



## Full wwPDB EM Validation Report ⓘ

Jul 14, 2025 – 05:40 pm BST

PDB ID : 9FXO / pdb\_00009fxo  
EMDB ID : EMD-50852  
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME  
WITH A/P/E-SITE TRNA AND MRNA : LM32CS1C1 M2 OE MUTANT  
Authors : Rajan, K.S.; Yonath, A.  
Deposited on : 2024-07-02  
Resolution : 2.25 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

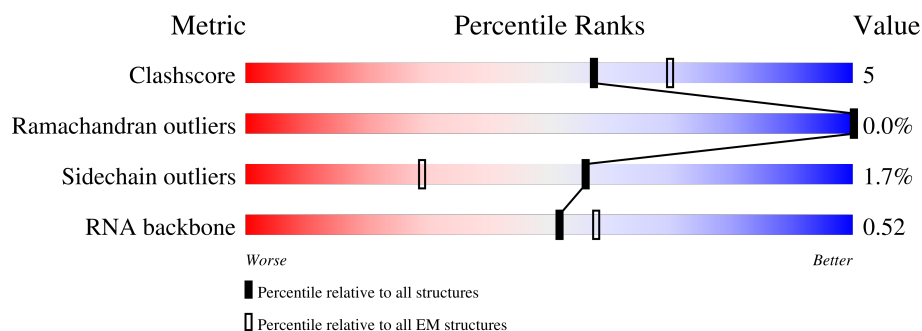
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.25 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	L1	1782	
2	L2	1526	
3	L3	216	
4	L4	184	
5	L5	135	
6	L6	73	
7	L7	171	


























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Mol	Chain	Length	Quality of chain
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	
29	LU	129	
30	LV	145	
31	LW	143	
32	LX	124	






















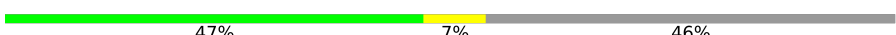



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Mol	Chain	Length	Quality of chain
33	LY	134	 90% 10% .
34	LZ	147	 81% 17% ..
35	La	127	 85% 13% ..
36	Lb	70	 84% 13% .
37	Lc	252	 81% 10% 9%
38	Ld	104	 75% 15% . 8%
39	Le	188	 87% 12% .
40	Lf	133	 89% 7% .
41	Lg	144	 85% 14% ..
42	Lh	168	 64% 11% . 24%
43	Li	105	 90% 7% .
44	Lj	83	 84% 13% .
45	Lk	83	 84% 10% 6%
46	Ll	51	 86% 12% .
47	Lm	128	 34% 7% 59%
48	Ln	34	 85% 12% .
49	Lo	92	 86% 11% .
50	Lp	106	 75% 15% . 8%
51	S1	2204	 55% 23% 6% 16%
52	S2	76	 11% 8% . 80%
52	S4	76	 39% 38% 12% 11%
53	S3	77	 68% 27% . .
54	SA	264	 79% 11% 10%
55	SB	246	 72% 14% 14%
56	SC	219	 79% 17% .

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Mol	Chain	Length	Quality of chain
57	SD	190	
58	SE	273	
59	SF	265	
60	SG	249	
61	SH	190	
62	SI	200	
63	SJ	130	
64	SK	220	
65	SL	149	
66	SM	116	
67	SN	168	
68	SO	144	
69	SP	143	
70	SQ	141	
71	SR	153	
72	SS	57	
73	ST	151	
74	SU	173	
75	SV	143	
76	SW	152	
77	SX	161	
78	SY	164	
79	SZ	137	
80	Sa	120	
81	Sb	112	

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Mol	Chain	Length	Quality of chain
82	Sc	86	
83	Sd	87	
84	Se	66	
85	Sf	152	
86	Sg	312	
87	Sh	235	
88	S5	13	

## 2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 218491 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	1684	Total	C	N	O	P	0	0
			36117	16147	6602	11684	1684		

- Molecule 2 is a RNA chain called LSUb\_rRNA\_chain\_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	1160	Total	C	N	O	P	0	0
			24815	11110	4470	8075	1160		

- 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
			3880	1736	672	1289	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	121	Total	C	N	O	P	0	0
			2578	1150	460	847	121		

- Molecule 6 is a RNA chain called SR6\_chain\_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	71	Total	C	N	O	P	1	0
			1526	684	274	496	72		

- 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
			3534	1584	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	1	0
			1972	1229	403	330	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
			2826	1765	562	484	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
			1391	878	262	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	151	Total	C	N	O	S	0	0
			1169	743	220	204	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	1	0
			1895	1190	376	322	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
			1329	827	263	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	200	Total	C	N	O	S	0	0
			1626	1025	323	264	14		

- 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	1	0
			2339	1486	440	407	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	1	0
			1692	1041	370	275	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
			1221	762	241	207	11		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LY	133	Total	C	N	O	S	0	0
			1065	683	215	164	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	96	Total	C	N	O	S	0	0
			730	455	133	137	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	1	0
			1159	720	243	191	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Li	101	Total	C	N	O	S	0	0
			798	503	162	131	2		

- Molecule 44 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lj	81	Total	C	N	O	S	0	0
			668	406	153	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
			416	263	85	64	4		

- Molecule 48 is a protein called Ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ln	33	Total	C	N	O	S	0	0
			292	178	75	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	1852	Total	C	N	O	P	1	0
			39635	17733	7147	12902	1853		

- Molecule 52 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S2	15	Total	C	N	O	P	0	0
			325	149	58	102	15		
52	S4	68	Total	C	N	O	P	0	0
			1446	646	258	475	67		

- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	75	Total	C	N	O	P	0	0
			1599	713	290	521	75		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SA	238	Total	C	N	O	S	0	0
			1909	1194	366	338	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SB	211	Total	C	N	O	S	0	0
			1662	1055	303	292	12		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SG	234	Total	C	N	O	S	0	0
			1866	1163	383	317	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SH	183	Total	C	N	O	S	0	0
			1441	896	276	262	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SK	197	Total	C	N	O	S	0	0
			1582	986	326	268	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SM	103	Total	C	N	O	S	0	0
			805	503	146	154	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SN	107	Total	C	N	O	S	0	0
			874	560	152	155	7		

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

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

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



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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
70	SQ	97	Total	C	N	O	0	0
			480	286	97	97		

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

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

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

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

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

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

- Molecule 74 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SU	153	Total	C	N	O	S	0	0
			1260	796	251	208	5		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SY	88	Total	C	N	O	S	1	0
			673	415	124	130	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sa	83	Total	C	N	O	S	0	0
			650	412	118	117	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sc	85	Total	C	N	O	S	0	0
			661	410	127	119	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Se	59	Total	C	N	O	S	0	0
			449	281	95	72	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sf	75	Total	C	N	O	S	0	0
			465	293	88	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Sg	303	Total	C	N	O	S	0	0
			2343	1469	418	443	13		

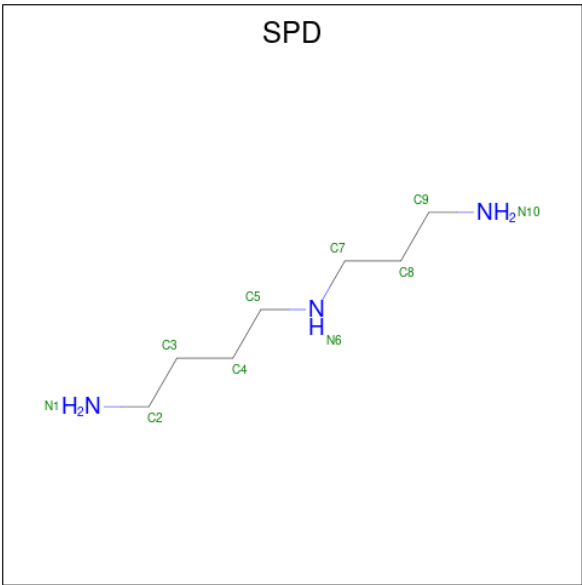
- Molecule 87 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Sh	171	Total	C	N	O	S	0	0
			1212	769	224	216	3		

- Molecule 88 is a RNA chain called mRNA.

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

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	
89	L1	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
89	L1	1	Total	C	N	0
			10	7	3	
89	L2	1	Total	C	N	0
			10	7	3	
89	L2	1	Total	C	N	0
			10	7	3	
89	LM	1	Total	C	N	0
			10	7	3	
89	S1	1	Total	C	N	0
			10	7	3	
89	S1	1	Total	C	N	0
			10	7	3	
89	S1	1	Total	C	N	0
			10	7	3	

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

Mol	Chain	Residues	Atoms		AltConf
90	L1	120	Total	Mg	0
			120	120	
90	L2	94	Total	Mg	0
			94	94	
90	L3	5	Total	Mg	0
			5	5	
90	L4	10	Total	Mg	0
			10	10	
90	L5	6	Total	Mg	0
			6	6	
90	L6	2	Total	Mg	0
			2	2	
90	L7	4	Total	Mg	0
			4	4	
90	L8	6	Total	Mg	0
			6	6	
90	LA	2	Total	Mg	0
			2	2	
90	LG	1	Total	Mg	0
			1	1	
90	LJ	1	Total	Mg	0
			1	1	
90	LN	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
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	2	Total 2	Mg 2	0
90	S1	109	Total 109	Mg 109	0
90	S3	1	Total 1	Mg 1	0
90	SG	1	Total 1	Mg 1	0
90	SO	1	Total 1	Mg 1	0
90	ST	1	Total 1	Mg 1	0
90	SX	1	Total 1	Mg 1	0
90	Sb	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
91	L1	15	Total 15	Na 15	0
91	L2	12	Total 12	Na 12	0
91	L3	1	Total 1	Na 1	0
91	L4	3	Total 3	Na 3	0
91	L7	2	Total 2	Na 2	0
91	LN	1	Total 1	Na 1	0
91	Lf	1	Total 1	Na 1	0
91	S1	12	Total 12	Na 12	0

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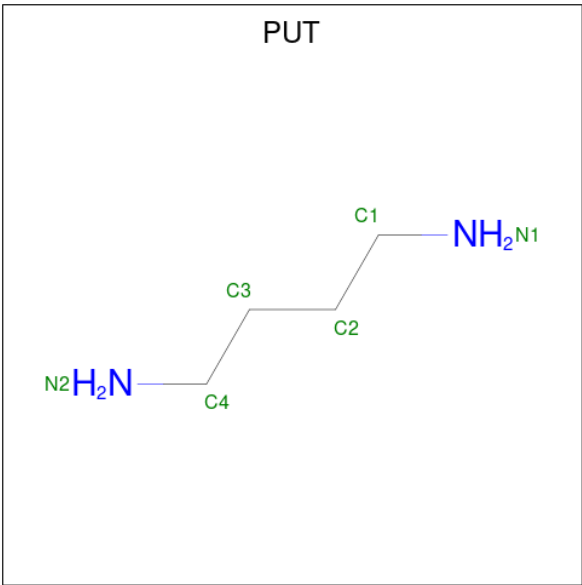
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Mol	Chain	Residues	Atoms		AltConf
91	SS	1	Total 1	Na 1	0

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

Mol	Chain	Residues	Atoms		AltConf
92	L1	20	Total 20	K 20	0
92	L2	14	Total 14	K 14	0
92	L4	4	Total 4	K 4	0
92	L7	1	Total 1	K 1	0
92	LB	1	Total 1	K 1	0
92	LC	2	Total 2	K 2	0
92	LM	1	Total 1	K 1	0
92	LV	1	Total 1	K 1	0
92	Le	1	Total 1	K 1	0
92	Ll	1	Total 1	K 1	0
92	S1	19	Total 19	K 19	0

- Molecule 93 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
93	L1	1	Total	C	N	0
			6	4	2	
93	L1	1	Total	C	N	0
			6	4	2	
93	L1	1	Total	C	N	0
			6	4	2	
93	L1	1	Total	C	N	0
			6	4	2	
93	L1	1	Total	C	N	0
			6	4	2	
93	L1	1	Total	C	N	0
			6	4	2	
93	L2	1	Total	C	N	0
			6	4	2	
93	L2	1	Total	C	N	0
			6	4	2	
93	L2	1	Total	C	N	0
			6	4	2	
93	L2	1	Total	C	N	0
			6	4	2	
93	L4	1	Total	C	N	0
			6	4	2	
93	L5	1	Total	C	N	0
			6	4	2	

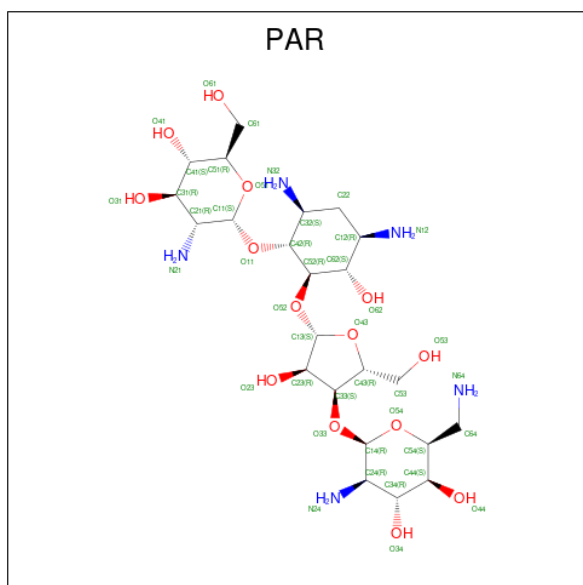
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Mol	Chain	Residues	Atoms			AltConf
93	S1	1	Total	C	N	0
			6	4	2	
93	S1	1	Total	C	N	0
			6	4	2	

- Molecule 94 is PAROMOMYCIN (CCD ID: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms				AltConf
94	L1	1	Total	C	N	O	0
			42	23	5	14	
94	L2	1	Total	C	N	O	0
			42	23	5	14	
94	L2	1	Total	C	N	O	0
			42	23	5	14	
94	L7	1	Total	C	N	O	0
			42	23	5	14	
94	S1	1	Total	C	N	O	0
			42	23	5	14	
94	S1	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 95 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
95	LK	1	Total	Zn	0
			1	1	

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

- Molecule 96 is water.

Mol	Chain	Residues	Atoms		AltConf
96	L1	762	Total 762	O 762	0
96	L2	787	Total 787	O 787	0
96	L3	49	Total 49	O 49	0
96	L4	55	Total 55	O 55	0
96	L5	22	Total 22	O 22	0
96	L7	24	Total 24	O 24	0
96	LA	46	Total 46	O 46	0
96	LB	42	Total 42	O 42	0
96	LC	27	Total 27	O 27	0
96	LD	1	Total 1	O 1	0
96	LG	1	Total 1	O 1	0
96	LH	6	Total 6	O 6	0
96	LI	11	Total 11	O 11	0

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Mol	Chain	Residues	Atoms		AltConf
96	LJ	5	Total 5	O 5	0
96	LL	15	Total 15	O 15	0
96	LM	26	Total 26	O 26	0
96	LN	2	Total 2	O 2	0
96	LO	1	Total 1	O 1	0
96	LP	9	Total 9	O 9	0
96	LQ	11	Total 11	O 11	0
96	LS	4	Total 4	O 4	0
96	LT	15	Total 15	O 15	0
96	LU	1	Total 1	O 1	0
96	LV	2	Total 2	O 2	0
96	LW	5	Total 5	O 5	0
96	LX	2	Total 2	O 2	0
96	LY	2	Total 2	O 2	0
96	La	1	Total 1	O 1	0
96	Lb	5	Total 5	O 5	0
96	Lc	2	Total 2	O 2	0
96	Ld	4	Total 4	O 4	0
96	Le	6	Total 6	O 6	0
96	Lf	3	Total 3	O 3	0
96	Lg	3	Total 3	O 3	0

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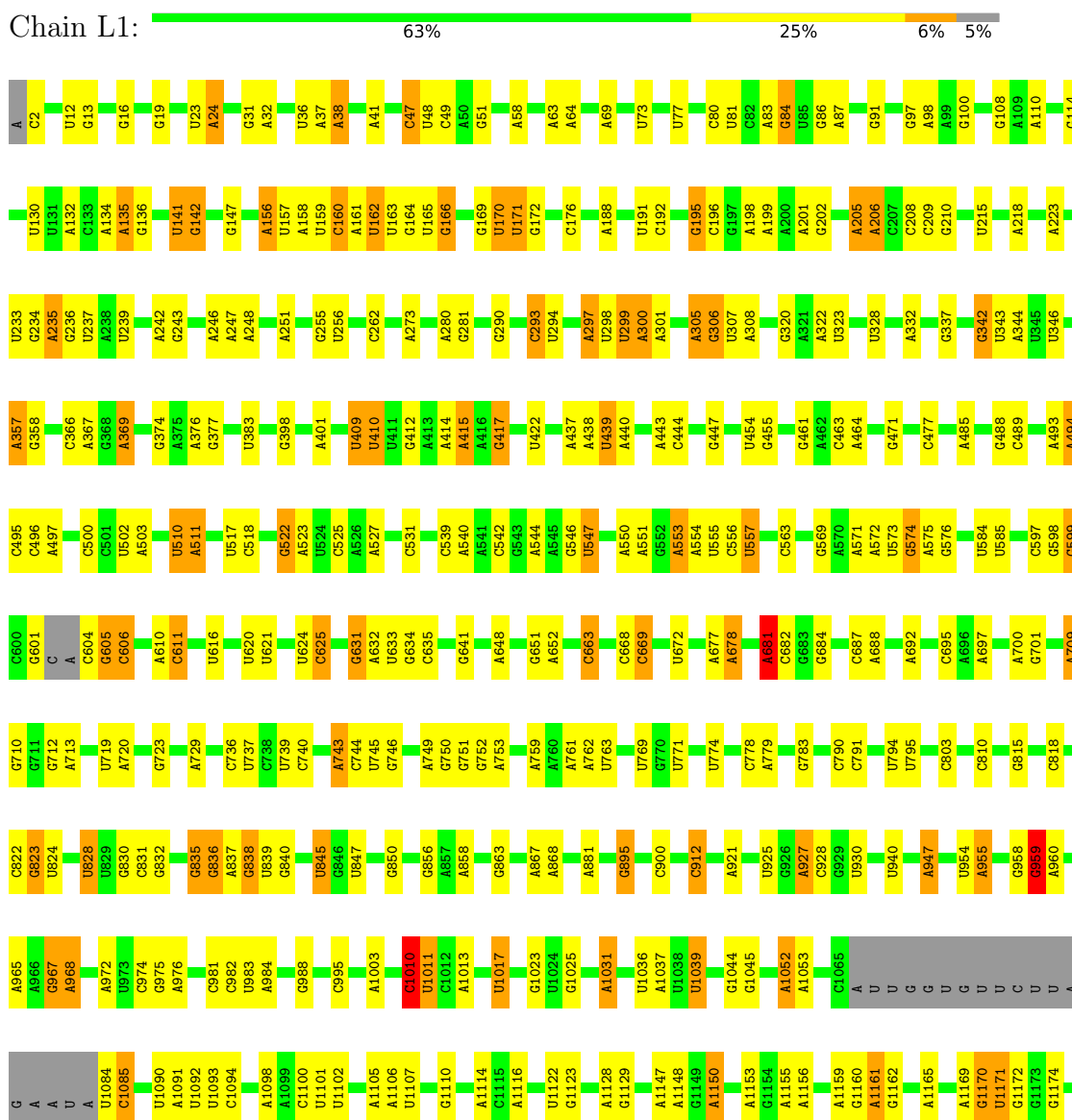
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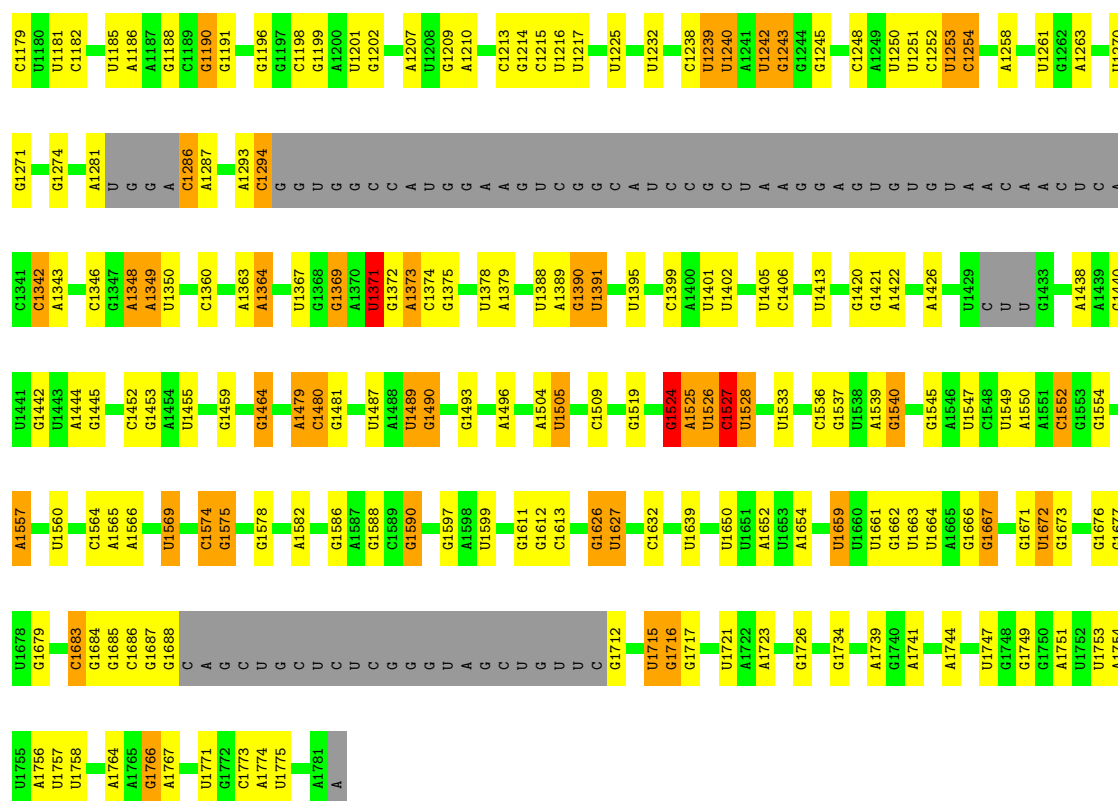
Mol	Chain	Residues	Atoms		AltConf
96	Lh	12	Total 12	O 12	0
96	Lj	18	Total 18	O 18	0
96	Ln	9	Total 9	O 9	0
96	Lo	23	Total 23	O 23	0
96	Lp	14	Total 14	O 14	0
96	S1	595	Total 595	O 595	0
96	S2	1	Total 1	O 1	0
96	S3	6	Total 6	O 6	0
96	S4	15	Total 15	O 15	0
96	SA	6	Total 6	O 6	0
96	SF	1	Total 1	O 1	0
96	SJ	1	Total 1	O 1	0
96	SK	19	Total 19	O 19	0
96	SO	9	Total 9	O 9	0
96	SP	4	Total 4	O 4	0
96	ST	14	Total 14	O 14	0
96	SU	9	Total 9	O 9	0
96	Sb	9	Total 9	O 9	0
96	Sc	1	Total 1	O 1	0
96	Sg	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.

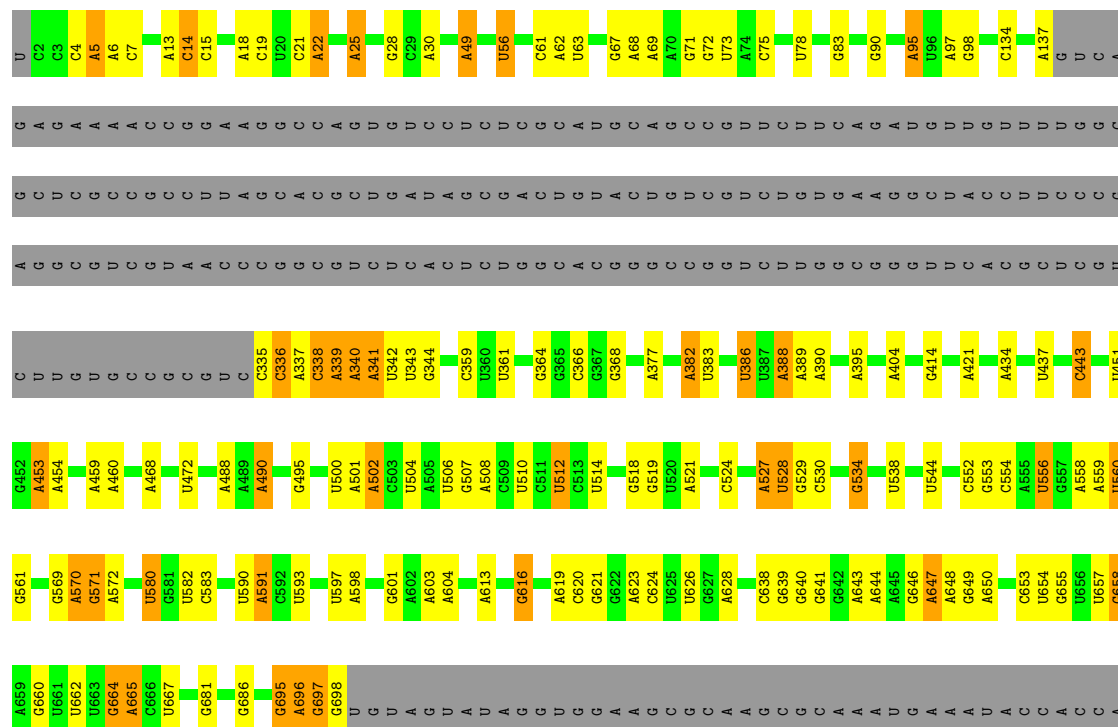
#### • Molecule 1: LSUa\_rRNA\_chain\_1

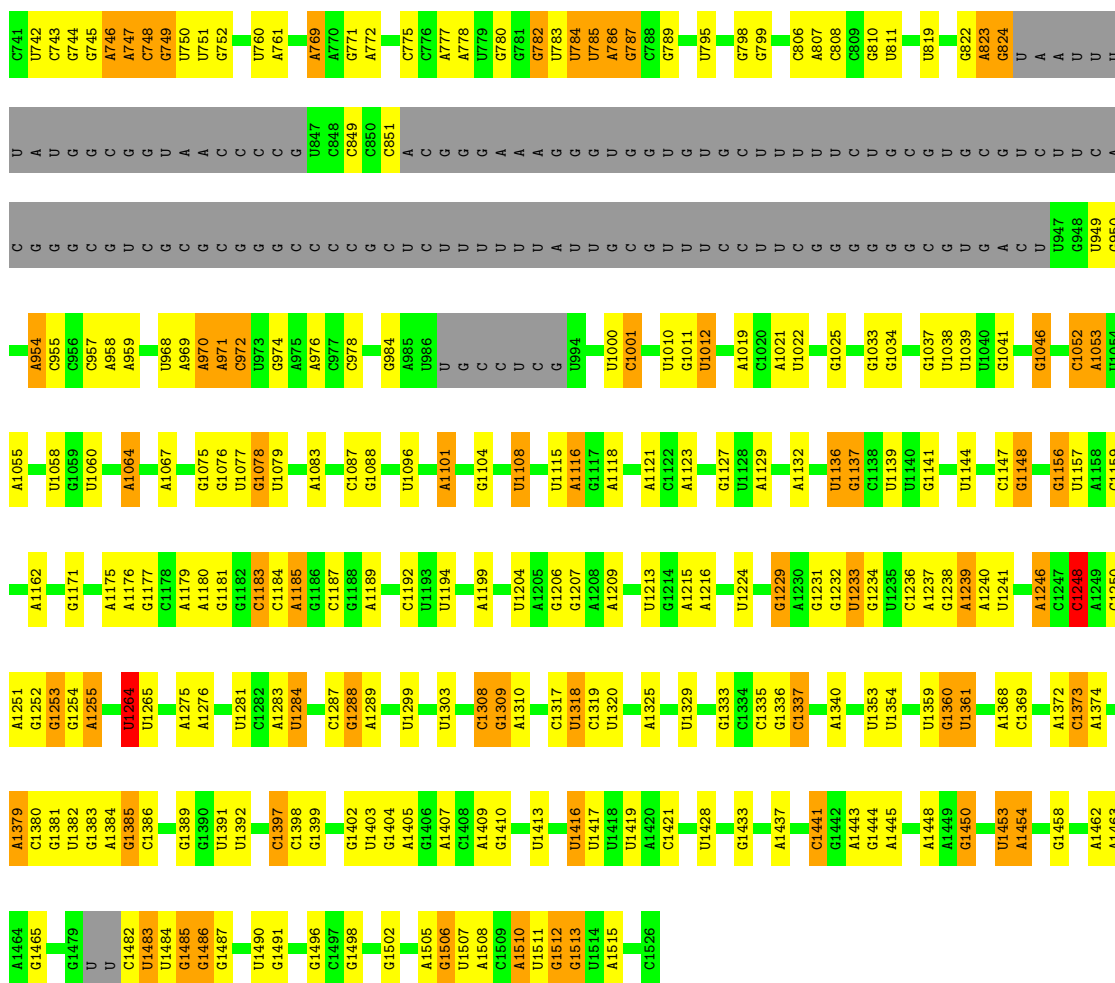




• Molecule 2: LSub\_rRNA\_chain\_2

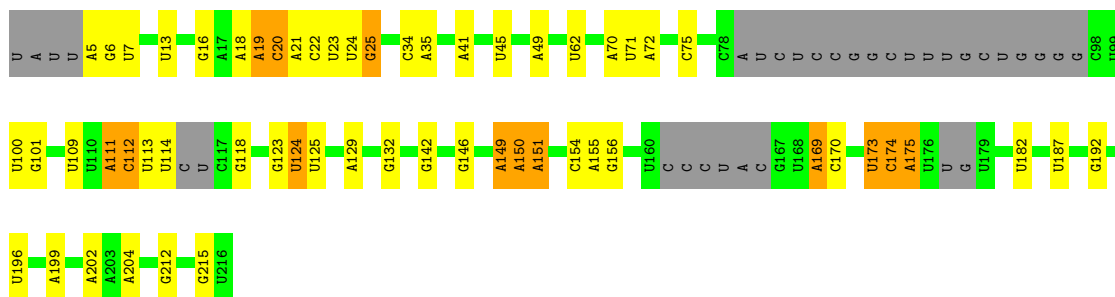
Chain L2: 50% 20% 6% 24%





• Molecule 3: SR1\_chain\_3

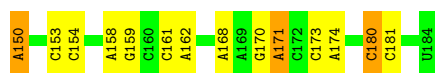
Chain L3: 58% 21% 6% 15%



• Molecule 4: SR2\_chain\_4

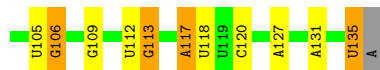
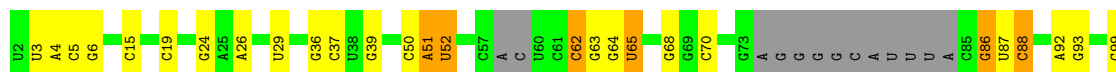
Chain L4: 73% 23% 4%





• Molecule 5: SR4\_chain\_5

Chain L5: 61% 21% 7% 10%



• Molecule 6: SR6\_chain\_6

Chain L6: 49% 37% 11% .



• Molecule 7: 5.8S\_rRNA\_chain\_7

Chain L7: 69% 21% 7% .



• Molecule 8: 5S\_rRNA\_chain\_8

Chain L8: 76% 20% . .



• Molecule 9: Putative 60S ribosomal protein L2

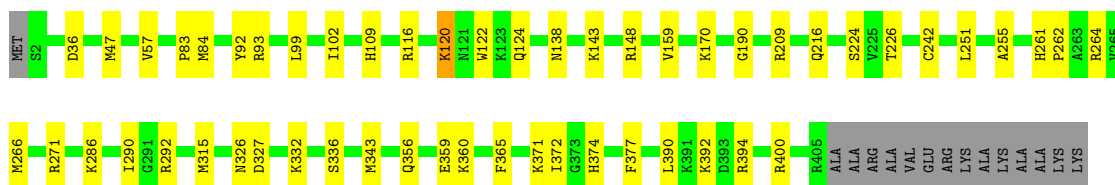
Chain LA: 89% 10% .



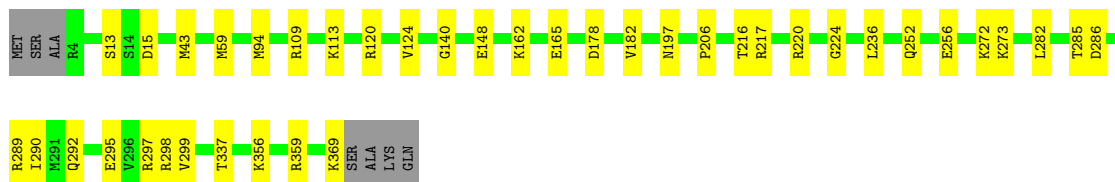
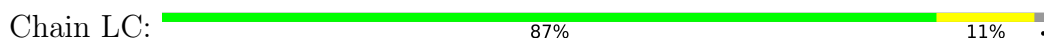
• Molecule 10: Putative ribosomal protein L3

Chain LB: 84% 12% .

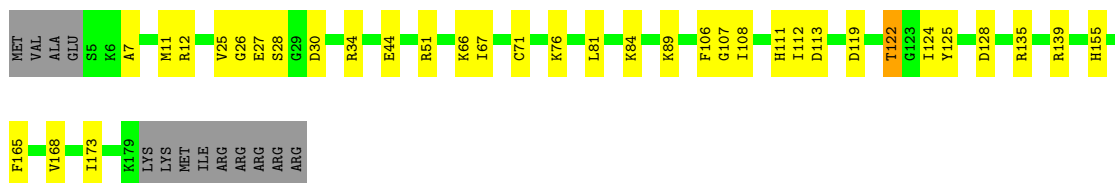
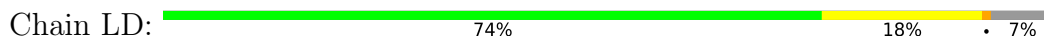




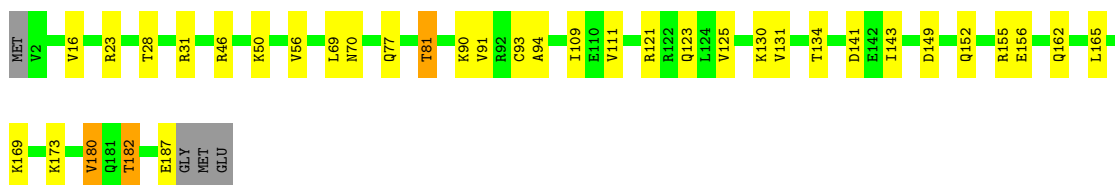
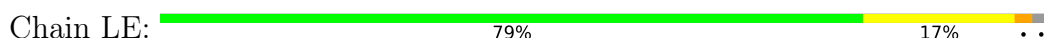
- Molecule 11: Putative ribosomal protein L1a



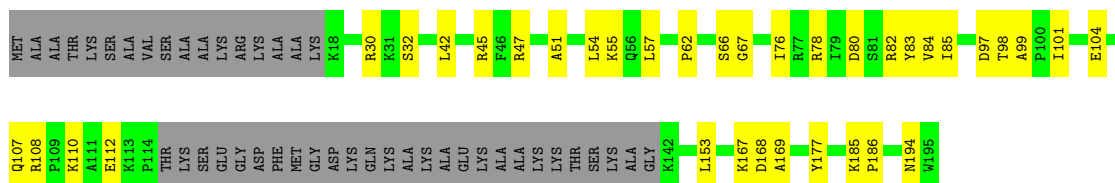
- Molecule 12: 60S ribosomal protein L11



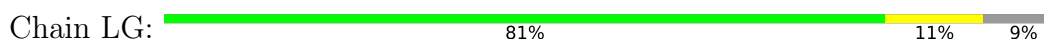
- Molecule 13: Putative 60S ribosomal protein L9



- Molecule 14: Putative 60S ribosomal protein L6



- Molecule 15: 60S ribosomal protein L7a





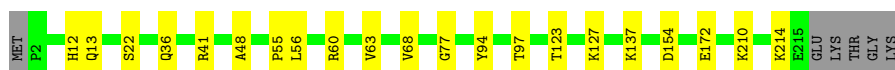
- Molecule 16: Putative 60S ribosomal protein L13a

Chain LH: 86% 14%



- Molecule 17: Putative 60S ribosomal protein L13

Chain LI: 88% 10% .



- Molecule 18: Putative 60S ribosomal protein L23

Chain LJ: 83% 14% .



- Molecule 19: Putative 40S ribosomal protein L14

Chain LK: 81% 15% ..



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

Chain LL: 81% 18% .




- Molecule 21: Ribosomal protein L15

Chain LM: 89% 10%




- Molecule 22: Putative 60S ribosomal protein L10

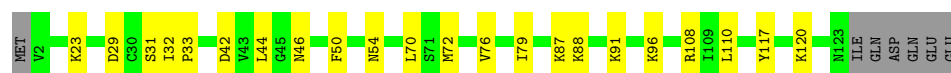


Chain LT:  83% 9% 8%




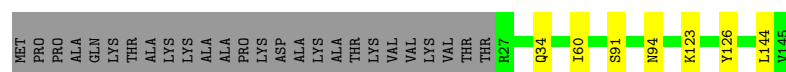
- Molecule 29: Putative 60S ribosomal protein L22

Chain LU:  78% 17% 5%



- Molecule 30: Putative 60S ribosomal protein L23a

Chain LV:  77% 5% 18%



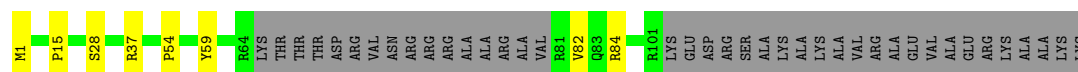
- Molecule 31: Putative 60S ribosomal protein L26

Chain LW:  71% 14% 15%



- Molecule 32: Putative ribosomal protein L24

Chain LX:  62% 6% 31%




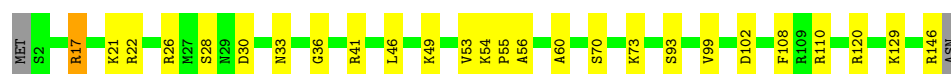
- Molecule 33: 60S ribosomal protein L27

Chain LY:  90% 10% 0%




- Molecule 34: Putative 60S ribosomal protein L28

Chain LZ:  81% 17% 2%




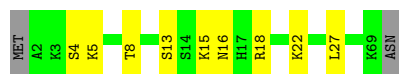
- Molecule 35: Putative 60S ribosomal protein L35

Chain La:  85% 13% ..




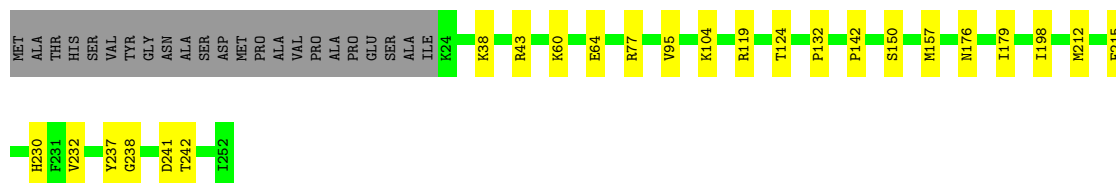
- Molecule 36: 60S ribosomal protein L29

Chain Lb:  84% 13% .




- Molecule 37: Putative 60S ribosomal protein L7

Chain Lc:  81% 10% 9%




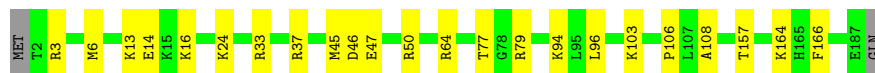
- Molecule 38: 60S ribosomal protein L30

Chain Ld:  75% 15% 8%




- Molecule 39: Putative 60S ribosomal subunit protein L31

Chain Le:  87% 12% .




- Molecule 40: 60S ribosomal protein L32

Chain Lf:  89% 7% .

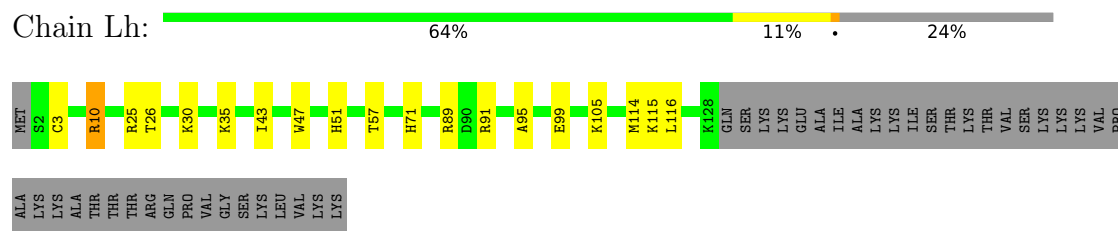


- Molecule 41: Putative ribosomal protein l35a

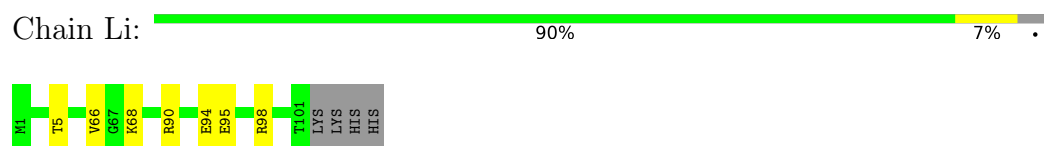
Chain Lg:  85% 14% ..



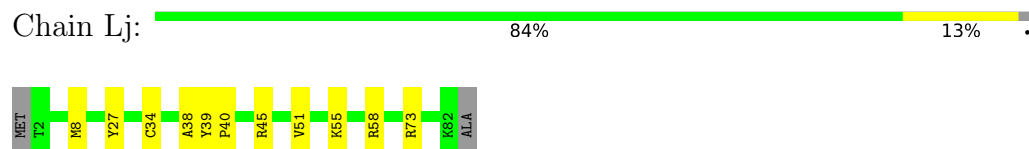
## • Molecule 42: Putative 60S ribosomal protein L34



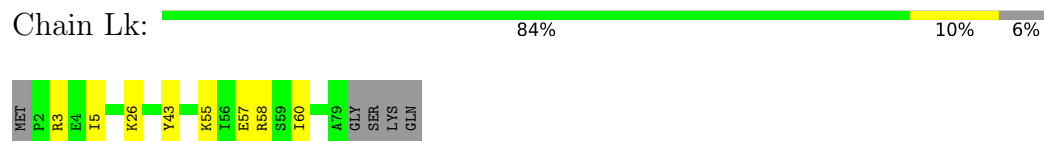
## • Molecule 43: Putative 60S Ribosomal protein L36



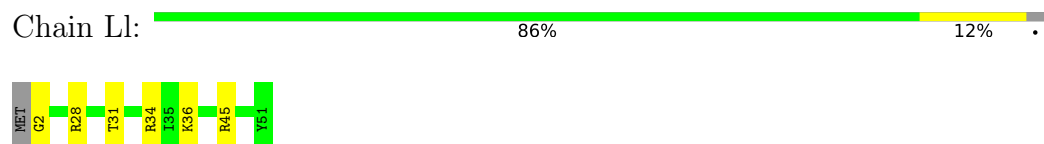
## • Molecule 44: Ribosomal protein L37



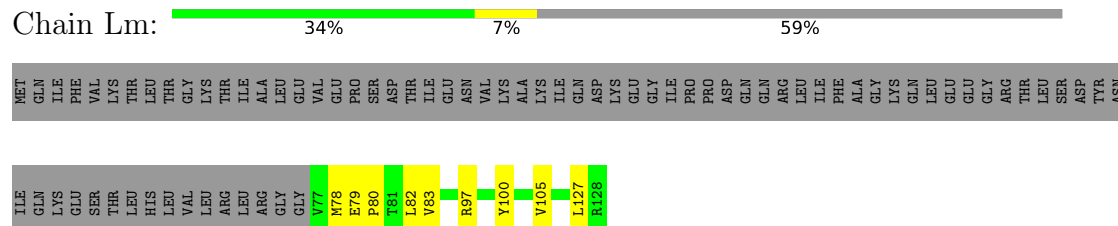
## • Molecule 45: Putative ribosomal protein L38



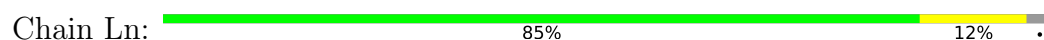
## • Molecule 46: Putative 60S ribosomal protein L39



## • Molecule 47: Ubiquitin-60S ribosomal protein L40



## • Molecule 48: Ribosomal protein L41





- Molecule 49: 60S ribosomal protein L37a

Chain Lo: 86% 11%



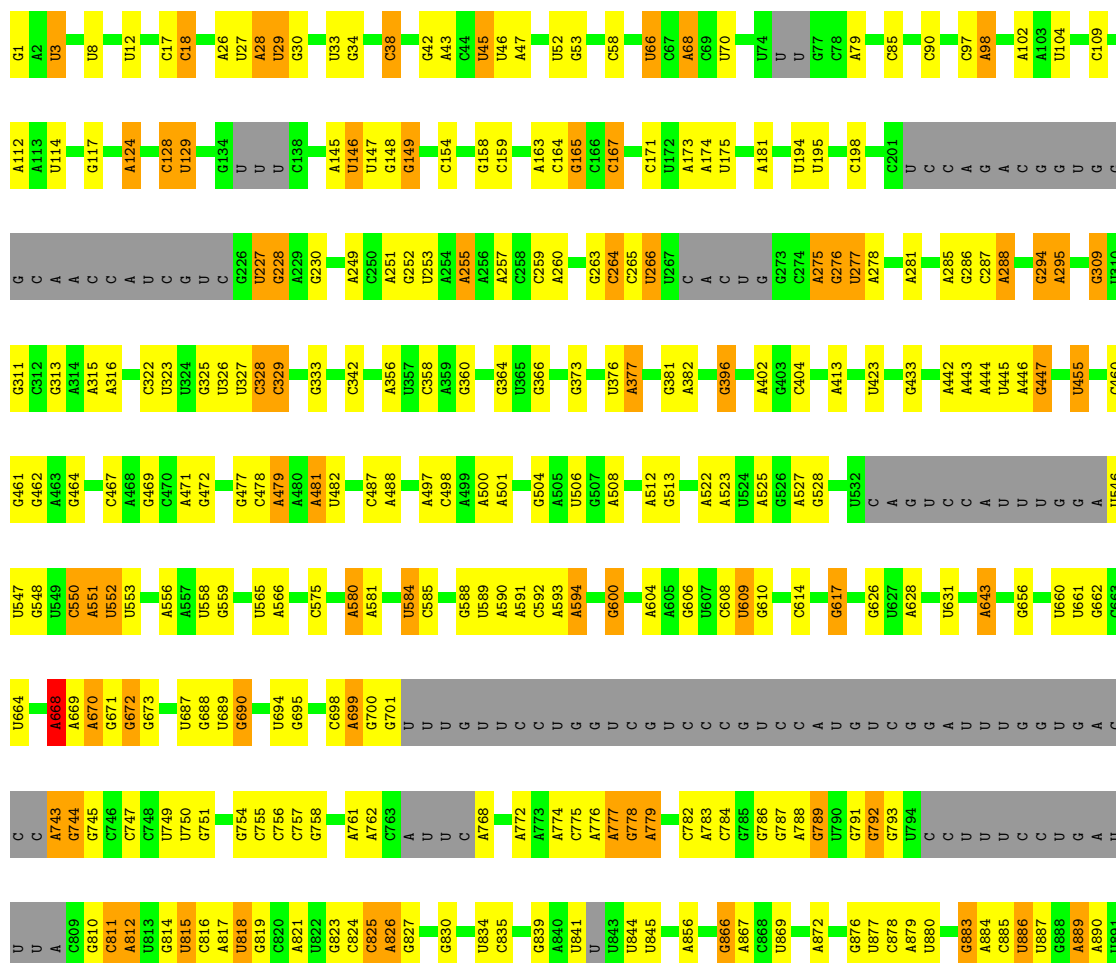
- Molecule 50: Putative 60S ribosomal protein L44

Chain Lp: 75% 15% 8%



- Molecule 51: SSU\_rRNA\_chain\_S1

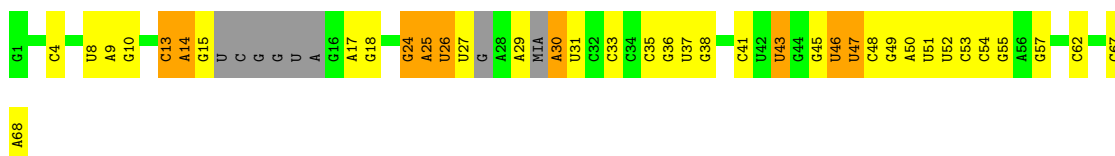
Chain S1: 55% 23% 6% 16%







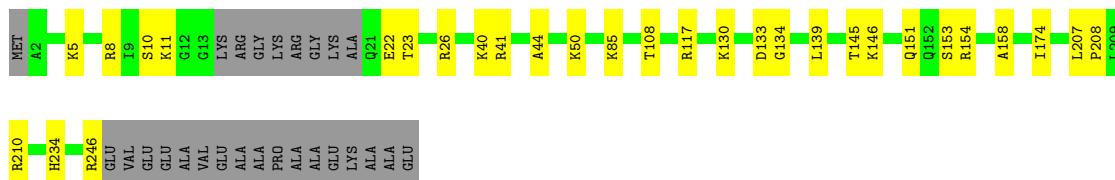
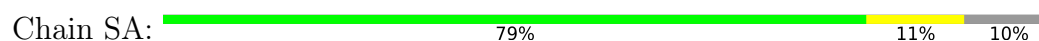
- Molecule 52: tRNA



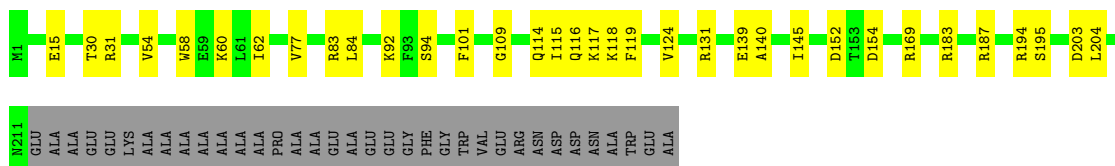
- Molecule 53: tRNA



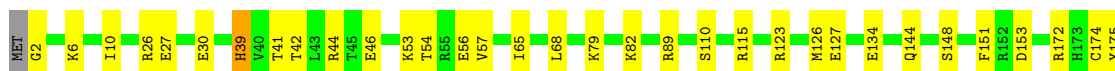
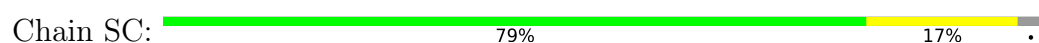
- Molecule 54: 40S ribosomal protein S3a

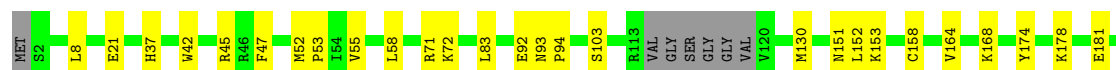


- Molecule 55: 40S ribosomal protein SA




- Molecule 56: Putative 40S ribosomal protein S3








- Molecule 68: 40S ribosomal protein S14

Chain SO:  83% 12% 5%



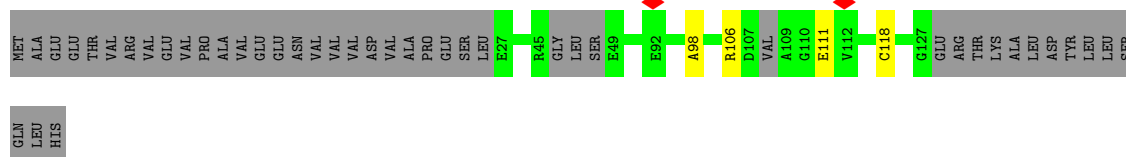
- Molecule 69: Putative 40S ribosomal protein S23

Chain SP:  84% 15% 1%




- Molecule 70: 40S ribosomal protein S12

Chain SQ:  66% 31% 3%




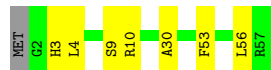
- Molecule 71: Putative 40S ribosomal protein S18

Chain SR:  78% 14% 7%




- Molecule 72: Putative ribosomal protein S29

Chain SS:  86% 12% 2%




- Molecule 73: Putative 40S ribosomal protein S13

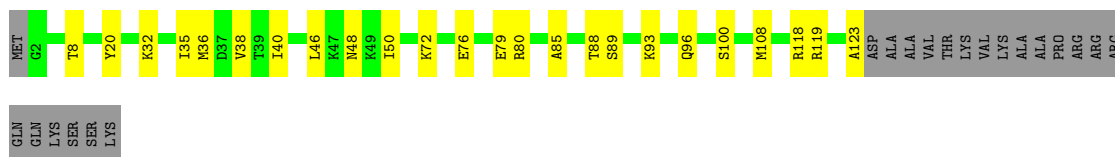
Chain ST:  87% 8% 5%



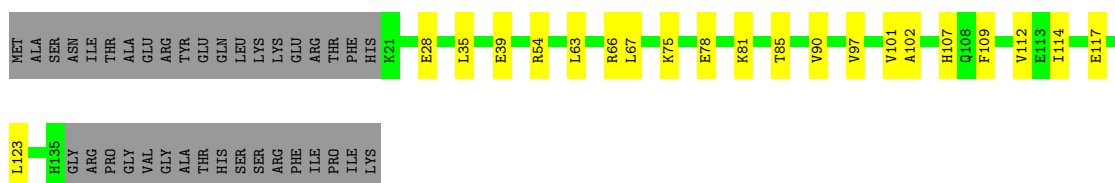
- Molecule 74: Putative 40S ribosomal protein S11

Chain SU:  81% 7% 12%

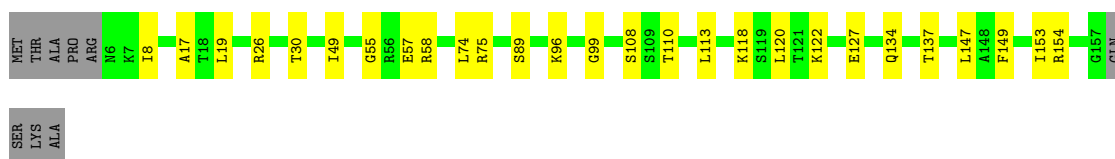
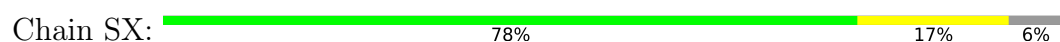
- Molecule 75: Putative 40S ribosomal protein S17



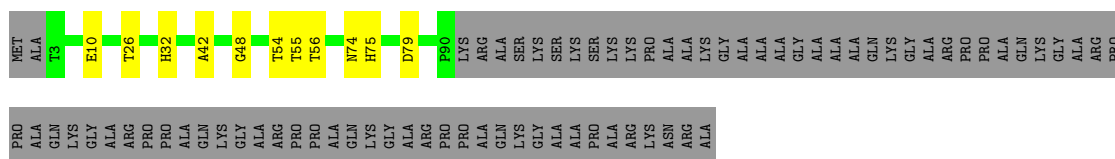
- Molecule 76: Putative 40S ribosomal protein S15



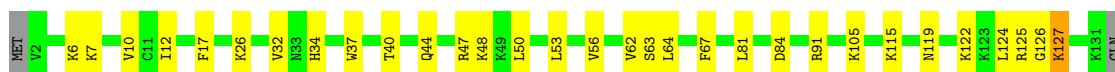
- Molecule 77: 40S ribosomal protein S19-like protein



- Molecule 78: Putative 40S ribosomal protein S21



- Molecule 79: 40S ribosomal protein S24





- 
- A diagram showing a 4x4 grid. The columns are labeled C1, C4, U8, U9, and A12. The rows are labeled A and A. The grid is divided into four quadrants by a vertical line between C4 and U8, and a horizontal line between A and A. The top-left quadrant (C1, C4, U8, U9) is green. The top-right quadrant (C1, C4, U8, U9) is orange. The bottom-left quadrant (C1, C4, U8, U9) is yellow. The bottom-right quadrant (C1, C4, U8, U9) is grey.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150124	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 ( $e^-/\text{\AA}^2$ )	0.92	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.201	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.005	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: MIA, 5MC, 7MG, OMC, ZN, MG, A2M, PAR, SPD, PSU, OMU, PUT, 1MA, NA, MA6, K, B8N, OMG

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	0.15	2/39379 (0.0%)	0.24	0/61402
2	L2	0.17	5/26133 (0.0%)	0.25	0/40729
3	L3	0.13	0/4306	0.24	0/6694
4	L4	0.09	0/4376	0.22	0/6822
5	L5	0.10	0/2878	0.25	0/4479
6	L6	0.10	0/1705	0.24	0/2652
7	L7	0.17	0/3804	0.26	0/5923
8	L8	0.08	0/2851	0.18	0/4439
9	LA	0.11	0/2018	0.30	0/2712
10	LB	0.11	0/3283	0.27	0/4412
11	LC	0.09	0/2876	0.26	0/3868
12	LD	0.09	0/1414	0.25	0/1888
13	LE	0.09	0/1497	0.24	0/2017
14	LF	0.11	0/1191	0.31	0/1608
15	LG	0.08	0/1921	0.24	0/2588
16	LH	0.08	0/1803	0.25	0/2422
17	LI	0.09	0/1728	0.26	0/2313
18	LJ	0.10	0/1029	0.30	0/1388
19	LK	0.08	0/1348	0.22	0/1808
20	LL	0.10	0/1151	0.28	0/1538
21	LM	0.09	0/1751	0.24	0/2338
22	LN	0.08	0/1658	0.26	0/2217
23	LO	0.09	0/2381	0.26	0/3187
24	LP	0.08	0/1564	0.24	0/2092
25	LQ	0.08	0/1712	0.22	0/2265
26	LR	0.09	0/1489	0.24	0/2008
27	LS	0.10	0/1290	0.26	0/1736
28	LT	0.10	0/1245	0.29	0/1670
29	LU	0.08	0/976	0.24	0/1303
30	LV	0.09	0/968	0.26	0/1302
31	LW	0.08	0/981	0.26	0/1310

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LX	0.09	0/735	0.25	0/989
33	LY	0.07	0/1086	0.21	0/1452
34	LZ	0.09	0/1133	0.22	0/1516
35	La	0.09	0/1054	0.24	0/1399
36	Lb	0.08	0/557	0.23	0/743
37	Lc	0.09	0/1896	0.25	0/2540
38	Ld	0.10	0/740	0.26	0/1003
39	Le	0.08	0/1488	0.22	0/1979
40	Lf	0.08	0/1066	0.26	0/1424
41	Lg	0.09	0/1183	0.25	0/1588
42	Lh	0.10	0/1045	0.28	0/1390
43	Li	0.11	0/813	0.29	0/1088
44	Lj	0.10	0/682	0.30	0/911
45	Lk	0.09	0/617	0.26	0/828
46	Ll	0.08	0/463	0.23	0/617
47	Lm	0.09	0/422	0.28	0/562
48	Ln	0.11	0/296	0.29	0/386
49	Lo	0.11	0/705	0.33	0/940
50	Lp	0.10	0/797	0.25	0/1053
51	S1	0.13	2/43029 (0.0%)	0.23	0/67033
52	S2	0.09	0/328	0.25	0/503
52	S4	0.11	0/1613	0.27	0/2508
53	S3	0.08	0/1785	0.18	0/2778
54	SA	0.10	0/1933	0.28	0/2596
55	SB	0.10	0/1696	0.28	0/2293
56	SC	0.08	0/1674	0.22	0/2240
57	SD	0.09	0/1536	0.24	0/2059
58	SE	0.09	0/2092	0.27	0/2819
59	SF	0.09	0/1744	0.25	0/2362
60	SG	0.09	0/1889	0.24	0/2523
61	SH	0.08	0/1463	0.23	0/1963
62	SI	0.10	0/1679	0.28	0/2255
63	SJ	0.09	0/1038	0.25	0/1391
64	SK	0.09	0/1605	0.25	0/2150
65	SL	0.08	0/1161	0.24	0/1559
66	SM	0.09	0/815	0.24	0/1105
67	SN	0.46	2/899 (0.2%)	0.89	5/1217 (0.4%)
68	SO	0.10	0/1039	0.30	0/1395
69	SP	0.09	0/1120	0.25	0/1500
70	SQ	0.08	0/477	0.24	0/660
71	SR	0.08	0/1158	0.23	0/1553
72	SS	0.08	0/458	0.25	0/607
73	ST	0.09	0/1190	0.27	0/1594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	SU	0.09	0/1289	0.27	0/1731
75	SV	0.08	0/1002	0.22	0/1334
76	SW	0.09	0/948	0.22	0/1275
77	SX	0.08	0/1237	0.24	0/1661
78	SY	0.09	0/684	0.25	0/928
79	SZ	0.09	0/1071	0.27	0/1425
80	Sa	0.08	0/657	0.24	0/882
81	Sb	0.09	0/842	0.25	0/1127
82	Sc	0.08	0/675	0.23	0/907
83	Sd	0.08	0/498	0.31	0/668
84	Se	0.09	0/457	0.26	0/609
85	Sf	0.07	0/472	0.25	0/640
86	Sg	0.08	0/2400	0.26	0/3260
87	Sh	0.09	0/1231	0.27	0/1671
88	S5	0.08	0/279	0.21	0/431
All	All	0.13	11/226647 (0.0%)	0.25	5/332750 (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
28	LT	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	SN	100	PRO	CG-CD	-11.35	1.12	1.50
67	SN	100	PRO	CB-CG	-5.79	1.20	1.49
2	L2	527	A2M	O3'-P	5.36	1.61	1.56
2	L2	1384	A2M	O3'-P	5.20	1.61	1.56
51	S1	668	A2M	O3'-P	5.17	1.61	1.56
1	L1	1253	OMU	O3'-P	5.12	1.61	1.56
2	L2	604	A2M	O3'-P	5.11	1.61	1.56
2	L2	1372	A2M	O3'-P	5.11	1.61	1.56
1	L1	1039	OMU	O3'-P	5.08	1.61	1.56
51	S1	98	A2M	O3'-P	5.05	1.61	1.56
2	L2	572	A2M	O3'-P	5.05	1.61	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	SN	100	PRO	N-CD-CG	-19.68	73.69	103.20
67	SN	100	PRO	CA-CB-CG	-17.99	70.31	104.50
67	SN	100	PRO	CB-CG-CD	8.34	132.79	106.10
67	SN	100	PRO	N-CA-CB	-6.44	97.40	103.19
67	SN	100	PRO	CA-N-CD	-6.41	103.03	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	LT	135	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	36117	0	18210	264	0
2	L2	24815	0	12579	193	0
3	L3	3880	0	1967	29	0
4	L4	3937	0	1989	19	0
5	L5	2578	0	1309	23	0
6	L6	1526	0	779	23	0
7	L7	3534	0	1793	30	0
8	L8	2551	0	1293	14	0
9	LA	1972	0	2018	21	0
10	LB	3216	0	3334	47	0
11	LC	2826	0	2942	24	0
12	LD	1391	0	1436	21	0
13	LE	1477	0	1558	22	0
14	LF	1169	0	1242	26	0
15	LG	1895	0	1993	18	0
16	LH	1767	0	1872	20	0
17	LI	1695	0	1764	15	0
18	LJ	1012	0	1057	12	0
19	LK	1329	0	1381	17	0
20	LL	1124	0	1151	22	0
21	LM	1711	0	1790	20	0
22	LN	1626	0	1696	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	LO	2339	0	2424	25	0
24	LP	1539	0	1648	21	0
25	LQ	1692	0	1807	16	0
26	LR	1455	0	1492	13	0
27	LS	1261	0	1311	13	0
28	LT	1221	0	1256	11	0
29	LU	960	0	987	15	0
30	LV	953	0	1016	5	0
31	LW	967	0	1040	15	0
32	LX	714	0	727	6	0
33	LY	1065	0	1135	8	0
34	LZ	1117	0	1165	18	0
35	La	1043	0	1142	11	0
36	Lb	546	0	575	5	0
37	Lc	1862	0	1959	16	0
38	Ld	730	0	743	10	0
39	Le	1469	0	1599	17	0
40	Lf	1046	0	1106	6	0
41	Lg	1159	0	1209	16	0
42	Lh	1029	0	1084	17	0
43	Li	798	0	853	3	0
44	Lj	668	0	672	8	0
45	Lk	608	0	641	5	0
46	Ll	450	0	483	6	0
47	Lm	416	0	446	7	0
48	Ln	292	0	331	4	0
49	Lo	693	0	712	7	0
50	Lp	784	0	841	13	0
51	S1	39635	0	20030	303	0
52	S2	325	0	175	3	0
52	S4	1446	0	738	16	0
53	S3	1599	0	816	9	0
54	SA	1909	0	1999	18	0
55	SB	1662	0	1692	22	0
56	SC	1646	0	1716	26	0
57	SD	1508	0	1582	29	0
58	SE	2054	0	2148	19	0
59	SF	1708	0	1754	17	0
60	SG	1866	0	1990	32	0
61	SH	1441	0	1469	19	0
62	SI	1649	0	1752	26	0
63	SJ	1021	0	1050	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	SK	1582	0	1652	21	0
65	SL	1140	0	1197	16	0
66	SM	805	0	844	16	0
67	SN	874	0	860	13	0
68	SO	1024	0	1052	13	0
69	SP	1100	0	1146	15	0
70	SQ	480	0	229	2	0
71	SR	1138	0	1186	12	0
72	SS	452	0	459	5	0
73	ST	1167	0	1243	9	0
74	SU	1260	0	1301	7	0
75	SV	992	0	1065	20	0
76	SW	928	0	955	13	0
77	SX	1206	0	1231	16	0
78	SY	673	0	664	8	0
79	SZ	1051	0	1130	17	0
80	Sa	650	0	688	12	0
81	Sb	825	0	859	7	0
82	Sc	661	0	647	10	0
83	Sd	496	0	511	4	0
84	Se	449	0	475	8	0
85	Sf	465	0	353	14	0
86	Sg	2343	0	2256	41	0
87	Sh	1212	0	1139	29	0
88	S5	251	0	130	1	0
89	L1	150	0	285	14	0
89	L2	20	0	36	1	0
89	LM	10	0	19	3	0
89	S1	30	0	57	5	0
90	L1	120	0	0	0	0
90	L2	94	0	0	0	0
90	L3	5	0	0	0	0
90	L4	10	0	0	0	0
90	L5	6	0	0	0	0
90	L6	2	0	0	0	0
90	L7	4	0	0	0	0
90	L8	6	0	0	0	0
90	LA	2	0	0	0	0
90	LG	1	0	0	0	0
90	LJ	1	0	0	0	0
90	LN	1	0	0	0	0
90	LS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	LT	1	0	0	0	0
90	Lf	1	0	0	0	0
90	Lh	2	0	0	0	0
90	S1	109	0	0	0	0
90	S3	1	0	0	0	0
90	SG	1	0	0	0	0
90	SO	1	0	0	0	0
90	ST	1	0	0	0	0
90	SX	1	0	0	0	0
90	Sb	1	0	0	0	0
91	L1	15	0	0	0	0
91	L2	12	0	0	0	0
91	L3	1	0	0	0	0
91	L4	3	0	0	0	0
91	L7	2	0	0	0	0
91	LN	1	0	0	0	0
91	Lf	1	0	0	0	0
91	S1	12	0	0	0	0
91	SS	1	0	0	0	0
92	L1	20	0	0	0	0
92	L2	14	0	0	0	0
92	L4	4	0	0	0	0
92	L7	1	0	0	0	0
92	LB	1	0	0	0	0
92	LC	2	0	0	0	0
92	LM	1	0	0	0	0
92	LV	1	0	0	0	0
92	Le	1	0	0	0	0
92	Ll	1	0	0	0	0
92	S1	19	0	0	0	0
93	L1	42	0	82	1	0
93	L2	30	0	60	1	0
93	L4	6	0	12	0	0
93	L5	6	0	12	0	0
93	S1	12	0	24	0	0
94	L1	42	0	45	3	0
94	L2	84	0	90	6	0
94	L7	42	0	45	4	0
94	S1	84	0	89	5	0
95	LK	1	0	0	0	0
95	Lj	1	0	0	0	0
95	Lm	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	Lo	1	0	0	0	0
95	Lp	1	0	0	0	0
95	SS	1	0	0	0	0
95	Sb	1	0	0	0	0
96	L1	762	0	0	4	0
96	L2	787	0	0	4	0
96	L3	49	0	0	0	0
96	L4	55	0	0	1	0
96	L5	22	0	0	0	0
96	L7	24	0	0	0	0
96	LA	46	0	0	1	0
96	LB	42	0	0	0	0
96	LC	27	0	0	0	0
96	LD	1	0	0	0	0
96	LG	1	0	0	0	0
96	LH	6	0	0	0	0
96	LI	11	0	0	0	0
96	LJ	5	0	0	0	0
96	LL	15	0	0	0	0
96	LM	26	0	0	0	0
96	LN	2	0	0	0	0
96	LO	1	0	0	0	0
96	LP	9	0	0	0	0
96	LQ	11	0	0	0	0
96	LS	4	0	0	0	0
96	LT	15	0	0	0	0
96	LU	1	0	0	0	0
96	LV	2	0	0	0	0
96	LW	5	0	0	1	0
96	LX	2	0	0	0	0
96	LY	2	0	0	0	0
96	La	1	0	0	0	0
96	Lb	5	0	0	0	0
96	Lc	2	0	0	0	0
96	Ld	4	0	0	0	0
96	Le	6	0	0	0	0
96	Lf	3	0	0	0	0
96	Lg	3	0	0	0	0
96	Lh	12	0	0	0	0
96	Lj	18	0	0	0	0
96	Ln	9	0	0	0	0
96	Lo	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
96	Lp	14	0	0	0	0
96	S1	595	0	0	3	0
96	S2	1	0	0	0	0
96	S3	6	0	0	0	0
96	S4	15	0	0	0	0
96	SA	6	0	0	0	0
96	SF	1	0	0	0	0
96	SJ	1	0	0	0	0
96	SK	19	0	0	0	0
96	SO	9	0	0	0	0
96	SP	4	0	0	0	0
96	ST	14	0	0	0	0
96	SU	9	0	0	0	0
96	Sb	9	0	0	0	0
96	Sc	1	0	0	0	0
96	Sg	1	0	0	0	0
All	All	218491	0	158596	1688	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1688) 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)
94:L2:1729:PAR:O43	94:L2:1729:PAR:C13	1.65	1.24
94:S1:2445:PAR:C13	94:S1:2445:PAR:O43	1.65	1.24
94:L2:1728:PAR:O43	94:L2:1728:PAR:C13	1.65	1.19
94:L7:208:PAR:O43	94:L7:208:PAR:C13	1.65	1.17
94:L1:1978:PAR:O43	94:L1:1978:PAR:C13	1.65	1.12
94:S1:2446:PAR:O43	94:S1:2446:PAR:C13	1.65	1.12
51:S1:955:A:HO2'	51:S1:956:A:H8	1.04	0.94
51:S1:1281:C:HO2'	63:SJ:2:THR:N	1.73	0.86
2:L2:1441:C:H5	6:L6:6:G:H1	1.22	0.86
87:Sh:163:GLN:HE21	87:Sh:178:ASP:HA	1.40	0.86
2:L2:1078:OMG:N2	2:L2:1236:C:O2	2.10	0.82
51:S1:264:C:O2	51:S1:275:A:N6	2.14	0.81
2:L2:1139:U:HO2'	2:L2:1171:G:HO2'	1.31	0.78
2:L2:1502:G:OP2	39:Le:33:ARG:NH1	2.18	0.77
2:L2:134:C:H5	2:L2:344:G:H1	1.34	0.76
5:L5:65:U:H3	5:L5:93:G:H1	1.33	0.75
1:L1:1182:C:O2	1:L1:1190:OMG:N2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L8:55:G:H21	12:LD:11:MET:HE3	1.52	0.74
51:S1:694:U:H3	51:S1:751:G:H1	1.33	0.74
2:L2:569:G:O2'	2:L2:571:G:OP2	2.05	0.74
8:L8:67:C:N4	22:LN:210:ASN:O	2.21	0.74
2:L2:1458:G:OP1	10:LB:148:ARG:NH1	2.21	0.73
19:LK:43:ASP:HB3	19:LK:46:MET:HB2	1.71	0.73
31:LW:28:MET:HB3	31:LW:98:PRO:HG2	1.69	0.72
64:SK:113:TYR:OH	64:SK:169:HIS:NE2	2.18	0.72
94:L2:1729:PAR:O44	94:L2:1729:PAR:N64	2.23	0.72
51:S1:1114:G:H1	51:S1:1207:U:H3	1.36	0.72
1:L1:599:G:H1	1:L1:606:C:H5	1.37	0.72
51:S1:779:A:H62	51:S1:839:G:H1	1.37	0.72
1:L1:242:A:H5''	34:LZ:146:ARG:HD3	1.71	0.71
87:Sh:136:SER:OG	87:Sh:177:LEU:O	2.09	0.71
1:L1:1685:G:H22	1:L1:1715:U:H3	1.37	0.71
8:L8:111:A:OP1	23:LO:289:ARG:NH1	2.23	0.71
52:S4:43:U:H3	52:S4:55:G:H1	1.39	0.71
51:S1:1767:G:OP1	51:S1:1767:G:N2	2.23	0.70
5:L5:37:C:OP2	10:LB:392:LYS:NZ	2.25	0.70
1:L1:1527:OMC:HM22	1:L1:1528:PSU:H5''	1.73	0.70
48:Ln:3:THR:HG22	51:S1:2196:G:H5''	1.74	0.70
84:Se:25:GLU:OE2	84:Se:25:GLU:N	2.26	0.69
1:L1:611:C:OP2	11:LC:359:ARG:NH1	2.26	0.69
51:S1:1543:B8N:O3'	65:SL:148:TYR:O	2.10	0.69
85:Sf:123:PRO:HA	85:Sf:127:ALA:HB2	1.74	0.69
1:L1:1588:G:O2'	1:L1:1590:G:OP2	2.10	0.69
57:SD:51:MET:HE3	57:SD:75:ILE:HD11	1.75	0.69
2:L2:782:G:H1	2:L2:807:A:H61	1.40	0.68
11:LC:113:LYS:HG2	21:LM:203:LYS:HB3	1.75	0.68
78:SY:10:GLU:OE2	78:SY:10:GLU:N	2.25	0.68
1:L1:1250:U:OP2	16:LH:67:ARG:NH1	2.25	0.68
51:S1:159:C:OP1	60:SG:2:LYS:NZ	2.26	0.68
56:SC:207:ILE:HD13	75:SV:50:ILE:HD11	1.75	0.68
87:Sh:67:VAL:HG12	87:Sh:70:ALA:H	1.58	0.68
51:S1:878:C:H2'	51:S1:879:A:H8	1.58	0.68
2:L2:743:C:H2'	2:L2:744:G:H8	1.59	0.68
67:SN:94:MET:HE3	67:SN:98:GLN:HB3	1.76	0.68
1:L1:1684:G:H22	1:L1:1716:G:H1	1.40	0.68
51:S1:927:G:H1	51:S1:959:U:H3	1.40	0.68
5:L5:62:C:H3'	5:L5:63:G:H21	1.59	0.67
5:L5:64:G:OP2	5:L5:64:G:N2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S4:26:U:O2	52:S4:30:A:N6	2.27	0.67
74:SU:36:PRO:HB3	74:SU:47:ILE:HD11	1.75	0.67
3:L3:212:G:H5'	33:LY:131:ARG:HH22	1.60	0.67
51:S1:1980:U:H4'	51:S1:2019:OMC:H4'	1.75	0.67
21:LM:195:ASN:O	89:LM:301:SPD:N10	2.27	0.67
14:LF:42:LEU:HD11	14:LF:85:ILE:HG13	1.75	0.67
58:SE:97:ARG:HB2	58:SE:111:LEU:HD11	1.76	0.66
2:L2:1402:G:N2	2:L2:1405:A:OP2	2.28	0.66
35:La:92:THR:HG22	35:La:95:ARG:H	1.60	0.66
2:L2:67:G:O6	39:Le:103:LYS:NZ	2.28	0.66
1:L1:306:G:H5''	21:LM:14:LYS:HE3	1.76	0.66
51:S1:695:G:H1	51:S1:750:U:H3	1.43	0.66
59:SF:138:ARG:HA	59:SF:141:MET:HE2	1.77	0.66
68:SO:106:GLN:HG2	81:Sb:47:LEU:HD23	1.76	0.66
1:L1:601:G:H1'	1:L1:604:C:H5	1.60	0.66
1:L1:1679:G:H1	1:L1:1721:U:H3	1.42	0.66
7:L7:93:C:O2'	7:L7:94:G:OP1	2.13	0.66
86:Sg:123:VAL:HG22	86:Sg:133:VAL:HG22	1.78	0.66
1:L1:1715:U:H2'	1:L1:1716:G:H8	1.61	0.66
51:S1:255:A:H5''	51:S1:943:U:H1'	1.76	0.66
54:SA:151:GLN:HE21	54:SA:153:SER:HB2	1.60	0.66
1:L1:983:U:O2'	89:L1:1813:SPD:N1	2.29	0.65
4:L4:126:G:O2'	4:L4:127:G:N2	2.29	0.65
7:L7:71:A:H3'	31:LW:48:ARG:HB2	1.77	0.65
64:SK:57:ALA:HB2	64:SK:196:GLY:HA2	1.79	0.65
69:SP:60:LYS:HG3	69:SP:116:PRO:HG3	1.78	0.65
76:SW:75:LYS:HE3	76:SW:78:GLU:HB2	1.78	0.65
51:S1:1207:U:H5'	73:ST:55:ARG:HD3	1.78	0.65
70:SQ:106:ARG:HA	70:SQ:111:GLU:HA	1.78	0.65
58:SE:84:MET:HE2	58:SE:120:LEU:H	1.62	0.65
14:LF:54:LEU:HD11	14:LF:66:SER:HB3	1.77	0.65
15:LG:106:ARG:HG3	15:LG:109:ARG:HH21	1.62	0.65
2:L2:1108:U:H5'	12:LD:67:ILE:HD11	1.76	0.65
43:Li:95:GLU:OE1	43:Li:98:ARG:NH2	2.30	0.65
51:S1:761:A:H62	51:S1:768:A:H61	1.42	0.65
51:S1:1539:PSU:O4	51:S1:1550:OMG:N2	2.28	0.65
86:Sg:38:ALA:HB3	86:Sg:61:LEU:HB2	1.78	0.65
93:L2:1727:PUT:H31	10:LB:242:CYS:HB2	1.79	0.65
5:L5:113:G:OP2	39:Le:64:ARG:N	2.20	0.65
56:SC:177:ARG:NH1	84:Se:63:GLY:O	2.30	0.64
81:Sb:48:ASP:OD1	81:Sb:51:SER:OG	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SC:207:ILE:HD11	75:SV:46:LEU:HD13	1.77	0.64
62:SI:2:GLN:HB2	62:SI:5:LEU:HD13	1.80	0.64
51:S1:1724:G:OP2	51:S1:1724:G:N2	2.26	0.64
2:L2:1284:PSU:H2'	47:Lm:97:ARG:HD3	1.79	0.64
2:L2:1353:U:O2'	2:L2:1373:C:O2	2.15	0.64
13:LE:46:ARG:NH2	19:LK:6:TYR:OH	2.27	0.64
86:Sg:238:ILE:HA	86:Sg:254:THR:HG22	1.79	0.64
9:LA:18:VAL:O	96:LA:401:HOH:O	2.15	0.64
51:S1:689[A]:U:O2'	51:S1:690:G:OP2	2.11	0.64
52:S4:9:A:O2'	52:S4:10:G:N7	2.29	0.64
66:SM:77:PHE:HB3	72:SS:53:PHE:HB3	1.79	0.64
27:LS:51:GLY:HA3	27:LS:92:ARG:HG3	1.80	0.64
51:S1:227:U:O3'	64:SK:164:ARG:NH2	2.30	0.63
1:L1:684:G:H4'	89:L1:1806:SPD:H82	1.80	0.63
12:LD:112:ILE:HD11	12:LD:124:ILE:HG12	1.81	0.63
86:Sg:188:ARG:HH22	86:Sg:223:LEU:HA	1.62	0.63
6:L6:67:C:OP1	41:Lg:96:ARG:NH2	2.31	0.63
51:S1:1493:A:OP1	96:S1:2501:HOH:O	2.14	0.63
54:SA:154:ARG:HG2	54:SA:154:ARG:HH11	1.62	0.63
2:L2:984:G:H1	2:L2:1000:U:H3	1.45	0.63
20:LL:29:GLU:CD	20:LL:29:GLU:H	2.07	0.63
51:S1:171:C:OP1	60:SG:134:ARG:NH1	2.32	0.63
51:S1:1589:G:H1	51:S1:1600:C:H5	1.44	0.63
2:L2:1510:A:H62	10:LB:326:ASN:HB3	1.64	0.62
54:SA:207:LEU:HD12	54:SA:208:PRO:HD2	1.80	0.62
13:LE:90:LYS:HB2	13:LE:182:THR:HG23	1.82	0.62
1:L1:1525:A:H5'	1:L1:1526:U:C5'	2.30	0.62
62:SI:183:ARG:HG2	62:SI:183:ARG:HH11	1.64	0.62
87:Sh:148:THR:HG23	87:Sh:196:ARG:HE	1.65	0.62
4:L4:154:C:H4'	13:LE:155:ARG:HE	1.64	0.62
79:SZ:34:HIS:HB2	79:SZ:37:TRP:HB2	1.82	0.62
1:L1:166:G:OP1	17:LI:137:LYS:NZ	2.32	0.62
2:L2:823:A:O2'	2:L2:824:G:N2	2.32	0.62
1:L1:836:G:OP2	24:LP:98:ARG:NH2	2.32	0.62
3:L3:5:A:N6	3:L3:215:G:O2'	2.33	0.62
51:S1:886:U:H5'	58:SE:238:LYS:HZ1	1.65	0.62
77:SX:74:LEU:HD12	77:SX:120:LEU:HD22	1.82	0.62
2:L2:974:G:H4'	42:Lh:91:ARG:HG2	1.82	0.61
51:S1:1905:C:O2'	51:S1:1906:G:O5'	2.15	0.61
56:SC:174:CYS:HB2	56:SC:181:ILE:HB	1.81	0.61
1:L1:927:A2M:HM'2	1:L1:928:C:H5'	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:771:G:N7	9:LA:67:TYR:OH	2.25	0.61
7:L7:94:G:OP2	44:Lj:73:ARG:NH1	2.32	0.61
51:S1:128:C:H4'	51:S1:129:U:O5'	1.99	0.61
51:S1:821:A:O2'	60:SG:225:GLN:OE1	2.17	0.61
79:SZ:125:ARG:HG3	79:SZ:126:GLY:H	1.64	0.61
34:LZ:22:ARG:HB3	40:Lf:76:PRO:HG2	1.82	0.61
38:Ld:55:ARG:O	38:Ld:59:GLU:HG3	2.01	0.61
80:Sa:91:LEU:HD21	80:Sa:94:CYS:HB2	1.82	0.61
12:LD:26:GLY:HA2	12:LD:67:ILE:HB	1.81	0.61
55:SB:131:ARG:NH2	55:SB:154:ASP:O	2.34	0.61
2:L2:335:C:H3'	2:L2:336:C:H5''	1.82	0.61
3:L3:155:A:H61	3:L3:174:C:H42	1.48	0.61
51:S1:689[A]:U:H4'	51:S1:690:G:H5''	1.83	0.61
2:L2:786:A:H4'	2:L2:787:G:OP1	2.00	0.61
36:Lb:5:LYS:HE2	36:Lb:8:THR:HB	1.82	0.61
7:L7:9:G:OP2	94:L7:208:PAR:N64	2.34	0.60
7:L7:31:A:O2'	7:L7:33:U:OP2	2.14	0.60
2:L2:1012:U:OP1	15:LG:49[B]:ARG:NH2	2.34	0.60
39:Le:47:GLU:OE2	39:Le:50:ARG:NH1	2.34	0.60
1:L1:77:U:H5''	21:LM:186:PRO:HG3	1.84	0.60
37:Lc:60:LYS:NZ	37:Lc:64:GLU:OE2	2.34	0.60
52:S4:50:A:O2'	52:S4:52:U:OP2	2.11	0.60
23:LO:134:THR:HG22	23:LO:136:LYS:H	1.67	0.60
52:S4:25:A:H3'	52:S4:26:U:H5''	1.82	0.60
1:L1:485:A:O5'	14:LF:110:LYS:NZ	2.34	0.60
5:L5:70:C:H41	5:L5:88:C:H42	1.49	0.60
7:L7:93:C:H2'	7:L7:94:G:H5''	1.84	0.60
51:S1:1119:U:H5'	51:S1:1120:U:H5'	1.84	0.60
61:SH:83:LEU:HD22	61:SH:94:PRO:HB2	1.83	0.60
2:L2:1052:C:O2'	2:L2:1053:A:O5'	2.17	0.60
15:LG:142:ARG:HG2	15:LG:146:LYS:HE2	1.82	0.60
48:Ln:25:ARG:HH22	51:S1:2152:A:H4'	1.67	0.60
51:S1:1108:A:H5''	73:ST:16:LEU:HD12	1.84	0.60
1:L1:494:A:OP1	14:LF:82:ARG:NE	2.33	0.60
2:L2:512:PSU:OP1	53:S3:25:U:O2'	2.20	0.60
2:L2:695:G:H2'	2:L2:696:A:C8	2.37	0.60
51:S1:913:G:OP2	51:S1:913:G:N2	2.29	0.60
65:SL:100:GLN:HB2	65:SL:108:LYS:HE3	1.83	0.60
86:Sg:13:TRP:HB2	86:Sg:34:ARG:HG3	1.84	0.60
86:Sg:132:ARG:HG2	86:Sg:143:GLU:HG2	1.84	0.60
1:L1:556:C:H5''	1:L1:557:U:H5''	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:23:U:O2'	3:L3:25:G:OP1	2.19	0.60
20:LL:72:THR:HG22	20:LL:108:LYS:HB3	1.83	0.60
2:L2:1510:A:N6	10:LB:327:ASP:H	2.00	0.59
5:L5:127:A:OP1	39:Le:79:ARG:NH2	2.35	0.59
54:SA:146:LYS:HB3	54:SA:210:ARG:HB2	1.84	0.59
80:Sa:60:ILE:HB	80:Sa:101:TYR:HB2	1.84	0.59
1:L1:663:C:OP1	16:LH:111:LYS:NZ	2.35	0.59
1:L1:1105:A:H5''	2:L2:1064:A:H61	1.65	0.59
1:L1:1209:G:OP2	1:L1:1209:G:N2	2.29	0.59
64:SK:162:TRP:HB3	64:SK:166:ARG:HH21	1.67	0.59
2:L2:28:G:H4'	44:Lj:8:MET:HG3	1.83	0.59
42:Lh:10:ARG:HG2	42:Lh:10:ARG:HH11	1.66	0.59
1:L1:1281:A:O2'	1:L1:1348:A:N6	2.35	0.59
1:L1:1372:G:H2'	1:L1:1373:A2M:H8	1.84	0.59
6:L6:67:C:N4	41:Lg:96:ARG:O	2.30	0.59
13:LE:155:ARG:NH1	13:LE:156:GLU:OE2	2.34	0.59
51:S1:478:C:H5''	69:SP:48:LYS:HE3	1.83	0.59
53:S3:8:U:O2'	53:S3:22:A:N6	2.35	0.59
85:Sf:140:CYS:SG	85:Sf:141:GLY:N	2.75	0.59
1:L1:130:U:H2'	1:L1:132:A:H62	1.67	0.59
1:L1:982:C:OP1	89:L1:1813:SPD:N10	2.35	0.59
2:L2:1329:U:O2'	4:L4:42:A:OP1	2.18	0.59
41:Lg:74:ARG:HG2	41:Lg:141:PRO:HD3	1.83	0.59
1:L1:1493:G:N2	1:L1:1496:A:OP2	2.28	0.59
71:SR:88:GLN:HA	71:SR:96:THR:HG23	1.83	0.59
1:L1:1487:U:OP1	94:L7:208:PAR:N24	2.36	0.59
6:L6:49:C:N4	41:Lg:29:LYS:O	2.36	0.59
1:L1:1084:U:H3'	1:L1:1085:C:H5''	1.84	0.59
3:L3:156:G:H1	3:L3:173:U:H3	1.49	0.59
18:LJ:111:MET:HE1	18:LJ:116:ILE:HG13	1.85	0.59
61:SH:8:LEU:HD21	61:SH:55:VAL:HG11	1.84	0.59
6:L6:70:G:HO2'	6:L6:71:A:H8	1.50	0.59
27:LS:82:THR:HG22	36:Lb:16:ASN:HA	1.83	0.59
51:S1:2010:G:H1	51:S1:2026:U:H3	1.50	0.59
67:SN:3:THR:HB	67:SN:51:GLN:HG3	1.84	0.59
1:L1:1667:G:OP2	21:LM:34:HIS:NE2	2.25	0.58
51:S1:672:G:N1	51:S1:1217:A:OP1	2.32	0.58
2:L2:1136:U:H2'	2:L2:1137:G:C8	2.38	0.58
2:L2:1253:OMG:HM21	2:L2:1255:A:H2'	1.84	0.58
2:L2:1335:C:H2'	2:L2:1337:C:H5''	1.85	0.58
2:L2:1510:A:N7	10:LB:326:ASN:ND2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:105:LEU:HD13	25:LQ:135:LYS:HE3	1.85	0.58
51:S1:1788:U:H5'	75:SV:48:ASN:HB3	1.84	0.58
57:SD:4:TYR:O	58:SE:19:LYS:NZ	2.33	0.58
14:LF:194:ASN:O	19:LK:110:ARG:NH2	2.37	0.58
51:S1:1234:G:N3	89:S1:2301:SPD:N1	2.51	0.58
1:L1:912:C:OP1	96:L1:2001:HOH:O	2.17	0.58
2:L2:1404:G:H5''	9:LA:220:GLY:HA3	1.84	0.58
3:L3:174:C:H2'	3:L3:175:A:C8	2.38	0.58
60:SG:129:ASP:OD1	60:SG:129:ASP:N	2.37	0.58
11:LC:178:ASP:HB3	11:LC:206:PRO:HD3	1.85	0.58
20:LL:39:HIS:O	20:LL:40:HIS:ND1	2.35	0.58
51:S1:1781:U:O2'	51:S1:1782:G:N7	2.33	0.58
51:S1:816:C:OP1	87:Sh:174:TYR:OH	2.21	0.58
61:SH:181:GLU:OE1	61:SH:184:ARG:NH2	2.37	0.58
79:SZ:63:SER:HB3	79:SZ:81:LEU:HB2	1.84	0.58
16:LH:79:ARG:HA	16:LH:88:PRO:HD2	1.85	0.58
24:LP:23:ASN:HB3	24:LP:26:ILE:HB	1.83	0.58
70:SQ:98:ALA:HB2	70:SQ:118:CYS:H	1.68	0.58
13:LE:31:ARG:NH1	13:LE:187:GLU:OE2	2.37	0.58
51:S1:1632:C:O2	51:S1:1829:OMG:N2	2.19	0.58
3:L3:154:C:H42	3:L3:175:A:H61	1.52	0.58
31:LW:71:TYR:O	96:LW:201:HOH:O	2.17	0.58
32:LX:84:ARG:NH1	60:SG:132:ALA:O	2.37	0.58
51:S1:1362:A:OP1	82:Sc:17:ARG:NH2	2.37	0.58
1:L1:493:A:O2'	14:LF:80:ASP:OD2	2.22	0.57
11:LC:282:LEU:HD11	24:LP:29:LEU:HG	1.85	0.57
45:Lk:55:LYS:HD2	45:Lk:58:ARG:HH22	1.68	0.57
55:SB:15:GLU:OE1	75:SV:118:ARG:NH2	2.37	0.57
55:SB:60:LYS:NZ	78:SY:74:ASN:OD1	2.33	0.57
56:SC:27:GLU:HG2	56:SC:68:LEU:HD21	1.86	0.57
1:L1:631:G:O6	37:Lc:43:ARG:NE	2.36	0.57
2:L2:623:A:H5''	2:L2:624:C:H5	1.68	0.57
11:LC:43:MET:HB3	11:LC:236:LEU:HD21	1.86	0.57
86:Sg:178:VAL:O	86:Sg:187:GLU:N	2.37	0.57
5:L5:51:A:H1'	5:L5:52:U:H2'	1.85	0.57
6:L6:68:A:N6	41:Lg:34:TYR:OH	2.37	0.57
10:LB:138:ASN:HA	10:LB:143:LYS:HZ3	1.69	0.57
51:S1:1572:C:H41	51:S1:1615:G:H1	1.52	0.57
2:L2:558:A:OP1	2:L2:560:OMU:H5	2.05	0.57
66:SM:39:ARG:NH2	66:SM:97:LYS:O	2.37	0.57
1:L1:141:U:H1'	1:L1:142:G:H5'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1391:U:H2'	2:L2:1392:U:H6	1.68	0.57
56:SC:56:GLU:OE1	56:SC:56:GLU:N	2.38	0.57
47:Lm:78:MET:HE3	47:Lm:83:VAL:HA	1.86	0.57
51:S1:479:A2M:O5'	51:S1:479:A2M:H8	2.04	0.57
56:SC:123:ARG:O	56:SC:127:GLU:HG3	2.05	0.57
2:L2:646:G:H5'	2:L2:647:A:OP2	2.04	0.57
2:L2:1486:G:H2'	2:L2:1487:G:H8	1.70	0.57
10:LB:93:ARG:HB3	10:LB:102:ILE:HD11	1.87	0.57
75:SV:32:LYS:O	75:SV:36:MET:HG2	2.04	0.57
1:L1:604:C:O2'	1:L1:605:G:O4'	2.23	0.57
2:L2:1407:A:N7	9:LA:215:ASN:ND2	2.53	0.57
4:L4:24:A:H5''	16:LH:7:LYS:HB2	1.87	0.57
64:SK:76:VAL:HG12	64:SK:108:PRO:HG2	1.85	0.57
69:SP:11:ARG:NH2	74:SU:117:LYS:O	2.34	0.57
82:Sc:34:MET:HE2	82:Sc:49:SER:HA	1.87	0.57
7:L7:60:U:O4	35:La:63:ASN:ND2	2.33	0.57
51:S1:1885:A:H5'	65:SL:20:THR:HG21	1.86	0.57
51:S1:1914:U:OP1	77:SX:134:GLN:NE2	2.35	0.56
1:L1:1242:U:OP1	19:LK:17:ARG:NH2	2.38	0.56
2:L2:421:A:N7	96:L2:1832:HOH:O	2.32	0.56
5:L5:26:A:OP2	10:LB:116:ARG:NH2	2.38	0.56
10:LB:216:GLN:OE1	10:LB:360:LYS:NZ	2.39	0.56
13:LE:123:GLN:NE2	13:LE:156:GLU:OE1	2.32	0.56
16:LH:65:GLU:OE1	16:LH:69:LYS:NZ	2.29	0.56
34:LZ:21:LYS:HG2	34:LZ:26:ARG:HG2	1.87	0.56
57:SD:58:LEU:HD22	57:SD:68:ARG:HA	1.86	0.56
57:SD:77:ARG:NH1	57:SD:81:GLU:OE2	2.36	0.56
1:L1:100:G:OP2	1:L1:100:G:N2	2.35	0.56
1:L1:837:A:H4'	1:L1:838:G:H5'	1.85	0.56
1:L1:1599:U:O2	1:L1:1626:OMG:N2	2.37	0.56
2:L2:1379:A:H5''	2:L2:1381:G:H4'	1.86	0.56
13:LE:125:VAL:HG13	13:LE:156:GLU:HG3	1.86	0.56
59:SF:55:VAL:HG21	59:SF:78:ILE:HG23	1.88	0.56
59:SF:182:VAL:HB	59:SF:209:TYR:HB2	1.87	0.56
64:SK:68:ALA:HB2	64:SK:201:ILE:HD11	1.88	0.56
87:Sh:165:LEU:O	87:Sh:166:ARG:NH1	2.38	0.56
1:L1:2:C:H5'	7:L7:169:A:H2	1.71	0.56
5:L5:131:A:OP1	28:LT:43:LYS:NZ	2.38	0.56
8:L8:32:C:H5'	12:LD:139:ARG:HD3	1.88	0.56
53:S3:1:C:H42	53:S3:73:A:H61	1.53	0.56
86:Sg:262:ASP:HB2	86:Sg:269:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:286:G:H1'	60:SG:217:ALA:HB1	1.87	0.56
51:S1:701:G:H22	51:S1:745:G:H22	1.54	0.56
94:S1:2445:PAR:N64	94:S1:2445:PAR:O44	2.38	0.56
1:L1:206:A:OP2	34:LZ:54:LYS:NZ	2.38	0.56
60:SG:2:LYS:HB2	60:SG:111:LEU:HD12	1.88	0.56
1:L1:1238:C:H5''	1:L1:1239:U:H5'	1.86	0.56
51:S1:263:G:H5'	87:Sh:169:ARG:HG3	1.87	0.56
51:S1:396:G:O6	69:SP:15:ARG:NH2	2.39	0.56
51:S1:994:U:H3	51:S1:1018:G:H1	1.54	0.56
51:S1:2150:G:N7	94:S1:2446:PAR:O44	2.39	0.56
66:SM:17:VAL:HG11	66:SM:95:VAL:HG11	1.88	0.56
82:Sc:11:PRO:HB2	82:Sc:16:GLU:HG2	1.86	0.56
25:LQ:15:LEU:HD13	25:LQ:52:ARG:HB2	1.87	0.56
87:Sh:177:LEU:HD12	87:Sh:183:ALA:HA	1.88	0.56
1:L1:1092:U:O2'	22:LN:196:HIS:NE2	2.35	0.55
1:L1:1153:A:H2'	1:L1:1155:A:H62	1.70	0.55
5:L5:127:A:C5	39:Le:13:LYS:HD3	2.41	0.55
21:LM:198:ILE:HD13	89:LM:301:SPD:H81	1.88	0.55
51:S1:1619:G:HO2'	51:S1:1849:G:HO2'	1.54	0.55
51:S1:617:G:H4'	69:SP:88:ASP:HB3	1.87	0.55
87:Sh:160:VAL:HG21	87:Sh:186:PHE:HD2	1.71	0.55
28:LT:112:MET:HE3	28:LT:150:MET:HG3	1.88	0.55
51:S1:789:G:OP1	58:SE:173:ARG:NH1	2.39	0.55
51:S1:79:A:O2'	51:S1:501:A:N1	2.32	0.55
86:Sg:148:GLY:HA2	86:Sg:179:TRP:HH2	1.71	0.55
51:S1:1911:U:H5	51:S1:1928:G:H1	1.54	0.55
51:S1:1961:G:O2'	51:S1:1987:G:N2	2.40	0.55
57:SD:47:THR:O	57:SD:51:MET:HG3	2.06	0.55
76:SW:35:LEU:HG	76:SW:39:GLU:HB2	1.89	0.55
1:L1:97:G:N7	17:LI:12:HIS:NE2	2.54	0.55
12:LD:111:HIS:HD2	12:LD:125:TYR:H	1.52	0.55
2:L2:978:C:OP1	15:LG:33:LYS:NZ	2.37	0.55
20:LL:80:ARG:NH2	20:LL:106:TYR:OH	2.38	0.55
22:LN:88:ARG:HG2	22:LN:90:ARG:HG2	1.89	0.55
51:S1:228:G:OP2	64:SK:160:ARG:NE	2.35	0.55
51:S1:878:C:H2'	51:S1:879:A:C8	2.42	0.55
52:S4:31:U:H4'	68:SO:59:ARG:HH22	1.71	0.55
54:SA:44:ALA:HB2	68:SO:40:MET:HE2	1.88	0.55
86:Sg:89:ILE:HB	86:Sg:103:PHE:HB2	1.88	0.55
1:L1:170:U:O2	35:La:107:LYS:NZ	2.38	0.55
1:L1:398:G:N2	1:L1:401:A:OP2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:746:A:H2'	2:L2:747:A:C8	2.42	0.55
2:L2:1281:U:O4	2:L2:1336:G:N2	2.40	0.55
51:S1:1684:U:H3	51:S1:1820:G:H22	1.55	0.55
55:SB:77:VAL:HG22	55:SB:124:VAL:HB	1.87	0.55
78:SY:42:ALA:HA	78:SY:54:THR:HG22	1.88	0.55
1:L1:1017:PSU:OP1	20:LL:44:ASN:ND2	2.38	0.55
2:L2:849:C:H42	2:L2:949:U:H3	1.55	0.55
20:LL:134:ILE:HG21	20:LL:141:VAL:HG23	1.88	0.55
29:LU:42:ASP:O	29:LU:46:ASN:ND2	2.39	0.55
39:Le:96:LEU:HD11	39:Le:108:ALA:HB2	1.88	0.55
51:S1:1360:U:H4'	51:S1:1361:U:O5'	2.06	0.55
1:L1:1683:C:H2'	1:L1:1684:G:C8	2.43	0.54
51:S1:594:A:H61	51:S1:643:A:H5''	1.72	0.54
64:SK:26:LYS:HG2	64:SK:29:LEU:HD23	1.89	0.54
1:L1:510:U:O2'	1:L1:511:A:OP1	2.24	0.54
3:L3:62:U:O4	29:LU:96:LYS:NZ	2.40	0.54
12:LD:89:LYS:HE3	12:LD:106:PHE:HB2	1.88	0.54
51:S1:1273:A:N7	51:S1:2175:C:O2'	2.38	0.54
51:S1:1961:G:H5'	77:SX:99:GLY:HA2	1.87	0.54
2:L2:382:A2M:O5'	2:L2:382:A2M:H8	2.07	0.54
4:L4:149:U:H1'	4:L4:150:A:H5''	1.89	0.54
8:L8:16:C:OP2	8:L8:71:C:O2'	2.25	0.54
22:LN:44:ASP:OD1	22:LN:185:ARG:NH1	2.39	0.54
44:Lj:27:TYR:HA	44:Lj:34:CYS:HA	1.90	0.54
51:S1:68:A:OP1	60:SG:175:LYS:NZ	2.39	0.54
52:S4:46:U:O2'	52:S4:47:U:O5'	2.24	0.54
61:SH:47:PHE:HD1	61:SH:130:MET:HE2	1.71	0.54
66:SM:23:SER:HB3	66:SM:29:VAL:HB	1.88	0.54
1:L1:1688:G:H22	1:L1:1712:G:H22	1.55	0.54
45:Lk:57:GLU:HA	45:Lk:60:ILE:HD12	1.88	0.54
60:SG:162:ARG:HG2	60:SG:176:ALA:HB2	1.89	0.54
74:SU:30:ASN:HB3	74:SU:33:MET:HG2	1.88	0.54
62:SI:55:PRO:O	62:SI:170:ARG:NH2	2.41	0.54
85:Sf:120:CYS:HA	85:Sf:131:MET:HE2	1.88	0.54
1:L1:1348:A:H2'	1:L1:1349:A:H4'	1.88	0.54
10:LB:209:ARG:HH22	10:LB:292:ARG:HD2	1.72	0.54
62:SI:40:GLU:OE1	62:SI:43:ARG:NH2	2.41	0.54
63:SJ:18:GLU:HG3	63:SJ:69:LEU:HD23	1.88	0.54
1:L1:1213:C:OP2	37:Lc:104:LYS:NZ	2.41	0.54
2:L2:1450:G:O2'	6:L6:14:A:N6	2.30	0.54
11:LC:162:LYS:HB2	11:LC:165:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:37:MIA:H2'	52:S2:38:A:O4'	2.08	0.54
2:L2:1360:OMG:HN21	52:S2:75:C:H42	1.55	0.54
51:S1:701:G:H1	51:S1:745:G:H22	1.56	0.54
54:SA:5:LYS:NZ	68:SO:58:ASP:OD2	2.39	0.54
2:L2:954:A:C8	42:Lh:114:MET:HE1	2.43	0.54
3:L3:173:U:H2'	3:L3:174:C:C6	2.43	0.54
63:SJ:80:ASP:HA	63:SJ:124:LYS:HA	1.89	0.54
89:L1:1815:SPD:H22	21:LM:83:LYS:HG3	1.90	0.54
2:L2:14:OMC:HM22	2:L2:15:C:O4'	2.08	0.54
2:L2:646:G:N7	2:L2:647:A:N6	2.55	0.54
50:Lp:74:CYS:SG	50:Lp:77:CYS:HB2	2.47	0.54
51:S1:1551:G:H5''	72:SS:30:ALA:HB2	1.90	0.54
1:L1:1363:A:H4'	1:L1:1364:A:H5''	1.89	0.53
1:L1:1773:C:O2'	7:L7:139:A:N3	2.37	0.53
7:L7:71:A:H4'	7:L7:72:A:O5'	2.08	0.53
1:L1:1243:G:OP2	26:LR:2:VAL:N	2.42	0.53
6:L6:24[B]:C:OP1	13:LE:23:ARG:NH1	2.33	0.53
19:LK:16:LEU:HD21	19:LK:57:GLU:HB2	1.90	0.53
44:Lj:55:LYS:HA	44:Lj:58:ARG:HD2	1.90	0.53
51:S1:461:G:O2'	60:SG:60:ASP:OD2	2.25	0.53
51:S1:810:G:OP1	87:Sh:125:THR:OG1	2.26	0.53
51:S1:955:A:O2'	51:S1:956:A:O5'	2.25	0.53
51:S1:1358:A:N6	78:SY:79:ASP:OD1	2.39	0.53
51:S1:1869:U:O2'	51:S1:1961:G:OP1	2.26	0.53
1:L1:73:U:H5''	17:LI:63:VAL:HB	1.90	0.53
51:S1:266:U:H5''	87:Sh:164:ARG:NH2	2.24	0.53
54:SA:154:ARG:HG2	54:SA:154:ARG:NH1	2.24	0.53
56:SC:134:GLU:OE1	56:SC:186:LYS:NZ	2.41	0.53
3:L3:19:A:H2	3:L3:215:G:H21	1.55	0.53
14:LF:168:ASP:OD1	14:LF:169:ALA:N	2.42	0.53
51:S1:167:C:OP1	60:SG:84:GLY:N	2.32	0.53
60:SG:214:ARG:HH11	60:SG:214:ARG:HG3	1.73	0.53
62:SI:132:MET:HE2	62:SI:175:VAL:HG12	1.91	0.53
1:L1:959:OMG:N1	2:L2:660:G:OP1	2.33	0.53
2:L2:19:C:O2'	2:L2:25:A:N1	2.34	0.53
25:LQ:69:ALA:HA	25:LQ:72:MET:HE2	1.90	0.53
39:Le:6:MET:HG2	39:Le:16:LYS:HE3	1.89	0.53
51:S1:754:G:OP2	51:S1:754:G:N2	2.36	0.53
51:S1:1908:A:H5'	51:S1:1909:C:H5	1.72	0.53
87:Sh:195:PHE:HB3	87:Sh:200:LEU:HD13	1.91	0.53
1:L1:1052:A:N1	8:L8:106:C:O2'	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1105:A:H5''	2:L2:1064:A:N6	2.24	0.53
2:L2:603:A:H5'	28:LT:137:THR:HG23	1.91	0.53
2:L2:1276:A:H4'	22:LN:74:LYS:HG2	1.89	0.53
23:LO:142:ASP:N	23:LO:142:ASP:OD1	2.38	0.53
50:Lp:2:VAL:N	50:Lp:90:HIS:O	2.42	0.53
71:SR:85:LEU:HD12	71:SR:96:THR:HG22	1.89	0.53
77:SX:19:LEU:HD11	77:SX:75:ARG:HG3	1.90	0.53
4:L4:21:C:O2'	5:L5:135:U:O4	2.26	0.53
51:S1:90:C:O2'	89:S1:2302:SPD:N1	2.41	0.53
51:S1:934:U:O2'	51:S1:936:U:OP2	2.26	0.53
51:S1:1836:G:O6	67:SN:71:TYR:OH	2.21	0.53
1:L1:1627:U:OP1	30:LV:126:TYR:OH	2.24	0.53
51:S1:277:U:H3	51:S1:945:G:HO2'	1.57	0.53
51:S1:792:G:H3'	51:S1:793:G:H21	1.74	0.53
51:S1:1019:U:H4'	62:SI:80:ALA:HA	1.91	0.53
51:S1:1889:G:H3'	51:S1:1932:A:N6	2.24	0.53
79:SZ:64:LEU:HB3	79:SZ:67:PHE:HE2	1.73	0.53
85:Sf:102:LYS:N	85:Sf:114:GLU:O	2.41	0.53
1:L1:1626:OMG:N2	2:L2:18:A:N3	2.57	0.53
51:S1:1603:U:O2	85:Sf:139:TYR:OH	2.22	0.53
57:SD:87:GLU:CD	57:SD:87:GLU:H	2.16	0.53
66:SM:53:LEU:HD23	66:SM:83:LYS:HG2	1.91	0.53
68:SO:75:VAL:HG22	68:SO:117:MET:HG3	1.89	0.53
1:L1:1003:A:OP1	36:Lb:18:ARG:NH1	2.30	0.53
1:L1:1574:C:H2'	1:L1:1575:G:C8	2.44	0.53
2:L2:954:A:H5'	2:L2:955:C:H5'	1.91	0.53
23:LO:162:GLY:HA2	23:LO:187:PRO:HD3	1.91	0.53
51:S1:323:U:O2'	51:S1:325:G:N2	2.42	0.53
1:L1:24:A:N3	1:L1:366:C:O2'	2.41	0.52
1:L1:31:G:H21	1:L1:49:C:H5	1.55	0.52
2:L2:644:A:OP1	96:L2:1801:HOH:O	2.18	0.52
2:L2:1101:A:H5''	12:LD:107:GLY:HA3	1.91	0.52
2:L2:1510:A:H2	10:LB:209:ARG:HE	1.56	0.52
51:S1:969:A2M:H61	62:SI:101:GLN:N	2.07	0.52
55:SB:204:LEU:HD21	75:SV:85:ALA:HB2	1.91	0.52
64:SK:161:GLU:OE1	64:SK:164:ARG:NH1	2.42	0.52
11:LC:148:GLU:HG3	34:LZ:73:LYS:HD3	1.91	0.52
14:LF:55:LYS:HD2	14:LF:98:THR:HG23	1.91	0.52
80:Sa:65:ILE:HG13	80:Sa:80:LEU:HD21	1.91	0.52
1:L1:1650:U:H5''	21:LM:67:ARG:HD2	1.91	0.52
2:L2:1383:G:O2'	2:L2:1386:C:OP2	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:118:G:OP1	25:LQ:118:HIS:ND1	2.43	0.52
51:S1:146:U:H4'	60:SG:183:ILE:HD13	1.90	0.52
51:S1:1209:C:O2'	51:S1:1210:C:OP1	2.26	0.52
51:S1:1619:G:O2'	51:S1:1849:G:O2'	2.26	0.52
1:L1:51:G:H4'	1:L1:863:G:H4'	1.90	0.52
2:L2:97:A:O2'	2:L2:366:C:O2	2.22	0.52
3:L3:7:U:OP1	33:LY:47:LYS:NZ	2.35	0.52
5:L5:117:A:H1'	10:LB:400:ARG:HH12	1.75	0.52
12:LD:7:ALA:HA	12:LD:12:ARG:HD3	1.92	0.52
33:LY:23:ALA:HA	33:LY:45:GLY:HA2	1.92	0.52
68:SO:86:LEU:HG	68:SO:117:MET:HE2	1.91	0.52
86:Sg:102:LYS:HD2	86:Sg:104:LEU:HD11	1.92	0.52
1:L1:1715:U:H2'	1:L1:1716:G:C8	2.42	0.52
51:S1:1530:G:H5'	51:S1:1542:C:H42	1.74	0.52
83:Sd:21:ALA:HA	83:Sd:76:MET:HA	1.91	0.52
2:L2:1127:G:H5''	27:LS:17:LYS:HG2	1.90	0.52
17:L1:172:GLU:HG2	20:LL:98:VAL:HG21	1.91	0.52
51:S1:979:U:H3	51:S1:1094:G:H1	1.58	0.52
83:Sd:30:LEU:HD12	83:Sd:41:GLN:HG2	1.92	0.52
1:L1:1524:OMG:N2	96:L1:2015:HOH:O	2.30	0.52
51:S1:1160:A:OP1	54:SA:10:SER:OG	2.28	0.52
51:S1:1397:A:O2'	51:S1:1399:G:OP2	2.21	0.52
51:S1:1539:PSU:HN3	51:S1:1550:OMG:HN1	1.57	0.52
1:L1:38:A:H5''	20:LL:35:ALA:HB1	1.91	0.52
6:L6:48:C:C2	14:LF:185:LYS:HD3	2.45	0.52
22:LN:48:VAL:HG22	22:LN:178:ARG:HH12	1.75	0.52
51:S1:889:A:OP2	58:SE:105:ARG:NH2	2.42	0.52
1:L1:839:U:H2'	1:L1:840:G:C8	2.45	0.51
1:L1:1764:A:H3'	1:L1:1766:G:OP2	2.09	0.51
2:L2:590:U:H2'	2:L2:591:A2M:H8	1.91	0.51
14:LF:30:ARG:NH2	41:Lg:144:ILE:OXT	2.37	0.51
22:LN:206:ILE:HD13	23:LO:296:VAL:HG23	1.92	0.51
51:S1:294:G:O2'	51:S1:295:A:OP1	2.27	0.51
51:S1:558:U:H2'	51:S1:559:G:C8	2.45	0.51
71:SR:103:MET:HE3	71:SR:103:MET:HA	1.91	0.51
6:L6:64:U:OP2	14:LF:78:ARG:NE	2.36	0.51
9:LA:32:LEU:HD13	9:LA:163:ARG:HD3	1.91	0.51
13:LE:173:LYS:HB2	47:Lm:127:LEU:HD11	1.92	0.51
86:Sg:240:GLN:HG2	86:Sg:285:ILE:HG12	1.92	0.51
86:Sg:256:ARG:HG2	86:Sg:256:ARG:HH11	1.75	0.51
1:L1:1741:A:O2'	3:L3:204:A:N1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LB:57:VAL:HB	10:LB:365:PHE:HB3	1.92	0.51
19:LK:27:ILE:O	19:LK:29:ASP:N	2.39	0.51
1:L1:1489:U:H2'	1:L1:1490:G:C8	2.45	0.51
2:L2:1233:U:OP2	50:Lp:63:LYS:HG2	2.09	0.51
6:L6:23:A:H4'	6:L6:24[B]:C:H5''	1.92	0.51
10:LB:92:TYR:HB2	10:LB:159:VAL:HB	1.92	0.51
22:LN:48:VAL:HG11	22:LN:145:VAL:HG22	1.93	0.51
60:SG:80:ARG:HG2	60:SG:87:THR:HA	1.90	0.51
66:SM:48:HIS:HB2	66:SM:87:ASP:HB2	1.92	0.51
1:L1:687:C:H2'	1:L1:688:A:C8	2.45	0.51
41:Lg:75:VAL:HG11	41:Lg:119:VAL:HG11	1.93	0.51
55:SB:114:GLN:HG2	55:SB:115:ILE:HG23	1.93	0.51
1:L1:1185:U:H2'	1:L1:1186:A:O4'	2.10	0.51
1:L1:1293:A:O2'	1:L1:1294:C:H5'	2.10	0.51
11:LC:292:GLN:HG2	11:LC:297:ARG:NH2	2.26	0.51
14:LF:80:ASP:HB3	14:LF:83:TYR:HD2	1.74	0.51
50:Lp:55:LYS:NZ	52:S4:67:C:O2	2.44	0.51
51:S1:342:C:H1'	58:SE:30:PRO:HG3	1.92	0.51
59:SF:250:ASP:OD2	59:SF:252:THR:OG1	2.27	0.51
51:S1:1858:G:N2	51:S1:1978:A:OP2	2.43	0.51
1:L1:162:U:H3	1:L1:293:C:H42	1.59	0.51
1:L1:759:A:H2	1:L1:761:A:H61	1.58	0.51
2:L2:25:A:H5''	46:L1:45:ARG:HH21	1.76	0.51
2:L2:1156:G:H5''	27:LS:83:ARG:NH2	2.25	0.51
4:L4:77:U:H4'	10:LB:371:LYS:HE3	1.93	0.51
20:LL:116:GLN:HB3	24:LP:100:ALA:HB2	1.92	0.51
51:S1:373:G:H5'	64:SK:98:LYS:HB3	1.92	0.51
51:S1:617:G:OP2	69:SP:68:LYS:NZ	2.44	0.51
1:L1:83:A:H61	1:L1:98:A:H3'	1.76	0.51
10:LB:356:GLN:CD	10:LB:356:GLN:H	2.18	0.51
11:LC:299:VAL:HG21	24:LP:138:PRO:HB2	1.92	0.51
51:S1:972:A:H61	51:S1:1100:U:H2'	1.76	0.51
51:S1:1718:A:O2'	51:S1:1949:A:N6	2.43	0.51
54:SA:41:ARG:NH2	54:SA:234:HIS:O	2.41	0.51
67:SN:5:VAL:HG11	67:SN:52:LEU:HD21	1.93	0.51
2:L2:696:A:H4'	2:L2:697:G:OP1	2.11	0.51
2:L2:782:G:O2'	2:L2:786:A:O5'	2.28	0.51
25:LQ:105:LEU:HD22	25:LQ:135:LYS:HG3	1.93	0.51
51:S1:17:C:O2'	51:S1:1489:A:N1	2.40	0.51
51:S1:251:A:H1'	51:S1:784:C:H1'	1.92	0.51
51:S1:2008:OMG:HM21	61:SH:71:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SF:66:ILE:HA	59:SF:71:MET:HE3	1.93	0.51
1:L1:1160:G:OP1	37:Lc:119:ARG:NH2	2.43	0.50
18:LJ:8:VAL:HB	18:LJ:127:LEU:HD22	1.93	0.50
23:LO:152:LEU:HD22	23:LO:169:LEU:HD22	1.93	0.50
29:LU:108:ARG:NH1	29:LU:110:LEU:HD21	2.26	0.50
33:LY:14:THR:HB	42:Lh:89:ARG:HG3	1.93	0.50
57:SD:27:MET:HG3	84:Se:44:PHE:HE2	1.75	0.50
1:L1:779:A:N1	24:LP:74:LYS:NZ	2.59	0.50
16:LH:217:LYS:HG2	16:LH:222:ALA:HB3	1.94	0.50
35:La:72:MET:O	35:La:72:MET:HE3	2.11	0.50
2:L2:1398:C:H2'	2:L2:1399:G:C8	2.46	0.50
6:L6:63:A:C6	14:LF:108:ARG:HD3	2.46	0.50
31:LW:35:GLU:H	31:LW:35:GLU:CD	2.19	0.50
59:SF:177:VAL:HG11	59:SF:222:LEU:HA	1.93	0.50
1:L1:1342:C:H2'	1:L1:1343:A:C8	2.46	0.50
2:L2:341:A:OP2	25:LQ:114:LYS:NZ	2.42	0.50
40:Lf:42:PRO:HB2	40:Lf:50:GLN:HG3	1.93	0.50
51:S1:1369:U:H3	51:S1:1401:G:H1	1.59	0.50
66:SM:63:ARG:HH21	66:SM:65:THR:HG21	1.77	0.50
1:L1:377:G:OP2	11:LC:197:ASN:ND2	2.25	0.50
1:L1:409:U:H5	46:Ll:34:ARG:HB3	1.77	0.50
1:L1:1525:A:H5'	1:L1:1526:U:H5'	1.94	0.50
2:L2:957:C:H2'	2:L2:958:A:H8	1.77	0.50
37:Lc:95:VAL:HG21	37:Lc:157:MET:HE1	1.94	0.50
39:Le:45:MET:O	39:Le:50:ARG:NH2	2.44	0.50
59:SF:83:ILE:HG21	59:SF:88:LEU:HD13	1.93	0.50
80:Sa:81:LYS:O	80:Sa:85:ARG:HG3	2.12	0.50
1:L1:881:A:O2'	2:L2:49:A:OP1	2.27	0.50
1:L1:1085:C:H4'	1:L1:1085:C:OP1	2.11	0.50
10:LB:92:TYR:HB3	10:LB:99:LEU:HD22	1.92	0.50
10:LB:315:MET:HE1	10:LB:377:PHE:HB2	1.94	0.50
51:S1:967:A:OP1	62:SI:9:ARG:NH2	2.43	0.50
51:S1:2198:A:H5'	81:Sb:83:ILE:HD11	1.94	0.50
20:LL:75:LEU:HG	20:LL:111:GLY:HA2	1.94	0.50
37:Lc:230:HIS:CE1	37:Lc:238:GLY:HA3	2.46	0.50
51:S1:506:U:OP1	79:SZ:115:LYS:NZ	2.45	0.50
51:S1:1923:A:HO2'	51:S1:1969:A:HO2'	1.60	0.50
51:S1:1948:U:OP2	77:SX:26:ARG:NH2	2.41	0.50
15:LG:187:LEU:HB3	15:LG:196:ALA:HB3	1.93	0.50
51:S1:124:A:OP2	60:SG:201:LYS:NZ	2.34	0.50
2:L2:1410:G:N7	96:L2:1843:HOH:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Lh:10:ARG:HH21	42:Lh:35:LYS:HD3	1.77	0.50
51:S1:1860:C:OP2	71:SR:137:THR:OG1	2.25	0.50
2:L2:972:C:N4	38:Ld:49:ASN:O	2.45	0.49
7:L7:93:C:HO2'	7:L7:94:G:P	2.33	0.49
51:S1:566:A:N3	79:SZ:40:THR:OG1	2.45	0.49
51:S1:1360:U:H5	62:SI:199:THR:H	1.59	0.49
1:L1:1254:C:O2'	1:L1:1360:C:OP1	2.27	0.49
55:SB:30:THR:O	55:SB:31:ARG:HG2	2.11	0.49
2:L2:389:A:OP2	2:L2:570:A2M:H8	2.12	0.49
22:LN:30:LYS:HG2	22:LN:63:GLU:HB3	1.94	0.49
51:S1:869:U:C2	57:SD:142:ILE:HG12	2.46	0.49
76:SW:117:GLU:CD	76:SW:117:GLU:H	2.19	0.49
14:LF:57:LEU:HD12	14:LF:62:PRO:HG2	1.94	0.49
14:LF:66:SER:HB2	14:LF:76:ILE:HG12	1.94	0.49
14:LF:104:GLU:HA	14:LF:107:GLN:HG2	1.94	0.49
25:LQ:171:ASN:OD1	25:LQ:174:ARG:NH1	2.45	0.49
51:S1:810:G:HO2'	51:S1:811:C:H6	1.56	0.49
51:S1:1605:U:O4	85:Sf:90:HIS:NE2	2.44	0.49
54:SA:8:ARG:HD3	54:SA:11:LYS:HA	1.93	0.49
59:SF:50:LYS:HD2	59:SF:259:LEU:HD13	1.93	0.49
15:LG:117:LYS:NZ	15:LG:123:LYS:O	2.37	0.49
43:Li:66:VAL:HG23	43:Li:68:LYS:HG3	1.94	0.49
51:S1:327:U:H2'	51:S1:328:C:H5''	1.95	0.49
51:S1:498:C:O2'	79:SZ:91:ARG:O	2.30	0.49
51:S1:1527:U:H2'	51:S1:1528:G:C8	2.48	0.49
51:S1:1967:G:OP2	51:S1:1967:G:N2	2.36	0.49
53:S3:9:G:O2'	53:S3:10:G:N7	2.46	0.49
57:SD:150:SER:HA	57:SD:153:ARG:HH12	1.78	0.49
67:SN:11:ASP:HA	67:SN:14:TYR:HB2	1.94	0.49
1:L1:235:A2M:O5'	1:L1:235:A2M:H8	2.13	0.49
7:L7:29:C:OP1	17:LI:36:GLN:NE2	2.42	0.49
19:LK:147:MET:HE1	41:Lg:13:LYS:HG3	1.94	0.49
2:L2:386:U:O2'	2:L2:1416:U:H5''	2.12	0.49
2:L2:658:G:OP1	96:L2:1803:HOH:O	2.20	0.49
6:L6:43:A:N6	16:LH:220:GLY:O	2.40	0.49
16:LH:29:LEU:HD13	16:LH:59:LEU:HD11	1.95	0.49
19:LK:13:VAL:HG12	19:LK:58:PRO:HA	1.94	0.49
31:LW:3:SER:O	31:LW:3:SER:OG	2.23	0.49
51:S1:777:A:H4'	51:S1:778:G:O5'	2.12	0.49
51:S1:1649:G:N2	51:S1:1652:A:OP2	2.45	0.49
76:SW:97:VAL:HA	76:SW:114:ILE:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Sg:98:GLN:O	86:Sg:100:GLN:NE2	2.42	0.49
1:L1:984:A:OP2	89:L1:1813:SPD:H52	2.12	0.49
2:L2:968:U:O4	2:L2:969:A:N6	2.45	0.49
13:LE:93:CYS:HB2	13:LE:141:ASP:HB3	1.94	0.49
28:LT:67:ILE:HD11	28:LT:80:LYS:HB3	1.94	0.49
41:Lg:34:TYR:CE1	41:Lg:136:ARG:HG2	2.47	0.49
44:Lj:39:TYR:CD1	44:Lj:40:PRO:HA	2.48	0.49
51:S1:1837:A:HO2'	56:SC:175:TYR:HH	1.60	0.49
77:SX:30:THR:HB	77:SX:147:LEU:HD21	1.94	0.49
2:L2:1482:C:H3'	2:L2:1483:U:H5''	1.95	0.49
3:L3:72:A:H5'	42:Lh:26:THR:HA	1.95	0.49
30:LV:144:LEU:HA	35:La:38:THR:HG21	1.94	0.49
51:S1:876:G:H1	51:S1:885:C:H5	1.61	0.49
51:S1:916:G:H22	73:ST:133:LYS:HB2	1.77	0.49
86:Sg:214:LYS:HD2	86:Sg:237:PRO:HB3	1.95	0.49
2:L2:1515:A:H5''	10:LB:109:HIS:CD2	2.48	0.49
9:LA:42:ARG:HG2	9:LA:42:ARG:HH11	1.78	0.49
10:LB:266:MET:HG2	16:LH:82:THR:HG22	1.95	0.49
23:LO:284:SER:OG	23:LO:287:GLU:OE1	2.26	0.49
51:S1:29:OMU:HM21	69:SP:123:VAL:HG11	1.95	0.49
62:SI:61:VAL:HG11	62:SI:175:VAL:HG21	1.95	0.49
71:SR:87:ARG:HD2	71:SR:99:LEU:HD11	1.95	0.49
77:SX:57:GLU:HG3	77:SX:58:ARG:HG3	1.95	0.49
51:S1:2198:A:N6	81:Sb:9:GLY:HA3	2.28	0.48
64:SK:210:PHE:O	64:SK:214:ARG:HG2	2.13	0.48
1:L1:369:A:O2'	44:Lj:58:ARG:NH2	2.46	0.48
1:L1:412:G:N1	1:L1:415:A:OP2	2.46	0.48
1:L1:835:G:H2'	1:L1:835:G:N3	2.27	0.48
1:L1:1684:G:N2	1:L1:1716:G:H1	2.08	0.48
2:L2:782:G:H8	2:L2:782:G:OP2	1.95	0.48
9:LA:62:GLU:OE1	9:LA:71:ARG:HD2	2.12	0.48
9:LA:178:PRO:HG2	49:Lo:26:ALA:HB2	1.94	0.48
15:LG:183:ASP:HB3	15:LG:186:ARG:H	1.78	0.48
51:S1:38:OMC:O2'	57:SD:5:ASN:ND2	2.46	0.48
51:S1:377:A:H5'	64:SK:48:ALA:HB1	1.95	0.48
51:S1:1202:A:OP1	73:ST:2:VAL:HG23	2.13	0.48
65:SL:23:ALA:HB2	65:SL:75:VAL:HG13	1.95	0.48
68:SO:90:MET:HE1	68:SO:105:ALA:HB1	1.95	0.48
73:ST:110:ASP:O	73:ST:114:ARG:HG2	2.12	0.48
2:L2:1246:A:H5''	2:L2:1248:OMC:O5'	2.13	0.48
23:LO:107:ARG:HH21	23:LO:110:LEU:HD12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LU:44:LEU:HG	29:LU:72:MET:HE2	1.95	0.48
29:LU:91:LYS:HB2	29:LU:117:TYR:CE2	2.49	0.48
51:S1:522:A:H5'	57:SD:143:PRO:HD2	1.95	0.48
51:S1:784:C:H41	51:S1:834:U:H3	1.60	0.48
51:S1:969:A2M:H2	62:SI:118:SER:HB2	1.95	0.48
86:Sg:234:VAL:HG21	86:Sg:254:THR:HG21	1.95	0.48
1:L1:1147:A:O2'	1:L1:1150:A:N1	2.45	0.48
1:L1:1683:C:H2'	1:L1:1684:G:H8	1.78	0.48
38:Ld:18:LEU:HD13	38:Ld:100:SER:HA	1.94	0.48
52:S2:74:C:H2'	52:S2:75:C:O4'	2.13	0.48
57:SD:31:GLY:HA3	84:Se:40:TYR:CG	2.49	0.48
86:Sg:67:PHE:HB2	86:Sg:85:TRP:CG	2.48	0.48
2:L2:1485:G:N3	19:LK:164:MET:HG2	2.29	0.48
2:L2:1510:A:HO2'	10:LB:170:LYS:HZ1	1.57	0.48
6:L6:66:A:OP1	14:LF:47:ARG:NH2	2.45	0.48
7:L7:47:C:H1'	7:L7:61:A:H2'	1.95	0.48
12:LD:25:VAL:HG12	12:LD:27:GLU:HG2	1.93	0.48
51:S1:1:G:OP1	57:SD:49:SER:OG	2.30	0.48
51:S1:251:A:N1	51:S1:835:C:O2'	2.43	0.48
51:S1:1523:A:H2'	51:S1:1524:G:C8	2.48	0.48
86:Sg:237:PRO:HD2	86:Sg:255:GLU:HG2	1.94	0.48
2:L2:1250:C:H2'	2:L2:1251:A:C8	2.48	0.48
11:LC:286:ASP:OD2	11:LC:289:ARG:NH1	2.46	0.48
26:LR:70:LYS:O	26:LR:74:ARG:NH2	2.44	0.48
51:S1:527:A:H4'	57:SD:119:LYS:HG3	1.96	0.48
51:S1:656:G:H5'	51:S1:662:G:N2	2.28	0.48
51:S1:1123:G:H1'	51:S1:1191:A:O4'	2.13	0.48
85:Sf:103:VAL:HA	85:Sf:113:VAL:HA	1.95	0.48
1:L1:1371:OMU:HM23	1:L1:1371:OMU:H1'	1.72	0.48
3:L3:174:C:O2'	3:L3:175:A:OP1	2.29	0.48
19:LK:25:GLY:HA2	19:LK:40:ASN:HB2	1.96	0.48
56:SC:210:ILE:HD11	75:SV:40:ILE:HD11	1.96	0.48
84:Se:64:LYS:HB3	84:Se:64:LYS:HE3	1.68	0.48
7:L7:142:C:O3'	30:LV:94:ASN:ND2	2.47	0.48
23:LO:206:PHE:CE1	23:LO:250:LYS:HG2	2.49	0.48
38:Ld:20:MET:HG3	38:Ld:83:CYS:O	2.13	0.48
41:Lg:32:ARG:NH1	41:Lg:36:LYS:HG3	2.29	0.48
74:SU:14:ASP:OD2	74:SU:67:LYS:NZ	2.44	0.48
86:Sg:222:ASP:OD2	86:Sg:224:SER:OG	2.20	0.48
1:L1:297:A:H1'	1:L1:298:U:C5	2.49	0.48
1:L1:1611:G:N7	96:L1:2024:HOH:O	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:638:C:O2'	10:LB:271:ARG:NH1	2.45	0.48
7:L7:70:C:OP1	31:LW:118:ARG:NH2	2.36	0.48
51:S1:1614:U:H2'	51:S1:1615:G:C8	2.47	0.48
1:L1:159:U:O2'	1:L1:160:C:H5'	2.14	0.48
9:LA:48:ILE:HG21	49:Lo:65:ALA:HB2	1.96	0.48
51:S1:1853:U:OP1	72:SS:10:ARG:NH2	2.46	0.48
64:SK:150:ASP:OD1	64:SK:150:ASP:N	2.41	0.48
77:SX:110:THR:HA	77:SX:113:LEU:HD12	1.95	0.48
1:L1:215:U:OP1	34:LZ:129:LYS:NZ	2.46	0.47
6:L6:60:A:OP1	14:LF:45:ARG:NH2	2.47	0.47
58:SE:95:ARG:HH21	58:SE:112:SER:HA	1.79	0.47
60:SG:34:GLY:HA2	60:SG:52:ARG:HE	1.79	0.47
79:SZ:6:LYS:NZ	79:SZ:7:LYS:O	2.46	0.47
1:L1:205:A:C6	34:LZ:55:PRO:HG3	2.49	0.47
2:L2:1484:U:N3	2:L2:1486:G:O4'	2.48	0.47
13:LE:91:VAL:HG22	13:LE:143:ILE:HB	1.96	0.47
51:S1:2006:A:OP1	65:SL:139:SER:OG	2.29	0.47
94:S1:2446:PAR:H24	94:S1:2446:PAR:H33	1.68	0.47
57:SD:50:LYS:O	57:SD:54:THR:HG22	2.14	0.47
86:Sg:135:ASN:HD22	86:Sg:137:ALA:H	1.59	0.47
2:L2:664:G:H5'	2:L2:664:G:N3	2.29	0.47
2:L2:1486:G:H2'	2:L2:1487:G:C8	2.49	0.47
8:L8:121:U:OP1	23:LO:266:LYS:NZ	2.48	0.47
51:S1:1250:A:O2'	51:S1:1252:A:N7	2.45	0.47
51:S1:1974:A:OP2	76:SW:54:ARG:NH1	2.47	0.47
58:SE:84:MET:HE3	58:SE:97:ARG:HD3	1.97	0.47
60:SG:121:ASP:N	60:SG:121:ASP:OD1	2.47	0.47
67:SN:86:TYR:HD1	67:SN:87:LEU:HD23	1.79	0.47
69:SP:53:GLU:OE2	69:SP:71:ARG:NH1	2.43	0.47
77:SX:55:GLY:HA2	77:SX:96:LYS:HD2	1.95	0.47
79:SZ:47:ARG:HG3	79:SZ:62:VAL:HB	1.96	0.47
1:L1:746:G:N2	1:L1:749:A:OP2	2.43	0.47
2:L2:1239:A:O2'	2:L2:1240:A:H2'	2.14	0.47
4:L4:174:A:H5'	16:LH:3:PHE:HB2	1.96	0.47
9:LA:59:ALA:HB2	9:LA:78:ALA:HB2	1.95	0.47
20:LL:51:GLY:HA2	24:LP:182:ARG:N	2.30	0.47
25:LQ:89:MET:HE2	25:LQ:94:LEU:HG	1.96	0.47
1:L1:553:A:C8	11:LC:337:THR:HG21	2.50	0.47
94:L7:208:PAR:O43	94:L7:208:PAR:O62	2.25	0.47
11:LC:290:ILE:HG23	24:LP:135:MET:SD	2.54	0.47
13:LE:91:VAL:HA	13:LE:180:VAL:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:2:VAL:HG23	25:LQ:33:GLN:HG3	1.95	0.47
51:S1:1433:G:H4'	63:SJ:19:ARG:HH21	1.79	0.47
51:S1:1932:A:O2'	51:S1:1934:A:OP2	2.28	0.47
1:L1:1238:C:C5'	1:L1:1239:U:H5'	2.45	0.47
1:L1:1766:G:H2'	1:L1:1767:A:C8	2.49	0.47
6:L6:6:G:H5''	6:L6:7:A:OP2	2.15	0.47
10:LB:286:LYS:NZ	10:LB:359:GLU:O	2.48	0.47
43:Li:90:ARG:O	43:Li:94:GLU:HG3	2.14	0.47
51:S1:3:U:O2	57:SD:16:ARG:NH2	2.42	0.47
51:S1:1714:C:H5''	77:SX:8:ILE:HD11	1.96	0.47
71:SR:25:ARG:HB2	71:SR:30:ALA:HB2	1.97	0.47
80:Sa:41:MET:HE2	80:Sa:41:MET:HB3	1.85	0.47
1:L1:633:U:H4'	1:L1:634:G:H5''	1.97	0.47
1:L1:1023:G:OP2	89:L1:1808:SPD:N6	2.32	0.47
2:L2:638:C:O2'	10:LB:271:ARG:NH2	2.47	0.47
3:L3:71:U:O2'	3:L3:149:A:N1	2.44	0.47
32:LX:82:VAL:HG11	60:SG:9:ARG:HG2	1.97	0.47
51:S1:1566:PSU:OP1	51:S1:1598:U:O2'	2.26	0.47
67:SN:80:ILE:HA	67:SN:83:MET:HB2	1.96	0.47
1:L1:1686:C:H2'	1:L1:1687:G:C8	2.50	0.47
2:L2:772:A:OP1	9:LA:37:ARG:NH2	2.48	0.47
4:L4:75:C:H5'	10:LB:336:SER:HA	1.97	0.47
45:Lk:5:ILE:HD11	45:Lk:43:TYR:HB3	1.97	0.47
65:SL:11:GLN:HG3	65:SL:28:THR:HB	1.97	0.47
85:Sf:139:TYR:H	85:Sf:139:TYR:HD2	1.61	0.47
86:Sg:82:THR:HG22	86:Sg:92:TRP:HE1	1.79	0.47
1:L1:47:C:O2	93:L1:1977:PUT:N1	2.40	0.47
1:L1:700:A:H2'	1:L1:701:G:C8	2.50	0.47
1:L1:967:G:H5'	1:L1:968:A:OP1	2.15	0.47
5:L5:106:G:N3	39:Le:94:LYS:HA	2.30	0.47
10:LB:374:HIS:O	32:LX:37:ARG:NH2	2.47	0.47
17:LI:60:ARG:HD2	17:LI:77:GLY:O	2.14	0.47
51:S1:701:G:H1	51:S1:745:G:H1	1.62	0.47
51:S1:1931:G:O6	56:SC:2:GLY:N	2.48	0.47
53:S3:51:U:H3	53:S3:65:G:H1	1.63	0.47
55:SB:114:GLN:HA	55:SB:119:PHE:CG	2.49	0.47
58:SE:178:VAL:HG12	58:SE:224:VAL:HA	1.96	0.47
59:SF:190:ILE:HD12	59:SF:201:GLU:HG3	1.97	0.47
61:SH:92:GLU:CD	61:SH:93:ASN:H	2.23	0.47
75:SV:72:LYS:HE3	75:SV:72:LYS:HB3	1.66	0.47
1:L1:262:C:H5'	31:LW:31:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:574:G:O2'	1:L1:576:G:H2'	2.15	0.47
2:L2:1264:PSU:H5'	2:L2:1264:PSU:H6	1.78	0.47
7:L7:71:A:OP1	31:LW:25:ARG:NH1	2.48	0.47
26:LR:95:GLU:OE1	26:LR:138:HIS:ND1	2.47	0.47
40:Lf:3:LYS:HE2	40:Lf:4:PRO:HD2	1.97	0.47
51:S1:1227:G:H4'	51:S1:2179:A:H4'	1.96	0.47
51:S1:1800:U:H2'	51:S1:1801:G:O4'	2.15	0.47
53:S3:7:G:P	53:S3:16:C:H42	2.38	0.47
69:SP:88:ASP:OD2	84:Se:15:LYS:HB2	2.14	0.47
1:L1:1526:U:H5''	1:L1:1527:OMC:H5'	1.96	0.46
1:L1:1597:G:O6	46:Ll:2:GLY:N	2.48	0.46
33:LY:35:GLU:H	33:LY:35:GLU:CD	2.23	0.46
51:S1:904:G:OP2	51:S1:904:G:N2	2.40	0.46
56:SC:210:ILE:O	75:SV:20:TYR:OH	2.30	0.46
61:SH:21:GLU:HG3	61:SH:103:SER:HB3	1.97	0.46
62:SI:25:LYS:HB3	62:SI:25:LYS:NZ	2.30	0.46
76:SW:67:LEU:HD21	76:SW:101:VAL:HG22	1.95	0.46
81:Sb:93:VAL:HG22	81:Sb:96:ARG:NH2	2.30	0.46
86:Sg:125:ALA:HB1	86:Sg:153:VAL:HB	1.97	0.46
2:L2:1512:G:H1'	2:L2:1513:G:OP2	2.15	0.46
4:L4:125:C:OP1	10:LB:332:LYS:NZ	2.45	0.46
4:L4:126:G:N7	96:L4:302:HOH:O	2.36	0.46
22:LN:47:PRO:HB3	22:LN:171:TRP:CZ2	2.50	0.46
29:LU:70:LEU:HD23	29:LU:79:ILE:HG12	1.96	0.46
51:S1:366:G:N7	96:S1:2524:HOH:O	2.36	0.46
51:S1:1692:G:H5'	86:Sg:65:THR:HG21	1.97	0.46
51:S1:1788:U:H5'	75:SV:48:ASN:CB	2.45	0.46
61:SH:174:TYR:CZ	61:SH:178:LYS:HE3	2.50	0.46
86:Sg:134:TRP:N	86:Sg:134:TRP:CD1	2.83	0.46
2:L2:949:U:H2'	2:L2:950:G:C8	2.50	0.46
7:L7:167:C:OP1	15:LG:182:LYS:NZ	2.42	0.46
37:Lc:198:ILE:HD11	37:Lc:212:MET:HE1	1.98	0.46
51:S1:52:U:H2'	51:S1:53:G:C8	2.51	0.46
51:S1:1793:U:H3'	51:S1:1794:U:H5''	1.98	0.46
56:SC:115:ARG:HG2	56:SC:151:PHE:CE2	2.50	0.46
75:SV:35:ILE:HA	75:SV:38:VAL:HG22	1.96	0.46
75:SV:88:THR:O	75:SV:93:LYS:NZ	2.48	0.46
76:SW:66:ARG:HH11	76:SW:66:ARG:HB3	1.80	0.46
83:Sd:60:VAL:HG12	83:Sd:82:ALA:HB3	1.98	0.46
87:Sh:182:ALA:HA	87:Sh:185:LYS:HG2	1.98	0.46
1:L1:1525:A:H5'	1:L1:1526:U:H5''	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1667:G:N2	2:L2:769:A:OP1	2.34	0.46
9:LA:83:PHE:HB3	49:Lo:64:VAL:HG22	1.97	0.46
29:LU:87:LYS:HE2	29:LU:117:TYR:CZ	2.50	0.46
34:LZ:49:LYS:HE2	34:LZ:99:VAL:HG13	1.97	0.46
51:S1:442:A:OP1	64:SK:49:ARG:NH2	2.49	0.46
51:S1:1862:C:H2'	51:S1:1863:G:H8	1.80	0.46
65:SL:99:PHE:HB3	65:SL:108:LYS:HB2	1.98	0.46
75:SV:35:ILE:HD13	75:SV:50:ILE:HG22	1.97	0.46
87:Sh:161:LYS:HE3	87:Sh:178:ASP:CG	2.41	0.46
1:L1:171:U:H2'	1:L1:172:G:C8	2.50	0.46
3:L3:169:A:H5'	3:L3:170:C:H5'	1.98	0.46
15:LG:101:GLU:HG3	15:LG:106:ARG:HB2	1.98	0.46
51:S1:1145:A:H5''	68:SO:53:MET:HE3	1.98	0.46
51:S1:1581:G:H3'	85:Sf:92:LEU:HD11	1.96	0.46
78:SY:75:HIS:ND1	82:Sc:5:ASP:OD2	2.37	0.46
82:Sc:35:ASP:CG	82:Sc:83:LYS:HZ3	2.24	0.46
1:L1:412:G:H4'	1:L1:437:A:N1	2.30	0.46
1:L1:547:U:H4'	26:LR:65:VAL:HG21	1.98	0.46
1:L1:1390:G:H4'	1:L1:1391:U:O5'	2.16	0.46
1:L1:1564:C:H5''	5:L5:127:A:N6	2.30	0.46
2:L2:414:G:OP2	2:L2:414:G:N2	2.38	0.46
4:L4:4:G:H1	4:L4:20:U:H3	1.64	0.46
10:LB:47:MET:HB2	10:LB:84:MET:HE3	1.98	0.46
29:LU:50:PHE:O	29:LU:54:ASN:HB2	2.16	0.46
51:S1:917:C:O2'	51:S1:918:A:H4'	2.15	0.46
51:S1:1699:A:H2	51:S1:1778:C:H42	1.64	0.46
54:SA:246:ARG:NH2	68:SO:11:GLY:O	2.39	0.46
61:SH:52:MET:HG2	61:SH:53:PRO:HD2	1.98	0.46
64:SK:177:ASP:O	64:SK:181:GLU:HG2	2.15	0.46
76:SW:90:VAL:HB	76:SW:123:LEU:HD12	1.97	0.46
1:L1:1650:U:OP1	21:LM:67:ARG:NH1	2.41	0.46
1:L1:1652:A:OP1	21:LM:71:ARG:NH1	2.49	0.46
10:LB:93:ARG:HD3	10:LB:102:ILE:HG12	1.98	0.46
16:LH:131:VAL:HG12	16:LH:132:ARG:HG3	1.98	0.46
51:S1:2200:A:C6	81:Sb:88:VAL:HG22	2.51	0.46
65:SL:104:ASN:ND2	65:SL:106:VAL:HG23	2.30	0.46
67:SN:37:LEU:HD13	67:SN:42:PHE:CE1	2.51	0.46
86:Sg:81:LEU:HD11	86:Sg:122:ILE:HG12	1.97	0.46
2:L2:590:U:H2'	2:L2:591:A2M:C8	2.45	0.46
41:Lg:20:LYS:HB2	41:Lg:20:LYS:HE3	1.59	0.46
42:Lh:115:LYS:HB2	42:Lh:115:LYS:HZ3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:98:A2M:HM'3	51:S1:98:A2M:H1'	1.84	0.46
51:S1:784:C:N4	51:S1:834:U:H3	2.14	0.46
51:S1:1511:C:N4	51:S1:1637:A:O5'	2.47	0.46
51:S1:1527:U:H2'	51:S1:1528:G:H8	1.81	0.46
65:SL:28:THR:HG23	65:SL:70:ARG:HB3	1.98	0.46
69:SP:17:ARG:NH1	69:SP:17:ARG:HA	2.30	0.46
82:Sc:3:PHE:HD1	82:Sc:4:PHE:H	1.62	0.46
86:Sg:191:LYS:HB3	86:Sg:191:LYS:HE3	1.76	0.46
1:L1:719:U:O2'	1:L1:720:A:H5''	2.16	0.46
2:L2:957:C:H2'	2:L2:958:A:C8	2.50	0.46
51:S1:17:C:H2'	51:S1:18:OMC:C6	2.51	0.46
51:S1:756:C:H42	51:S1:772:A:H62	1.64	0.46
54:SA:26:ARG:O	54:SA:50:LYS:HG3	2.16	0.46
64:SK:119:ILE:HD11	64:SK:166:ARG:HD3	1.96	0.46
2:L2:501:A:N1	51:S1:2064:C:O2'	2.46	0.46
2:L2:507:G:H21	2:L2:508:A:N6	2.14	0.46
2:L2:1336:G:H5''	2:L2:1337:C:H5'	1.98	0.46
2:L2:1510:A:H61	10:LB:327:ASP:H	1.63	0.46
3:L3:20:C:H5	42:Lh:71:HIS:NE2	2.14	0.46
10:LB:390:LEU:O	10:LB:394:ARG:HG3	2.15	0.46
14:LF:101:ILE:HG12	14:LF:153:LEU:HD11	1.98	0.46
51:S1:45:U:O2'	51:S1:46:U:H2'	2.16	0.46
51:S1:546:U:C2	51:S1:547:U:H1'	2.51	0.46
51:S1:878:C:H5	51:S1:883:G:H1	1.64	0.46
63:SJ:67:GLY:HA3	78:SY:26:THR:HB	1.98	0.46
80:Sa:60:ILE:HG23	80:Sa:65:ILE:HD11	1.98	0.46
87:Sh:185:LYS:HG3	87:Sh:186:PHE:N	2.31	0.46
1:L1:84:G:O6	89:LM:301:SPD:H91	2.16	0.45
1:L1:358:G:N7	89:L1:1811:SPD:N6	2.63	0.45
18:LJ:106:ASN:OD1	18:LJ:110:GLU:N	2.50	0.45
51:S1:328:C:O2'	51:S1:329:C:OP1	2.32	0.45
69:SP:95:GLU:O	69:SP:98:ASP:HB2	2.15	0.45
1:L1:163:U:H2'	1:L1:164:G:C8	2.51	0.45
1:L1:678:A2M:HM'3	1:L1:678:A2M:H1'	1.86	0.45
1:L1:1039:OMU:HM23	1:L1:1039:OMU:H1'	1.64	0.45
2:L2:83:G:O2'	2:L2:580:U:O4	2.28	0.45
2:L2:488:A:H5''	9:LA:244:GLY:HA3	1.97	0.45
12:LD:111:HIS:CD2	12:LD:124:ILE:HA	2.51	0.45
12:LD:165:PHE:HD2	12:LD:173:ILE:HD11	1.81	0.45
22:LN:69:ARG:HG3	22:LN:70:ILE:N	2.32	0.45
51:S1:811:C:HO2'	51:S1:812:A:H8	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:824:C:H5'	51:S1:825:C:H5'	1.98	0.45
51:S1:933:G:N2	96:S1:2579:HOH:O	2.49	0.45
52:S4:54:C:H2'	52:S4:55:G:H8	1.82	0.45
57:SD:91:LYS:HB2	57:SD:94:TYR:CE2	2.52	0.45
60:SG:59:LYS:HD3	60:SG:110:ALA:HB2	1.97	0.45
1:L1:531:C:H1'	26:LR:132:PRO:HG3	1.98	0.45
2:L2:1192:C:O3'	50:Lp:39:GLY:HA3	2.17	0.45
12:LD:30:ASP:OD1	12:LD:34:ARG:NE	2.37	0.45
13:LE:56:VAL:HG22	13:LE:69:LEU:HD23	1.98	0.45
18:LJ:19:LEU:HD13	18:LJ:25:VAL:HG11	1.98	0.45
32:LX:84:ARG:H	60:SG:134:ARG:NH2	2.14	0.45
51:S1:29:OMU:H2'	51:S1:30:G:H8	1.81	0.45
58:SE:138:THR:OG1	58:SE:140:ASP:OD1	2.30	0.45
86:Sg:135:ASN:ND2	86:Sg:137:ALA:H	2.15	0.45
1:L1:1753:U:O4	1:L1:1754:A:N6	2.49	0.45
2:L2:382:A2M:HM'3	2:L2:382:A2M:H1'	1.85	0.45
2:L2:1333:G:O2'	47:Lm:100:TYR:O	2.25	0.45
2:L2:1368:A:O2'	18:LJ:40:SER:OG	2.28	0.45
7:L7:83:A:O2'	7:L7:84:U:O5'	2.29	0.45
15:LG:163:LEU:HD23	21:LM:7:LEU:HD21	1.99	0.45
20:LL:72:THR:HB	20:LL:110:LEU:HG	1.98	0.45
23:LO:83:LEU:HB3	23:LO:88:ILE:HB	1.98	0.45
42:Lh:10:ARG:HG2	42:Lh:10:ARG:NH1	2.29	0.45
50:Lp:7:LYS:HD3	50:Lp:24:LYS:HA	1.97	0.45
54:SA:85:LYS:NZ	54:SA:108:THR:HA	2.32	0.45
62:SI:95:MET:HE1	62:SI:172:VAL:HA	1.98	0.45
76:SW:63:LEU:HD13	76:SW:85:THR:HB	1.98	0.45
94:L2:1729:PAR:H24	94:L2:1729:PAR:H33	1.80	0.45
18:LJ:29:ASP:HB3	18:LJ:31:THR:HG23	1.97	0.45
19:LK:39:GLU:OE1	19:LK:48:ARG:HB2	2.17	0.45
51:S1:309:G:O2'	51:S1:311:G:OP2	2.21	0.45
1:L1:195:G:H1'	1:L1:196:C:C6	2.52	0.45
1:L1:1286:C:H1'	1:L1:1348:A:H61	1.82	0.45
1:L1:1672:U:H2'	1:L1:1673:G:O4'	2.16	0.45
1:L1:1766:G:H2'	1:L1:1767:A:H8	1.80	0.45
2:L2:806:C:H2'	2:L2:807:A:O4'	2.17	0.45
2:L2:1224:U:OP1	50:Lp:38:ARG:N	2.35	0.45
8:L8:52:G:OP2	23:LO:94:ASN:HB3	2.17	0.45
33:LY:77:HIS:HB3	38:Ld:37:ARG:HD3	1.99	0.45
55:SB:183:ARG:HD3	55:SB:187:ARG:CZ	2.47	0.45
56:SC:126:MET:HE2	56:SC:153:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SG:33:LEU:HD11	60:SG:64:MET:HB2	1.97	0.45
62:SI:41:LEU:N	62:SI:42:PRO:HD2	2.31	0.45
77:SX:17:ALA:HB3	77:SX:149:PHE:HA	1.99	0.45
85:Sf:85:LYS:HG3	85:Sf:86:PRO:HD2	1.99	0.45
1:L1:1037:A:O2'	37:Lc:132:PRO:O	2.35	0.45
2:L2:1404:G:C5'	9:LA:220:GLY:HA3	2.47	0.45
22:LN:38:ARG:HG3	22:LN:83:ASP:HA	1.98	0.45
2:L2:383:U:OP2	2:L2:388:A:N6	2.39	0.45
2:L2:1510:A:C6	10:LB:83:PRO:HD3	2.51	0.45
15:LG:73:PRO:HG3	21:LM:18:VAL:HA	1.98	0.45
51:S1:528:G:H1	51:S1:553:U:H3	1.65	0.45
51:S1:1598:U:OP2	72:SS:3:HIS:ND1	2.38	0.45
55:SB:194:ARG:HE	78:SY:48:GLY:HA3	1.82	0.45
60:SG:59:LYS:HG2	60:SG:108:ASP:O	2.16	0.45
79:SZ:12:ILE:HG21	79:SZ:50:LEU:HG	1.98	0.45
86:Sg:21:GLN:HA	86:Sg:289:ALA:HB2	1.98	0.45
87:Sh:150:LYS:HA	87:Sh:167:MET:HE1	1.98	0.45
2:L2:4:C:O2	3:L3:18:A:O2'	2.28	0.45
2:L2:748:C:N4	2:L2:749:G:O6	2.49	0.45
37:Lc:142:PRO:HA	37:Lc:237:TYR:CG	2.51	0.45
37:Lc:230:HIS:ND1	37:Lc:232:VAL:HG22	2.32	0.45
80:Sa:71:ILE:HB	80:Sa:75:ILE:HD11	1.98	0.45
1:L1:921:A:C5	89:L1:1802:SPD:H32	2.52	0.45
2:L2:25:A:H5''	46:Ll:45:ARG:NH2	2.31	0.45
3:L3:111:A:O2'	3:L3:112:C:H5''	2.17	0.45
3:L3:123:G:N2	3:L3:124:U:O4	2.49	0.45
8:L8:109:U:H2'	8:L8:110:G:H8	1.81	0.45
18:LJ:106:ASN:ND2	18:LJ:110:GLU:HB2	2.32	0.45
19:LK:141:LYS:HA	19:LK:141:LYS:HD3	1.71	0.45
24:LP:92:ASP:OD1	24:LP:92:ASP:N	2.50	0.45
51:S1:29:OMU:HM23	51:S1:29:OMU:H1'	1.63	0.45
51:S1:481:A:O2'	51:S1:513:G:N2	2.33	0.45
51:S1:2015:U:H5''	51:S1:2016:C:H5	1.82	0.45
58:SE:121:MET:HB3	58:SE:138:THR:HB	1.99	0.45
65:SL:66:TYR:HA	65:SL:69:LEU:HD12	1.99	0.45
87:Sh:81:VAL:H	87:Sh:94:PHE:C	2.25	0.45
1:L1:196:C:O2'	1:L1:198:A:OP2	2.35	0.44
1:L1:550:A:OP1	37:Lc:150:SER:OG	2.25	0.44
1:L1:752:G:OP1	20:LL:128:LYS:HG2	2.17	0.44
1:L1:1479:A:H4'	1:L1:1480:C:O5'	2.16	0.44
10:LB:226:THR:HG22	10:LB:336:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Lb:22:LYS:HA	36:Lb:22:LYS:HD3	1.79	0.44
51:S1:664:U:O2'	51:S1:670:A:N1	2.42	0.44
51:S1:1449:U:C4	59:SF:213:ARG:HD3	2.52	0.44
51:S1:2198:A:N6	81:Sb:36:LYS:HE3	2.31	0.44
59:SF:164:HIS:ND1	59:SF:207:ASP:OD2	2.49	0.44
66:SM:21:ILE:HG22	66:SM:29:VAL:HG23	1.98	0.44
4:L4:24:A:N1	4:L4:181:C:O2'	2.49	0.44
18:LJ:86:SER:HA	18:LJ:96:TYR:HB3	1.99	0.44
27:LS:48:VAL:HG12	27:LS:50:GLU:H	1.82	0.44
61:SH:58:LEU:HD23	61:SH:58:LEU:HA	1.88	0.44
75:SV:96:GLN:HA	75:SV:119:ARG:HH21	1.82	0.44
1:L1:743:A:H4'	1:L1:744:C:H5'	2.00	0.44
2:L2:1187:C:N3	50:Lp:63:LYS:HE3	2.32	0.44
10:LB:224:SER:HB3	10:LB:343:MET:HG2	2.00	0.44
22:LN:75:TYR:CZ	22:LN:79:ARG:HG3	2.52	0.44
25:LQ:105:LEU:HD23	25:LQ:138:LEU:HD23	1.99	0.44
51:S1:701:G:H22	51:S1:745:G:N2	2.15	0.44
51:S1:1518:C:H2'	51:S1:1519:G:O4'	2.17	0.44
76:SW:102:ALA:HB1	76:SW:109:PHE:HB3	1.99	0.44
86:Sg:283:ILE:HD11	86:Sg:299:LYS:HE3	1.99	0.44
1:L1:409:U:H5'	1:L1:410:U:H2'	1.99	0.44
1:L1:597:C:H2'	1:L1:598:G:H8	1.82	0.44
1:L1:824:U:O2'	1:L1:1128:A:N6	2.30	0.44
2:L2:5:A:H2'	2:L2:6:A:C8	2.52	0.44
6:L6:51:A:C6	41:Lg:23:ARG:HD2	2.52	0.44
7:L7:106:G:H4'	7:L7:149:A:H5'	1.98	0.44
31:LW:108:LEU:HD13	31:LW:113:LYS:HD3	2.00	0.44
51:S1:580:A:H8	51:S1:584:U:H5''	1.82	0.44
51:S1:1502:G:H22	88:S5:4:C:H3'	1.82	0.44
51:S1:1603:U:O2'	85:Sf:132:ALA:HB1	2.18	0.44
51:S1:1916:G:H3'	51:S1:1917:A:H8	1.83	0.44
51:S1:2015:U:H5'	51:S1:2016:C:OP2	2.18	0.44
57:SD:88:GLU:CD	57:SD:88:GLU:H	2.26	0.44
59:SF:63:LEU:HD12	59:SF:83:ILE:HD11	2.00	0.44
68:SO:24:VAL:HB	68:SO:86:LEU:HD13	1.99	0.44
86:Sg:33:SER:OG	86:Sg:34:ARG:N	2.51	0.44
87:Sh:170:GLN:HB2	87:Sh:172:PHE:CD1	2.52	0.44
1:L1:447:G:N2	7:L7:15:G:O2'	2.50	0.44
3:L3:109:U:O2'	3:L3:111:A:H8	2.01	0.44
8:L8:87:G:O2'	8:L8:89:C:OP1	2.33	0.44
60:SG:165:VAL:HB	60:SG:173:ARG:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SH:151:ASN:OD1	61:SH:152:LEU:N	2.51	0.44
62:SI:21:GLU:O	62:SI:25:LYS:HG3	2.17	0.44
62:SI:100:ARG:HH22	62:SI:131:ASP:CG	2.25	0.44
66:SM:33:THR:HG23	66:SM:86:ILE:HD11	2.00	0.44
79:SZ:44:GLN:O	79:SZ:48:LYS:HG2	2.18	0.44
79:SZ:84:ASP:N	79:SZ:84:ASP:OD1	2.51	0.44
1:L1:1632:C:H5''	42:Lh:10:ARG:HH12	1.82	0.44
2:L2:538:U:O2'	51:S1:2076:U:O2'	2.34	0.44
2:L2:1116:A:H2'	2:L2:1116:A:N3	2.33	0.44
5:L5:39:G:H4'	10:LB:372:ILE:O	2.17	0.44
10:LB:261:HIS:HA	10:LB:262:PRO:C	2.42	0.44
28:LT:43:LYS:HE3	28:LT:43:LYS:HB3	1.63	0.44
51:S1:2132:C:H2'	51:S1:2133:G:O4'	2.18	0.44
56:SC:205:ASP:OD1	56:SC:205:ASP:N	2.50	0.44
58:SE:258:GLU:HA	58:SE:258:GLU:OE2	2.16	0.44
61:SH:42:TRP:CE2	61:SH:52:MET:HG3	2.53	0.44
61:SH:45:ARG:HG3	61:SH:45:ARG:HH11	1.83	0.44
65:SL:96:ILE:HG23	65:SL:108:LYS:HG2	1.99	0.44
1:L1:165:U:H3	1:L1:290:G:H1	1.66	0.44
2:L2:1076:G:N3	2:L2:1185:A2M:H2	2.33	0.44
2:L2:1175:A:H5'	23:LO:181:HIS:HA	1.99	0.44
15:LG:177:PRO:HA	15:LG:224:LEU:HD22	1.98	0.44
34:LZ:120:ARG:HD3	40:Lf:117:ASP:HB2	2.00	0.44
51:S1:285:A:N1	51:S1:815:U:H5''	2.33	0.44
55:SB:94:SER:OG	55:SB:101:PHE:HB3	2.17	0.44
66:SM:47:ILE:HG22	66:SM:88:LEU:HB3	1.99	0.44
76:SW:28:GLU:N	76:SW:28:GLU:OE1	2.51	0.44
86:Sg:172:TRP:HA	86:Sg:196:TYR:HB2	2.00	0.44
1:L1:1216:U:O5'	1:L1:1402:U:H4'	2.18	0.44
2:L2:337:A:HO2'	2:L2:338:C:P	2.41	0.44
2:L2:1360:OMG:H1'	2:L2:1389:G:N3	2.33	0.44
4:L4:141:A:H4'	13:LE:70:ASN:HB3	2.00	0.44
9:LA:42:ARG:HG2	9:LA:42:ARG:NH1	2.31	0.44
18:LJ:106:ASN:HD21	18:LJ:110:GLU:HB2	1.83	0.44
27:LS:57:TYR:HA	27:LS:60:ARG:HG3	2.00	0.44
28:LT:16:LYS:HG2	28:LT:149:PHE:HB3	2.00	0.44
51:S1:198:C:H4'	87:Sh:196:ARG:HH12	1.83	0.44
55:SB:109:GLY:N	55:SB:139:GLU:OE2	2.40	0.44
87:Sh:164:ARG:HB3	87:Sh:176:TYR:HB2	1.99	0.44
1:L1:751:G:O2'	1:L1:815:G:H5''	2.17	0.44
1:L1:752:G:OP1	20:LL:128:LYS:NZ	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:845:OMU:HM23	1:L1:845:OMU:H1'	1.82	0.44
1:L1:1369:G:OP1	16:LH:78:LYS:NZ	2.40	0.44
1:L1:1749:G:OP2	42:Lh:30:LYS:NZ	2.50	0.44
2:L2:613:A:OP1	10:LB:264:ARG:NH2	2.51	0.44
14:LF:97:ASP:C	14:LF:99:ALA:H	2.26	0.44
17:LI:55:PRO:HB3	17:LI:154:ASP:HB3	2.00	0.44
19:LK:7:ILE:HD11	19:LK:58:PRO:HG3	2.00	0.44
35:La:20:LYS:O	35:La:24:GLU:HG3	2.16	0.44
39:Le:164:LYS:HG2	39:Le:166:PHE:CE1	2.53	0.44
51:S1:700:G:H2'	51:S1:701:G:C8	2.53	0.44
51:S1:969:A2M:N6	62:SI:101:GLN:O	2.51	0.44
51:S1:2182:G:OP2	51:S1:2182:G:N2	2.38	0.44
56:SC:53:LYS:O	56:SC:57:VAL:HG12	2.18	0.44
1:L1:947:A:H5'	9:LA:183:GLY:HA2	2.00	0.43
2:L2:1318:PSU:H1'	10:LB:255:ALA:HB3	1.99	0.43
2:L2:1490:U:H2'	2:L2:1491:G:H8	1.83	0.43
11:LC:252:GLN:O	11:LC:256:GLU:HG3	2.17	0.43
14:LF:112:GLU:OE1	14:LF:112:GLU:N	2.42	0.43
16:LH:22:PRO:HG2	16:LH:24:ILE:HD11	1.99	0.43
17:LI:48:ALA:HB2	17:LI:56:LEU:HD22	1.99	0.43
27:LS:83:ARG:NE	27:LS:85:LEU:HD21	2.33	0.43
32:LX:1:MET:HG3	32:LX:15:PRO:HG3	2.00	0.43
51:S1:2015:U:H5''	51:S1:2016:C:C5	2.53	0.43
56:SC:89:ARG:HG3	56:SC:89:ARG:HH11	1.82	0.43
86:Sg:185:LYS:HE2	86:Sg:185:LYS:HB2	1.90	0.43
1:L1:1010:OMC:HN42	2:L2:1239:A:H5''	1.84	0.43
12:LD:51:ARG:HA	12:LD:66:LYS:HA	2.00	0.43
25:LQ:198:GLN:HA	25:LQ:201:LYS:HD2	1.99	0.43
42:Lh:10:ARG:HH11	42:Lh:10:ARG:CG	2.31	0.43
42:Lh:95:ALA:O	42:Lh:99:GLU:HG3	2.18	0.43
51:S1:98:A2M:O5'	51:S1:98:A2M:H8	2.18	0.43
51:S1:866:G:C6	57:SD:148:ARG:HG3	2.52	0.43
51:S1:1439:G:O2'	51:S1:1445:A:N1	2.49	0.43
60:SG:184:THR:O	60:SG:188:LYS:HG3	2.18	0.43
82:Sc:39:PRO:HA	82:Sc:42:ARG:HH11	1.83	0.43
1:L1:320:G:O6	1:L1:342:G:H1'	2.18	0.43
1:L1:447:G:H1'	7:L7:15:G:N2	2.33	0.43
1:L1:745:U:OP1	1:L1:831:C:O2'	2.32	0.43
2:L2:382:A2M:H2	2:L2:389:A:N7	2.33	0.43
2:L2:1308:5MC:H6	2:L2:1308:5MC:H2'	1.75	0.43
4:L4:92:U:H2'	4:L4:93:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LV:91:SER:HA	30:LV:123:LYS:HB2	2.01	0.43
42:Lh:43:ILE:HD12	42:Lh:57:THR:HB	2.01	0.43
47:Lm:79:GLU:HG3	47:Lm:82:LEU:H	1.83	0.43
51:S1:288:A:H5'	60:SG:213:LEU:HD22	2.00	0.43
51:S1:1870:A:H4'	51:S1:1960:G:H4'	2.01	0.43
54:SA:22:GLU:OE1	54:SA:23:THR:N	2.52	0.43
57:SD:125:ARG:HD2	84:Se:33:ARG:HD3	2.00	0.43
58:SE:99:MET:HE2	58:SE:99:MET:HB3	1.72	0.43
62:SI:9:ARG:HG3	62:SI:12:LYS:HG2	1.99	0.43
1:L1:37:A:H5''	20:LL:35:ALA:HB2	2.00	0.43
1:L1:307:U:H2'	1:L1:308:A:H8	1.82	0.43
1:L1:678:A2M:H5''	96:L1:2728:HOH:O	2.19	0.43
2:L2:1038:U:H2'	2:L2:1039:U:C6	2.53	0.43
94:L2:1729:PAR:H62	94:L2:1729:PAR:H13	1.68	0.43
3:L3:100:U:H2'	3:L3:101:G:C8	2.54	0.43
7:L7:32:U:H5''	7:L7:33:U:OP2	2.18	0.43
8:L8:30:C:H5''	23:LO:56:THR:HG21	2.00	0.43
11:LC:140:GLY:HA2	34:LZ:17:ARG:HD2	2.00	0.43
12:LD:113:ASP:OD2	71:SR:15:ARG:NH2	2.51	0.43
16:LH:161:CYS:HA	16:LH:164:VAL:HG22	2.01	0.43
23:LO:40:ASP:HB2	23:LO:43:LYS:HG3	2.00	0.43
29:LU:32:ILE:HB	29:LU:33:PRO:HD3	2.01	0.43
29:LU:96:LYS:HB3	29:LU:96:LYS:HE3	1.80	0.43
30:LV:60:ILE:HD12	35:La:26:LYS:HE3	1.99	0.43
35:La:27:LYS:O	35:La:31:GLN:HG3	2.17	0.43
46:Ll:28:ARG:HD3	46:Ll:36:LYS:HD2	1.99	0.43
51:S1:699:A:N6	51:S1:747:C:H42	2.17	0.43
51:S1:783:A:H61	51:S1:835:C:H42	1.65	0.43
51:S1:1637:A:H62	51:S1:1822:A:N6	2.17	0.43
51:S1:1982:G:OP1	77:SX:96:LYS:NZ	2.41	0.43
53:S3:11:A:H2'	53:S3:12:G:C8	2.53	0.43
56:SC:6:LYS:O	56:SC:10:ILE:HD12	2.17	0.43
61:SH:164:VAL:HG12	61:SH:168:LYS:HE3	2.01	0.43
66:SM:19:LEU:O	66:SM:85:ILE:HA	2.18	0.43
84:Se:56:HIS:HB3	84:Se:59:LYS:HB2	2.00	0.43
2:L2:601:G:OP2	28:LT:25:HIS:NE2	2.47	0.43
6:L6:30:C:H3'	13:LE:50:LYS:HD3	2.00	0.43
7:L7:162:A2M:H1'	7:L7:162:A2M:HM'3	1.77	0.43
49:Lo:55:TRP:NE1	49:Lo:66:GLY:O	2.51	0.43
51:S1:124:A:OP2	51:S1:124:A:H8	2.01	0.43
51:S1:826:A:H2'	51:S1:827:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SB:140:ALA:HB1	55:SB:145:ILE:HB	2.00	0.43
55:SB:152:ASP:OD2	55:SB:169:ARG:NH1	2.50	0.43
56:SC:30:GLU:H	56:SC:30:GLU:CD	2.26	0.43
59:SF:156:TRP:CE2	59:SF:185:PRO:HG3	2.53	0.43
62:SI:146:ARG:HA	63:SJ:49:GLU:HG3	2.00	0.43
79:SZ:17:PHE:HZ	79:SZ:26:LYS:HD2	1.83	0.43
20:LL:70:LYS:HD2	20:LL:125:TYR:CE1	2.54	0.43
22:LN:40:ARG:HG3	22:LN:40:ARG:HH11	1.84	0.43
51:S1:1672:C:H4'	51:S1:1673:A:OP1	2.18	0.43
51:S1:1921:A:N3	51:S1:1982:G:O2'	2.43	0.43
65:SL:108:LYS:NZ	86:Sg:62:GLU:OE2	2.50	0.43
1:L1:299:U:HO2'	1:L1:300:A:H8	1.64	0.43
1:L1:496:C:H2'	1:L1:497:A:C8	2.53	0.43
1:L1:709:A:OP1	24:LP:115:SER:OG	2.35	0.43
1:L1:1102:U:H5''	27:LS:19:PHE:HB2	2.00	0.43
2:L2:1397:OMC:HM22	2:L2:1398:C:O4'	2.19	0.43
4:L4:180:C:H1'	5:L5:5:C:H1'	2.00	0.43
12:LD:28:SER:HB2	12:LD:66:LYS:O	2.19	0.43
12:LD:119:ASP:HB3	12:LD:122:THR:HG23	2.01	0.43
13:LE:94:ALA:HB1	47:Lm:78:MET:SD	2.58	0.43
38:Ld:26:VAL:HG12	38:Ld:93:SER:HB3	2.01	0.43
51:S1:550:C:H2'	51:S1:551:A:C8	2.53	0.43
51:S1:552:U:H2'	51:S1:553:U:O4'	2.18	0.43
51:S1:918:A:H3'	51:S1:919:G:C8	2.54	0.43
51:S1:1718:A:C8	80:Sa:85:ARG:HG2	2.53	0.43
54:SA:130:LYS:NZ	54:SA:134:GLY:O	2.48	0.43
61:SH:45:ARG:HG3	61:SH:45:ARG:NH1	2.33	0.43
64:SK:72:ILE:HG21	64:SK:112:TRP:CZ2	2.54	0.43
86:Sg:7:LEU:HB2	86:Sg:303:ILE:HB	2.00	0.43
1:L1:981:C:P	89:L1:1813:SPD:H42	2.59	0.43
1:L1:1574:C:O2'	1:L1:1575:G:OP1	2.30	0.43
2:L2:521:A:OP1	94:L2:1729:PAR:N24	2.51	0.43
3:L3:75:C:O2'	45:Lk:3:ARG:NH1	2.51	0.43
12:LD:76:LYS:HB2	12:LD:76:LYS:HE3	1.73	0.43
15:LG:184:MET:HE3	15:LG:195:THR:HG21	2.00	0.43
15:LG:224:LEU:HD12	15:LG:224:LEU:HA	1.81	0.43
50:Lp:74:CYS:HB3	50:Lp:77:CYS:HB2	2.01	0.43
51:S1:500:A:OP1	79:SZ:105:LYS:NZ	2.51	0.43
51:S1:750:U:H2'	51:S1:751:G:C8	2.54	0.43
89:L1:1814:SPD:H41	2:L2:1037:G:OP1	2.18	0.43
2:L2:453:A:H1'	51:S1:1160:A:C5	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L2:1087:C:H2'	2:L2:1088:G:C8	2.54	0.43
11:LC:120:ARG:HG2	11:LC:272:LYS:HE3	2.01	0.43
27:LS:80:VAL:HG12	27:LS:81:ARG:HG2	1.99	0.43
29:LU:87:LYS:HG2	29:LU:117:TYR:CE2	2.54	0.43
46:LI:36:LYS:HD2	46:LI:36:LYS:HA	1.75	0.43
51:S1:1450:A:OP1	59:SF:171:THR:OG1	2.33	0.43
55:SB:83:ARG:O	55:SB:84:LEU:HB3	2.19	0.43
80:Sa:51:ARG:NH1	80:Sa:86:GLU:OE1	2.52	0.43
1:L1:247:A:N3	11:LC:217:ARG:HD2	2.34	0.43
1:L1:684:G:O2'	89:L1:1806:SPD:H41	2.19	0.43
1:L1:1110:G:H5'	27:LS:60:ARG:NH1	2.34	0.43
1:L1:1232:U:H5''	16:LH:43:LYS:HD3	2.01	0.43
1:L1:1452:C:H2'	1:L1:1453:G:H8	1.84	0.43
1:L1:1686:C:H2'	1:L1:1687:G:H8	1.84	0.43
2:L2:528:U:O2	2:L2:556:U:H4'	2.19	0.43
8:L8:30:C:H2'	8:L8:31:A:O4'	2.19	0.43
10:LB:120:LYS:HA	10:LB:120:LYS:HD2	1.75	0.43
22:LN:46:PHE:HE1	22:LN:141:LYS:HE2	1.83	0.43
23:LO:41:LYS:HA	23:LO:41:LYS:HD2	1.68	0.43
23:LO:166:PHE:HA	23:LO:169:LEU:HB3	2.00	0.43
26:LR:19:GLU:CD	26:LR:19:GLU:H	2.27	0.43
31:LW:74:LYS:HB2	31:LW:76:VAL:HG22	2.00	0.43
36:Lb:15:LYS:HB3	36:Lb:15:LYS:HE2	1.86	0.43
51:S1:1271:C:O2'	51:S1:2177:G:O3'	2.36	0.43
51:S1:2198:A:O2'	51:S1:2200:A:N7	2.39	0.43
67:SN:27:LYS:HG3	67:SN:71:TYR:CE2	2.54	0.43
69:SP:77:ASN:ND2	69:SP:79:LYS:HD2	2.34	0.43
1:L1:135:A:N7	1:L1:171:U:H4'	2.34	0.42
1:L1:255:G:OP1	31:LW:57:ARG:NH2	2.52	0.42
1:L1:1537:G:O2'	2:L2:601:G:O6	2.33	0.42
2:L2:14:OMC:HM21	7:L7:113:G:H5'	2.00	0.42
2:L2:795:U:O2'	2:L2:798:G:O6	2.27	0.42
2:L2:1127:G:O2'	2:L2:1132:A:N1	2.45	0.42
4:L4:161:C:H2'	4:L4:162:A:C8	2.54	0.42
7:L7:161:C:H2'	7:L7:162:A2M:H8	2.01	0.42
14:LF:177:TYR:OH	19:LK:107:ASP:OD2	2.26	0.42
51:S1:29:OMU:H2'	51:S1:30:G:C8	2.54	0.42
51:S1:2129:C:H2'	51:S1:2130:A:C8	2.53	0.42
62:SI:183:ARG:HG2	62:SI:183:ARG:NH1	2.30	0.42
67:SN:76:ASN:O	67:SN:80:ILE:HG22	2.19	0.42
71:SR:27:VAL:O	71:SR:31:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:ST:2:VAL:HG22	73:ST:3:ARG:HG2	2.01	0.42
1:L1:1405:U:H2'	1:L1:1406:C:C6	2.55	0.42
1:L1:1569:U:C2	28:LT:46:GLN:HG3	2.55	0.42
2:L2:56:OMU:HM23	2:L2:56:OMU:H1'	1.84	0.42
2:L2:1183:C:H2'	2:L2:1184:C:O4'	2.18	0.42
26:LR:48:ARG:HG3	26:LR:54:LYS:HD2	2.01	0.42
39:Le:13:LYS:HA	39:Le:13:LYS:HD2	1.69	0.42
51:S1:66:U:H1'	60:SG:163:ARG:HH21	1.83	0.42
51:S1:701:G:N2	51:S1:745:G:H22	2.17	0.42
51:S1:2098:G:C6	51:S1:2099:G:C6	3.07	0.42
57:SD:16:ARG:HB2	57:SD:19:GLU:OE2	2.18	0.42
66:SM:26:ALA:HB2	66:SM:82:TYR:CZ	2.54	0.42
66:SM:27:LYS:HB2	66:SM:27:LYS:NZ	2.33	0.42
69:SP:17:ARG:HA	69:SP:17:ARG:HH11	1.84	0.42
74:SU:20:GLU:C	74:SU:22:ALA:H	2.28	0.42
1:L1:108:G:N1	35:La:120:LYS:HB3	2.34	0.42
1:L1:357:A:N7	89:L1:1811:SPD:H71	2.35	0.42
1:L1:624:U:O2'	1:L1:625:C:H4'	2.19	0.42
1:L1:823:G:N3	1:L1:823:G:H2'	2.35	0.42
2:L2:1354:U:H1'	18:LJ:46:GLY:HA3	2.00	0.42
2:L2:1453:U:H4'	2:L2:1454:A:H5''	2.01	0.42
5:L5:62:C:H3'	5:L5:63:G:N2	2.28	0.42
9:LA:106:GLN:HE21	9:LA:106:GLN:HA	1.83	0.42
10:LB:356:GLN:CD	10:LB:356:GLN:N	2.77	0.42
22:LN:153:ARG:HD2	22:LN:153:ARG:C	2.44	0.42
23:LO:231:GLN:HG3	23:LO:232:PHE:CD2	2.54	0.42
31:LW:109:THR:H	31:LW:112:ARG:HB3	1.85	0.42
38:Ld:10:ASP:OD1	38:Ld:11:THR:N	2.51	0.42
40:Lf:96:VAL:HG22	40:Lf:121:ALA:HB3	2.00	0.42
51:S1:471:A:H2'	51:S1:472:G:O4'	2.18	0.42
53:S3:44:A:H2'	53:S3:45:A:C8	2.55	0.42
57:SD:28:LYS:HE2	57:SD:28:LYS:HB2	1.89	0.42
65:SL:55:MET:HB3	65:SL:55:MET:HE3	1.80	0.42
75:SV:100:SER:HB3	75:SV:123:ALA:HB2	2.01	0.42
1:L1:80:C:H2'	1:L1:81:U:O4'	2.20	0.42
1:L1:1775:U:O2'	7:L7:127:C:OP1	2.34	0.42
94:L1:1978:PAR:N24	94:L1:1978:PAR:O44	2.52	0.42
2:L2:1309:G:H5''	2:L2:1310:A:H5''	2.01	0.42
7:L7:43:A2M:HM'3	7:L7:43:A2M:H1'	1.92	0.42
13:LE:77:GLN:O	13:LE:81:THR:HG22	2.20	0.42
21:LM:146:PRO:HG3	35:La:106:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:54:PRO:HA	32:LX:59:TYR:CG	2.54	0.42
51:S1:1560:A:H5''	51:S1:1561:C:OP2	2.20	0.42
51:S1:1686:C:H4'	72:SS:56:LEU:HD13	2.00	0.42
51:S1:1905:C:HO2'	51:S1:1906:G:P	2.39	0.42
52:S4:33:C:H4'	61:SH:184:ARG:HE	1.84	0.42
54:SA:145:THR:HG21	54:SA:158:ALA:HB2	2.00	0.42
56:SC:39:HIS:ND1	56:SC:39:HIS:C	2.77	0.42
58:SE:84:MET:HE2	58:SE:120:LEU:HB2	2.00	0.42
61:SH:37:HIS:CD2	61:SH:72:LYS:HG2	2.53	0.42
62:SI:117:ARG:HA	62:SI:117:ARG:HD2	1.84	0.42
1:L1:610:A:C2	37:Lc:77:ARG:HB3	2.54	0.42
1:L1:739:U:H2'	1:L1:740:C:C6	2.54	0.42
2:L2:1101:A:H8	12:LD:128:ASP:OD2	2.02	0.42
2:L2:1319:C:H2'	2:L2:1320:U:C6	2.55	0.42
9:LA:206:PRO:HD3	9:LA:213:GLY:CA	2.50	0.42
21:LM:54:LYS:HD3	21:LM:54:LYS:HA	1.90	0.42
34:LZ:41:ARG:HH11	34:LZ:102:ASP:HB2	1.85	0.42
41:Lg:61:VAL:HG13	41:Lg:66:ASP:HB3	2.00	0.42
55:SB:117:LYS:HD2	55:SB:117:LYS:O	2.20	0.42
1:L1:328:U:OP1	21:LM:68:ARG:HD2	2.19	0.42
1:L1:1170:G:H4'	1:L1:1459:G:H5'	2.02	0.42
2:L2:1000:U:H5'	2:L2:1001:C:OP2	2.19	0.42
2:L2:1513:G:N7	39:Le:37:ARG:NH2	2.66	0.42
3:L3:174:C:H2'	3:L3:175:A:H8	1.83	0.42
5:L5:5:C:H2'	5:L5:6:G:O4'	2.20	0.42
5:L5:36:G:OP1	10:LB:392:LYS:HE3	2.19	0.42
6:L6:44:G:H2'	6:L6:45:G:C8	2.54	0.42
7:L7:169:A:OP2	7:L7:169:A:H8	2.03	0.42
11:LC:94:MET:HE3	11:LC:94:MET:HB3	1.95	0.42
21:LM:75:VAL:HG23	21:LM:78:GLY:HA2	2.01	0.42
24:LP:36:LEU:O	24:LP:40:THR:OG1	2.31	0.42
25:LQ:77:GLY:O	25:LQ:81:ARG:HG3	2.18	0.42
51:S1:376:U:H5''	64:SK:31:ARG:HH11	1.85	0.42
51:S1:462:G:H5'	60:SG:73:ARG:HH21	1.84	0.42
51:S1:1978:A:H5''	71:SR:134:GLY:HA3	2.01	0.42
87:Sh:67:VAL:HG12	87:Sh:70:ALA:N	2.31	0.42
1:L1:114:G:H4'	21:LM:49:ARG:HG2	2.01	0.42
1:L1:984:A:OP1	17:LI:22:SER:HB3	2.20	0.42
2:L2:1369:C:N3	2:L2:1373:C:H5	2.18	0.42
2:L2:1385:G:H4'	2:L2:1385:G:OP2	2.20	0.42
2:L2:1485:G:OP2	19:LK:171:ARG:NH2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LC:356:LYS:HE3	11:LC:356:LYS:HB3	1.86	0.42
14:LF:51:ALA:HA	14:LF:67:GLY:HA3	2.01	0.42
20:LL:36:GLY:O	20:LL:41:HIS:HB2	2.19	0.42
23:LO:262:LYS:HB2	23:LO:262:LYS:HE2	1.81	0.42
37:Lc:176:ASN:HA	37:Lc:179:ILE:HD12	2.02	0.42
48:Ln:3:THR:HG23	51:S1:2174:G:H1'	2.02	0.42
49:Lo:49:ARG:HG3	49:Lo:55:TRP:CE2	2.55	0.42
51:S1:58:C:OP1	51:S1:504:G:O2'	2.38	0.42
51:S1:230:G:O2'	87:Sh:198:HIS:NE2	2.47	0.42
51:S1:1409:U:H2'	51:S1:1410:C:C6	2.55	0.42
52:S4:45:G:H2'	52:S4:46:U:H5'	2.02	0.42
60:SG:14:LYS:HD3	60:SG:14:LYS:HA	1.95	0.42
62:SI:191:ASN:HB3	62:SI:196:GLN:HB2	2.02	0.42
1:L1:510:U:O2'	26:LR:67:LYS:HE2	2.19	0.42
1:L1:517:U:H2'	1:L1:518:C:C6	2.55	0.42
2:L2:72:G:OP1	10:LB:251:LEU:N	2.52	0.42
6:L6:68:A:H5'	14:LF:47:ARG:NH2	2.34	0.42
6:L6:68:A:H2'	6:L6:70:G:C5	2.54	0.42
16:LH:65:GLU:HG3	16:LH:155:THR:HG23	2.01	0.42
16:LH:72:TYR:OH	16:LH:91:HIS:O	2.36	0.42
21:LM:103:GLU:OE2	21:LM:118:SER:OG	2.34	0.42
41:Lg:69:TRP:HZ2	41:Lg:144:ILE:HD11	1.85	0.42
49:Lo:67:GLY:HA3	49:Lo:70:THR:O	2.20	0.42
50:Lp:11:HIS:HA	50:Lp:20:HIS:HA	2.01	0.42
51:S1:1:G:OP2	57:SD:52:ARG:NH2	2.53	0.42
51:S1:148:G:H2'	51:S1:149:G:C8	2.54	0.42
51:S1:315:A:H5''	51:S1:333:G:H22	1.84	0.42
51:S1:969:A2M:H8	51:S1:969:A2M:H2'	1.80	0.42
54:SA:11:LYS:O	54:SA:11:LYS:HG2	2.20	0.42
73:ST:47:PRO:HG3	73:ST:75:LEU:HD12	2.01	0.42
1:L1:246:A:H4'	1:L1:248:A:N7	2.35	0.42
1:L1:687:C:H2'	1:L1:688:A:H8	1.83	0.42
1:L1:958:G:H5'	1:L1:960:A:H1'	2.02	0.42
1:L1:1659:OMU:H6	1:L1:1659:OMU:O5'	2.20	0.42
2:L2:459:A:H2'	2:L2:460:A:C8	2.54	0.42
2:L2:1507:U:H2'	2:L2:1508:A:C8	2.54	0.42
6:L6:11:G:C8	14:LF:186:PRO:HG2	2.55	0.42
12:LD:135:ARG:NH2	12:LD:155:HIS:O	2.48	0.42
15:LG:88:ARG:HD2	15:LG:92:LEU:HD22	2.01	0.42
20:LL:51:GLY:C	24:LP:179:GLU:HA	2.44	0.42
22:LN:115:MET:HA	22:LN:118:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:89:MET:HE1	25:LQ:93:GLU:HB3	2.01	0.42
26:LR:68:ASP:OD1	26:LR:100:SER:HB2	2.20	0.42
38:Ld:9:VAL:HG23	38:Ld:73:SER:HB2	2.01	0.42
44:Lj:38:ALA:HB2	44:Lj:45:ARG:HG3	2.02	0.42
51:S1:259:C:H2'	51:S1:260:A:H8	1.85	0.42
51:S1:826:A:H2'	51:S1:827:G:C8	2.55	0.42
55:SB:15:GLU:OE2	75:SV:118:ARG:HB2	2.20	0.42
59:SF:200:LEU:HD13	59:SF:208:VAL:HG11	2.02	0.42
64:SK:171:VAL:O	74:SU:7:TYR:HA	2.19	0.42
1:L1:1574:C:HO2'	1:L1:1575:G:P	2.41	0.42
1:L1:1685:G:H1	1:L1:1715:U:H3	1.68	0.42
2:L2:490:A:H5''	9:LA:243:THR:HB	2.01	0.42
2:L2:771:G:H4'	15:LG:50:PHE:CE1	2.55	0.42
2:L2:1175:A:OP1	23:LO:182:ARG:HD3	2.20	0.42
6:L6:70:G:O2'	6:L6:71:A:H8	2.02	0.42
9:LA:36:GLU:OE2	9:LA:90:CYS:HB3	2.20	0.42
13:LE:149:ASP:HB3	13:LE:152:GLN:HB2	2.01	0.42
34:LZ:53:VAL:HB	34:LZ:110:ARG:HG2	2.02	0.42
34:LZ:56:ALA:HB3	34:LZ:60:ALA:HB3	2.01	0.42
41:Lg:85:LYS:HG3	41:Lg:101:ARG:NH2	2.34	0.42
42:Lh:47:TRP:HA	42:Lh:51:HIS:HB2	2.02	0.42
44:Lj:51:VAL:HG12	44:Lj:55:LYS:HD2	2.02	0.42
51:S1:27:U:H2'	51:S1:28:A2M:H8	2.02	0.42
51:S1:259:C:H2'	51:S1:260:A:C8	2.55	0.42
51:S1:1972:G:N1	51:S1:1975:A:OP2	2.52	0.42
55:SB:116:GLN:C	55:SB:118:LYS:H	2.28	0.42
59:SF:250:ASP:CG	59:SF:252:THR:HG1	2.26	0.42
65:SL:107:GLU:O	65:SL:108:LYS:HB3	2.20	0.42
66:SM:18:ARG:HD3	66:SM:87:ASP:OD2	2.19	0.42
66:SM:96:LYS:HE3	66:SM:96:LYS:HB2	1.87	0.42
67:SN:79:GLY:O	67:SN:83:MET:HB2	2.20	0.42
73:ST:19:ARG:HB2	82:Sc:86:HIS:NE2	2.35	0.42
77:SX:118:LYS:HG2	77:SX:122:LYS:HE2	2.01	0.42
1:L1:307:U:H2'	1:L1:308:A:C8	2.55	0.41
1:L1:836:G:N1	24:LP:96:ASP:HA	2.35	0.41
1:L1:921:A:N3	89:L1:1802:SPD:H51	2.35	0.41
1:L1:1031:A:N1	1:L1:1161:A:O2'	2.52	0.41
1:L1:1106:A:H5''	8:L8:102:G:O2'	2.20	0.41
4:L4:170:G:H4'	4:L4:171:A:H3'	2.02	0.41
8:L8:109:U:H2'	8:L8:110:G:C8	2.55	0.41
11:LC:295:GLU:HG3	11:LC:298:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LF:32:SER:OG	41:Lg:144:ILE:O	2.33	0.41
26:LR:29:PHE:CE2	26:LR:31:VAL:HB	2.55	0.41
51:S1:402:A:H4'	69:SP:33:PHE:HZ	1.84	0.41
51:S1:1535:A:C2	76:SW:107:HIS:HB3	2.55	0.41
51:S1:1637:A:H1'	51:S1:1638:U:C6	2.55	0.41
51:S1:1915:U:H2'	51:S1:1916:G:O4'	2.20	0.41
57:SD:70:LEU:HD12	58:SE:247:ILE:HG12	2.02	0.41
66:SM:64:LYS:HE2	66:SM:75:ASP:OD1	2.20	0.41
86:Sg:243:PHE:CE1	86:Sg:263:LEU:HD11	2.55	0.41
1:L1:159:U:H1'	1:L1:160:C:H5'	2.02	0.41
1:L1:169:G:H4'	1:L1:170:U:H3'	2.02	0.41
1:L1:454:U:H2'	1:L1:455:G:C8	2.55	0.41
1:L1:1044:G:N3	2:L2:1064:A:H2'	2.35	0.41
1:L1:1578:G:H4'	25:LQ:26:PRO:HD3	2.02	0.41
2:L2:653:C:H2'	2:L2:654:U:C6	2.56	0.41
2:L2:822:G:O2'	2:L2:823:A:H5'	2.20	0.41
2:L2:970:A:HO2'	2:L2:971:A:H8	1.66	0.41
2:L2:1232:G:O2'	2:L2:1233:U:OP2	2.27	0.41
2:L2:1385:G:C2	10:LB:255:ALA:HB1	2.55	0.41
18:LJ:47:ARG:HD2	18:LJ:48:LEU:H	1.85	0.41
31:LW:32:LEU:HB2	31:LW:37:ARG:HG3	2.02	0.41
39:Le:24:LYS:HE2	39:Le:24:LYS:HB3	1.78	0.41
51:S1:792:G:H5'	51:S1:792:G:N3	2.35	0.41
51:S1:1114:G:OP1	73:ST:121:ARG:NE	2.52	0.41
51:S1:2119:C:H1'	51:S1:2120:C:O5'	2.20	0.41
55:SB:194:ARG:NE	78:SY:48:GLY:HA3	2.35	0.41
58:SE:118:ILE:HG23	58:SE:158:VAL:HG23	2.02	0.41
87:Sh:165:LEU:HD23	87:Sh:165:LEU:HA	1.86	0.41
2:L2:21:C:H5''	2:L2:22:A:H5'	2.01	0.41
20:LL:110:LEU:O	20:LL:130:ALA:HB2	2.21	0.41
47:Lm:79:GLU:OE1	47:Lm:80:PRO:HD2	2.21	0.41
51:S1:668:A2M:H8	51:S1:668:A2M:H2'	1.90	0.41
51:S1:1281:C:O2'	63:SJ:2:THR:N	2.45	0.41
51:S1:1859:A:H2'	51:S1:1859:A:N3	2.35	0.41
52:S4:17:A:H2'	52:S4:18:G:C8	2.56	0.41
55:SB:54:VAL:HG22	75:SV:108:MET:SD	2.60	0.41
60:SG:4:ASN:ND2	60:SG:111:LEU:HD11	2.35	0.41
63:SJ:3:MET:HE3	63:SJ:3:MET:HB2	1.77	0.41
71:SR:113:GLU:HA	71:SR:116:LYS:HG2	2.02	0.41
85:Sf:92:LEU:HD12	85:Sf:92:LEU:HA	1.89	0.41
86:Sg:4:GLU:O	86:Sg:47:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:Sh:75:SER:HA	87:Sh:78:GLY:O	2.20	0.41
1:L1:156:A:H8	1:L1:156:A:OP2	2.03	0.41
1:L1:712:G:H2'	1:L1:713:A:O4'	2.21	0.41
2:L2:742:U:H2'	2:L2:743:C:C6	2.56	0.41
2:L2:784:U:H1'	2:L2:785:U:OP2	2.20	0.41
10:LB:116:ARG:HG2	10:LB:122:TRP:CG	2.55	0.41
11:LC:216:THR:O	11:LC:220:ARG:HG3	2.20	0.41
22:LN:46:PHE:HB2	22:LN:139:ARG:HG2	2.02	0.41
23:LO:187:PRO:HG2	23:LO:201:HIS:CD2	2.56	0.41
39:Le:103:LYS:C	39:Le:106:PRO:HD2	2.45	0.41
42:Lh:105:LYS:HE2	42:Lh:105:LYS:HB3	1.76	0.41
51:S1:43:A:O2'	51:S1:97:C:OP1	2.35	0.41
51:S1:1166:C:H2'	51:S1:1167:A:C8	2.55	0.41
51:S1:1715:C:O2'	77:SX:154:ARG:NH1	2.52	0.41
51:S1:1873:A:H5'	51:S1:1875:G:O4'	2.20	0.41
51:S1:2058:G:H2'	51:S1:2059:OMC:O4'	2.21	0.41
53:S3:7:G:OP1	53:S3:16:C:N4	2.38	0.41
76:SW:81:LYS:HB3	76:SW:81:LYS:HE2	1.81	0.41
79:SZ:119:ASN:HA	79:SZ:122:LYS:HE3	2.02	0.41
1:L1:12:U:H2'	1:L1:13:G:H8	1.85	0.41
1:L1:540:A:N6	26:LR:68:ASP:O	2.47	0.41
1:L1:895:G:N7	94:L1:1978:PAR:H221	2.36	0.41
1:L1:954:U:H2'	1:L1:955:A2M:H8	2.02	0.41
1:L1:1549:U:H2'	1:L1:1550:A:C8	2.55	0.41
1:L1:1554:G:N1	1:L1:1557:A:OP1	2.53	0.41
2:L2:958:A:H2'	2:L2:959:A:C8	2.55	0.41
5:L5:19:C:O2'	28:LT:69:ARG:O	2.32	0.41
7:L7:70:C:H5''	31:LW:25:ARG:CZ	2.51	0.41
11:LC:369:LYS:HE2	11:LC:369:LYS:HB3	1.86	0.41
12:LD:84:LYS:HZ3	12:LD:84:LYS:HG3	1.80	0.41
16:LH:30:LYS:HG2	16:LH:31:ASP:OD2	2.21	0.41
17:LI:13:GLN:HE21	17:LI:13:GLN:HB2	1.67	0.41
20:LL:51:GLY:N	24:LP:182:ARG:O	2.48	0.41
22:LN:12:CYS:SG	22:LN:59:GLN:HG3	2.61	0.41
34:LZ:30:ASP:HB3	34:LZ:33:ASN:HB2	2.03	0.41
51:S1:889:A:C2	58:SE:16:MET:HG2	2.56	0.41
57:SD:87:GLU:CD	57:SD:87:GLU:N	2.78	0.41
64:SK:172:GLU:HG3	64:SK:175:ILE:HD13	2.02	0.41
75:SV:88:THR:HG23	75:SV:93:LYS:NZ	2.36	0.41
87:Sh:81:VAL:HG12	87:Sh:82:LYS:HG3	2.03	0.41
3:L3:71:U:H5	3:L3:150:A:N7	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L3:151:A:H5'	45:Lk:26:LYS:HE2	2.02	0.41
7:L7:68:A:H2'	7:L7:69:PSU:O4'	2.20	0.41
15:LG:166:TRP:CD1	15:LG:166:TRP:H	2.38	0.41
17:LI:94:TYR:O	17:LI:97:THR:OG1	2.37	0.41
19:LK:148:LEU:HD12	19:LK:148:LEU:HA	1.85	0.41
29:LU:88:LYS:HE2	29:LU:88:LYS:HB3	1.91	0.41
38:Ld:102:ILE:HD12	38:Ld:102:ILE:HA	1.84	0.41
51:S1:275:A:O2'	51:S1:276:G:H8	2.03	0.41
51:S1:818:U:O2	87:Sh:67:VAL:HG22	2.20	0.41
52:S4:24:G:H2'	52:S4:25:A:H8	1.86	0.41
56:SC:44:ARG:HG3	56:SC:46:GLU:HG3	2.02	0.41
62:SI:61:VAL:HG22	62:SI:93:LEU:HB2	2.02	0.41
65:SL:107:GLU:C	65:SL:109:ALA:H	2.29	0.41
68:SO:27:PHE:HB3	68:SO:34:PHE:HB2	2.02	0.41
79:SZ:10:VAL:HG13	79:SZ:32:VAL:HG13	2.02	0.41
82:Sc:39:PRO:HG3	82:Sc:78:CYS:N	2.36	0.41
83:Sd:72:MET:HE3	83:Sd:72:MET:HB2	1.95	0.41
1:L1:601:G:N1	1:L1:605:G:O6	2.53	0.41
1:L1:1687:G:H2'	1:L1:1688:G:C8	2.55	0.41
29:LU:29:ASP:HA	29:LU:76:VAL:HG12	2.02	0.41
33:LY:123:GLY:HA2	33:LY:126:MET:HE3	2.02	0.41
35:La:49:ARG:HB3	35:La:50:PRO:HD3	2.02	0.41
51:S1:1605:U:O4'	85:Sf:141:GLY:HA3	2.21	0.41
51:S1:1662:OMU:H1'	51:S1:1662:OMU:HM23	1.63	0.41
55:SB:58:TRP:O	55:SB:62:ILE:HG12	2.20	0.41
56:SC:65:ILE:HD12	56:SC:65:ILE:HA	1.83	0.41
61:SH:153:LYS:HG2	61:SH:158:CYS:SG	2.61	0.41
65:SL:99:PHE:O	65:SL:103:HIS:HB2	2.20	0.41
68:SO:75:VAL:HG21	68:SO:115:ALA:HB3	2.02	0.41
85:Sf:74:LYS:HE2	85:Sf:74:LYS:HB3	1.89	0.41
87:Sh:149:THR:O	87:Sh:153:VAL:HG23	2.21	0.41
1:L1:719:U:OP2	17:LI:41:ARG:NH1	2.49	0.41
1:L1:791:C:OP2	37:Lc:38:LYS:HD3	2.21	0.41
1:L1:1240:U:OP1	26:LR:159:LYS:NZ	2.38	0.41
1:L1:1252:C:O3'	1:L1:1253:OMU:H6	2.21	0.41
2:L2:95:A2M:O5'	2:L2:95:A2M:H8	2.21	0.41
2:L2:443:OMC:N4	2:L2:488:A:O5'	2.48	0.41
2:L2:1254:G:O4'	2:L2:1308:5MC:HM52	2.20	0.41
2:L2:1340:A:OP1	13:LE:169:LYS:NZ	2.50	0.41
16:LH:31:ASP:HA	16:LH:60:ASN:OD1	2.21	0.41
21:LM:47:LYS:HA	21:LM:47:LYS:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:166:VAL:HG21	27:LS:159:TYR:CD1	2.56	0.41
23:LO:41:LYS:NZ	27:LS:30:ILE:O	2.54	0.41
34:LZ:46:LEU:HD12	34:LZ:46:LEU:HA	1.87	0.41
51:S1:1597:G:N1	51:S1:1601:U:O4	2.53	0.41
51:S1:2008:OMG:HM23	51:S1:2008:OMG:H1'	1.81	0.41
60:SG:214:ARG:HG3	60:SG:214:ARG:NH1	2.35	0.41
62:SI:196:GLN:HG3	82:Sc:13:VAL:HG22	2.03	0.41
71:SR:120:ALA:O	71:SR:124:VAL:HG23	2.20	0.41
86:Sg:196:TYR:CZ	86:Sg:214:LYS:HB2	2.56	0.41
86:Sg:261:TYR:CE2	86:Sg:268:VAL:HG22	2.55	0.41
1:L1:23:U:H4'	1:L1:24:A:N7	2.36	0.41
1:L1:205:A:N6	34:LZ:55:PRO:HG3	2.36	0.41
1:L1:346:U:H1'	2:L2:468:A:N3	2.35	0.41
1:L1:669:OMC:HM23	1:L1:678:A2M:H4'	2.03	0.41
1:L1:828:U:O5'	2:L2:1148:G:H4'	2.21	0.41
1:L1:1161:A:N6	24:LP:13:ARG:HD2	2.35	0.41
1:L1:1190:OMG:HM22	1:L1:1191:G:H5'	2.03	0.41
1:L1:1524:OMG:H8	1:L1:1524:OMG:H2'	1.41	0.41
2:L2:339:A:H1'	2:L2:341:A:H2'	2.03	0.41
2:L2:340:A:H4'	2:L2:341:A:H5'	2.02	0.41
2:L2:591:A2M:H8	2:L2:591:A2M:O5'	2.20	0.41
2:L2:598:A:H5''	28:LT:83:TRP:O	2.20	0.41
2:L2:775:C:H1'	2:L2:811:U:C4	2.56	0.41
2:L2:1248:OMC:H1'	2:L2:1248:OMC:HM23	1.77	0.41
5:L5:112:U:H6	5:L5:112:U:H2'	1.66	0.41
9:LA:40:TYR:HA	9:LA:91:GLY:HA3	2.03	0.41
10:LB:124:GLN:O	39:Le:3:ARG:HD3	2.21	0.41
13:LE:109:ILE:HD11	13:LE:131:VAL:HG21	2.03	0.41
13:LE:111:VAL:HB	13:LE:121:ARG:HB2	2.02	0.41
17:LI:137:LYS:HB3	17:LI:137:LYS:HE2	1.57	0.41
22:LN:54:SER:HB2	22:LN:135:LEU:HD11	2.02	0.41
23:LO:107:ARG:NH2	23:LO:119:PHE:O	2.54	0.41
29:LU:23:LYS:HB3	29:LU:23:LYS:HE2	1.82	0.41
29:LU:120:LYS:HE3	29:LU:120:LYS:HB3	1.68	0.41
31:LW:77:ILE:HG23	31:LW:98:PRO:HG3	2.02	0.41
38:Ld:53:ILE:HD12	38:Ld:53:ILE:HA	1.93	0.41
50:Lp:22:SER:O	50:Lp:75:SER:OG	2.39	0.41
51:S1:447:G:H4'	60:SG:91:TYR:HE2	1.86	0.41
51:S1:498:C:H4'	58:SE:60:MET:HE2	2.02	0.41
51:S1:695:G:H22	51:S1:750:U:H3	1.68	0.41
51:S1:784:C:H3'	51:S1:787:G:H1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S1:1014:C:H2'	51:S1:1015:G:C8	2.56	0.41
51:S1:1588:A:H2'	51:S1:1589:G:C8	2.56	0.41
51:S1:1615:G:H2'	51:S1:1616:A:O4'	2.21	0.41
51:S1:1983:U:H2'	51:S1:1984:C:C6	2.56	0.41
51:S1:2008:OMG:O6	89:S1:2447:SPD:H21	2.21	0.41
52:S4:17:A:H2'	52:S4:18:G:H8	1.85	0.41
56:SC:41:THR:HG23	56:SC:44:ARG:H	1.85	0.41
56:SC:79:LYS:HB2	56:SC:82:LYS:HG3	2.03	0.41
62:SI:86:GLU:HG3	62:SI:94:VAL:HG23	2.02	0.41
75:SV:76:GLU:O	75:SV:80:ARG:HG3	2.21	0.41
75:SV:76:GLU:HA	75:SV:79:GLU:HG3	2.02	0.41
80:Sa:26:LYS:HA	80:Sa:26:LYS:HD3	1.84	0.41
86:Sg:22:GLN:H	86:Sg:22:GLN:HG2	1.66	0.41
1:L1:19:G:OP2	1:L1:19:G:N2	2.48	0.41
1:L1:522:G:H8	1:L1:522:G:OP2	2.04	0.41
2:L2:976:A:OP2	2:L2:976:A:H8	2.04	0.41
2:L2:1287:C:O2'	2:L2:1288:G:O5'	2.39	0.41
11:LC:182:VAL:HG11	11:LC:224:GLY:HA2	2.02	0.41
51:S1:328:C:H2'	51:S1:329:C:C6	2.56	0.41
51:S1:743:A:O2'	51:S1:744:G:OP1	2.32	0.41
51:S1:2135:U:H2'	51:S1:2136:A:C8	2.55	0.41
52:S4:13:C:H4'	52:S4:14:A:OP1	2.21	0.41
67:SN:63:LYS:HB3	67:SN:63:LYS:HE3	1.75	0.41
74:SU:73:CYS:O	74:SU:77:SER:OG	2.31	0.41
1:L1:415:A:O2'	1:L1:417:G:H5'	2.20	0.40
1:L1:1090:U:H2'	1:L1:1091:A:C8	2.57	0.40
1:L1:1198:C:H2'	1:L1:1199:G:O4'	2.22	0.40
1:L1:1374:C:H2'	1:L1:1375:G:O4'	2.22	0.40
1:L1:1390:G:O2'	19:LK:50:VAL:N	2.45	0.40
1:L1:1574:C:H2'	1:L1:1575:G:H8	1.86	0.40
2:L2:1250:C:H2'	2:L2:1251:A:H8	1.86	0.40
2:L2:1275:A:N7	89:L2:1602:SPD:H81	2.35	0.40
2:L2:1505:A:H2'	2:L2:1506:G:C8	2.56	0.40
23:LO:248:MET:HE3	23:LO:248:MET:HB3	1.72	0.40
24:LP:67:ILE:O	24:LP:71:MET:HG2	2.21	0.40
51:S1:163:A:H2'	51:S1:165:G:O4'	2.21	0.40
51:S1:447:G:H5''	89:S1:2302:SPD:HN6	1.86	0.40
51:S1:1796:U:H2'	51:S1:1797:A:O4'	2.21	0.40
52:S4:33:C:O2'	61:SH:184:ARG:NH2	2.54	0.40
54:SA:139:LEU:HG	54:SA:174:ILE:HG21	2.03	0.40
57:SD:112:VAL:HG13	57:SD:117:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Sg:158:PHE:CE1	86:Sg:181:VAL:HG11	2.57	0.40
87:Sh:110:GLU:H	87:Sh:119:LEU:HD13	1.86	0.40
1:L1:305:A2M:H5''	21:LM:47:LYS:NZ	2.37	0.40
1:L1:357:A:N7	89:L1:1811:SPD:N10	2.62	0.40
1:L1:681:A2M:HM'2	1:L1:682:C:O4'	2.22	0.40
1:L1:830:G:OP1	24:LP:192:ARG:NH2	2.55	0.40
1:L1:1442:G:H3'	1:L1:1464:G:N2	2.35	0.40
1:L1:1452:C:H2'	1:L1:1453:G:C8	2.57	0.40
1:L1:1749:G:H2'	1:L1:1751:A:N7	2.35	0.40
2:L2:1416:U:O2'	2:L2:1417:U:H5'	2.21	0.40
3:L3:129:A:C6	49:Lo:42:CYS:HA	2.57	0.40
5:L5:86:G:H8	5:L5:86:G:OP2	2.04	0.40
11:LC:59:MET:HE3	11:LC:59:MET:HB3	1.97	0.40
17:LI:123:THR:O	17:LI:127:LYS:HG2	2.20	0.40
23:LO:106:ALA:O	23:LO:110:LEU:HG	2.21	0.40
25:LQ:66:MET:SD	25:LQ:70:LYS:HE3	2.62	0.40
25:LQ:84:SER:O	25:LQ:88:ARG:HG3	2.21	0.40
50:Lp:46:LYS:HE3	50:Lp:54:THR:HB	2.02	0.40
62:SI:143:TRP:HZ3	63:SJ:54:ASP:HB2	1.85	0.40
71:SR:6:ILE:HA	80:Sa:41:MET:HE2	2.03	0.40
1:L1:447:G:OP1	1:L1:1505:U:O2'	2.39	0.40
1:L1:1245:G:N3	26:LR:114:SER:HB2	2.35	0.40
1:L1:1493:G:O6	40:Lf:17:ARG:NH1	2.54	0.40
1:L1:1552:OMC:HM23	1:L1:1552:OMC:H1'	1.64	0.40
2:L2:616:G:OP2	2:L2:616:G:H8	2.04	0.40
4:L4:8:U:H4'	28:LT:7:LYS:HG2	2.03	0.40
10:LB:36:ASP:O	10:LB:190:GLY:HA2	2.21	0.40
15:LG:65:VAL:O	15:LG:69:ARG:HG2	2.22	0.40
34:LZ:28:SER:N	34:LZ:36:GLY:O	2.55	0.40
34:LZ:93:SER:HB2	34:LZ:108:PHE:HB2	2.04	0.40
37:Lc:241:ASP:OD2	37:Lc:242:THR:HG23	2.21	0.40
50:Lp:74:CYS:CB	50:Lp:77:CYS:HB2	2.51	0.40
51:S1:70:U:OP1	60:SG:167:LYS:NZ	2.34	0.40
56:SC:26:ARG:HD2	67:SN:67:ALA:HB2	2.03	0.40
56:SC:172:ARG:HD3	56:SC:172:ARG:HA	1.95	0.40
57:SD:12:LYS:HE3	57:SD:12:LYS:HB3	1.86	0.40
64:SK:157:LYS:HE2	64:SK:157:LYS:HB3	1.87	0.40
1:L1:36:U:H4'	20:LL:32:ARG:HD2	2.04	0.40
1:L1:170:U:H1'	1:L1:171:U:OP2	2.21	0.40
1:L1:836:G:H1	24:LP:96:ASP:HA	1.86	0.40
1:L1:1214:G:H2'	1:L1:1215:C:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1232:U:H1'	16:LH:105:MET:HG2	2.04	0.40
3:L3:45:U:OP1	42:Lh:25:ARG:NH2	2.47	0.40
17:LI:210:LYS:O	17:LI:214:LYS:HG2	2.22	0.40
18:LJ:12:ARG:HG2	18:LJ:13:PHE:O	2.21	0.40
20:LL:64:LYS:HB2	20:LL:64:LYS:HE3	1.91	0.40
27:LS:123:LYS:HE2	27:LS:123:LYS:HB2	1.88	0.40
37:Lc:124:THR:HB	37:Lc:215:PHE:HB2	2.02	0.40
39:Le:46:ASP:O	39:Le:50:ARG:HB2	2.22	0.40
51:S1:154:C:OP1	79:SZ:127:LYS:HB2	2.22	0.40
51:S1:275:A:O2'	51:S1:276:G:H5'	2.20	0.40
51:S1:556:A:H5''	57:SD:172:LYS:HE3	2.03	0.40
51:S1:823:G:N7	87:Sh:86:ARG:NH2	2.69	0.40
51:S1:877:U:H3	51:S1:884:A:H62	1.70	0.40
51:S1:1272:A:H2'	51:S1:1274:A:H5''	2.03	0.40
57:SD:96:LEU:HB3	59:SF:186:ARG:O	2.21	0.40
68:SO:129:PRO:HB2	68:SO:131:ASP:O	2.20	0.40
77:SX:127:GLU:HG2	77:SX:137:THR:HG22	2.03	0.40
80:Sa:58:LYS:HG3	80:Sa:103:ARG:NH2	2.37	0.40
1:L1:438:A:H4'	1:L1:439:U:H3'	2.03	0.40
13:LE:162:GLN:O	13:LE:165:LEU:HG	2.21	0.40
24:LP:74:LYS:O	24:LP:78:THR:OG1	2.33	0.40
24:LP:145:LEU:HD12	24:LP:145:LEU:HA	1.94	0.40
24:LP:178:LYS:HG3	24:LP:179:GLU:N	2.36	0.40
33:LY:54:VAL:H	33:LY:57:MET:HE2	1.87	0.40
48:Ln:28:ARG:HG3	48:Ln:28:ARG:HH11	1.87	0.40
51:S1:2026:U:C4	89:S1:2447:SPD:H71	2.56	0.40
51:S1:2140:OMC:H1'	51:S1:2140:OMC:HM23	1.86	0.40
55:SB:92:LYS:HB3	55:SB:92:LYS:HE2	1.96	0.40
69:SP:51:VAL:HG13	69:SP:70:VAL:HB	2.03	0.40
77:SX:89:SER:HB2	77:SX:108:SER:O	2.21	0.40
86:Sg:118:ASP:OD1	86:Sg:118:ASP:N	2.43	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	257/260 (99%)	248 (96%)	9 (4%)	0	100	100
10	LB	402/419 (96%)	398 (99%)	4 (1%)	0	100	100
11	LC	364/373 (98%)	355 (98%)	9 (2%)	0	100	100
12	LD	173/188 (92%)	171 (99%)	2 (1%)	0	100	100
13	LE	184/190 (97%)	178 (97%)	6 (3%)	0	100	100
14	LF	147/195 (75%)	141 (96%)	6 (4%)	0	100	100
15	LG	240/264 (91%)	237 (99%)	3 (1%)	0	100	100
16	LH	219/222 (99%)	217 (99%)	2 (1%)	0	100	100
17	LI	212/220 (96%)	207 (98%)	5 (2%)	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%)	137 (96%)	5 (4%)	0	100	100
21	LM	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
22	LN	196/213 (92%)	189 (96%)	7 (4%)	0	100	100
23	LO	295/305 (97%)	292 (99%)	3 (1%)	0	100	100
24	LP	195/198 (98%)	190 (97%)	5 (3%)	0	100	100
25	LQ	200/254 (79%)	200 (100%)	0	0	100	100
26	LR	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
27	LS	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
28	LT	150/166 (90%)	149 (99%)	1 (1%)	0	100	100
29	LU	120/129 (93%)	119 (99%)	1 (1%)	0	100	100
30	LV	117/145 (81%)	116 (99%)	1 (1%)	0	100	100
31	LW	119/143 (83%)	116 (98%)	3 (2%)	0	100	100
32	LX	81/124 (65%)	78 (96%)	3 (4%)	0	100	100
33	LY	131/134 (98%)	130 (99%)	1 (1%)	0	100	100
34	LZ	143/147 (97%)	142 (99%)	1 (1%)	0	100	100
35	La	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
36	Lb	66/70 (94%)	66 (100%)	0	0	100	100
37	Lc	227/252 (90%)	222 (98%)	5 (2%)	0	100	100
38	Ld	94/104 (90%)	94 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Le	184/188 (98%)	183 (100%)	1 (0%)	0	100	100
40	Lf	126/133 (95%)	123 (98%)	3 (2%)	0	100	100
41	Lg	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
42	Lh	125/168 (74%)	124 (99%)	1 (1%)	0	100	100
43	Li	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
44	Lj	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
45	Lk	76/83 (92%)	76 (100%)	0	0	100	100
46	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
47	Lm	50/128 (39%)	50 (100%)	0	0	100	100
48	Ln	31/34 (91%)	31 (100%)	0	0	100	100
49	Lo	87/92 (95%)	82 (94%)	5 (6%)	0	100	100
50	Lp	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
54	SA	234/264 (89%)	229 (98%)	5 (2%)	0	100	100
55	SB	209/246 (85%)	205 (98%)	4 (2%)	0	100	100
56	SC	211/219 (96%)	208 (99%)	3 (1%)	0	100	100
57	SD	181/190 (95%)	180 (99%)	1 (1%)	0	100	100
58	SE	258/273 (94%)	255 (99%)	3 (1%)	0	100	100
59	SF	220/265 (83%)	218 (99%)	2 (1%)	0	100	100
60	SG	232/249 (93%)	229 (99%)	3 (1%)	0	100	100
61	SH	179/190 (94%)	176 (98%)	3 (2%)	0	100	100
62	SI	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
63	SJ	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
64	SK	193/220 (88%)	191 (99%)	2 (1%)	0	100	100
65	SL	142/149 (95%)	139 (98%)	3 (2%)	0	100	100
66	SM	101/116 (87%)	99 (98%)	2 (2%)	0	100	100
67	SN	105/168 (62%)	103 (98%)	2 (2%)	0	100	100
68	SO	135/144 (94%)	131 (97%)	3 (2%)	1 (1%)	19	18
69	SP	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
70	SQ	91/141 (64%)	89 (98%)	2 (2%)	0	100	100
71	SR	140/153 (92%)	137 (98%)	3 (2%)	0	100	100
72	SS	54/57 (95%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	ST	141/151 (93%)	137 (97%)	4 (3%)	0	100	100
74	SU	151/173 (87%)	146 (97%)	5 (3%)	0	100	100
75	SV	120/143 (84%)	119 (99%)	1 (1%)	0	100	100
76	SW	113/152 (74%)	111 (98%)	2 (2%)	0	100	100
77	SX	150/161 (93%)	146 (97%)	4 (3%)	0	100	100
78	SY	87/164 (53%)	83 (95%)	4 (5%)	0	100	100
79	SZ	128/137 (93%)	125 (98%)	3 (2%)	0	100	100
80	Sa	81/120 (68%)	81 (100%)	0	0	100	100
81	Sb	102/112 (91%)	99 (97%)	3 (3%)	0	100	100
82	Sc	83/86 (96%)	83 (100%)	0	0	100	100
83	Sd	64/87 (74%)	62 (97%)	2 (3%)	0	100	100
84	Se	57/66 (86%)	56 (98%)	1 (2%)	0	100	100
85	Sf	71/152 (47%)	68 (96%)	3 (4%)	0	100	100
86	Sg	297/312 (95%)	284 (96%)	13 (4%)	0	100	100
87	Sh	167/235 (71%)	158 (95%)	9 (5%)	0	100	100
All	All	11533/12926 (89%)	11308 (98%)	224 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
68	SO	131	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	LA	201/204 (98%)	200 (100%)	1 (0%)	86	91
10	LB	337/351 (96%)	335 (99%)	2 (1%)	84	89
11	LC	293/301 (97%)	287 (98%)	6 (2%)	50	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	LD	148/162 (91%)	142 (96%)	6 (4%)	26	30
13	LE	166/172 (96%)	159 (96%)	7 (4%)	25	29
14	LF	124/153 (81%)	122 (98%)	2 (2%)	58	69
15	LG	193/221 (87%)	191 (99%)	2 (1%)	73	80
16	LH	182/188 (97%)	181 (100%)	1 (0%)	86	91
17	LI	178/183 (97%)	177 (99%)	1 (1%)	84	89
18	LJ	106/111 (96%)	104 (98%)	2 (2%)	52	62
19	LK	136/145 (94%)	131 (96%)	5 (4%)	29	35
20	LL	113/114 (99%)	112 (99%)	1 (1%)	75	83
21	LM	178/180 (99%)	177 (99%)	1 (1%)	84	89
22	LN	170/179 (95%)	168 (99%)	2 (1%)	67	76
23	LO	233/242 (96%)	227 (97%)	6 (3%)	41	50
24	LP	163/164 (99%)	162 (99%)	1 (1%)	84	89
25	LQ	171/198 (86%)	170 (99%)	1 (1%)	84	89
26	LR	157/159 (99%)	154 (98%)	3 (2%)	52	62
27	LS	132/134 (98%)	132 (100%)	0	100	100
28	LT	129/143 (90%)	128 (99%)	1 (1%)	79	86
29	LU	93/114 (82%)	92 (99%)	1 (1%)	70	79
30	LV	102/124 (82%)	101 (99%)	1 (1%)	73	80
31	LW	104/122 (85%)	103 (99%)	1 (1%)	73	80
32	LX	74/104 (71%)	73 (99%)	1 (1%)	62	72
33	LY	110/116 (95%)	108 (98%)	2 (2%)	54	64
34	LZ	114/118 (97%)	112 (98%)	2 (2%)	54	64
35	La	114/118 (97%)	111 (97%)	3 (3%)	41	50
36	Lb	56/58 (97%)	53 (95%)	3 (5%)	18	18
37	Lc	191/209 (91%)	191 (100%)	0	100	100
38	Ld	82/89 (92%)	78 (95%)	4 (5%)	21	23
39	Le	154/158 (98%)	151 (98%)	3 (2%)	52	62
40	Lf	111/115 (96%)	111 (100%)	0	100	100
41	Lg	121/121 (100%)	118 (98%)	3 (2%)	42	52
42	Lh	107/146 (73%)	104 (97%)	3 (3%)	38	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Li	82/88 (93%)	81 (99%)	1 (1%)	67	76
44	Lj	67/70 (96%)	67 (100%)	0	100	100
45	Lk	65/74 (88%)	65 (100%)	0	100	100
46	Ll	46/47 (98%)	45 (98%)	1 (2%)	47	56
47	Lm	42/113 (37%)	41 (98%)	1 (2%)	44	53
48	Ln	30/32 (94%)	29 (97%)	1 (3%)	33	41
49	Lo	69/74 (93%)	68 (99%)	1 (1%)	62	72
50	Lp	83/92 (90%)	81 (98%)	2 (2%)	44	53
54	SA	205/222 (92%)	202 (98%)	3 (2%)	60	70
55	SB	179/202 (89%)	177 (99%)	2 (1%)	70	79
56	SC	176/184 (96%)	170 (97%)	6 (3%)	32	40
57	SD	159/164 (97%)	156 (98%)	3 (2%)	52	62
58	SE	216/225 (96%)	214 (99%)	2 (1%)	75	83
59	SF	182/208 (88%)	179 (98%)	3 (2%)	58	69
60	SG	194/208 (93%)	191 (98%)	3 (2%)	60	70
61	SH	152/159 (96%)	152 (100%)	0	100	100
62	SI	181/186 (97%)	180 (99%)	1 (1%)	84	89
63	SJ	110/111 (99%)	109 (99%)	1 (1%)	75	83
64	SK	159/176 (90%)	159 (100%)	0	100	100
65	SL	116/120 (97%)	112 (97%)	4 (3%)	32	40
66	SM	93/104 (89%)	92 (99%)	1 (1%)	70	79
67	SN	95/128 (74%)	92 (97%)	3 (3%)	34	42
68	SO	104/113 (92%)	103 (99%)	1 (1%)	73	80
69	SP	114/117 (97%)	111 (97%)	3 (3%)	41	50
71	SR	120/130 (92%)	114 (95%)	6 (5%)	20	22
72	SS	47/49 (96%)	45 (96%)	2 (4%)	25	28
73	ST	126/132 (96%)	125 (99%)	1 (1%)	79	86
74	SU	136/152 (90%)	134 (98%)	2 (2%)	60	70
75	SV	109/126 (86%)	107 (98%)	2 (2%)	54	64
76	SW	98/130 (75%)	97 (99%)	1 (1%)	73	80
77	SX	122/131 (93%)	120 (98%)	2 (2%)	58	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	SY	73/116 (63%)	69 (94%)	4 (6%)	18	18
79	SZ	111/118 (94%)	107 (96%)	4 (4%)	30	37
80	Sa	71/95 (75%)	70 (99%)	1 (1%)	62	72
81	Sb	85/93 (91%)	82 (96%)	3 (4%)	31	38
82	Sc	70/76 (92%)	69 (99%)	1 (1%)	62	72
83	Sd	52/75 (69%)	52 (100%)	0	100	100
84	Se	44/54 (82%)	43 (98%)	1 (2%)	45	54
85	Sf	26/126 (21%)	25 (96%)	1 (4%)	28	34
86	Sg	255/265 (96%)	248 (97%)	7 (3%)	40	48
87	Sh	104/177 (59%)	100 (96%)	4 (4%)	28	34
All	All	9611/10678 (90%)	9448 (98%)	163 (2%)	56	66

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	LA	208	GLU
10	LB	120	LYS
10	LB	290	ILE
11	LC	13	SER
11	LC	15	ASP
11	LC	109	ARG
11	LC	124	VAL
11	LC	273	LYS
11	LC	285	THR
12	LD	44	GLU
12	LD	71	CYS
12	LD	81	LEU
12	LD	108	ILE
12	LD	122	THR
12	LD	168	VAL
13	LE	16	VAL
13	LE	28	THR
13	LE	81	THR
13	LE	130	LYS
13	LE	134	THR
13	LE	180	VAL
13	LE	182	THR
14	LF	84	VAL

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Mol	Chain	Res	Type
14	LF	167	LYS
15	LG	148	GLN
15	LG	211	THR
16	LH	85	THR
17	LI	68	VAL
18	LJ	124	SER
18	LJ	133	THR
19	LK	4	SER
19	LK	66	SER
19	LK	72	LYS
19	LK	148	LEU
19	LK	156	SER
20	LL	132	LYS
21	LM	117	ASN
22	LN	189	LYS
22	LN	198	LYS
23	LO	66	GLN
23	LO	132	VAL
23	LO	233	SER
23	LO	244	SER
23	LO	273	VAL
23	LO	289	ARG
24	LP	57	SER
25	LQ	183	LYS
26	LR	2	VAL
26	LR	161	THR
26	LR	173	THR
28	LT	11	SER
29	LU	31	SER
30	LV	34	GLN
31	LW	101	VAL
32	LX	28	SER
33	LY	89	MET
33	LY	99	VAL
34	LZ	17	ARG
34	LZ	70	SER
35	La	43	THR
35	La	92	THR
35	La	109	SER
36	Lb	4	SER
36	Lb	13	SER
36	Lb	27	LEU

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Mol	Chain	Res	Type
38	Ld	9	VAL
38	Ld	26	VAL
38	Ld	90	CYS
38	Ld	101	ASP
39	Le	14	GLU
39	Le	77	THR
39	Le	157	THR
41	Lg	38	THR
41	Lg	50	THR
41	Lg	75	VAL
42	Lh	3	CYS
42	Lh	10	ARG
42	Lh	116	LEU
43	Li	5	THR
46	Ll	31	THR
47	Lm	105	VAL
48	Ln	6	ARG
49	Lo	41	PHE
50	Lp	20	HIS
50	Lp	72	LEU
54	SA	40	LYS
54	SA	117	ARG
54	SA	133	ASP
55	SB	195	SER
55	SB	203	ASP
56	SC	39	HIS
56	SC	42	THR
56	SC	54	THR
56	SC	110	SER
56	SC	144	GLN
56	SC	148	SER
57	SD	54	THR
57	SD	60	THR
57	SD	150	SER
58	SE	158	VAL
58	SE	249	GLU
59	SF	210	THR
59	SF	244	ASP
59	SF	248	SER
60	SG	121	ASP
60	SG	129	ASP
60	SG	232	HIS

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Mol	Chain	Res	Type
62	SI	167	SER
63	SJ	16	SER
65	SL	28	THR
65	SL	56	GLU
65	SL	75	VAL
65	SL	106	VAL
66	SM	88	LEU
67	SN	22	VAL
67	SN	36	THR
67	SN	44	VAL
68	SO	45	THR
69	SP	115	ILE
69	SP	119	ARG
69	SP	137	LYS
71	SR	6	ILE
71	SR	9	HIS
71	SR	32	ARG
71	SR	61	THR
71	SR	93	THR
71	SR	100	SER
72	SS	4	LEU
72	SS	9	SER
73	ST	87	ASP
74	SU	67	LYS
74	SU	71	ARG
75	SV	8	THR
75	SV	89	SER
76	SW	112	VAL
77	SX	49	ILE
77	SX	153	ILE
78	SY	32[A]	HIS
78	SY	32[B]	HIS
78	SY	55	THR
78	SY	56	THR
79	SZ	53	LEU
79	SZ	56	VAL
79	SZ	124	LEU
79	SZ	127	LYS
80	Sa	33	ARG
81	Sb	32	THR
81	Sb	88	VAL
81	Sb	97	LYS

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Mol	Chain	Res	Type
82	Sc	3	PHE
84	Se	39	LYS
85	Sf	143	CYS
86	Sg	134	TRP
86	Sg	142	HIS
86	Sg	167	VAL
86	Sg	179	TRP
86	Sg	199	THR
86	Sg	225	THR
86	Sg	285	ILE
87	Sh	80	VAL
87	Sh	165	LEU
87	Sh	187	VAL
87	Sh	212	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
9	LA	38	HIS
9	LA	106	GLN
9	LA	205	ASN
10	LB	11	HIS
10	LB	109	HIS
10	LB	248	HIS
11	LC	40	HIS
11	LC	64	HIS
11	LC	145	ASN
11	LC	158	GLN
11	LC	212	ASN
13	LE	51	ASN
13	LE	108	ASN
13	LE	181	GLN
14	LF	154	GLN
15	LG	78	GLN
15	LG	169	ASN
16	LH	74	GLN
16	LH	187	HIS
17	LI	93	GLN
18	LJ	26	ASN
18	LJ	134	HIS
19	LK	68	ASN
20	LL	112	ASN

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Mol	Chain	Res	Type
22	LN	73	ASN
23	LO	35	GLN
23	LO	90	HIS
25	LQ	34	ASN
25	LQ	143	HIS
25	LQ	176	GLN
26	LR	116	HIS
26	LR	121	HIS
28	LT	111	GLN
30	LV	51	ASN
30	LV	133	HIS
31	LW	83	ASN
33	LY	67	GLN
34	LZ	15	ASN
34	LZ	83	HIS
35	La	114	GLN
36	Lb	9	ASN
37	Lc	82	HIS
37	Lc	84	ASN
37	Lc	184	ASN
39	Le	44	ASN
40	Lf	21	HIS
40	Lf	89	GLN
42	Lh	123	ASN
43	Li	18	HIS
43	Li	26	GLN
43	Li	30	ASN
48	Ln	15	HIS
49	Lo	75	ASN
50	Lp	90	HIS
54	SA	103	HIS
54	SA	228	GLN
56	SC	73	GLN
57	SD	45	ASN
58	SE	240	GLN
59	SF	147	ASN
60	SG	86	ASN
61	SH	74	GLN
62	SI	99	GLN
62	SI	178	GLN
62	SI	196	GLN
63	SJ	9	ASN

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Mol	Chain	Res	Type
63	SJ	56	HIS
63	SJ	120	ASN
65	SL	11	GLN
65	SL	76	HIS
65	SL	138	HIS
67	SN	70	HIS
67	SN	98	GLN
72	SS	38	ASN
73	ST	49	GLN
74	SU	24	GLN
74	SU	32	ASN
74	SU	40	HIS
74	SU	91	HIS
74	SU	104	ASN
74	SU	113	GLN
75	SV	110	GLN
77	SX	34	HIS
77	SX	114	HIS
77	SX	141	HIS
79	SZ	36	HIS
81	Sb	27	ASN
82	Sc	43	GLN
86	Sg	135	ASN
87	Sh	163	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1678/1782 (94%)	320 (19%)	14 (0%)
2	L2	1153/1526 (75%)	207 (17%)	6 (0%)
3	L3	178/216 (82%)	34 (19%)	2 (1%)
4	L4	183/184 (99%)	31 (16%)	1 (0%)
5	L5	118/135 (87%)	24 (20%)	0
51	S1	1831/2204 (83%)	354 (19%)	18 (0%)
52	S2	13/76 (17%)	3 (23%)	1 (7%)
52	S4	65/76 (85%)	24 (36%)	3 (4%)
53	S3	73/77 (94%)	10 (13%)	0
6	L6	69/73 (94%)	22 (31%)	0
7	L7	164/171 (95%)	22 (13%)	3 (1%)
8	L8	119/124 (95%)	11 (9%)	0
88	S5	11/13 (84%)	3 (27%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5655/6657 (84%)	1065 (18%)	48 (0%)

All (1065) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	16	G
1	L1	24	A
1	L1	32	A
1	L1	38	A
1	L1	41	A
1	L1	47	C
1	L1	58	A
1	L1	63	A
1	L1	64	A
1	L1	84	G
1	L1	86	G
1	L1	87	A
1	L1	91	G
1	L1	110	A
1	L1	134	A
1	L1	135	A
1	L1	136	G
1	L1	141	U
1	L1	142	G
1	L1	147	G
1	L1	156	A
1	L1	158	A
1	L1	160	C
1	L1	161	A
1	L1	162	U
1	L1	166	G
1	L1	170	U
1	L1	171	U
1	L1	176	C
1	L1	188	A
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	205	A

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Mol	Chain	Res	Type
1	L1	206	A
1	L1	209	C
1	L1	210	G
1	L1	218	A
1	L1	223	A
1	L1	233	U
1	L1	234	G
1	L1	236	G
1	L1	237	U
1	L1	243	G
1	L1	251	A
1	L1	256	U
1	L1	273	A
1	L1	280	A
1	L1	281	G
1	L1	293	C
1	L1	294	U
1	L1	297	A
1	L1	299	U
1	L1	300	A
1	L1	301	A
1	L1	306	G
1	L1	322	A
1	L1	323	U
1	L1	332	A
1	L1	337	G
1	L1	342	G
1	L1	343	U
1	L1	344	A
1	L1	357	A
1	L1	367	A
1	L1	369	A
1	L1	374	G
1	L1	376	A
1	L1	383	U
1	L1	409	U
1	L1	410	U
1	L1	414	A
1	L1	415	A
1	L1	417	G
1	L1	439	U
1	L1	440	A

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Mol	Chain	Res	Type
1	L1	443	A
1	L1	444	C
1	L1	461	G
1	L1	463	C
1	L1	464	A
1	L1	471	G
1	L1	477	C
1	L1	488	G
1	L1	489	C
1	L1	494	A
1	L1	495	C
1	L1	500	C
1	L1	502	U
1	L1	503	A
1	L1	511	A
1	L1	522	G
1	L1	523	A
1	L1	525	C
1	L1	527	A
1	L1	539	C
1	L1	542	C
1	L1	544	A
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	563	C
1	L1	569	G
1	L1	571	A
1	L1	572	A
1	L1	573	U
1	L1	575	A
1	L1	585	U
1	L1	599	G
1	L1	605	G
1	L1	606	C
1	L1	611	C
1	L1	616	U
1	L1	620	U

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Mol	Chain	Res	Type
1	L1	621	U
1	L1	625	C
1	L1	631	G
1	L1	632	A
1	L1	635	C
1	L1	641	G
1	L1	648	A
1	L1	651	G
1	L1	652	A
1	L1	663	C
1	L1	668	C
1	L1	681	A2M
1	L1	692	A
1	L1	709	A
1	L1	710	G
1	L1	723	G
1	L1	729	A
1	L1	736	C
1	L1	737	U
1	L1	743	A
1	L1	750	G
1	L1	753	A
1	L1	762	A
1	L1	763	U
1	L1	769	U
1	L1	771	U
1	L1	778	C
1	L1	783	G
1	L1	790	C
1	L1	794	U
1	L1	795	U
1	L1	803	C
1	L1	810	C
1	L1	818	C
1	L1	822	C
1	L1	823	G
1	L1	828	U
1	L1	832	G
1	L1	836	G
1	L1	838	G
1	L1	850	G
1	L1	867	A

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Mol	Chain	Res	Type
1	L1	868	A
1	L1	895	G
1	L1	900	C
1	L1	912	C
1	L1	925	U
1	L1	930	U
1	L1	947	A
1	L1	959	OMG
1	L1	965	A
1	L1	967	G
1	L1	968	A
1	L1	972	A
1	L1	974	C
1	L1	975	G
1	L1	976	A
1	L1	988	G
1	L1	995	C
1	L1	1010	OMC
1	L1	1011	PSU
1	L1	1013	A
1	L1	1025	G
1	L1	1031	A
1	L1	1036	U
1	L1	1045	G
1	L1	1052	A
1	L1	1053	A
1	L1	1085	C
1	L1	1094	C
1	L1	1098	A
1	L1	1100	C
1	L1	1101	U
1	L1	1114	A
1	L1	1116	A
1	L1	1122	U
1	L1	1123	G
1	L1	1129	G
1	L1	1148	A
1	L1	1150	A
1	L1	1156	A
1	L1	1159	A
1	L1	1161	A
1	L1	1162	G

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Mol	Chain	Res	Type
1	L1	1165	A
1	L1	1169	A
1	L1	1170	G
1	L1	1171	PSU
1	L1	1172	G
1	L1	1174	G
1	L1	1179	C
1	L1	1188	G
1	L1	1196	G
1	L1	1201	U
1	L1	1202	G
1	L1	1207	A
1	L1	1210	A
1	L1	1217	U
1	L1	1225	U
1	L1	1239	U
1	L1	1240	U
1	L1	1242	U
1	L1	1243	G
1	L1	1248	C
1	L1	1251	U
1	L1	1254	C
1	L1	1258	A
1	L1	1261	U
1	L1	1263	A
1	L1	1270	U
1	L1	1271	G
1	L1	1274	G
1	L1	1286	C
1	L1	1287	A
1	L1	1294	C
1	L1	1342	C
1	L1	1346	C
1	L1	1348	A
1	L1	1349	A
1	L1	1350	U
1	L1	1364	A
1	L1	1367	U
1	L1	1369	G
1	L1	1371	OMU
1	L1	1378	U
1	L1	1379	A

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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	1413	U
1	L1	1420	G
1	L1	1421	G
1	L1	1422	A
1	L1	1426	A
1	L1	1438	A
1	L1	1440	G
1	L1	1444	A
1	L1	1445	G
1	L1	1455	U
1	L1	1464	G
1	L1	1480	C
1	L1	1481	G
1	L1	1489	U
1	L1	1490	G
1	L1	1504	A
1	L1	1505	U
1	L1	1509	C
1	L1	1519	G
1	L1	1524	OMG
1	L1	1525	A
1	L1	1526	U
1	L1	1527	OMC
1	L1	1536	C
1	L1	1540	OMG
1	L1	1545	G
1	L1	1547	U
1	L1	1557	A
1	L1	1560	U
1	L1	1566	A
1	L1	1569	U
1	L1	1574	C
1	L1	1575	G
1	L1	1582	A
1	L1	1586	G

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Mol	Chain	Res	Type
1	L1	1590	G
1	L1	1612	G
1	L1	1613	C
1	L1	1627	U
1	L1	1639	U
1	L1	1654	A
1	L1	1661	U
1	L1	1662	G
1	L1	1663	U
1	L1	1666	G
1	L1	1667	G
1	L1	1671	G
1	L1	1672	U
1	L1	1676	G
1	L1	1677	G
1	L1	1683	C
1	L1	1715	U
1	L1	1716	G
1	L1	1717	G
1	L1	1723	A
1	L1	1726	G
1	L1	1734	G
1	L1	1739	A
1	L1	1744	A
1	L1	1747	U
1	L1	1756	A
1	L1	1757	U
1	L1	1758	U
1	L1	1766	G
1	L1	1771	U
1	L1	1774	A
2	L2	5	A
2	L2	7	C
2	L2	13	A
2	L2	22	A
2	L2	25	A
2	L2	30	A
2	L2	49	A
2	L2	61	C
2	L2	62	A
2	L2	63	U
2	L2	68	A

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Mol	Chain	Res	Type
2	L2	69	A
2	L2	75	C
2	L2	90	G
2	L2	98	G
2	L2	137	A
2	L2	336	C
2	L2	338	C
2	L2	339	A
2	L2	340	A
2	L2	341	A
2	L2	342	U
2	L2	343	U
2	L2	361	U
2	L2	364	G
2	L2	368	G
2	L2	377	A
2	L2	386	U
2	L2	388	A
2	L2	390	A
2	L2	395	A
2	L2	404	A
2	L2	434	A
2	L2	451	U
2	L2	453	A
2	L2	454	A
2	L2	490	A
2	L2	495	G
2	L2	502	A2M
2	L2	514	U
2	L2	518	G
2	L2	519	G
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

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Mol	Chain	Res	Type
2	L2	561	G
2	L2	571	G
2	L2	580	U
2	L2	582	U
2	L2	616	G
2	L2	619	A
2	L2	620	C
2	L2	621	G
2	L2	639	G
2	L2	640	G
2	L2	643	A
2	L2	647	A
2	L2	648	A
2	L2	649	G
2	L2	650	A
2	L2	657	U
2	L2	658	G
2	L2	664	G
2	L2	665	A2M
2	L2	681	G
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
2	L2	750	U
2	L2	751	U
2	L2	752	G
2	L2	760	U
2	L2	761	A
2	L2	769	A
2	L2	777	A
2	L2	778	A
2	L2	780	G
2	L2	782	G
2	L2	783	U
2	L2	785	U
2	L2	787	G
2	L2	789	G

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Mol	Chain	Res	Type
2	L2	799	G
2	L2	808	C
2	L2	810	G
2	L2	819	U
2	L2	823	A
2	L2	824	G
2	L2	851	C
2	L2	954	A
2	L2	970	A
2	L2	971	A
2	L2	972	C
2	L2	1001	C
2	L2	1010	U
2	L2	1011	G
2	L2	1012	U
2	L2	1019	A
2	L2	1021	A
2	L2	1022	U
2	L2	1025	G
2	L2	1033	G
2	L2	1034	G
2	L2	1041	G
2	L2	1046	OMG
2	L2	1053	A
2	L2	1055	A
2	L2	1064	A
2	L2	1075	G
2	L2	1079	U
2	L2	1083	A
2	L2	1096	U
2	L2	1101	A
2	L2	1104	G
2	L2	1108	U
2	L2	1115	U
2	L2	1116	A
2	L2	1118	A
2	L2	1121	A
2	L2	1123	A
2	L2	1129	A
2	L2	1137	G
2	L2	1141	G
2	L2	1147	C

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Mol	Chain	Res	Type
2	L2	1148	G
2	L2	1156	G
2	L2	1157	U
2	L2	1162	A
2	L2	1176	A
2	L2	1177	G
2	L2	1179	A
2	L2	1180	A
2	L2	1181	G
2	L2	1183	C
2	L2	1189	A
2	L2	1199	A
2	L2	1204	U
2	L2	1206	G
2	L2	1207	G
2	L2	1209	A
2	L2	1215	A
2	L2	1216	A
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	1241	U
2	L2	1246	A
2	L2	1248	OMC
2	L2	1252	G
2	L2	1255	A
2	L2	1264	PSU
2	L2	1283	A
2	L2	1288	G
2	L2	1289	A
2	L2	1299	U
2	L2	1309	G
2	L2	1325	A
2	L2	1337	C
2	L2	1361	PSU
2	L2	1373	C
2	L2	1374	A
2	L2	1379	A
2	L2	1380	C

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Mol	Chain	Res	Type
2	L2	1385	G
2	L2	1409	A
2	L2	1416	U
2	L2	1421	C
2	L2	1428	U
2	L2	1433	G
2	L2	1437	A
2	L2	1441	C
2	L2	1443	A
2	L2	1444	G
2	L2	1445	A
2	L2	1448	A
2	L2	1450	G
2	L2	1453	U
2	L2	1454	A
2	L2	1462	A
2	L2	1463	A
2	L2	1465	G
2	L2	1483	U
2	L2	1485	G
2	L2	1486	G
2	L2	1496	G
2	L2	1498	G
2	L2	1506	G
2	L2	1510	A
2	L2	1511	U
2	L2	1512	G
2	L2	1513	G
3	L3	6	G
3	L3	16	G
3	L3	19	A
3	L3	20	C
3	L3	21	A
3	L3	22	C
3	L3	24	U
3	L3	25	G
3	L3	34	C
3	L3	35	A
3	L3	41	A
3	L3	49	A
3	L3	70	A
3	L3	111	A

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Mol	Chain	Res	Type
3	L3	112	C
3	L3	113	U
3	L3	114	U
3	L3	124	U
3	L3	125	U
3	L3	132	G
3	L3	142	G
3	L3	146	G
3	L3	149	A
3	L3	150	A
3	L3	151	A
3	L3	169	A
3	L3	174	C
3	L3	175	A
3	L3	182	U
3	L3	187	U
3	L3	192	G
3	L3	196	U
3	L3	199	A
3	L3	202	A
4	L4	8	U
4	L4	9	G
4	L4	10	U
4	L4	20	U
4	L4	24	A
4	L4	40	G
4	L4	50	G
4	L4	60	A
4	L4	61	A
4	L4	83	U
4	L4	85	C
4	L4	86	U
4	L4	87	G
4	L4	89	G
4	L4	102	G
4	L4	106	G
4	L4	114	A
4	L4	120	U
4	L4	121	C
4	L4	128	U
4	L4	133	C
4	L4	144	G

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Mol	Chain	Res	Type
4	L4	148	C
4	L4	150	A
4	L4	153	C
4	L4	158	A
4	L4	159	G
4	L4	168	A
4	L4	171	A
4	L4	173	C
4	L4	180	C
5	L5	3	U
5	L5	4	A
5	L5	15	C
5	L5	24	G
5	L5	29	U
5	L5	50	C
5	L5	51	A
5	L5	52	U
5	L5	62	C
5	L5	65	U
5	L5	68	G
5	L5	86	G
5	L5	87	U
5	L5	88	C
5	L5	92	A
5	L5	99	G
5	L5	105	U
5	L5	106	G
5	L5	109	G
5	L5	113	G
5	L5	117	A
5	L5	118	U
5	L5	120	C
5	L5	135	U
6	L6	7	A
6	L6	14	A
6	L6	15	C
6	L6	22	G
6	L6	25	U
6	L6	26	G
6	L6	31	U
6	L6	33	G
6	L6	41	G

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Mol	Chain	Res	Type
6	L6	42	A
6	L6	43	A
6	L6	52	G
6	L6	54	A
6	L6	55	U
6	L6	56	A
6	L6	64	U
6	L6	67	C
6	L6	68	A
6	L6	70	G
6	L6	71	A
6	L6	72	C
6	L6	73	A
7	L7	16	A
7	L7	33	U
7	L7	59	A
7	L7	62	A
7	L7	63	G
7	L7	72	A
7	L7	80	A
7	L7	81	U
7	L7	82	C
7	L7	84	U
7	L7	94	G
7	L7	101	OMU
7	L7	102	G
7	L7	103	A
7	L7	105	C
7	L7	110	A
7	L7	120	G
7	L7	124	A
7	L7	125	A
7	L7	127	C
7	L7	157	U
7	L7	158	U
8	L8	11	G
8	L8	26	A
8	L8	37	U
8	L8	52	G
8	L8	57	U
8	L8	58	A
8	L8	63	C

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Mol	Chain	Res	Type
8	L8	68	A
8	L8	95	U
8	L8	104	A
8	L8	114	G
51	S1	3	U
51	S1	26	A
51	S1	34	G
51	S1	42	G
51	S1	45	U
51	S1	47	A
51	S1	66	U
51	S1	68	A
51	S1	85	C
51	S1	102	A
51	S1	109	C
51	S1	112	A
51	S1	114	U
51	S1	117	G
51	S1	124	A
51	S1	129	U
51	S1	145	A
51	S1	146	U
51	S1	147	U
51	S1	149	G
51	S1	158	G
51	S1	164	C
51	S1	165	G
51	S1	167	C
51	S1	173	A
51	S1	174	A
51	S1	175	U
51	S1	181	A
51	S1	194	U
51	S1	195	U
51	S1	227	U
51	S1	228	G
51	S1	249	A
51	S1	252	G
51	S1	253	U
51	S1	255	A
51	S1	257	A
51	S1	264	C

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Mol	Chain	Res	Type
51	S1	265	C
51	S1	266	U
51	S1	275	A
51	S1	276	G
51	S1	277	U
51	S1	278	A
51	S1	281	A
51	S1	287	C
51	S1	288	A
51	S1	295	A
51	S1	309	G
51	S1	313	G
51	S1	316	A
51	S1	322	C
51	S1	326	U
51	S1	329	C
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	396	G
51	S1	404	C
51	S1	413	A
51	S1	423	U
51	S1	433	G
51	S1	443	A
51	S1	444	A
51	S1	445	U
51	S1	446	A
51	S1	447	G
51	S1	455	PSU
51	S1	460	C
51	S1	464	G
51	S1	467	C
51	S1	469	G
51	S1	477	G
51	S1	481	A
51	S1	482	U
51	S1	487	C

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Mol	Chain	Res	Type
51	S1	488	A
51	S1	497	A
51	S1	508	A
51	S1	523	A
51	S1	525	A
51	S1	548	G
51	S1	551	A
51	S1	552	U
51	S1	565	U
51	S1	575	C
51	S1	580	A
51	S1	581	A
51	S1	584	U
51	S1	585	C
51	S1	588	G
51	S1	589	U
51	S1	590	A
51	S1	591	A
51	S1	592	C
51	S1	593	A
51	S1	594	A
51	S1	600	OMG
51	S1	604	A
51	S1	606	G
51	S1	608	C
51	S1	609	PSU
51	S1	610	G
51	S1	614	C
51	S1	617	G
51	S1	626	G
51	S1	628	A
51	S1	631	U
51	S1	643	A
51	S1	660	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	687	U
51	S1	688	G

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Mol	Chain	Res	Type
51	S1	690	G
51	S1	698	C
51	S1	699	A
51	S1	744	G
51	S1	749	U
51	S1	755	C
51	S1	757	C
51	S1	758	G
51	S1	762	A
51	S1	774	A
51	S1	775	C
51	S1	776	A
51	S1	778	G
51	S1	779	A
51	S1	782	C
51	S1	786	G
51	S1	788	A
51	S1	789	G
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	817	A
51	S1	818	U
51	S1	819	G
51	S1	825	C
51	S1	826	A
51	S1	830	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	872	A
51	S1	880	U
51	S1	883	G
51	S1	886	U
51	S1	887	U
51	S1	890	A

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Mol	Chain	Res	Type
51	S1	892	U
51	S1	914	G
51	S1	919	G
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	951	U
51	S1	954	A
51	S1	956	A
51	S1	959	U
51	S1	967	A
51	S1	970	U
51	S1	972	A
51	S1	1101	A
51	S1	1102	G
51	S1	1105	A
51	S1	1109	A
51	S1	1119	U
51	S1	1123	G
51	S1	1133	U
51	S1	1139	G
51	S1	1180	A
51	S1	1181	C
51	S1	1182	A
51	S1	1191	A
51	S1	1207	U
51	S1	1210	C
51	S1	1213	A
51	S1	1217	A
51	S1	1232	G
51	S1	1235	A
51	S1	1239	A
51	S1	1251	A
51	S1	1252	A
51	S1	1271	C
51	S1	1272	A

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Mol	Chain	Res	Type
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	1366	A
51	S1	1371	U
51	S1	1398	C
51	S1	1399	G
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	1490	A
51	S1	1502	G
51	S1	1510	C
51	S1	1516	G
51	S1	1537	U
51	S1	1543	B8N
51	S1	1546	A
51	S1	1548	A
51	S1	1551	G
51	S1	1552	G
51	S1	1554	A
51	S1	1555	A
51	S1	1559	U
51	S1	1560	A
51	S1	1564	G
51	S1	1569	G
51	S1	1570	G
51	S1	1580	G
51	S1	1581	G
51	S1	1591	U
51	S1	1595	G
51	S1	1597	G
51	S1	1603	U
51	S1	1604	C
51	S1	1608	A
51	S1	1609	U

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Mol	Chain	Res	Type
51	S1	1611	C
51	S1	1612	C
51	S1	1613	C
51	S1	1614	U
51	S1	1622	G
51	S1	1637	A
51	S1	1638	U
51	S1	1653	U
51	S1	1658	U
51	S1	1659	U
51	S1	1666	U
51	S1	1667	U
51	S1	1673	A
51	S1	1677	G
51	S1	1699	A
51	S1	1706	A
51	S1	1712	G
51	S1	1713	C
51	S1	1715	C
51	S1	1720	G
51	S1	1723	A
51	S1	1725	C
51	S1	1762	A
51	S1	1766	G
51	S1	1768	U
51	S1	1769	C
51	S1	1770	G
51	S1	1773	U
51	S1	1784	G
51	S1	1788	U
51	S1	1789	U
51	S1	1790	C
51	S1	1794	U
51	S1	1795	G
51	S1	1799	U
51	S1	1800	U
51	S1	1806	A
51	S1	1814	U
51	S1	1816	U
51	S1	1823	A
51	S1	1826	G
51	S1	1828	A

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Mol	Chain	Res	Type
51	S1	1829	OMG
51	S1	1833	OMU
51	S1	1836	G
51	S1	1839	G
51	S1	1846	A
51	S1	1847	A
51	S1	1860	C
51	S1	1872	A
51	S1	1874	U
51	S1	1884	A
51	S1	1887	A
51	S1	1889	G
51	S1	1890	A
51	S1	1891	A
51	S1	1893	A
51	S1	1896	G
51	S1	1898	C
51	S1	1904	U
51	S1	1906	G
51	S1	1907	A
51	S1	1916	G
51	S1	1917	A
51	S1	1918	U
51	S1	1923	A
51	S1	1933	A
51	S1	1938	C
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	2003	C
51	S1	2004	G
51	S1	2010	G
51	S1	2015	U
51	S1	2021	A2M

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Mol	Chain	Res	Type
51	S1	2031	A
51	S1	2097	C
51	S1	2101	C
51	S1	2118	G
51	S1	2119	C
51	S1	2120	C
51	S1	2121	C
51	S1	2134	A
51	S1	2158	A
51	S1	2163	G
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	34	G
52	S2	35	A
52	S2	76	A
53	S3	10	G
53	S3	16	C
53	S3	18	U
53	S3	23	G
53	S3	47	A
53	S3	48	U
53	S3	49	C
53	S3	50	G
53	S3	75	C
53	S3	77	A
52	S4	4	C
52	S4	8	U
52	S4	14	A
52	S4	15	G
52	S4	24	G
52	S4	25	A
52	S4	26	U

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Mol	Chain	Res	Type
52	S4	27	U
52	S4	29	A
52	S4	30	A
52	S4	36	G
52	S4	37	U
52	S4	38	G
52	S4	41	C
52	S4	43	U
52	S4	46	U
52	S4	47	U
52	S4	48	C
52	S4	49	G
52	S4	51	U
52	S4	53	C
52	S4	57	G
52	S4	62	C
52	S4	68	A
88	S5	4	C
88	S5	8	U
88	S5	9	U

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	157	U
1	L1	170	U
1	L1	208	C
1	L1	510	U
1	L1	574	G
1	L1	584	U
1	L1	835	G
1	L1	967	G
1	L1	1390	G
1	L1	1479	A
1	L1	1524	OMG
1	L1	1565	A
1	L1	1574	C
1	L1	1662	G
2	L2	748	C
2	L2	784	U
2	L2	786	A
2	L2	1052	C

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Mol	Chain	Res	Type
2	L2	1136	U
2	L2	1512	G
3	L3	173	U
3	L3	174	C
4	L4	149	U
7	L7	71	A
7	L7	83	A
7	L7	93	C
51	S1	128	C
51	S1	276	G
51	S1	294	G
51	S1	328	C
51	S1	550	C
51	S1	743	A
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	1799	U
51	S1	1889	G
51	S1	1915	U
51	S1	2119	C
52	S2	34	G
52	S4	13	C
52	S4	35	C
52	S4	37	U

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

175 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	B8N	S1	1543	51	24,29,30	3.15	8 (33%)	29,42,45	1.71	5 (17%)
2	PSU	L2	662	90,2	18,21,22	4.61	8 (44%)	22,30,33	1.88	5 (22%)
1	PSU	L1	940	1	18,21,22	4.55	7 (38%)	22,30,33	1.77	5 (22%)
51	OMG	S1	600	51	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
2	PSU	L2	1194	2	18,21,22	4.55	7 (38%)	22,30,33	1.77	5 (22%)
2	PSU	L2	1264	2	18,21,22	4.65	9 (50%)	22,30,33	1.79	4 (18%)
51	PSU	S1	2048	51	18,21,22	4.54	7 (38%)	22,30,33	1.79	5 (22%)
2	PSU	L2	1144	2	18,21,22	4.54	7 (38%)	22,30,33	1.80	5 (22%)
1	PSU	L1	774	1	18,21,22	4.56	7 (38%)	22,30,33	1.82	5 (22%)
1	1MA	L1	677	1,90	16,25,26	3.92	4 (25%)	18,37,40	1.40	3 (16%)
51	PSU	S1	1246	51	18,21,22	4.55	7 (38%)	22,30,33	1.81	5 (22%)
7	OMU	L7	101	7	19,22,23	4.57	14 (73%)	26,31,34	1.96	6 (23%)
51	OMG	S1	1829	51,90	18,26,27	2.41	8 (44%)	19,38,41	1.19	3 (15%)
51	OMU	S1	29	51	19,22,23	3.04	8 (42%)	26,31,34	1.70	5 (19%)
7	A2M	L7	43	7	18,25,26	4.28	7 (38%)	18,36,39	2.65	3 (16%)
2	PSU	L2	506	2	18,21,22	4.56	7 (38%)	22,30,33	1.78	5 (22%)
51	A2M	S1	2021	51	18,25,26	4.24	7 (38%)	18,36,39	2.71	4 (22%)
2	A2M	L2	572	2	18,25,26	4.24	7 (38%)	18,36,39	2.67	3 (16%)
1	OMU	L1	1253	1	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)
1	A2M	L1	681	1	18,25,26	4.26	7 (38%)	18,36,39	2.59	3 (16%)
2	OMU	L2	667	2	19,22,23	3.05	8 (42%)	26,31,34	1.71	4 (15%)
51	PSU	S1	1292	51,90	18,21,22	4.55	7 (38%)	22,30,33	1.75	5 (22%)
2	PSU	L2	1060	2	18,21,22	4.53	7 (38%)	22,30,33	1.83	5 (22%)
1	A2M	L1	1539	1,2,90	18,25,26	4.33	7 (38%)	18,36,39	2.59	3 (16%)
2	OMG	L2	641	2	18,26,27	2.42	8 (44%)	19,38,41	1.27	3 (15%)
52	MIA	S2	37	52	24,31,32	2.44	3 (12%)	26,44,47	4.98	9 (34%)
2	A2M	L2	1384	90,2	18,25,26	4.33	7 (38%)	18,36,39	2.44	3 (16%)
2	A2M	L2	502	90,2	18,25,26	4.26	7 (38%)	18,36,39	2.65	3 (16%)
2	PSU	L2	500	2	18,21,22	4.56	7 (38%)	22,30,33	1.83	5 (22%)
51	OMU	S1	1621	51,90	19,22,23	3.04	8 (42%)	26,31,34	1.69	5 (19%)
2	OMU	L2	73	2	19,22,23	3.02	8 (42%)	26,31,34	1.64	4 (15%)
1	PSU	L1	422	1	18,21,22	4.56	7 (38%)	22,30,33	1.79	5 (22%)
2	PSU	L2	1413	2	18,21,22	4.66	7 (38%)	22,30,33	1.89	5 (22%)
2	A2M	L2	604	1,2	18,25,26	4.26	7 (38%)	18,36,39	2.64	3 (16%)
2	OMG	L2	1360	2,52	18,26,27	2.58	8 (44%)	19,38,41	1.48	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMC	L2	1159	2	19,22,23	3.05	8 (42%)	26,31,34	0.75	0
51	OMU	S1	1662	51	19,22,23	3.06	8 (42%)	26,31,34	1.68	4 (15%)
2	OMG	L2	1046	2,53	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
2	OMG	L2	1231	2	18,26,27	2.56	8 (44%)	19,38,41	1.51	5 (26%)
51	OMC	S1	2059	51,90	19,22,23	3.05	8 (42%)	26,31,34	0.76	0
1	PSU	L1	1011	1,2	18,21,22	4.61	7 (38%)	22,30,33	1.63	4 (18%)
1	PSU	L1	1533	1,2	18,21,22	4.54	7 (38%)	22,30,33	1.77	5 (22%)
1	OMU	L1	1107	1	19,22,23	3.01	8 (42%)	26,31,34	1.76	5 (19%)
2	PSU	L2	593	2	18,21,22	4.56	7 (38%)	22,30,33	1.77	5 (22%)
3	OMU	L3	13	3	19,22,23	3.03	8 (42%)	26,31,34	1.70	5 (19%)
2	OMU	L2	56	1,2	19,22,23	3.05	8 (42%)	26,31,34	1.71	5 (19%)
7	OMG	L7	75	7	18,26,27	2.60	8 (44%)	19,38,41	1.52	4 (21%)
2	A2M	L2	1372	2	18,25,26	4.23	7 (38%)	18,36,39	2.70	3 (16%)
1	OMC	L1	695	1	19,22,23	3.05	8 (42%)	26,31,34	0.70	0
2	OMC	L2	1397	2	19,22,23	3.06	8 (42%)	26,31,34	0.74	0
51	OMG	S1	1550	51	18,26,27	2.42	8 (44%)	19,38,41	1.18	3 (15%)
2	PSU	L2	597	2	18,21,22	4.55	7 (38%)	22,30,33	1.83	5 (22%)
2	OMU	L2	1419	2	19,22,23	3.04	8 (42%)	26,31,34	1.65	4 (15%)
51	OMU	S1	1777	51	19,22,23	3.06	8 (42%)	26,31,34	1.68	4 (15%)
51	OMU	S1	661	51	19,22,23	3.11	8 (42%)	26,31,34	1.70	4 (15%)
2	PSU	L2	512	2	18,21,22	4.54	7 (38%)	22,30,33	1.78	5 (22%)
51	OMC	S1	38	51	19,22,23	3.05	8 (42%)	26,31,34	0.72	0
51	A2M	S1	668	51,90	18,25,26	4.14	6 (33%)	18,36,39	2.69	4 (22%)
51	PSU	S1	1539	51	18,21,22	4.66	7 (38%)	22,30,33	1.85	5 (22%)
1	A2M	L1	858	1	18,25,26	4.33	7 (38%)	18,36,39	2.67	3 (16%)
2	PSU	L2	1058	2	18,21,22	4.63	7 (38%)	22,30,33	1.93	5 (22%)
2	PSU	L2	1265	90,2	18,21,22	4.50	8 (44%)	22,30,33	1.69	5 (22%)
1	OMU	L1	1371	1	19,22,23	3.04	8 (42%)	26,31,34	1.67	4 (15%)
2	PSU	L2	1403	2	18,21,22	4.65	7 (38%)	22,30,33	1.79	6 (27%)
1	A2M	L1	305	1	18,25,26	4.17	7 (38%)	18,36,39	2.67	3 (16%)
1	OMU	L1	845	1	19,22,23	3.04	8 (42%)	26,31,34	1.67	4 (15%)
1	OMC	L1	1552	1	19,22,23	3.04	8 (42%)	26,31,34	0.75	0
51	PSU	S1	455	51	18,21,22	4.56	7 (38%)	22,30,33	1.73	5 (22%)
51	5MC	S1	1544	51	18,22,23	3.60	7 (38%)	26,32,35	1.01	1 (3%)
1	OMG	L1	1540	1,2	18,26,27	2.44	8 (44%)	19,38,41	1.18	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	5MC	S1	2061	51	18,22,23	3.59	7 (38%)	26,32,35	0.94	1 (3%)
1	OMU	L1	1659	1,90	19,22,23	3.05	8 (42%)	26,31,34	1.67	5 (19%)
2	OMC	L2	14	1,2	19,22,23	3.05	8 (42%)	26,31,34	0.72	0
1	PSU	L1	1171	1,91,92	18,21,22	4.62	8 (44%)	22,30,33	1.90	5 (22%)
51	PSU	S1	12	51	18,21,22	4.55	7 (38%)	22,30,33	1.80	5 (22%)
1	OMG	L1	1524	1	18,26,27	2.40	8 (44%)	19,38,41	1.17	3 (15%)
2	OMU	L2	1077	2	19,22,23	3.08	8 (42%)	26,31,34	1.68	4 (15%)
51	OMC	S1	2019	51	19,22,23	3.05	8 (42%)	26,31,34	0.71	0
1	PSU	L1	1093	1	18,21,22	4.56	7 (38%)	22,30,33	1.77	5 (22%)
2	PSU	L2	1213	2	18,21,22	4.56	7 (38%)	22,30,33	1.81	5 (22%)
2	PSU	L2	1303	2	18,21,22	4.57	7 (38%)	22,30,33	1.84	6 (27%)
2	OMC	L2	1317	2	19,22,23	3.03	8 (42%)	26,31,34	0.66	0
51	OMC	S1	2140	51	19,22,23	3.06	8 (42%)	26,31,34	0.73	0
2	5MC	L2	1308	90,2	18,21,23	4.62	12 (66%)	25,30,35	1.39	3 (12%)
51	PSU	S1	33	51	18,21,22	4.57	7 (38%)	22,30,33	1.79	5 (22%)
51	PSU	S1	2046	51	18,21,22	4.56	7 (38%)	22,30,33	1.82	5 (22%)
51	OMG	S1	1865	91,51	18,26,27	2.61	8 (44%)	19,38,41	1.53	4 (21%)
2	5MC	L2	524	90,2	18,22,23	3.57	7 (38%)	26,32,35	1.04	2 (7%)
1	A2M	L1	955	1	18,25,26	4.25	7 (38%)	18,36,39	2.74	3 (16%)
2	OMG	L2	1078	2	18,26,27	2.56	8 (44%)	19,38,41	1.68	5 (26%)
51	A2M	S1	28	51,90	18,25,26	4.28	7 (38%)	18,36,39	2.63	3 (16%)
51	A2M	S1	512	51,90	18,25,26	4.24	8 (44%)	18,36,39	2.69	3 (16%)
51	A2M	S1	969	51	18,25,26	4.20	6 (33%)	18,36,39	2.86	4 (22%)
51	OMC	S1	1866	51	19,22,23	3.05	8 (42%)	26,31,34	0.75	0
2	PSU	L2	1361	2,52	18,21,22	4.54	7 (38%)	22,30,33	1.88	5 (22%)
51	OMC	S1	18	51	19,22,23	3.02	8 (42%)	26,31,34	0.68	0
1	A2M	L1	69	1	18,25,26	4.13	6 (33%)	18,36,39	2.69	3 (16%)
2	PSU	L2	626	2	18,21,22	4.55	7 (38%)	22,30,33	1.83	5 (22%)
1	A2M	L1	697	1	18,25,26	4.26	7 (38%)	18,36,39	2.66	3 (16%)
1	A2M	L1	678	1,2	18,25,26	4.22	7 (38%)	18,36,39	2.64	3 (16%)
51	PSU	S1	1192	51	18,21,22	4.56	7 (38%)	22,30,33	1.65	4 (18%)
51	OMG	S1	1647	51	18,26,27	2.62	8 (44%)	19,38,41	1.58	4 (21%)
2	A2M	L2	665	2	18,25,26	4.27	7 (38%)	18,36,39	2.68	3 (16%)
1	A2M	L1	927	1,90	18,25,26	4.34	8 (44%)	18,36,39	2.47	3 (16%)
51	PSU	S1	1566	51	18,21,22	4.57	7 (38%)	22,30,33	1.74	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMC	L2	1248	2	19,22,23	3.06	8 (42%)	26,31,34	0.71	0
51	PSU	S1	609	51	18,21,22	4.56	7 (38%)	22,30,33	1.79	5 (22%)
51	OMG	S1	2151	51	18,26,27	2.59	8 (44%)	19,38,41	1.56	3 (15%)
7	A2M	L7	162	7,1	18,25,26	4.24	7 (38%)	18,36,39	2.69	3 (16%)
51	A2M	S1	479	51	18,25,26	4.25	7 (38%)	18,36,39	2.67	3 (16%)
2	OMG	L2	1229	2	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
2	PSU	L2	510	2	18,21,22	4.57	7 (38%)	22,30,33	1.76	5 (22%)
51	OMG	S1	1623	51	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)
2	OMG	L2	534	2	18,26,27	2.57	8 (44%)	19,38,41	1.50	4 (21%)
51	OMG	S1	2008	51	18,26,27	2.60	8 (44%)	19,38,41	1.61	4 (21%)
51	PSU	S1	1533	51	18,21,22	4.56	7 (38%)	22,30,33	1.78	5 (22%)
2	A2M	L2	1067	2	18,25,26	4.26	7 (38%)	18,36,39	2.62	3 (16%)
2	PSU	L2	504	2	18,21,22	4.56	7 (38%)	22,30,33	1.81	6 (27%)
2	A2M	L2	382	2	18,25,26	4.36	8 (44%)	18,36,39	2.47	3 (16%)
51	OMG	S1	1478	51	18,26,27	2.57	8 (44%)	19,38,41	1.54	5 (26%)
2	PSU	L2	1382	90,2,92	18,21,22	4.64	7 (38%)	22,30,33	1.90	6 (27%)
51	PSU	S1	1841	51	18,21,22	4.56	7 (38%)	22,30,33	1.83	5 (22%)
1	OMU	L1	1039	1	19,22,23	3.07	8 (42%)	26,31,34	1.70	4 (15%)
2	PSU	L2	78	2	18,21,22	4.56	7 (38%)	22,30,33	1.75	5 (22%)
1	OMC	L1	1527	1	19,22,23	3.08	8 (42%)	26,31,34	0.78	1 (3%)
1	PSU	L1	239	1	18,21,22	4.55	7 (38%)	22,30,33	1.77	5 (22%)
51	MA6	S1	2185	51	18,26,27	1.04	2 (11%)	19,38,41	4.02	2 (10%)
51	7MG	S1	1995	51,53	22,26,27	4.33	10 (45%)	29,39,42	2.05	9 (31%)
2	A2M	L2	1185	2	18,25,26	4.38	8 (44%)	18,36,39	2.68	3 (16%)
1	OMG	L1	1190	1	18,26,27	2.60	8 (44%)	19,38,41	1.64	6 (31%)
2	OMC	L2	359	2	19,22,23	3.07	8 (42%)	26,31,34	0.68	0
51	PSU	S1	1156	51	18,21,22	4.56	7 (38%)	22,30,33	1.78	5 (22%)
2	OMC	L2	583	2	19,22,23	3.05	8 (42%)	26,31,34	0.74	0
2	OMU	L2	1359	90,2	19,22,23	3.05	8 (42%)	26,31,34	1.69	5 (19%)
2	PSU	L2	1284	2	18,21,22	4.56	7 (38%)	22,30,33	1.77	5 (22%)
2	OMC	L2	443	91,2	19,22,23	3.01	8 (42%)	26,31,34	0.63	0
1	OMG	L1	1626	1,92	18,26,27	2.41	8 (44%)	19,38,41	1.16	3 (15%)
51	A2M	S1	98	51,90	18,25,26	4.26	7 (38%)	18,36,39	2.58	3 (16%)
51	OMU	S1	1833	51	19,22,23	3.06	8 (42%)	26,31,34	1.74	4 (15%)
51	PSU	S1	104	51	18,21,22	4.55	7 (38%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	L2	686	2	18,26,27	2.61	8 (44%)	19,38,41	1.54	4 (21%)
1	OMC	L1	669	1	19,22,23	2.97	8 (42%)	26,31,34	0.59	0
1	PSU	L1	1664	1	18,21,22	4.55	8 (44%)	22,30,33	1.72	5 (22%)
1	A2M	L1	1373	1	18,25,26	4.26	7 (38%)	18,36,39	2.65	3 (16%)
51	OMU	S1	1979	51	19,22,23	3.05	8 (42%)	26,31,34	1.68	4 (15%)
1	A2M	L1	235	1	18,25,26	4.26	7 (38%)	18,36,39	2.65	3 (16%)
1	PSU	L1	672	1,90	18,21,22	4.63	7 (38%)	22,30,33	1.87	4 (18%)
51	MA6	S1	2184	51	18,26,27	1.04	2 (11%)	19,38,41	3.90	2 (10%)
2	OMG	L2	655	2,92	18,26,27	2.59	8 (44%)	19,38,41	1.56	3 (15%)
2	A2M	L2	591	2	18,25,26	4.24	7 (38%)	18,36,39	2.62	3 (16%)
2	OMG	L2	1253	2	18,26,27	2.43	8 (44%)	19,38,41	1.19	3 (15%)
4	OMG	L4	74	4	18,26,27	2.58	8 (44%)	19,38,41	1.53	5 (26%)
2	PSU	L2	437	2,92	18,21,22	4.56	7 (38%)	22,30,33	1.77	5 (22%)
2	A2M	L2	628	2	18,25,26	4.26	7 (38%)	18,36,39	2.68	3 (16%)
51	OMU	S1	8	51	19,22,23	3.04	8 (42%)	26,31,34	1.74	5 (19%)
2	A2M	L2	95	2	18,25,26	4.26	7 (38%)	18,36,39	2.67	3 (16%)
1	OMU	L1	48	1	19,22,23	3.03	8 (42%)	26,31,34	1.67	5 (19%)
1	OMU	L1	847	1	19,22,23	3.05	8 (42%)	26,31,34	1.68	4 (15%)
7	PSU	L7	74	7	18,21,22	4.56	7 (38%)	22,30,33	1.83	5 (22%)
1	OMG	L1	856	1	18,26,27	2.39	8 (44%)	19,38,41	1.19	3 (15%)
51	PSU	S1	2202	51	18,21,22	4.55	8 (44%)	22,30,33	1.71	5 (22%)
1	OMC	L1	1010	1,90	19,22,23	3.07	8 (42%)	26,31,34	0.75	0
2	OMG	L2	71	2	18,26,27	2.43	8 (44%)	19,38,41	1.24	3 (15%)
7	PSU	L7	69	7,90	18,21,22	4.61	7 (38%)	22,30,33	1.85	6 (27%)
1	PSU	L1	1528	1,92	18,21,22	4.66	7 (38%)	22,30,33	1.82	5 (22%)
2	A2M	L2	570	1,2	18,25,26	4.28	7 (38%)	18,36,39	2.71	3 (16%)
2	PSU	L2	1318	2	18,21,22	4.56	7 (38%)	22,30,33	1.78	5 (22%)
1	PSU	L1	1181	1	18,21,22	4.56	7 (38%)	22,30,33	1.82	5 (22%)
51	PSU	S1	1657	51	18,21,22	4.55	7 (38%)	22,30,33	1.77	5 (22%)
1	OMG	L1	959	1	18,26,27	2.59	8 (44%)	19,38,41	1.48	4 (21%)
2	A2M	L2	527	90,2	18,25,26	3.98	7 (38%)	18,36,39	2.64	3 (16%)
1	PSU	L1	1017	1,91	18,21,22	4.65	7 (38%)	22,30,33	1.85	5 (22%)
2	PSU	L2	472	2	18,21,22	4.55	7 (38%)	22,30,33	1.78	5 (22%)
51	A2M	S1	897	51	18,25,26	4.28	7 (38%)	18,36,39	2.65	3 (16%)
2	OMU	L2	560	90,2	19,22,23	3.09	8 (42%)	26,31,34	1.81	4 (15%)



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	B8N	S1	1543	51	-	4/16/34/35	0/2/2/2
2	PSU	L2	662	90,2	-	0/7/25/26	0/2/2/2
1	PSU	L1	940	1	-	0/7/25/26	0/2/2/2
51	OMG	S1	600	51	-	2/5/27/28	0/3/3/3
2	PSU	L2	1194	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1264	2	-	2/7/25/26	0/2/2/2
51	PSU	S1	2048	51	-	0/7/25/26	0/2/2/2
2	PSU	L2	1144	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	774	1	-	0/7/25/26	0/2/2/2
1	1MA	L1	677	1,90	-	0/3/25/26	0/3/3/3
51	PSU	S1	1246	51	-	0/7/25/26	0/2/2/2
7	OMU	L7	101	7	-	0/9/27/28	0/2/2/2
51	OMG	S1	1829	51,90	-	2/5/27/28	0/3/3/3
51	OMU	S1	29	51	-	1/9/27/28	0/2/2/2
7	A2M	L7	43	7	-	0/5/27/28	0/3/3/3
2	PSU	L2	506	2	-	0/7/25/26	0/2/2/2
51	A2M	S1	2021	51	-	1/5/27/28	0/3/3/3
2	A2M	L2	572	2	-	0/5/27/28	0/3/3/3
1	OMU	L1	1253	1	-	0/9/27/28	0/2/2/2
1	A2M	L1	681	1	-	3/5/27/28	0/3/3/3
2	OMU	L2	667	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1292	51,90	-	0/7/25/26	0/2/2/2
2	PSU	L2	1060	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	1539	1,2,90	-	0/5/27/28	0/3/3/3
2	OMG	L2	641	2	-	0/5/27/28	0/3/3/3
52	MIA	S2	37	52	-	4/11/33/34	0/3/3/3
2	A2M	L2	1384	90,2	-	1/5/27/28	0/3/3/3
2	A2M	L2	502	90,2	-	1/5/27/28	0/3/3/3
2	PSU	L2	500	2	-	0/7/25/26	0/2/2/2
51	OMU	S1	1621	51,90	-	0/9/27/28	0/2/2/2
2	OMU	L2	73	2	-	0/9/27/28	0/2/2/2
1	PSU	L1	422	1	-	0/7/25/26	0/2/2/2
2	PSU	L2	1413	2	-	0/7/25/26	0/2/2/2
2	A2M	L2	604	1,2	-	1/5/27/28	0/3/3/3
2	OMG	L2	1360	2,52	-	0/5/27/28	0/3/3/3
2	OMC	L2	1159	2	-	0/9/27/28	0/2/2/2
51	OMU	S1	1662	51	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L2	1046	2,53	-	3/5/27/28	0/3/3/3
2	OMG	L2	1231	2	-	0/5/27/28	0/3/3/3
51	OMC	S1	2059	51,90	-	1/9/27/28	0/2/2/2
1	PSU	L1	1011	1,2	-	4/7/25/26	0/2/2/2
1	PSU	L1	1533	1,2	-	0/7/25/26	0/2/2/2
1	OMU	L1	1107	1	-	0/9/27/28	0/2/2/2
2	PSU	L2	593	2	-	0/7/25/26	0/2/2/2
3	OMU	L3	13	3	-	0/9/27/28	0/2/2/2
2	OMU	L2	56	1,2	-	0/9/27/28	0/2/2/2
7	OMG	L7	75	7	-	0/5/27/28	0/3/3/3
2	A2M	L2	1372	2	-	0/5/27/28	0/3/3/3
1	OMC	L1	695	1	-	0/9/27/28	0/2/2/2
2	OMC	L2	1397	2	-	0/9/27/28	0/2/2/2
51	OMG	S1	1550	51	-	0/5/27/28	0/3/3/3
2	PSU	L2	597	2	-	0/7/25/26	0/2/2/2
2	OMU	L2	1419	2	-	0/9/27/28	0/2/2/2
51	OMU	S1	1777	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	512	2	-	0/7/25/26	0/2/2/2
51	OMC	S1	38	51	-	0/9/27/28	0/2/2/2
51	A2M	S1	668	51,90	-	3/5/27/28	0/3/3/3
51	PSU	S1	1539	51	-	0/7/25/26	0/2/2/2
1	A2M	L1	858	1	-	0/5/27/28	0/3/3/3
2	PSU	L2	1058	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1265	90,2	-	0/7/25/26	0/2/2/2
1	OMU	L1	1371	1	-	3/9/27/28	0/2/2/2
2	PSU	L2	1403	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	305	1	-	0/5/27/28	0/3/3/3
1	OMU	L1	845	1	-	0/9/27/28	0/2/2/2
1	OMC	L1	1552	1	-	1/9/27/28	0/2/2/2
51	PSU	S1	455	51	-	2/7/25/26	0/2/2/2
51	5MC	S1	1544	51	-	1/7/25/26	0/2/2/2
1	OMG	L1	1540	1,2	-	2/5/27/28	0/3/3/3
51	5MC	S1	2061	51	-	0/7/25/26	0/2/2/2
1	OMU	L1	1659	1,90	-	0/9/27/28	0/2/2/2
2	OMC	L2	14	1,2	-	0/9/27/28	0/2/2/2
1	PSU	L1	1171	1,91,92	-	2/7/25/26	0/2/2/2
51	PSU	S1	12	51	-	0/7/25/26	0/2/2/2
1	OMG	L1	1524	1	-	3/5/27/28	0/3/3/3
2	OMU	L2	1077	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	OMC	S1	2019	51	-	0/9/27/28	0/2/2/2
1	PSU	L1	1093	1	-	0/7/25/26	0/2/2/2
2	PSU	L2	1213	2	-	0/7/25/26	0/2/2/2
2	PSU	L2	1303	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	1317	2	-	0/9/27/28	0/2/2/2
51	OMC	S1	2140	51	-	0/9/27/28	0/2/2/2
2	5MC	L2	1308	90,2	-	4/6/24/26	0/2/2/2
51	PSU	S1	33	51	-	0/7/25/26	0/2/2/2
51	PSU	S1	2046	51	-	0/7/25/26	0/2/2/2
51	OMG	S1	1865	91,51	-	0/5/27/28	0/3/3/3
2	5MC	L2	524	90,2	-	0/7/25/26	0/2/2/2
1	A2M	L1	955	1	-	1/5/27/28	0/3/3/3
2	OMG	L2	1078	2	-	0/5/27/28	0/3/3/3
51	A2M	S1	28	51,90	-	0/5/27/28	0/3/3/3
51	A2M	S1	512	51,90	-	2/5/27/28	0/3/3/3
51	A2M	S1	969	51	-	1/5/27/28	0/3/3/3
51	OMC	S1	1866	51	-	0/9/27/28	0/2/2/2
2	PSU	L2	1361	2,52	-	3/7/25/26	0/2/2/2
51	OMC	S1	18	51	-	0/9/27/28	0/2/2/2
1	A2M	L1	69	1	-	0/5/27/28	0/3/3/3
2	PSU	L2	626	2	-	0/7/25/26	0/2/2/2
1	A2M	L1	697	1	-	0/5/27/28	0/3/3/3
1	A2M	L1	678	1,2	-	0/5/27/28	0/3/3/3
51	PSU	S1	1192	51	-	0/7/25/26	0/2/2/2
51	OMG	S1	1647	51	-	0/5/27/28	0/3/3/3
2	A2M	L2	665	2	-	3/5/27/28	0/3/3/3
1	A2M	L1	927	1,90	-	0/5/27/28	0/3/3/3
51	PSU	S1	1566	51	-	0/7/25/26	0/2/2/2
2	OMC	L2	1248	2	-	2/9/27/28	0/2/2/2
51	PSU	S1	609	51	-	0/7/25/26	0/2/2/2
51	OMG	S1	2151	51	-	0/5/27/28	0/3/3/3
7	A2M	L7	162	7,1	-	1/5/27/28	0/3/3/3
51	A2M	S1	479	51	-	0/5/27/28	0/3/3/3
2	OMG	L2	1229	2	-	2/5/27/28	0/3/3/3
2	PSU	L2	510	2	-	0/7/25/26	0/2/2/2
51	OMG	S1	1623	51	-	1/5/27/28	0/3/3/3
2	OMG	L2	534	2	-	2/5/27/28	0/3/3/3
51	OMG	S1	2008	51	-	0/5/27/28	0/3/3/3
51	PSU	S1	1533	51	-	0/7/25/26	0/2/2/2
2	A2M	L2	1067	2	-	0/5/27/28	0/3/3/3
2	PSU	L2	504	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	L2	382	2	-	0/5/27/28	0/3/3/3
51	OMG	S1	1478	51	-	1/5/27/28	0/3/3/3
2	PSU	L2	1382	90,2,92	-	1/7/25/26	0/2/2/2
51	PSU	S1	1841	51	-	0/7/25/26	0/2/2/2
1	OMU	L1	1039	1	-	1/9/27/28	0/2/2/2
2	PSU	L2	78	2	-	0/7/25/26	0/2/2/2
1	OMC	L1	1527	1	-	2/9/27/28	0/2/2/2
1	PSU	L1	239	1	-	0/7/25/26	0/2/2/2
51	MA6	S1	2185	51	-	1/7/29/30	0/3/3/3
51	7MG	S1	1995	51,53	-	2/7/37/38	0/3/3/3
2	A2M	L2	1185	2	-	3/5/27/28	0/3/3/3
1	OMG	L1	1190	1	-	0/5/27/28	0/3/3/3
2	OMC	L2	359	2	-	0/9/27/28	0/2/2/2
51	PSU	S1	1156	51	-	0/7/25/26	0/2/2/2
2	OMC	L2	583	2	-	0/9/27/28	0/2/2/2
2	OMU	L2	1359	90,2	-	0/9/27/28	0/2/2/2
2	PSU	L2	1284	2	-	0/7/25/26	0/2/2/2
2	OMC	L2	443	91,2	-	4/9/27/28	0/2/2/2
1	OMG	L1	1626	1,92	-	0/5/27/28	0/3/3/3
51	A2M	S1	98	51,90	-	2/5/27/28	0/3/3/3
51	OMU	S1	1833	51	-	1/9/27/28	0/2/2/2
51	PSU	S1	104	51	-	0/7/25/26	0/2/2/2
2	OMG	L2	686	2	-	0/5/27/28	0/3/3/3
1	OMC	L1	669	1	-	1/9/27/28	0/2/2/2
1	PSU	L1	1664	1	-	0/7/25/26	0/2/2/2
1	A2M	L1	1373	1	-	0/5/27/28	0/3/3/3
51	OMU	S1	1979	51	-	0/9/27/28	0/2/2/2
1	A2M	L1	235	1	-	0/5/27/28	0/3/3/3
1	PSU	L1	672	1,90	-	0/7/25/26	0/2/2/2
51	MA6	S1	2184	51	-	0/7/29/30	0/3/3/3
2	OMG	L2	655	2,92	-	0/5/27/28	0/3/3/3
2	A2M	L2	591	2	-	1/5/27/28	0/3/3/3
2	OMG	L2	1253	2	-	0/5/27/28	0/3/3/3
4	OMG	L4	74	4	-	1/5/27/28	0/3/3/3
2	PSU	L2	437	2,92	-	0/7/25/26	0/2/2/2
2	A2M	L2	628	2	-	0/5/27/28	0/3/3/3
51	OMU	S1	8	51	-	5/9/27/28	0/2/2/2
2	A2M	L2	95	2	-	0/5/27/28	0/3/3/3
1	OMU	L1	48	1	-	0/9/27/28	0/2/2/2
1	OMU	L1	847	1	-	0/9/27/28	0/2/2/2
7	PSU	L7	74	7	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L1	856	1	-	0/5/27/28	0/3/3/3
51	PSU	S1	2202	51	-	1/7/25/26	0/2/2/2
1	OMC	L1	1010	1,90	-	3/9/27/28	0/2/2/2
2	OMG	L2	71	2	-	0/5/27/28	0/3/3/3
7	PSU	L7	69	7,90	-	0/7/25/26	0/2/2/2
1	PSU	L1	1528	1,92	-	0/7/25/26	0/2/2/2
2	A2M	L2	570	1,2	-	2/5/27/28	0/3/3/3
2	PSU	L2	1318	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	1181	1	-	0/7/25/26	0/2/2/2
51	PSU	S1	1657	51	-	1/7/25/26	0/2/2/2
1	OMG	L1	959	1	-	0/5/27/28	0/3/3/3
2	A2M	L2	527	90,2	-	1/5/27/28	0/3/3/3
1	PSU	L1	1017	1,91	-	0/7/25/26	0/2/2/2
2	PSU	L2	472	2	-	0/7/25/26	0/2/2/2
51	A2M	S1	897	51	-	0/5/27/28	0/3/3/3
2	OMU	L2	560	90,2	-	1/9/27/28	0/2/2/2

All (1303) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	382	A2M	O4'-C1'	15.97	1.63	1.41
2	L2	1185	A2M	O4'-C1'	15.90	1.63	1.41
2	L2	1384	A2M	O4'-C1'	15.80	1.63	1.41
1	L1	927	A2M	O4'-C1'	15.78	1.63	1.41
1	L1	1539	A2M	O4'-C1'	15.74	1.63	1.41
1	L1	858	A2M	O4'-C1'	15.66	1.62	1.41
51	S1	897	A2M	O4'-C1'	15.50	1.62	1.41
1	L1	681	A2M	O4'-C1'	15.49	1.62	1.41
2	L2	570	A2M	O4'-C1'	15.49	1.62	1.41
51	S1	28	A2M	O4'-C1'	15.46	1.62	1.41
7	L7	43	A2M	O4'-C1'	15.46	1.62	1.41
2	L2	1067	A2M	O4'-C1'	15.41	1.62	1.41
2	L2	665	A2M	O4'-C1'	15.39	1.62	1.41
51	S1	98	A2M	O4'-C1'	15.39	1.62	1.41
2	L2	628	A2M	O4'-C1'	15.39	1.62	1.41
1	L1	697	A2M	O4'-C1'	15.38	1.62	1.41
1	L1	1373	A2M	O4'-C1'	15.38	1.62	1.41
2	L2	502	A2M	O4'-C1'	15.38	1.62	1.41
2	L2	604	A2M	O4'-C1'	15.38	1.62	1.41
51	S1	479	A2M	O4'-C1'	15.36	1.62	1.41
2	L2	572	A2M	O4'-C1'	15.35	1.62	1.41
2	L2	95	A2M	O4'-C1'	15.34	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	512	A2M	O4'-C1'	15.32	1.62	1.41
1	L1	955	A2M	O4'-C1'	15.32	1.62	1.41
7	L7	162	A2M	O4'-C1'	15.28	1.62	1.41
1	L1	235	A2M	O4'-C1'	15.28	1.62	1.41
2	L2	591	A2M	O4'-C1'	15.27	1.62	1.41
1	L1	678	A2M	O4'-C1'	15.24	1.62	1.41
51	S1	2021	A2M	O4'-C1'	15.23	1.62	1.41
2	L2	1372	A2M	O4'-C1'	15.19	1.62	1.41
51	S1	969	A2M	O4'-C1'	15.09	1.62	1.41
1	L1	305	A2M	O4'-C1'	15.00	1.62	1.41
1	L1	69	A2M	O4'-C1'	14.91	1.61	1.41
51	S1	668	A2M	O4'-C1'	14.84	1.61	1.41
2	L2	527	A2M	O4'-C1'	14.19	1.60	1.41
1	L1	677	1MA	C2-N3	14.01	1.46	1.29
2	L2	1264	PSU	C6-C5	12.32	1.49	1.35
2	L2	1413	PSU	C6-C5	12.19	1.49	1.35
1	L1	1528	PSU	C6-C5	12.17	1.49	1.35
1	L1	1011	PSU	C6-C5	12.14	1.49	1.35
51	S1	1539	PSU	C6-C5	12.12	1.49	1.35
1	L1	1017	PSU	C6-C5	12.07	1.49	1.35
1	L1	672	PSU	C6-C5	12.07	1.49	1.35
2	L2	1382	PSU	C6-C5	12.04	1.49	1.35
2	L2	1058	PSU	C6-C5	12.02	1.49	1.35
2	L2	1403	PSU	C6-C5	12.00	1.49	1.35
1	L1	1171	PSU	C6-C5	11.97	1.49	1.35
51	S1	455	PSU	C6-C5	11.96	1.49	1.35
51	S1	1192	PSU	C6-C5	11.93	1.49	1.35
2	L2	510	PSU	C6-C5	11.90	1.49	1.35
2	L2	593	PSU	C6-C5	11.87	1.49	1.35
2	L2	1194	PSU	C6-C5	11.87	1.49	1.35
2	L2	662	PSU	C6-C5	11.87	1.49	1.35
1	L1	422	PSU	C6-C5	11.87	1.49	1.35
51	S1	1156	PSU	C6-C5	11.87	1.49	1.35
51	S1	104	PSU	C6-C5	11.87	1.49	1.35
2	L2	1318	PSU	C6-C5	11.86	1.49	1.35
2	L2	504	PSU	C6-C5	11.86	1.49	1.35
51	S1	33	PSU	C6-C5	11.85	1.49	1.35
2	L2	626	PSU	C6-C5	11.85	1.49	1.35
2	L2	437	PSU	C6-C5	11.84	1.49	1.35
1	L1	774	PSU	C6-C5	11.84	1.49	1.35
7	L7	69	PSU	C6-C5	11.84	1.49	1.35
51	S1	1292	PSU	C6-C5	11.84	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	940	PSU	C6-C5	11.84	1.49	1.35
51	S1	1533	PSU	C6-C5	11.84	1.49	1.35
2	L2	78	PSU	C6-C5	11.84	1.49	1.35
1	L1	1093	PSU	C6-C5	11.83	1.49	1.35
2	L2	1303	PSU	C6-C5	11.83	1.49	1.35
2	L2	597	PSU	C6-C5	11.83	1.49	1.35
1	L1	1181	PSU	C6-C5	11.82	1.49	1.35
51	S1	609	PSU	C6-C5	11.82	1.49	1.35
2	L2	506	PSU	C6-C5	11.82	1.49	1.35
51	S1	1566	PSU	C6-C5	11.82	1.49	1.35
51	S1	2046	PSU	C6-C5	11.81	1.49	1.35
51	S1	2048	PSU	C6-C5	11.81	1.49	1.35
1	L1	239	PSU	C6-C5	11.81	1.49	1.35
1	L1	1664	PSU	C6-C5	11.81	1.49	1.35
2	L2	1213	PSU	C6-C5	11.81	1.49	1.35
2	L2	1284	PSU	C6-C5	11.81	1.49	1.35
7	L7	74	PSU	C6-C5	11.80	1.49	1.35
51	S1	12	PSU	C6-C5	11.79	1.49	1.35
51	S1	2202	PSU	C6-C5	11.78	1.49	1.35
51	S1	1246	PSU	C6-C5	11.78	1.49	1.35
1	L1	1533	PSU	C6-C5	11.77	1.49	1.35
2	L2	500	PSU	C6-C5	11.76	1.49	1.35
2	L2	1144	PSU	C6-C5	11.76	1.49	1.35
2	L2	1361	PSU	C6-C5	11.76	1.49	1.35
51	S1	1841	PSU	C6-C5	11.75	1.49	1.35
2	L2	1060	PSU	C6-C5	11.75	1.49	1.35
2	L2	472	PSU	C6-C5	11.75	1.49	1.35
2	L2	1265	PSU	C6-C5	11.73	1.49	1.35
2	L2	512	PSU	C6-C5	11.72	1.49	1.35
51	S1	1657	PSU	C6-C5	11.72	1.49	1.35
51	S1	1995	7MG	C8-N9	11.33	1.52	1.46
2	L2	1403	PSU	C2-N1	10.14	1.50	1.36
51	S1	1539	PSU	C2-N1	10.13	1.50	1.36
1	L1	1017	PSU	C2-N1	10.12	1.50	1.36
2	L2	1413	PSU	C2-N1	10.11	1.50	1.36
2	L2	662	PSU	C2-N1	10.10	1.50	1.36
2	L2	1058	PSU	C2-N1	10.10	1.50	1.36
1	L1	1528	PSU	C2-N1	10.09	1.50	1.36
1	L1	672	PSU	C2-N1	10.09	1.50	1.36
2	L2	1382	PSU	C2-N1	10.07	1.50	1.36
1	L1	1171	PSU	C2-N1	10.00	1.50	1.36
7	L7	69	PSU	C2-N1	10.00	1.50	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1264	PSU	C2-N1	9.96	1.50	1.36
1	L1	1011	PSU	C2-N1	9.95	1.50	1.36
51	S1	1841	PSU	C2-N1	9.87	1.50	1.36
7	L7	74	PSU	C2-N1	9.86	1.50	1.36
2	L2	1213	PSU	C2-N1	9.86	1.50	1.36
51	S1	1156	PSU	C2-N1	9.86	1.50	1.36
51	S1	33	PSU	C2-N1	9.86	1.50	1.36
1	L1	1093	PSU	C2-N1	9.85	1.50	1.36
2	L2	500	PSU	C2-N1	9.85	1.50	1.36
2	L2	78	PSU	C2-N1	9.85	1.50	1.36
2	L2	1318	PSU	C2-N1	9.83	1.50	1.36
51	S1	1566	PSU	C2-N1	9.83	1.50	1.36
2	L2	510	PSU	C2-N1	9.83	1.50	1.36
1	L1	774	PSU	C2-N1	9.83	1.50	1.36
2	L2	1303	PSU	C2-N1	9.83	1.50	1.36
1	L1	1181	PSU	C2-N1	9.82	1.50	1.36
51	S1	1657	PSU	C2-N1	9.82	1.50	1.36
51	S1	1533	PSU	C2-N1	9.82	1.50	1.36
2	L2	1144	PSU	C2-N1	9.82	1.50	1.36
2	L2	1284	PSU	C2-N1	9.81	1.50	1.36
2	L2	437	PSU	C2-N1	9.81	1.50	1.36
2	L2	506	PSU	C2-N1	9.81	1.50	1.36
1	L1	422	PSU	C2-N1	9.80	1.50	1.36
51	S1	2046	PSU	C2-N1	9.80	1.50	1.36
2	L2	472	PSU	C2-N1	9.79	1.50	1.36
2	L2	597	PSU	C2-N1	9.79	1.50	1.36
1	L1	940	PSU	C2-N1	9.79	1.50	1.36
2	L2	512	PSU	C2-N1	9.79	1.50	1.36
51	S1	1246	PSU	C2-N1	9.79	1.50	1.36
1	L1	239	PSU	C2-N1	9.79	1.50	1.36
1	L1	1664	PSU	C2-N1	9.79	1.50	1.36
2	L2	626	PSU	C2-N1	9.78	1.50	1.36
51	S1	1292	PSU	C2-N1	9.78	1.50	1.36
51	S1	12	PSU	C2-N1	9.78	1.50	1.36
2	L2	504	PSU	C2-N1	9.77	1.49	1.36
2	L2	1060	PSU	C2-N1	9.77	1.49	1.36
2	L2	593	PSU	C2-N1	9.76	1.49	1.36
51	S1	2202	PSU	C2-N1	9.75	1.49	1.36
51	S1	609	PSU	C2-N1	9.75	1.49	1.36
51	S1	104	PSU	C2-N1	9.75	1.49	1.36
1	L1	1533	PSU	C2-N1	9.74	1.49	1.36
51	S1	1192	PSU	C2-N1	9.74	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1361	PSU	C2-N1	9.73	1.49	1.36
2	L2	1194	PSU	C2-N1	9.73	1.49	1.36
51	S1	2048	PSU	C2-N1	9.73	1.49	1.36
51	S1	455	PSU	C2-N1	9.66	1.49	1.36
51	S1	1995	7MG	C5-N7	9.51	1.46	1.35
2	L2	1265	PSU	C2-N1	9.43	1.49	1.36
51	S1	1544	5MC	C6-C5	9.23	1.49	1.34
2	L2	524	5MC	C6-C5	9.22	1.49	1.34
51	S1	2061	5MC	C6-C5	9.10	1.49	1.34
2	L2	1308	5MC	C6-C5	9.03	1.49	1.34
2	L2	1308	5MC	C3'-C4'	-8.83	1.30	1.53
52	S2	37	MIA	C2-S10	8.75	1.83	1.75
7	L7	101	OMU	C3'-C2'	-8.51	1.34	1.52
51	S1	1543	B8N	C6-N1	7.88	1.56	1.36
2	L2	560	OMU	C2-N1	7.75	1.50	1.38
51	S1	1995	7MG	C4-N9	7.75	1.46	1.37
2	L2	500	PSU	C2-N3	7.70	1.50	1.37
51	S1	609	PSU	C2-N3	7.69	1.50	1.37
2	L2	1361	PSU	C2-N3	7.68	1.50	1.37
1	L1	1528	PSU	C2-N3	7.68	1.50	1.37
2	L2	504	PSU	C2-N3	7.67	1.50	1.37
2	L2	1303	PSU	C2-N3	7.67	1.50	1.37
51	S1	1841	PSU	C2-N3	7.67	1.50	1.37
2	L2	1264	PSU	C2-N3	7.67	1.50	1.37
2	L2	506	PSU	C2-N3	7.66	1.50	1.37
2	L2	1077	OMU	C2-N1	7.66	1.50	1.38
51	S1	1246	PSU	C2-N3	7.66	1.50	1.37
51	S1	1566	PSU	C2-N3	7.65	1.50	1.37
51	S1	661	OMU	C2-N1	7.65	1.50	1.38
1	L1	1533	PSU	C2-N3	7.65	1.50	1.37
51	S1	1657	PSU	C2-N3	7.65	1.50	1.37
2	L2	472	PSU	C2-N3	7.65	1.50	1.37
51	S1	1192	PSU	C2-N3	7.64	1.50	1.37
51	S1	1533	PSU	C2-N3	7.63	1.50	1.37
51	S1	33	PSU	C2-N3	7.63	1.50	1.37
2	L2	512	PSU	C2-N3	7.63	1.50	1.37
51	S1	2046	PSU	C2-N3	7.63	1.50	1.37
7	L7	74	PSU	C2-N3	7.63	1.50	1.37
51	S1	455	PSU	C2-N3	7.63	1.50	1.37
2	L2	1284	PSU	C2-N3	7.63	1.50	1.37
51	S1	2048	PSU	C2-N3	7.62	1.50	1.37
1	L1	774	PSU	C2-N3	7.62	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	593	PSU	C2-N3	7.62	1.50	1.37
2	L2	1213	PSU	C2-N3	7.62	1.50	1.37
1	L1	239	PSU	C2-N3	7.61	1.50	1.37
1	L1	1039	OMU	C2-N1	7.61	1.50	1.38
1	L1	1093	PSU	C2-N3	7.61	1.50	1.37
51	S1	104	PSU	C2-N3	7.61	1.50	1.37
51	S1	1292	PSU	C2-N3	7.61	1.50	1.37
1	L1	1181	PSU	C2-N3	7.61	1.50	1.37
2	L2	626	PSU	C2-N3	7.61	1.50	1.37
51	S1	2202	PSU	C2-N3	7.60	1.50	1.37
2	L2	1194	PSU	C2-N3	7.60	1.50	1.37
1	L1	940	PSU	C2-N3	7.60	1.50	1.37
2	L2	1413	PSU	C2-N3	7.60	1.50	1.37
51	S1	1543	B8N	C4-N3	-7.60	1.26	1.40
1	L1	1664	PSU	C2-N3	7.60	1.50	1.37
51	S1	12	PSU	C2-N3	7.59	1.50	1.37
2	L2	597	PSU	C2-N3	7.59	1.50	1.37
1	L1	1017	PSU	C2-N3	7.59	1.50	1.37
2	L2	437	PSU	C2-N3	7.59	1.50	1.37
2	L2	510	PSU	C2-N3	7.58	1.50	1.37
1	L1	422	PSU	C2-N3	7.57	1.50	1.37
51	S1	1156	PSU	C2-N3	7.57	1.50	1.37
2	L2	1060	PSU	C2-N3	7.57	1.50	1.37
1	L1	1011	PSU	C2-N3	7.56	1.50	1.37
2	L2	1058	PSU	C2-N3	7.56	1.50	1.37
2	L2	1144	PSU	C2-N3	7.56	1.50	1.37
2	L2	1318	PSU	C2-N3	7.55	1.50	1.37
7	L7	69	PSU	C2-N3	7.53	1.50	1.37
51	S1	1539	PSU	C2-N3	7.53	1.50	1.37
2	L2	78	PSU	C2-N3	7.53	1.50	1.37
2	L2	1382	PSU	C2-N3	7.52	1.50	1.37
2	L2	1403	PSU	C2-N3	7.51	1.50	1.37
2	L2	662	PSU	C2-N3	7.49	1.50	1.37
2	L2	1265	PSU	C2-N3	7.47	1.50	1.37
1	L1	1171	PSU	C2-N3	7.44	1.50	1.37
7	L7	101	OMU	O4'-C1'	7.42	1.59	1.42
1	L1	672	PSU	C2-N3	7.40	1.50	1.37
2	L2	1308	5MC	O4'-C4'	7.38	1.61	1.45
7	L7	101	OMU	C2-N1	7.24	1.50	1.38
51	S1	1833	OMU	C2-N1	7.21	1.50	1.38
51	S1	1662	OMU	C2-N1	7.12	1.49	1.38
51	S1	1777	OMU	C2-N1	7.11	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	847	OMU	C2-N1	7.10	1.49	1.38
2	L2	667	OMU	C2-N1	7.09	1.49	1.38
1	L1	1253	OMU	C2-N1	7.08	1.49	1.38
51	S1	1979	OMU	C2-N1	7.07	1.49	1.38
1	L1	1659	OMU	C2-N1	7.06	1.49	1.38
2	L2	1419	OMU	C2-N1	7.06	1.49	1.38
1	L1	845	OMU	C2-N1	7.06	1.49	1.38
2	L2	56	OMU	C2-N1	7.05	1.49	1.38
51	S1	1621	OMU	C2-N1	7.04	1.49	1.38
1	L1	1371	OMU	C2-N1	7.03	1.49	1.38
51	S1	8	OMU	C2-N1	7.02	1.49	1.38
51	S1	29	OMU	C2-N1	7.01	1.49	1.38
2	L2	1359	OMU	C2-N1	7.01	1.49	1.38
1	L1	48	OMU	C2-N1	6.98	1.49	1.38
2	L2	73	OMU	C2-N1	6.96	1.49	1.38
3	L3	13	OMU	C2-N1	6.95	1.49	1.38
51	S1	1777	OMU	C2-N3	6.93	1.50	1.38
1	L1	1253	OMU	C2-N3	6.93	1.50	1.38
1	L1	1107	OMU	C2-N1	6.92	1.49	1.38
51	S1	661	OMU	C2-N3	6.88	1.50	1.38
1	L1	1659	OMU	C2-N3	6.88	1.50	1.38
2	L2	1359	OMU	C2-N3	6.88	1.50	1.38
51	S1	1662	OMU	C2-N3	6.88	1.50	1.38
51	S1	1979	OMU	C2-N3	6.88	1.50	1.38
51	S1	1621	OMU	C2-N3	6.87	1.50	1.38
2	L2	667	OMU	C2-N3	6.85	1.50	1.38
2	L2	56	OMU	C2-N3	6.85	1.50	1.38
51	S1	8	OMU	C2-N3	6.84	1.50	1.38
1	L1	845	OMU	C2-N3	6.83	1.50	1.38
51	S1	29	OMU	C2-N3	6.83	1.50	1.38
1	L1	847	OMU	C2-N3	6.82	1.50	1.38
3	L3	13	OMU	C2-N3	6.81	1.50	1.38
2	L2	1419	OMU	C2-N3	6.80	1.50	1.38
7	L7	101	OMU	C2-N3	6.80	1.50	1.38
1	L1	1371	OMU	C2-N3	6.79	1.50	1.38
1	L1	48	OMU	C2-N3	6.78	1.50	1.38
1	L1	1039	OMU	C2-N3	6.76	1.50	1.38
2	L2	73	OMU	C2-N3	6.75	1.50	1.38
1	L1	1107	OMU	C2-N3	6.74	1.50	1.38
2	L2	1077	OMU	C2-N3	6.72	1.49	1.38
2	L2	560	OMU	C2-N3	6.71	1.49	1.38
52	S2	37	MIA	C6-N6	6.66	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1833	OMU	C2-N3	6.57	1.49	1.38
51	S1	2061	5MC	C4-N3	6.55	1.45	1.34
1	L1	858	A2M	O4'-C4'	-6.51	1.30	1.45
51	S1	1544	5MC	C4-N3	6.50	1.45	1.34
2	L2	359	OMC	C2-N3	6.48	1.49	1.36
51	S1	1543	B8N	C6-C5	6.46	1.44	1.34
2	L2	1185	A2M	O4'-C4'	-6.44	1.30	1.45
51	S1	668	A2M	O4'-C4'	-6.41	1.30	1.45
51	S1	2140	OMC	C2-N3	6.38	1.49	1.36
51	S1	1995	7MG	C2-N3	6.38	1.48	1.33
51	S1	2059	OMC	C2-N3	6.37	1.49	1.36
2	L2	524	5MC	C4-N3	6.37	1.44	1.34
1	L1	1552	OMC	C2-N3	6.36	1.49	1.36
1	L1	695	OMC	C2-N3	6.36	1.49	1.36
51	S1	18	OMC	C2-N3	6.35	1.49	1.36
2	L2	1317	OMC	C2-N3	6.35	1.49	1.36
1	L1	235	A2M	O4'-C4'	-6.35	1.30	1.45
2	L2	14	OMC	C2-N3	6.35	1.49	1.36
51	S1	1866	OMC	C2-N3	6.34	1.49	1.36
51	S1	38	OMC	C2-N3	6.34	1.49	1.36
2	L2	1159	OMC	C2-N3	6.34	1.49	1.36
2	L2	443	OMC	C6-C5	6.32	1.49	1.35
1	L1	1010	OMC	C2-N3	6.31	1.49	1.36
1	L1	1010	OMC	C6-C5	6.31	1.49	1.35
51	S1	2019	OMC	C2-N3	6.31	1.49	1.36
1	L1	1527	OMC	C6-C5	6.31	1.49	1.35
2	L2	583	OMC	C2-N3	6.31	1.49	1.36
2	L2	443	OMC	C2-N3	6.30	1.49	1.36
2	L2	1372	A2M	O4'-C4'	-6.30	1.30	1.45
2	L2	628	A2M	O4'-C4'	-6.29	1.30	1.45
51	S1	969	A2M	O4'-C4'	-6.29	1.30	1.45
2	L2	665	A2M	O4'-C4'	-6.29	1.30	1.45
1	L1	1539	A2M	O4'-C4'	-6.29	1.31	1.45
2	L2	1397	OMC	C6-C5	6.28	1.49	1.35
51	S1	2021	A2M	O4'-C4'	-6.28	1.31	1.45
1	L1	1527	OMC	C2-N3	6.27	1.49	1.36
2	L2	1248	OMC	C2-N3	6.25	1.49	1.36
2	L2	1397	OMC	C2-N3	6.24	1.49	1.36
1	L1	669	OMC	C2-N3	6.24	1.49	1.36
2	L2	1248	OMC	C6-C5	6.23	1.49	1.35
7	L7	162	A2M	O4'-C4'	-6.23	1.31	1.45
1	L1	678	A2M	O4'-C4'	-6.23	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	955	A2M	O4'-C4'	-6.22	1.31	1.45
51	S1	98	A2M	O4'-C4'	-6.22	1.31	1.45
2	L2	95	A2M	O4'-C4'	-6.22	1.31	1.45
2	L2	591	A2M	O4'-C4'	-6.21	1.31	1.45
1	L1	69	A2M	O4'-C4'	-6.20	1.31	1.45
51	S1	28	A2M	O4'-C4'	-6.20	1.31	1.45
1	L1	927	A2M	O4'-C4'	-6.19	1.31	1.45
51	S1	479	A2M	O4'-C4'	-6.19	1.31	1.45
1	L1	697	A2M	O4'-C4'	-6.18	1.31	1.45
51	S1	897	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	1373	A2M	O4'-C4'	-6.18	1.31	1.45
1	L1	669	OMC	C6-C5	6.18	1.49	1.35
7	L7	101	OMU	O4'-C4'	-6.17	1.31	1.45
7	L7	43	A2M	O4'-C4'	-6.17	1.31	1.45
2	L2	570	A2M	O4'-C4'	-6.16	1.31	1.45
51	S1	1544	5MC	C2-N3	6.16	1.48	1.36
2	L2	1067	A2M	O4'-C4'	-6.16	1.31	1.45
2	L2	502	A2M	O4'-C4'	-6.15	1.31	1.45
2	L2	604	A2M	O4'-C4'	-6.15	1.31	1.45
2	L2	1384	A2M	O4'-C4'	-6.13	1.31	1.45
51	S1	2019	OMC	C6-C5	6.13	1.49	1.35
2	L2	527	A2M	O4'-C4'	-6.13	1.31	1.45
51	S1	38	OMC	C6-C5	6.12	1.49	1.35
51	S1	512	A2M	O4'-C4'	-6.12	1.31	1.45
51	S1	2061	5MC	C2-N3	6.11	1.48	1.36
2	L2	359	OMC	C6-C5	6.11	1.49	1.35
1	L1	305	A2M	O4'-C4'	-6.10	1.31	1.45
1	L1	1552	OMC	C6-C5	6.10	1.49	1.35
51	S1	1866	OMC	C6-C5	6.09	1.49	1.35
2	L2	14	OMC	C6-C5	6.09	1.49	1.35
2	L2	1159	OMC	C6-C5	6.09	1.49	1.35
2	L2	572	A2M	O4'-C4'	-6.09	1.31	1.45
51	S1	2140	OMC	C6-C5	6.08	1.49	1.35
2	L2	583	OMC	C6-C5	6.07	1.49	1.35
51	S1	2059	OMC	C6-C5	6.06	1.49	1.35
1	L1	695	OMC	C6-C5	6.05	1.49	1.35
51	S1	1543	B8N	C2-N1	6.05	1.57	1.39
2	L2	1317	OMC	C6-C5	6.05	1.49	1.35
2	L2	382	A2M	O4'-C4'	-6.04	1.31	1.45
2	L2	524	5MC	C2-N3	6.04	1.48	1.36
51	S1	18	OMC	C6-C5	6.02	1.49	1.35
1	L1	681	A2M	O4'-C4'	-5.97	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1403	PSU	C6-N1	5.96	1.46	1.36
51	S1	1539	PSU	C6-N1	5.84	1.45	1.36
2	L2	1308	5MC	C2-N3	5.82	1.48	1.36
51	S1	1833	OMU	C6-C5	5.82	1.48	1.35
7	L7	69	PSU	C6-N1	5.80	1.45	1.36
1	L1	1017	PSU	C6-N1	5.78	1.45	1.36
7	L7	101	OMU	C6-C5	5.78	1.48	1.35
1	L1	1171	PSU	C6-N1	5.75	1.45	1.36
2	L2	1308	5MC	C4-N3	5.75	1.43	1.34
2	L2	1382	PSU	C6-N1	5.75	1.45	1.36
1	L1	1371	OMU	C6-C5	5.74	1.48	1.35
51	S1	1979	OMU	C6-C5	5.74	1.48	1.35
51	S1	8	OMU	C6-C5	5.74	1.48	1.35
51	S1	1662	OMU	C6-C5	5.74	1.48	1.35
51	S1	1621	OMU	C6-C5	5.73	1.48	1.35
1	L1	672	PSU	C6-N1	5.73	1.45	1.36
2	L2	1359	OMU	C6-C5	5.73	1.48	1.35
1	L1	847	OMU	C6-C5	5.73	1.48	1.35
1	L1	48	OMU	C6-C5	5.73	1.48	1.35
2	L2	56	OMU	C6-C5	5.72	1.48	1.35
2	L2	667	OMU	C6-C5	5.72	1.48	1.35
1	L1	1253	OMU	C6-C5	5.72	1.48	1.35
1	L1	1011	PSU	C6-N1	5.72	1.45	1.36
51	S1	29	OMU	C6-C5	5.71	1.48	1.35
1	L1	845	OMU	C6-C5	5.71	1.48	1.35
1	L1	1659	OMU	C6-C5	5.71	1.48	1.35
51	S1	1777	OMU	C6-C5	5.70	1.48	1.35
2	L2	1419	OMU	C6-C5	5.70	1.48	1.35
2	L2	662	PSU	C6-N1	5.70	1.45	1.36
2	L2	73	OMU	C6-C5	5.69	1.48	1.35
2	L2	1058	PSU	C6-N1	5.69	1.45	1.36
2	L2	1413	PSU	C6-N1	5.68	1.45	1.36
3	L3	13	OMU	C6-C5	5.68	1.48	1.35
1	L1	1107	OMU	C6-C5	5.65	1.48	1.35
1	L1	1528	PSU	C6-N1	5.62	1.45	1.36
51	S1	1995	7MG	C4-N3	5.52	1.47	1.34
2	L2	560	OMU	C6-C5	5.52	1.47	1.35
2	L2	78	PSU	C6-N1	5.50	1.45	1.36
1	L1	1039	OMU	C6-C5	5.50	1.47	1.35
51	S1	661	OMU	C6-C5	5.50	1.47	1.35
51	S1	1566	PSU	C6-N1	5.49	1.45	1.36
1	L1	1664	PSU	C6-N1	5.48	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1841	PSU	C6-N1	5.47	1.45	1.36
2	L2	1077	OMU	C6-C5	5.46	1.47	1.35
2	L2	510	PSU	C6-N1	5.46	1.45	1.36
51	S1	1156	PSU	C6-N1	5.46	1.45	1.36
51	S1	2046	PSU	C6-N1	5.45	1.45	1.36
51	S1	1623	OMG	C2-N3	5.45	1.46	1.33
2	L2	437	PSU	C6-N1	5.44	1.45	1.36
51	S1	33	PSU	C6-N1	5.44	1.45	1.36
2	L2	506	PSU	C6-N1	5.44	1.45	1.36
2	L2	1284	PSU	C6-N1	5.44	1.45	1.36
2	L2	1318	PSU	C6-N1	5.44	1.45	1.36
1	L1	1093	PSU	C6-N1	5.44	1.45	1.36
1	L1	422	PSU	C6-N1	5.43	1.45	1.36
7	L7	74	PSU	C6-N1	5.43	1.45	1.36
2	L2	500	PSU	C6-N1	5.43	1.45	1.36
1	L1	239	PSU	C6-N1	5.43	1.45	1.36
1	L1	940	PSU	C6-N1	5.43	1.45	1.36
51	S1	12	PSU	C6-N1	5.43	1.45	1.36
2	L2	1213	PSU	C6-N1	5.43	1.45	1.36
51	S1	1533	PSU	C6-N1	5.43	1.45	1.36
1	L1	774	PSU	C6-N1	5.42	1.45	1.36
51	S1	1865	OMG	C2-N3	5.42	1.46	1.33
1	L1	959	OMG	C2-N3	5.42	1.46	1.33
1	L1	1181	PSU	C6-N1	5.41	1.45	1.36
51	S1	1657	PSU	C6-N1	5.41	1.45	1.36
2	L2	1265	PSU	C6-N1	5.40	1.45	1.36
2	L2	1060	PSU	C6-N1	5.40	1.45	1.36
2	L2	472	PSU	C6-N1	5.40	1.45	1.36
2	L2	626	PSU	C6-N1	5.40	1.45	1.36
2	L2	597	PSU	C6-N1	5.40	1.45	1.36
51	S1	1292	PSU	C6-N1	5.40	1.45	1.36
2	L2	504	PSU	C6-N1	5.40	1.45	1.36
2	L2	1144	PSU	C6-N1	5.39	1.45	1.36
51	S1	2202	PSU	C6-N1	5.38	1.45	1.36
2	L2	512	PSU	C6-N1	5.38	1.45	1.36
51	S1	609	PSU	C6-N1	5.37	1.45	1.36
2	L2	1046	OMG	C2-N3	5.37	1.46	1.33
2	L2	1303	PSU	C6-N1	5.37	1.45	1.36
2	L2	1360	OMG	C2-N3	5.37	1.46	1.33
51	S1	600	OMG	C2-N3	5.37	1.46	1.33
2	L2	1229	OMG	C2-N3	5.36	1.46	1.33
51	S1	1192	PSU	C6-N1	5.36	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1647	OMG	C2-N3	5.36	1.46	1.33
51	S1	1246	PSU	C6-N1	5.36	1.45	1.36
1	L1	1533	PSU	C6-N1	5.36	1.45	1.36
2	L2	1264	PSU	C6-N1	5.36	1.45	1.36
2	L2	686	OMG	C2-N3	5.35	1.46	1.33
51	S1	104	PSU	C6-N1	5.35	1.45	1.36
2	L2	655	OMG	C2-N3	5.35	1.46	1.33
2	L2	593	PSU	C6-N1	5.35	1.45	1.36
2	L2	1194	PSU	C6-N1	5.35	1.45	1.36
51	S1	455	PSU	C6-N1	5.34	1.45	1.36
51	S1	2048	PSU	C6-N1	5.34	1.45	1.36
2	L2	1361	PSU	C6-N1	5.33	1.45	1.36
2	L2	359	OMC	C4-N3	5.30	1.45	1.34
2	L2	534	OMG	C2-N3	5.30	1.46	1.33
7	L7	75	OMG	C2-N3	5.29	1.46	1.33
51	S1	2151	OMG	C2-N3	5.29	1.46	1.33
51	S1	2008	OMG	C2-N3	5.27	1.46	1.33
2	L2	1231	OMG	C2-N3	5.26	1.46	1.33
4	L4	74	OMG	C2-N3	5.24	1.45	1.33
1	L1	695	OMC	C4-N3	5.24	1.45	1.34
2	L2	1159	OMC	C4-N3	5.24	1.45	1.34
1	L1	1552	OMC	C4-N3	5.23	1.45	1.34
51	S1	2059	OMC	C4-N3	5.23	1.45	1.34
51	S1	2140	OMC	C4-N3	5.23	1.45	1.34
51	S1	2019	OMC	C4-N3	5.22	1.45	1.34
51	S1	38	OMC	C4-N3	5.22	1.45	1.34
2	L2	14	OMC	C4-N3	5.22	1.45	1.34
51	S1	1866	OMC	C4-N3	5.22	1.45	1.34
7	L7	101	OMU	C1'-N1	-5.21	1.32	1.47
51	S1	18	OMC	C4-N3	5.21	1.45	1.34
2	L2	583	OMC	C4-N3	5.18	1.44	1.34
2	L2	1317	OMC	C4-N3	5.17	1.44	1.34
51	S1	1478	OMG	C2-N3	5.16	1.45	1.33
2	L2	71	OMG	C2-N3	5.15	1.45	1.33
1	L1	1190	OMG	C2-N3	5.14	1.45	1.33
1	L1	1524	OMG	C2-N3	5.09	1.45	1.33
2	L2	1253	OMG	C2-N3	5.07	1.45	1.33
2	L2	359	OMC	C4-N4	5.06	1.45	1.33
51	S1	2140	OMC	C4-N4	5.05	1.45	1.33
2	L2	1248	OMC	C4-N3	5.04	1.44	1.34
1	L1	1010	OMC	C4-N4	5.03	1.45	1.33
2	L2	583	OMC	C4-N4	5.03	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1626	OMG	C2-N3	5.02	1.45	1.33
1	L1	856	OMG	C2-N3	5.02	1.45	1.33
1	L1	1527	OMC	C4-N3	5.02	1.44	1.34
51	S1	2059	OMC	C4-N4	5.02	1.45	1.33
1	L1	1527	OMC	C2-N1	5.01	1.50	1.40
51	S1	1866	OMC	C4-N4	5.01	1.45	1.33
51	S1	38	OMC	C4-N4	5.00	1.45	1.33
1	L1	695	OMC	C4-N4	5.00	1.45	1.33
51	S1	1550	OMG	C2-N3	5.00	1.45	1.33
2	L2	1078	OMG	C2-N3	5.00	1.45	1.33
51	S1	1865	OMG	C4-N3	5.00	1.49	1.37
1	L1	1552	OMC	C4-N4	5.00	1.45	1.33
2	L2	14	OMC	C4-N4	5.00	1.45	1.33
51	S1	2019	OMC	C4-N4	4.99	1.45	1.33
1	L1	1540	OMG	C2-N3	4.99	1.45	1.33
2	L2	1159	OMC	C4-N4	4.98	1.45	1.33
51	S1	1623	OMG	C4-N3	4.97	1.49	1.37
1	L1	959	OMG	C4-N3	4.96	1.49	1.37
2	L2	1317	OMC	C4-N4	4.96	1.45	1.33
51	S1	18	OMC	C4-N4	4.96	1.45	1.33
51	S1	1647	OMG	C4-N3	4.95	1.49	1.37
2	L2	1229	OMG	C4-N3	4.95	1.49	1.37
2	L2	1046	OMG	C4-N3	4.95	1.49	1.37
2	L2	641	OMG	C2-N3	4.94	1.45	1.33
2	L2	655	OMG	C4-N3	4.94	1.49	1.37
1	L1	669	OMC	C4-N3	4.94	1.44	1.34
2	L2	1397	OMC	C4-N3	4.94	1.44	1.34
1	L1	1010	OMC	C4-N3	4.94	1.44	1.34
7	L7	75	OMG	C4-N3	4.93	1.49	1.37
2	L2	443	OMC	C4-N3	4.93	1.44	1.34
2	L2	686	OMG	C4-N3	4.93	1.49	1.37
2	L2	1360	OMG	C4-N3	4.92	1.49	1.37
51	S1	1829	OMG	C2-N3	4.91	1.45	1.33
51	S1	600	OMG	C4-N3	4.91	1.49	1.37
1	L1	856	OMG	C4-N3	4.89	1.49	1.37
2	L2	71	OMG	C4-N3	4.89	1.49	1.37
51	S1	2008	OMG	C4-N3	4.88	1.49	1.37
51	S1	2151	OMG	C4-N3	4.87	1.49	1.37
2	L2	1253	OMG	C4-N3	4.87	1.49	1.37
1	L1	1626	OMG	C4-N3	4.87	1.49	1.37
2	L2	1308	5MC	C4-N4	4.87	1.46	1.34
1	L1	1540	OMG	C4-N3	4.84	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	534	OMG	C4-N3	4.84	1.49	1.37
51	S1	1550	OMG	C4-N3	4.83	1.49	1.37
1	L1	1524	OMG	C4-N3	4.82	1.49	1.37
2	L2	1231	OMG	C4-N3	4.82	1.49	1.37
4	L4	74	OMG	C4-N3	4.82	1.49	1.37
2	L2	1397	OMC	C4-N4	4.82	1.45	1.33
2	L2	641	OMG	C4-N3	4.81	1.49	1.37
2	L2	1248	OMC	C2-N1	4.79	1.50	1.40
1	L1	669	OMC	C4-N4	4.78	1.45	1.33
2	L2	1248	OMC	C4-N4	4.78	1.45	1.33
2	L2	1397	OMC	C2-N1	4.77	1.50	1.40
51	S1	1829	OMG	C4-N3	4.77	1.48	1.37
1	L1	1527	OMC	C4-N4	4.77	1.45	1.33
1	L1	1190	OMG	C4-N3	4.76	1.48	1.37
2	L2	1360	OMG	C2-N2	4.76	1.45	1.34
51	S1	1478	OMG	C4-N3	4.76	1.48	1.37
51	S1	1647	OMG	C2-N2	4.76	1.45	1.34
1	L1	959	OMG	C2-N2	4.76	1.45	1.34
2	L2	1229	OMG	C2-N2	4.75	1.45	1.34
7	L7	75	OMG	C2-N2	4.75	1.45	1.34
51	S1	1865	OMG	C2-N2	4.75	1.45	1.34
2	L2	655	OMG	C2-N2	4.74	1.45	1.34
2	L2	686	OMG	C2-N2	4.74	1.45	1.34
51	S1	1623	OMG	C2-N2	4.73	1.45	1.34
2	L2	1046	OMG	C2-N2	4.73	1.45	1.34
51	S1	2008	OMG	C2-N2	4.72	1.45	1.34
51	S1	2061	5MC	C6-N1	4.72	1.46	1.38
51	S1	600	OMG	C2-N2	4.70	1.45	1.34
4	L4	74	OMG	C2-N2	4.69	1.45	1.34
51	S1	2151	OMG	C2-N2	4.68	1.45	1.34
1	L1	1190	OMG	C2-N2	4.68	1.45	1.34
2	L2	443	OMC	C4-N4	4.67	1.44	1.33
2	L2	534	OMG	C2-N2	4.65	1.45	1.34
2	L2	524	5MC	C6-N1	4.65	1.46	1.38
2	L2	1231	OMG	C2-N2	4.65	1.45	1.34
51	S1	1478	OMG	C2-N2	4.64	1.45	1.34
51	S1	1544	5MC	C6-N1	4.63	1.46	1.38
7	L7	69	PSU	C1'-C5	-4.63	1.39	1.50
1	L1	1010	OMC	C2-N1	4.61	1.50	1.40
2	L2	1078	OMG	C2-N2	4.61	1.45	1.34
2	L2	14	OMC	C2-N1	4.60	1.50	1.40
2	L2	1382	PSU	C1'-C5	-4.59	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	1078	OMG	C4-N3	4.59	1.48	1.37
1	L1	677	1MA	C2-N1	4.59	1.44	1.35
51	S1	2140	OMC	C2-N1	4.59	1.49	1.40
51	S1	1866	OMC	C2-N1	4.58	1.49	1.40
51	S1	2059	OMC	C2-N1	4.57	1.49	1.40
2	L2	583	OMC	C2-N1	4.57	1.49	1.40
2	L2	1058	PSU	C1'-C5	-4.56	1.39	1.50
2	L2	662	PSU	C1'-C5	-4.55	1.39	1.50
1	L1	672	PSU	C1'-C5	-4.54	1.39	1.50
51	S1	1539	PSU	C1'-C5	-4.54	1.39	1.50
2	L2	443	OMC	C2-N1	4.53	1.49	1.40
1	L1	1552	OMC	C2-N1	4.53	1.49	1.40
2	L2	359	OMC	C2-N1	4.53	1.49	1.40
51	S1	2019	OMC	C2-N1	4.53	1.49	1.40
2	L2	1159	OMC	C2-N1	4.52	1.49	1.40
51	S1	38	OMC	C2-N1	4.52	1.49	1.40
2	L2	1317	OMC	C2-N1	4.51	1.49	1.40
2	L2	1413	PSU	C1'-C5	-4.50	1.39	1.50
1	L1	695	OMC	C2-N1	4.50	1.49	1.40
2	L2	1403	PSU	C1'-C5	-4.50	1.39	1.50
1	L1	1017	PSU	C1'-C5	-4.49	1.39	1.50
51	S1	18	OMC	C2-N1	4.48	1.49	1.40
1	L1	1171	PSU	C1'-C5	-4.47	1.40	1.50
1	L1	1528	PSU	C1'-C5	-4.43	1.40	1.50
1	L1	1540	OMG	C2-N2	4.38	1.44	1.34
51	S1	1544	5MC	C4-N4	4.38	1.45	1.34
51	S1	1841	PSU	C1'-C5	-4.37	1.40	1.50
51	S1	1657	PSU	C1'-C5	-4.36	1.40	1.50
2	L2	1253	OMG	C2-N2	4.36	1.44	1.34
1	L1	1626	OMG	C2-N2	4.35	1.44	1.34
1	L1	669	OMC	C2-N1	4.34	1.49	1.40
2	L2	1060	PSU	C1'-C5	-4.34	1.40	1.50
51	S1	1550	OMG	C2-N2	4.34	1.44	1.34
51	S1	2061	5MC	C4-N4	4.34	1.45	1.34
1	L1	1181	PSU	C1'-C5	-4.33	1.40	1.50
2	L2	71	OMG	C2-N2	4.33	1.44	1.34
2	L2	1361	PSU	C1'-C5	-4.33	1.40	1.50
2	L2	524	5MC	C4-N4	4.32	1.45	1.34
1	L1	1524	OMG	C2-N2	4.32	1.44	1.34
1	L1	774	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	500	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	1213	PSU	C1'-C5	-4.31	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	2046	PSU	C1'-C5	-4.31	1.40	1.50
2	L2	1144	PSU	C1'-C5	-4.31	1.40	1.50
51	S1	1544	5MC	C2-N1	4.31	1.49	1.40
1	L1	239	PSU	C1'-C5	-4.30	1.40	1.50
51	S1	1246	PSU	C1'-C5	-4.30	1.40	1.50
2	L2	593	PSU	C1'-C5	-4.29	1.40	1.50
51	S1	33	PSU	C1'-C5	-4.29	1.40	1.50
51	S1	2048	PSU	C1'-C5	-4.29	1.40	1.50
2	L2	472	PSU	C1'-C5	-4.29	1.40	1.50
1	L1	940	PSU	C1'-C5	-4.29	1.40	1.50
51	S1	104	PSU	C1'-C5	-4.28	1.40	1.50
51	S1	1829	OMG	C2-N2	4.28	1.44	1.34
2	L2	1303	PSU	C1'-C5	-4.28	1.40	1.50
2	L2	512	PSU	C1'-C5	-4.28	1.40	1.50
2	L2	1194	PSU	C1'-C5	-4.28	1.40	1.50
2	L2	626	PSU	C1'-C5	-4.27	1.40	1.50
51	S1	1533	PSU	C1'-C5	-4.27	1.40	1.50
51	S1	1292	PSU	C1'-C5	-4.27	1.40	1.50
7	L7	74	PSU	C1'-C5	-4.27	1.40	1.50
2	L2	506	PSU	C1'-C5	-4.27	1.40	1.50
1	L1	1093	PSU	C1'-C5	-4.27	1.40	1.50
2	L2	597	PSU	C1'-C5	-4.26	1.40	1.50
51	S1	1156	PSU	C1'-C5	-4.26	1.40	1.50
1	L1	422	PSU	C1'-C5	-4.26	1.40	1.50
2	L2	641	OMG	C2-N2	4.25	1.44	1.34
1	L1	856	OMG	C2-N2	4.25	1.44	1.34
2	L2	1318	PSU	C1'-C5	-4.25	1.40	1.50
2	L2	524	5MC	C2-N1	4.24	1.49	1.40
2	L2	510	PSU	C1'-C5	-4.24	1.40	1.50
51	S1	609	PSU	C1'-C5	-4.24	1.40	1.50
2	L2	504	PSU	C1'-C5	-4.23	1.40	1.50
2	L2	1308	5MC	O4'-C1'	-4.23	1.32	1.42
1	L1	1533	PSU	C1'-C5	-4.22	1.40	1.50
51	S1	1777	OMU	C4-N3	4.22	1.46	1.38
2	L2	78	PSU	C1'-C5	-4.21	1.40	1.50
2	L2	1284	PSU	C1'-C5	-4.20	1.40	1.50
51	S1	1566	PSU	C1'-C5	-4.20	1.40	1.50
51	S1	2202	PSU	C1'-C5	-4.20	1.40	1.50
1	L1	1107	OMU	C4-N3	4.19	1.46	1.38
51	S1	12	PSU	C1'-C5	-4.18	1.40	1.50
2	L2	437	PSU	C1'-C5	-4.18	1.40	1.50
2	L2	1419	OMU	C4-N3	4.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1253	OMU	C4-N3	4.18	1.46	1.38
51	S1	2061	5MC	C2-N1	4.17	1.49	1.40
51	S1	1621	OMU	C4-N3	4.17	1.46	1.38
7	L7	101	OMU	C3'-C4'	4.17	1.63	1.53
3	L3	13	OMU	C4-N3	4.16	1.46	1.38
51	S1	1979	OMU	C4-N3	4.16	1.46	1.38
1	L1	1659	OMU	C4-N3	4.16	1.46	1.38
51	S1	29	OMU	C4-N3	4.15	1.46	1.38
1	L1	1664	PSU	C1'-C5	-4.15	1.40	1.50
51	S1	1662	OMU	C4-N3	4.15	1.46	1.38
1	L1	677	1MA	C4-N3	4.15	1.50	1.37
2	L2	1308	5MC	C6-N1	4.14	1.45	1.38
2	L2	56	OMU	C4-N3	4.14	1.46	1.38
2	L2	1359	OMU	C4-N3	4.14	1.46	1.38
2	L2	1265	PSU	C1'-C5	-4.14	1.40	1.50
51	S1	661	OMU	C4-N3	4.14	1.46	1.38
1	L1	845	OMU	C4-N3	4.13	1.46	1.38
2	L2	1308	5MC	C2-N1	4.12	1.48	1.40
51	S1	455	PSU	C1'-C5	-4.11	1.40	1.50
7	L7	101	OMU	C4-N3	4.11	1.45	1.38
1	L1	48	OMU	C4-N3	4.11	1.45	1.38
2	L2	667	OMU	C4-N3	4.10	1.45	1.38
1	L1	847	OMU	C4-N3	4.09	1.45	1.38
1	L1	1371	OMU	C4-N3	4.09	1.45	1.38
2	L2	504	PSU	C4-N3	4.08	1.46	1.38
51	S1	8	OMU	C4-N3	4.08	1.45	1.38
2	L2	1264	PSU	C1'-C5	-4.08	1.40	1.50
1	L1	1190	OMG	C6-N1	4.07	1.43	1.37
2	L2	1078	OMG	C6-N1	4.06	1.43	1.37
51	S1	1192	PSU	C1'-C5	-4.06	1.40	1.50
2	L2	560	OMU	C4-N3	4.06	1.45	1.38
2	L2	512	PSU	C4-N3	4.05	1.46	1.38
51	S1	1192	PSU	C4-N3	4.05	1.46	1.38
2	L2	73	OMU	C4-N3	4.05	1.45	1.38
51	S1	609	PSU	C4-N3	4.04	1.46	1.38
51	S1	1566	PSU	C4-N3	4.04	1.46	1.38
2	L2	500	PSU	C4-N3	4.03	1.46	1.38
2	L2	437	PSU	C4-N3	4.01	1.46	1.38
2	L2	1284	PSU	C4-N3	4.01	1.46	1.38
51	S1	455	PSU	C4-N3	4.01	1.46	1.38
2	L2	1077	OMU	C4-N3	4.01	1.45	1.38
1	L1	1533	PSU	C4-N3	4.01	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1533	PSU	C4-N3	4.00	1.46	1.38
51	S1	33	PSU	C4-N3	4.00	1.46	1.38
2	L2	506	PSU	C4-N3	4.00	1.46	1.38
2	L2	472	PSU	C4-N3	3.99	1.46	1.38
51	S1	1657	PSU	C4-N3	3.99	1.46	1.38
51	S1	2046	PSU	C4-N3	3.99	1.46	1.38
2	L2	1303	PSU	C4-N3	3.99	1.46	1.38
51	S1	1292	PSU	C4-N3	3.99	1.46	1.38
7	L7	74	PSU	C4-N3	3.99	1.46	1.38
51	S1	12	PSU	C4-N3	3.98	1.46	1.38
51	S1	2048	PSU	C4-N3	3.98	1.46	1.38
51	S1	1841	PSU	C4-N3	3.98	1.46	1.38
51	S1	1246	PSU	C4-N3	3.98	1.46	1.38
51	S1	2202	PSU	C4-N3	3.98	1.46	1.38
1	L1	1664	PSU	C4-N3	3.98	1.46	1.38
1	L1	1011	PSU	C1'-C5	-3.97	1.41	1.50
2	L2	593	PSU	C4-N3	3.97	1.46	1.38
1	L1	1093	PSU	C4-N3	3.97	1.46	1.38
2	L2	1318	PSU	C4-N3	3.96	1.46	1.38
51	S1	104	PSU	C4-N3	3.96	1.46	1.38
1	L1	239	PSU	C4-N3	3.96	1.46	1.38
2	L2	626	PSU	C4-N3	3.96	1.46	1.38
2	L2	597	PSU	C4-N3	3.96	1.46	1.38
1	L1	422	PSU	C4-N3	3.96	1.46	1.38
2	L2	1213	PSU	C4-N3	3.96	1.46	1.38
51	S1	1833	OMU	C4-N3	3.95	1.45	1.38
2	L2	1194	PSU	C4-N3	3.95	1.46	1.38
1	L1	1039	OMU	C4-N3	3.95	1.45	1.38
2	L2	510	PSU	C4-N3	3.94	1.46	1.38
2	L2	1361	PSU	C4-N3	3.93	1.46	1.38
1	L1	774	PSU	C4-N3	3.92	1.46	1.38
1	L1	940	PSU	C4-N3	3.92	1.46	1.38
2	L2	78	PSU	C4-N3	3.91	1.46	1.38
51	S1	1156	PSU	C4-N3	3.91	1.46	1.38
2	L2	686	OMG	C6-N1	3.90	1.43	1.37
4	L4	74	OMG	C6-N1	3.90	1.43	1.37
1	L1	1181	PSU	C4-N3	3.90	1.46	1.38
2	L2	1060	PSU	C4-N3	3.89	1.46	1.38
2	L2	1144	PSU	C4-N3	3.89	1.46	1.38
51	S1	1478	OMG	C6-N1	3.88	1.43	1.37
2	L2	1265	PSU	C4-N3	3.87	1.46	1.38
51	S1	1647	OMG	C6-N1	3.86	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	2008	OMG	C6-N1	3.86	1.43	1.37
51	S1	600	OMG	C6-N1	3.82	1.43	1.37
51	S1	2151	OMG	C6-N1	3.82	1.43	1.37
7	L7	75	OMG	C6-N1	3.80	1.43	1.37
2	L2	534	OMG	C6-N1	3.80	1.43	1.37
1	L1	1011	PSU	C4-N3	3.80	1.45	1.38
2	L2	1264	PSU	C4-N3	3.78	1.45	1.38
51	S1	1623	OMG	C6-N1	3.77	1.43	1.37
2	L2	1231	OMG	C6-N1	3.77	1.43	1.37
51	S1	1865	OMG	C6-N1	3.76	1.43	1.37
2	L2	1046	OMG	C6-N1	3.75	1.43	1.37
1	L1	1528	PSU	C4-N3	3.73	1.45	1.38
2	L2	1229	OMG	C6-N1	3.73	1.43	1.37
7	L7	69	PSU	C4-N3	3.73	1.45	1.38
2	L2	1397	OMC	C6-N1	3.72	1.47	1.38
1	L1	1017	PSU	C4-N3	3.71	1.45	1.38
2	L2	1248	OMC	C6-N1	3.71	1.46	1.38
2	L2	1360	OMG	C6-N1	3.70	1.43	1.37
1	L1	959	OMG	C6-N1	3.69	1.43	1.37
1	L1	1527	OMC	C6-N1	3.69	1.46	1.38
2	L2	1403	PSU	C4-N3	3.68	1.45	1.38
2	L2	655	OMG	C6-N1	3.68	1.43	1.37
1	L1	1171	PSU	C4-N3	3.67	1.45	1.38
2	L2	662	PSU	C4-N3	3.65	1.45	1.38
51	S1	1995	7MG	C6-N1	3.64	1.45	1.38
2	L2	1382	PSU	C4-N3	3.64	1.45	1.38
51	S1	1539	PSU	C4-N3	3.64	1.45	1.38
2	L2	1413	PSU	C4-N3	3.63	1.45	1.38
51	S1	1543	B8N	C1'-C5	3.59	1.58	1.50
2	L2	1058	PSU	C4-N3	3.58	1.45	1.38
51	S1	1995	7MG	C2-N1	3.56	1.46	1.37
51	S1	1995	7MG	C5-C6	3.51	1.52	1.43
1	L1	672	PSU	C4-N3	3.49	1.45	1.38
1	L1	1010	OMC	C6-N1	3.45	1.46	1.38
1	L1	927	A2M	O3'-C3'	-3.35	1.35	1.43
1	L1	695	OMC	C6-N1	3.35	1.46	1.38
51	S1	1995	7MG	C2-N2	3.35	1.42	1.34
2	L2	359	OMC	C6-N1	3.34	1.46	1.38
1	L1	1539	A2M	O3'-C3'	-3.34	1.35	1.43
2	L2	583	OMC	C6-N1	3.34	1.46	1.38
51	S1	2140	OMC	C6-N1	3.33	1.46	1.38
2	L2	1317	OMC	C6-N1	3.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	382	A2M	O3'-C3'	-3.32	1.35	1.43
51	S1	1866	OMC	C6-N1	3.31	1.46	1.38
51	S1	2151	OMG	C5-C6	3.31	1.54	1.47
2	L2	1159	OMC	C6-N1	3.30	1.46	1.38
2	L2	1185	A2M	O3'-C3'	-3.30	1.35	1.43
51	S1	38	OMC	C6-N1	3.30	1.46	1.38
1	L1	1039	OMU	C6-N1	3.29	1.45	1.38
51	S1	2019	OMC	C6-N1	3.29	1.45	1.38
51	S1	661	OMU	C6-N1	3.29	1.45	1.38
2	L2	655	OMG	C5-C6	3.29	1.54	1.47
1	L1	1552	OMC	C6-N1	3.28	1.45	1.38
2	L2	1078	OMG	C5-C6	3.27	1.54	1.47
1	L1	1190	OMG	C5-C6	3.27	1.54	1.47
2	L2	14	OMC	C6-N1	3.27	1.45	1.38
51	S1	1829	OMG	C5-C6	3.26	1.54	1.47
51	S1	2059	OMC	C6-N1	3.26	1.45	1.38
51	S1	18	OMC	C6-N1	3.26	1.45	1.38
2	L2	686	OMG	C5-C6	3.25	1.54	1.47
1	L1	681	A2M	O3'-C3'	-3.23	1.35	1.43
7	L7	75	OMG	C5-C6	3.21	1.53	1.47
51	S1	2008	OMG	C5-C6	3.21	1.53	1.47
2	L2	1077	OMU	C6-N1	3.21	1.45	1.38
51	S1	1647	OMG	C5-C6	3.20	1.53	1.47
51	S1	1623	OMG	C5-C6	3.19	1.53	1.47
1	L1	858	A2M	O3'-C3'	-3.19	1.35	1.43
51	S1	1865	OMG	C5-C6	3.19	1.53	1.47
2	L2	534	OMG	C5-C6	3.18	1.53	1.47
2	L2	1384	A2M	O3'-C3'	-3.18	1.35	1.43
2	L2	443	OMC	C6-N1	3.18	1.45	1.38
51	S1	600	OMG	C5-C6	3.17	1.53	1.47
2	L2	641	OMG	C5-C6	3.16	1.53	1.47
2	L2	502	A2M	C6-N6	3.16	1.45	1.34
4	L4	74	OMG	C5-C6	3.16	1.53	1.47
51	S1	1478	OMG	C5-C6	3.16	1.53	1.47
51	S1	28	A2M	C6-N6	3.14	1.45	1.34
2	L2	591	A2M	C6-N6	3.13	1.45	1.34
51	S1	479	A2M	C6-N6	3.13	1.45	1.34
2	L2	1372	A2M	C6-N6	3.13	1.45	1.34
51	S1	512	A2M	C6-N6	3.13	1.45	1.34
1	L1	235	A2M	C6-N6	3.13	1.45	1.34
51	S1	2021	A2M	O2'-C2'	3.13	1.50	1.42
51	S1	98	A2M	C6-N6	3.12	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L7	162	A2M	C6-N6	3.12	1.45	1.34
2	L2	665	A2M	C6-N6	3.12	1.45	1.34
51	S1	2021	A2M	C6-N6	3.12	1.45	1.34
1	L1	1540	OMG	C5-C6	3.12	1.53	1.47
51	S1	897	A2M	C6-N6	3.12	1.45	1.34
2	L2	570	A2M	C6-N6	3.12	1.45	1.34
2	L2	1067	A2M	C6-N6	3.11	1.45	1.34
2	L2	628	A2M	C6-N6	3.11	1.45	1.34
1	L1	959	OMG	C5-C6	3.11	1.53	1.47
2	L2	95	A2M	C6-N6	3.11	1.45	1.34
1	L1	1373	A2M	C6-N6	3.11	1.45	1.34
1	L1	955	A2M	C6-N6	3.11	1.45	1.34
51	S1	897	A2M	O3'-C3'	-3.11	1.35	1.43
1	L1	305	A2M	C6-N6	3.11	1.45	1.34
2	L2	604	A2M	C6-N6	3.11	1.45	1.34
7	L7	43	A2M	C6-N6	3.11	1.45	1.34
1	L1	678	A2M	C6-N6	3.10	1.45	1.34
51	S1	1833	OMU	C6-N1	3.10	1.45	1.38
2	L2	1229	OMG	C5-C6	3.10	1.53	1.47
2	L2	1253	OMG	C5-C6	3.09	1.53	1.47
2	L2	572	A2M	C6-N6	3.08	1.45	1.34
2	L2	1360	OMG	C5-C6	3.08	1.53	1.47
2	L2	1231	OMG	C5-C6	3.08	1.53	1.47
1	L1	697	A2M	C6-N6	3.08	1.45	1.34
2	L2	1046	OMG	C5-C6	3.08	1.53	1.47
2	L2	1308	5MC	O3'-C3'	3.07	1.50	1.43
1	L1	669	OMC	C6-N1	3.06	1.45	1.38
2	L2	1067	A2M	O3'-C3'	-3.06	1.35	1.43
51	S1	969	A2M	C6-N6	3.06	1.45	1.34
51	S1	512	A2M	O3'-C3'	-3.05	1.35	1.43
2	L2	1185	A2M	O2'-C2'	3.05	1.50	1.42
2	L2	1308	5MC	O2'-C2'	-3.05	1.35	1.43
51	S1	668	A2M	O3'-C3'	-3.05	1.35	1.43
7	L7	43	A2M	O3'-C3'	-3.04	1.35	1.43
51	S1	8	OMU	O4-C4	-3.03	1.18	1.24
51	S1	1995	7MG	O6-C6	-3.03	1.17	1.23
2	L2	560	OMU	C6-N1	3.02	1.45	1.38
1	L1	1626	OMG	C5-C6	3.02	1.53	1.47
2	L2	95	A2M	O3'-C3'	-3.01	1.35	1.43
51	S1	28	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	955	A2M	O3'-C3'	-3.01	1.35	1.43
2	L2	73	OMU	O4-C4	-3.01	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	71	OMG	C5-C6	3.01	1.53	1.47
1	L1	235	A2M	O3'-C3'	-3.01	1.35	1.43
1	L1	48	OMU	O4-C4	-3.01	1.18	1.24
51	S1	1833	OMU	O4-C4	-3.01	1.18	1.24
2	L2	665	A2M	O3'-C3'	-3.00	1.35	1.43
2	L2	570	A2M	O3'-C3'	-3.00	1.35	1.43
1	L1	1540	OMG	C6-N1	3.00	1.42	1.37
7	L7	162	A2M	O3'-C3'	-3.00	1.35	1.43
1	L1	681	A2M	O2'-C2'	3.00	1.50	1.42
2	L2	502	A2M	O3'-C3'	-2.99	1.35	1.43
1	L1	1539	A2M	O2'-C2'	2.99	1.50	1.42
1	L1	69	A2M	O3'-C3'	-2.99	1.35	1.43
1	L1	697	A2M	O3'-C3'	-2.99	1.35	1.43
2	L2	604	A2M	O3'-C3'	-2.98	1.35	1.43
7	L7	101	OMU	O4-C4	-2.98	1.18	1.24
2	L2	382	A2M	O2'-C2'	2.98	1.50	1.42
51	S1	1829	OMG	C6-N1	2.97	1.42	1.37
51	S1	98	A2M	O3'-C3'	-2.97	1.36	1.43
1	L1	1107	OMU	O4-C4	-2.96	1.18	1.24
2	L2	570	A2M	O2'-C2'	2.96	1.50	1.42
1	L1	1371	OMU	O4-C4	-2.96	1.18	1.24
1	L1	1373	A2M	O3'-C3'	-2.96	1.36	1.43
3	L3	13	OMU	O4-C4	-2.96	1.18	1.24
2	L2	628	A2M	O3'-C3'	-2.96	1.36	1.43
2	L2	591	A2M	O3'-C3'	-2.96	1.36	1.43
2	L2	56	OMU	O4-C4	-2.96	1.18	1.24
2	L2	1419	OMU	O4-C4	-2.96	1.18	1.24
1	L1	847	OMU	O4-C4	-2.95	1.18	1.24
2	L2	604	A2M	O2'-C2'	2.95	1.50	1.42
51	S1	1550	OMG	C5-C6	2.95	1.53	1.47
7	L7	101	OMU	C6-N1	2.95	1.45	1.38
51	S1	1550	OMG	C6-N1	2.95	1.42	1.37
51	S1	29	OMU	O4-C4	-2.95	1.18	1.24
1	L1	847	OMU	C6-N1	2.94	1.45	1.38
2	L2	667	OMU	O4-C4	-2.94	1.18	1.24
2	L2	1384	A2M	O2'-C2'	2.94	1.50	1.42
1	L1	927	A2M	O2'-C2'	2.94	1.50	1.42
2	L2	1419	OMU	C6-N1	2.94	1.45	1.38
2	L2	1185	A2M	C6-N6	2.94	1.44	1.34
51	S1	2021	A2M	O3'-C3'	-2.93	1.36	1.43
2	L2	56	OMU	C6-N1	2.93	1.45	1.38
2	L2	73	OMU	C6-N1	2.93	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L7	162	A2M	O2'-C2'	2.93	1.50	1.42
1	L1	955	A2M	O2'-C2'	2.93	1.50	1.42
2	L2	572	A2M	O3'-C3'	-2.92	1.36	1.43
1	L1	845	OMU	C6-N1	2.92	1.45	1.38
3	L3	13	OMU	C6-N1	2.92	1.45	1.38
1	L1	48	OMU	C6-N1	2.91	1.45	1.38
2	L2	665	A2M	O2'-C2'	2.91	1.50	1.42
51	S1	1662	OMU	O4-C4	-2.91	1.18	1.24
51	S1	969	A2M	O3'-C3'	-2.91	1.36	1.43
2	L2	1359	OMU	O4-C4	-2.91	1.18	1.24
1	L1	305	A2M	O3'-C3'	-2.91	1.36	1.43
2	L2	95	A2M	O2'-C2'	2.91	1.50	1.42
2	L2	1359	OMU	C6-N1	2.91	1.45	1.38
1	L1	1659	OMU	O4-C4	-2.91	1.18	1.24
51	S1	1979	OMU	C6-N1	2.91	1.45	1.38
51	S1	1777	OMU	O4-C4	-2.91	1.18	1.24
1	L1	235	A2M	O2'-C2'	2.90	1.50	1.42
1	L1	1371	OMU	C6-N1	2.90	1.45	1.38
51	S1	1662	OMU	C6-N1	2.90	1.45	1.38
51	S1	1621	OMU	O4-C4	-2.90	1.18	1.24
2	L2	591	A2M	O2'-C2'	2.90	1.50	1.42
51	S1	668	A2M	C6-N6	2.90	1.44	1.34
51	S1	1979	OMU	O4-C4	-2.90	1.18	1.24
1	L1	845	OMU	O4-C4	-2.90	1.18	1.24
2	L2	1078	OMG	C2-N1	2.90	1.44	1.37
51	S1	1777	OMU	C6-N1	2.89	1.45	1.38
51	S1	479	A2M	O2'-C2'	2.89	1.50	1.42
2	L2	667	OMU	C6-N1	2.89	1.45	1.38
1	L1	858	A2M	O2'-C2'	2.89	1.50	1.42
2	L2	1372	A2M	O2'-C2'	2.88	1.50	1.42
51	S1	668	A2M	O2'-C2'	2.88	1.50	1.42
2	L2	1372	A2M	O3'-C3'	-2.88	1.36	1.43
51	S1	479	A2M	O3'-C3'	-2.88	1.36	1.43
2	L2	641	OMG	C6-N1	2.88	1.42	1.37
1	L1	1659	OMU	C6-N1	2.88	1.44	1.38
1	L1	1190	OMG	C2-N1	2.87	1.44	1.37
51	S1	1621	OMU	C6-N1	2.87	1.44	1.38
51	S1	8	OMU	C6-N1	2.87	1.44	1.38
51	S1	29	OMU	C6-N1	2.86	1.44	1.38
1	L1	697	A2M	O2'-C2'	2.86	1.49	1.42
7	L7	43	A2M	O2'-C2'	2.86	1.49	1.42
51	S1	969	A2M	O2'-C2'	2.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1107	OMU	C6-N1	2.86	1.44	1.38
2	L2	1253	OMG	C6-N1	2.86	1.42	1.37
51	S1	98	A2M	O2'-C2'	2.85	1.49	1.42
1	L1	1253	OMU	C6-N1	2.85	1.44	1.38
2	L2	572	A2M	O2'-C2'	2.85	1.49	1.42
2	L2	628	A2M	O2'-C2'	2.85	1.49	1.42
1	L1	1253	OMU	O4-C4	-2.85	1.19	1.24
1	L1	1524	OMG	C5-C6	2.84	1.53	1.47
51	S1	512	A2M	O2'-C2'	2.84	1.49	1.42
51	S1	1478	OMG	C2-N1	2.84	1.44	1.37
2	L2	502	A2M	O2'-C2'	2.84	1.49	1.42
1	L1	1373	A2M	O2'-C2'	2.84	1.49	1.42
2	L2	1231	OMG	C2-N1	2.84	1.44	1.37
1	L1	69	A2M	C6-N6	2.83	1.44	1.34
1	L1	858	A2M	C6-N6	2.83	1.44	1.34
1	L1	856	OMG	C5-C6	2.83	1.53	1.47
2	L2	686	OMG	C2-N1	2.83	1.44	1.37
1	L1	1626	OMG	C6-N1	2.83	1.42	1.37
1	L1	678	A2M	O3'-C3'	-2.83	1.36	1.43
51	S1	28	A2M	O2'-C2'	2.83	1.49	1.42
2	L2	527	A2M	O2'-C2'	2.82	1.49	1.42
7	L7	75	OMG	C2-N1	2.82	1.44	1.37
1	L1	678	A2M	O2'-C2'	2.82	1.49	1.42
51	S1	600	OMG	C2-N1	2.82	1.44	1.37
2	L2	1067	A2M	O2'-C2'	2.81	1.49	1.42
51	S1	1647	OMG	C2-N1	2.81	1.44	1.37
2	L2	534	OMG	C2-N1	2.81	1.44	1.37
1	L1	1039	OMU	O4-C4	-2.81	1.19	1.24
4	L4	74	OMG	C2-N1	2.81	1.44	1.37
2	L2	1046	OMG	C2-N1	2.81	1.44	1.37
1	L1	1539	A2M	C6-N6	2.80	1.44	1.34
2	L2	1078	OMG	C5-C4	-2.80	1.35	1.43
1	L1	959	OMG	C2-N1	2.79	1.44	1.37
51	S1	2151	OMG	C2-N1	2.79	1.44	1.37
51	S1	2059	OMC	O2-C2	-2.78	1.18	1.23
51	S1	1865	OMG	C2-N1	2.78	1.44	1.37
51	S1	1623	OMG	C2-N1	2.78	1.44	1.37
2	L2	1229	OMG	C2-N1	2.78	1.44	1.37
51	S1	897	A2M	O2'-C2'	2.78	1.49	1.42
1	L1	927	A2M	C6-N6	2.78	1.44	1.34
1	L1	1190	OMG	C5-C4	-2.77	1.36	1.43
2	L2	443	OMC	C5-C4	2.77	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	2008	OMG	C2-N1	2.77	1.44	1.37
1	L1	681	A2M	C6-N6	2.77	1.44	1.34
51	S1	2008	OMG	C5-C4	-2.76	1.36	1.43
2	L2	527	A2M	C6-N6	2.76	1.44	1.34
2	L2	1384	A2M	C6-N6	2.76	1.44	1.34
1	L1	69	A2M	O2'-C2'	2.75	1.49	1.42
2	L2	1360	OMG	C2-N1	2.75	1.44	1.37
51	S1	661	OMU	O4-C4	-2.75	1.19	1.24
2	L2	382	A2M	C6-N6	2.75	1.44	1.34
2	L2	560	OMU	O4-C4	-2.75	1.19	1.24
1	L1	1010	OMC	C5-C4	2.75	1.49	1.42
2	L2	655	OMG	C2-N1	2.75	1.44	1.37
1	L1	305	A2M	O2'-C2'	2.75	1.49	1.42
2	L2	71	OMG	C6-N1	2.74	1.42	1.37
51	S1	1478	OMG	C5-C4	-2.74	1.36	1.43
2	L2	1077	OMU	O4-C4	-2.74	1.19	1.24
1	L1	1524	OMG	C6-N1	2.74	1.41	1.37
51	S1	38	OMC	O2-C2	-2.72	1.18	1.23
1	L1	1373	A2M	C5-C4	-2.71	1.33	1.40
1	L1	235	A2M	C5-C4	-2.71	1.33	1.40
2	L2	95	A2M	C5-C4	-2.70	1.33	1.40
2	L2	1372	A2M	C5-C4	-2.70	1.33	1.40
1	L1	856	OMG	C6-N1	2.70	1.41	1.37
51	S1	2061	5MC	O2-C2	-2.70	1.18	1.23
2	L2	583	OMC	O2-C2	-2.70	1.18	1.23
2	L2	604	A2M	C5-C4	-2.69	1.33	1.40
2	L2	570	A2M	C5-C4	-2.69	1.33	1.40
51	S1	897	A2M	C5-C4	-2.69	1.33	1.40
1	L1	669	OMC	C5-C4	2.68	1.49	1.42
2	L2	572	A2M	C5-C4	-2.68	1.33	1.40
1	L1	678	A2M	C5-C4	-2.68	1.33	1.40
51	S1	969	A2M	C5-C4	-2.68	1.33	1.40
1	L1	695	OMC	O2-C2	-2.68	1.18	1.23
2	L2	527	A2M	O3'-C3'	-2.67	1.36	1.43
2	L2	1067	A2M	C5-C4	-2.67	1.33	1.40
7	L7	43	A2M	C5-C4	-2.67	1.33	1.40
1	L1	305	A2M	C5-C4	-2.67	1.33	1.40
2	L2	502	A2M	C5-C4	-2.67	1.33	1.40
2	L2	591	A2M	C5-C4	-2.66	1.33	1.40
1	L1	697	A2M	C5-C4	-2.66	1.33	1.40
51	S1	2021	A2M	C5-C4	-2.66	1.33	1.40
51	S1	1647	OMG	C5-C4	-2.66	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	665	A2M	C5-C4	-2.66	1.33	1.40
7	L7	162	A2M	C5-C4	-2.66	1.33	1.40
2	L2	1248	OMC	C5-C4	2.66	1.49	1.42
51	S1	98	A2M	C5-C4	-2.66	1.33	1.40
2	L2	1159	OMC	O2-C2	-2.65	1.18	1.23
4	L4	74	OMG	C5-C4	-2.65	1.36	1.43
51	S1	28	A2M	C5-C4	-2.65	1.33	1.40
2	L2	628	A2M	C5-C4	-2.65	1.33	1.40
2	L2	14	OMC	O2-C2	-2.64	1.18	1.23
2	L2	78	PSU	O4-C4	-2.64	1.18	1.23
51	S1	18	OMC	O2-C2	-2.64	1.18	1.23
2	L2	641	OMG	C5-C4	-2.64	1.36	1.43
2	L2	1229	OMG	C5-C4	-2.64	1.36	1.43
2	L2	524	5MC	O2-C2	-2.64	1.18	1.23
1	L1	955	A2M	C5-C4	-2.64	1.34	1.40
51	S1	512	A2M	C5-C4	-2.64	1.34	1.40
7	L7	75	OMG	C5-C4	-2.63	1.36	1.43
51	S1	479	A2M	C5-C4	-2.63	1.34	1.40
51	S1	1866	OMC	O2-C2	-2.63	1.18	1.23
2	L2	686	OMG	C5-C4	-2.62	1.36	1.43
2	L2	1397	OMC	C5-C4	2.62	1.48	1.42
51	S1	2019	OMC	O2-C2	-2.62	1.18	1.23
51	S1	2151	OMG	C5-C4	-2.62	1.36	1.43
2	L2	1317	OMC	O2-C2	-2.61	1.18	1.23
2	L2	1361	PSU	O4-C4	-2.61	1.18	1.23
2	L2	1284	PSU	O4-C4	-2.61	1.18	1.23
51	S1	2140	OMC	O2-C2	-2.61	1.18	1.23
51	S1	1544	5MC	O2-C2	-2.60	1.18	1.23
2	L2	534	OMG	C5-C4	-2.60	1.36	1.43
1	L1	1540	OMG	C5-C4	-2.60	1.36	1.43
1	L1	1527	OMC	C5-C4	2.60	1.48	1.42
2	L2	359	OMC	O2-C2	-2.60	1.18	1.23
51	S1	2019	OMC	C5-C4	2.60	1.48	1.42
1	L1	669	OMC	O2-C2	-2.60	1.18	1.23
1	L1	1010	OMC	O2-C2	-2.59	1.18	1.23
2	L2	1231	OMG	C5-C4	-2.59	1.36	1.43
51	S1	38	OMC	C5-C4	2.59	1.48	1.42
51	S1	600	OMG	C5-C4	-2.59	1.36	1.43
2	L2	1046	OMG	C5-C4	-2.59	1.36	1.43
1	L1	1552	OMC	O2-C2	-2.58	1.18	1.23
2	L2	1194	PSU	O4-C4	-2.58	1.18	1.23
51	S1	1865	OMG	C5-C4	-2.58	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L2	626	PSU	O4-C4	-2.58	1.18	1.23
2	L2	1213	PSU	O4-C4	-2.58	1.18	1.23
1	L1	1524	OMG	C2-N1	2.58	1.44	1.37
2	L2	1360	OMG	C5-C4	-2.58	1.36	1.43
51	S1	2140	OMC	C5-C4	2.58	1.48	1.42
1	L1	422	PSU	O4-C4	-2.58	1.18	1.23
51	S1	12	PSU	O4-C4	-2.58	1.18	1.23
51	S1	1550	OMG	C2-N1	2.57	1.44	1.37
2	L2	1318	PSU	O4-C4	-2.57	1.18	1.23
1	L1	940	PSU	O4-C4	-2.57	1.18	1.23
51	S1	1292	PSU	O4-C4	-2.57	1.18	1.23
2	L2	14	OMC	C5-C4	2.57	1.48	1.42
2	L2	1159	OMC	C5-C4	2.57	1.48	1.42
2	L2	437	PSU	O4-C4	-2.57	1.18	1.23
51	S1	2059	OMC	C5-C4	2.57	1.48	1.42
51	S1	1156	PSU	O4-C4	-2.56	1.18	1.23
51	S1	1657	PSU	O4-C4	-2.56	1.18	1.23
1	L1	1664	PSU	O4-C4	-2.56	1.18	1.23
2	L2	1317	OMC	C5-C4	2.56	1.48	1.42
51	S1	2048	PSU	O4-C4	-2.56	1.18	1.23
2	L2	443	OMC	O2-C2	-2.56	1.19	1.23
1	L1	1552	OMC	C5-C4	2.56	1.48	1.42
51	S1	1833	OMU	O2-C2	-2.56	1.18	1.23
1	L1	1181	PSU	O4-C4	-2.56	1.18	1.23
1	L1	1626	OMG	C2-N1	2.55	1.44	1.37
51	S1	609	PSU	O4-C4	-2.55	1.18	1.23
2	L2	583	OMC	C5-C4	2.55	1.48	1.42
51	S1	1550	OMG	C5-C4	-2.55	1.36	1.43
1	L1	239	PSU	O4-C4	-2.55	1.18	1.23
1	L1	1093	PSU	O4-C4	-2.55	1.18	1.23
51	S1	1623	OMG	C5-C4	-2.55	1.36	1.43
51	S1	1866	OMC	C5-C4	2.55	1.48	1.42
51	S1	2202	PSU	O4-C4	-2.55	1.18	1.23
2	L2	655	OMG	C5-C4	-2.55	1.36	1.43
2	L2	506	PSU	O4-C4	-2.55	1.18	1.23
2	L2	1253	OMG	C5-C4	-2.54	1.36	1.43
51	S1	1192	PSU	O4-C4	-2.54	1.18	1.23
1	L1	774	PSU	O4-C4	-2.54	1.18	1.23
51	S1	1246	PSU	O4-C4	-2.54	1.18	1.23
1	L1	856	OMG	C5-C4	-2.54	1.36	1.43
2	L2	597	PSU	O4-C4	-2.54	1.18	1.23
2	L2	359	OMC	C5-C4	2.54	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	1829	OMG	C2-N1	2.54	1.43	1.37
2	L2	1144	PSU	O4-C4	-2.53	1.18	1.23
7	L7	74	PSU	O4-C4	-2.53	1.18	1.23
2	L2	71	OMG	C2-N1	2.53	1.43	1.37
1	L1	1540	OMG	C2-N1	2.53	1.43	1.37
51	S1	104	PSU	O4-C4	-2.53	1.18	1.23
51	S1	2046	PSU	O4-C4	-2.53	1.18	1.23
1	L1	695	OMC	C5-C4	2.53	1.48	1.42
51	S1	2184	MA6	C5-C4	-2.52	1.34	1.40
2	L2	512	PSU	O4-C4	-2.52	1.18	1.23
2	L2	500	PSU	O4-C4	-2.52	1.18	1.23
51	S1	1833	OMU	C5-C4	2.52	1.49	1.43
2	L2	1248	OMC	O2-C2	-2.52	1.19	1.23
2	L2	510	PSU	O4-C4	-2.52	1.18	1.23
1	L1	1533	PSU	O4-C4	-2.51	1.18	1.23
1	L1	959	OMG	C5-C4	-2.51	1.36	1.43
51	S1	33	PSU	O4-C4	-2.51	1.18	1.23
51	S1	1829	OMG	C5-C4	-2.51	1.36	1.43
51	S1	1841	PSU	O4-C4	-2.51	1.18	1.23
2	L2	472	PSU	O4-C4	-2.51	1.18	1.23
2	L2	1060	PSU	O4-C4	-2.51	1.18	1.23
51	S1	1566	PSU	O4-C4	-2.51	1.18	1.23
52	S2	37	MIA	C5-C4	-2.51	1.34	1.40
51	S1	2184	MA6	C2-N3	2.51	1.36	1.32
51	S1	455	PSU	O4-C4	-2.50	1.18	1.23
2	L2	1397	OMC	O2-C2	-2.50	1.19	1.23
1	L1	856	OMG	O6-C6	-2.50	1.18	1.23
51	S1	1533	PSU	O4-C4	-2.50	1.18	1.23
2	L2	504	PSU	O4-C4	-2.50	1.18	1.23
2	L2	71	OMG	C5-C4	-2.49	1.36	1.43
2	L2	1253	OMG	C2-N1	2.49	1.43	1.37
1	L1	1626	OMG	C5-C4	-2.49	1.36	1.43
51	S1	2185	MA6	C5-C4	-2.49	1.34	1.40
51	S1	18	OMC	C5-C4	2.48	1.48	1.42
2	L2	593	PSU	O4-C4	-2.48	1.18	1.23
2	L2	1303	PSU	O4-C4	-2.48	1.18	1.23
2	L2	1265	PSU	O4-C4	-2.47	1.18	1.23
2	L2	641	OMG	C2-N1	2.46	1.43	1.37
1	L1	677	1MA	C5-C4	-2.46	1.36	1.43
2	L2	1253	OMG	O6-C6	-2.46	1.18	1.23
2	L2	560	OMU	C5-C4	2.45	1.49	1.43
51	S1	2185	MA6	C2-N3	2.45	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	856	OMG	C2-N1	2.44	1.43	1.37
1	L1	1171	PSU	O4-C4	-2.44	1.19	1.23
1	L1	48	OMU	C5-C4	2.43	1.49	1.43
2	L2	1413	PSU	O4-C4	-2.43	1.19	1.23
1	L1	1524	OMG	O6-C6	-2.43	1.18	1.23
1	L1	1527	OMC	O2-C2	-2.42	1.19	1.23
2	L2	1382	PSU	O4-C4	-2.41	1.19	1.23
1	L1	1107	OMU	C5-C4	2.40	1.49	1.43
2	L2	641	OMG	O6-C6	-2.40	1.18	1.23
2	L2	1359	OMU	C5-C4	2.40	1.48	1.43
51	S1	8	OMU	C5-C4	2.39	1.48	1.43
2	L2	667	OMU	C5-C4	2.39	1.48	1.43
1	L1	1253	OMU	C5-C4	2.39	1.48	1.43
51	S1	29	OMU	C5-C4	2.39	1.48	1.43
1	L1	1371	OMU	C5-C4	2.38	1.48	1.43
2	L2	71	OMG	O6-C6	-2.38	1.18	1.23
7	L7	101	OMU	C5-C4	2.38	1.48	1.43
51	S1	1662	OMU	C5-C4	2.38	1.48	1.43
3	L3	13	OMU	C5-C4	2.38	1.48	1.43
2	L2	1077	OMU	C5-C4	2.38	1.48	1.43
1	L1	1017	PSU	O4-C4	-2.38	1.19	1.23
1	L1	672	PSU	O4-C4	-2.38	1.19	1.23
51	S1	1621	OMU	C5-C4	2.37	1.48	1.43
2	L2	667	OMU	O2-C2	-2.37	1.18	1.23
1	L1	1528	PSU	O4-C4	-2.37	1.19	1.23
2	L2	662	PSU	O4-C4	-2.37	1.19	1.23
3	L3	13	OMU	O2-C2	-2.37	1.18	1.23
51	S1	1979	OMU	C5-C4	2.37	1.48	1.43
1	L1	1659	OMU	C5-C4	2.37	1.48	1.43
2	L2	1264	PSU	O4-C4	-2.37	1.19	1.23
2	L2	527	A2M	C5-C4	-2.36	1.34	1.40
1	L1	48	OMU	O2-C2	-2.36	1.18	1.23
2	L2	56	OMU	C5-C4	2.36	1.48	1.43
1	L1	845	OMU	C5-C4	2.36	1.48	1.43
2	L2	1058	PSU	O4-C4	-2.36	1.19	1.23
2	L2	1419	OMU	C5-C4	2.36	1.48	1.43
1	L1	858	A2M	C5-C4	-2.35	1.34	1.40
51	S1	1539	PSU	O4-C4	-2.35	1.19	1.23
1	L1	1253	OMU	O2-C2	-2.35	1.18	1.23
1	L1	847	OMU	C5-C4	2.35	1.48	1.43
2	L2	1359	OMU	O2-C2	-2.35	1.18	1.23
1	L1	845	OMU	O2-C2	-2.35	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	1540	OMG	O6-C6	-2.34	1.18	1.23
2	L2	73	OMU	C5-C4	2.34	1.48	1.43
51	S1	661	OMU	C5-C4	2.34	1.48	1.43
1	L1	1659	OMU	O2-C2	-2.34	1.18	1.23
51	S1	1777	OMU	C5-C4	2.34	1.48	1.43
51	S1	8	OMU	O2-C2	-2.34	1.18	1.23
2	L2	1419	OMU	O2-C2	-2.34	1.18	1.23
1	L1	1524	OMG	C5-C4	-2.34	1.37	1.43
1	L1	1626	OMG	O6-C6	-2.34	1.18	1.23
1	L1	847	OMU	O2-C2	-2.33	1.18	1.23
2	L2	1264	PSU	O4'-C1'	-2.33	1.40	1.43
2	L2	56	OMU	O2-C2	-2.33	1.18	1.23
1	L1	1371	OMU	O2-C2	-2.32	1.18	1.23
51	S1	1621	OMU	O2-C2	-2.32	1.18	1.23
2	L2	73	OMU	O2-C2	-2.31	1.18	1.23
7	L7	101	OMU	O2-C2	-2.31	1.18	1.23
51	S1	1979	OMU	O2-C2	-2.31	1.18	1.23
51	S1	29	OMU	O2-C2	-2.31	1.18	1.23
1	L1	1011	PSU	O4-C4	-2.30	1.19	1.23
2	L2	1403	PSU	O4-C4	-2.30	1.19	1.23
51	S1	1662	OMU	O2-C2	-2.30	1.18	1.23
51	S1	2008	OMG	O6-C6	-2.30	1.18	1.23
51	S1	1829	OMG	O6-C6	-2.30	1.18	1.23
1	L1	1107	OMU	O2-C2	-2.29	1.18	1.23
2	L2	1384	A2M	C5-C4	-2.29	1.34	1.40
4	L4	74	OMG	O6-C6	-2.29	1.18	1.23
51	S1	1777	OMU	O2-C2	-2.28	1.18	1.23
1	L1	1539	A2M	C5-C4	-2.28	1.34	1.40
1	L1	1039	OMU	C5-C4	2.28	1.48	1.43
51	S1	1478	OMG	O6-C6	-2.28	1.18	1.23
7	L7	69	PSU	O4-C4	-2.28	1.19	1.23
1	L1	69	A2M	C5-C4	-2.27	1.34	1.40
51	S1	1550	OMG	O6-C6	-2.27	1.18	1.23
2	L2	1046	OMG	O6-C6	-2.27	1.18	1.23
51	S1	668	A2M	C5-C4	-2.26	1.35	1.40
1	L1	681	A2M	C5-C4	-2.25	1.35	1.40
2	L2	655	OMG	O6-C6	-2.25	1.18	1.23
2	L2	560	OMU	O2-C2	-2.25	1.18	1.23
51	S1	1543	B8N	O2-C2	-2.25	1.18	1.22
1	L1	959	OMG	O6-C6	-2.24	1.18	1.23
2	L2	382	A2M	C5-C4	-2.24	1.35	1.40
2	L2	534	OMG	O6-C6	-2.23	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S1	2151	OMG	O6-C6	-2.22	1.18	1.23
1	L1	927	A2M	C2-N3	2.22	1.35	1.32
2	L2	1360	OMG	O6-C6	-2.22	1.18	1.23
1	L1	927	A2M	C5-C4	-2.22	1.35	1.40
51	S1	661	OMU	O2-C2	-2.22	1.19	1.23
51	S1	479	A2M	C2-N3	2.22	1.35	1.32
1	L1	1190	OMG	O6-C6	-2.22	1.18	1.23
51	S1	98	A2M	C2-N3	2.21	1.35	1.32
2	L2	1077	OMU	O2-C2	-2.21	1.19	1.23
51	S1	1865	OMG	O6-C6	-2.21	1.18	1.23
2	L2	1078	OMG	O6-C6	-2.21	1.18	1.23
2	L2	1231	OMG	O6-C6	-2.21	1.18	1.23
2	L2	1229	OMG	O6-C6	-2.20	1.18	1.23
51	S1	1647	OMG	O6-C6	-2.20	1.18	1.23
2	L2	1265	PSU	C4-C5	2.19	1.50	1.44
1	L1	305	A2M	C2-N3	2.19	1.35	1.32
51	S1	28	A2M	C2-N3	2.19	1.35	1.32
2	L2	502	A2M	C2-N3	2.19	1.35	1.32
51	S1	2021	A2M	C2-N3	2.19	1.35	1.32
51	S1	1543	B8N	O4-C4	-2.19	1.18	1.23
7	L7	75	OMG	O6-C6	-2.18	1.18	1.23
51	S1	600	OMG	O6-C6	-2.18	1.18	1.23
51	S1	1623	OMG	O6-C6	-2.17	1.18	1.23
1	L1	1039	OMU	O2-C2	-2.16	1.19	1.23
2	L2	686	OMG	O6-C6	-2.16	1.18	1.23
2	L2	1067	A2M	C2-N3	2.15	1.35	1.32
2	L2	382	A2M	O5'-C5'	-2.15	1.39	1.44
1	L1	235	A2M	C2-N3	2.15	1.35	1.32
7	L7	43	A2M	C2-N3	2.14	1.35	1.32
51	S1	897	A2M	C2-N3	2.14	1.35	1.32
7	L7	162	A2M	C2-N3	2.13	1.35	1.32
2	L2	604	A2M	C2-N3	2.13	1.35	1.32
2	L2	95	A2M	C2-N3	2.13	1.35	1.32
1	L1	1373	A2M	C2-N3	2.12	1.35	1.32
51	S1	512	A2M	C2-N3	2.12	1.35	1.32
51	S1	1543	B8N	C2-N3	2.11	1.42	1.38
2	L2	591	A2M	C2-N3	2.11	1.35	1.32
2	L2	1384	A2M	O5'-C5'	-2.10	1.39	1.44
2	L2	1185	A2M	C5-C4	-2.10	1.35	1.40
7	L7	101	OMU	O2'-C2'	2.10	1.48	1.42
2	L2	1308	5MC	O2-C2	-2.09	1.19	1.23
2	L2	628	A2M	C2-N3	2.09	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L1	678	A2M	C2-N3	2.09	1.35	1.32
1	L1	697	A2M	C2-N3	2.09	1.35	1.32
2	L2	572	A2M	C2-N3	2.08	1.35	1.32
2	L2	665	A2M	C2-N3	2.07	1.35	1.32
1	L1	955	A2M	C2-N3	2.07	1.35	1.32
1	L1	681	A2M	C2-N3	2.07	1.35	1.32
2	L2	1372	A2M	C2-N3	2.07	1.35	1.32
2	L2	527	A2M	O5'-C5'	-2.06	1.39	1.44
2	L2	1185	A2M	O5'-C5'	-2.06	1.39	1.44
2	L2	662	PSU	C4-C5	2.06	1.50	1.44
1	L1	1539	A2M	O5'-C5'	-2.05	1.39	1.44
1	L1	1171	PSU	C4-C5	2.05	1.50	1.44
51	S1	512	A2M	O5'-C5'	-2.05	1.39	1.44
2	L2	570	A2M	C2-N3	2.04	1.35	1.32
1	L1	858	A2M	O5'-C5'	-2.04	1.39	1.44
2	L2	1264	PSU	C4-C5	2.04	1.50	1.44
2	L2	382	A2M	C2-N3	2.02	1.35	1.32
2	L2	1185	A2M	C2-N3	2.02	1.35	1.32
51	S1	2202	PSU	C4-C5	2.01	1.49	1.44
1	L1	1664	PSU	C4-C5	2.01	1.49	1.44
1	L1	927	A2M	O5'-C5'	-2.00	1.39	1.44

All (656) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	37	MIA	C1'-N9-C4	18.64	159.40	126.64
51	S1	2185	MA6	N1-C6-N6	-16.43	99.76	117.06
51	S1	2184	MA6	N1-C6-N6	-15.94	100.28	117.06
52	S2	37	MIA	C11-S10-C2	9.89	109.65	102.27
52	S2	37	MIA	S10-C2-N3	9.45	148.89	116.10
51	S1	969	A2M	C5-C6-N6	8.35	133.03	120.35
2	L2	1185	A2M	C5-C6-N6	8.27	132.91	120.35
1	L1	955	A2M	C5-C6-N6	8.18	132.78	120.35
1	L1	69	A2M	C5-C6-N6	8.11	132.68	120.35
51	S1	668	A2M	C5-C6-N6	8.02	132.54	120.35
51	S1	512	A2M	C5-C6-N6	8.01	132.52	120.35
2	L2	628	A2M	C5-C6-N6	7.99	132.50	120.35
1	L1	681	A2M	C5-C6-N6	7.98	132.48	120.35
2	L2	570	A2M	C5-C6-N6	7.97	132.47	120.35
2	L2	1372	A2M	C5-C6-N6	7.97	132.46	120.35
1	L1	1539	A2M	C5-C6-N6	7.96	132.45	120.35
7	L7	162	A2M	C5-C6-N6	7.96	132.45	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	572	A2M	C5-C6-N6	7.95	132.44	120.35
2	L2	665	A2M	C5-C6-N6	7.92	132.39	120.35
7	L7	43	A2M	C5-C6-N6	7.91	132.37	120.35
1	L1	858	A2M	C5-C6-N6	7.90	132.36	120.35
1	L1	697	A2M	C5-C6-N6	7.90	132.35	120.35
51	S1	897	A2M	C5-C6-N6	7.86	132.30	120.35
51	S1	479	A2M	C5-C6-N6	7.86	132.30	120.35
2	L2	502	A2M	C5-C6-N6	7.86	132.29	120.35
2	L2	604	A2M	C5-C6-N6	7.85	132.28	120.35
51	S1	2021	A2M	C5-C6-N6	7.85	132.28	120.35
1	L1	1373	A2M	C5-C6-N6	7.84	132.26	120.35
51	S1	28	A2M	C5-C6-N6	7.81	132.22	120.35
1	L1	305	A2M	C5-C6-N6	7.80	132.21	120.35
2	L2	527	A2M	C5-C6-N6	7.80	132.21	120.35
2	L2	1067	A2M	C5-C6-N6	7.80	132.20	120.35
2	L2	95	A2M	C5-C6-N6	7.78	132.18	120.35
2	L2	591	A2M	C5-C6-N6	7.77	132.16	120.35
1	L1	235	A2M	C5-C6-N6	7.75	132.12	120.35
51	S1	98	A2M	C5-C6-N6	7.65	131.98	120.35
1	L1	678	A2M	C5-C6-N6	7.64	131.96	120.35
2	L2	382	A2M	C5-C6-N6	7.63	131.94	120.35
1	L1	927	A2M	C5-C6-N6	7.57	131.86	120.35
2	L2	1384	A2M	C5-C6-N6	7.56	131.84	120.35
52	S2	37	MIA	S10-C2-N1	-7.24	90.99	116.01
2	L2	560	OMU	C4-N3-C2	-5.81	118.92	126.58
1	L1	955	A2M	N3-C2-N1	-5.71	119.75	128.68
2	L2	527	A2M	N6-C6-N1	-5.69	106.77	118.57
1	L1	858	A2M	N6-C6-N1	-5.69	106.77	118.57
1	L1	69	A2M	N6-C6-N1	-5.68	106.78	118.57
51	S1	512	A2M	N3-C2-N1	-5.65	119.85	128.68
1	L1	678	A2M	N3-C2-N1	-5.65	119.85	128.68
2	L2	570	A2M	N3-C2-N1	-5.64	119.86	128.68
2	L2	572	A2M	N3-C2-N1	-5.64	119.86	128.68
1	L1	1373	A2M	N3-C2-N1	-5.64	119.87	128.68
2	L2	591	A2M	N3-C2-N1	-5.61	119.90	128.68
2	L2	604	A2M	N3-C2-N1	-5.60	119.92	128.68
7	L7	162	A2M	N3-C2-N1	-5.60	119.92	128.68
1	L1	235	A2M	N3-C2-N1	-5.60	119.93	128.68
51	S1	969	A2M	N6-C6-N1	-5.59	106.96	118.57
7	L7	43	A2M	N3-C2-N1	-5.58	119.96	128.68
2	L2	1185	A2M	N6-C6-N1	-5.57	107.01	118.57
1	L1	697	A2M	N3-C2-N1	-5.57	119.98	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	28	A2M	N3-C2-N1	-5.55	120.00	128.68
51	S1	1833	OMU	C4-N3-C2	-5.55	119.26	126.58
2	L2	665	A2M	N3-C2-N1	-5.55	120.00	128.68
51	S1	897	A2M	N3-C2-N1	-5.55	120.00	128.68
2	L2	95	A2M	N3-C2-N1	-5.55	120.00	128.68
51	S1	2021	A2M	N3-C2-N1	-5.54	120.02	128.68
2	L2	502	A2M	N3-C2-N1	-5.54	120.03	128.68
2	L2	628	A2M	N3-C2-N1	-5.53	120.03	128.68
1	L1	305	A2M	N3-C2-N1	-5.52	120.06	128.68
2	L2	1372	A2M	N3-C2-N1	-5.51	120.07	128.68
51	S1	479	A2M	N3-C2-N1	-5.50	120.08	128.68
2	L2	1067	A2M	N3-C2-N1	-5.49	120.09	128.68
51	S1	98	A2M	N3-C2-N1	-5.47	120.12	128.68
1	L1	1107	OMU	C4-N3-C2	-5.46	119.38	126.58
51	S1	2185	MA6	N3-C2-N1	-5.46	120.15	128.68
1	L1	681	A2M	N6-C6-N1	-5.43	107.30	118.57
1	L1	955	A2M	N6-C6-N1	-5.42	107.32	118.57
51	S1	668	A2M	N6-C6-N1	-5.42	107.32	118.57
51	S1	2184	MA6	N3-C2-N1	-5.41	120.22	128.68
51	S1	969	A2M	N3-C2-N1	-5.39	120.25	128.68
1	L1	1539	A2M	N6-C6-N1	-5.39	107.38	118.57
51	S1	661	OMU	C4-N3-C2	-5.38	119.49	126.58
51	S1	8	OMU	C4-N3-C2	-5.37	119.49	126.58
2	L2	1077	OMU	C4-N3-C2	-5.36	119.51	126.58
2	L2	570	A2M	N6-C6-N1	-5.36	107.46	118.57
51	S1	512	A2M	N6-C6-N1	-5.34	107.49	118.57
2	L2	572	A2M	N6-C6-N1	-5.30	107.57	118.57
2	L2	628	A2M	N6-C6-N1	-5.30	107.57	118.57
1	L1	1039	OMU	C4-N3-C2	-5.29	119.60	126.58
7	L7	162	A2M	N6-C6-N1	-5.29	107.60	118.57
2	L2	665	A2M	N6-C6-N1	-5.28	107.60	118.57
2	L2	604	A2M	N6-C6-N1	-5.28	107.62	118.57
7	L7	43	A2M	N6-C6-N1	-5.27	107.63	118.57
51	S1	479	A2M	N6-C6-N1	-5.27	107.63	118.57
2	L2	56	OMU	C4-N3-C2	-5.27	119.63	126.58
51	S1	29	OMU	C4-N3-C2	-5.26	119.64	126.58
51	S1	2021	A2M	N6-C6-N1	-5.26	107.66	118.57
1	L1	697	A2M	N6-C6-N1	-5.26	107.66	118.57
1	L1	48	OMU	C4-N3-C2	-5.25	119.65	126.58
2	L2	502	A2M	N6-C6-N1	-5.24	107.69	118.57
51	S1	897	A2M	N6-C6-N1	-5.24	107.70	118.57
2	L2	667	OMU	C4-N3-C2	-5.24	119.67	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	1621	OMU	C4-N3-C2	-5.24	119.67	126.58
2	L2	1372	A2M	N6-C6-N1	-5.23	107.71	118.57
2	L2	95	A2M	N6-C6-N1	-5.23	107.72	118.57
51	S1	28	A2M	N6-C6-N1	-5.22	107.73	118.57
1	L1	305	A2M	N6-C6-N1	-5.22	107.74	118.57
1	L1	1373	A2M	N6-C6-N1	-5.21	107.76	118.57
1	L1	235	A2M	N6-C6-N1	-5.21	107.77	118.57
51	S1	1979	OMU	C4-N3-C2	-5.19	119.73	126.58
3	L3	13	OMU	C4-N3-C2	-5.19	119.73	126.58
1	L1	1253	OMU	C4-N3-C2	-5.19	119.74	126.58
2	L2	382	A2M	N6-C6-N1	-5.18	107.82	118.57
1	L1	1371	OMU	C4-N3-C2	-5.17	119.75	126.58
1	L1	927	A2M	N6-C6-N1	-5.17	107.84	118.57
51	S1	1777	OMU	C4-N3-C2	-5.17	119.77	126.58
1	L1	1659	OMU	C4-N3-C2	-5.16	119.77	126.58
51	S1	1662	OMU	C4-N3-C2	-5.16	119.77	126.58
7	L7	101	OMU	C4-N3-C2	-5.14	119.80	126.58
2	L2	1067	A2M	N6-C6-N1	-5.14	107.91	118.57
2	L2	1359	OMU	C4-N3-C2	-5.13	119.81	126.58
1	L1	847	OMU	C4-N3-C2	-5.12	119.83	126.58
2	L2	1384	A2M	N6-C6-N1	-5.12	107.95	118.57
1	L1	678	A2M	N6-C6-N1	-5.11	107.97	118.57
51	S1	98	A2M	N6-C6-N1	-5.10	107.98	118.57
2	L2	1419	OMU	C4-N3-C2	-5.07	119.89	126.58
1	L1	845	OMU	C4-N3-C2	-5.07	119.90	126.58
2	L2	591	A2M	N6-C6-N1	-5.06	108.07	118.57
51	S1	1543	B8N	C5-C4-N3	5.05	125.52	116.17
2	L2	73	OMU	C4-N3-C2	-5.04	119.94	126.58
51	S1	1995	7MG	C5-C6-N1	4.95	119.71	110.99
2	L2	527	A2M	N3-C2-N1	-4.86	121.08	128.68
51	S1	668	A2M	N3-C2-N1	-4.81	121.17	128.68
1	L1	69	A2M	N3-C2-N1	-4.67	121.37	128.68
1	L1	927	A2M	N3-C2-N1	-4.66	121.39	128.68
1	L1	858	A2M	N3-C2-N1	-4.61	121.47	128.68
2	L2	1361	PSU	C4-N3-C2	-4.60	119.70	126.34
7	L7	74	PSU	C4-N3-C2	-4.59	119.72	126.34
1	L1	1171	PSU	C4-N3-C2	-4.56	119.77	126.34
2	L2	1058	PSU	C4-N3-C2	-4.56	119.77	126.34
51	S1	1246	PSU	C4-N3-C2	-4.55	119.78	126.34
2	L2	500	PSU	C4-N3-C2	-4.54	119.80	126.34
2	L2	1060	PSU	C4-N3-C2	-4.53	119.81	126.34
51	S1	1841	PSU	C4-N3-C2	-4.53	119.81	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	2046	PSU	C4-N3-C2	-4.53	119.81	126.34
1	L1	774	PSU	C4-N3-C2	-4.53	119.81	126.34
51	S1	1657	PSU	C4-N3-C2	-4.53	119.82	126.34
1	L1	1181	PSU	C4-N3-C2	-4.52	119.82	126.34
2	L2	1284	PSU	C4-N3-C2	-4.52	119.83	126.34
1	L1	681	A2M	N3-C2-N1	-4.52	121.62	128.68
2	L2	597	PSU	C4-N3-C2	-4.50	119.85	126.34
2	L2	626	PSU	C4-N3-C2	-4.49	119.88	126.34
2	L2	437	PSU	C4-N3-C2	-4.48	119.88	126.34
2	L2	1413	PSU	C4-N3-C2	-4.48	119.89	126.34
2	L2	1318	PSU	C4-N3-C2	-4.48	119.89	126.34
51	S1	104	PSU	C4-N3-C2	-4.48	119.89	126.34
2	L2	78	PSU	C4-N3-C2	-4.47	119.89	126.34
1	L1	672	PSU	N1-C2-N3	4.47	120.19	115.13
2	L2	1213	PSU	C4-N3-C2	-4.47	119.90	126.34
51	S1	12	PSU	C4-N3-C2	-4.47	119.90	126.34
2	L2	1382	PSU	C4-N3-C2	-4.47	119.90	126.34
2	L2	512	PSU	C4-N3-C2	-4.47	119.90	126.34
2	L2	472	PSU	C4-N3-C2	-4.46	119.91	126.34
2	L2	1303	PSU	C4-N3-C2	-4.46	119.91	126.34
2	L2	1144	PSU	C4-N3-C2	-4.46	119.92	126.34
1	L1	1539	A2M	N3-C2-N1	-4.46	121.71	128.68
51	S1	1533	PSU	C4-N3-C2	-4.45	119.92	126.34
51	S1	2048	PSU	C4-N3-C2	-4.45	119.93	126.34
1	L1	422	PSU	C4-N3-C2	-4.45	119.93	126.34
51	S1	33	PSU	C4-N3-C2	-4.45	119.93	126.34
51	S1	609	PSU	C4-N3-C2	-4.44	119.95	126.34
2	L2	506	PSU	C4-N3-C2	-4.44	119.95	126.34
2	L2	1185	A2M	N3-C2-N1	-4.43	121.76	128.68
51	S1	1995	7MG	C2-N3-C4	4.43	120.19	112.30
2	L2	1194	PSU	C4-N3-C2	-4.42	119.97	126.34
51	S1	1156	PSU	C4-N3-C2	-4.42	119.97	126.34
1	L1	1171	PSU	N1-C2-N3	4.42	120.13	115.13
2	L2	504	PSU	C4-N3-C2	-4.41	119.98	126.34
1	L1	940	PSU	C4-N3-C2	-4.41	119.99	126.34
1	L1	672	PSU	C4-N3-C2	-4.41	119.99	126.34
1	L1	1093	PSU	C4-N3-C2	-4.41	119.99	126.34
1	L1	1017	PSU	C4-N3-C2	-4.40	120.00	126.34
2	L2	662	PSU	C4-N3-C2	-4.40	120.00	126.34
2	L2	1058	PSU	N1-C2-N3	4.40	120.12	115.13
1	L1	239	PSU	C4-N3-C2	-4.40	120.00	126.34
2	L2	510	PSU	C4-N3-C2	-4.39	120.01	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1533	PSU	C4-N3-C2	-4.38	120.03	126.34
2	L2	662	PSU	N1-C2-N3	4.37	120.08	115.13
1	L1	1528	PSU	C4-N3-C2	-4.36	120.05	126.34
2	L2	593	PSU	C4-N3-C2	-4.35	120.07	126.34
51	S1	1566	PSU	C4-N3-C2	-4.35	120.07	126.34
51	S1	1539	PSU	C4-N3-C2	-4.35	120.07	126.34
1	L1	1664	PSU	C4-N3-C2	-4.35	120.08	126.34
51	S1	2202	PSU	C4-N3-C2	-4.34	120.09	126.34
51	S1	1292	PSU	C4-N3-C2	-4.32	120.11	126.34
2	L2	1361	PSU	N1-C2-N3	4.32	120.02	115.13
2	L2	1413	PSU	N1-C2-N3	4.32	120.02	115.13
2	L2	1382	PSU	N1-C2-N3	4.30	120.00	115.13
7	L7	69	PSU	C4-N3-C2	-4.29	120.16	126.34
2	L2	1308	5MC	C5-C6-N1	-4.28	118.94	123.34
2	L2	1403	PSU	C4-N3-C2	-4.28	120.17	126.34
51	S1	1539	PSU	N1-C2-N3	4.28	119.97	115.13
2	L2	1264	PSU	N1-C2-N3	4.27	119.97	115.13
51	S1	455	PSU	C4-N3-C2	-4.25	120.21	126.34
2	L2	1303	PSU	N1-C2-N3	4.24	119.93	115.13
1	L1	1528	PSU	N1-C2-N3	4.23	119.93	115.13
2	L2	1144	PSU	N1-C2-N3	4.23	119.92	115.13
2	L2	626	PSU	N1-C2-N3	4.23	119.92	115.13
2	L2	1264	PSU	C4-N3-C2	-4.23	120.25	126.34
2	L2	1060	PSU	N1-C2-N3	4.22	119.92	115.13
1	L1	1017	PSU	N1-C2-N3	4.22	119.91	115.13
2	L2	1384	A2M	N3-C2-N1	-4.22	122.08	128.68
1	L1	774	PSU	N1-C2-N3	4.22	119.91	115.13
2	L2	597	PSU	N1-C2-N3	4.22	119.91	115.13
1	L1	1011	PSU	C4-N3-C2	-4.21	120.27	126.34
51	S1	1995	7MG	C5-C4-N3	-4.20	120.12	128.13
7	L7	74	PSU	N1-C2-N3	4.20	119.89	115.13
51	S1	12	PSU	N1-C2-N3	4.20	119.89	115.13
51	S1	2048	PSU	N1-C2-N3	4.20	119.88	115.13
1	L1	1181	PSU	N1-C2-N3	4.19	119.88	115.13
2	L2	382	A2M	N3-C2-N1	-4.19	122.13	128.68
7	L7	69	PSU	N1-C2-N3	4.18	119.87	115.13
51	S1	2046	PSU	N1-C2-N3	4.17	119.86	115.13
2	L2	504	PSU	N1-C2-N3	4.17	119.85	115.13
51	S1	104	PSU	N1-C2-N3	4.17	119.85	115.13
2	L2	500	PSU	N1-C2-N3	4.16	119.84	115.13
51	S1	609	PSU	N1-C2-N3	4.15	119.83	115.13
51	S1	1246	PSU	N1-C2-N3	4.15	119.83	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	422	PSU	N1-C2-N3	4.15	119.83	115.13
2	L2	560	OMU	N3-C2-N1	4.14	120.39	114.89
2	L2	1213	PSU	N1-C2-N3	4.14	119.82	115.13
51	S1	1657	PSU	N1-C2-N3	4.13	119.81	115.13
51	S1	1841	PSU	N1-C2-N3	4.13	119.81	115.13
51	S1	2202	PSU	N1-C2-N3	4.13	119.81	115.13
51	S1	1156	PSU	N1-C2-N3	4.13	119.80	115.13
2	L2	593	PSU	N1-C2-N3	4.12	119.80	115.13
2	L2	1284	PSU	N1-C2-N3	4.12	119.80	115.13
51	S1	455	PSU	N1-C2-N3	4.11	119.79	115.13
2	L2	1318	PSU	N1-C2-N3	4.11	119.79	115.13
51	S1	33	PSU	N1-C2-N3	4.11	119.78	115.13
1	L1	1093	PSU	N1-C2-N3	4.10	119.77	115.13
1	L1	1533	PSU	N1-C2-N3	4.09	119.76	115.13
2	L2	506	PSU	N1-C2-N3	4.09	119.76	115.13
2	L2	1194	PSU	N1-C2-N3	4.08	119.76	115.13
2	L2	512	PSU	N1-C2-N3	4.08	119.75	115.13
2	L2	510	PSU	N1-C2-N3	4.08	119.75	115.13
51	S1	1533	PSU	N1-C2-N3	4.08	119.75	115.13
2	L2	472	PSU	N1-C2-N3	4.07	119.75	115.13
2	L2	437	PSU	N1-C2-N3	4.07	119.74	115.13
51	S1	1543	B8N	C4-N3-C2	-4.07	120.31	125.46
51	S1	1192	PSU	C4-N3-C2	-4.05	120.50	126.34
2	L2	1265	PSU	N1-C2-N3	4.05	119.72	115.13
1	L1	239	PSU	N1-C2-N3	4.03	119.70	115.13
1	L1	940	PSU	N1-C2-N3	4.03	119.70	115.13
51	S1	1292	PSU	N1-C2-N3	4.00	119.66	115.13
51	S1	1566	PSU	N1-C2-N3	4.00	119.66	115.13
2	L2	78	PSU	N1-C2-N3	3.98	119.64	115.13
1	L1	1664	PSU	N1-C2-N3	3.98	119.64	115.13
2	L2	1265	PSU	C4-N3-C2	-3.96	120.64	126.34
2	L2	1403	PSU	N1-C2-N3	3.95	119.61	115.13
51	S1	1833	OMU	N3-C2-N1	3.88	120.04	114.89
2	L2	56	OMU	N3-C2-N1	3.87	120.03	114.89
51	S1	1192	PSU	N1-C2-N3	3.85	119.49	115.13
51	S1	8	OMU	N3-C2-N1	3.84	119.99	114.89
2	L2	1359	OMU	N3-C2-N1	3.82	119.97	114.89
2	L2	667	OMU	N3-C2-N1	3.80	119.93	114.89
51	S1	1979	OMU	N3-C2-N1	3.79	119.92	114.89
51	S1	1621	OMU	N3-C2-N1	3.78	119.90	114.89
51	S1	1833	OMU	C5-C4-N3	3.77	120.47	114.84
1	L1	845	OMU	N3-C2-N1	3.77	119.89	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	1253	OMU	N3-C2-N1	3.76	119.88	114.89
7	L7	101	OMU	N3-C2-N1	3.76	119.88	114.89
1	L1	847	OMU	N3-C2-N1	3.74	119.85	114.89
52	S2	37	MIA	N3-C2-N1	-3.73	120.12	126.98
1	L1	1371	OMU	N3-C2-N1	3.73	119.83	114.89
1	L1	1659	OMU	N3-C2-N1	3.72	119.83	114.89
51	S1	661	OMU	N3-C2-N1	3.72	119.83	114.89
51	S1	29	OMU	N3-C2-N1	3.72	119.82	114.89
51	S1	1662	OMU	N3-C2-N1	3.72	119.82	114.89
1	L1	1107	OMU	N3-C2-N1	3.68	119.78	114.89
51	S1	1777	OMU	N3-C2-N1	3.67	119.76	114.89
1	L1	48	OMU	N3-C2-N1	3.67	119.76	114.89
2	L2	1419	OMU	N3-C2-N1	3.66	119.75	114.89
1	L1	1011	PSU	N1-C2-N3	3.62	119.23	115.13
1	L1	1039	OMU	N3-C2-N1	3.62	119.70	114.89
1	L1	677	1MA	N1-C2-N3	-3.61	121.81	126.02
3	L3	13	OMU	N3-C2-N1	3.61	119.68	114.89
2	L2	1077	OMU	N3-C2-N1	3.59	119.66	114.89
2	L2	73	OMU	N3-C2-N1	3.59	119.65	114.89
2	L2	1077	OMU	C5-C4-N3	3.58	120.20	114.84
2	L2	524	5MC	C5-C6-N1	-3.58	119.66	123.34
1	L1	1107	OMU	C5-C4-N3	3.54	120.14	114.84
1	L1	1039	OMU	C5-C4-N3	3.54	120.13	114.84
1	L1	677	1MA	C5-C6-N1	3.53	119.17	113.90
51	S1	661	OMU	C5-C4-N3	3.52	120.11	114.84
2	L2	560	OMU	C5-C4-N3	3.51	120.09	114.84
2	L2	1264	PSU	C6-N1-C2	-3.47	119.14	122.68
1	L1	48	OMU	C5-C4-N3	3.46	120.01	114.84
2	L2	1382	PSU	C6-C5-C4	3.45	120.61	118.20
51	S1	2008	OMG	C5-C6-N1	3.45	120.04	113.95
2	L2	1058	PSU	C6-C5-C4	3.43	120.59	118.20
51	S1	8	OMU	C5-C4-N3	3.42	119.96	114.84
1	L1	1190	OMG	C5-C6-N1	3.40	119.96	113.95
51	S1	1647	OMG	C5-C6-N1	3.40	119.95	113.95
2	L2	686	OMG	C5-C6-N1	3.40	119.95	113.95
51	S1	1623	OMG	C5-C6-N1	3.40	119.95	113.95
52	S2	37	MIA	C2-N3-C4	3.39	120.00	115.32
3	L3	13	OMU	C5-C4-N3	3.38	119.89	114.84
51	S1	1865	OMG	C5-C6-N1	3.38	119.92	113.95
51	S1	29	OMU	C5-C4-N3	3.38	119.89	114.84
2	L2	73	OMU	C5-C4-N3	3.37	119.89	114.84
2	L2	655	OMG	C5-C6-N1	3.37	119.91	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	1478	OMG	C5-C6-N1	3.37	119.90	113.95
51	S1	2151	OMG	C5-C6-N1	3.37	119.90	113.95
1	L1	1371	OMU	C5-C4-N3	3.36	119.87	114.84
4	L4	74	OMG	C5-C6-N1	3.36	119.88	113.95
1	L1	959	OMG	C5-C6-N1	3.35	119.87	113.95
2	L2	1046	OMG	C5-C6-N1	3.35	119.87	113.95
2	L2	1360	OMG	C5-C6-N1	3.35	119.86	113.95
7	L7	101	OMU	C5-C4-N3	3.34	119.83	114.84
52	S2	37	MIA	C12-C13-C14	-3.33	120.65	127.14
51	S1	600	OMG	C5-C6-N1	3.33	119.84	113.95
51	S1	1777	OMU	C5-C4-N3	3.33	119.82	114.84
2	L2	1231	OMG	C5-C6-N1	3.32	119.81	113.95
51	S1	1662	OMU	C5-C4-N3	3.32	119.80	114.84
2	L2	56	OMU	C5-C4-N3	3.31	119.80	114.84
2	L2	534	OMG	C5-C6-N1	3.31	119.79	113.95
51	S1	1621	OMU	C5-C4-N3	3.30	119.78	114.84
2	L2	1229	OMG	C5-C6-N1	3.30	119.78	113.95
1	L1	1659	OMU	C5-C4-N3	3.30	119.78	114.84
1	L1	1253	OMU	C5-C4-N3	3.30	119.77	114.84
2	L2	662	PSU	C6-C5-C4	3.30	120.50	118.20
7	L7	75	OMG	C5-C6-N1	3.29	119.77	113.95
2	L2	1419	OMU	C5-C4-N3	3.29	119.77	114.84
2	L2	667	OMU	C5-C4-N3	3.29	119.76	114.84
51	S1	1979	OMU	C5-C4-N3	3.29	119.76	114.84
1	L1	847	OMU	C5-C4-N3	3.28	119.75	114.84
51	S1	1544	5MC	C5-C6-N1	-3.27	119.97	123.34
2	L2	1078	OMG	C5-C6-N1	3.26	119.72	113.95
2	L2	1413	PSU	C6-C5-C4	3.26	120.48	118.20
7	L7	69	PSU	C6-C5-C4	3.26	120.47	118.20
51	S1	1995	7MG	C4-C5-N7	3.23	110.02	105.53
2	L2	1359	OMU	C5-C4-N3	3.22	119.65	114.84
1	L1	845	OMU	C5-C4-N3	3.21	119.65	114.84
1	L1	672	PSU	C6-C5-C4	3.21	120.44	118.20
51	S1	1192	PSU	C6-N1-C2	-3.18	119.43	122.68
51	S1	455	PSU	C6-N1-C2	-3.18	119.44	122.68
1	L1	672	PSU	C6-N1-C2	-3.14	119.47	122.68
51	S1	1539	PSU	C6-C5-C4	3.13	120.38	118.20
1	L1	1528	PSU	C6-N1-C2	-3.12	119.50	122.68
51	S1	1539	PSU	C6-N1-C2	-3.12	119.50	122.68
1	L1	1171	PSU	C6-C5-C4	3.11	120.37	118.20
1	L1	1017	PSU	C6-C5-C4	3.10	120.36	118.20
2	L2	1361	PSU	C6-N1-C2	-3.06	119.55	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	1995	7MG	C5-C4-N9	3.06	110.31	106.35
2	L2	504	PSU	C6-N1-C2	-3.04	119.57	122.68
1	L1	1107	OMU	O4-C4-C5	-3.04	119.82	125.16
2	L2	1403	PSU	C6-C5-C4	3.03	120.32	118.20
1	L1	1190	OMG	C8-N7-C5	3.02	108.74	102.99
2	L2	1413	PSU	C6-N1-C2	-3.01	119.60	122.68
51	S1	2048	PSU	C6-N1-C2	-3.01	119.61	122.68
51	S1	609	PSU	C6-N1-C2	-3.00	119.61	122.68
51	S1	2008	OMG	C8-N7-C5	3.00	108.71	102.99
1	L1	1017	PSU	C6-N1-C2	-3.00	119.61	122.68
2	L2	662	PSU	C6-N1-C2	-3.00	119.61	122.68
2	L2	1058	PSU	C6-N1-C2	-3.00	119.62	122.68
7	L7	69	PSU	C6-N1-C2	-2.99	119.62	122.68
2	L2	1078	OMG	C8-N7-C5	2.99	108.69	102.99
2	L2	626	PSU	C6-N1-C2	-2.97	119.64	122.68
51	S1	2202	PSU	C6-N1-C2	-2.96	119.65	122.68
51	S1	2061	5MC	C5-C6-N1	-2.96	120.29	123.34
51	S1	2151	OMG	C8-N7-C5	2.96	108.63	102.99
51	S1	1841	PSU	C6-C5-C4	2.95	120.26	118.20
51	S1	1647	OMG	C8-N7-C5	2.95	108.61	102.99
2	L2	1144	PSU	C6-N1-C2	-2.95	119.67	122.68
1	L1	1533	PSU	C6-N1-C2	-2.95	119.67	122.68
51	S1	1292	PSU	C6-N1-C2	-2.95	119.67	122.68
2	L2	1303	PSU	C6-N1-C2	-2.94	119.67	122.68
51	S1	1777	OMU	O4-C4-C5	-2.94	120.00	125.16
7	L7	75	OMG	C8-N7-C5	2.93	108.58	102.99
2	L2	1213	PSU	C6-N1-C2	-2.93	119.69	122.68
1	L1	774	PSU	C6-N1-C2	-2.92	119.70	122.68
2	L2	1361	PSU	C6-C5-C4	2.91	120.23	118.20
51	S1	33	PSU	C6-N1-C2	-2.91	119.71	122.68
1	L1	422	PSU	C6-N1-C2	-2.91	119.71	122.68
2	L2	655	OMG	C8-N7-C5	2.91	108.53	102.99
1	L1	1093	PSU	C6-N1-C2	-2.90	119.72	122.68
2	L2	686	OMG	C8-N7-C5	2.90	108.52	102.99
51	S1	1829	OMG	C8-N7-C5	2.90	108.52	102.99
51	S1	1566	PSU	C6-N1-C2	-2.90	119.72	122.68
2	L2	1265	PSU	C6-N1-C2	-2.90	119.72	122.68
3	L3	13	OMU	O4-C4-C5	-2.90	120.07	125.16
2	L2	1194	PSU	C6-N1-C2	-2.89	119.72	122.68
51	S1	1156	PSU	C6-N1-C2	-2.89	119.72	122.68
2	L2	593	PSU	C6-N1-C2	-2.89	119.72	122.68
2	L2	1303	PSU	C6-C5-C4	2.89	120.22	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S1	12	PSU	C6-N1-C2	-2.89	119.73	122.68
51	S1	29	OMU	O4-C4-C5	-2.89	120.08	125.16
2	L2	1229	OMG	C8-N7-C5	2.88	108.48	102.99
51	S1	1995	7MG	C2-N1-C6	-2.88	119.84	125.10
51	S1	104	PSU	C6-N1-C2	-2.88	119.74	122.68
2	L2	1382	PSU	C6-N1-C2	-2.88	119.74	122.68
1	L1	1181	PSU	C6-C5-C4	2.87	120.21	118.20
2	L2	641	OMG	C8-N7-C5	2.87	108.46	102.99
51	S1	1865	OMG	C8-N7-C5	2.87	108.46	102.99
2	L2	500	PSU	C6-C5-C4	2.87	120.20	118.20
2	L2	512	PSU	C6-N1-C2	-2.87	119.75	122.68
51	S1	1623	OMG	C2-N1-C6	-2.86	119.82	125.10
2	L2	1419	OMU	O4-C4-C5	-2.86	120.13	125.16
4	L4	74	OMG	C8-N7-C5	2.86	108.44	102.99
2	L2	1284	PSU	C6-N1-C2	-2.86	119.76	122.68
51	S1	1478	OMG	C8-N7-C5	2.86	108.44	102.99
51	S1	1543	B8N	N3-C2-N1	2.86	120.80	116.76
51	S1	1657	PSU	C6-N1-C2	-2.85	119.76	122.68
1	L1	1540	OMG	C8-N7-C5	2.85	108.43	102.99
1	L1	1253	OMU	O4-C4-C5	-2.85	120.14	125.16
2	L2	510	PSU	C6-N1-C2	-2.85	119.77	122.68
2	L2	597	PSU	C6-N1-C2	-2.85	119.77	122.68
51	S1	2046	PSU	C6-N1-C2	-2.85	119.77	122.68
2	L2	56	OMU	O4-C4-C5	-2.85	120.15	125.16
2	L2	506	PSU	C6-N1-C2	-2.85	119.77	122.68
2	L2	1231	OMG	C2-N1-C6	-2.85	119.86	125.10
51	S1	1657	PSU	C6-C5-C4	2.84	120.19	118.20
51	S1	600	OMG	C8-N7-C5	2.84	108.40	102.99
51	S1	600	OMG	C2-N1-C6	-2.84	119.87	125.10
2	L2	1265	PSU	O2-C2-N1	-2.84	119.67	122.79
51	S1	1979	OMU	O4-C4-C5	-2.84	120.17	125.16
1	L1	1171	PSU	C6-N1-C2	-2.84	119.78	122.68
7	L7	74	PSU	C6-N1-C2	-2.84	119.78	122.68
51	S1	1623	OMG	C8-N7-C5	2.83	108.39	102.99
2	L2	534	OMG	C8-N7-C5	2.83	108.38	102.99
1	L1	845	OMU	O4-C4-C5	-2.83	120.18	125.16
51	S1	1621	OMU	O4-C4-C5	-2.83	120.19	125.16
2	L2	686	OMG	C2-N1-C6	-2.83	119.89	125.10
51	S1	1662	OMU	O4-C4-C5	-2.83	120.19	125.16
2	L2	597	PSU	C6-C5-C4	2.82	120.17	118.20
2	L2	500	PSU	C6-N1-C2	-2.82	119.80	122.68
2	L2	534	OMG	C2-N1-C6	-2.82	119.91	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1060	PSU	C6-N1-C2	-2.82	119.80	122.68
51	S1	1841	PSU	C6-N1-C2	-2.82	119.80	122.68
1	L1	959	OMG	C2-N1-C6	-2.82	119.91	125.10
1	L1	847	OMU	O4-C4-C5	-2.82	120.21	125.16
1	L1	940	PSU	C6-N1-C2	-2.81	119.81	122.68
2	L2	1060	PSU	C6-C5-C4	2.81	120.16	118.20
1	L1	1659	OMU	O4-C4-C5	-2.81	120.22	125.16
2	L2	1046	OMG	C2-N1-C6	-2.81	119.92	125.10
2	L2	667	OMU	O4-C4-C5	-2.81	120.23	125.16
2	L2	1265	PSU	C6-C5-C4	2.80	120.16	118.20
51	S1	8	OMU	O4-C4-C5	-2.80	120.24	125.16
2	L2	1046	OMG	C8-N7-C5	2.80	108.32	102.99
51	S1	1246	PSU	C6-C5-C4	2.79	120.15	118.20
1	L1	1181	PSU	C6-N1-C2	-2.79	119.83	122.68
2	L2	1360	OMG	C8-N7-C5	2.78	108.29	102.99
1	L1	1664	PSU	C6-N1-C2	-2.78	119.84	122.68
2	L2	1213	PSU	C6-C5-C4	2.78	120.14	118.20
51	S1	1533	PSU	C6-N1-C2	-2.78	119.84	122.68
2	L2	472	PSU	C6-N1-C2	-2.78	119.84	122.68
1	L1	774	PSU	C6-C5-C4	2.78	120.14	118.20
2	L2	1359	OMU	O4-C4-C5	-2.78	120.28	125.16
2	L2	1144	PSU	C6-C5-C4	2.78	120.14	118.20
1	L1	1371	OMU	O4-C4-C5	-2.78	120.28	125.16
51	S1	2151	OMG	C2-N1-C6	-2.77	119.99	125.10
7	L7	74	PSU	C6-C5-C4	2.77	120.14	118.20
51	S1	2046	PSU	C6-C5-C4	2.77	120.14	118.20
1	L1	239	PSU	C6-N1-C2	-2.77	119.85	122.68
51	S1	1647	OMG	C2-N1-C6	-2.77	120.01	125.10
2	L2	1078	OMG	C2-N1-C6	-2.76	120.01	125.10
1	L1	1190	OMG	C2-N1-C6	-2.76	120.01	125.10
1	L1	48	OMU	O4-C4-C5	-2.76	120.30	125.16
51	S1	1865	OMG	C2-N1-C6	-2.76	120.01	125.10
51	S1	1246	PSU	C6-N1-C2	-2.76	119.86	122.68
2	L2	73	OMU	O4-C4-C5	-2.75	120.32	125.16
2	L2	1318	PSU	C6-N1-C2	-2.75	119.87	122.68
2	L2	1403	PSU	C6-N1-C2	-2.75	119.87	122.68
2	L2	1231	OMG	C8-N7-C5	2.75	108.23	102.99
51	S1	1478	OMG	C2-N1-C6	-2.75	120.04	125.10
2	L2	626	PSU	C6-C5-C4	2.74	120.12	118.20
4	L4	74	OMG	C2-N1-C6	-2.74	120.05	125.10
1	L1	239	PSU	C6-C5-C4	2.74	120.11	118.20
2	L2	71	OMG	C8-N7-C5	2.74	108.21	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	655	OMG	C2-N1-C6	-2.74	120.05	125.10
51	S1	1995	7MG	N9-C4-N3	2.74	129.56	125.47
2	L2	472	PSU	C6-C5-C4	2.73	120.11	118.20
1	L1	959	OMG	C8-N7-C5	2.73	108.20	102.99
2	L2	593	PSU	C6-C5-C4	2.73	120.11	118.20
51	S1	1995	7MG	O6-C6-C5	-2.73	120.84	127.54
1	L1	1528	PSU	C6-C5-C4	2.72	120.10	118.20
2	L2	437	PSU	C6-N1-C2	-2.72	119.90	122.68
51	S1	661	OMU	O4-C4-C5	-2.72	120.38	125.16
51	S1	2008	OMG	C2-N1-C6	-2.70	120.12	125.10
2	L2	1253	OMG	C8-N7-C5	2.70	108.14	102.99
2	L2	1360	OMG	C2-N1-C6	-2.70	120.12	125.10
51	S1	1543	B8N	O4-C4-N3	-2.70	115.39	119.98
7	L7	101	OMU	O4-C4-C5	-2.70	120.42	125.16
2	L2	1308	5MC	C4'-O4'-C1'	-2.70	103.52	109.47
1	L1	1011	PSU	C6-N1-C2	-2.69	119.94	122.68
7	L7	75	OMG	C2-N1-C6	-2.68	120.17	125.10
51	S1	1156	PSU	C6-C5-C4	2.68	120.07	118.20
1	L1	1171	PSU	O2-C2-N1	-2.67	119.85	122.79
2	L2	560	OMU	O4-C4-C5	-2.67	120.46	125.16
2	L2	1318	PSU	C6-C5-C4	2.67	120.07	118.20
2	L2	1229	OMG	C2-N1-C6	-2.66	120.19	125.10
1	L1	1039	OMU	O4-C4-C5	-2.66	120.49	125.16
2	L2	1361	PSU	O2-C2-N1	-2.66	119.87	122.79
1	L1	1093	PSU	C6-C5-C4	2.65	120.05	118.20
1	L1	1626	OMG	C8-N7-C5	2.65	108.03	102.99
2	L2	78	PSU	C6-N1-C2	-2.64	119.98	122.68
51	S1	1550	OMG	C8-N7-C5	2.64	108.02	102.99
51	S1	33	PSU	C6-C5-C4	2.63	120.04	118.20
2	L2	1078	OMG	N2-C2-N1	2.63	122.30	116.71
2	L2	506	PSU	C6-C5-C4	2.62	120.03	118.20
1	L1	422	PSU	C6-C5-C4	2.62	120.03	118.20
51	S1	104	PSU	C6-C5-C4	2.61	120.02	118.20
51	S1	1533	PSU	C6-C5-C4	2.60	120.02	118.20
51	S1	609	PSU	C6-C5-C4	2.60	120.01	118.20
2	L2	504	PSU	C6-C5-C4	2.60	120.01	118.20
1	L1	856	OMG	C8-N7-C5	2.59	107.93	102.99
51	S1	12	PSU	C6-C5-C4	2.58	120.00	118.20
2	L2	504	PSU	O2-C2-N1	-2.58	119.95	122.79
51	S1	609	PSU	O2-C2-N1	-2.57	119.96	122.79
51	S1	2048	PSU	C6-C5-C4	2.57	120.00	118.20
1	L1	940	PSU	C6-C5-C4	2.57	119.99	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	597	PSU	O2-C2-N1	-2.56	119.97	122.79
7	L7	69	PSU	O2-C2-N1	-2.56	119.97	122.79
2	L2	510	PSU	C6-C5-C4	2.56	119.98	118.20
51	S1	455	PSU	O2-C2-N1	-2.55	119.98	122.79
2	L2	512	PSU	C6-C5-C4	2.54	119.98	118.20
2	L2	500	PSU	O2-C2-N1	-2.53	120.00	122.79
2	L2	71	OMG	C2-N1-C6	-2.53	120.45	125.10
2	L2	1382	PSU	O2-C2-N1	-2.52	120.01	122.79
1	L1	1528	PSU	O2-C2-N1	-2.52	120.01	122.79
2	L2	1077	OMU	O4-C4-C5	-2.52	120.72	125.16
51	S1	2202	PSU	C6-C5-C4	2.52	119.96	118.20
2	L2	1058	PSU	O2-C2-N1	-2.52	120.02	122.79
51	S1	1292	PSU	C6-C5-C4	2.52	119.96	118.20
2	L2	662	PSU	O2-C2-N1	-2.51	120.03	122.79
1	L1	1533	PSU	C6-C5-C4	2.50	119.95	118.20
51	S1	104	PSU	O2-C2-N1	-2.48	120.06	122.79
2	L2	78	PSU	C6-C5-C4	2.48	119.93	118.20
2	L2	1194	PSU	C6-C5-C4	2.48	119.93	118.20
2	L2	1264	PSU	O2-C2-N1	-2.48	120.06	122.79
2	L2	626	PSU	O2-C2-N1	-2.48	120.06	122.79
1	L1	1533	PSU	O2-C2-N1	-2.48	120.06	122.79
2	L2	437	PSU	C6-C5-C4	2.47	119.93	118.20
51	S1	1246	PSU	O2-C2-N1	-2.47	120.08	122.79
1	L1	1017	PSU	O2-C2-N1	-2.46	120.08	122.79
51	S1	1833	OMU	O4-C4-C5	-2.46	120.83	125.16
2	L2	1284	PSU	C6-C5-C4	2.45	119.91	118.20
2	L2	1303	PSU	O2-C2-N1	-2.45	120.09	122.79
51	S1	2048	PSU	O2-C2-N1	-2.45	120.10	122.79
1	L1	677	1MA	C8-N7-C5	2.45	107.65	102.99
2	L2	1413	PSU	O2-C2-N1	-2.45	120.10	122.79
2	L2	512	PSU	O2-C2-N1	-2.44	120.10	122.79
51	S1	12	PSU	O2-C2-N1	-2.44	120.11	122.79
7	L7	74	PSU	O2-C2-N1	-2.44	120.11	122.79
51	S1	1995	7MG	N9-C8-N7	2.44	106.86	103.38
51	S1	1192	PSU	O2-C2-N1	-2.43	120.12	122.79
51	S1	668	A2M	C3'-C2'-C1'	2.43	107.45	102.89
51	S1	1566	PSU	C6-C5-C4	2.42	119.89	118.20
1	L1	1190	OMG	N2-C2-N1	2.42	121.87	116.71
51	S1	2046	PSU	O2-C2-N1	-2.42	120.12	122.79
2	L2	1194	PSU	O2-C2-N1	-2.42	120.13	122.79
51	S1	1533	PSU	O2-C2-N1	-2.42	120.13	122.79
2	L2	641	OMG	C5-C6-N1	2.41	118.21	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	472	PSU	O2-C2-N1	-2.41	120.14	122.79
51	S1	2202	PSU	O2-C2-N1	-2.40	120.15	122.79
51	S1	1657	PSU	O2-C2-N1	-2.40	120.15	122.79
51	S1	33	PSU	O2-C2-N1	-2.40	120.15	122.79
51	S1	1841	PSU	O2-C2-N1	-2.39	120.16	122.79
2	L2	593	PSU	O2-C2-N1	-2.39	120.16	122.79
1	L1	239	PSU	O2-C2-N1	-2.39	120.17	122.79
1	L1	774	PSU	O2-C2-N1	-2.38	120.17	122.79
51	S1	1543	B8N	C32-C31-N3	-2.38	107.53	112.00
2	L2	1253	OMG	C2-N1-C6	-2.38	120.71	125.10
1	L1	1524	OMG	C8-N7-C5	2.38	107.52	102.99
1	L1	1626	OMG	C2-N1-C6	-2.38	120.72	125.10
1	L1	1181	PSU	O2-C2-N1	-2.38	120.17	122.79
2	L2	1284	PSU	O2-C2-N1	-2.37	120.18	122.79
52	S2	37	MIA	C16-C14-C15	2.37	119.84	114.60
1	L1	856	OMG	C2-N1-C6	-2.37	120.74	125.10
1	L1	856	OMG	C5-C6-N1	2.37	118.13	113.95
2	L2	1060	PSU	O2-C2-N1	-2.36	120.19	122.79
2	L2	641	OMG	C2-N1-C6	-2.36	120.75	125.10
7	L7	101	OMU	O3'-C3'-C2'	2.36	117.86	111.17
1	L1	1011	PSU	O2-C2-N1	-2.35	120.20	122.79
51	S1	1292	PSU	O2-C2-N1	-2.35	120.20	122.79
2	L2	1253	OMG	C5-C6-N1	2.35	118.09	113.95
2	L2	437	PSU	O2-C2-N1	-2.33	120.22	122.79
2	L2	1403	PSU	O2-C2-N1	-2.33	120.22	122.79
1	L1	1093	PSU	O2-C2-N1	-2.33	120.22	122.79
1	L1	422	PSU	O2-C2-N1	-2.32	120.23	122.79
2	L2	506	PSU	O2-C2-N1	-2.31	120.25	122.79
51	S1	1539	PSU	O2-C2-N1	-2.31	120.25	122.79
1	L1	1540	OMG	C2-N1-C6	-2.31	120.85	125.10
1	L1	1540	OMG	C5-C6-N1	2.31	118.03	113.95
51	S1	1829	OMG	C2-N1-C6	-2.31	120.85	125.10
51	S1	1566	PSU	O2-C2-N1	-2.30	120.25	122.79
1	L1	940	PSU	O2-C2-N1	-2.30	120.26	122.79
51	S1	1550	OMG	C2-N1-C6	-2.29	120.88	125.10
2	L2	1213	PSU	O2-C2-N1	-2.27	120.29	122.79
2	L2	1144	PSU	O2-C2-N1	-2.26	120.30	122.79
1	L1	1664	PSU	C6-C5-C4	2.26	119.78	118.20
51	S1	1478	OMG	N2-C2-N1	2.26	121.52	116.71
2	L2	71	OMG	C5-C6-N1	2.25	117.93	113.95
1	L1	1664	PSU	O2-C2-N1	-2.24	120.33	122.79
2	L2	1318	PSU	O2-C2-N1	-2.21	120.36	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L2	1046	OMG	O6-C6-C5	-2.21	120.06	124.37
1	L1	1524	OMG	C2-N1-C6	-2.21	121.03	125.10
1	L1	1527	OMC	O2-C2-N3	-2.20	118.75	122.33
1	L1	1626	OMG	C5-C6-N1	2.20	117.83	113.95
3	L3	13	OMU	O2-C2-N1	-2.19	119.87	122.79
51	S1	8	OMU	O2-C2-N1	-2.19	119.88	122.79
2	L2	1231	OMG	O6-C6-C5	-2.18	120.11	124.37
7	L7	101	OMU	C2'-C1'-N1	-2.18	110.00	114.22
2	L2	510	PSU	O2-C2-N1	-2.18	120.39	122.79
2	L2	1359	OMU	O2-C2-N1	-2.16	119.91	122.79
51	S1	29	OMU	O2-C2-N1	-2.15	119.93	122.79
51	S1	2021	A2M	O2'-C2'-C1'	2.15	113.36	109.09
1	L1	959	OMG	O6-C6-C5	-2.14	120.18	124.37
51	S1	1829	OMG	C5-C6-N1	2.13	117.72	113.95
51	S1	1478	OMG	O6-C6-C5	-2.13	120.20	124.37
2	L2	1078	OMG	O6-C6-C5	-2.13	120.21	124.37
2	L2	1303	PSU	O4'-C1'-C2'	2.13	108.15	105.14
51	S1	1550	OMG	C5-C6-N1	2.13	117.71	113.95
2	L2	1308	5MC	C5-C4-N3	-2.13	119.38	121.67
2	L2	1229	OMG	O6-C6-C5	-2.13	120.22	124.37
7	L7	69	PSU	O4'-C1'-C2'	2.12	108.14	105.14
1	L1	1190	OMG	O6-C6-C5	-2.12	120.23	124.37
51	S1	600	OMG	O6-C6-C5	-2.12	120.24	124.37
4	L4	74	OMG	O6-C6-C5	-2.12	120.24	124.37
51	S1	1647	OMG	O6-C6-C5	-2.11	120.24	124.37
2	L2	56	OMU	O2-C2-N1	-2.11	119.98	122.79
2	L2	686	OMG	O6-C6-C5	-2.11	120.25	124.37
51	S1	1623	OMG	O6-C6-C5	-2.11	120.25	124.37
2	L2	78	PSU	O2-C2-N1	-2.11	120.47	122.79
1	L1	1524	OMG	C5-C6-N1	2.10	117.67	113.95
2	L2	1360	OMG	O6-C6-C5	-2.10	120.27	124.37
51	S1	1156	PSU	O2-C2-N1	-2.09	120.49	122.79
2	L2	1382	PSU	O4'-C1'-C2'	2.08	108.08	105.14
2	L2	1403	PSU	O4'-C1'-C2'	2.08	108.07	105.14
51	S1	1865	OMG	O6-C6-C5	-2.08	120.32	124.37
2	L2	534	OMG	O6-C6-C5	-2.07	120.32	124.37
52	S2	37	MIA	C12-N6-C6	-2.07	119.48	122.55
51	S1	1621	OMU	O2-C2-N1	-2.07	120.04	122.79
1	L1	1107	OMU	O2-C2-N1	-2.05	120.06	122.79
4	L4	74	OMG	N2-C2-N1	2.05	121.07	116.71
2	L2	1231	OMG	N2-C2-N1	2.04	121.06	116.71
1	L1	1659	OMU	O2-C2-N1	-2.02	120.10	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	48	OMU	O2-C2-N1	-2.02	120.10	122.79
51	S1	2008	OMG	N1-C2-N3	-2.02	119.55	123.32
1	L1	1190	OMG	N1-C2-N3	-2.02	119.55	123.32
51	S1	455	PSU	C6-C5-C4	2.02	119.61	118.20
7	L7	75	OMG	O6-C6-C5	-2.01	120.44	124.37
1	L1	1253	OMU	O2-C2-N1	-2.01	120.11	122.79
2	L2	524	5MC	CM5-C5-C6	-2.01	120.17	122.85
2	L2	504	PSU	O4'-C1'-C2'	2.00	107.97	105.14
51	S1	969	A2M	C3'-C2'-C1'	2.00	106.66	102.89

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L1	681	A2M	O4'-C4'-C5'-O5'
1	L1	681	A2M	C3'-C4'-C5'-O5'
1	L1	955	A2M	C1'-C2'-O2'-CM'
1	L1	1010	OMC	C1'-C2'-O2'-CM2
1	L1	1011	PSU	C2'-C1'-C5-C4
1	L1	1011	PSU	C2'-C1'-C5-C6
1	L1	1039	OMU	C1'-C2'-O2'-CM2
1	L1	1171	PSU	C3'-C4'-C5'-O5'
1	L1	1171	PSU	O4'-C4'-C5'-O5'
1	L1	1371	OMU	C1'-C2'-O2'-CM2
1	L1	1371	OMU	C3'-C4'-C5'-O5'
1	L1	1540	OMG	O4'-C4'-C5'-O5'
1	L1	1540	OMG	C3'-C4'-C5'-O5'
1	L1	1552	OMC	C1'-C2'-O2'-CM2
2	L2	534	OMG	O4'-C4'-C5'-O5'
2	L2	534	OMG	C3'-C4'-C5'-O5'
2	L2	591	A2M	C1'-C2'-O2'-CM'
2	L2	604	A2M	C1'-C2'-O2'-CM'
2	L2	665	A2M	C1'-C2'-O2'-CM'
2	L2	1046	OMG	O4'-C4'-C5'-O5'
2	L2	1185	A2M	C1'-C2'-O2'-CM'
2	L2	1229	OMG	O4'-C4'-C5'-O5'
2	L2	1229	OMG	C3'-C4'-C5'-O5'
2	L2	1248	OMC	C1'-C2'-O2'-CM2
2	L2	1264	PSU	C3'-C4'-C5'-O5'
2	L2	1308	5MC	C2'-C1'-N1-C6
2	L2	1361	PSU	C3'-C4'-C5'-O5'
7	L7	162	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
51	S1	29	OMU	C1'-C2'-O2'-CM2
51	S1	98	A2M	C1'-C2'-O2'-CM'
51	S1	455	PSU	C3'-C4'-C5'-O5'
51	S1	668	A2M	O4'-C4'-C5'-O5'
51	S1	668	A2M	C1'-C2'-O2'-CM'
51	S1	1543	B8N	O4'-C4'-C5'-O5'
51	S1	1543	B8N	C3'-C4'-C5'-O5'
51	S1	1543	B8N	N34-C33-C34-O35
51	S1	1662	OMU	C1'-C2'-O2'-CM2
51	S1	2021	A2M	C1'-C2'-O2'-CM'
51	S1	2202	PSU	O4'-C1'-C5-C6
52	S2	37	MIA	N1-C2-S10-C11
52	S2	37	MIA	N3-C2-S10-C11
2	L2	1308	5MC	C2'-C1'-N1-C2
2	L2	1046	OMG	C3'-C4'-C5'-O5'
2	L2	1361	PSU	O4'-C4'-C5'-O5'
51	S1	600	OMG	O4'-C4'-C5'-O5'
2	L2	665	A2M	O4'-C4'-C5'-O5'
2	L2	665	A2M	C3'-C4'-C5'-O5'
51	S1	455	PSU	O4'-C4'-C5'-O5'
51	S1	668	A2M	C3'-C4'-C5'-O5'
2	L2	443	OMC	C2'-C1'-N1-C6
51	S1	1543	B8N	N34-C33-C34-O36
1	L1	1371	OMU	O4'-C4'-C5'-O5'
2	L2	1264	PSU	O4'-C4'-C5'-O5'
51	S1	600	OMG	C3'-C4'-C5'-O5'
1	L1	1524	OMG	O4'-C4'-C5'-O5'
51	S1	512	A2M	C3'-C4'-C5'-O5'
51	S1	1995	7MG	O4'-C4'-C5'-O5'
51	S1	1995	7MG	C3'-C4'-C5'-O5'
2	L2	443	OMC	C2'-C1'-N1-C2
1	L1	1010	OMC	O4'-C4'-C5'-O5'
1	L1	1524	OMG	C3'-C4'-C5'-O5'
2	L2	570	A2M	O4'-C4'-C5'-O5'
51	S1	8	OMU	C2'-C1'-N1-C6
2	L2	570	A2M	C3'-C4'-C5'-O5'
2	L2	443	OMC	O4'-C1'-N1-C6
2	L2	1308	5MC	O4'-C1'-N1-C6
1	L1	681	A2M	C4'-C5'-O5'-P
51	S1	2185	MA6	C4'-C5'-O5'-P
4	L4	74	OMG	C3'-C4'-C5'-O5'
2	L2	560	OMU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
51	S1	98	A2M	O4'-C4'-C5'-O5'
52	S2	37	MIA	C5-C6-N6-C12
2	L2	1308	5MC	O4'-C1'-N1-C2
51	S1	512	A2M	O4'-C4'-C5'-O5'
51	S1	1544	5MC	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C1'-N1-C6
2	L2	443	OMC	O4'-C1'-N1-C2
2	L2	1248	OMC	C4'-C5'-O5'-P
1	L1	1524	OMG	C3'-C2'-O2'-CM2
52	S2	37	MIA	N1-C6-N6-C12
2	L2	1361	PSU	C4'-C5'-O5'-P
51	S1	1478	OMG	C4'-C5'-O5'-P
51	S1	1829	OMG	C4'-C5'-O5'-P
1	L1	1011	PSU	O4'-C1'-C5-C4
2	L2	1382	PSU	O4'-C1'-C5-C4
51	S1	1657	PSU	O4'-C1'-C5-C4
2	L2	502	A2M	C3'-C2'-O2'-CM'
51	S1	1833	OMU	O4'-C4'-C5'-O5'
51	S1	1829	OMG	O4'-C4'-C5'-O5'
51	S1	2059	OMC	O4'-C4'-C5'-O5'
51	S1	8	OMU	O4'-C1'-N1-C2
1	L1	1010	OMC	C3'-C4'-C5'-O5'
2	L2	1046	OMG	C1'-C2'-O2'-CM2
2	L2	1384	A2M	C1'-C2'-O2'-CM'
1	L1	1011	PSU	O4'-C1'-C5-C6
2	L2	1185	A2M	C4'-C5'-O5'-P
51	S1	8	OMU	O4'-C4'-C5'-O5'
51	S1	1623	OMG	O4'-C4'-C5'-O5'
51	S1	8	OMU	C2'-C1'-N1-C2
1	L1	1527	OMC	C3'-C2'-O2'-CM2
51	S1	969	A2M	C3'-C2'-O2'-CM'
1	L1	669	OMC	O4'-C4'-C5'-O5'
1	L1	1527	OMC	O4'-C4'-C5'-O5'
2	L2	527	A2M	O4'-C4'-C5'-O5'
2	L2	1185	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

63 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S1	1543	B8N	1	0
2	L2	1264	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	S1	1829	OMG	1	0
51	S1	29	OMU	4	0
7	L7	43	A2M	1	0
1	L1	1253	OMU	1	0
1	L1	681	A2M	1	0
52	S2	37	MIA	1	0
2	L2	1360	OMG	2	0
51	S1	1662	OMU	1	0
51	S1	2059	OMC	1	0
2	L2	56	OMU	1	0
2	L2	1397	OMC	1	0
51	S1	1550	OMG	2	0
2	L2	512	PSU	1	0
51	S1	38	OMC	1	0
51	S1	668	A2M	1	0
51	S1	1539	PSU	2	0
1	L1	1371	OMU	1	0
1	L1	305	A2M	1	0
1	L1	845	OMU	1	0
1	L1	1552	OMC	1	0
1	L1	1659	OMU	1	0
2	L2	14	OMC	2	0
1	L1	1524	OMG	2	0
51	S1	2019	OMC	1	0
51	S1	2140	OMC	1	0
2	L2	1308	5MC	2	0
1	L1	955	A2M	1	0
2	L2	1078	OMG	1	0
51	S1	28	A2M	1	0
51	S1	969	A2M	4	0
51	S1	18	OMC	1	0
1	L1	678	A2M	3	0
1	L1	927	A2M	1	0
51	S1	1566	PSU	1	0
2	L2	1248	OMC	2	0
7	L7	162	A2M	2	0
51	S1	479	A2M	1	0
51	S1	2008	OMG	3	0
2	L2	382	A2M	3	0
1	L1	1039	OMU	1	0
1	L1	1527	OMC	2	0
2	L2	1185	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L1	1190	OMG	2	0
2	L2	1284	PSU	1	0
2	L2	443	OMC	1	0
1	L1	1626	OMG	2	0
51	S1	98	A2M	2	0
1	L1	669	OMC	1	0
1	L1	1373	A2M	1	0
1	L1	235	A2M	1	0
2	L2	591	A2M	3	0
2	L2	1253	OMG	1	0
2	L2	95	A2M	1	0
1	L1	1010	OMC	1	0
7	L7	69	PSU	1	0
1	L1	1528	PSU	1	0
2	L2	570	A2M	1	0
2	L2	1318	PSU	1	0
1	L1	959	OMG	1	0
1	L1	1017	PSU	1	0
2	L2	560	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 535 ligands modelled in this entry, 492 are monoatomic - leaving 43 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	$\# Z  > 2$
94	PAR	L1	1978	-	45,45,45	3.57	11 (24%)	64,67,67	1.13	4 (6%)
94	PAR	L7	208	-	45,45,45	3.47	11 (24%)	64,67,67	1.36	12 (18%)
89	SPD	L1	1806	-	9,9,9	0.44	0	8,8,8	0.39	0
93	PUT	L5	207	-	5,5,5	0.24	0	4,4,4	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
89	SPD	L1	1808	-	9,9,9	0.43	0	8,8,8	0.37	0
93	PUT	L1	1975	-	5,5,5	0.24	0	4,4,4	0.17	0
93	PUT	L2	1726	-	5,5,5	0.24	0	4,4,4	0.15	0
89	SPD	L2	1601	-	9,9,9	0.44	0	8,8,8	0.18	0
93	PUT	L2	1724	-	5,5,5	0.24	0	4,4,4	0.18	0
93	PUT	L1	1973	-	5,5,5	0.24	0	4,4,4	0.16	0
89	SPD	L1	1804	-	9,9,9	0.43	0	8,8,8	0.34	0
94	PAR	L2	1729	-	45,45,45	3.52	10 (22%)	64,67,67	1.36	10 (15%)
93	PUT	S1	2444	-	5,5,5	0.24	0	4,4,4	0.16	0
89	SPD	S1	2301	-	9,9,9	0.44	0	8,8,8	0.27	0
94	PAR	S1	2445	92	45,45,45	3.59	11 (24%)	64,67,67	1.05	6 (9%)
89	SPD	L1	1814	-	9,9,9	0.44	0	8,8,8	0.24	0
89	SPD	L1	1805	-	9,9,9	0.46	0	8,8,8	0.24	0
89	SPD	L1	1815	-	9,9,9	0.44	0	8,8,8	0.25	0
89	SPD	L2	1602	2	9,9,9	0.45	0	8,8,8	0.21	0
89	SPD	L1	1802	-	9,9,9	0.43	0	8,8,8	0.21	0
89	SPD	L1	1811	-	9,9,9	0.42	0	8,8,8	0.41	0
93	PUT	L1	1976	-	5,5,5	0.24	0	4,4,4	0.18	0
89	SPD	L1	1812	-	9,9,9	0.45	0	8,8,8	0.22	0
89	SPD	L1	1801	-	9,9,9	0.42	0	8,8,8	0.44	0
93	PUT	S1	2443	-	5,5,5	0.24	0	4,4,4	0.16	0
89	SPD	L1	1809	-	9,9,9	0.44	0	8,8,8	0.28	0
93	PUT	L1	1977	-	5,5,5	0.24	0	4,4,4	0.16	0
89	SPD	L1	1813	-	9,9,9	0.44	0	8,8,8	0.19	0
89	SPD	L1	1803	-	9,9,9	0.43	0	8,8,8	0.26	0
94	PAR	S1	2446	-	45,45,45	3.56	11 (24%)	64,67,67	1.15	6 (9%)
93	PUT	L4	218	-	5,5,5	0.24	0	4,4,4	0.16	0
93	PUT	L2	1725	-	5,5,5	0.24	0	4,4,4	0.17	0
89	SPD	S1	2302	-	9,9,9	0.44	0	8,8,8	0.34	0
93	PUT	L1	1974	-	5,5,5	0.24	0	4,4,4	0.17	0
89	SPD	LM	301	-	9,9,9	0.44	0	8,8,8	0.16	0
89	SPD	L1	1807	-	9,9,9	0.42	0	8,8,8	0.36	0
93	PUT	L1	1971	-	5,5,5	0.24	0	4,4,4	0.17	0
93	PUT	L2	1727	-	5,5,5	0.23	0	4,4,4	0.22	0
93	PUT	L1	1972	1	5,5,5	0.25	0	4,4,4	0.09	0
89	SPD	L1	1810	-	9,9,9	0.42	0	8,8,8	0.31	0
94	PAR	L2	1728	-	45,45,45	3.54	10 (22%)	64,67,67	1.22	6 (9%)
89	SPD	S1	2447	-	9,9,9	0.44	0	8,8,8	0.31	0
93	PUT	L2	1723	-	5,5,5	0.23	0	4,4,4	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
94	PAR	L1	1978	-	-	8/18/94/94	0/4/4/4
94	PAR	L7	208	-	-	9/18/94/94	0/4/4/4
89	SPD	L1	1806	-	-	1/7/7/7	-
93	PUT	L5	207	-	-	0/3/3/3	-
89	SPD	L1	1808	-	-	0/7/7/7	-
93	PUT	L1	1975	-	-	1/3/3/3	-
93	PUT	L2	1726	-	-	0/3/3/3	-
89	SPD	L2	1601	-	-	1/7/7/7	-
93	PUT	L2	1724	-	-	1/3/3/3	-
93	PUT	L1	1973	-	-	0/3/3/3	-
89	SPD	L1	1804	-	-	2/7/7/7	-
94	PAR	L2	1729	-	-	11/18/94/94	0/4/4/4
93	PUT	S1	2444	-	-	1/3/3/3	-
89	SPD	S1	2301	-	-	2/7/7/7	-
94	PAR	S1	2445	92	-	6/18/94/94	0/4/4/4
89	SPD	L1	1814	-	-	0/7/7/7	-
89	SPD	L1	1805	-	-	2/7/7/7	-
89	SPD	L1	1815	-	-	0/7/7/7	-
89	SPD	L2	1602	2	-	1/7/7/7	-
89	SPD	L1	1802	-	-	1/7/7/7	-
89	SPD	L1	1811	-	-	2/7/7/7	-
93	PUT	L1	1976	-	-	0/3/3/3	-
89	SPD	L1	1812	-	-	2/7/7/7	-
89	SPD	L1	1801	-	-	3/7/7/7	-
93	PUT	S1	2443	-	-	1/3/3/3	-
89	SPD	L1	1809	-	-	2/7/7/7	-
93	PUT	L1	1977	-	-	0/3/3/3	-
89	SPD	L1	1813	-	-	1/7/7/7	-
89	SPD	L1	1803	-	-	0/7/7/7	-
94	PAR	S1	2446	-	-	10/18/94/94	0/4/4/4
93	PUT	L4	218	-	-	0/3/3/3	-
93	PUT	L2	1725	-	-	0/3/3/3	-
89	SPD	S1	2302	-	-	0/7/7/7	-
93	PUT	L1	1974	-	-	0/3/3/3	-
89	SPD	LM	301	-	-	0/7/7/7	-
89	SPD	L1	1807	-	-	2/7/7/7	-
93	PUT	L1	1971	-	-	0/3/3/3	-
93	PUT	L2	1727	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	PUT	L1	1972	1	-	0/3/3/3	-
89	SPD	L1	1810	-	-	0/7/7/7	-
94	PAR	L2	1728	-	-	6/18/94/94	0/4/4/4
89	SPD	S1	2447	-	-	2/7/7/7	-
93	PUT	L2	1723	-	-	1/3/3/3	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	S1	2445	PAR	C13-C23	-15.69	1.32	1.52
94	L1	1978	PAR	C13-C23	-15.62	1.32	1.52
94	S1	2446	PAR	C13-C23	-15.46	1.33	1.52
94	L2	1728	PAR	C13-C23	-15.18	1.33	1.52
94	L7	208	PAR	C13-C23	-14.99	1.33	1.52
94	L2	1729	PAR	C13-C23	-14.84	1.33	1.52
94	L2	1729	PAR	O43-C13	13.41	1.65	1.41
94	L2	1728	PAR	O43-C13	13.37	1.65	1.41
94	S1	2445	PAR	O43-C13	13.29	1.65	1.41
94	L1	1978	PAR	O43-C13	13.19	1.65	1.41
94	S1	2446	PAR	O43-C13	13.17	1.65	1.41
94	L7	208	PAR	O43-C13	13.07	1.65	1.41
94	L7	208	PAR	O43-C43	-6.30	1.30	1.45
94	L2	1729	PAR	O43-C43	-6.15	1.31	1.45
94	S1	2446	PAR	O43-C43	-6.07	1.31	1.45
94	L2	1728	PAR	O43-C43	-6.06	1.31	1.45
94	L1	1978	PAR	O43-C43	-5.88	1.31	1.45
94	S1	2445	PAR	O43-C43	-5.83	1.32	1.45
94	L1	1978	PAR	C34-C24	-4.73	1.47	1.53
94	L1	1978	PAR	O54-C14	4.41	1.53	1.41
94	S1	2445	PAR	O54-C14	4.40	1.53	1.41
94	L2	1728	PAR	O54-C14	4.38	1.53	1.41
94	L2	1729	PAR	O54-C14	4.38	1.53	1.41
94	S1	2446	PAR	C34-C24	-4.35	1.48	1.53
94	S1	2446	PAR	O54-C14	4.35	1.52	1.41
94	S1	2445	PAR	C34-C24	-4.30	1.48	1.53
94	L2	1728	PAR	C34-C24	-4.27	1.48	1.53
94	L2	1729	PAR	C34-C24	-4.27	1.48	1.53
94	L7	208	PAR	O54-C14	4.22	1.52	1.41
94	L2	1729	PAR	O51-C11	3.84	1.51	1.41
94	S1	2445	PAR	O51-C11	3.77	1.51	1.41
94	L1	1978	PAR	O51-C11	3.77	1.51	1.41
94	S1	2445	PAR	O33-C33	-3.76	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	L2	1729	PAR	O33-C33	-3.75	1.34	1.43
94	L2	1728	PAR	O51-C11	3.74	1.51	1.41
94	L1	1978	PAR	O33-C33	-3.71	1.34	1.43
94	L2	1728	PAR	O33-C33	-3.70	1.34	1.43
94	S1	2446	PAR	O51-C11	3.69	1.51	1.41
94	L7	208	PAR	O51-C11	3.67	1.51	1.41
94	L7	208	PAR	O33-C33	-3.65	1.34	1.43
94	S1	2446	PAR	O33-C33	-3.54	1.34	1.43
94	S1	2445	PAR	C31-C21	-3.48	1.49	1.53
94	L7	208	PAR	C24-N24	3.39	1.52	1.47
94	S1	2446	PAR	C31-C21	-3.36	1.49	1.53
94	S1	2445	PAR	C24-N24	3.30	1.52	1.47
94	S1	2446	PAR	C24-N24	3.29	1.52	1.47
94	L2	1728	PAR	C24-N24	3.25	1.52	1.47
94	L2	1729	PAR	C31-C21	-3.20	1.49	1.53
94	L2	1728	PAR	C31-C21	-3.20	1.49	1.53
94	L2	1729	PAR	C24-N24	3.20	1.52	1.47
94	L1	1978	PAR	C24-N24	3.17	1.52	1.47
94	L7	208	PAR	C34-C24	-3.13	1.49	1.53
94	L1	1978	PAR	C31-C21	-3.05	1.49	1.53
94	L7	208	PAR	C31-C21	-2.89	1.49	1.53
94	L2	1729	PAR	C64-C54	2.46	1.55	1.52
94	S1	2446	PAR	C33-C43	2.22	1.58	1.52
94	L7	208	PAR	C64-C54	2.22	1.55	1.52
94	L1	1978	PAR	C33-C43	2.18	1.58	1.52
94	S1	2446	PAR	C64-C54	2.17	1.55	1.52
94	S1	2445	PAR	C33-C43	2.14	1.58	1.52
94	L7	208	PAR	C33-C43	2.13	1.58	1.52
94	L1	1978	PAR	C64-C54	2.13	1.54	1.52
94	S1	2445	PAR	C64-C54	2.11	1.54	1.52
94	L2	1728	PAR	C64-C54	2.07	1.54	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
94	L1	1978	PAR	C14-O33-C33	-4.03	107.99	117.96
94	L7	208	PAR	C44-C34-C24	3.77	117.55	111.07
94	L2	1728	PAR	C14-O33-C33	-3.58	109.12	117.96
94	L2	1729	PAR	C34-C44-C54	3.12	115.81	110.24
94	L7	208	PAR	C11-O11-C42	-3.10	110.30	117.96
94	L2	1728	PAR	C13-C23-C33	3.04	105.76	102.10
94	L2	1728	PAR	C13-O52-C52	-3.04	110.44	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
94	L2	1729	PAR	C13-C23-C33	2.98	105.68	102.10
94	L2	1728	PAR	C11-O11-C42	-2.95	110.67	117.96
94	L1	1978	PAR	C11-O11-C42	-2.91	110.75	117.96
94	S1	2445	PAR	C13-O52-C52	-2.89	110.81	117.96
94	S1	2446	PAR	C13-C23-C33	2.87	105.56	102.10
94	L2	1729	PAR	O52-C13-O43	-2.83	108.37	111.43
94	L7	208	PAR	C14-C24-C34	2.82	117.60	110.21
94	L2	1729	PAR	C14-O33-C33	-2.81	111.02	117.96
94	S1	2446	PAR	C14-O33-C33	-2.80	111.03	117.96
94	L2	1729	PAR	C11-O11-C42	-2.79	111.07	117.96
94	S1	2445	PAR	C14-O33-C33	-2.78	111.09	117.96
94	L7	208	PAR	O52-C13-C23	2.77	113.70	107.96
94	L7	208	PAR	C14-O33-C33	-2.73	111.21	117.96
94	L2	1729	PAR	O52-C52-C62	2.73	114.53	107.28
94	S1	2446	PAR	C13-O52-C52	-2.66	111.37	117.96
94	L7	208	PAR	O52-C13-O43	2.60	114.24	111.43
94	L2	1729	PAR	C22-C12-C62	2.52	113.84	110.04
94	S1	2446	PAR	O51-C51-C41	2.49	114.22	109.69
94	L2	1728	PAR	O43-C13-C23	2.47	108.16	104.98
94	L1	1978	PAR	C13-O52-C52	-2.43	111.96	117.96
94	L7	208	PAR	C13-C23-C33	2.42	105.02	102.10
94	L2	1729	PAR	O54-C54-C44	2.34	113.95	109.69
94	S1	2445	PAR	C11-O11-C42	-2.31	112.25	117.96
94	L2	1728	PAR	C64-C54-C44	-2.28	108.61	113.10
94	L7	208	PAR	C52-C42-C32	2.24	115.34	111.16
94	S1	2445	PAR	O51-C51-C41	2.22	113.72	109.69
94	L7	208	PAR	O54-C54-C64	2.17	110.05	106.01
94	L1	1978	PAR	C64-C54-C44	-2.16	108.85	113.10
94	L7	208	PAR	C64-C54-C44	-2.16	108.86	113.10
94	L2	1729	PAR	C61-C51-C41	-2.14	107.98	113.00
94	L7	208	PAR	C34-C44-C54	2.09	113.96	110.24
94	S1	2446	PAR	O11-C42-C32	-2.07	104.25	109.18
94	S1	2445	PAR	C61-C51-C41	-2.05	108.20	113.00
94	S1	2445	PAR	C64-C54-C44	-2.04	109.09	113.10
94	L2	1729	PAR	O51-C11-C21	2.04	114.64	110.06
94	S1	2446	PAR	C64-C54-C44	-2.01	109.14	113.10
94	L7	208	PAR	C22-C32-C42	2.00	114.60	109.53

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	L1	1978	PAR	C23-C13-O52-C52
94	L1	1978	PAR	O43-C43-C53-O53
94	L1	1978	PAR	C44-C54-C64-N64
94	L1	1978	PAR	O54-C54-C64-N64
94	L2	1729	PAR	C23-C13-O52-C52
94	L2	1729	PAR	O43-C13-O52-C52
94	L2	1729	PAR	C24-C14-O33-C33
94	L2	1729	PAR	C44-C54-C64-N64
94	L2	1729	PAR	O54-C54-C64-N64
94	L7	208	PAR	C23-C13-O52-C52
94	L7	208	PAR	O43-C13-O52-C52
94	L7	208	PAR	O54-C54-C64-N64
94	S1	2445	PAR	O43-C43-C53-O53
94	S1	2446	PAR	C24-C14-O33-C33
94	S1	2446	PAR	O54-C14-O33-C33
94	L2	1729	PAR	C62-C52-O52-C13
94	L2	1729	PAR	O54-C14-O33-C33
94	L1	1978	PAR	C33-C43-C53-O53
94	S1	2445	PAR	C33-C43-C53-O53
94	S1	2445	PAR	O54-C14-O33-C33
89	L1	1801	SPD	N6-C7-C8-C9
89	L1	1809	SPD	N6-C7-C8-C9
94	L7	208	PAR	O43-C43-C53-O53
94	L7	208	PAR	C33-C43-C53-O53
94	L1	1978	PAR	O51-C51-C61-O61
94	L2	1728	PAR	O51-C51-C61-O61
94	L2	1728	PAR	C41-C51-C61-O61
94	S1	2446	PAR	O51-C51-C61-O61
94	L1	1978	PAR	C41-C51-C61-O61
94	L2	1728	PAR	O54-C14-O33-C33
94	S1	2446	PAR	C33-C43-C53-O53
89	L1	1811	SPD	C2-C3-C4-C5
94	S1	2446	PAR	C41-C51-C61-O61
89	S1	2301	SPD	C8-C7-N6-C5
94	L1	1978	PAR	O43-C13-O52-C52
94	S1	2446	PAR	O43-C43-C53-O53
94	S1	2446	PAR	O51-C11-O11-C42
89	L1	1811	SPD	C8-C7-N6-C5
94	L7	208	PAR	O51-C51-C61-O61
94	S1	2446	PAR	C44-C54-C64-N64
94	L2	1729	PAR	C33-C43-C53-O53
94	L2	1728	PAR	C23-C13-O52-C52
89	L1	1806	SPD	N1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
94	S1	2446	PAR	O54-C54-C64-N64
94	S1	2446	PAR	C52-C42-O11-C11
94	L7	208	PAR	O54-C14-O33-C33
94	L2	1728	PAR	O51-C11-O11-C42
89	L1	1802	SPD	C4-C5-N6-C7
94	S1	2445	PAR	C43-C33-O33-C14
93	L2	1724	PUT	C1-C2-C3-C4
89	L1	1804	SPD	N1-C2-C3-C4
89	L2	1602	SPD	C2-C3-C4-C5
89	S1	2301	SPD	C2-C3-C4-C5
89	L1	1801	SPD	C4-C5-N6-C7
94	L2	1729	PAR	C41-C51-C61-O61
94	L2	1729	PAR	O43-C43-C53-O53
89	L1	1807	SPD	C4-C5-N6-C7
94	L2	1729	PAR	O51-C11-O11-C42
93	L2	1723	PUT	C1-C2-C3-C4
93	S1	2444	PUT	C1-C2-C3-C4
89	L1	1801	SPD	C8-C7-N6-C5
89	S1	2447	SPD	C8-C7-N6-C5
89	S1	2447	SPD	N1-C2-C3-C4
93	L1	1975	PUT	C1-C2-C3-C4
94	L7	208	PAR	C62-C52-O52-C13
94	L7	208	PAR	C42-C52-O52-C13
89	L1	1804	SPD	C8-C7-N6-C5
89	L2	1601	SPD	C8-C7-N6-C5
89	L1	1813	SPD	C2-C3-C4-C5
89	L1	1805	SPD	C7-C8-C9-N10
89	L1	1805	SPD	C4-C5-N6-C7
93	S1	2443	PUT	C1-C2-C3-C4
89	L1	1807	SPD	C8-C7-N6-C5
89	L1	1809	SPD	C8-C7-N6-C5
89	L1	1812	SPD	C4-C5-N6-C7
94	L2	1728	PAR	C43-C33-O33-C14
94	S1	2445	PAR	C23-C33-O33-C14
94	S1	2445	PAR	O51-C11-O11-C42
89	L1	1812	SPD	C2-C3-C4-C5

There are no ring outliers.

20 monomers are involved in 43 short contacts:

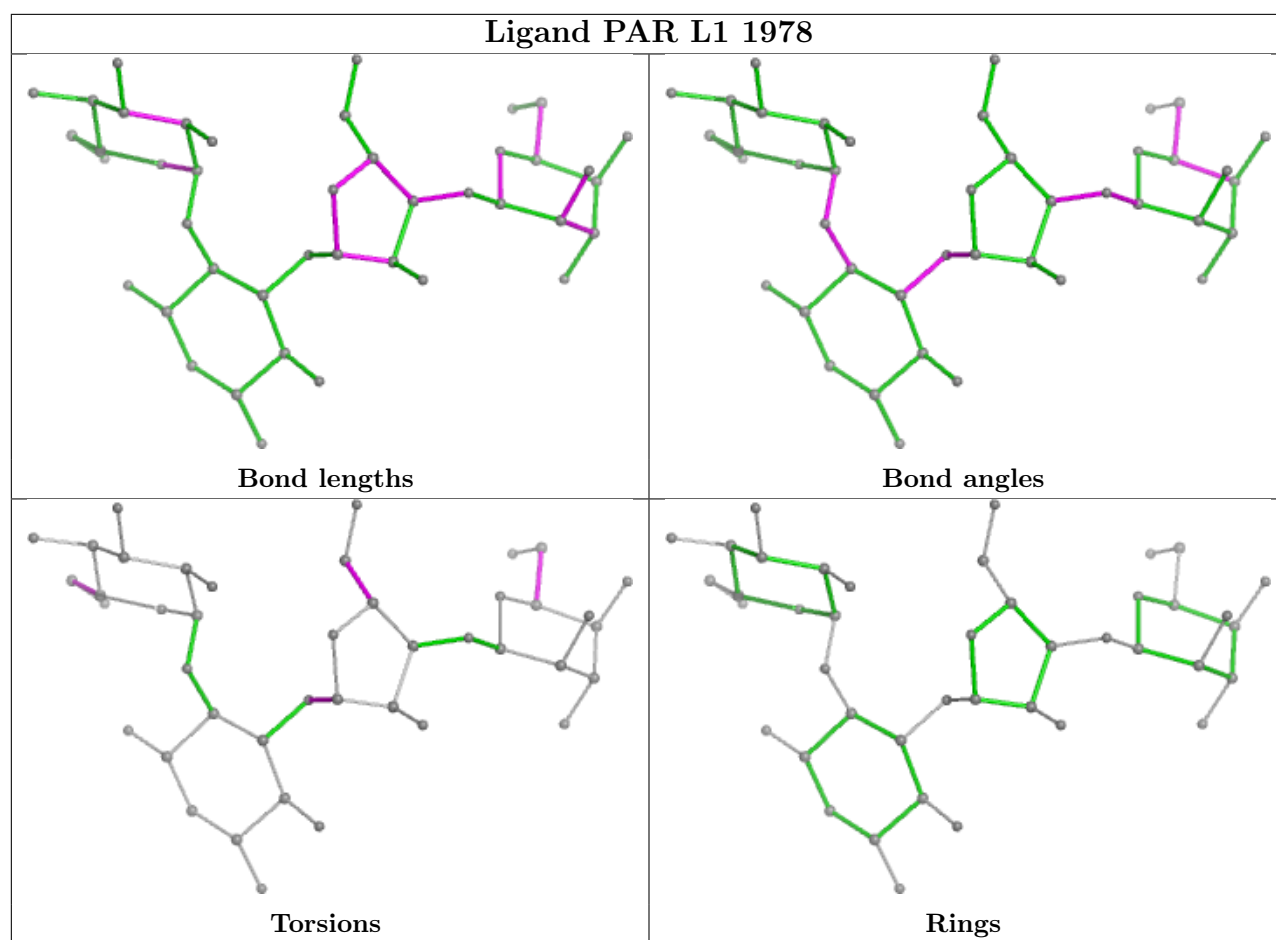
Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	L1	1978	PAR	3	0

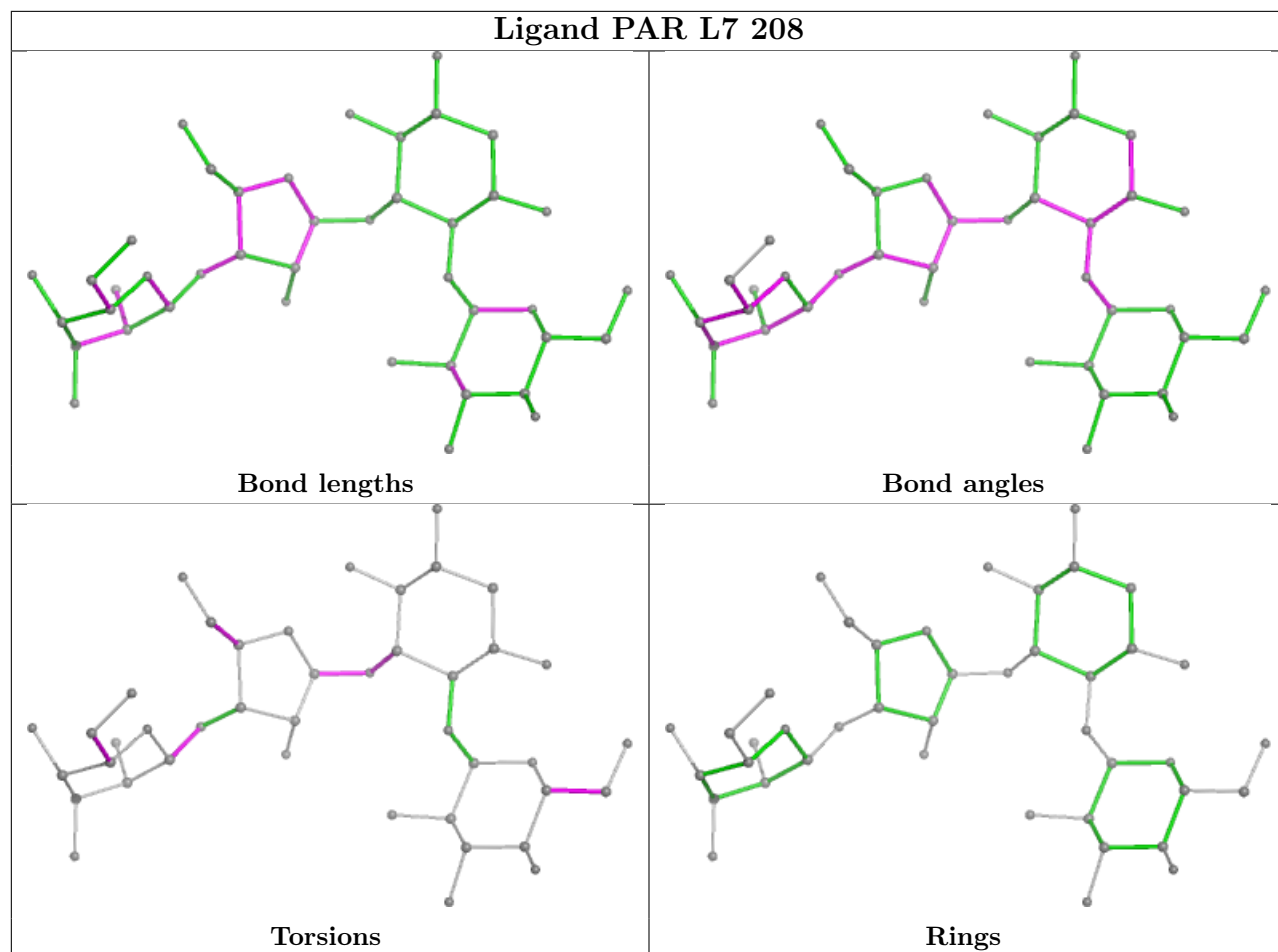
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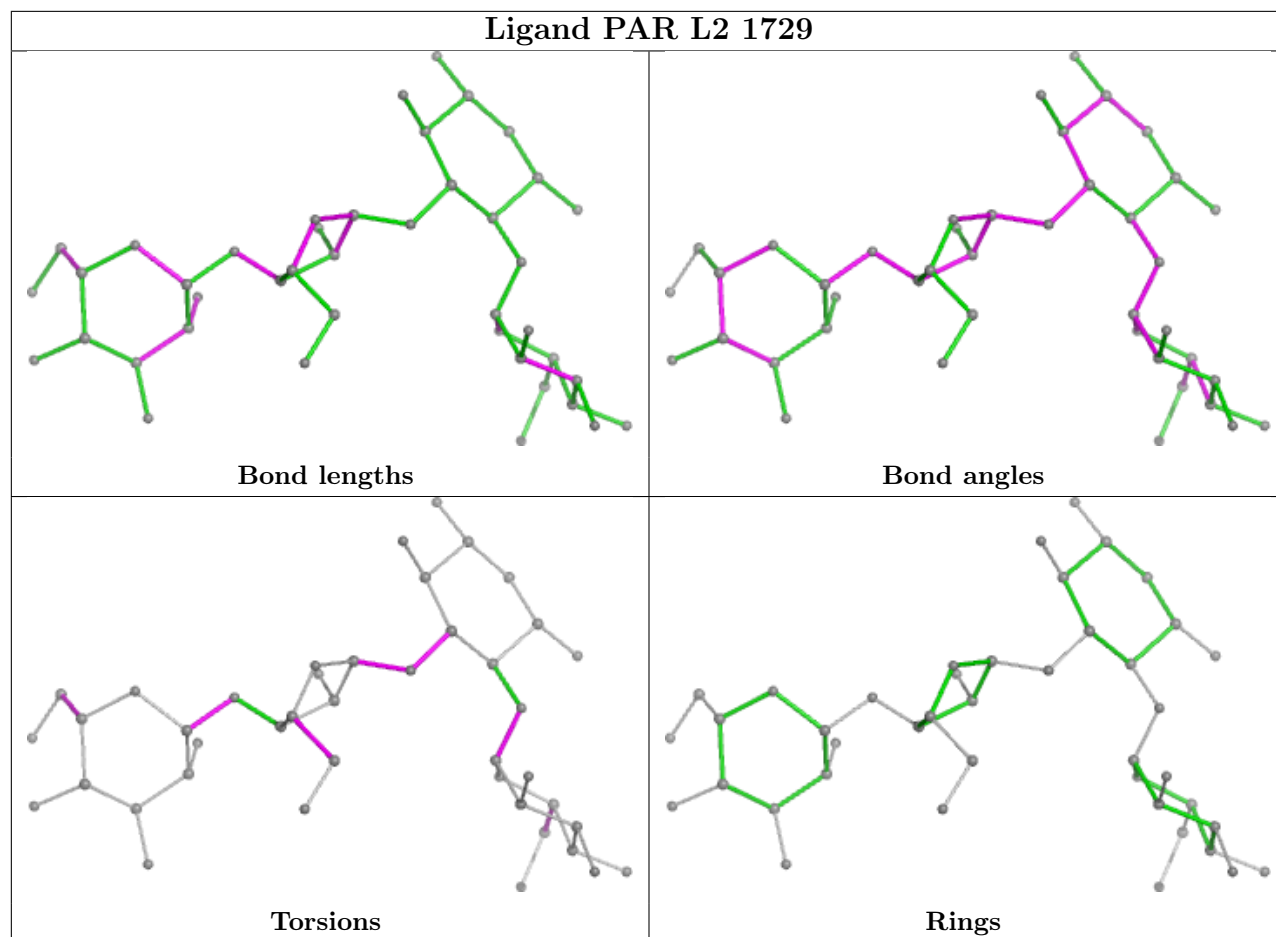
Mol	Chain	Res	Type	Clashes	Symm-Clashes
94	L7	208	PAR	4	0
89	L1	1806	SPD	2	0
89	L1	1808	SPD	1	0
94	L2	1729	PAR	5	0
89	S1	2301	SPD	1	0
94	S1	2445	PAR	2	0
89	L1	1814	SPD	1	0
89	L1	1815	SPD	1	0
89	L2	1602	SPD	1	0
89	L1	1802	SPD	2	0
89	L1	1811	SPD	3	0
93	L1	1977	PUT	1	0
89	L1	1813	SPD	4	0
94	S1	2446	PAR	3	0
89	S1	2302	SPD	2	0
89	LM	301	SPD	3	0
93	L2	1727	PUT	1	0
94	L2	1728	PAR	1	0
89	S1	2447	SPD	2	0

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

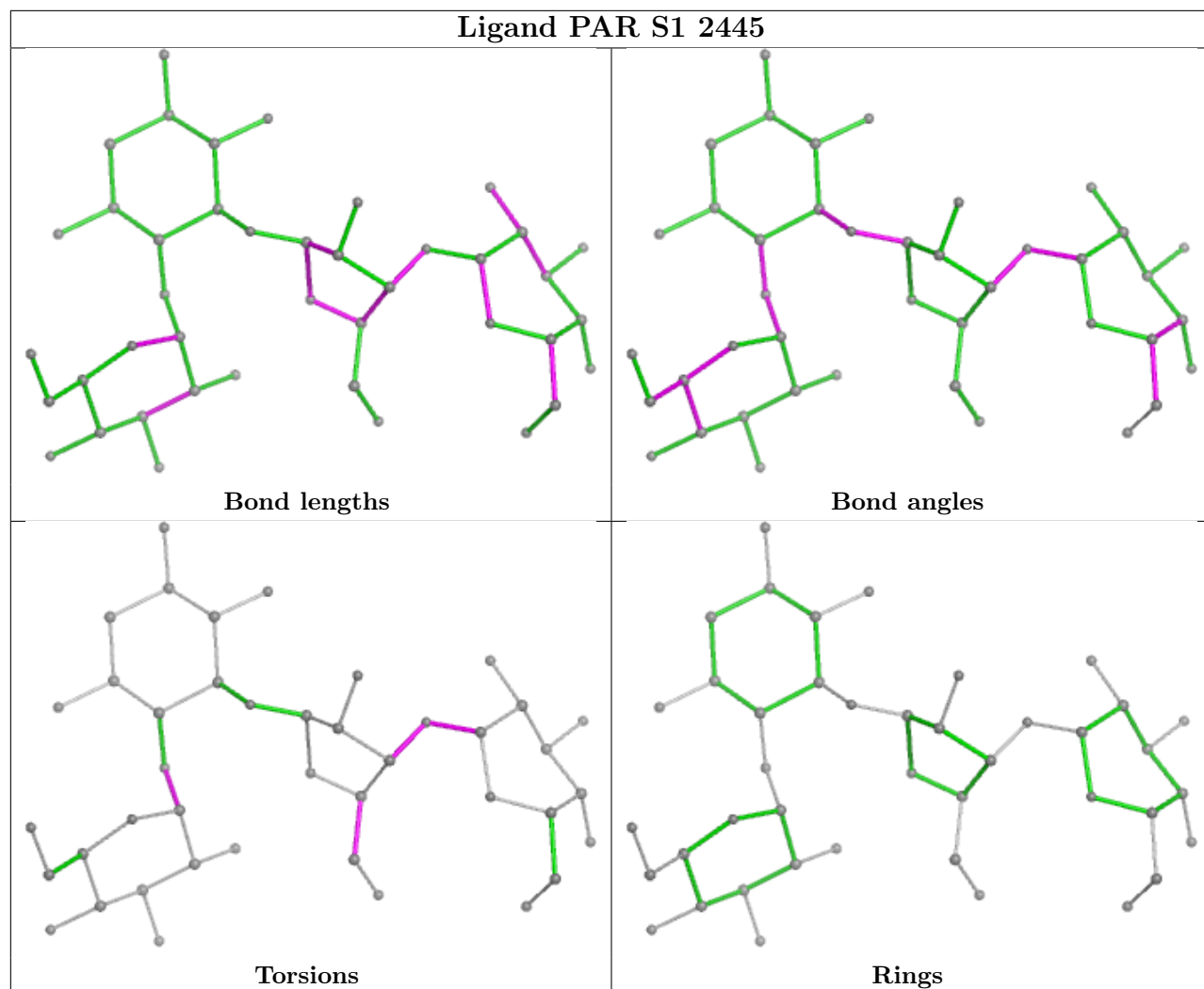


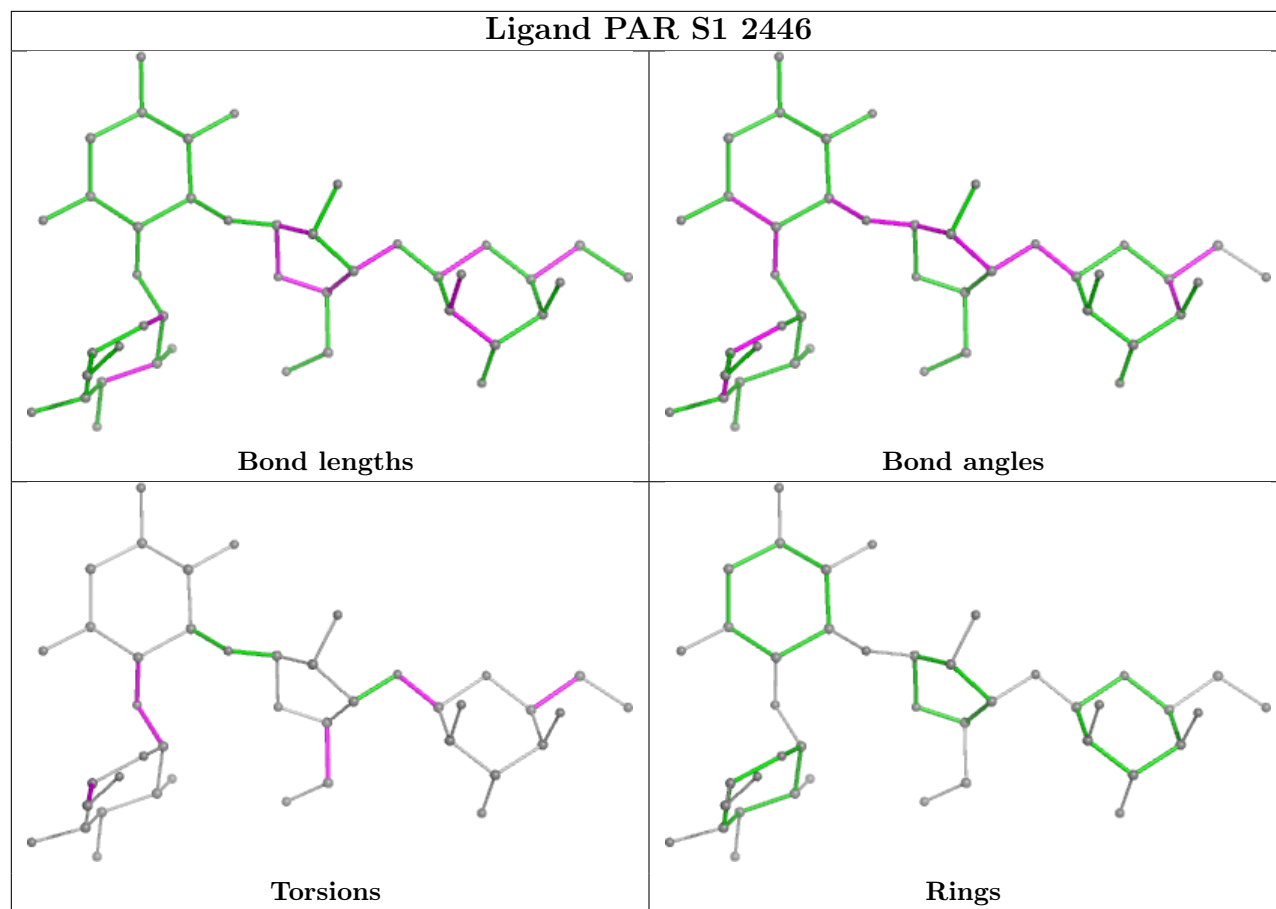


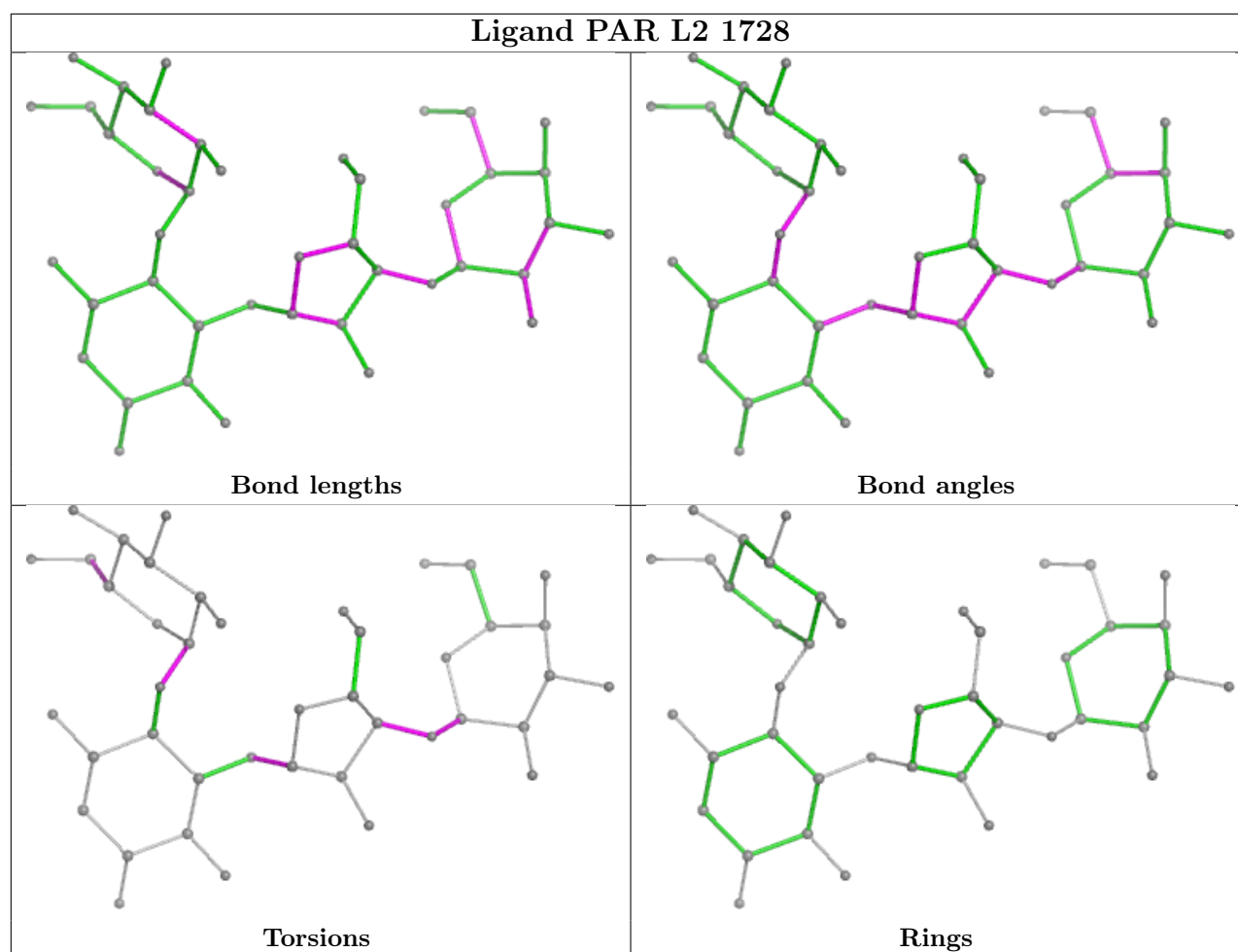




## Ligand PAR S1 2445







## 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	1

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	4.02

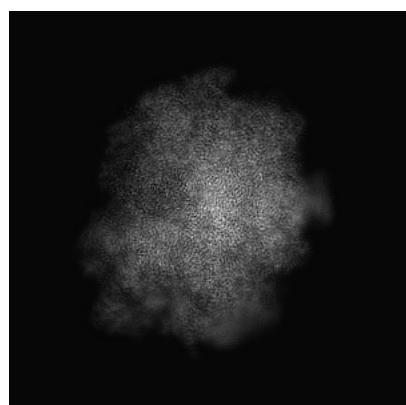
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50852. These allow visual inspection of the internal detail of the map and identification of artifacts.

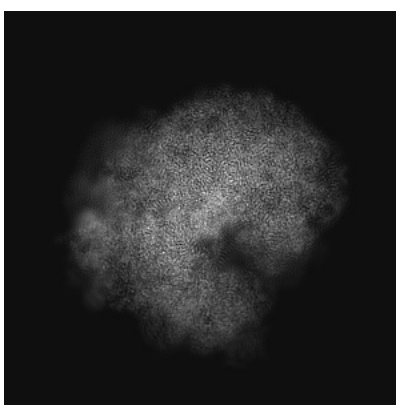
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

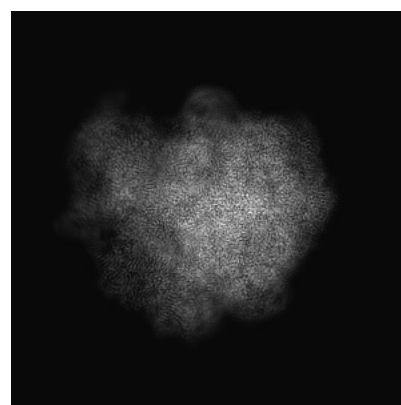
#### 6.1.1 Primary map



X



Y

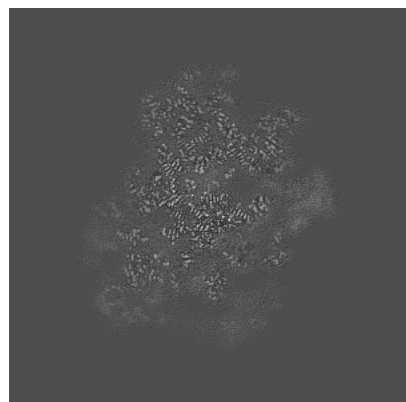


Z

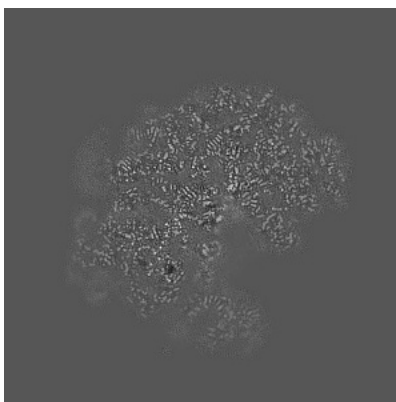
The images above show the map projected in three orthogonal directions.

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

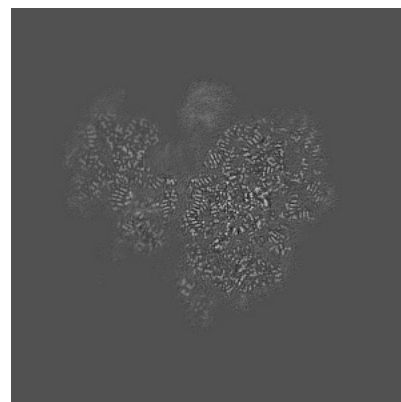
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

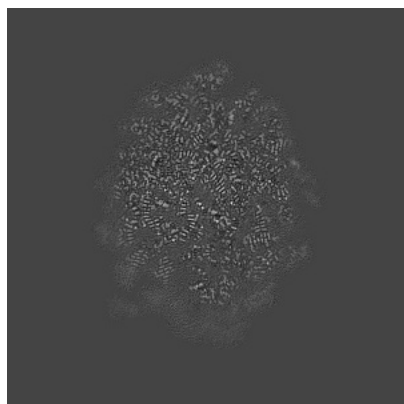


Z Index: 240

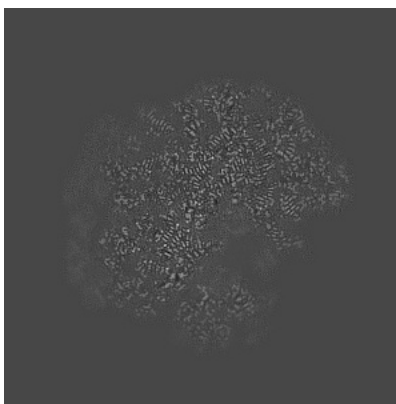
The images above show central slices of the map in three orthogonal directions.

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

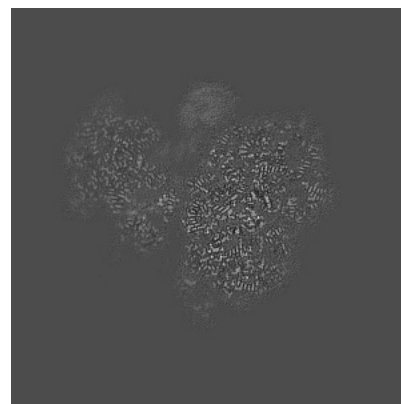
### 6.3.1 Primary map



X Index: 271



Y Index: 253

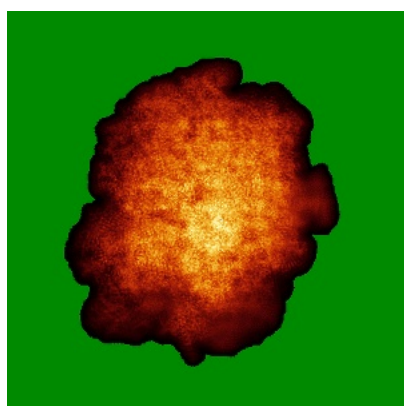


Z Index: 243

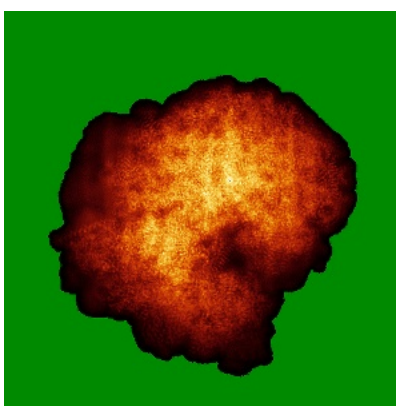
The images above show the largest variance slices of the map in three orthogonal directions.

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

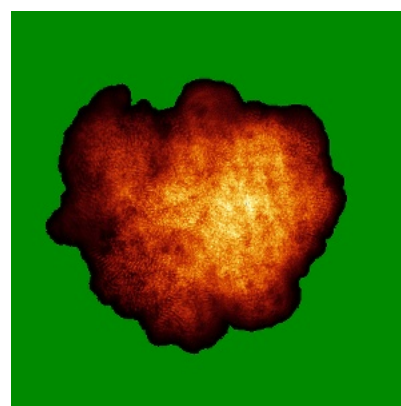
### 6.4.1 Primary map



X



Y

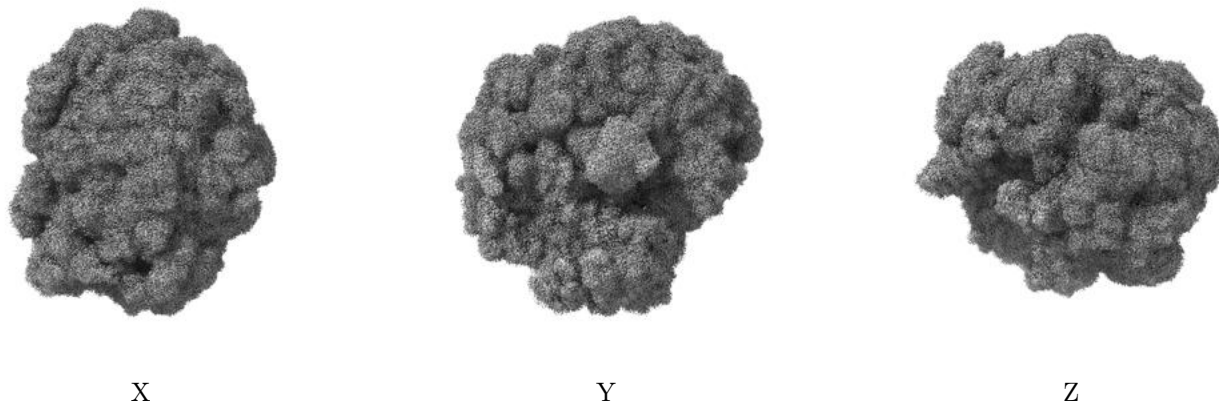


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

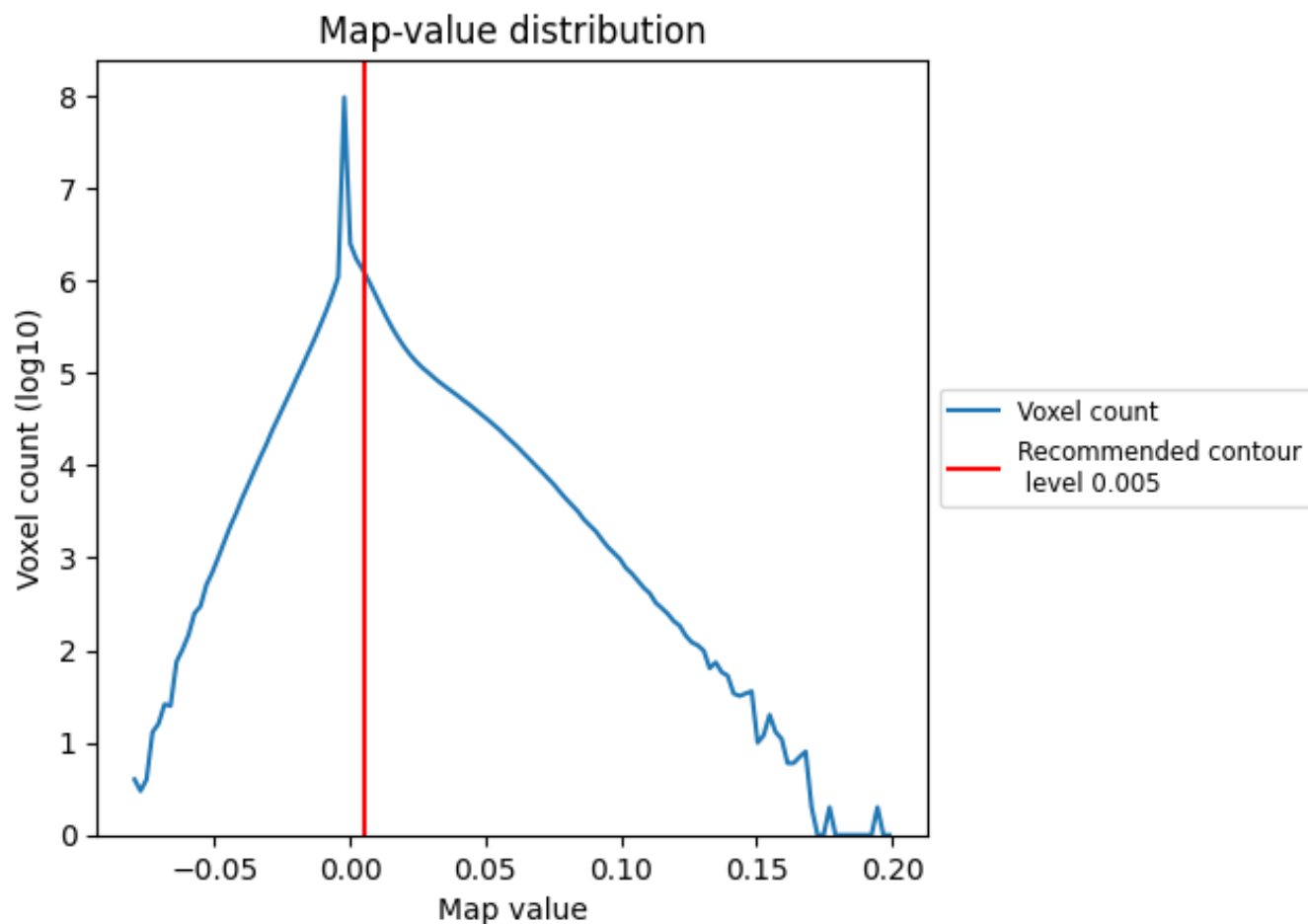
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

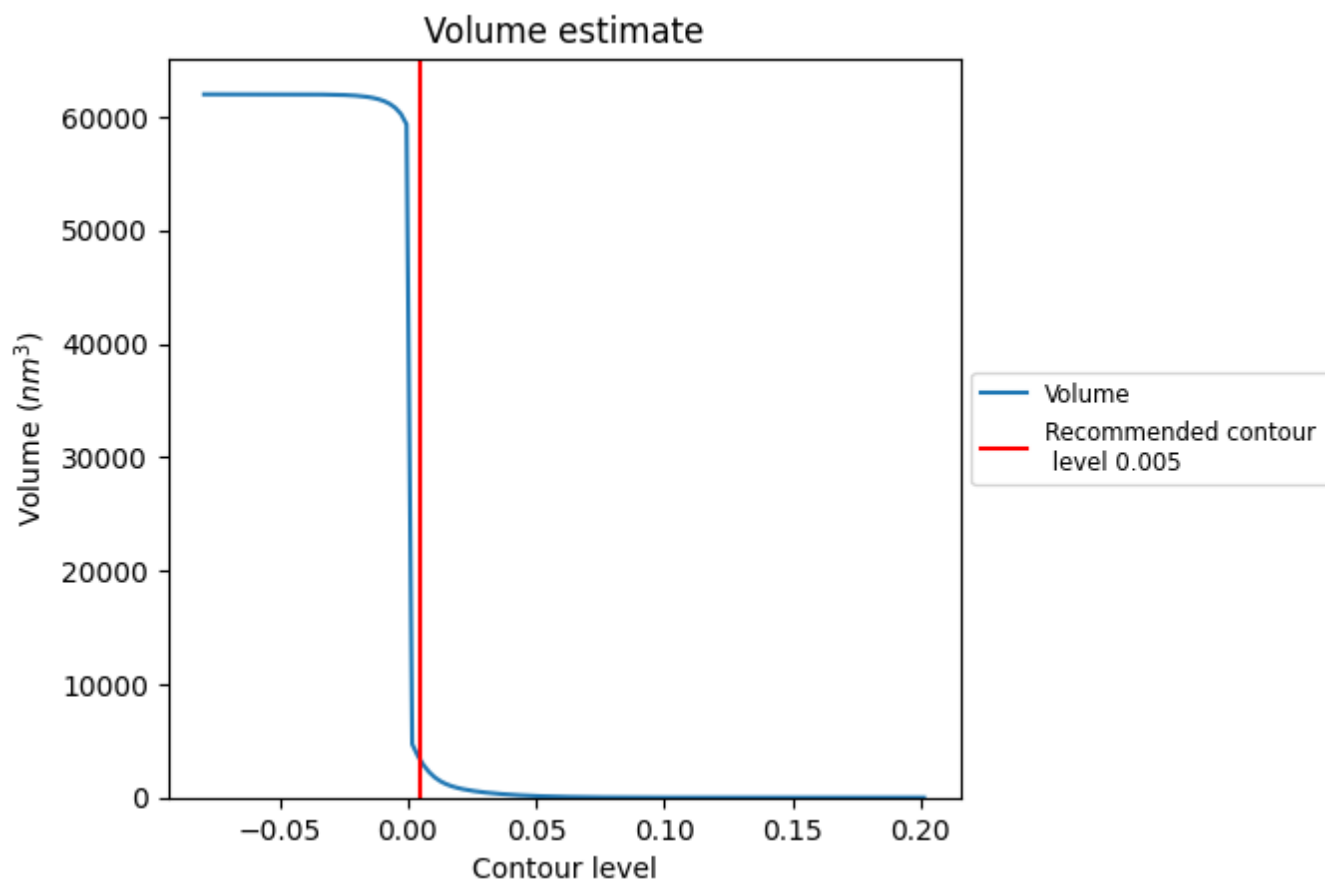
### 7.1 Map-value distribution [i](#)



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



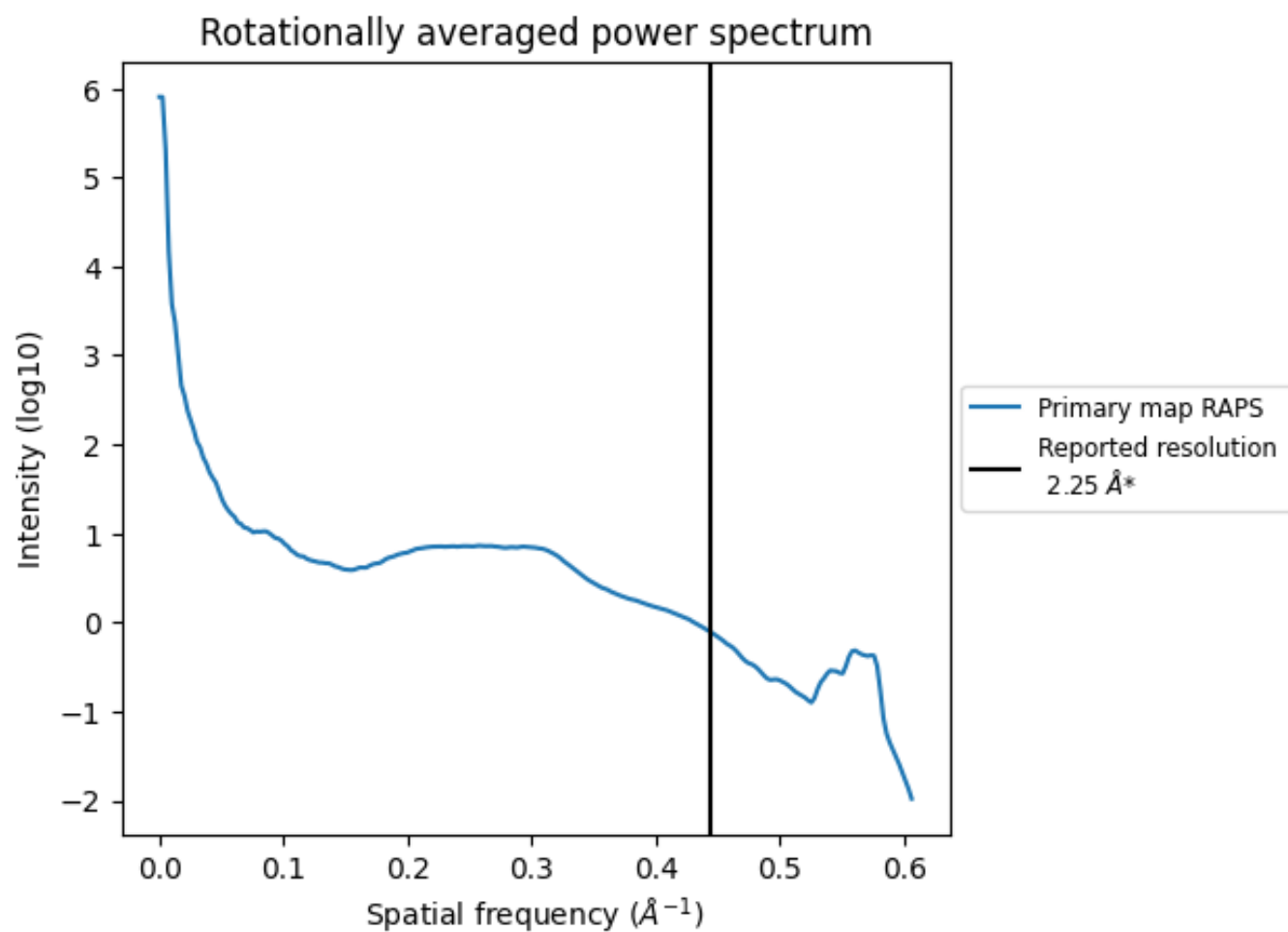
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3258  $\text{nm}^3$ ; this corresponds to an approximate mass of 2943 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 ⓘ

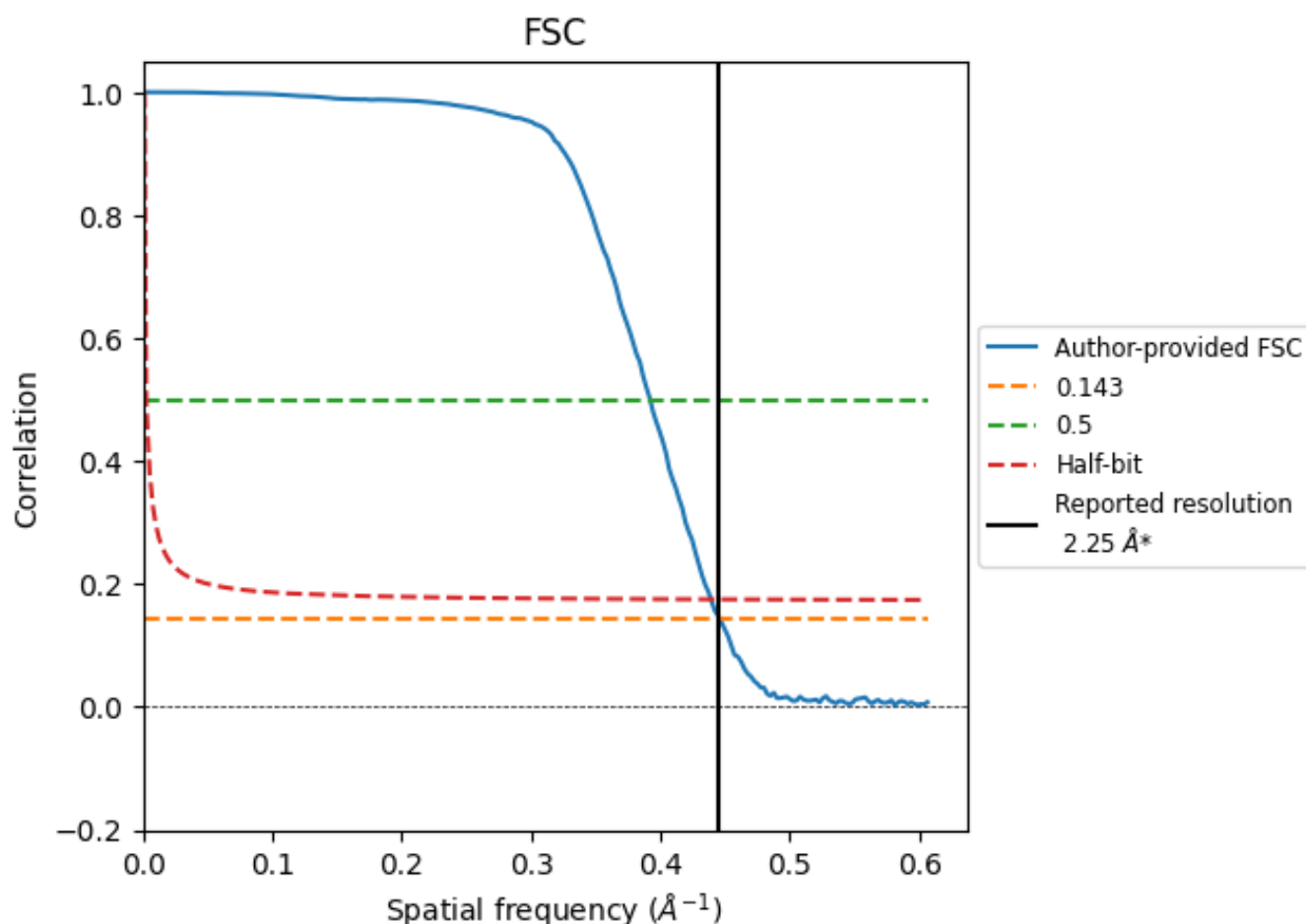


\*Reported resolution corresponds to spatial frequency of 0.444 Å<sup>-1</sup>

## 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 0.444 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

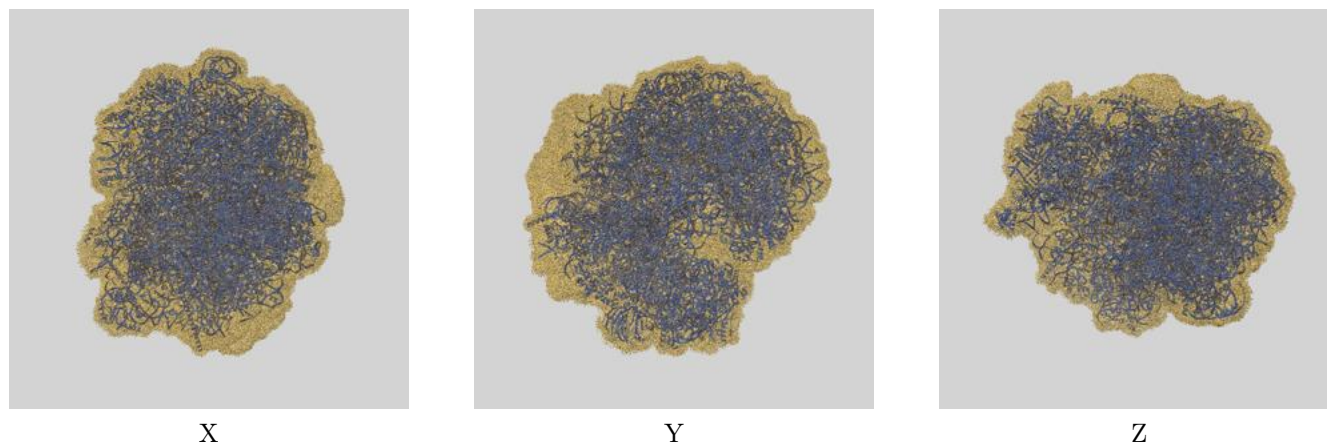
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.24	2.55	2.28
Unmasked-calculated*	-	-	-

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

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

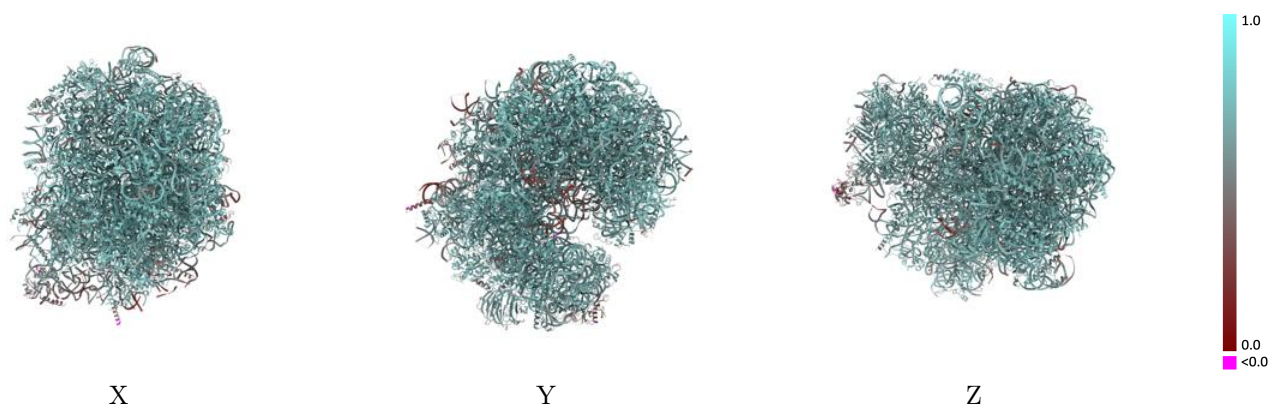
This section contains information regarding the fit between EMDB map EMD-50852 and PDB model 9FXO. Per-residue inclusion information can be found in section 3 on page 29.

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



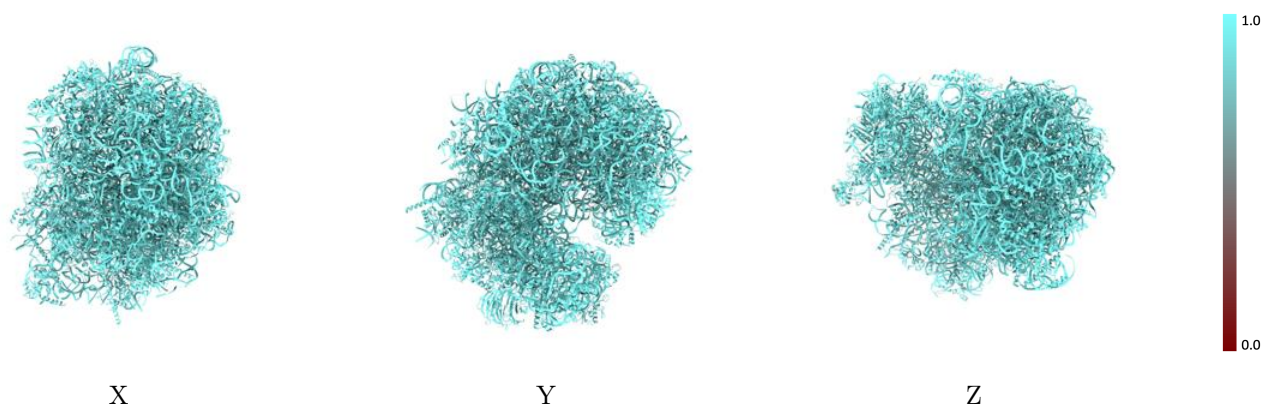
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



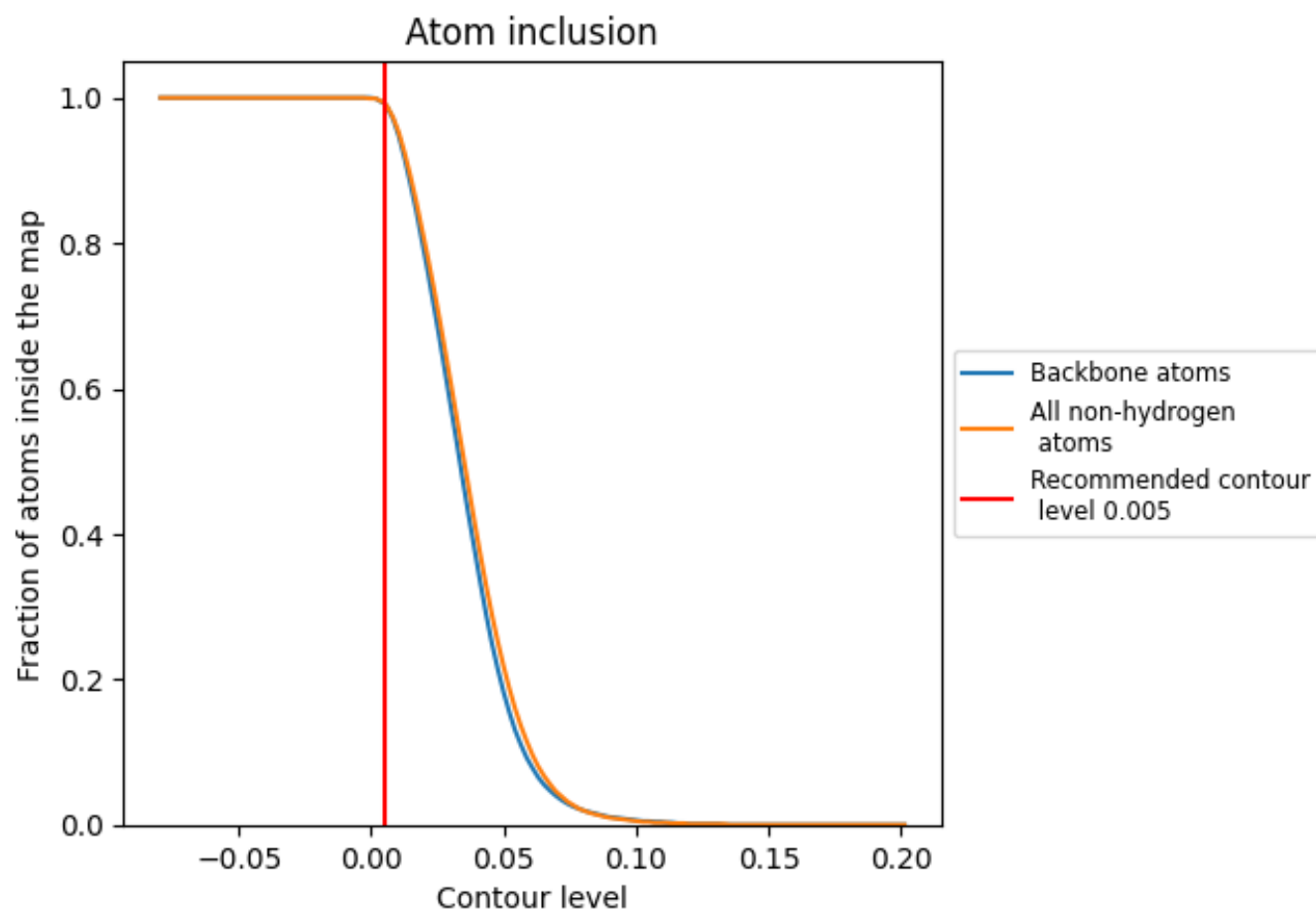
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.9930	 0.6730
L1	 0.9940	 0.6770
L2	 0.9960	 0.6770
L3	 0.9940	 0.6840
L4	 0.9980	 0.6920
L5	 0.9920	 0.6680
L6	 0.9900	 0.6410
L7	 0.9930	 0.6880
L8	 1.0000	 0.6770
LA	 0.9990	 0.7500
LB	 0.9970	 0.7260
LC	 0.9970	 0.7140
LD	 0.9960	 0.6380
LE	 0.9950	 0.6900
LF	 0.9890	 0.6570
LG	 0.9900	 0.6990
LH	 0.9990	 0.7100
LI	 0.9950	 0.7080
LJ	 0.9980	 0.7270
LK	 0.9950	 0.6650
LL	 0.9960	 0.7220
LM	 1.0000	 0.7500
LN	 0.9960	 0.6920
LO	 0.9870	 0.6550
LP	 0.9980	 0.7160
LQ	 0.9940	 0.6830
LR	 0.9980	 0.6970
LS	 0.9970	 0.6890
LT	 0.9980	 0.7340
LU	 0.9950	 0.6410
LV	 0.9980	 0.7280
LW	 0.9980	 0.7220
LX	 0.9930	 0.6910
LY	 0.9990	 0.7010
LZ	 1.0000	 0.7060



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Chain	Atom inclusion	Q-score
La	 0.9980	 0.7020
Lb	 0.9960	 0.7090
Lc	 0.9990	 0.7030
Ld	 0.9940	 0.7210
Le	 0.9900	 0.6880
Lf	 0.9980	 0.7080
Lg	 0.9980	 0.6990
Lh	 0.9920	 0.6980
Li	 0.9960	 0.6970
Lj	 0.9980	 0.7490
Lk	 0.9950	 0.6970
Ll	 1.0000	 0.7440
Lm	 0.9980	 0.6910
Ln	 1.0000	 0.7130
Lo	 0.9940	 0.7420
Lp	 0.9970	 0.6930
S1	 0.9910	 0.6530
S2	 0.9540	 0.4430
S3	 0.9860	 0.5550
S4	 0.9540	 0.3780
S5	 0.9560	 0.5120
SA	 0.9910	 0.7080
SB	 0.9930	 0.6860
SC	 0.9910	 0.6410
SD	 0.9950	 0.6930
SE	 0.9950	 0.7030
SF	 0.9890	 0.7090
SG	 0.9960	 0.6600
SH	 0.9930	 0.6860
SI	 0.9940	 0.6910
SJ	 0.9970	 0.7330
SK	 0.9960	 0.6880
SL	 0.9980	 0.6960
SM	 0.9870	 0.6450
SN	 0.9870	 0.5820
SO	 0.9960	 0.7270
SP	 0.9960	 0.7100
SQ	 0.8850	 0.3870
SR	 0.9940	 0.6490
SS	 0.9930	 0.6900
ST	 0.9960	 0.7330
SU	 0.9920	 0.6870

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Chain	Atom inclusion	Q-score
SV	 0.9810	 0.6380
SW	 0.9830	 0.6280
SX	 0.9950	 0.6700
SY	 0.9940	 0.6940
SZ	 0.9900	 0.6680
Sa	 0.9790	 0.6320
Sb	 0.9990	 0.7320
Sc	 0.9840	 0.6730
Sd	 0.9810	 0.6530
Se	 0.9790	 0.6280
Sf	 0.9180	 0.4020
Sg	 0.9740	 0.5940
Sh	 0.9220	 0.4270