655	OMG	C2-N3	5.16	1.45	1.33
2	L2	1264	PSU	C6-N1	5.15	1.44	1.36
51	S1	1866	OMC	C4-N3	5.15	1.44	1.34
7	L7	101	PSU	C6-N1	5.14	1.44	1.36
2	L2	534	OMG	C2-N3	5.13	1.45	1.33
2	L2	1265	PSU	C6-N1	5.12	1.44	1.36
2	L2	1231	OMG	C2-N3	5.12	1.45	1.33
2	L2	1060	PSU	C6-N1	5.11	1.44	1.36
1	L1	856	OMG	C2-N3	5.10	1.45	1.33
1	L1	313	PSU	C6-N1	5.10	1.44	1.36
1	L1	1171	PSU	C6-N1	5.09	1.44	1.36
2	L2	1229	OMG	C2-N3	5.09	1.45	1.33
1	L1	1017	PSU	C6-N1	5.08	1.44	1.36
51	S1	18	OMC	C4-N3	5.08	1.44	1.34
1	L1	1529	PSU	C6-N1	5.08	1.44	1.36
2	L2	1413	PSU	C6-N1	5.07	1.44	1.36
51	S1	2151	OMG	C2-N3	5.05	1.45	1.33
1	L1	695	OMC	C4-N3	5.04	1.44	1.34
2	L2	1397	OMC	C4-N3	5.04	1.44	1.34
2	L2	1248	OMC	C4-N3	5.03	1.44	1.34
2	L2	1308	5MC	O4'-C1'	-5.00	1.30	1.42
51	S1	2059	OMC	C4-N3	4.99	1.44	1.34
2	L2	1317	OMC	C4-N3	4.98	1.44	1.34
2	L2	1253	OMG	C2-N3	4.98	1.45	1.33
51	S1	1478	OMG	C2-N3	4.98	1.45	1.33
2	L2	641	OMG	C2-N3	4.92	1.45	1.33
51	S1	2059	OMC	C2-N1	4.92	1.50	1.40
2	L2	1078	OMG	C2-N3	4.80	1.44	1.33
51	S1	1865	OMG	C2-N2	4.79	1.45	1.34
1	L1	1190	OMG	C2-N3	4.78	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	71	OMG	C2-N2	4.77	1.45	1.34
51	S1	1647	OMG	C2-N2	4.75	1.45	1.34
51	S1	1543	B8N	C1'-C5	-4.74	1.39	1.50
2	L2	686	OMG	C2-N2	4.73	1.45	1.34
7	L7	75	OMG	C2-N2	4.73	1.45	1.34
2	L2	1229	OMG	C2-N2	4.72	1.45	1.34
2	L2	1360	OMG	C2-N2	4.72	1.45	1.34
2	L2	655	OMG	C2-N2	4.72	1.45	1.34
51	S1	1623	OMG	C2-N2	4.72	1.45	1.34
51	S1	600	OMG	C2-N2	4.70	1.45	1.34
51	S1	38	OMC	C4-N4	4.70	1.45	1.33
2	L2	359	OMC	C4-N4	4.70	1.45	1.33
2	L2	1046	OMG	C2-N2	4.69	1.45	1.34
51	S1	2059	OMC	C4-N4	4.68	1.45	1.33
51	S1	2151	OMG	C2-N2	4.68	1.45	1.34
51	S1	2140	OMC	C4-N4	4.68	1.45	1.33
2	L2	1060	PSU	C1'-C5	-4.67	1.39	1.50
51	S1	2140	OMC	C2-N1	4.67	1.49	1.40
1	L1	1527	OMC	C4-N4	4.67	1.45	1.33
1	L1	1524	OMG	C2-N2	4.67	1.45	1.34
51	S1	1866	OMC	C4-N4	4.67	1.45	1.33
2	L2	1231	OMG	C2-N2	4.66	1.45	1.34
51	S1	18	OMC	C4-N4	4.66	1.45	1.33
2	L2	534	OMG	C2-N2	4.66	1.45	1.34
2	L2	1397	OMC	C4-N4	4.64	1.45	1.33
51	S1	1478	OMG	C2-N2	4.64	1.45	1.34
2	L2	1058	PSU	C1'-C5	-4.64	1.39	1.50
2	L2	1248	OMC	C4-N4	4.64	1.45	1.33
2	L2	641	OMG	C2-N2	4.62	1.45	1.34
1	L1	1190	OMG	C2-N2	4.61	1.45	1.34
51	S1	38	OMC	C2-N1	4.59	1.49	1.40
1	L1	856	OMG	C2-N2	4.59	1.44	1.34
2	L2	1078	OMG	C2-N2	4.58	1.44	1.34
1	L1	695	OMC	C4-N4	4.58	1.45	1.33
7	L7	74	PSU	C1'-C5	-4.57	1.39	1.50
2	L2	583	OMC	C4-N4	4.57	1.45	1.33
2	L2	1308	5MC	C6-N1	4.57	1.45	1.38
2	L2	1248	OMC	C2-N1	4.56	1.49	1.40
2	L2	1317	OMC	C4-N4	4.54	1.44	1.33
2	L2	1413	PSU	C1'-C5	-4.53	1.40	1.50
1	L1	1526	PSU	C1'-C5	-4.53	1.40	1.50
1	L1	1017	PSU	C1'-C5	-4.51	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	2061	5MC	C6-N1	4.50	1.45	1.38
2	L2	1144	PSU	C1'-C5	-4.50	1.40	1.50
2	L2	1253	OMG	C2-N2	4.49	1.44	1.34
2	L2	1213	PSU	C1'-C5	-4.48	1.40	1.50
1	L1	940	PSU	C1'-C5	-4.48	1.40	1.50
51	S1	1539	PSU	C1'-C5	-4.48	1.40	1.50
2	L2	78	PSU	C1'-C5	-4.47	1.40	1.50
51	S1	1543	B8N	O4'-C1'	4.46	1.50	1.43
2	L2	802	PSU	C1'-C5	-4.46	1.40	1.50
1	L1	1181	PSU	C1'-C5	-4.46	1.40	1.50
7	L7	101	PSU	C1'-C5	-4.46	1.40	1.50
2	L2	597	PSU	C1'-C5	-4.45	1.40	1.50
2	L2	510	PSU	C1'-C5	-4.45	1.40	1.50
2	L2	1317	OMC	C2-N1	4.44	1.49	1.40
51	S1	1866	OMC	C2-N1	4.44	1.49	1.40
1	L1	1533	PSU	C1'-C5	-4.44	1.40	1.50
1	L1	422	PSU	C1'-C5	-4.43	1.40	1.50
1	L1	1529	PSU	C1'-C5	-4.43	1.40	1.50
2	L2	472	PSU	C1'-C5	-4.43	1.40	1.50
51	S1	18	OMC	C2-N1	4.43	1.49	1.40
51	S1	2061	5MC	C4-N4	4.43	1.45	1.34
51	S1	512	A2M	C6-N6	4.42	1.45	1.34
51	S1	479	A2M	C6-N6	4.41	1.45	1.34
1	L1	1177	PSU	C1'-C5	-4.41	1.40	1.50
2	L2	1403	PSU	C1'-C5	-4.41	1.40	1.50
51	S1	1292	PSU	C1'-C5	-4.41	1.40	1.50
1	L1	1527	OMC	C2-N1	4.41	1.49	1.40
2	L2	359	OMC	C2-N1	4.40	1.49	1.40
51	S1	1246	PSU	C1'-C5	-4.40	1.40	1.50
51	S1	1533	PSU	C1'-C5	-4.40	1.40	1.50
51	S1	2046	PSU	C1'-C5	-4.39	1.40	1.50
2	L2	1152	PSU	C1'-C5	-4.39	1.40	1.50
2	L2	1361	PSU	C1'-C5	-4.39	1.40	1.50
2	L2	500	PSU	C1'-C5	-4.39	1.40	1.50
2	L2	502	A2M	C6-N6	4.39	1.45	1.34
51	S1	1657	PSU	C1'-C5	-4.39	1.40	1.50
2	L2	662	PSU	C1'-C5	-4.38	1.40	1.50
2	L2	593	PSU	C1'-C5	-4.38	1.40	1.50
2	L2	95	A2M	C6-N6	4.37	1.45	1.34
2	L2	504	PSU	C1'-C5	-4.37	1.40	1.50
2	L2	1194	PSU	C1'-C5	-4.37	1.40	1.50
1	L1	858	A2M	C6-N6	4.37	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	28	A2M	C6-N6	4.36	1.45	1.34
51	S1	897	A2M	C6-N6	4.36	1.45	1.34
2	L2	1303	PSU	C1'-C5	-4.36	1.40	1.50
2	L2	1284	PSU	C1'-C5	-4.36	1.40	1.50
51	S1	1662	OMU	C4-N3	4.35	1.46	1.38
51	S1	1543	B8N	C6-C5	4.35	1.41	1.35
1	L1	69	A2M	C6-N6	4.35	1.45	1.34
2	L2	1372	A2M	C6-N6	4.35	1.45	1.34
51	S1	33	PSU	C1'-C5	-4.34	1.40	1.50
2	L2	1397	OMC	C2-N1	4.34	1.49	1.40
7	L7	162	A2M	C6-N6	4.34	1.45	1.34
51	S1	29	OMU	C4-N3	4.34	1.46	1.38
7	L7	69	PSU	C1'-C5	-4.34	1.40	1.50
2	L2	1185	A2M	C6-N6	4.34	1.45	1.34
7	L7	166	PSU	C1'-C5	-4.34	1.40	1.50
51	S1	1192	PSU	C1'-C5	-4.34	1.40	1.50
2	L2	512	PSU	C1'-C5	-4.34	1.40	1.50
2	L2	1318	PSU	C1'-C5	-4.33	1.40	1.50
51	S1	1621	OMU	C4-N3	4.33	1.46	1.38
2	L2	1308	5MC	C4-N4	4.33	1.45	1.34
1	L1	305	A2M	C6-N6	4.31	1.45	1.34
1	L1	927	A2M	C6-N6	4.31	1.45	1.34
2	L2	570	A2M	C6-N6	4.31	1.45	1.34
2	L2	1384	A2M	C6-N6	4.31	1.45	1.34
2	L2	572	A2M	C6-N6	4.31	1.45	1.34
2	L2	647	A2M	C6-N6	4.31	1.45	1.34
51	S1	668	A2M	C6-N6	4.30	1.45	1.34
1	L1	235	A2M	C6-N6	4.30	1.45	1.34
2	L2	626	PSU	C1'-C5	-4.30	1.40	1.50
2	L2	583	OMC	C2-N1	4.30	1.49	1.40
7	L7	43	A2M	C6-N6	4.29	1.45	1.34
2	L2	591	A2M	C6-N6	4.29	1.45	1.34
2	L2	665	A2M	C6-N6	4.29	1.45	1.34
2	L2	382	A2M	C6-N6	4.29	1.45	1.34
51	S1	98	A2M	C6-N6	4.29	1.45	1.34
2	L2	604	A2M	C6-N6	4.28	1.45	1.34
1	L1	695	OMC	C2-N1	4.28	1.49	1.40
51	S1	1833	OMU	C4-N3	4.28	1.45	1.38
1	L1	1528	PSU	C1'-C5	-4.27	1.40	1.50
1	L1	697	A2M	C6-N6	4.27	1.45	1.34
1	L1	407	A2M	C6-N6	4.25	1.45	1.34
51	S1	1543	B8N	C2'-C1'	4.24	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	661	OMU	C4-N3	4.23	1.45	1.38
1	L1	1539	A2M	C6-N6	4.23	1.45	1.34
3	L3	13	OMU	C4-N3	4.23	1.45	1.38
51	S1	455	PSU	C1'-C5	-4.23	1.40	1.50
51	S1	2202	PSU	C1'-C5	-4.23	1.40	1.50
2	L2	1077	OMU	C4-N3	4.22	1.45	1.38
51	S1	1566	PSU	C1'-C5	-4.22	1.40	1.50
1	L1	1373	A2M	C6-N6	4.21	1.45	1.34
2	L2	527	A2M	C6-N6	4.21	1.45	1.34
51	S1	1979	OMU	C4-N3	4.21	1.45	1.38
2	L2	73	OMU	C4-N3	4.21	1.45	1.38
2	L2	56	OMU	C4-N3	4.20	1.45	1.38
2	L2	1419	OMU	C4-N3	4.20	1.45	1.38
1	L1	1659	OMU	C4-N3	4.13	1.45	1.38
1	L1	313	PSU	C1'-C5	-4.12	1.41	1.50
2	L2	1359	OMU	C4-N3	4.12	1.45	1.38
2	L2	1265	PSU	C1'-C5	-4.08	1.41	1.50
1	L1	1107	OMU	C4-N3	4.08	1.45	1.38
2	L2	667	OMU	C4-N3	4.07	1.45	1.38
1	L1	1171	PSU	C1'-C5	-4.07	1.41	1.50
51	S1	2061	5MC	C2-N1	4.06	1.48	1.40
2	L2	1308	5MC	C2-N1	3.98	1.48	1.40
2	L2	504	PSU	C4-N3	3.97	1.46	1.38
1	L1	1371	OMU	C4-N3	3.97	1.45	1.38
51	S1	1566	PSU	C4-N3	3.96	1.46	1.38
2	L2	1264	PSU	C1'-C5	-3.92	1.41	1.50
2	L2	1284	PSU	C4-N3	3.91	1.46	1.38
51	S1	455	PSU	C4-N3	3.90	1.46	1.38
51	S1	1246	PSU	C4-N3	3.89	1.46	1.38
51	S1	2202	PSU	C4-N3	3.88	1.46	1.38
51	S1	33	PSU	C4-N3	3.88	1.46	1.38
51	S1	2185	MA6	C6-N6	3.88	1.47	1.36
51	S1	1192	PSU	C4-N3	3.87	1.46	1.38
51	S1	2184	MA6	C6-N6	3.85	1.47	1.36
1	L1	1181	PSU	C4-N3	3.84	1.46	1.38
2	L2	1264	PSU	C4-N3	3.83	1.46	1.38
2	L2	1265	PSU	C4-N3	3.83	1.46	1.38
2	L2	1361	PSU	C4-N3	3.83	1.46	1.38
2	L2	472	PSU	C4-N3	3.83	1.46	1.38
1	L1	1533	PSU	C4-N3	3.82	1.46	1.38
2	L2	500	PSU	C4-N3	3.81	1.46	1.38
7	L7	74	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	512	PSU	C4-N3	3.80	1.46	1.38
1	L1	422	PSU	C4-N3	3.80	1.46	1.38
7	L7	166	PSU	C4-N3	3.79	1.45	1.38
51	S1	1533	PSU	C4-N3	3.79	1.45	1.38
51	S1	1292	PSU	C4-N3	3.79	1.45	1.38
2	L2	802	PSU	C4-N3	3.79	1.45	1.38
51	S1	2046	PSU	C4-N3	3.78	1.45	1.38
51	S1	1657	PSU	C4-N3	3.78	1.45	1.38
2	L2	1194	PSU	C4-N3	3.77	1.45	1.38
1	L1	1526	PSU	C4-N3	3.77	1.45	1.38
51	S1	1539	PSU	C4-N3	3.77	1.45	1.38
2	L2	510	PSU	C4-N3	3.76	1.45	1.38
1	L1	1177	PSU	C4-N3	3.76	1.45	1.38
1	L1	1171	PSU	C4-N3	3.74	1.45	1.38
2	L2	1413	PSU	C4-N3	3.74	1.45	1.38
1	L1	1528	PSU	C4-N3	3.74	1.45	1.38
2	L2	78	PSU	C4-N3	3.73	1.45	1.38
2	L2	1403	PSU	C4-N3	3.73	1.45	1.38
1	L1	313	PSU	C4-N3	3.72	1.45	1.38
2	L2	662	PSU	C4-N3	3.72	1.45	1.38
2	L2	1213	PSU	C4-N3	3.72	1.45	1.38
2	L2	1303	PSU	C4-N3	3.72	1.45	1.38
2	L2	626	PSU	C4-N3	3.71	1.45	1.38
1	L1	940	PSU	C4-N3	3.71	1.45	1.38
1	L1	1529	PSU	C4-N3	3.70	1.45	1.38
7	L7	69	PSU	C4-N3	3.70	1.45	1.38
51	S1	1544	5MC	C5-C4	-3.70	1.41	1.44
2	L2	593	PSU	C4-N3	3.70	1.45	1.38
2	L2	1144	PSU	C4-N3	3.69	1.45	1.38
7	L7	101	PSU	C4-N3	3.69	1.45	1.38
2	L2	1318	PSU	C4-N3	3.68	1.45	1.38
2	L2	597	PSU	C4-N3	3.67	1.45	1.38
1	L1	1017	PSU	C4-N3	3.64	1.45	1.38
2	L2	1060	PSU	C4-N3	3.64	1.45	1.38
2	L2	1058	PSU	C4-N3	3.61	1.45	1.38
2	L2	1152	PSU	C4-N3	3.60	1.45	1.38
51	S1	1995	7MG	C2-N1	3.58	1.46	1.37
51	S1	1995	7MG	C5-C6	3.56	1.52	1.43
2	L2	524	5MC	C5-C4	-3.54	1.41	1.44
1	L1	510	PSU	C6-C5	3.50	1.39	1.35
51	S1	1995	7MG	C6-N1	3.50	1.45	1.38
2	L2	565	PSU	C6-C5	3.47	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	12	PSU	C6-C5	3.47	1.39	1.35
1	L1	1664	PSU	C6-C5	3.45	1.39	1.35
51	S1	2048	PSU	C6-C5	3.45	1.39	1.35
1	L1	239	PSU	C6-C5	3.44	1.39	1.35
1	L1	774	PSU	C6-C5	3.39	1.39	1.35
51	S1	1995	7MG	C2-N2	3.36	1.42	1.34
51	S1	2140	OMC	C6-N1	3.32	1.46	1.38
1	L1	672	PSU	C6-C5	3.32	1.39	1.35
2	L2	527	A2M	C5-C4	-3.31	1.33	1.39
2	L2	359	OMC	C6-N1	3.28	1.45	1.38
2	L2	437	PSU	C6-C5	3.28	1.38	1.35
1	L1	1011	PSU	C6-C5	3.28	1.38	1.35
2	L2	647	A2M	O2'-C2'	3.24	1.50	1.42
7	L7	43	A2M	C5-C4	-3.23	1.33	1.39
2	L2	1248	OMC	C6-N1	3.23	1.45	1.38
1	L1	1527	OMC	C6-N1	3.21	1.45	1.38
2	L2	665	A2M	C5-C4	-3.20	1.33	1.39
2	L2	583	OMC	C6-N1	3.20	1.45	1.38
1	L1	697	A2M	C5-C4	-3.19	1.33	1.39
2	L2	570	A2M	C5-C4	-3.17	1.33	1.39
2	L2	1397	OMC	C6-N1	3.16	1.45	1.38
51	S1	1866	OMC	C6-N1	3.16	1.45	1.38
51	S1	2059	OMC	C6-N1	3.16	1.45	1.38
7	L7	162	A2M	C5-C4	-3.15	1.33	1.39
51	S1	668	A2M	C5-C4	-3.15	1.33	1.39
2	L2	1384	A2M	C5-C4	-3.15	1.33	1.39
51	S1	38	OMC	C6-N1	3.15	1.45	1.38
1	L1	1373	A2M	C5-C4	-3.14	1.33	1.39
2	L2	1317	OMC	C6-N1	3.14	1.45	1.38
2	L2	572	A2M	C5-C4	-3.13	1.33	1.39
1	L1	407	A2M	C5-C4	-3.13	1.33	1.39
2	L2	591	A2M	C5-C4	-3.12	1.33	1.39
1	L1	858	A2M	C5-C4	-3.11	1.33	1.39
51	S1	1833	OMU	O4-C4	-3.11	1.18	1.24
3	L3	13	OMU	O4-C4	-3.11	1.18	1.24
2	L2	1185	A2M	C5-C4	-3.11	1.33	1.39
51	S1	98	A2M	C5-C4	-3.10	1.33	1.39
1	L1	1539	A2M	C5-C4	-3.10	1.33	1.39
2	L2	1372	A2M	C5-C4	-3.09	1.33	1.39
2	L2	382	A2M	C5-C4	-3.09	1.33	1.39
1	L1	305	A2M	C5-C4	-3.09	1.33	1.39
2	L2	667	OMU	O4-C4	-3.08	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	604	A2M	C5-C4	-3.07	1.33	1.39
51	S1	18	OMC	C6-N1	3.07	1.45	1.38
51	S1	897	A2M	C5-C4	-3.07	1.33	1.39
51	S1	1995	7MG	O6-C6	-3.06	1.17	1.23
1	L1	695	OMC	C6-N1	3.05	1.45	1.38
51	S1	661	OMU	O4-C4	-3.05	1.18	1.24
51	S1	28	A2M	C5-C4	-3.04	1.33	1.39
1	L1	927	A2M	C5-C4	-3.04	1.33	1.39
2	L2	56	OMU	O4-C4	-3.04	1.18	1.24
1	L1	69	A2M	C5-C4	-3.03	1.33	1.39
51	S1	668	A2M	O2'-C2'	3.03	1.50	1.42
1	L1	1659	OMU	O4-C4	-3.03	1.18	1.24
1	L1	1107	OMU	O4-C4	-3.03	1.18	1.24
52	S2	37	MIA	C5-C4	-3.02	1.33	1.39
2	L2	502	A2M	C5-C4	-3.02	1.33	1.39
2	L2	95	A2M	C5-C4	-3.01	1.33	1.39
51	S1	2185	MA6	C5-C4	-3.01	1.33	1.39
51	S1	2184	MA6	C5-C4	-3.01	1.33	1.39
2	L2	527	A2M	O2'-C2'	3.01	1.50	1.42
7	L7	162	A2M	O2'-C2'	3.01	1.50	1.42
1	L1	1371	OMU	O4-C4	-3.01	1.18	1.24
2	L2	570	A2M	O2'-C2'	3.00	1.50	1.42
51	S1	512	A2M	C5-C4	-3.00	1.33	1.39
2	L2	1419	OMU	O4-C4	-2.99	1.18	1.24
1	L1	235	A2M	C5-C4	-2.99	1.33	1.39
51	S1	1979	OMU	O4-C4	-2.99	1.18	1.24
2	L2	1077	OMU	O4-C4	-2.98	1.18	1.24
2	L2	73	OMU	O4-C4	-2.97	1.18	1.24
7	L7	43	A2M	O3'-C3'	-2.97	1.35	1.43
51	S1	2059	OMC	O2-C2	-2.97	1.18	1.23
2	L2	95	A2M	O2'-C2'	2.97	1.49	1.42
2	L2	382	A2M	O3'-C3'	-2.96	1.35	1.43
51	S1	1662	OMU	O4-C4	-2.95	1.18	1.24
1	L1	1371	OMU	C6-N1	2.95	1.45	1.38
2	L2	591	A2M	C5-N7	-2.95	1.33	1.39
2	L2	1359	OMU	O4-C4	-2.95	1.18	1.24
51	S1	897	A2M	O3'-C3'	-2.94	1.35	1.43
2	L2	382	A2M	O2'-C2'	2.94	1.49	1.42
2	L2	1372	A2M	O2'-C2'	2.94	1.49	1.42
51	S1	512	A2M	O3'-C3'	-2.93	1.35	1.43
51	S1	512	A2M	O2'-C2'	2.93	1.49	1.42
7	L7	162	A2M	O3'-C3'	-2.93	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	502	A2M	O3'-C3'	-2.93	1.35	1.43
51	S1	1621	OMU	O4-C4	-2.93	1.18	1.24
2	L2	572	A2M	O3'-C3'	-2.92	1.35	1.43
2	L2	591	A2M	O2'-C2'	2.92	1.49	1.42
1	L1	858	A2M	O3'-C3'	-2.92	1.35	1.43
2	L2	1308	5MC	O2-C2	-2.92	1.18	1.23
1	L1	927	A2M	O3'-C3'	-2.91	1.35	1.43
51	S1	479	A2M	C5-C4	-2.91	1.33	1.39
2	L2	604	A2M	O2'-C2'	2.91	1.49	1.42
1	L1	1373	A2M	O2'-C2'	2.91	1.49	1.42
2	L2	1384	A2M	O2'-C2'	2.91	1.49	1.42
51	S1	98	A2M	O2'-C2'	2.91	1.49	1.42
2	L2	502	A2M	O2'-C2'	2.90	1.49	1.42
51	S1	1979	OMU	C6-N1	2.90	1.45	1.38
51	S1	600	OMG	C2-N1	2.90	1.44	1.37
2	L2	665	A2M	O2'-C2'	2.90	1.49	1.42
51	S1	28	A2M	O3'-C3'	-2.90	1.35	1.43
2	L2	1372	A2M	C5-N7	-2.89	1.33	1.39
1	L1	1373	A2M	O3'-C3'	-2.89	1.35	1.43
51	S1	1621	OMU	C6-N1	2.89	1.45	1.38
2	L2	1185	A2M	O2'-C2'	2.89	1.49	1.42
1	L1	235	A2M	O2'-C2'	2.89	1.49	1.42
1	L1	697	A2M	O3'-C3'	-2.88	1.35	1.43
1	L1	1539	A2M	C5-N7	-2.88	1.33	1.39
1	L1	927	A2M	O2'-C2'	2.88	1.49	1.42
2	L2	95	A2M	O3'-C3'	-2.88	1.35	1.43
2	L2	641	OMG	C2-N1	2.88	1.44	1.37
7	L7	75	OMG	C2-N1	2.88	1.44	1.37
1	L1	1190	OMG	C2-N1	2.88	1.44	1.37
3	L3	13	OMU	C6-N1	2.88	1.44	1.38
51	S1	661	OMU	C6-N1	2.88	1.44	1.38
2	L2	686	OMG	C2-N1	2.87	1.44	1.37
2	L2	1185	A2M	C5-N7	-2.87	1.33	1.39
2	L2	1317	OMC	O2-C2	-2.87	1.18	1.23
2	L2	591	A2M	O3'-C3'	-2.87	1.35	1.43
51	S1	479	A2M	O2'-C2'	2.87	1.49	1.42
1	L1	407	A2M	O3'-C3'	-2.86	1.35	1.43
51	S1	29	OMU	O4-C4	-2.86	1.18	1.24
1	L1	858	A2M	O2'-C2'	2.86	1.49	1.42
2	L2	1359	OMU	C6-N1	2.86	1.44	1.38
51	S1	1662	OMU	C6-N1	2.86	1.44	1.38
2	L2	73	OMU	C6-N1	2.86	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	583	OMC	O2-C2	-2.86	1.18	1.23
1	L1	407	A2M	O2'-C2'	2.86	1.49	1.42
2	L2	665	A2M	O3'-C3'	-2.85	1.35	1.43
1	L1	1539	A2M	O2'-C2'	2.85	1.49	1.42
51	S1	98	A2M	O3'-C3'	-2.85	1.35	1.43
2	L2	1078	OMG	C2-N1	2.85	1.44	1.37
1	L1	235	A2M	C5-N7	-2.85	1.33	1.39
51	S1	1865	OMG	C2-N1	2.85	1.44	1.37
2	L2	1397	OMC	O2-C2	-2.85	1.18	1.23
2	L2	382	A2M	C5-N7	-2.85	1.33	1.39
1	L1	69	A2M	O2'-C2'	2.85	1.49	1.42
1	L1	697	A2M	O2'-C2'	2.85	1.49	1.42
51	S1	28	A2M	O2'-C2'	2.84	1.49	1.42
2	L2	1229	OMG	C2-N1	2.84	1.44	1.37
1	L1	1107	OMU	C6-N1	2.83	1.44	1.38
2	L2	95	A2M	C5-N7	-2.83	1.33	1.39
7	L7	43	A2M	O2'-C2'	2.83	1.49	1.42
51	S1	1478	OMG	C2-N1	2.82	1.44	1.37
1	L1	1190	OMG	C4-N9	-2.82	1.30	1.38
2	L2	534	OMG	C5-N7	-2.82	1.33	1.39
51	S1	98	A2M	C5-N7	-2.82	1.33	1.39
2	L2	1077	OMU	C6-N1	2.82	1.44	1.38
2	L2	1384	A2M	C5-N7	-2.81	1.33	1.39
2	L2	534	OMG	C2-N1	2.81	1.44	1.37
51	S1	1623	OMG	C2-N1	2.81	1.44	1.37
1	L1	697	A2M	C5-N7	-2.81	1.33	1.39
51	S1	29	OMU	C6-N1	2.81	1.44	1.38
1	L1	235	A2M	O3'-C3'	-2.81	1.36	1.43
7	L7	101	PSU	O4-C4	-2.81	1.18	1.23
2	L2	572	A2M	O2'-C2'	2.81	1.49	1.42
2	L2	1360	OMG	C5-N7	-2.81	1.33	1.39
2	L2	527	A2M	O3'-C3'	-2.81	1.36	1.43
2	L2	1185	A2M	O3'-C3'	-2.80	1.36	1.43
1	L1	856	OMG	C2-N1	2.80	1.44	1.37
2	L2	1308	5MC	O3'-C3'	2.80	1.49	1.43
2	L2	1046	OMG	C5-N7	-2.80	1.33	1.39
2	L2	1360	OMG	C2-N1	2.80	1.44	1.37
51	S1	2151	OMG	C2-N1	2.80	1.44	1.37
51	S1	1833	OMU	C6-N1	2.80	1.44	1.38
1	L1	1373	A2M	C5-N7	-2.80	1.34	1.39
51	S1	1647	OMG	C2-N1	2.79	1.44	1.37
2	L2	359	OMC	O2-C2	-2.79	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	570	A2M	O3'-C3'	-2.79	1.36	1.43
2	L2	604	A2M	O3'-C3'	-2.79	1.36	1.43
2	L2	647	A2M	C5-C4	-2.79	1.34	1.39
2	L2	1078	OMG	C4-N9	-2.79	1.31	1.38
1	L1	1527	OMC	O2-C2	-2.79	1.18	1.23
2	L2	1308	5MC	O2'-C2'	-2.78	1.36	1.43
2	L2	78	PSU	O4-C4	-2.78	1.18	1.23
51	S1	1623	OMG	C5-N7	-2.78	1.33	1.39
1	L1	1524	OMG	C5-N7	-2.78	1.33	1.39
2	L2	570	A2M	C5-N7	-2.78	1.34	1.39
2	L2	667	OMU	C6-N1	2.78	1.44	1.38
2	L2	655	OMG	C2-N1	2.77	1.44	1.37
2	L2	1253	OMG	C5-N7	-2.77	1.33	1.39
2	L2	1372	A2M	O3'-C3'	-2.77	1.36	1.43
2	L2	1231	OMG	C2-N1	2.77	1.44	1.37
1	L1	1017	PSU	O4-C4	-2.77	1.18	1.23
2	L2	56	OMU	C6-N1	2.77	1.44	1.38
1	L1	927	A2M	C5-N7	-2.76	1.34	1.39
7	L7	43	A2M	C5-N7	-2.76	1.34	1.39
2	L2	604	A2M	C5-N7	-2.76	1.34	1.39
1	L1	1539	A2M	O3'-C3'	-2.76	1.36	1.43
2	L2	665	A2M	C5-N7	-2.76	1.34	1.39
1	L1	1524	OMG	C2-N1	2.76	1.44	1.37
2	L2	1253	OMG	C2-N1	2.76	1.44	1.37
1	L1	305	A2M	O2'-C2'	2.76	1.49	1.42
2	L2	1229	OMG	C5-N7	-2.76	1.33	1.39
2	L2	1194	PSU	O4-C4	-2.75	1.18	1.23
51	S1	600	OMG	C5-N7	-2.75	1.33	1.39
51	S1	897	A2M	O2'-C2'	2.75	1.49	1.42
1	L1	1659	OMU	C6-N1	2.75	1.44	1.38
1	L1	695	OMC	O2-C2	-2.75	1.18	1.23
51	S1	1647	OMG	C5-N7	-2.75	1.33	1.39
2	L2	1046	OMG	C2-N1	2.74	1.44	1.37
1	L1	856	OMG	C5-N7	-2.74	1.33	1.39
2	L2	1318	PSU	O4-C4	-2.74	1.18	1.23
1	L1	858	A2M	C5-N7	-2.74	1.34	1.39
2	L2	1419	OMU	C6-N1	2.74	1.44	1.38
2	L2	647	A2M	O3'-C3'	-2.74	1.36	1.43
51	S1	668	A2M	C5-N7	-2.73	1.34	1.39
2	L2	686	OMG	C5-N7	-2.73	1.33	1.39
2	L2	647	A2M	C5-N7	-2.73	1.34	1.39
2	L2	71	OMG	C2-N1	2.73	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	527	A2M	C5-N7	-2.73	1.34	1.39
51	S1	18	OMC	O2-C2	-2.73	1.18	1.23
2	L2	655	OMG	C5-N7	-2.73	1.33	1.39
2	L2	1231	OMG	C5-N7	-2.73	1.33	1.39
51	S1	2151	OMG	C5-N7	-2.73	1.33	1.39
2	L2	572	A2M	C5-N7	-2.73	1.34	1.39
51	S1	38	OMC	O2-C2	-2.73	1.18	1.23
7	L7	162	A2M	C5-N7	-2.73	1.34	1.39
2	L2	1384	A2M	O3'-C3'	-2.72	1.36	1.43
1	L1	1526	PSU	O4-C4	-2.72	1.18	1.23
51	S1	1865	OMG	C5-N7	-2.72	1.33	1.39
1	L1	407	A2M	C5-N7	-2.72	1.34	1.39
2	L2	1303	PSU	O4-C4	-2.72	1.18	1.23
1	L1	940	PSU	O4-C4	-2.72	1.18	1.23
51	S1	2140	OMC	O2-C2	-2.72	1.18	1.23
2	L2	641	OMG	C5-N7	-2.72	1.33	1.39
7	L7	75	OMG	C5-N7	-2.71	1.33	1.39
1	L1	313	PSU	O4-C4	-2.71	1.18	1.23
51	S1	479	A2M	C5-N7	-2.71	1.34	1.39
2	L2	1248	OMC	O2-C2	-2.71	1.18	1.23
1	L1	305	A2M	C5-N7	-2.71	1.34	1.39
1	L1	305	A2M	O3'-C3'	-2.70	1.36	1.43
1	L1	1529	PSU	O4-C4	-2.69	1.18	1.23
2	L2	1361	PSU	O4-C4	-2.69	1.18	1.23
2	L2	641	OMG	C4-N9	-2.69	1.31	1.38
51	S1	1478	OMG	C5-N7	-2.69	1.33	1.39
2	L2	71	OMG	C5-N7	-2.69	1.33	1.39
2	L2	1152	PSU	O4-C4	-2.69	1.18	1.23
2	L2	1144	PSU	O4-C4	-2.69	1.18	1.23
2	L2	1253	OMG	O6-C6	-2.69	1.18	1.23
51	S1	1657	PSU	O4-C4	-2.68	1.18	1.23
1	L1	1190	OMG	C5-N7	-2.68	1.33	1.39
2	L2	71	OMG	O6-C6	-2.68	1.18	1.23
2	L2	1060	PSU	O4-C4	-2.68	1.18	1.23
51	S1	668	A2M	O3'-C3'	-2.68	1.36	1.43
2	L2	1403	PSU	O4-C4	-2.67	1.18	1.23
1	L1	69	A2M	C5-N7	-2.67	1.34	1.39
1	L1	1171	PSU	O4-C4	-2.67	1.18	1.23
51	S1	1246	PSU	O4-C4	-2.67	1.18	1.23
1	L1	422	PSU	O4-C4	-2.67	1.18	1.23
2	L2	662	PSU	O4-C4	-2.66	1.18	1.23
1	L1	856	OMG	O6-C6	-2.66	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1264	PSU	O4-C4	-2.66	1.18	1.23
51	S1	1478	OMG	O6-C6	-2.66	1.18	1.23
51	S1	1533	PSU	O4-C4	-2.66	1.18	1.23
2	L2	1265	PSU	O4-C4	-2.65	1.18	1.23
51	S1	1866	OMC	O2-C2	-2.65	1.18	1.23
7	L7	69	PSU	O4-C4	-2.65	1.18	1.23
51	S1	479	A2M	O3'-C3'	-2.65	1.36	1.43
2	L2	626	PSU	O4-C4	-2.65	1.18	1.23
2	L2	655	OMG	O6-C6	-2.65	1.18	1.23
51	S1	2184	MA6	C5-N7	-2.65	1.34	1.39
2	L2	512	PSU	O4-C4	-2.65	1.18	1.23
2	L2	1413	PSU	O4-C4	-2.65	1.18	1.23
51	S1	897	A2M	C5-N7	-2.64	1.34	1.39
7	L7	166	PSU	O4-C4	-2.64	1.18	1.23
51	S1	28	A2M	C5-N7	-2.64	1.34	1.39
2	L2	1229	OMG	O6-C6	-2.64	1.18	1.23
1	L1	1190	OMG	O6-C6	-2.64	1.18	1.23
2	L2	597	PSU	O4-C4	-2.63	1.18	1.23
51	S1	1292	PSU	O4-C4	-2.63	1.18	1.23
51	S1	1566	PSU	O4-C4	-2.63	1.18	1.23
51	S1	512	A2M	C5-N7	-2.63	1.34	1.39
7	L7	74	PSU	O4-C4	-2.62	1.18	1.23
1	L1	1181	PSU	O4-C4	-2.62	1.18	1.23
1	L1	1533	PSU	O4-C4	-2.62	1.18	1.23
2	L2	593	PSU	O4-C4	-2.62	1.18	1.23
2	L2	1078	OMG	O6-C6	-2.62	1.18	1.23
2	L2	1046	OMG	O6-C6	-2.62	1.18	1.23
2	L2	1213	PSU	O4-C4	-2.61	1.18	1.23
1	L1	1528	PSU	O4-C4	-2.61	1.18	1.23
51	S1	2061	5MC	O2-C2	-2.60	1.18	1.23
2	L2	1058	PSU	O4-C4	-2.60	1.18	1.23
2	L2	534	OMG	O6-C6	-2.60	1.18	1.23
2	L2	1284	PSU	O4-C4	-2.60	1.18	1.23
2	L2	502	A2M	C5-N7	-2.59	1.34	1.39
7	L7	75	OMG	O6-C6	-2.59	1.18	1.23
1	L1	1177	PSU	O4-C4	-2.59	1.18	1.23
1	L1	1659	OMU	O2-C2	-2.59	1.18	1.23
2	L2	1231	OMG	O6-C6	-2.59	1.18	1.23
2	L2	1078	OMG	C5-N7	-2.59	1.33	1.39
2	L2	802	PSU	O4-C4	-2.59	1.18	1.23
51	S1	2202	PSU	O4-C4	-2.59	1.18	1.23
2	L2	641	OMG	O6-C6	-2.59	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1478	OMG	C4-N9	-2.58	1.31	1.38
51	S1	1647	OMG	O6-C6	-2.58	1.18	1.23
51	S1	1192	PSU	O4-C4	-2.58	1.18	1.23
51	S1	2185	MA6	C5-N7	-2.58	1.34	1.39
51	S1	2151	OMG	O6-C6	-2.58	1.18	1.23
1	L1	1524	OMG	C5-C6	2.57	1.54	1.44
51	S1	2046	PSU	O4-C4	-2.57	1.18	1.23
51	S1	1539	PSU	O4-C4	-2.57	1.18	1.23
1	L1	1190	OMG	C6-N1	2.57	1.43	1.38
2	L2	1360	OMG	O6-C6	-2.56	1.18	1.23
2	L2	1359	OMU	O2-C2	-2.56	1.18	1.23
2	L2	510	PSU	O4-C4	-2.56	1.18	1.23
51	S1	455	PSU	O4-C4	-2.56	1.18	1.23
2	L2	500	PSU	O4-C4	-2.56	1.18	1.23
51	S1	661	OMU	O2-C2	-2.55	1.18	1.23
51	S1	33	PSU	O4-C4	-2.55	1.18	1.23
2	L2	472	PSU	O4-C4	-2.54	1.18	1.23
51	S1	1478	OMG	C6-N1	2.54	1.43	1.38
51	S1	1865	OMG	O6-C6	-2.54	1.18	1.23
2	L2	591	A2M	C8-N9	-2.54	1.33	1.37
51	S1	1543	B8N	O2'-C2'	2.53	1.49	1.43
51	S1	1623	OMG	O6-C6	-2.53	1.18	1.23
51	S1	600	OMG	O6-C6	-2.53	1.18	1.23
2	L2	1264	PSU	O4'-C1'	-2.53	1.40	1.43
2	L2	95	A2M	C8-N9	-2.53	1.33	1.37
2	L2	686	OMG	C5-C6	2.52	1.53	1.44
2	L2	686	OMG	O6-C6	-2.52	1.18	1.23
2	L2	73	OMU	O2-C2	-2.52	1.18	1.23
2	L2	1372	A2M	C8-N9	-2.52	1.33	1.37
2	L2	1078	OMG	C6-N1	2.52	1.43	1.38
2	L2	1078	OMG	C5-C6	2.52	1.53	1.44
51	S1	600	OMG	C5-C6	2.51	1.53	1.44
2	L2	641	OMG	C6-N1	2.51	1.43	1.38
1	L1	1371	OMU	O2-C2	-2.51	1.18	1.23
1	L1	1524	OMG	C6-N1	2.51	1.43	1.38
2	L2	504	PSU	O4-C4	-2.51	1.18	1.23
2	L2	1253	OMG	C4-N9	-2.51	1.31	1.38
2	L2	1231	OMG	C5-C6	2.50	1.53	1.44
3	L3	13	OMU	O2-C2	-2.50	1.18	1.23
2	L2	667	OMU	O2-C2	-2.50	1.18	1.23
2	L2	71	OMG	C5-C6	2.49	1.53	1.44
51	S1	2151	OMG	C5-C6	2.49	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	604	A2M	C8-N9	-2.49	1.33	1.37
51	S1	1647	OMG	C5-C6	2.49	1.53	1.44
1	L1	1524	OMG	O6-C6	-2.49	1.18	1.23
2	L2	1185	A2M	C8-N9	-2.49	1.33	1.37
7	L7	75	OMG	C5-C6	2.49	1.53	1.44
51	S1	1865	OMG	C5-C6	2.49	1.53	1.44
2	L2	534	OMG	C5-C6	2.48	1.53	1.44
2	L2	570	A2M	C8-N9	-2.48	1.33	1.37
51	S1	1478	OMG	C5-C6	2.47	1.53	1.44
2	L2	665	A2M	C8-N9	-2.47	1.33	1.37
2	L2	56	OMU	O2-C2	-2.47	1.18	1.23
2	L2	1229	OMG	C6-N1	2.46	1.43	1.38
51	S1	1979	OMU	O2-C2	-2.46	1.18	1.23
2	L2	686	OMG	C6-N1	2.46	1.43	1.38
51	S1	1543	B8N	O2-C2	-2.46	1.18	1.22
51	S1	1623	OMG	C6-N1	2.45	1.43	1.38
51	S1	29	OMU	C5-C4	2.45	1.49	1.43
51	S1	1623	OMG	C5-C6	2.45	1.53	1.44
51	S1	1833	OMU	O2-C2	-2.45	1.18	1.23
1	L1	856	OMG	C5-C6	2.45	1.53	1.44
2	L2	1229	OMG	C5-C6	2.45	1.53	1.44
1	L1	1107	OMU	O2-C2	-2.45	1.18	1.23
51	S1	1621	OMU	O2-C2	-2.45	1.18	1.23
2	L2	655	OMG	C5-C6	2.44	1.53	1.44
1	L1	1190	OMG	C5-C6	2.44	1.53	1.44
2	L2	534	OMG	C4-N9	-2.44	1.31	1.38
2	L2	1229	OMG	C4-N9	-2.44	1.31	1.38
2	L2	1360	OMG	C6-N1	2.44	1.43	1.38
1	L1	1171	PSU	O4'-C1'	-2.44	1.40	1.43
51	S1	98	A2M	C8-N9	-2.44	1.33	1.37
2	L2	1253	OMG	C5-C6	2.43	1.53	1.44
2	L2	641	OMG	C5-C6	2.43	1.53	1.44
51	S1	1865	OMG	C6-N1	2.43	1.43	1.38
51	S1	600	OMG	C6-N1	2.43	1.43	1.38
2	L2	1419	OMU	O2-C2	-2.42	1.18	1.23
51	S1	2140	OMC	C5-C4	2.42	1.48	1.42
51	S1	1662	OMU	O2-C2	-2.42	1.18	1.23
2	L2	655	OMG	C6-N1	2.41	1.43	1.38
2	L2	1360	OMG	C5-C6	2.41	1.53	1.44
2	L2	1077	OMU	O2-C2	-2.41	1.18	1.23
51	S1	1647	OMG	C6-N1	2.41	1.43	1.38
51	S1	38	OMC	C5-C4	2.41	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	534	OMG	C6-N1	2.41	1.43	1.38
1	L1	697	A2M	C8-N9	-2.41	1.33	1.37
1	L1	1539	A2M	C8-N9	-2.40	1.33	1.37
1	L1	858	A2M	C8-N9	-2.40	1.33	1.37
2	L2	71	OMG	C6-N1	2.40	1.43	1.38
2	L2	1046	OMG	C5-C6	2.39	1.53	1.44
7	L7	75	OMG	C6-N1	2.39	1.43	1.38
51	S1	2151	OMG	C6-N1	2.39	1.43	1.38
51	S1	2151	OMG	C4-N9	-2.39	1.32	1.38
2	L2	686	OMG	C4-N9	-2.38	1.32	1.38
2	L2	655	OMG	C4-N9	-2.37	1.32	1.38
1	L1	1107	OMU	C5-C4	2.37	1.48	1.43
2	L2	1253	OMG	C6-N1	2.37	1.43	1.38
51	S1	1621	OMU	C5-C4	2.37	1.48	1.43
1	L1	305	A2M	C8-N9	-2.37	1.33	1.37
2	L2	1046	OMG	C6-N1	2.36	1.43	1.38
2	L2	1397	OMC	C5-C4	2.35	1.48	1.42
2	L2	527	A2M	C8-N9	-2.35	1.33	1.37
2	L2	359	OMC	C5-C4	2.35	1.48	1.42
2	L2	1231	OMG	C6-N1	2.34	1.43	1.38
1	L1	856	OMG	C6-N1	2.34	1.43	1.38
2	L2	1360	OMG	C4-N9	-2.34	1.32	1.38
2	L2	1231	OMG	C4-N9	-2.34	1.32	1.38
51	S1	2059	OMC	C5-C4	2.34	1.48	1.42
51	S1	1866	OMC	C5-C4	2.34	1.48	1.42
1	L1	927	A2M	C8-N9	-2.34	1.33	1.37
2	L2	1248	OMC	C5-C4	2.34	1.48	1.42
7	L7	43	A2M	C8-N9	-2.33	1.33	1.37
51	S1	1979	OMU	C5-C4	2.33	1.48	1.43
1	L1	1373	A2M	C8-N9	-2.33	1.33	1.37
1	L1	856	OMG	C4-N9	-2.32	1.32	1.38
2	L2	667	OMU	C5-C4	2.32	1.48	1.43
51	S1	1662	OMU	C5-C4	2.32	1.48	1.43
1	L1	1371	OMU	C5-C4	2.31	1.48	1.43
2	L2	1077	OMU	C5-C4	2.31	1.48	1.43
2	L2	1384	A2M	C8-N9	-2.31	1.33	1.37
7	L7	75	OMG	C4-N9	-2.30	1.32	1.38
51	S1	661	OMU	C5-C4	2.30	1.48	1.43
2	L2	1317	OMC	C5-C4	2.30	1.48	1.42
1	L1	69	A2M	C8-N9	-2.29	1.33	1.37
2	L2	1359	OMU	C5-C4	2.29	1.48	1.43
2	L2	382	A2M	C8-N9	-2.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	583	OMC	C5-C4	2.29	1.48	1.42
51	S1	29	OMU	O2-C2	-2.28	1.19	1.23
2	L2	56	OMU	C5-C4	2.28	1.48	1.43
2	L2	1046	OMG	C4-N9	-2.28	1.32	1.38
2	L2	502	A2M	C8-N9	-2.28	1.33	1.37
51	S1	1833	OMU	C5-C4	2.28	1.48	1.43
51	S1	668	A2M	C8-N9	-2.28	1.33	1.37
2	L2	71	OMG	C4-N9	-2.27	1.32	1.38
51	S1	1647	OMG	C4-N9	-2.27	1.32	1.38
2	L2	73	OMU	C5-C4	2.27	1.48	1.43
51	S1	2185	MA6	C4-N9	-2.27	1.33	1.37
1	L1	1659	OMU	C5-C4	2.27	1.48	1.43
1	L1	1524	OMG	C4-N9	-2.25	1.32	1.38
1	L1	235	A2M	C8-N9	-2.25	1.33	1.37
51	S1	600	OMG	C4-N9	-2.25	1.32	1.38
7	L7	162	A2M	C8-N9	-2.24	1.33	1.37
51	S1	1865	OMG	C4-N9	-2.23	1.32	1.38
51	S1	1623	OMG	C4-N9	-2.23	1.32	1.38
51	S1	28	A2M	C8-N9	-2.23	1.33	1.37
51	S1	897	A2M	C8-N9	-2.23	1.33	1.37
1	L1	407	A2M	C8-N9	-2.23	1.33	1.37
51	S1	18	OMC	C5-C4	2.23	1.48	1.42
2	L2	572	A2M	C8-N9	-2.20	1.33	1.37
2	L2	1419	OMU	C5-C4	2.20	1.48	1.43
51	S1	479	A2M	C8-N9	-2.19	1.33	1.37
1	L1	695	OMC	C5-C4	2.18	1.48	1.42
51	S1	1543	B8N	O3'-C3'	2.18	1.48	1.43
51	S1	512	A2M	C8-N9	-2.16	1.33	1.37
3	L3	13	OMU	C5-C4	2.16	1.48	1.43
1	L1	1527	OMC	C5-C4	2.15	1.47	1.42
51	S1	1566	PSU	C4-C5	2.10	1.50	1.44
51	S1	2184	MA6	C4-N9	-2.10	1.33	1.37
51	S1	1543	B8N	O4-C4	-2.08	1.18	1.23
1	L1	1526	PSU	O4'-C1'	-2.08	1.41	1.43
2	L2	647	A2M	C8-N9	-2.07	1.34	1.37
51	S1	2185	MA6	C10-N6	2.07	1.50	1.45
7	L7	101	PSU	O4'-C1'	-2.07	1.41	1.43
52	S2	37	MIA	C5-N7	-2.03	1.35	1.39
51	S1	1995	7MG	C8-N7	2.01	1.52	1.42
51	S1	2184	MA6	C10-N6	2.01	1.50	1.45
51	S1	2202	PSU	C4-C5	2.00	1.49	1.44

All (965) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	37	MIA	C1'-N9-C8	-14.53	94.86	127.09
52	S2	37	MIA	C4-N9-C1'	12.87	156.72	126.63
52	S2	37	MIA	C11-S10-C2	11.51	110.89	102.25
51	S1	2185	MA6	N1-C6-N6	-10.44	104.14	116.86
51	S1	2184	MA6	N1-C6-N6	-9.46	105.33	116.86
52	S2	37	MIA	S10-C2-N3	8.98	147.02	116.04
51	S1	1623	OMG	C1'-N9-C8	-8.06	103.83	126.73
2	L2	534	OMG	C1'-N9-C8	-7.87	104.39	126.73
2	L2	1046	OMG	C1'-N9-C8	-7.83	104.48	126.73
2	L2	1360	OMG	C1'-N9-C8	-7.81	104.55	126.73
51	S1	600	OMG	C1'-N9-C8	-7.77	104.66	126.73
2	L2	686	OMG	C1'-N9-C8	-7.56	105.26	126.73
51	S1	2151	OMG	C1'-N9-C8	-7.50	105.43	126.73
2	L2	655	OMG	C1'-N9-C8	-7.50	105.43	126.73
51	S1	1865	OMG	C1'-N9-C8	-7.47	105.50	126.73
2	L2	1231	OMG	C1'-N9-C8	-7.45	105.56	126.73
2	L2	1253	OMG	C1'-N9-C8	-7.45	105.56	126.73
7	L7	75	OMG	C1'-N9-C8	-7.39	105.73	126.73
51	S1	1647	OMG	C1'-N9-C8	-7.38	105.76	126.73
2	L2	1229	OMG	C1'-N9-C8	-7.30	105.98	126.73
1	L1	856	OMG	C1'-N9-C8	-7.29	106.03	126.73
2	L2	71	OMG	C1'-N9-C8	-7.23	106.20	126.73
51	S1	1478	OMG	C1'-N9-C8	-7.09	106.58	126.73
2	L2	641	OMG	C1'-N9-C8	-7.04	106.73	126.73
1	L1	1524	OMG	C1'-N9-C8	-7.00	106.86	126.73
51	S1	1623	OMG	C1'-N9-C4	6.99	147.12	126.49
51	S1	2185	MA6	C5-C6-N6	6.86	136.18	125.33
2	L2	534	OMG	C1'-N9-C4	6.71	146.31	126.49
2	L2	1360	OMG	C1'-N9-C4	6.70	146.26	126.49
2	L2	1046	OMG	C1'-N9-C4	6.69	146.26	126.49
51	S1	600	OMG	C1'-N9-C4	6.64	146.11	126.49
52	S2	37	MIA	S10-C2-N1	-6.47	93.71	116.04
1	L1	1190	OMG	C1'-N9-C8	-6.47	108.34	126.73
2	L2	1253	OMG	C1'-N9-C4	6.43	145.49	126.49
2	L2	1078	OMG	C1'-N9-C8	-6.41	108.52	126.73
51	S1	2151	OMG	C1'-N9-C4	6.40	145.39	126.49
2	L2	686	OMG	C1'-N9-C4	6.40	145.38	126.49
2	L2	1231	OMG	C1'-N9-C4	6.35	145.25	126.49
7	L7	75	OMG	C1'-N9-C4	6.30	145.08	126.49
2	L2	655	OMG	C1'-N9-C4	6.29	145.07	126.49
51	S1	1865	OMG	C1'-N9-C4	6.28	145.04	126.49
2	L2	71	OMG	C1'-N9-C4	6.19	144.76	126.49
51	S1	1647	OMG	C1'-N9-C4	6.16	144.69	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L7	43	A2M	N3-C2-N1	-6.15	119.28	128.58
1	L1	856	OMG	C1'-N9-C4	6.14	144.61	126.49
2	L2	1229	OMG	C1'-N9-C4	6.09	144.48	126.49
1	L1	1524	OMG	C1'-N9-C4	6.02	144.27	126.49
51	S1	2184	MA6	C5-C6-N6	6.02	134.86	125.33
51	S1	1833	OMU	C4-N3-C2	-5.92	119.26	126.61
51	S1	1478	OMG	C1'-N9-C4	5.88	143.85	126.49
2	L2	572	A2M	N3-C2-N1	-5.83	119.76	128.58
2	L2	641	OMG	C1'-N9-C4	5.82	143.68	126.49
51	S1	512	A2M	N3-C2-N1	-5.82	119.78	128.58
51	S1	2185	MA6	N1-C2-N3	-5.81	119.78	128.58
7	L7	162	A2M	N3-C2-N1	-5.81	119.79	128.58
52	S2	37	MIA	C5-C4-N3	-5.80	121.07	127.18
2	L2	665	A2M	N3-C2-N1	-5.79	119.82	128.58
1	L1	1373	A2M	N3-C2-N1	-5.79	119.82	128.58
51	S1	2184	MA6	N1-C2-N3	-5.77	119.85	128.58
51	S1	28	A2M	N3-C2-N1	-5.76	119.87	128.58
1	L1	697	A2M	N3-C2-N1	-5.75	119.87	128.58
51	S1	897	A2M	N3-C2-N1	-5.72	119.92	128.58
2	L2	1372	A2M	N3-C2-N1	-5.71	119.94	128.58
1	L1	69	A2M	N3-C2-N1	-5.71	119.94	128.58
2	L2	1384	A2M	N3-C2-N1	-5.71	119.94	128.58
2	L2	667	OMU	C4-N3-C2	-5.71	119.53	126.61
2	L2	502	A2M	N3-C2-N1	-5.70	119.95	128.58
1	L1	1539	A2M	N3-C2-N1	-5.70	119.95	128.58
2	L2	570	A2M	N3-C2-N1	-5.67	120.00	128.58
2	L2	527	A2M	N3-C2-N1	-5.66	120.01	128.58
2	L2	1077	OMU	C4-N3-C2	-5.65	119.60	126.61
1	L1	1107	OMU	C4-N3-C2	-5.65	119.60	126.61
2	L2	56	OMU	C4-N3-C2	-5.65	119.60	126.61
51	S1	1621	OMU	C4-N3-C2	-5.64	119.61	126.61
2	L2	647	A2M	C5-C4-N3	-5.63	118.96	126.72
2	L2	1185	A2M	N3-C2-N1	-5.63	120.06	128.58
51	S1	479	A2M	N3-C2-N1	-5.62	120.08	128.58
51	S1	29	OMU	C4-N3-C2	-5.61	119.65	126.61
3	L3	13	OMU	C4-N3-C2	-5.60	119.65	126.61
1	L1	407	A2M	N3-C2-N1	-5.60	120.10	128.58
2	L2	591	A2M	N3-C2-N1	-5.59	120.13	128.58
1	L1	235	A2M	N3-C2-N1	-5.58	120.14	128.58
51	S1	98	A2M	N3-C2-N1	-5.58	120.14	128.58
1	L1	927	A2M	N3-C2-N1	-5.57	120.15	128.58
1	L1	305	A2M	N3-C2-N1	-5.56	120.17	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1359	OMU	C4-N3-C2	-5.53	119.74	126.61
51	S1	668	A2M	N3-C2-N1	-5.53	120.21	128.58
51	S1	661	OMU	C4-N3-C2	-5.53	119.75	126.61
2	L2	604	A2M	N3-C2-N1	-5.53	120.21	128.58
1	L1	858	A2M	N3-C2-N1	-5.53	120.22	128.58
51	S1	1662	OMU	C4-N3-C2	-5.51	119.77	126.61
51	S1	1979	OMU	C4-N3-C2	-5.51	119.78	126.61
2	L2	647	A2M	N3-C2-N1	-5.50	120.25	128.58
1	L1	1659	OMU	C4-N3-C2	-5.47	119.82	126.61
2	L2	95	A2M	N3-C2-N1	-5.43	120.36	128.58
2	L2	1419	OMU	C4-N3-C2	-5.39	119.93	126.61
2	L2	570	A2M	C5-C4-N3	-5.32	119.39	126.72
2	L2	73	OMU	C4-N3-C2	-5.31	120.02	126.61
1	L1	235	A2M	C5-C4-N3	-5.28	119.45	126.72
2	L2	382	A2M	N3-C2-N1	-5.24	120.65	128.58
1	L1	927	A2M	C5-C4-N3	-5.24	119.50	126.72
1	L1	1190	OMG	C1'-N9-C4	5.22	141.91	126.49
2	L2	1078	OMG	C1'-N9-C4	5.21	141.88	126.49
2	L2	665	A2M	C5-C4-N3	-5.19	119.57	126.72
2	L2	95	A2M	C5-C4-N3	-5.18	119.58	126.72
1	L1	69	A2M	C5-C4-N3	-5.16	119.61	126.72
1	L1	1371	OMU	C4-N3-C2	-5.16	120.21	126.61
51	S1	512	A2M	C5-C4-N3	-5.10	119.69	126.72
2	L2	604	A2M	C5-C4-N3	-5.09	119.71	126.72
1	L1	1539	A2M	N6-C6-N1	-5.08	107.07	118.38
51	S1	479	A2M	C5-C4-N3	-5.06	119.75	126.72
2	L2	591	A2M	C5-C4-N3	-5.06	119.75	126.72
2	L2	1185	A2M	C5-C4-N3	-5.05	119.77	126.72
2	L2	527	A2M	N6-C6-N1	-5.05	107.14	118.38
1	L1	407	A2M	C5-C4-N3	-5.02	119.80	126.72
7	L7	162	A2M	C5-C4-N3	-5.01	119.81	126.72
1	L1	697	A2M	C5-C4-N3	-5.01	119.82	126.72
2	L2	1058	PSU	N1-C2-N3	5.00	120.45	115.17
7	L7	43	A2M	N6-C6-N1	-5.00	107.24	118.38
1	L1	305	A2M	C5-C4-N3	-4.99	119.84	126.72
1	L1	1373	A2M	N6-C6-N1	-4.99	107.26	118.38
51	S1	98	A2M	C5-C4-N3	-4.98	119.86	126.72
51	S1	1995	7MG	C5-C6-N1	4.97	119.69	110.94
1	L1	858	A2M	C5-C4-N3	-4.96	119.89	126.72
51	S1	28	A2M	C5-C4-N3	-4.95	119.90	126.72
2	L2	382	A2M	C5-C4-N3	-4.94	119.92	126.72
2	L2	382	A2M	N6-C6-N1	-4.94	107.38	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	570	A2M	N6-C6-N1	-4.93	107.39	118.38
51	S1	897	A2M	C5-C4-N3	-4.93	119.93	126.72
2	L2	1384	A2M	C5-C4-N3	-4.92	119.94	126.72
2	L2	95	A2M	N6-C6-N1	-4.91	107.43	118.38
2	L2	502	A2M	C5-C4-N3	-4.90	119.96	126.72
51	S1	668	A2M	N6-C6-N1	-4.90	107.46	118.38
1	L1	235	A2M	N6-C6-N1	-4.89	107.48	118.38
51	S1	1543	B8N	C5-C4-N3	4.89	125.04	116.15
51	S1	897	A2M	N6-C6-N1	-4.89	107.48	118.38
1	L1	1533	PSU	C4-N3-C2	-4.88	119.65	126.37
1	L1	305	A2M	N6-C6-N1	-4.87	107.52	118.38
52	S2	37	MIA	N9-C8-N7	-4.87	107.03	113.94
2	L2	1318	PSU	C4-N3-C2	-4.87	119.67	126.37
1	L1	69	A2M	N6-C6-N1	-4.86	107.55	118.38
2	L2	1152	PSU	C4-N3-C2	-4.86	119.68	126.37
2	L2	604	A2M	N6-C6-N1	-4.86	107.56	118.38
2	L2	1060	PSU	C4-N3-C2	-4.86	119.68	126.37
1	L1	1539	A2M	C5-C4-N3	-4.86	120.03	126.72
51	S1	2184	MA6	C5-C4-N3	-4.85	120.03	126.72
2	L2	1185	A2M	N6-C6-N1	-4.85	107.57	118.38
2	L2	665	A2M	N6-C6-N1	-4.85	107.58	118.38
2	L2	502	A2M	N6-C6-N1	-4.84	107.59	118.38
2	L2	1144	PSU	C4-N3-C2	-4.84	119.71	126.37
51	S1	1246	PSU	C4-N3-C2	-4.83	119.71	126.37
1	L1	697	A2M	N6-C6-N1	-4.82	107.63	118.38
1	L1	858	A2M	N6-C6-N1	-4.82	107.63	118.38
2	L2	1372	A2M	N6-C6-N1	-4.82	107.64	118.38
1	L1	1373	A2M	C5-C4-N3	-4.82	120.08	126.72
1	L1	407	A2M	N6-C6-N1	-4.80	107.68	118.38
1	L1	940	PSU	C4-N3-C2	-4.80	119.75	126.37
2	L2	572	A2M	C5-C4-N3	-4.80	120.11	126.72
51	S1	479	A2M	N6-C6-N1	-4.80	107.69	118.38
2	L2	647	A2M	N6-C6-N1	-4.79	107.71	118.38
51	S1	1657	PSU	C4-N3-C2	-4.79	119.78	126.37
51	S1	668	A2M	C5-C4-N3	-4.79	120.12	126.72
2	L2	1372	A2M	C5-C4-N3	-4.79	120.13	126.72
1	L1	1526	PSU	C4-N3-C2	-4.79	119.78	126.37
2	L2	1303	PSU	C4-N3-C2	-4.78	119.78	126.37
2	L2	1384	A2M	N6-C6-N1	-4.78	107.72	118.38
2	L2	1403	PSU	C4-N3-C2	-4.78	119.78	126.37
51	S1	1533	PSU	C4-N3-C2	-4.78	119.79	126.37
2	L2	1058	PSU	C4-N3-C2	-4.78	119.79	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	78	PSU	C4-N3-C2	-4.78	119.79	126.37
2	L2	1194	PSU	C4-N3-C2	-4.78	119.79	126.37
7	L7	74	PSU	C4-N3-C2	-4.77	119.80	126.37
2	L2	572	A2M	N6-C6-N1	-4.76	107.77	118.38
2	L2	1213	PSU	C4-N3-C2	-4.76	119.82	126.37
1	L1	927	A2M	N6-C6-N1	-4.76	107.78	118.38
51	S1	98	A2M	N6-C6-N1	-4.75	107.80	118.38
2	L2	591	A2M	N6-C6-N1	-4.75	107.80	118.38
2	L2	527	A2M	C5-C4-N3	-4.75	120.18	126.72
51	S1	2046	PSU	C4-N3-C2	-4.75	119.83	126.37
1	L1	1529	PSU	C4-N3-C2	-4.75	119.83	126.37
1	L1	1017	PSU	C4-N3-C2	-4.74	119.84	126.37
2	L2	1060	PSU	N1-C2-N3	4.74	120.17	115.17
2	L2	1144	PSU	N1-C2-N3	4.73	120.16	115.17
51	S1	512	A2M	N6-C6-N1	-4.73	107.85	118.38
2	L2	1413	PSU	C4-N3-C2	-4.73	119.86	126.37
2	L2	1284	PSU	C4-N3-C2	-4.72	119.87	126.37
7	L7	162	A2M	N6-C6-N1	-4.72	107.87	118.38
2	L2	500	PSU	C4-N3-C2	-4.70	119.89	126.37
52	S2	37	MIA	N6-C6-N1	4.70	124.63	118.33
51	S1	1623	OMG	C5-C4-N3	-4.69	120.92	128.39
7	L7	101	PSU	C4-N3-C2	-4.69	119.91	126.37
2	L2	1361	PSU	C4-N3-C2	-4.69	119.91	126.37
2	L2	512	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	802	PSU	C4-N3-C2	-4.68	119.92	126.37
7	L7	166	PSU	C4-N3-C2	-4.67	119.94	126.37
1	L1	1181	PSU	C4-N3-C2	-4.67	119.94	126.37
51	S1	28	A2M	N6-C6-N1	-4.66	107.99	118.38
2	L2	71	OMG	C5-C4-N3	-4.66	120.98	128.39
2	L2	1318	PSU	N1-C2-N3	4.65	120.07	115.17
51	S1	1292	PSU	C4-N3-C2	-4.65	119.97	126.37
2	L2	504	PSU	C4-N3-C2	-4.63	119.99	126.37
2	L2	1152	PSU	N1-C2-N3	4.63	120.05	115.17
7	L7	43	A2M	C5-C4-N3	-4.63	120.35	126.72
51	S1	1539	PSU	C4-N3-C2	-4.62	120.01	126.37
51	S1	2185	MA6	C5-C4-N3	-4.62	120.36	126.72
2	L2	504	PSU	N1-C2-N3	4.62	120.04	115.17
1	L1	1524	OMG	C5-C4-N3	-4.61	121.05	128.39
1	L1	422	PSU	C4-N3-C2	-4.61	120.02	126.37
2	L2	1303	PSU	N1-C2-N3	4.61	120.03	115.17
51	S1	1995	7MG	C2-N3-C4	4.60	120.23	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	597	PSU	C4-N3-C2	-4.60	120.04	126.37
51	S1	33	PSU	C4-N3-C2	-4.59	120.05	126.37
51	S1	600	OMG	C5-C4-N3	-4.59	121.09	128.39
1	L1	1533	PSU	N1-C2-N3	4.58	120.00	115.17
2	L2	510	PSU	C4-N3-C2	-4.58	120.06	126.37
2	L2	472	PSU	C4-N3-C2	-4.56	120.09	126.37
51	S1	1647	OMG	C5-C4-N3	-4.56	121.14	128.39
1	L1	1528	PSU	N1-C2-N3	4.55	119.96	115.17
2	L2	1231	OMG	C5-C4-N3	-4.54	121.16	128.39
2	L2	626	PSU	C4-N3-C2	-4.54	120.11	126.37
2	L2	71	OMG	C2-N3-C4	4.54	120.11	112.30
51	S1	455	PSU	C4-N3-C2	-4.53	120.13	126.37
2	L2	662	PSU	C4-N3-C2	-4.53	120.14	126.37
2	L2	1046	OMG	C5-C4-N3	-4.52	121.19	128.39
7	L7	69	PSU	N1-C2-N3	4.52	119.94	115.17
51	S1	1543	B8N	C4-N3-C2	-4.52	120.06	125.62
51	S1	2202	PSU	C4-N3-C2	-4.51	120.16	126.37
7	L7	69	PSU	C4-N3-C2	-4.50	120.17	126.37
1	L1	1177	PSU	C4-N3-C2	-4.50	120.17	126.37
51	S1	2151	OMG	C5-C4-N3	-4.50	121.23	128.39
2	L2	1403	PSU	N1-C2-N3	4.50	119.91	115.17
2	L2	1360	OMG	C5-C4-N3	-4.49	121.24	128.39
1	L1	1181	PSU	N1-C2-N3	4.49	119.91	115.17
51	S1	1657	PSU	N1-C2-N3	4.49	119.91	115.17
2	L2	1213	PSU	N1-C2-N3	4.48	119.90	115.17
51	S1	2046	PSU	N1-C2-N3	4.48	119.89	115.17
1	L1	1529	PSU	N1-C2-N3	4.48	119.89	115.17
1	L1	1017	PSU	N1-C2-N3	4.47	119.89	115.17
2	L2	527	A2M	N9-C8-N7	-4.47	107.59	113.94
7	L7	166	PSU	N1-C2-N3	4.46	119.88	115.17
2	L2	1231	OMG	C2-N3-C4	4.46	119.98	112.30
51	S1	1192	PSU	C4-N3-C2	-4.45	120.24	126.37
51	S1	1647	OMG	C2-N3-C4	4.45	119.96	112.30
2	L2	655	OMG	C2-N3-C4	4.45	119.96	112.30
1	L1	1171	PSU	C4-N3-C2	-4.44	120.25	126.37
2	L2	78	PSU	N1-C2-N3	4.44	119.85	115.17
2	L2	1413	PSU	N1-C2-N3	4.44	119.85	115.17
7	L7	74	PSU	N1-C2-N3	4.44	119.85	115.17
1	L1	313	PSU	C4-N3-C2	-4.44	120.26	126.37
2	L2	1264	PSU	C4-N3-C2	-4.44	120.26	126.37
1	L1	1524	OMG	C2-N3-C4	4.44	119.94	112.30
2	L2	686	OMG	C5-C4-N3	-4.43	121.34	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	2151	OMG	C2-N3-C4	4.43	119.93	112.30
51	S1	1865	OMG	C5-C4-N3	-4.43	121.34	128.39
2	L2	1265	PSU	N1-C2-N3	4.43	119.84	115.17
2	L2	593	PSU	C4-N3-C2	-4.42	120.28	126.37
51	S1	33	PSU	N1-C2-N3	4.42	119.83	115.17
51	S1	1566	PSU	C4-N3-C2	-4.42	120.28	126.37
51	S1	1533	PSU	N1-C2-N3	4.41	119.82	115.17
1	L1	1171	PSU	N1-C2-N3	4.41	119.82	115.17
2	L2	1284	PSU	N1-C2-N3	4.41	119.82	115.17
2	L2	500	PSU	N1-C2-N3	4.40	119.81	115.17
7	L7	75	OMG	C5-C4-N3	-4.40	121.38	128.39
51	S1	600	OMG	C2-N3-C4	4.40	119.88	112.30
7	L7	101	PSU	N1-C2-N3	4.40	119.81	115.17
2	L2	1194	PSU	N1-C2-N3	4.39	119.80	115.17
2	L2	512	PSU	N1-C2-N3	4.39	119.80	115.17
51	S1	1246	PSU	N1-C2-N3	4.39	119.80	115.17
51	S1	1566	PSU	N1-C2-N3	4.39	119.80	115.17
51	S1	2202	PSU	N1-C2-N3	4.39	119.80	115.17
2	L2	655	OMG	C5-C4-N3	-4.38	121.41	128.39
2	L2	1253	OMG	C5-C4-N3	-4.38	121.42	128.39
1	L1	940	PSU	N1-C2-N3	4.38	119.79	115.17
2	L2	534	OMG	C5-C4-N3	-4.37	121.43	128.39
2	L2	1265	PSU	C4-N3-C2	-4.37	120.35	126.37
51	S1	1623	OMG	C2-N3-C4	4.37	119.83	112.30
2	L2	802	PSU	N1-C2-N3	4.36	119.77	115.17
1	L1	1526	PSU	N1-C2-N3	4.36	119.76	115.17
1	L1	313	PSU	N1-C2-N3	4.35	119.75	115.17
2	L2	1361	PSU	N1-C2-N3	4.35	119.75	115.17
51	S1	1539	PSU	N1-C2-N3	4.35	119.75	115.17
2	L2	472	PSU	N1-C2-N3	4.34	119.75	115.17
2	L2	510	PSU	N1-C2-N3	4.34	119.74	115.17
1	L1	1177	PSU	N1-C2-N3	4.33	119.74	115.17
51	S1	1865	OMG	C2-N3-C4	4.33	119.76	112.30
2	L2	597	PSU	N1-C2-N3	4.33	119.73	115.17
51	S1	1292	PSU	N1-C2-N3	4.33	119.73	115.17
2	L2	686	OMG	C2-N3-C4	4.32	119.75	112.30
1	L1	856	OMG	C2-N3-C4	4.32	119.73	112.30
2	L2	1046	OMG	C2-N3-C4	4.32	119.73	112.30
2	L2	1253	OMG	C2-N3-C4	4.31	119.72	112.30
7	L7	75	OMG	C2-N3-C4	4.30	119.71	112.30
2	L2	1360	OMG	C2-N3-C4	4.30	119.71	112.30
1	L1	856	OMG	C5-C4-N3	-4.30	121.54	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	662	PSU	N1-C2-N3	4.30	119.70	115.17
51	S1	1192	PSU	N1-C2-N3	4.30	119.70	115.17
51	S1	455	PSU	N1-C2-N3	4.29	119.70	115.17
2	L2	1229	OMG	C2-N3-C4	4.29	119.69	112.30
51	S1	1478	OMG	C2-N3-C4	4.29	119.68	112.30
2	L2	534	OMG	C2-N3-C4	4.29	119.68	112.30
1	L1	858	A2M	N9-C8-N7	-4.28	107.86	113.94
1	L1	1190	OMG	C2-N3-C4	4.27	119.66	112.30
2	L2	1078	OMG	C2-N3-C4	4.25	119.62	112.30
52	S2	37	MIA	N3-C2-N1	-4.24	119.27	127.00
2	L2	1229	OMG	C5-C4-N3	-4.23	121.65	128.39
2	L2	593	PSU	N1-C2-N3	4.23	119.63	115.17
1	L1	422	PSU	N1-C2-N3	4.23	119.62	115.17
2	L2	641	OMG	C2-N3-C4	4.20	119.54	112.30
51	S1	1995	7MG	C5-C4-N3	-4.20	120.25	128.13
2	L2	626	PSU	N1-C2-N3	4.19	119.59	115.17
51	S1	2185	MA6	N9-C8-N7	-4.19	107.99	113.94
51	S1	2184	MA6	N9-C8-N7	-4.19	107.99	113.94
2	L2	502	A2M	N9-C8-N7	-4.18	108.00	113.94
51	S1	668	A2M	N9-C8-N7	-4.17	108.02	113.94
2	L2	527	A2M	C4'-O4'-C1'	-4.15	100.30	109.47
7	L7	43	A2M	N9-C8-N7	-4.15	108.05	113.94
51	S1	1478	OMG	C5-C4-N3	-4.14	121.81	128.39
2	L2	665	A2M	N9-C8-N7	-4.13	108.07	113.94
51	S1	897	A2M	N9-C8-N7	-4.13	108.07	113.94
51	S1	512	A2M	N9-C8-N7	-4.12	108.09	113.94
51	S1	98	A2M	N9-C8-N7	-4.11	108.11	113.94
1	L1	305	A2M	N9-C8-N7	-4.09	108.14	113.94
2	L2	560	OMU	O3'-C3'-C4'	4.07	122.78	111.08
51	S1	28	A2M	N9-C8-N7	-4.07	108.16	113.94
2	L2	1264	PSU	N1-C2-N3	4.06	119.45	115.17
2	L2	572	A2M	N9-C8-N7	-4.06	108.18	113.94
2	L2	1185	A2M	N9-C8-N7	-4.04	108.21	113.94
51	S1	1995	7MG	C4-C5-N7	4.03	110.14	105.38
51	S1	1543	B8N	C1'-C5-C4	4.03	123.72	117.61
1	L1	1171	PSU	C6-N1-C2	-4.02	118.96	122.69
1	L1	1659	OMU	N3-C2-N1	3.99	120.09	114.89
1	L1	69	A2M	N9-C8-N7	-3.99	108.28	113.94
1	L1	407	A2M	N9-C8-N7	-3.98	108.28	113.94
2	L2	570	A2M	N9-C8-N7	-3.98	108.28	113.94
51	S1	1833	OMU	C5-C4-N3	3.97	120.36	114.80
1	L1	697	A2M	N9-C8-N7	-3.97	108.31	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L7	162	A2M	N9-C8-N7	-3.96	108.31	113.94
1	L1	1371	OMU	C1'-N1-C2	3.95	124.69	117.59
2	L2	647	A2M	N9-C8-N7	-3.95	108.33	113.94
2	L2	641	OMG	C5-C4-N3	-3.95	122.11	128.39
1	L1	1539	A2M	N9-C8-N7	-3.93	108.35	113.94
7	L7	43	A2M	C5-C6-N6	3.93	133.02	123.29
2	L2	1384	A2M	N9-C8-N7	-3.92	108.37	113.94
1	L1	1107	OMU	N3-C2-N1	3.92	120.00	114.89
2	L2	604	A2M	N9-C8-N7	-3.91	108.38	113.94
51	S1	2184	MA6	C4-C5-C6	3.91	119.95	115.91
1	L1	1371	OMU	N3-C2-N1	3.91	119.98	114.89
2	L2	667	OMU	N3-C2-N1	3.90	119.97	114.89
51	S1	479	A2M	N9-C8-N7	-3.90	108.41	113.94
2	L2	1359	OMU	N3-C2-N1	3.89	119.96	114.89
1	L1	1190	OMG	N9-C8-N7	-3.88	106.20	113.40
1	L1	1373	A2M	N9-C8-N7	-3.86	108.45	113.94
51	S1	661	OMU	N3-C2-N1	3.86	119.91	114.89
51	S1	1979	OMU	N3-C2-N1	3.85	119.91	114.89
2	L2	1058	PSU	C6-N1-C2	-3.85	119.12	122.69
1	L1	235	A2M	N9-C8-N7	-3.85	108.48	113.94
1	L1	927	A2M	N9-C8-N7	-3.85	108.48	113.94
2	L2	1078	OMG	N9-C8-N7	-3.85	106.27	113.40
51	S1	29	OMU	N3-C2-N1	3.82	119.86	114.89
51	S1	1543	B8N	N3-C2-N1	3.82	121.38	116.72
1	L1	1539	A2M	C5-C6-N6	3.82	132.74	123.29
2	L2	1372	A2M	N9-C8-N7	-3.81	108.53	113.94
3	L3	13	OMU	C5-C4-N3	3.81	120.14	114.80
2	L2	56	OMU	N3-C2-N1	3.81	119.85	114.89
2	L2	95	A2M	N9-C8-N7	-3.81	108.53	113.94
51	S1	1647	OMG	N9-C8-N7	-3.80	106.35	113.40
51	S1	1621	OMU	N3-C2-N1	3.80	119.84	114.89
2	L2	73	OMU	N3-C2-N1	3.79	119.83	114.89
2	L2	1077	OMU	C5-C4-N3	3.78	120.10	114.80
1	L1	1190	OMG	C5-C4-N3	-3.78	122.37	128.39
2	L2	1372	A2M	C5-C6-N6	3.78	132.64	123.29
2	L2	1185	A2M	C5-C6-N6	3.78	132.63	123.29
1	L1	1373	A2M	C5-C6-N6	3.77	132.63	123.29
2	L2	1265	PSU	C6-N1-C2	-3.77	119.19	122.69
2	L2	95	A2M	C5-C6-N6	3.76	132.59	123.29
51	S1	668	A2M	C5-C6-N6	3.76	132.58	123.29
1	L1	313	PSU	C6-N1-C2	-3.75	119.21	122.69
51	S1	1478	OMG	N9-C8-N7	-3.75	106.45	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L3	13	OMU	N3-C2-N1	3.74	119.76	114.89
2	L2	570	A2M	C5-C6-N6	3.73	132.53	123.29
2	L2	382	A2M	N9-C8-N7	-3.73	108.64	113.94
2	L2	1078	OMG	C5-C4-N3	-3.73	122.45	128.39
2	L2	1419	OMU	N3-C2-N1	3.72	119.74	114.89
2	L2	667	OMU	C5-C4-N3	3.72	120.01	114.80
2	L2	527	A2M	C5-C6-N6	3.72	132.49	123.29
2	L2	382	A2M	C5-C6-N6	3.72	132.49	123.29
2	L2	641	OMG	N9-C8-N7	-3.71	106.51	113.40
51	S1	1833	OMU	N3-C2-N1	3.71	119.72	114.89
1	L1	305	A2M	C5-C6-N6	3.70	132.46	123.29
2	L2	1229	OMG	N9-C8-N7	-3.70	106.53	113.40
51	S1	897	A2M	C5-C6-N6	3.70	132.46	123.29
51	S1	1662	OMU	N3-C2-N1	3.70	119.71	114.89
1	L1	1107	OMU	C5-C4-N3	3.70	119.98	114.80
51	S1	1543	B8N	C2'-C3'-C4'	3.68	109.72	102.61
51	S1	1621	OMU	C5-C4-N3	3.67	119.94	114.80
2	L2	502	A2M	C5-C6-N6	3.67	132.36	123.29
2	L2	647	A2M	N3-C4-N9	3.67	133.40	127.17
1	L1	858	A2M	C5-C6-N6	3.66	132.36	123.29
2	L2	1077	OMU	N3-C2-N1	3.66	119.65	114.89
51	S1	1979	OMU	C5-C4-N3	3.66	119.92	114.80
7	L7	69	PSU	C6-N1-C2	-3.66	119.30	122.69
2	L2	504	PSU	C6-N1-C2	-3.65	119.30	122.69
2	L2	1359	OMU	C5-C4-N3	3.65	119.92	114.80
51	S1	1662	OMU	C5-C4-N3	3.65	119.91	114.80
2	L2	604	A2M	C5-C6-N6	3.65	132.32	123.29
2	L2	572	A2M	C5-C6-N6	3.65	132.32	123.29
2	L2	1144	PSU	C6-N1-C2	-3.65	119.31	122.69
2	L2	655	OMG	N9-C8-N7	-3.64	106.64	113.40
2	L2	1384	A2M	C5-C6-N6	3.64	132.30	123.29
1	L1	235	A2M	C5-C6-N6	3.64	132.29	123.29
51	S1	661	OMU	C5-C4-N3	3.63	119.88	114.80
52	S2	37	MIA	C12-C13-C14	-3.63	120.50	127.01
51	S1	1543	B8N	C3'-C2'-C1'	3.63	105.97	101.69
1	L1	69	A2M	C5-C6-N6	3.62	132.25	123.29
2	L2	686	OMG	N9-C8-N7	-3.62	106.69	113.40
2	L2	591	A2M	N9-C8-N7	-3.62	108.80	113.94
2	L2	56	OMU	C5-C4-N3	3.62	119.87	114.80
1	L1	697	A2M	C5-C6-N6	3.61	132.22	123.29
1	L1	407	A2M	C5-C6-N6	3.61	132.22	123.29
2	L2	1308	5MC	C5-C6-N1	-3.60	119.40	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	479	A2M	C5-C6-N6	3.60	132.20	123.29
2	L2	591	A2M	C5-C6-N6	3.60	132.19	123.29
51	S1	1865	OMG	N9-C8-N7	-3.59	106.73	113.40
2	L2	665	A2M	C5-C6-N6	3.59	132.18	123.29
1	L1	927	A2M	C5-C6-N6	3.58	132.15	123.29
1	L1	856	OMG	N9-C8-N7	-3.58	106.76	113.40
51	S1	98	A2M	C5-C6-N6	3.58	132.14	123.29
51	S1	1192	PSU	C6-N1-C2	-3.57	119.38	122.69
2	L2	570	A2M	C2-N3-C4	3.57	120.55	111.83
51	S1	29	OMU	C5-C4-N3	3.56	119.79	114.80
52	S2	37	MIA	C5-C6-N6	-3.56	115.17	122.03
7	L7	162	A2M	C5-C6-N6	3.55	132.07	123.29
2	L2	647	A2M	C5-C6-N6	3.55	132.07	123.29
51	S1	512	A2M	C5-C6-N6	3.54	132.05	123.29
51	S1	600	OMG	N9-C8-N7	-3.54	106.83	113.40
2	L2	665	A2M	C2-N3-C4	3.54	120.47	111.83
51	S1	2185	MA6	C2-N1-C6	3.53	120.46	111.83
2	L2	647	A2M	C2-N3-C4	3.53	120.46	111.83
51	S1	2151	OMG	N9-C8-N7	-3.53	106.86	113.40
2	L2	1419	OMU	C5-C4-N3	3.53	119.74	114.80
51	S1	455	PSU	C6-N1-C2	-3.52	119.42	122.69
2	L2	1264	PSU	C6-N1-C2	-3.52	119.42	122.69
51	S1	512	A2M	C2-N3-C4	3.52	120.43	111.83
2	L2	73	OMU	C5-C4-N3	3.51	119.72	114.80
1	L1	235	A2M	C2-N3-C4	3.51	120.40	111.83
1	L1	69	A2M	C2-N3-C4	3.50	120.37	111.83
51	S1	2185	MA6	C4-C5-C6	3.48	119.51	115.91
51	S1	1833	OMU	O4-C4-C5	-3.48	119.16	125.16
51	S1	28	A2M	C5-C6-N6	3.48	131.90	123.29
1	L1	1528	PSU	C6-N1-C2	-3.48	119.46	122.69
2	L2	1060	PSU	C6-N1-C2	-3.48	119.46	122.69
2	L2	1231	OMG	N9-C8-N7	-3.47	106.97	113.40
1	L1	1524	OMG	N9-C8-N7	-3.47	106.97	113.40
1	L1	697	A2M	C2-N3-C4	3.46	120.29	111.83
2	L2	1413	PSU	C6-N1-C2	-3.46	119.48	122.69
51	S1	1566	PSU	C6-N1-C2	-3.45	119.49	122.69
1	L1	1371	OMU	C5-C4-N3	3.45	119.64	114.80
1	L1	1659	OMU	C5-C4-N3	3.45	119.63	114.80
7	L7	166	PSU	C6-N1-C2	-3.45	119.49	122.69
7	L7	162	A2M	C2-N3-C4	3.45	120.25	111.83
1	L1	1181	PSU	C6-N1-C2	-3.45	119.49	122.69
2	L2	647	A2M	C4'-O4'-C1'	-3.44	101.88	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	2184	MA6	C2-N1-C6	3.43	120.22	111.83
51	S1	2185	MA6	C2-N3-C4	3.43	120.21	111.83
51	S1	897	A2M	C2-N3-C4	3.43	120.20	111.83
7	L7	75	OMG	N9-C8-N7	-3.42	107.05	113.40
1	L1	927	A2M	C2-N3-C4	3.42	120.19	111.83
2	L2	534	OMG	N9-C8-N7	-3.42	107.06	113.40
2	L2	1046	OMG	N9-C8-N7	-3.42	107.06	113.40
1	L1	407	A2M	C2-N3-C4	3.42	120.18	111.83
51	S1	28	A2M	C2-N3-C4	3.42	120.17	111.83
2	L2	1152	PSU	C6-C5-C4	3.41	120.47	118.17
2	L2	604	A2M	C2-N3-C4	3.41	120.16	111.83
2	L2	1360	OMG	N9-C8-N7	-3.41	107.08	113.40
2	L2	71	OMG	N9-C8-N7	-3.41	107.08	113.40
2	L2	1284	PSU	C6-N1-C2	-3.40	119.53	122.69
51	S1	2202	PSU	C6-N1-C2	-3.40	119.53	122.69
51	S1	2184	MA6	C2-N3-C4	3.40	120.14	111.83
2	L2	1185	A2M	C2-N3-C4	3.40	120.13	111.83
51	S1	479	A2M	C2-N3-C4	3.40	120.13	111.83
2	L2	1318	PSU	C6-N1-C2	-3.40	119.54	122.69
1	L1	1177	PSU	C6-N1-C2	-3.39	119.55	122.69
7	L7	43	A2M	C2-N3-C4	3.39	120.11	111.83
2	L2	1253	OMG	N9-C8-N7	-3.38	107.12	113.40
2	L2	1303	PSU	C6-N1-C2	-3.38	119.55	122.69
2	L2	1384	A2M	C2-N3-C4	3.37	120.07	111.83
1	L1	1533	PSU	C6-N1-C2	-3.37	119.56	122.69
2	L2	510	PSU	C6-N1-C2	-3.37	119.56	122.69
1	L1	858	A2M	C2-N3-C4	3.37	120.06	111.83
51	S1	1657	PSU	C6-N1-C2	-3.37	119.57	122.69
1	L1	1373	A2M	C2-N3-C4	3.37	120.05	111.83
2	L2	572	A2M	C2-N3-C4	3.36	120.05	111.83
51	S1	1292	PSU	C6-N1-C2	-3.36	119.57	122.69
2	L2	1058	PSU	C6-C5-C4	3.36	120.44	118.17
2	L2	1194	PSU	C6-N1-C2	-3.36	119.57	122.69
1	L1	1539	A2M	C2-N3-C4	3.36	120.04	111.83
2	L2	591	A2M	C2-N3-C4	3.36	120.04	111.83
2	L2	95	A2M	C2-N3-C4	3.36	120.03	111.83
2	L2	597	PSU	C6-N1-C2	-3.35	119.58	122.69
1	L1	69	A2M	C2'-C1'-N9	-3.35	108.23	113.75
1	L1	305	A2M	C2-N3-C4	3.35	120.02	111.83
2	L2	502	A2M	C2-N3-C4	3.35	120.02	111.83
51	S1	1539	PSU	C6-N1-C2	-3.35	119.58	122.69
2	L2	1152	PSU	C6-N1-C2	-3.35	119.59	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	527	A2M	C2-N3-C4	3.34	120.00	111.83
51	S1	1623	OMG	N9-C8-N7	-3.34	107.21	113.40
51	S1	2046	PSU	C6-N1-C2	-3.33	119.60	122.69
7	L7	74	PSU	C6-N1-C2	-3.33	119.60	122.69
51	S1	98	A2M	C2-N3-C4	3.32	119.95	111.83
2	L2	1213	PSU	C6-N1-C2	-3.32	119.61	122.69
2	L2	512	PSU	C6-N1-C2	-3.32	119.61	122.69
2	L2	1403	PSU	C6-N1-C2	-3.32	119.61	122.69
51	S1	33	PSU	C6-N1-C2	-3.32	119.61	122.69
2	L2	662	PSU	C6-N1-C2	-3.31	119.62	122.69
2	L2	1361	PSU	C6-N1-C2	-3.31	119.62	122.69
51	S1	668	A2M	C2-N3-C4	3.30	119.90	111.83
2	L2	1060	PSU	C6-C5-C4	3.30	120.40	118.17
2	L2	1372	A2M	C2-N3-C4	3.30	119.89	111.83
2	L2	593	PSU	C6-N1-C2	-3.30	119.63	122.69
1	L1	1529	PSU	C6-N1-C2	-3.29	119.64	122.69
2	L2	472	PSU	C6-N1-C2	-3.28	119.65	122.69
7	L7	101	PSU	C6-N1-C2	-3.28	119.65	122.69
2	L2	626	PSU	C6-N1-C2	-3.27	119.66	122.69
1	L1	1017	PSU	C6-N1-C2	-3.26	119.66	122.69
1	L1	927	A2M	N3-C4-N9	3.25	132.69	127.17
2	L2	382	A2M	C2-N3-C4	3.24	119.75	111.83
1	L1	1526	PSU	C6-N1-C2	-3.24	119.69	122.69
1	L1	940	PSU	C6-N1-C2	-3.24	119.69	122.69
2	L2	527	A2M	O4'-C1'-N9	3.24	114.31	108.09
52	S2	37	MIA	C5-N7-C8	3.23	108.53	103.45
1	L1	422	PSU	C6-N1-C2	-3.23	119.70	122.69
51	S1	1533	PSU	C6-N1-C2	-3.22	119.70	122.69
2	L2	500	PSU	C6-N1-C2	-3.22	119.71	122.69
1	L1	858	A2M	C2'-C1'-N9	-3.21	108.47	113.75
2	L2	78	PSU	C6-N1-C2	-3.21	119.71	122.69
3	L3	13	OMU	O4-C4-C5	-3.20	119.65	125.16
51	S1	1995	7MG	C5-C4-N9	3.19	110.42	106.33
51	S1	1246	PSU	C6-N1-C2	-3.19	119.73	122.69
2	L2	802	PSU	C6-N1-C2	-3.19	119.73	122.69
2	L2	665	A2M	N3-C4-N9	3.18	132.57	127.17
7	L7	43	A2M	C2'-C1'-N9	-3.17	108.53	113.75
1	L1	407	A2M	C2'-C1'-N9	-3.16	108.55	113.75
51	S1	512	A2M	N3-C4-N9	3.14	132.51	127.17
51	S1	2059	OMC	O2-C2-N3	-3.12	117.41	122.33
1	L1	69	A2M	N3-C4-N9	3.12	132.47	127.17
2	L2	1253	OMG	C2-N1-C6	-3.12	119.46	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	37	MIA	C2-N3-C4	3.11	120.45	112.29
2	L2	95	A2M	N3-C4-N9	3.10	132.44	127.17
1	L1	959	OMG	O2'-C2'-C1'	3.09	114.85	108.99
2	L2	604	A2M	N3-C4-N9	3.08	132.41	127.17
51	S1	28	A2M	N3-C4-N9	3.08	132.40	127.17
51	S1	1979	OMU	O4-C4-C5	-3.07	119.87	125.16
2	L2	591	A2M	N3-C4-N9	3.05	132.35	127.17
1	L1	858	A2M	N3-C4-N9	3.04	132.34	127.17
51	S1	1662	OMU	O4-C4-C5	-3.04	119.91	125.16
1	L1	305	A2M	N3-C4-N9	3.04	132.34	127.17
2	L2	1077	OMU	O4-C4-C5	-3.04	119.92	125.16
2	L2	504	PSU	O2-C2-N1	-3.04	119.66	122.79
51	S1	2184	MA6	N3-C4-N9	3.04	132.33	127.17
51	S1	1621	OMU	O4-C4-C5	-3.03	119.93	125.16
1	L1	235	A2M	N3-C4-N9	3.03	132.33	127.17
2	L2	570	A2M	N3-C4-N9	3.03	132.32	127.17
7	L7	162	A2M	N3-C4-N9	3.02	132.31	127.17
2	L2	56	OMU	O4-C4-C5	-3.02	119.96	125.16
2	L2	1419	OMU	O4-C4-C5	-3.02	119.96	125.16
1	L1	858	A2M	C5-N7-C8	3.01	108.18	103.45
51	S1	2059	OMC	C1'-N1-C2	3.00	125.08	118.44
2	L2	73	OMU	O4-C4-C5	-3.00	119.99	125.16
1	L1	697	A2M	N3-C4-N9	3.00	132.27	127.17
51	S1	479	A2M	N3-C4-N9	3.00	132.26	127.17
1	L1	1524	OMG	C2-N1-C6	-2.98	119.70	125.11
2	L2	1403	PSU	C6-C5-C4	2.98	120.19	118.17
51	S1	1623	OMG	C2-N1-C6	-2.98	119.71	125.11
2	L2	802	PSU	C6-C5-C4	2.98	120.18	118.17
2	L2	527	A2M	C5-N7-C8	2.97	108.12	103.45
51	S1	98	A2M	N3-C4-N9	2.96	132.21	127.17
2	L2	1213	PSU	C6-C5-C4	2.96	120.17	118.17
2	L2	502	A2M	N3-C4-N9	2.96	132.21	127.17
1	L1	407	A2M	N3-C4-N9	2.96	132.20	127.17
1	L1	1533	PSU	O2-C2-N1	-2.96	119.74	122.79
2	L2	570	A2M	C5-N7-C8	2.95	108.09	103.45
2	L2	1185	A2M	N3-C4-N9	2.95	132.19	127.17
2	L2	665	A2M	C5-N7-C8	2.95	108.08	103.45
52	S2	37	MIA	C4-C5-N7	-2.94	107.22	110.58
1	L1	1526	PSU	C6-C5-C4	2.92	120.14	118.17
2	L2	1185	A2M	C5-N7-C8	2.92	108.03	103.45
2	L2	71	OMG	C2-N1-C6	-2.91	119.83	125.11
51	S1	668	A2M	C5-N7-C8	2.91	108.02	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	647	A2M	C5-N7-C8	2.91	108.02	103.45
2	L2	667	OMU	O4-C4-C5	-2.90	120.16	125.16
1	L1	1107	OMU	O4-C4-C5	-2.90	120.16	125.16
2	L2	1231	OMG	C2-N1-C6	-2.90	119.86	125.11
1	L1	305	A2M	C5-N7-C8	2.90	108.00	103.45
51	S1	1478	OMG	C2-N1-C6	-2.90	119.86	125.11
2	L2	1384	A2M	N3-C4-N9	2.89	132.09	127.17
2	L2	502	A2M	C5-N7-C8	2.89	107.99	103.45
51	S1	600	OMG	C2-N1-C6	-2.88	119.89	125.11
51	S1	98	A2M	C5-N7-C8	2.88	107.97	103.45
51	S1	2151	OMG	C2-N1-C6	-2.87	119.90	125.11
51	S1	2202	PSU	O2-C2-N1	-2.87	119.83	122.79
2	L2	1359	OMU	O4-C4-C5	-2.87	120.21	125.16
2	L2	604	A2M	C5-N7-C8	2.87	107.96	103.45
51	S1	1995	7MG	C2-N1-C6	-2.87	119.91	125.11
51	S1	33	PSU	C6-C5-C4	2.87	120.11	118.17
2	L2	686	OMG	C2-N1-C6	-2.87	119.92	125.11
51	S1	897	A2M	N3-C4-N9	2.86	132.04	127.17
2	L2	1078	OMG	C2-N1-C6	-2.86	119.92	125.11
2	L2	1413	PSU	O2-C2-N1	-2.86	119.84	122.79
51	S1	897	A2M	C5-N7-C8	2.86	107.94	103.45
7	L7	75	OMG	C2-N1-C6	-2.85	119.94	125.11
51	S1	661	OMU	O4-C4-C5	-2.85	120.25	125.16
51	S1	512	A2M	C5-N7-C8	2.85	107.92	103.45
2	L2	1144	PSU	O2-C2-N1	-2.84	119.86	122.79
51	S1	1647	OMG	C2-N1-C6	-2.84	119.97	125.11
51	S1	29	OMU	O4-C4-C5	-2.84	120.27	125.16
1	L1	1539	A2M	N3-C4-N9	2.84	131.99	127.17
1	L1	69	A2M	C5-N7-C8	2.83	107.90	103.45
1	L1	1171	PSU	O2-C2-N1	-2.83	119.87	122.79
1	L1	1533	PSU	C6-C5-C4	2.83	120.08	118.17
1	L1	1373	A2M	N3-C4-N9	2.82	131.97	127.17
2	L2	1046	OMG	C2-N1-C6	-2.82	119.99	125.11
51	S1	2184	MA6	C5-N7-C8	2.82	107.89	103.45
51	S1	2185	MA6	C5-N7-C8	2.82	107.88	103.45
1	L1	1659	OMU	O4-C4-C5	-2.82	120.30	125.16
2	L2	655	OMG	C2-N1-C6	-2.82	120.00	125.11
1	L1	235	A2M	C5-N7-C8	2.81	107.87	103.45
2	L2	1303	PSU	C6-C5-C4	2.81	120.07	118.17
1	L1	1190	OMG	C2-N1-C6	-2.81	120.02	125.11
51	S1	1246	PSU	C6-C5-C4	2.81	120.07	118.17
2	L2	572	A2M	N3-C4-N9	2.80	131.94	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1372	A2M	N3-C4-N9	2.80	131.94	127.17
2	L2	527	A2M	N3-C4-N9	2.80	131.92	127.17
51	S1	1657	PSU	O2-C2-N1	-2.79	119.91	122.79
1	L1	407	A2M	C5-N7-C8	2.79	107.84	103.45
7	L7	43	A2M	C5-N7-C8	2.79	107.83	103.45
2	L2	1360	OMG	C2-N1-C6	-2.78	120.06	125.11
51	S1	1566	PSU	O2-C2-N1	-2.78	119.92	122.79
51	S1	1865	OMG	C2-N1-C6	-2.78	120.06	125.11
7	L7	74	PSU	C6-C5-C4	2.78	120.05	118.17
2	L2	1284	PSU	O2-C2-N1	-2.78	119.92	122.79
1	L1	856	OMG	C2-N1-C6	-2.78	120.07	125.11
2	L2	1229	OMG	C2-N1-C6	-2.78	120.08	125.11
2	L2	572	A2M	C5-N7-C8	2.78	107.81	103.45
1	L1	1539	A2M	C5-N7-C8	2.77	107.80	103.45
51	S1	1995	7MG	O6-C6-C5	-2.77	120.83	127.62
7	L7	162	A2M	C5-N7-C8	2.77	107.80	103.45
1	L1	927	A2M	C5-N7-C8	2.76	107.79	103.45
2	L2	1078	OMG	N2-C2-N1	2.76	122.59	116.76
2	L2	1152	PSU	O2-C2-N1	-2.76	119.95	122.79
2	L2	500	PSU	C6-C5-C4	2.75	120.03	118.17
2	L2	1265	PSU	O2-C2-N1	-2.75	119.95	122.79
2	L2	641	OMG	C2-N1-C6	-2.75	120.12	125.11
51	S1	479	A2M	C5-N7-C8	2.75	107.77	103.45
1	L1	697	A2M	C5-N7-C8	2.75	107.77	103.45
2	L2	71	OMG	C5-C6-N1	2.74	120.24	113.25
51	S1	1539	PSU	C6-C5-C4	2.74	120.03	118.17
52	S2	37	MIA	C5-C4-N9	2.74	108.80	105.81
2	L2	95	A2M	C5-N7-C8	2.74	107.75	103.45
51	S1	1623	OMG	N9-C4-N3	2.74	131.43	125.95
2	L2	534	OMG	C2-N1-C6	-2.73	120.16	125.11
51	S1	28	A2M	C5-N7-C8	2.73	107.74	103.45
51	S1	2046	PSU	O2-C2-N1	-2.73	119.97	122.79
2	L2	382	A2M	N3-C4-N9	2.73	131.80	127.17
1	L1	1190	OMG	N2-C2-N1	2.72	122.51	116.76
51	S1	668	A2M	N3-C4-N9	2.72	131.80	127.17
2	L2	1253	OMG	C5-C6-N1	2.72	120.17	113.25
2	L2	1384	A2M	C5-N7-C8	2.72	107.72	103.45
2	L2	1361	PSU	O2-C2-N1	-2.72	119.99	122.79
2	L2	1303	PSU	O2-C2-N1	-2.71	119.99	122.79
2	L2	655	OMG	C5-C6-N1	2.71	120.15	113.25
1	L1	1529	PSU	O2-C2-N1	-2.71	120.00	122.79
2	L2	1372	A2M	C5-N7-C8	2.70	107.70	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L7	43	A2M	N3-C4-N9	2.70	131.76	127.17
2	L2	1046	OMG	N9-C4-N3	2.69	131.34	125.95
2	L2	1361	PSU	C6-C5-C4	2.69	119.99	118.17
51	S1	1533	PSU	C6-C5-C4	2.68	119.98	118.17
2	L2	1078	OMG	C5-C6-N1	2.67	120.06	113.25
7	L7	166	PSU	O2-C2-N1	-2.67	120.03	122.79
1	L1	313	PSU	O2-C2-N1	-2.67	120.03	122.79
1	L1	1017	PSU	O2-C2-N1	-2.67	120.03	122.79
51	S1	1543	B8N	O4-C4-N3	-2.67	115.66	119.99
1	L1	856	OMG	C5-C6-N1	2.67	120.04	113.25
51	S1	1865	OMG	C5-C6-N1	2.67	120.04	113.25
2	L2	382	A2M	C5-N7-C8	2.66	107.64	103.45
2	L2	510	PSU	O2-C2-N1	-2.66	120.04	122.79
1	L1	1181	PSU	O2-C2-N1	-2.66	120.04	122.79
1	L1	1524	OMG	C5-C6-N1	2.66	120.02	113.25
51	S1	1647	OMG	C5-C6-N1	2.65	120.01	113.25
1	L1	1371	OMU	O4-C4-C5	-2.65	120.59	125.16
51	S1	1995	7MG	N9-C8-N7	2.65	107.12	103.37
7	L7	69	PSU	O2-C2-N1	-2.65	120.06	122.79
7	L7	75	OMG	C5-C6-N1	2.65	119.99	113.25
1	L1	1190	OMG	C5-C6-N1	2.64	119.98	113.25
2	L2	500	PSU	O2-C2-N1	-2.64	120.06	122.79
51	S1	1623	OMG	C5-C6-N1	2.64	119.98	113.25
1	L1	1373	A2M	C5-N7-C8	2.64	107.60	103.45
1	L1	1017	PSU	C6-C5-C4	2.64	119.96	118.17
51	S1	1995	7MG	N9-C4-N3	2.64	129.33	125.46
2	L2	1046	OMG	C5-C6-N1	2.64	119.96	113.25
2	L2	1231	OMG	C5-C6-N1	2.63	119.96	113.25
51	S1	2151	OMG	C5-C6-N1	2.63	119.95	113.25
2	L2	472	PSU	O2-C2-N1	-2.63	120.07	122.79
51	S1	1192	PSU	O2-C2-N1	-2.63	120.08	122.79
2	L2	593	PSU	O2-C2-N1	-2.62	120.08	122.79
7	L7	101	PSU	O2-C2-N1	-2.62	120.08	122.79
51	S1	600	OMG	N9-C4-N3	2.62	131.20	125.95
51	S1	1478	OMG	C5-C6-N1	2.62	119.92	113.25
2	L2	504	PSU	C6-C5-C4	2.62	119.94	118.17
2	L2	1229	OMG	C5-C6-N1	2.61	119.91	113.25
51	S1	1865	OMG	N9-C4-N3	2.61	131.18	125.95
51	S1	455	PSU	O2-C2-N1	-2.61	120.10	122.79
2	L2	686	OMG	C5-C6-N1	2.60	119.88	113.25
51	S1	33	PSU	O2-C2-N1	-2.60	120.10	122.79
2	L2	512	PSU	C6-C5-C4	2.60	119.93	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1318	PSU	C6-C5-C4	2.60	119.93	118.17
7	L7	69	PSU	C6-C5-C4	2.59	119.92	118.17
2	L2	597	PSU	O2-C2-N1	-2.59	120.11	122.79
2	L2	1360	OMG	N9-C4-N3	2.59	131.14	125.95
2	L2	71	OMG	N9-C4-N3	2.59	131.13	125.95
51	S1	600	OMG	C5-C6-N1	2.59	119.84	113.25
7	L7	101	PSU	C6-C5-C4	2.59	119.92	118.17
51	S1	1647	OMG	C8-N7-C5	2.58	108.86	104.26
2	L2	1360	OMG	C5-C6-N1	2.58	119.82	113.25
2	L2	1144	PSU	C6-C5-C4	2.58	119.92	118.17
2	L2	1264	PSU	O2-C2-N1	-2.58	120.13	122.79
2	L2	78	PSU	C6-C5-C4	2.58	119.91	118.17
2	L2	647	A2M	O4'-C1'-N9	2.57	113.03	108.09
2	L2	1194	PSU	O2-C2-N1	-2.57	120.14	122.79
2	L2	1318	PSU	O2-C2-N1	-2.57	120.14	122.79
51	S1	1533	PSU	O2-C2-N1	-2.56	120.14	122.79
2	L2	534	OMG	C5-C6-N1	2.56	119.78	113.25
2	L2	802	PSU	O2-C2-N1	-2.56	120.15	122.79
2	L2	591	A2M	C5-N7-C8	2.56	107.47	103.45
2	L2	78	PSU	O2-C2-N1	-2.56	120.15	122.79
51	S1	1647	OMG	N9-C4-N3	2.56	131.07	125.95
1	L1	305	A2M	O2'-C2'-C1'	2.55	113.84	108.99
1	L1	1177	PSU	O2-C2-N1	-2.55	120.16	122.79
2	L2	527	A2M	C4-N9-C8	2.55	108.41	105.74
52	S2	37	MIA	C4-N9-C8	2.55	108.41	105.74
2	L2	1231	OMG	N9-C4-N3	2.54	131.04	125.95
2	L2	641	OMG	C5-C6-N1	2.54	119.72	113.25
51	S1	1657	PSU	C6-C5-C4	2.53	119.88	118.17
2	L2	534	OMG	N9-C4-N3	2.53	131.01	125.95
2	L2	641	OMG	N2-C2-N1	2.53	122.10	116.76
1	L1	1190	OMG	C2'-C1'-N9	-2.53	109.44	114.24
2	L2	1253	OMG	O6-C6-C5	-2.52	119.87	126.53
2	L2	570	A2M	C4-C5-N7	-2.52	107.70	110.58
2	L2	1060	PSU	O2-C2-N1	-2.52	120.19	122.79
51	S1	897	A2M	C2'-C1'-N9	-2.52	109.61	113.75
7	L7	74	PSU	O2-C2-N1	-2.52	120.19	122.79
51	S1	1246	PSU	O2-C2-N1	-2.51	120.20	122.79
51	S1	1292	PSU	O2-C2-N1	-2.51	120.20	122.79
1	L1	1528	PSU	O2-C2-N1	-2.50	120.21	122.79
2	L2	1403	PSU	O2-C2-N1	-2.50	120.21	122.79
1	L1	1529	PSU	C6-C5-C4	2.50	119.86	118.17
2	L2	1284	PSU	C6-C5-C4	2.49	119.85	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	512	PSU	O2-C2-N1	-2.49	120.22	122.79
7	L7	75	OMG	N9-C4-N3	2.49	130.93	125.95
1	L1	940	PSU	O2-C2-N1	-2.49	120.22	122.79
51	S1	1623	OMG	O6-C6-C5	-2.48	119.97	126.53
2	L2	655	OMG	N9-C4-N3	2.48	130.91	125.95
2	L2	1213	PSU	O2-C2-N1	-2.48	120.23	122.79
52	S2	37	MIA	N3-C4-N9	2.48	130.13	126.99
51	S1	2061	5MC	C5-C6-N1	-2.47	120.63	123.31
1	L1	1181	PSU	C6-C5-C4	2.47	119.84	118.17
2	L2	510	PSU	C6-C5-C4	2.47	119.84	118.17
2	L2	662	PSU	O2-C2-N1	-2.46	120.25	122.79
51	S1	1865	OMG	O6-C6-C5	-2.46	120.03	126.53
2	L2	472	PSU	C6-C5-C4	2.46	119.83	118.17
2	L2	1360	OMG	O6-C6-C5	-2.45	120.06	126.53
51	S1	1478	OMG	O6-C6-C5	-2.45	120.07	126.53
2	L2	686	OMG	N9-C4-N3	2.45	130.85	125.95
1	L1	858	A2M	C4'-O4'-C1'	-2.44	104.07	109.47
2	L2	71	OMG	O6-C6-C5	-2.44	120.09	126.53
2	L2	560	OMU	O4'-C4'-C3'	-2.44	100.31	105.15
2	L2	1308	5MC	C4'-O4'-C1'	-2.44	104.09	109.47
7	L7	166	PSU	C6-C5-C4	2.43	119.82	118.17
51	S1	2046	PSU	C6-C5-C4	2.43	119.82	118.17
51	S1	2185	MA6	N3-C4-N9	2.43	131.30	127.17
2	L2	1185	A2M	C2'-C1'-N9	-2.43	109.75	113.75
2	L2	647	A2M	C6-C5-C4	2.43	120.49	117.18
2	L2	686	OMG	O6-C6-C5	-2.42	120.13	126.53
51	S1	1292	PSU	C6-C5-C4	2.42	119.81	118.17
2	L2	1046	OMG	O6-C6-C5	-2.42	120.14	126.53
51	S1	2151	OMG	N9-C4-N3	2.42	130.78	125.95
7	L7	75	OMG	O6-C6-C5	-2.41	120.16	126.53
51	S1	2184	MA6	C4-N9-C8	2.41	108.27	105.74
1	L1	1190	OMG	C8-N7-C5	2.41	108.55	104.26
2	L2	1229	OMG	O6-C6-C5	-2.41	120.18	126.53
2	L2	1253	OMG	N2-C2-N1	2.40	121.83	116.76
1	L1	1524	OMG	O2'-C2'-C1'	2.40	113.55	108.99
2	L2	655	OMG	O6-C6-C5	-2.40	120.19	126.53
1	L1	697	A2M	C2'-C1'-N9	-2.40	109.80	113.75
1	L1	858	A2M	C4-N9-C8	2.40	108.26	105.74
2	L2	641	OMG	O6-C6-C5	-2.40	120.20	126.53
1	L1	1526	PSU	O2-C2-N1	-2.40	120.31	122.79
2	L2	1413	PSU	C6-C5-C4	2.40	119.79	118.17
1	L1	940	PSU	C6-C5-C4	2.39	119.79	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	48	OMU	C1'-N1-C2	2.39	121.89	117.59
2	L2	662	PSU	C6-C5-C4	2.39	119.79	118.17
1	L1	1190	OMG	O6-C6-C5	-2.39	120.23	126.53
51	S1	600	OMG	C8-N7-C5	2.39	108.51	104.26
51	S1	1539	PSU	O2-C2-N1	-2.39	120.33	122.79
51	S1	2202	PSU	C6-C5-C4	2.39	119.78	118.17
51	S1	2151	OMG	O6-C6-C5	-2.38	120.25	126.53
2	L2	1231	OMG	O6-C6-C5	-2.38	120.25	126.53
2	L2	686	OMG	C8-N7-C5	2.38	108.50	104.26
51	S1	1478	OMG	C8-N7-C5	2.37	108.49	104.26
1	L1	856	OMG	N9-C4-N3	2.37	130.70	125.95
51	S1	1647	OMG	O6-C6-C5	-2.37	120.27	126.53
1	L1	1524	OMG	C8-N7-C5	2.37	108.48	104.26
1	L1	1524	OMG	N9-C4-N3	2.37	130.69	125.95
51	S1	2185	MA6	C4-C5-N7	-2.37	107.88	110.58
1	L1	422	PSU	O2-C2-N1	-2.36	120.36	122.79
2	L2	1229	OMG	C8-N7-C5	2.36	108.46	104.26
2	L2	655	OMG	C8-N7-C5	2.36	108.46	104.26
51	S1	600	OMG	O6-C6-C5	-2.35	120.32	126.53
2	L2	1185	A2M	C4-C5-N7	-2.35	107.89	110.58
2	L2	641	OMG	C8-N7-C5	2.35	108.45	104.26
51	S1	668	A2M	C4-C5-N7	-2.35	107.89	110.58
1	L1	1528	PSU	C6-C5-C4	2.35	119.76	118.17
51	S1	1865	OMG	C8-N7-C5	2.35	108.44	104.26
1	L1	422	PSU	C6-C5-C4	2.35	119.76	118.17
1	L1	856	OMG	O6-C6-C5	-2.35	120.34	126.53
2	L2	1078	OMG	C8-N7-C5	2.35	108.44	104.26
1	L1	856	OMG	C8-N7-C5	2.34	108.43	104.26
2	L2	534	OMG	O6-C6-C5	-2.34	120.35	126.53
1	L1	1524	OMG	O6-C6-C5	-2.34	120.37	126.53
2	L2	1058	PSU	O2-C2-N1	-2.33	120.38	122.79
1	L1	858	A2M	O4'-C1'-N9	2.33	112.56	108.09
2	L2	1229	OMG	N9-C4-N3	2.33	130.60	125.95
2	L2	597	PSU	C6-C5-C4	2.33	119.74	118.17
51	S1	2185	MA6	C5-C4-N9	2.32	108.34	105.81
51	S1	1478	OMG	N2-C2-N1	2.32	121.65	116.76
51	S1	2151	OMG	C8-N7-C5	2.32	108.39	104.26
2	L2	1078	OMG	O6-C6-C5	-2.32	120.42	126.53
1	L1	858	A2M	C4-C5-N7	-2.32	107.93	110.58
2	L2	1078	OMG	C6-C5-N7	2.31	134.49	130.29
2	L2	502	A2M	C4-N9-C8	2.30	108.15	105.74
1	L1	235	A2M	C4-C5-N7	-2.30	107.96	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	665	A2M	C4-C5-N7	-2.29	107.97	110.58
2	L2	604	A2M	C4-C5-N7	-2.28	107.97	110.58
2	L2	527	A2M	C4-C5-N7	-2.28	107.98	110.58
51	S1	897	A2M	C4-C5-N7	-2.28	107.98	110.58
2	L2	1403	PSU	O4'-C1'-C2'	2.28	108.30	105.15
51	S1	98	A2M	C4-C5-N7	-2.28	107.98	110.58
2	L2	1253	OMG	N9-C4-N3	2.28	130.50	125.95
2	L2	570	A2M	C5-C4-N9	2.27	108.29	105.81
1	L1	48	OMU	O4'-C1'-N1	2.27	113.50	108.36
2	L2	1046	OMG	C8-N7-C5	2.27	108.30	104.26
1	L1	1526	PSU	O4'-C1'-C2'	2.26	108.28	105.15
2	L2	382	A2M	C5-C4-N9	2.26	108.28	105.81
1	L1	1177	PSU	C6-C5-C4	2.26	119.70	118.17
51	S1	28	A2M	C4-N9-C8	2.26	108.11	105.74
2	L2	95	A2M	C4-C5-N7	-2.26	108.00	110.58
2	L2	1231	OMG	C8-N7-C5	2.25	108.27	104.26
51	S1	668	A2M	C3'-C2'-C1'	2.25	107.12	102.81
1	L1	305	A2M	C4-C5-N7	-2.25	108.01	110.58
2	L2	382	A2M	C4-C5-N7	-2.24	108.02	110.58
1	L1	305	A2M	O4'-C1'-C2'	-2.24	102.73	106.59
2	L2	502	A2M	C4-C5-N7	-2.24	108.02	110.58
2	L2	71	OMG	C8-N7-C5	2.24	108.25	104.26
1	L1	69	A2M	C4-C5-N7	-2.23	108.03	110.58
7	L7	43	A2M	C4-N9-C8	2.23	108.08	105.74
1	L1	1190	OMG	C6-C5-N7	2.23	134.34	130.29
51	S1	8	OMU	C3'-C2'-C1'	-2.22	98.55	102.81
1	L1	235	A2M	C5-C4-N9	2.22	108.23	105.81
51	S1	1623	OMG	C8-N7-C5	2.21	108.19	104.26
1	L1	69	A2M	C3'-C2'-C1'	2.21	107.03	102.81
7	L7	75	OMG	C8-N7-C5	2.20	108.19	104.26
2	L2	1360	OMG	C8-N7-C5	2.20	108.18	104.26
2	L2	95	A2M	C6-C5-C4	2.20	120.18	117.18
2	L2	527	A2M	O4'-C1'-C2'	-2.19	102.82	106.59
1	L1	407	A2M	C4-C5-N7	-2.19	108.08	110.58
51	S1	1833	OMU	O2-C2-N1	-2.19	119.95	122.80
2	L2	626	PSU	O2-C2-N1	-2.19	120.53	122.79
2	L2	534	OMG	C8-N7-C5	2.19	108.16	104.26
1	L1	305	A2M	C4-N9-C8	2.18	108.03	105.74
2	L2	570	A2M	C6-C5-C4	2.18	120.15	117.18
1	L1	1539	A2M	C4-C5-N7	-2.18	108.09	110.58
51	S1	479	A2M	C4-C5-N7	-2.18	108.09	110.58
2	L2	1372	A2M	C4-C5-N7	-2.18	108.09	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	665	A2M	C4-N9-C8	2.17	108.02	105.74
51	S1	512	A2M	C4-N9-C8	2.17	108.02	105.74
2	L2	1253	OMG	C8-N7-C5	2.17	108.13	104.26
7	L7	101	PSU	O4'-C1'-C2'	2.17	108.15	105.15
1	L1	927	A2M	C6-C5-C4	2.17	120.14	117.18
51	S1	98	A2M	C4-N9-C8	2.17	108.01	105.74
51	S1	29	OMU	O2-C2-N1	-2.16	119.98	122.80
51	S1	2151	OMG	N2-C2-N1	2.16	121.33	116.76
2	L2	14	OMC	O3'-C3'-C2'	2.16	117.23	111.19
1	L1	774	PSU	C2'-C3'-C4'	-2.16	98.44	102.61
2	L2	1185	A2M	C4'-O4'-C1'	-2.15	104.71	109.47
51	S1	1543	B8N	C5'-C4'-C3'	-2.15	107.47	115.21
51	S1	1192	PSU	C6-C5-C4	2.15	119.62	118.17
52	S2	37	MIA	C4-C5-C6	2.15	118.57	116.78
51	S1	1621	OMU	O2-C2-N1	-2.14	120.01	122.80
51	S1	668	A2M	C4-N9-C8	2.14	107.98	105.74
2	L2	572	A2M	C4-C5-N7	-2.14	108.14	110.58
2	L2	1185	A2M	C6-C5-C4	2.14	120.10	117.18
2	L2	1303	PSU	O4'-C1'-C2'	2.13	108.11	105.15
2	L2	1078	OMG	C4-C5-N7	-2.13	107.29	110.67
1	L1	1190	OMG	C4-C5-N7	-2.13	107.29	110.67
7	L7	43	A2M	C4-C5-N7	-2.13	108.15	110.58
51	S1	897	A2M	C4-N9-C8	2.13	107.97	105.74
52	S2	37	MIA	C16-C14-C15	2.12	119.47	114.59
1	L1	235	A2M	C6-C5-C4	2.12	120.07	117.18
51	S1	512	A2M	C4-C5-N7	-2.11	108.16	110.58
51	S1	98	A2M	C6-C5-C4	2.11	120.06	117.18
51	S1	1478	OMG	N9-C4-N3	2.11	130.18	125.95
2	L2	593	PSU	C6-C5-C4	2.11	119.60	118.17
1	L1	697	A2M	C4-C5-N7	-2.11	108.17	110.58
2	L2	1384	A2M	C4-C5-N7	-2.11	108.17	110.58
51	S1	1543	B8N	C31-N3-C4	2.11	120.16	117.18
2	L2	802	PSU	O4'-C1'-C2'	2.10	108.06	105.15
2	L2	591	A2M	C6-C5-C4	2.09	120.04	117.18
51	S1	1478	OMG	C2'-C1'-N9	-2.09	110.27	114.24
1	L1	927	A2M	C4-C5-N7	-2.09	108.19	110.58
7	L7	162	A2M	C4-C5-N7	-2.08	108.20	110.58
51	S1	668	A2M	C5-C4-N9	2.08	108.08	105.81
2	L2	560	OMU	C2'-C3'-C4'	-2.08	97.52	101.99
51	S1	98	A2M	C2'-C1'-N9	-2.07	110.34	113.75
2	L2	572	A2M	C4-N9-C8	2.07	107.91	105.74
51	S1	2185	MA6	C4-N9-C8	2.07	107.91	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	2184	MA6	C4-C5-N7	-2.07	108.22	110.58
2	L2	655	OMG	N1-C2-N3	-2.07	119.54	123.32
2	L2	686	OMG	N2-C2-N1	2.06	121.12	116.76
1	L1	305	A2M	C6-C5-C4	2.06	119.99	117.18
51	S1	661	OMU	O2-C2-N1	-2.06	120.12	122.80
1	L1	69	A2M	O3'-C3'-C4'	2.06	116.99	111.08
1	L1	1371	OMU	O2-C2-N3	-2.06	117.70	121.49
7	L7	69	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	L2	655	OMG	N2-C2-N1	2.05	121.09	116.76
2	L2	560	OMU	C2'-C1'-N1	-2.05	110.34	114.24
2	L2	1185	A2M	C5-C4-N9	2.05	108.05	105.81
1	L1	1373	A2M	C4-C5-N7	-2.05	108.24	110.58
2	L2	667	OMU	O2-C2-N1	-2.05	120.13	122.80
51	S1	897	A2M	C5-C4-N9	2.04	108.04	105.81
2	L2	647	A2M	C4-C5-N7	-2.04	108.25	110.58
51	S1	479	A2M	C6-C5-C4	2.04	119.96	117.18
1	L1	856	OMG	N2-C2-N1	2.04	121.07	116.76
2	L2	626	PSU	C6-C5-C4	2.04	119.55	118.17
2	L2	1231	OMG	N2-C2-N1	2.04	121.06	116.76
2	L2	604	A2M	C6-C5-C4	2.03	119.96	117.18
51	S1	512	A2M	C6-C5-C4	2.03	119.96	117.18
2	L2	572	A2M	C2'-C1'-N9	-2.03	110.41	113.75
1	L1	1190	OMG	N1-C2-N3	-2.03	119.60	123.32
1	L1	69	A2M	C4-N9-C8	2.03	107.87	105.74
51	S1	1647	OMG	C4-C5-N7	-2.02	107.46	110.67
51	S1	455	PSU	C6-C5-C4	2.02	119.53	118.17
1	L1	1524	OMG	C4-C5-N7	-2.02	107.48	110.67
1	L1	69	A2M	C5'-C4'-C3'	-2.01	107.97	115.21
1	L1	1524	OMG	N2-C2-N1	2.01	121.00	116.76
1	L1	407	A2M	C5-C4-N9	2.01	108.00	105.81
1	L1	697	A2M	C4-N9-C8	2.00	107.84	105.74
51	S1	28	A2M	C4-C5-N7	-2.00	108.29	110.58
2	L2	382	A2M	C6-C5-C4	2.00	119.91	117.18
51	S1	1865	OMG	N1-C2-N3	-2.00	119.66	123.32
7	L7	162	A2M	C6-C5-C4	2.00	119.91	117.18
1	L1	1107	OMU	O2-C2-N1	-2.00	120.19	122.80
51	S1	1566	PSU	C6-C5-C4	2.00	119.52	118.17
51	S1	1647	OMG	N1-C2-N3	-2.00	119.66	123.32
2	L2	641	OMG	C4-C5-N7	-2.00	107.50	110.67
1	L1	858	A2M	O4'-C4'-C3'	-2.00	101.18	105.15

There are no chirality outliers.

All (161) 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	305	A2M	O4'-C4'-C5'-O5'
1	L1	681	A2M	O4'-C4'-C5'-O5'
1	L1	681	A2M	C1'-C2'-O2'-CM'
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	955	A2M	C1'-C2'-O2'-CM'
1	L1	959	OMG	C1'-C2'-O2'-CM2
1	L1	1371	OMU	O4'-C1'-N1-C2
1	L1	1371	OMU	O4'-C1'-N1-C6
1	L1	1524	OMG	C1'-C2'-O2'-CM2
1	L1	1540	OMG	O4'-C4'-C5'-O5'
2	L2	95	A2M	C1'-C2'-O2'-CM'
2	L2	443	OMC	C2'-C1'-N1-C6
2	L2	502	A2M	O4'-C4'-C5'-O5'
2	L2	534	OMG	O4'-C4'-C5'-O5'
2	L2	560	OMU	C1'-C2'-O2'-CM2
2	L2	647	A2M	O4'-C4'-C5'-O5'
2	L2	647	A2M	C1'-C2'-O2'-CM'
2	L2	686	OMG	O4'-C4'-C5'-O5'
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	1229	OMG	O4'-C4'-C5'-O5'
2	L2	1264	PSU	C3'-C4'-C5'-O5'
2	L2	1264	PSU	O4'-C4'-C5'-O5'
51	S1	18	OMC	C1'-C2'-O2'-CM2
51	S1	29	OMU	C1'-C2'-O2'-CM2
51	S1	512	A2M	C1'-C2'-O2'-CM'
51	S1	600	OMG	O4'-C4'-C5'-O5'
51	S1	668	A2M	C1'-C2'-O2'-CM'
51	S1	1543	B8N	N34-C33-C34-O35
51	S1	1543	B8N	C31-C32-C33-N34
51	S1	1566	PSU	O4'-C4'-C5'-O5'
51	S1	1662	OMU	C1'-C2'-O2'-CM2
51	S1	1829	OMG	C1'-C2'-O2'-CM2
51	S1	2021	A2M	C1'-C2'-O2'-CM'
51	S1	2059	OMC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
51	S1	2059	OMC	O4'-C1'-N1-C6
2	L2	443	OMC	C2'-C1'-N1-C2
1	L1	1010	OMC	O4'-C4'-C5'-O5'
1	L1	1171	PSU	C3'-C4'-C5'-O5'
1	L1	1528	PSU	O4'-C4'-C5'-O5'
2	L2	14	OMC	C3'-C4'-C5'-O5'
2	L2	502	A2M	C3'-C4'-C5'-O5'
2	L2	534	OMG	C3'-C4'-C5'-O5'
2	L2	686	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'
51	S1	455	PSU	C3'-C4'-C5'-O5'
51	S1	668	A2M	O4'-C4'-C5'-O5'
51	S1	668	A2M	C3'-C4'-C5'-O5'
51	S1	1566	PSU	C3'-C4'-C5'-O5'
51	S1	1543	B8N	N34-C33-C34-O36
1	L1	305	A2M	C3'-C4'-C5'-O5'
1	L1	313	PSU	C3'-C4'-C5'-O5'
1	L1	681	A2M	C3'-C4'-C5'-O5'
1	L1	1171	PSU	O4'-C4'-C5'-O5'
1	L1	1540	OMG	C3'-C4'-C5'-O5'
2	L2	14	OMC	O4'-C4'-C5'-O5'
2	L2	665	A2M	C3'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C4'-C5'-O5'
51	S1	98	A2M	O4'-C4'-C5'-O5'
51	S1	1995	7MG	C3'-C4'-C5'-O5'
51	S1	2061	5MC	O4'-C4'-C5'-O5'
51	S1	2061	5MC	C3'-C4'-C5'-O5'
51	S1	2151	OMG	C3'-C4'-C5'-O5'
2	L2	1046	OMG	C3'-C4'-C5'-O5'
51	S1	600	OMG	C3'-C4'-C5'-O5'
51	S1	8	OMU	C2'-C1'-N1-C6
1	L1	1010	OMC	C3'-C4'-C5'-O5'
1	L1	1664	PSU	C3'-C4'-C5'-O5'
2	L2	647	A2M	C3'-C4'-C5'-O5'
4	L4	74	OMG	C3'-C4'-C5'-O5'
51	S1	1995	7MG	O4'-C4'-C5'-O5'
1	L1	313	PSU	O4'-C4'-C5'-O5'
1	L1	1664	PSU	O4'-C4'-C5'-O5'
2	L2	665	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	L2	1185	A2M	C3'-C4'-C5'-O5'
51	S1	455	PSU	O4'-C4'-C5'-O5'
51	S1	2151	OMG	O4'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C6
1	L1	1017	PSU	O4'-C4'-C5'-O5'
1	L1	69	A2M	C3'-C4'-C5'-O5'
1	L1	1017	PSU	C3'-C4'-C5'-O5'
51	S1	8	OMU	C3'-C4'-C5'-O5'
51	S1	1543	B8N	C3'-C4'-C5'-O5'
51	S1	1543	B8N	C32-C33-C34-O35
1	L1	959	OMG	O4'-C4'-C5'-O5'
1	L1	1528	PSU	C3'-C4'-C5'-O5'
51	S1	1543	B8N	C32-C33-C34-O36
2	L2	570	A2M	C2'-C1'-N9-C8
1	L1	69	A2M	O4'-C4'-C5'-O5'
1	L1	959	OMG	C3'-C4'-C5'-O5'
51	S1	2140	OMC	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C31-C32-C33-C34
2	L2	527	A2M	C3'-C4'-C5'-O5'
51	S1	668	A2M	C2'-C1'-N9-C8
51	S1	8	OMU	O4'-C1'-N1-C6
51	S1	512	A2M	C3'-C4'-C5'-O5'
51	S1	1543	B8N	N3-C31-C32-C33
4	L4	74	OMG	O4'-C4'-C5'-O5'
51	S1	33	PSU	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C4'-C5'-O5'-P
51	S1	8	OMU	C2'-C1'-N1-C2
1	L1	1526	PSU	C3'-C4'-C5'-O5'
2	L2	560	OMU	C3'-C4'-C5'-O5'
2	L2	1078	OMG	O4'-C4'-C5'-O5'
2	L2	443	OMC	O4'-C1'-N1-C2
2	L2	1308	5MC	O4'-C1'-N1-C6
1	L1	681	A2M	C4'-C5'-O5'-P
1	L1	510	PSU	O4'-C1'-C5-C4
1	L1	1526	PSU	O4'-C1'-C5-C4
2	L2	1361	PSU	O4'-C1'-C5-C4
51	S1	1657	PSU	O4'-C1'-C5-C4
2	L2	570	A2M	C2'-C1'-N9-C4
51	S1	1192	PSU	C3'-C4'-C5'-O5'
2	L2	443	OMC	O4'-C1'-N1-C6
2	L2	1308	5MC	C2'-C1'-N1-C2
51	S1	2185	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
1	L1	1371	OMU	C3'-C4'-C5'-O5'
51	S1	1192	PSU	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C1'-N1-C2
2	L2	527	A2M	C3'-C2'-O2'-CM'
51	S1	8	OMU	C3'-C2'-O2'-CM2
51	S1	1550	OMG	C3'-C2'-O2'-CM2
2	L2	1248	OMC	C4'-C5'-O5'-P
51	S1	1478	OMG	C4'-C5'-O5'-P
1	L1	1526	PSU	O4'-C4'-C5'-O5'
2	L2	1078	OMG	C3'-C4'-C5'-O5'
51	S1	1543	B8N	O4'-C4'-C5'-O5'
51	S1	2059	OMC	O4'-C4'-C5'-O5'
51	S1	668	A2M	O4'-C1'-N9-C8
2	L2	560	OMU	C4'-C5'-O5'-P
2	L2	1361	PSU	C4'-C5'-O5'-P
51	S1	1829	OMG	C4'-C5'-O5'-P
2	L2	527	A2M	O4'-C4'-C5'-O5'
4	L4	74	OMG	C1'-C2'-O2'-CM2
51	S1	2140	OMC	C1'-C2'-O2'-CM2
2	L2	1308	5MC	O4'-C1'-N1-C2
2	L2	1361	PSU	O4'-C1'-C5-C6
51	S1	2202	PSU	O4'-C1'-C5-C6
51	S1	1979	OMU	C4'-C5'-O5'-P
2	L2	56	OMU	O4'-C4'-C5'-O5'
51	S1	98	A2M	C3'-C4'-C5'-O5'
2	L2	570	A2M	O4'-C1'-N9-C8
2	L2	1185	A2M	O4'-C4'-C5'-O5'
2	L2	527	A2M	C2'-C1'-N9-C8
2	L2	647	A2M	O4'-C1'-N9-C8
1	L1	1526	PSU	C4'-C5'-O5'-P
1	L1	1539	A2M	C3'-C2'-O2'-CM'
51	S1	668	A2M	C2'-C1'-N9-C4
51	S1	1833	OMU	O4'-C4'-C5'-O5'
1	L1	858	A2M	O4'-C1'-N9-C8
51	S1	1539	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

64 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S1	2059	OMC	1	0
51	S1	1292	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S1	1829	OMG	1	0
1	L1	422	PSU	1	0
2	L2	14	OMC	3	0
1	L1	856	OMG	1	0
2	L2	512	PSU	1	0
7	L7	166	PSU	1	0
2	L2	604	A2M	2	0
1	L1	1527	OMC	1	0
2	L2	1046	OMG	1	0
51	S1	1478	OMG	1	0
2	L2	1060	PSU	1	0
1	L1	1539	A2M	1	0
1	L1	955	A2M	1	0
1	L1	69	A2M	1	0
2	L2	382	A2M	2	0
2	L2	591	A2M	2	0
2	L2	1372	A2M	2	0
51	S1	29	OMU	3	0
7	L7	162	A2M	1	0
1	L1	695	OMC	2	0
2	L2	665	A2M	1	0
2	L2	1360	OMG	2	0
1	L1	48	OMU	1	0
2	L2	1384	A2M	2	0
51	S1	600	OMG	1	0
1	L1	1190	OMG	1	0
2	L2	1253	OMG	2	0
51	S1	1662	OMU	1	0
51	S1	2048	PSU	1	0
1	L1	845	OMU	4	0
51	S1	1995	7MG	2	0
2	L2	1317	OMC	1	0
51	S1	479	A2M	1	0
2	L2	1413	PSU	1	0
51	S1	1621	OMU	1	0
1	L1	1171	PSU	1	0
2	L2	1152	PSU	1	0
2	L2	597	PSU	2	0
2	L2	1264	PSU	1	0
51	S1	512	A2M	2	0
1	L1	959	OMG	1	0
2	L2	1318	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S1	1539	PSU	1	0
7	L7	43	A2M	1	0
1	L1	681	A2M	1	0
1	L1	1373	A2M	1	0
51	S1	18	OMC	3	0
2	L2	560	OMU	2	0
51	S1	1623	OMG	1	0
2	L2	570	A2M	1	0
2	L2	1078	OMG	2	0
51	S1	38	OMC	2	0
51	S1	2202	PSU	1	0
1	L1	1533	PSU	1	0
2	L2	95	A2M	1	0
51	S1	2151	OMG	1	0
7	L7	101	PSU	1	0
7	L7	75	OMG	1	0
2	L2	1308	5MC	1	0
51	S1	661	OMU	1	0
2	L2	1303	PSU	1	0
2	L2	1185	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 520 ligands modelled in this entry, 519 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	$\# Z > 2$
93	A1H4F	L2	1601	-	32,32,32	4.46	11 (34%)	39,42,42	1.40	5 (12%)

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
93	A1H4F	L2	1601	-	-	9/26/39/39	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	L2	1601	A1H4F	C03-C02	-18.01	1.28	1.53
93	L2	1601	A1H4F	C27-C05	-12.18	1.29	1.53
93	L2	1601	A1H4F	C02-C27	6.50	1.65	1.53
93	L2	1601	A1H4F	C13-N14	6.09	1.46	1.34
93	L2	1601	A1H4F	C05-N04	3.96	1.55	1.47
93	L2	1601	A1H4F	O28-C29	3.86	1.43	1.35
93	L2	1601	A1H4F	C06-C05	3.12	1.59	1.53
93	L2	1601	A1H4F	C03-N04	2.72	1.56	1.47
93	L2	1601	A1H4F	C06-C07	2.55	1.57	1.51
93	L2	1601	A1H4F	O11-C10	2.25	1.42	1.37
93	L2	1601	A1H4F	C12-C13	2.05	1.55	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	L2	1601	A1H4F	O28-C29-C30	5.16	120.30	111.09
93	L2	1601	A1H4F	C12-C13-N14	3.01	121.61	116.41
93	L2	1601	A1H4F	C12-O11-C10	-2.83	112.57	117.63
93	L2	1601	A1H4F	O23-C21-C15	2.19	120.92	113.51
93	L2	1601	A1H4F	O23-C21-O22	-2.08	119.36	124.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

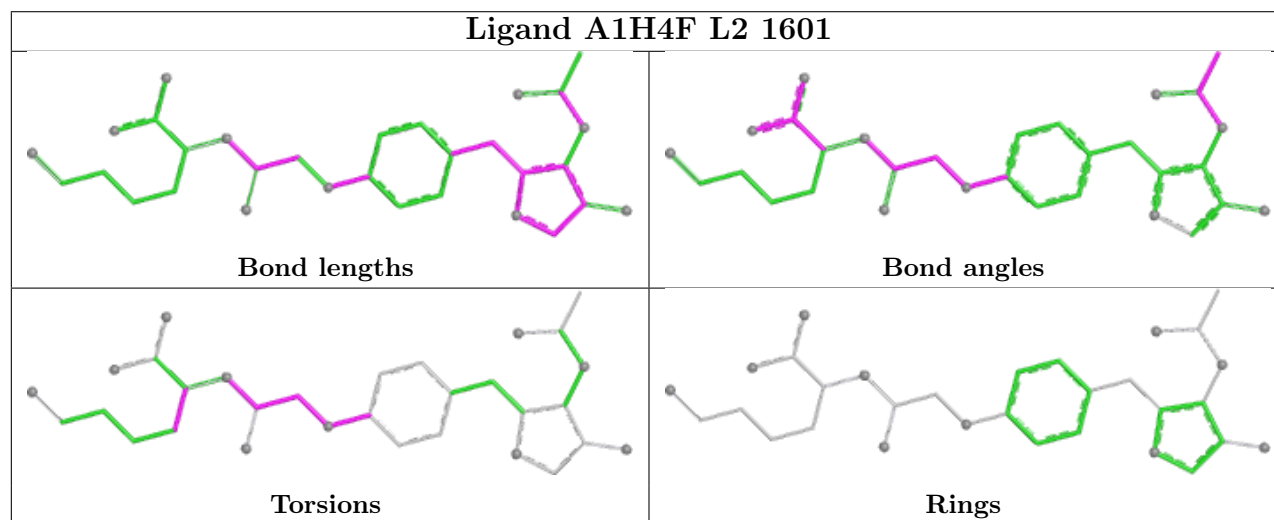
Mol	Chain	Res	Type	Atoms
93	L2	1601	A1H4F	C12-C13-N14-C15
93	L2	1601	A1H4F	O24-C13-N14-C15
93	L2	1601	A1H4F	C09-C10-O11-C12
93	L2	1601	A1H4F	C25-C10-O11-C12
93	L2	1601	A1H4F	N14-C15-C16-C17
93	L2	1601	A1H4F	C21-C15-C16-C17
93	L2	1601	A1H4F	O11-C12-C13-N14
93	L2	1601	A1H4F	O11-C12-C13-O24
93	L2	1601	A1H4F	C13-C12-O11-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
93	L2	1601	A1H4F	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	S1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S1	1543:B8N	O3'	1544:5MC	P	3.54
1	S1	1542:C	O3'	1543:B8N	P	2.98

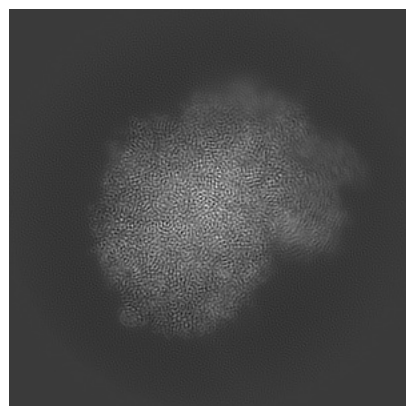
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19576. These allow visual inspection of the internal detail of the map and identification of artifacts.

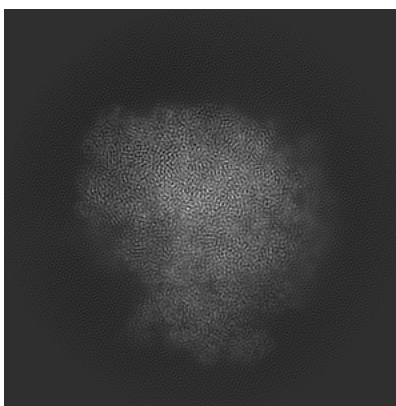
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

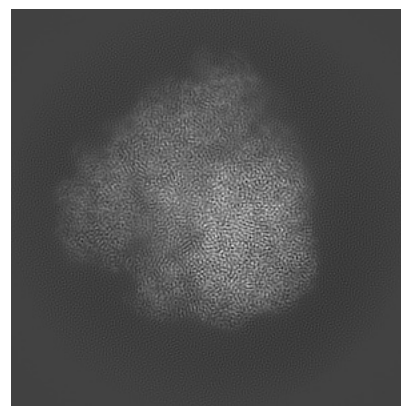
6.1.1 Primary map



X

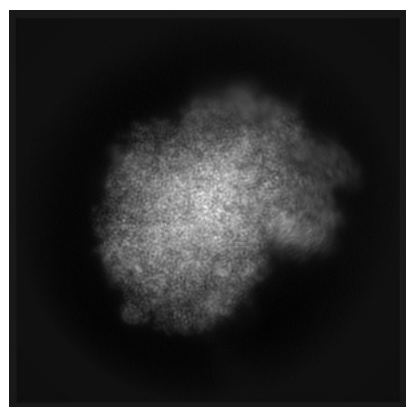


Y

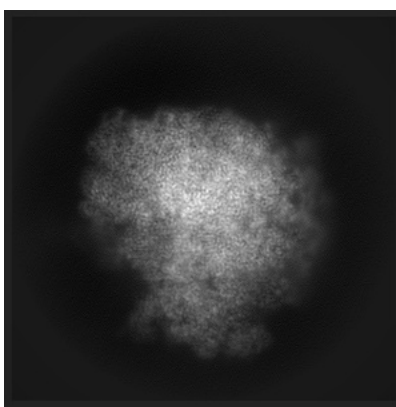


Z

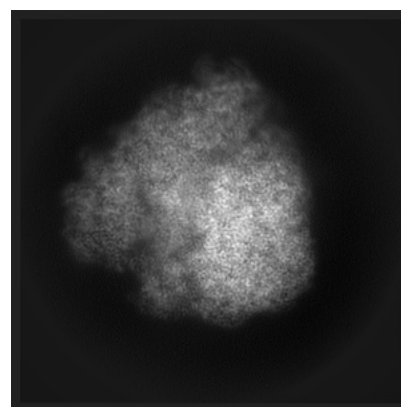
6.1.2 Raw map



X



Y

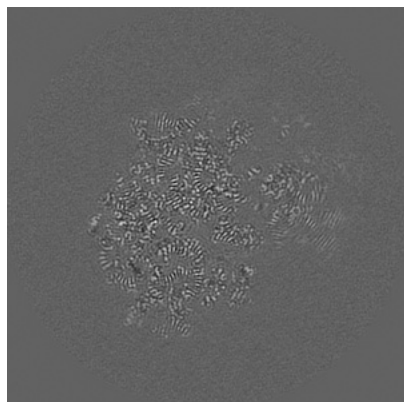


Z

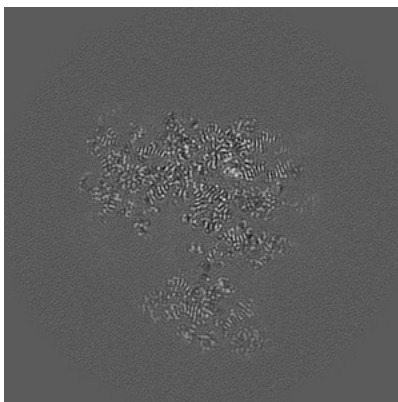
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

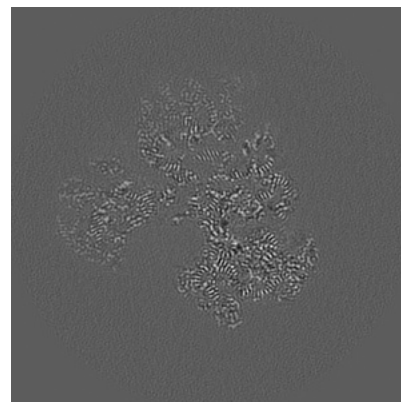
6.2.1 Primary map



X Index: 240

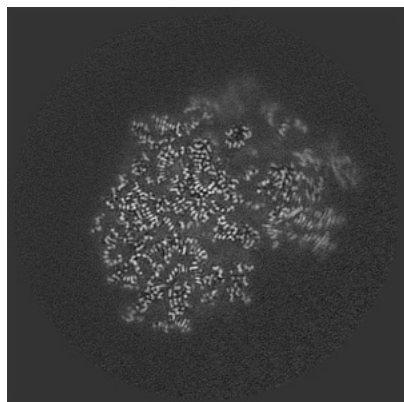


Y Index: 240

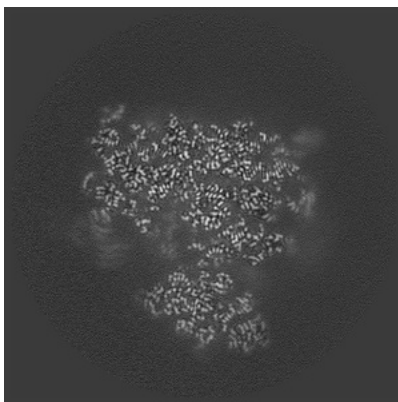


Z Index: 240

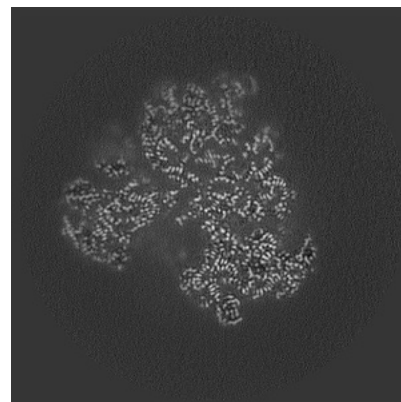
6.2.2 Raw map



X Index: 240



Y Index: 240

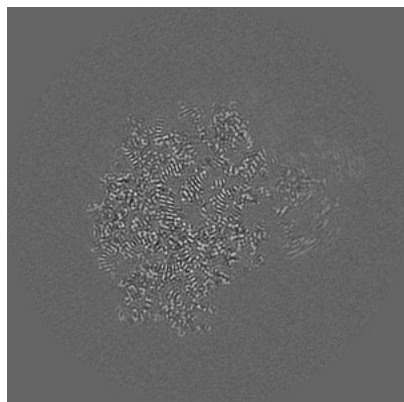


Z Index: 240

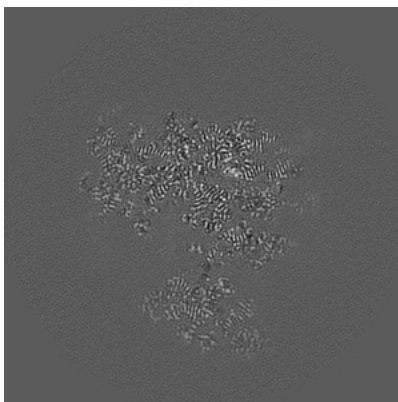
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

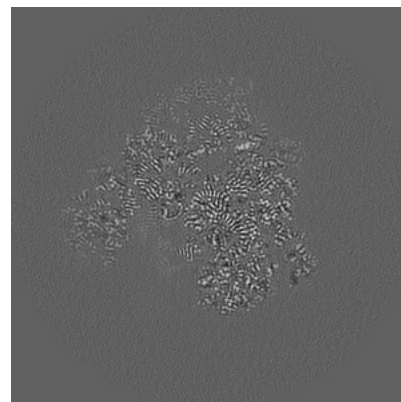
6.3.1 Primary map



X Index: 270

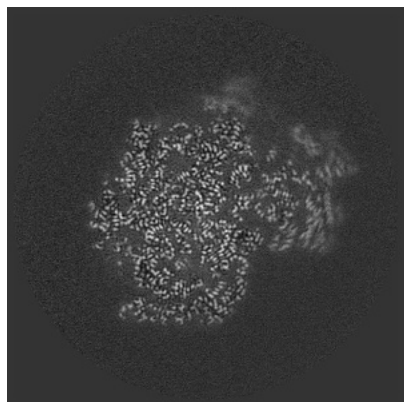


Y Index: 240

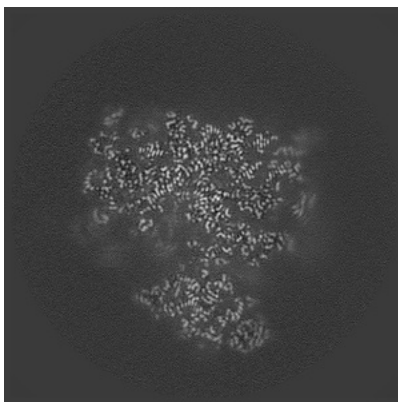


Z Index: 259

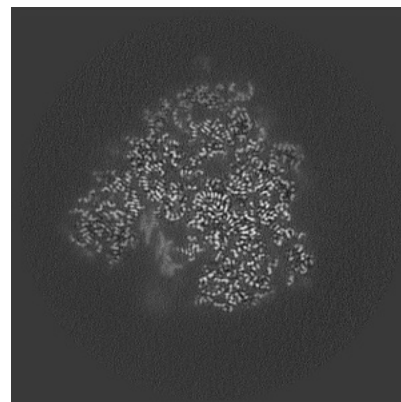
6.3.2 Raw map



X Index: 255



Y Index: 236

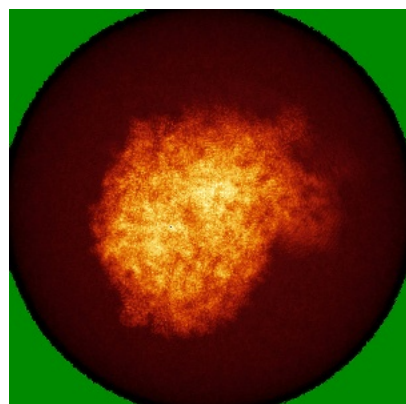


Z Index: 259

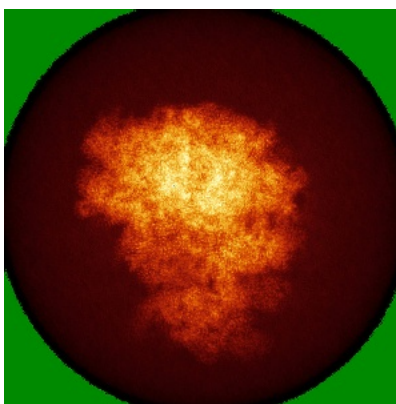
The images above show the largest variance slices of the map in three orthogonal directions.

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

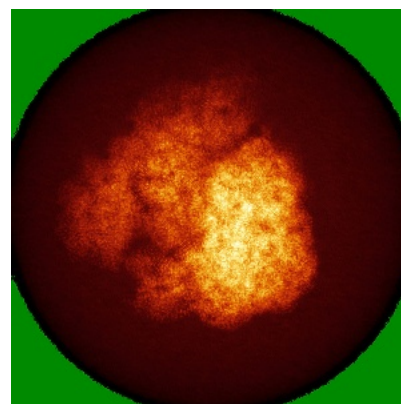
6.4.1 Primary map



X

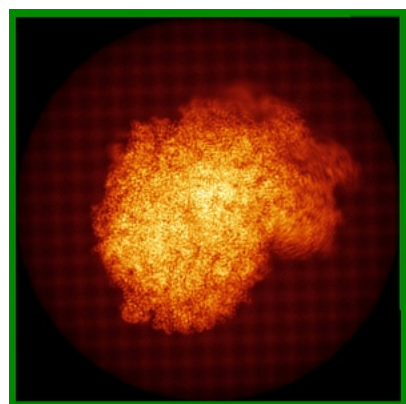


Y

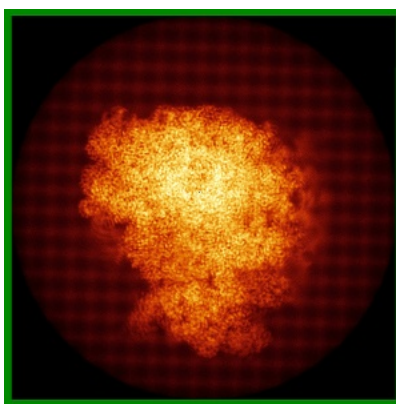


Z

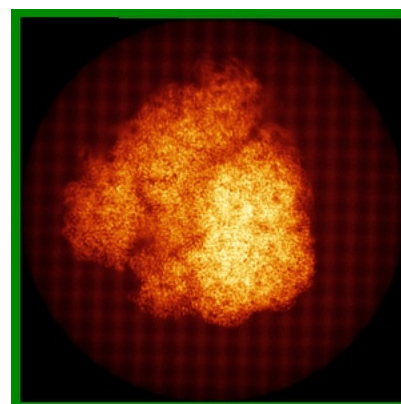
6.4.2 Raw map



X



Y

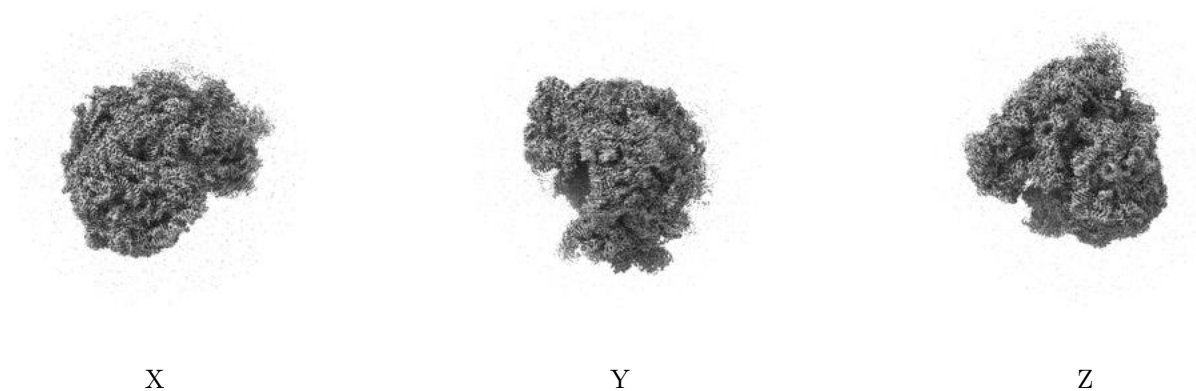


Z

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

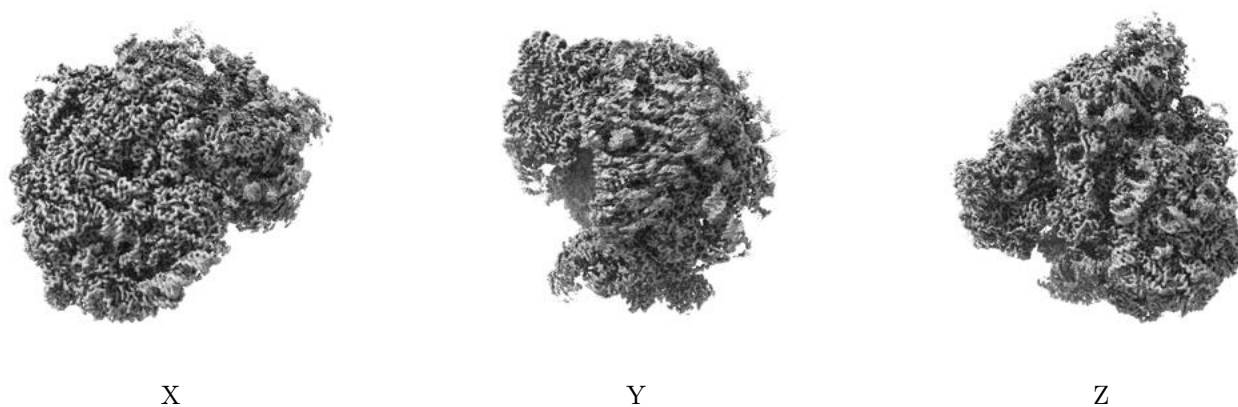
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

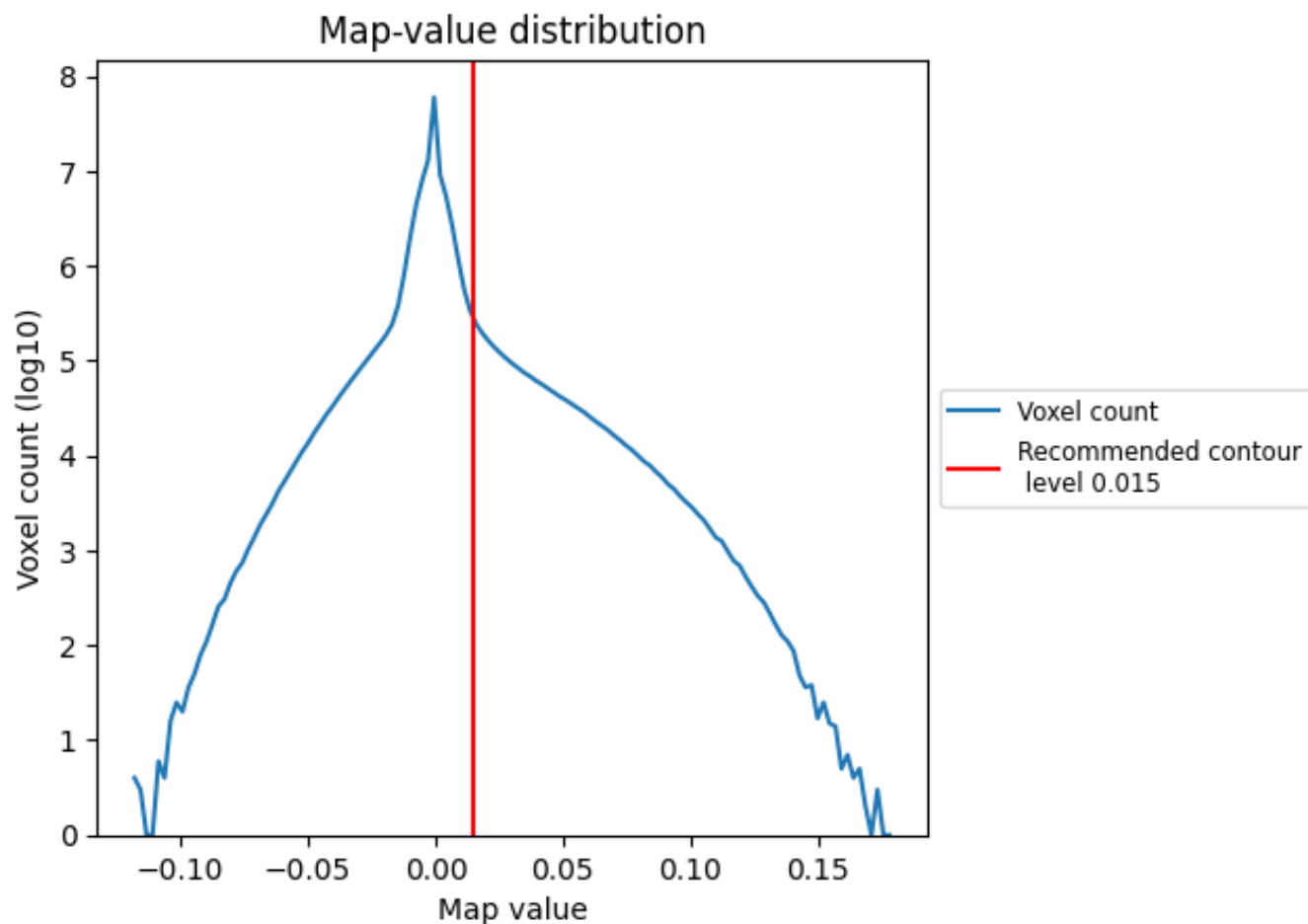
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

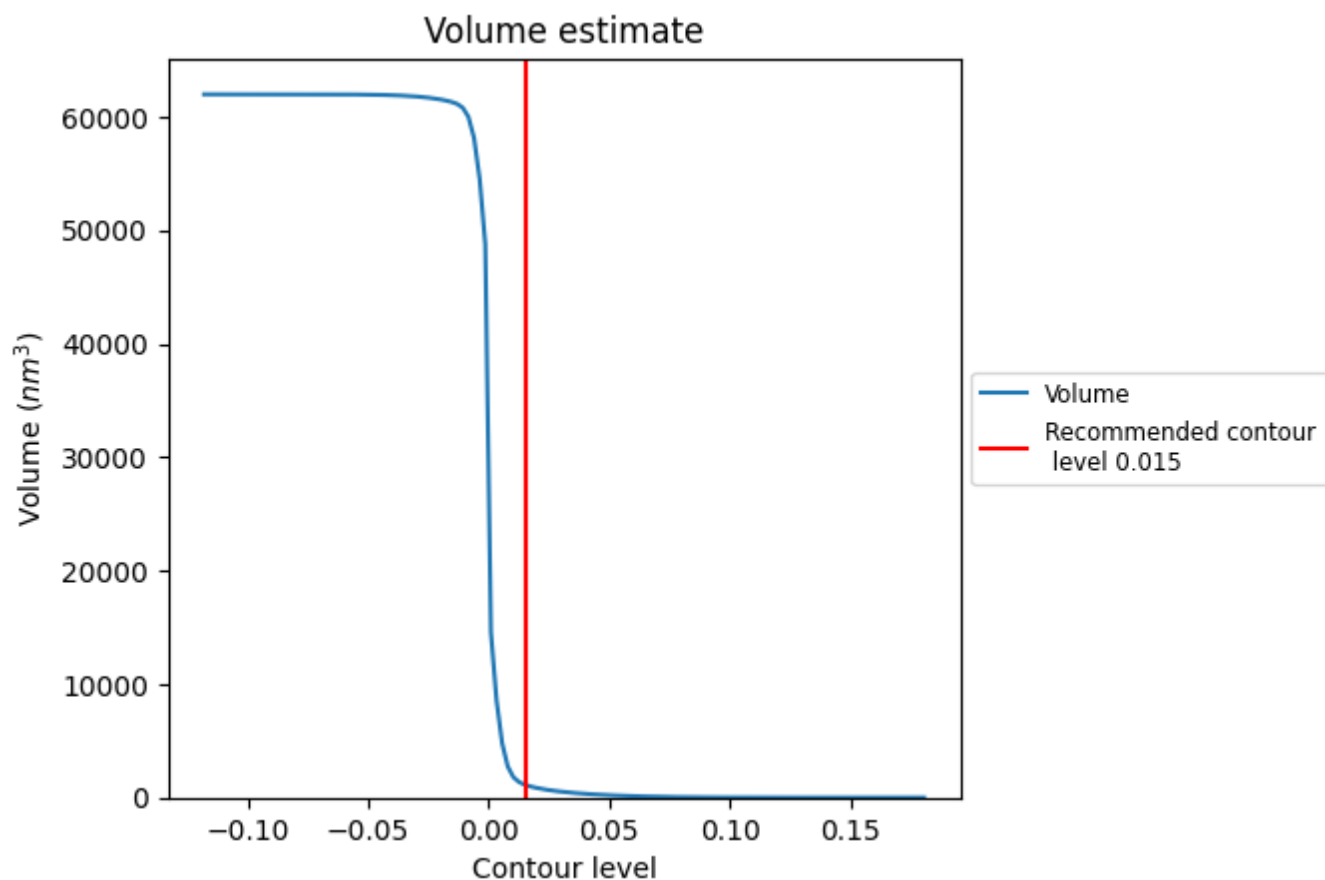
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

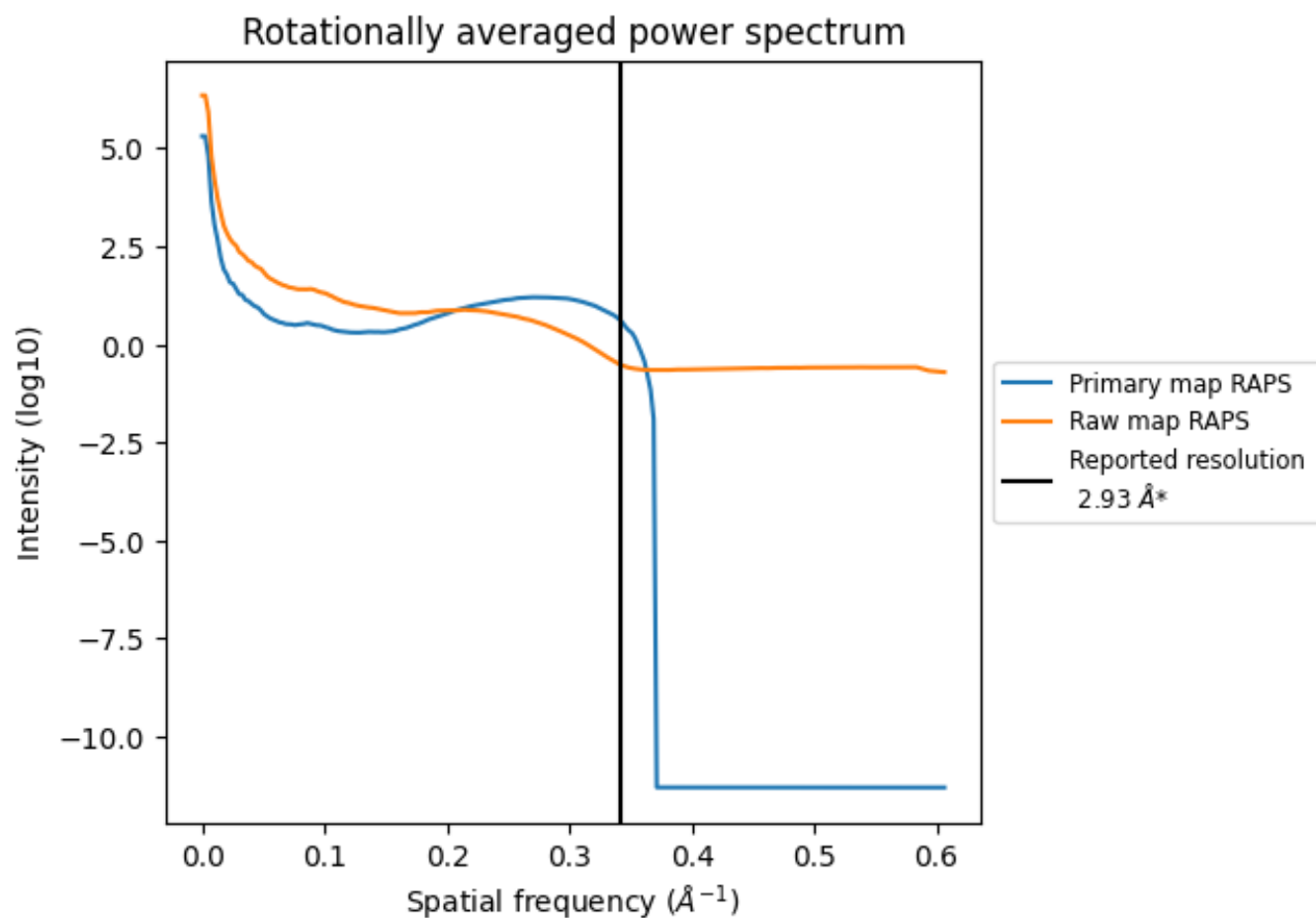
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm³; this corresponds to an approximate mass of 1022 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 ⓘ

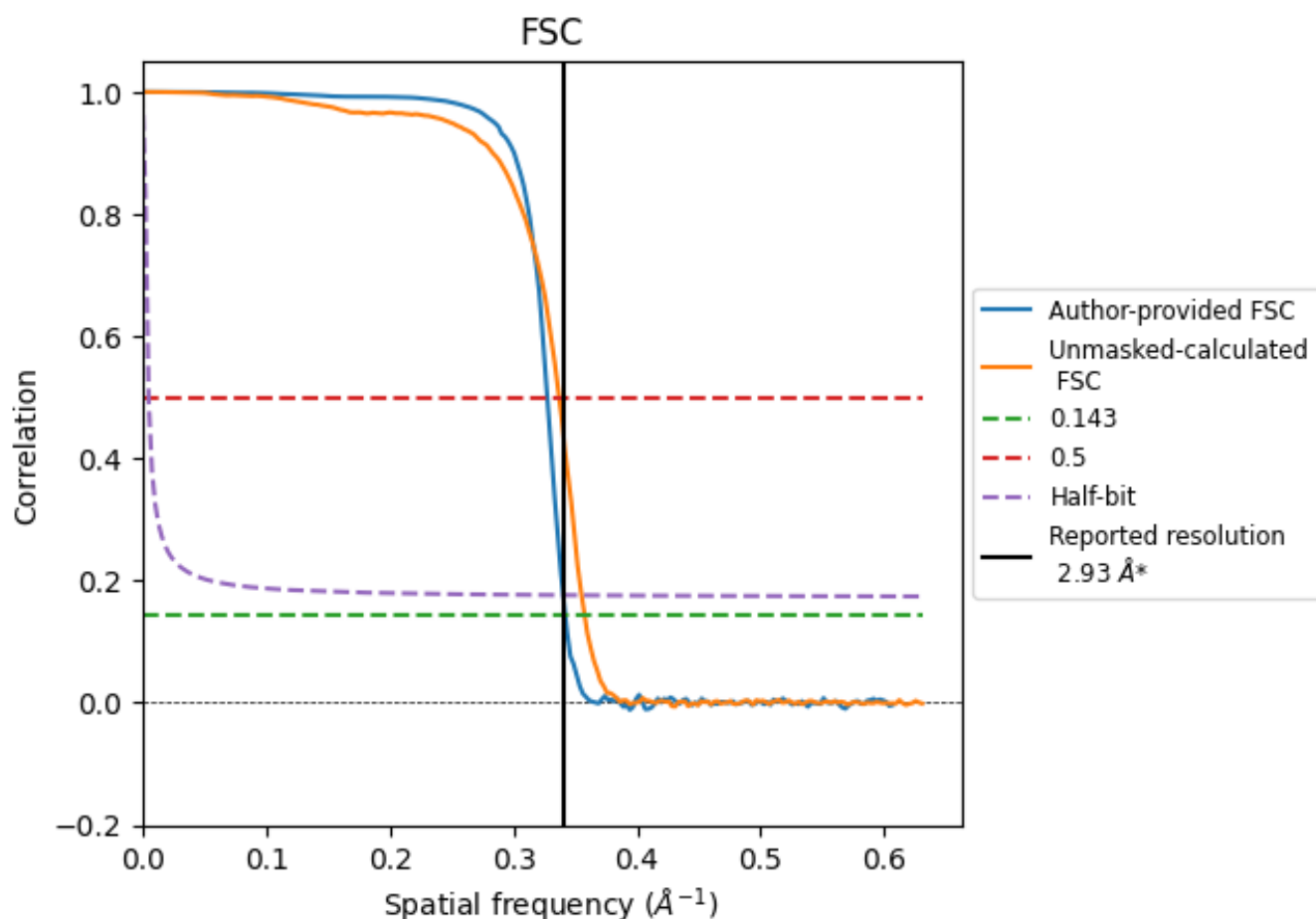


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.341 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

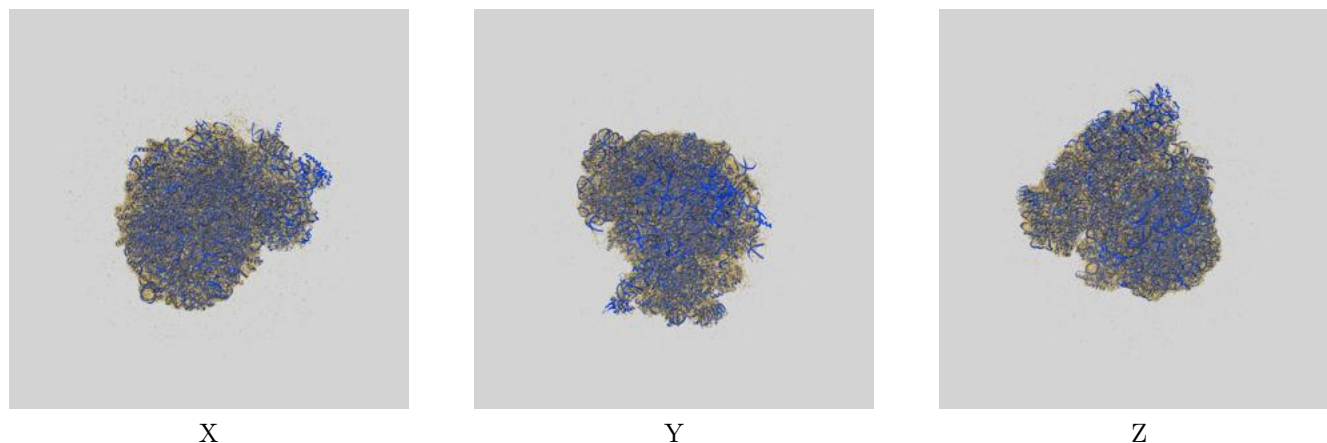
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.92	3.05	2.94
Unmasked-calculated*	2.80	2.97	2.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

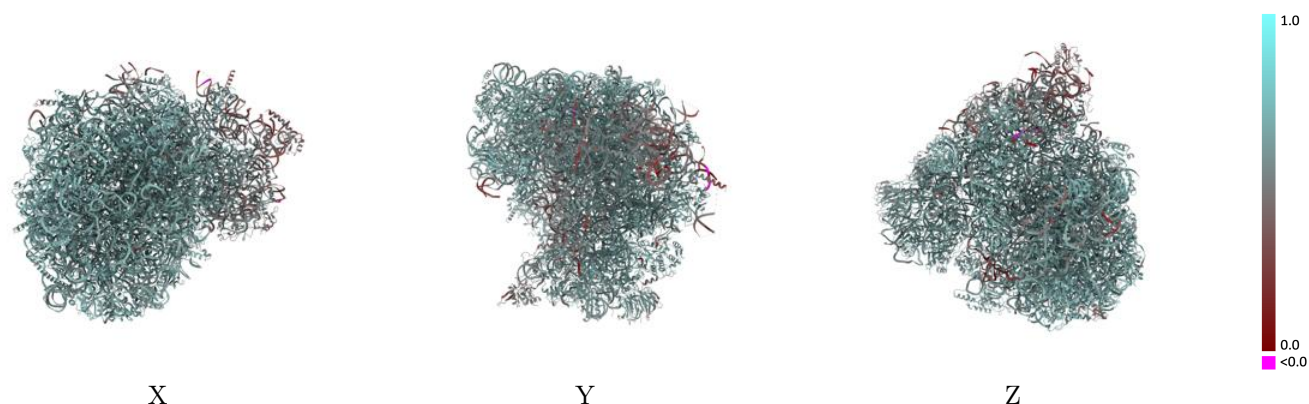
This section contains information regarding the fit between EMDB map EMD-19576 and PDB model 8RXH. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



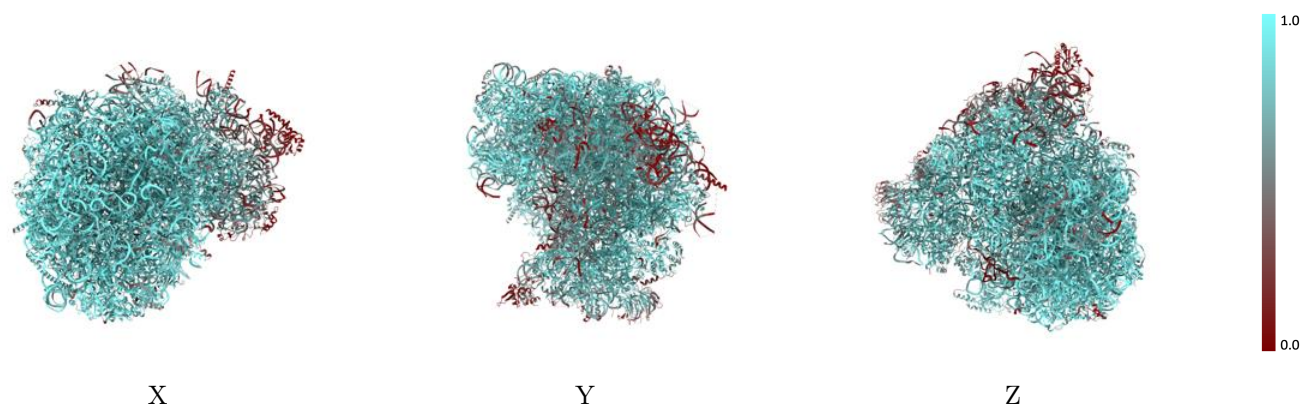
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



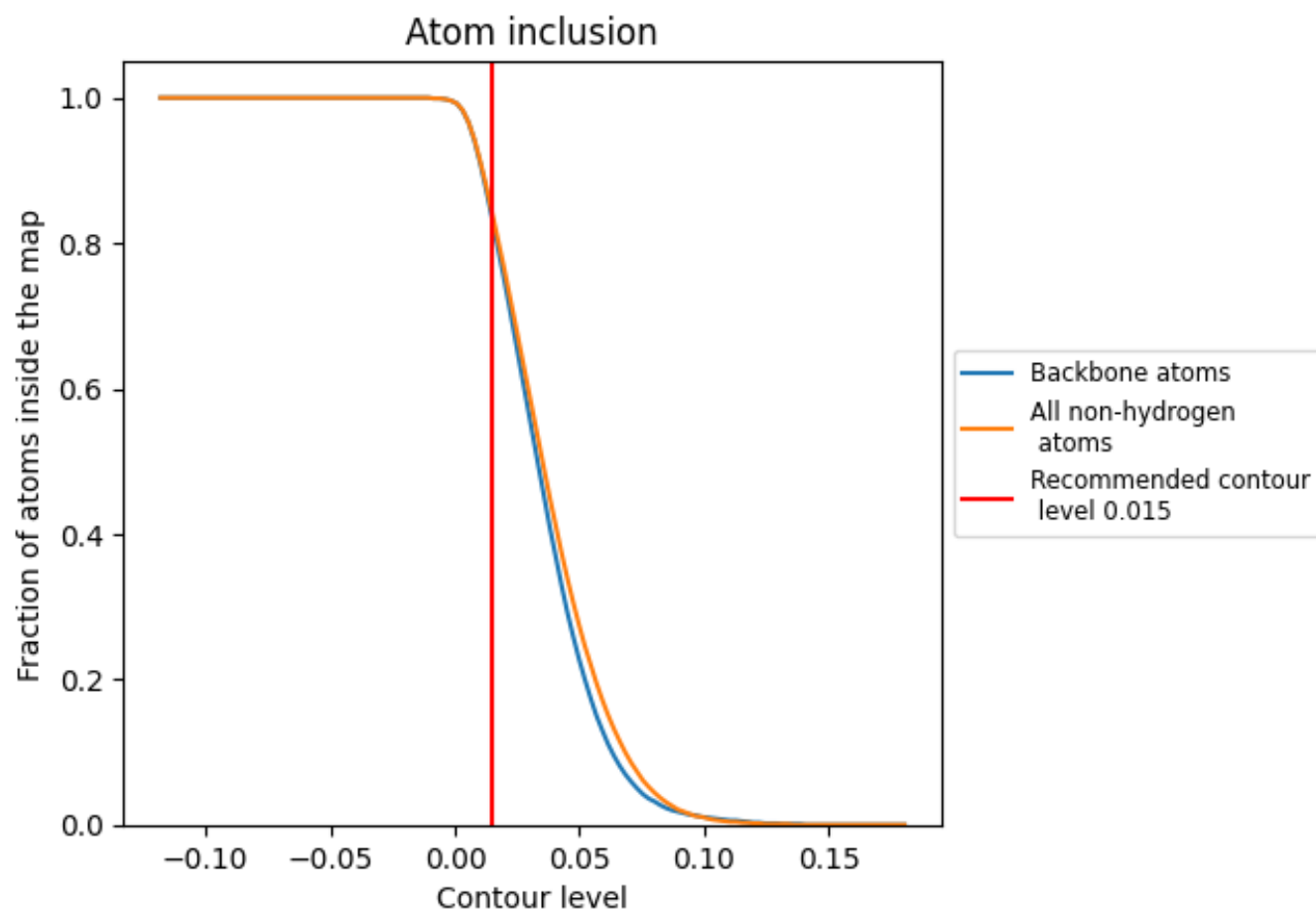
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.6030
L1	 0.9320	 0.6220
L2	 0.9180	 0.6170
L3	 0.8960	 0.6070
L4	 0.9590	 0.6350
L5	 0.8820	 0.6040
L6	 0.8930	 0.6060
L7	 0.9420	 0.6280
L8	 0.9610	 0.6320
LA	 0.9610	 0.6540
LB	 0.9350	 0.6480
LC	 0.9460	 0.6480
LD	 0.7950	 0.6200
LE	 0.9070	 0.6430
LF	 0.8420	 0.6220
LG	 0.8390	 0.6190
LH	 0.9400	 0.6510
LI	 0.8920	 0.6400
LJ	 0.9370	 0.6450
LK	 0.8420	 0.6300
LL	 0.9530	 0.6560
LM	 0.9800	 0.6600
LN	 0.8920	 0.6370
LO	 0.8180	 0.6190
LP	 0.9580	 0.6520
LQ	 0.7810	 0.6070
LR	 0.9520	 0.6510
LS	 0.9180	 0.6380
LT	 0.9700	 0.6580
LU	 0.6830	 0.6010
LV	 0.9440	 0.6490
LW	 0.9420	 0.6530
LX	 0.7440	 0.5880
LY	 0.8830	 0.6370
LZ	 0.9170	 0.6470



Continued on next page...

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Chain	Atom inclusion	Q-score
La	 0.9080	 0.6420
Lb	 0.9470	 0.6470
Lc	 0.9490	 0.6530
Ld	 0.8790	 0.6220
Le	 0.8420	 0.6300
Lf	 0.9300	 0.6430
Lg	 0.9470	 0.6540
Lh	 0.8720	 0.6250
Li	 0.8480	 0.6220
Lj	 0.9760	 0.6570
Lk	 0.8260	 0.6310
Ll	 0.9600	 0.6520
Lm	 0.9080	 0.6390
Ln	 0.9080	 0.6330
Lo	 0.9340	 0.6380
Lp	 0.9490	 0.6520
S1	 0.7820	 0.5580
S2	 0.2470	 0.3850
S3	 0.6870	 0.5430
S4	 0.3680	 0.3940
S5	 0.8180	 0.5790
SA	 0.8530	 0.6310
SB	 0.8440	 0.6220
SC	 0.7350	 0.6070
SD	 0.5680	 0.5300
SE	 0.5580	 0.5210
SF	 0.8710	 0.6360
SG	 0.4640	 0.5130
SH	 0.8320	 0.6220
SI	 0.8130	 0.6140
SJ	 0.9330	 0.6430
SK	 0.7710	 0.5930
SL	 0.8580	 0.6210
SM	 0.6760	 0.5900
SN	 0.6840	 0.5830
SO	 0.9080	 0.6360
SP	 0.7980	 0.5820
SQ	 0.1990	 0.4560
SR	 0.7420	 0.6060
SS	 0.8920	 0.6250
ST	 0.9080	 0.6310
SU	 0.8270	 0.6090

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Chain	Atom inclusion	Q-score
SV	 0.6950	 0.6010
SW	 0.7130	 0.6020
SX	 0.8310	 0.6170
SY	 0.8420	 0.6210
SZ	 0.3880	 0.4940
Sa	 0.6330	 0.5710
Sb	 0.9210	 0.6410
Sc	 0.8460	 0.6120
Sd	 0.7370	 0.6000
Se	 0.5230	 0.4940
Sf	 0.2880	 0.4960
Sg	 0.5490	 0.5650
Sh	 0.0860	 0.4150