



Full wwPDB EM Validation Report ⓘ

May 6, 2026 – 08:28 pm BST

PDB ID : 9RUC / pdb_00009ruc
EMDB ID : EMD-54269
Title : WT-HEK 80S ribosome bound to H2B mRNA (WT-H2B)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

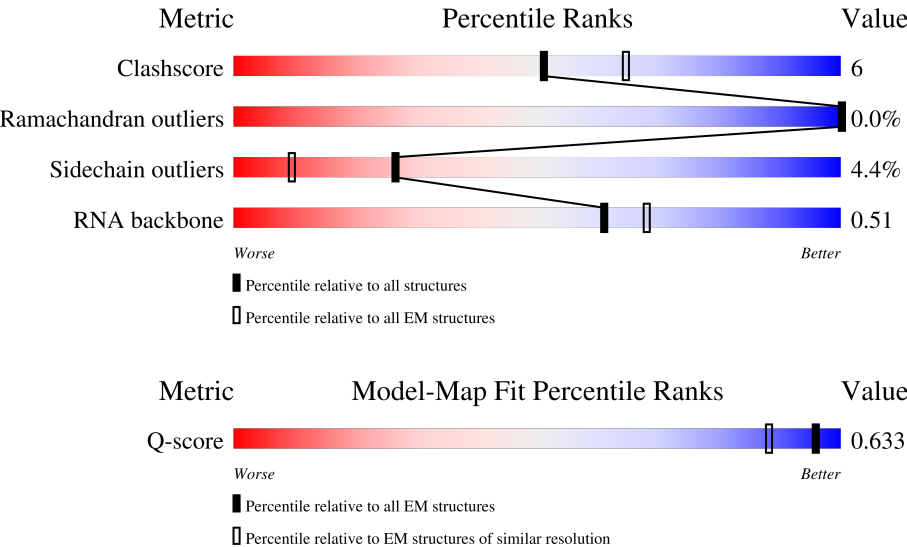
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





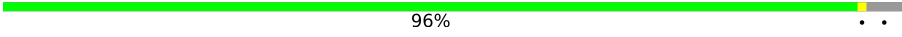





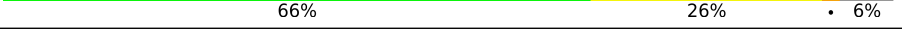

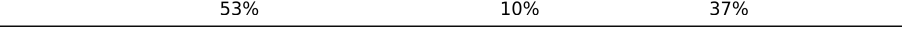
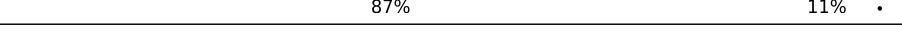

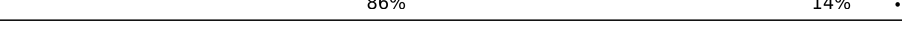


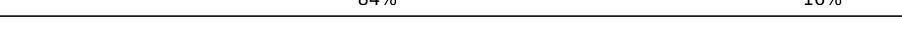

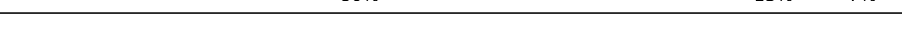






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	L7	120	
2	L8	156	
3	LA	254	








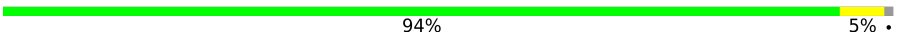
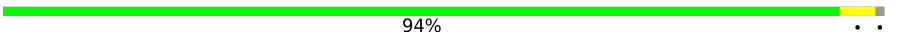
















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Mol	Chain	Length	Quality of chain
4	LB	396	 86% 12% ..
5	LC	427	 74% 10% 16%
6	LD	297	 96% ..
7	LE	288	 54% 14% 32%
8	LF	248	 84% 6% 9%
9	LG	266	 70% 9% 21%
10	LH	189	 78% 21% .
11	LI	213	 77% 17% 6%
12	LJ	178	 66% 26% . 6%
13	LL	211	 85% 9% . 5%
14	LM	215	 53% 10% 37%
15	LN	204	 87% 11% .
16	LO	203	 86% 13% .
17	LP	154	 86% 14% .
18	LQ	188	 90% 9% .
19	LR	196	 70% 8% 21%
20	LS	176	 84% 16%
21	LT	160	 86% 13% ..
22	LV	140	 80% 13% 7%
23	LW	157	 38% . 60%
24	LX	156	 64% 12% 24%
25	LY	145	 76% 14% 10%
26	LZ	136	 79% 18% ..
27	La	148	 86% 14% .
28	Lb	159	 53% 8% 39%



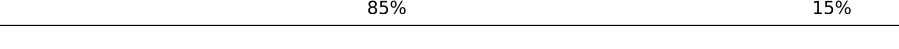
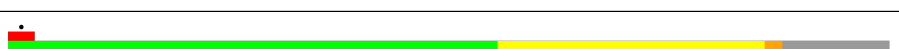



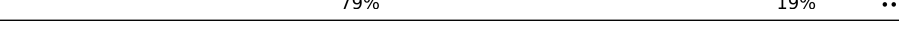



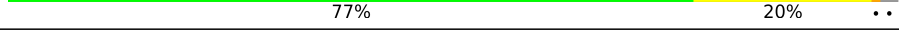

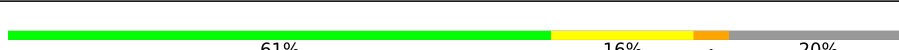


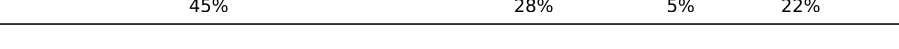

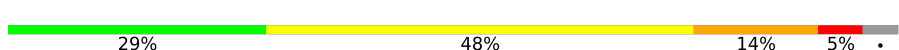





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Mol	Chain	Length	Quality of chain
29	Lc	115	
30	Ld	125	
31	Le	129	
32	Lf	110	
33	Lg	117	
34	Lh	123	
35	Li	105	
36	Lj	87	
37	Lk	70	
38	Ll	51	
39	Lm	127	
40	Ln	25	
41	Lo	105	
42	Lp	92	
43	Lr	137	
44	Pt	77	
45	SA	295	
46	SB	264	
47	SC	293	
48	SF	204	
49	SI	208	
50	mR	27	
51	SD	243	
52	SE	263	
53	SH	194	



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Mol	Chain	Length	Quality of chain
54	SK	165	
55	SL	158	
56	SN	151	
57	SO	151	
58	SP	145	
59	SQ	146	
60	SR	135	
61	SS	152	
62	ST	145	
63	SU	119	
64	SV	84	
65	SW	130	
66	SY	133	
67	SX	143	
68	Sb	84	
69	Sc	69	
70	Sd	56	
71	Se	133	
72	Sg	317	
73	S2	1869	
74	L5	5069	
75	Sa	115	
76	S6	77	
77	SG	249	
78	LU	128	

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Mol	Chain	Length	Quality of chain
79	SZ	125	
80	SJ	194	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 192496 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 5S rRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	150	Total	C	N	O	P	0	0
			3193	1425	565	1053	150		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LA	247	Total	C	N	O	S	0	0
			1888	1182	387	313	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LA	254	LYS	GLU	conflict	UNP P62917

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LB	390	Total	C	N	O	S	0	0
			3091	1968	575	534	14		

- Molecule 5 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LC	357	Total	C	N	O	S	0	0
			2829	1783	563	470	13		

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	LD	286	Total	C	N	O		
			1419	846	286	287	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LE	196	Total	C	N	O	S		
			1561	1006	295	256	4	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LF	225	Total	C	N	O	S		
			1845	1187	351	298	9	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LG	211	Total	C	N	O	S		
			1598	1015	308	271	4	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LH	189	Total	C	N	O	S		
			1441	909	269	257	6	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LI	201	Total	C	N	O	S		
			1623	1032	314	265	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LJ	168	Total	C	N	O	S		
			1242	780	234	222	6	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LL	201	Total	C	N	O	S	0	0
			1570	981	327	258	4		

- Molecule 14 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LM	135	Total	C	N	O	S	0	0
			1080	693	207	173	7		

- Molecule 15 is a protein called 60S ribosomal protein L15.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LO	201	Total	C	N	O	S	0	0
			1634	1055	315	259	5		

- Molecule 17 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LP	153	Total	C	N	O	S	0	0
			1234	771	240	214	9		

- Molecule 18 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LQ	187	Total	C	N	O	S	0	0
			1497	934	310	248	5		

- Molecule 19 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LR	154	Total	C	N	O	S	0	0
			1251	780	272	190	9		

- Molecule 20 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LS	176	Total	C	N	O	S	0	0
			1456	927	283	235	11		

- Molecule 21 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LT	159	Total	C	N	O	S	0	0
			1293	820	251	216	6		

- Molecule 22 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LV	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

- Molecule 23 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LW	63	Total	C	N	O	S	0	0
			517	329	101	85	2		

- Molecule 24 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LX	118	Total	C	N	O	S	1	0
			977	624	184	168	1		

- Molecule 25 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LY	130	Total	C	N	O	S	0	0
			1084	681	220	180	3		

- Molecule 26 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LZ	135	Total	C	N	O	S	0	0
			1034	668	195	168	3		

- Molecule 27 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	La	147	Total	C	N	O	S	0	0
			1155	730	235	187	3		

- Molecule 28 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Lb	97	Total	C	N	O	S	0	0
			723	450	154	118	1		

- Molecule 29 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lc	98	Total	C	N	O	S	0	0
			738	467	131	134	6		

- Molecule 30 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ld	105	Total	C	N	O	S	0	0
			854	543	167	142	2		

- Molecule 31 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Le	128	Total	C	N	O	S	0	0
			1029	650	209	165	5		

- Molecule 32 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lf	109	Total	C	N	O	S	0	0
			875	555	174	143	3		

- Molecule 33 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lg	106	Total	C	N	O	S	0	0
			825	512	172	135	6		

- Molecule 34 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lh	121	Total	C	N	O	S	1	0
			1012	638	206	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Li	97	Total	C	N	O	S	0	0
			793	497	167	124	5		

- Molecule 36 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 37 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lk	69	Total	C	N	O	S	0	0
			450	285	85	79	1		

- Molecule 38 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ll	48	Total	C	N	O	S	0	0
			417	266	90	60	1		

- Molecule 39 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lm	50	Total	C	N	O	S	0	0
			400	245	85	64	6		

- Molecule 40 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ln	25	Total	C	N	O	S	0	0
			224	137	58	27	2		

- Molecule 41 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lo	97	Total	C	N	O	S	1	0
			786	494	161	125	6		

- Molecule 42 is a protein called 60S ribosomal protein L37a.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lr	126	Total	C	N	O	S	0	0
			988	611	204	169	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	2	ACE	-	acetylation	UNP P46779

- Molecule 44 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	Pt	75	Total	C	N	O	P	S	0	0
			1605	716	294	519	75	1		

- Molecule 45 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SA	209	Total	C	N	O	S	0	0
			1624	1036	287	293	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	1	ACE	-	acetylation	UNP A0A2J8WY29

- Molecule 46 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SB	219	Total	C	N	O	S	0	0
			1724	1093	313	304	14		

- Molecule 47 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SC	214	Total	C	N	O	S	0	0
			1605	1038	276	282	9		

- Molecule 48 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SF	185	Total	C	N	O	S	0	0
			1362	860	258	237	7		

- Molecule 49 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SI	163	Total	C	N	O	S	0	0
			1123	699	235	187	2		

- Molecule 50 is a RNA chain called Histone H2B mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	mR	8	Total	C	N	O	P	0	0
			172	77	31	56	8		

- Molecule 51 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	202	Total	C	N	O	S	0	0
			1350	852	248	243	7		

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	258	Total	C	N	O	S	0	0
			2029	1296	375	350	8		

- Molecule 53 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	SH	164	Total	C	N	O	0	0
			1133	716	212	205		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SK	47	Total	C	N	O	S	0	0
			339	216	62	57	4		

- Molecule 55 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	130	Total	C	N	O	S	0	0
			1011	646	189	170	6		

- Molecule 56 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SN	150	Total	C	N	O	S	0	0
			1160	745	220	194	1		

- Molecule 57 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SO	129	Total	C	N	O	S	0	0
			956	587	190	173	6		

- Molecule 58 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	127	Total	C	N	O	S	0	0
			963	611	178	168	6		

- Molecule 59 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	141	Total	C	N	O	S	0	0
			1099	702	207	187	3		

- Molecule 60 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SR	133	Total	C	N	O	S	0	0
			867	540	172	152	3		

- Molecule 61 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS	147	Total	C	N	O	S	0	0
			1146	724	230	191	1		

- Molecule 62 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	ST	144	Total	C	N	O	S	0	0
			1043	656	201	183	3		

- Molecule 63 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	SU	75	Total	C	N	O	0	0
			383	230	75	78		

- Molecule 64 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SV	83	Total	C	N	O	S	0	0
			610	376	115	114	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SV	0	ACE	-	acetylation	UNP P63220

- Molecule 65 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SW	129	Total	C	N	O	S	0	0
			1014	649	189	170	6		

- Molecule 66 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SY	121	Total	C	N	O	S	0	0
			952	605	183	159	5		

- Molecule 67 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SX	140	Total	C	N	O	S	0	0
			1082	683	215	181	3		

- Molecule 68 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	Sb	71	Total	C	N	O	0	0
			461	285	93	83		

- Molecule 69 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Sc	64	Total	C	N	O	S	0	0
			484	297	93	92	2		

- Molecule 70 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sd	45	Total	C	N	O	S	0	0
			351	217	71	58	5		

- Molecule 71 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Se	49	Total	C	N	O	S	0	0
			371	226	83	61	1		

- Molecule 72 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	Sg	261	Total	C	N	O	0	0
			1284	762	261	261		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sg	56	ASN	GLN	conflict	UNP P63244

- Molecule 73 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	S2	1455	Total	C	N	O	P	0	0
			31042	13867	5577	10144	1454		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	140	C	U	conflict	GB 151415227
S2	338	A	G	conflict	GB 151415227
S2	582	C	U	conflict	GB 151415227
S2	583	C	A	conflict	GB 151415227
S2	584	G	A	conflict	GB 151415227
S2	1095	U	C	conflict	GB 151415227

- Molecule 74 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	L5	3192	Total	C	N	O	P	1	0
			68538	30571	12545	22230	3192		

- Molecule 75 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sa	102	Total	C	N	O	S	0	0
			776	484	162	127	3		

- Molecule 76 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	S6	74	Total	C	N	O	P	S	0	0
			1582	705	288	514	74	1		

- Molecule 77 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SG	214	Total	C	N	O	S	0	0
			1157	700	229	226	2		

- Molecule 78 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	LU	98	Total	C	N	O	S	0	0
			671	423	121	126	1		

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
79	SZ	77	Total	C	N	O	0	0
			540	347	101	92		

- Molecule 80 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SJ	178	Total	C	N	O	S	0	0
			1441	922	286	231	2		

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	L7	3	Total	Mg	0
			3	3	
81	L8	4	Total	Mg	0
			4	4	
81	LA	1	Total	Mg	0
			1	1	
81	LB	1	Total	Mg	0
			1	1	
81	LH	2	Total	Mg	0
			2	2	
81	LM	1	Total	Mg	0
			1	1	
81	LN	2	Total	Mg	0
			2	2	
81	LP	1	Total	Mg	0
			1	1	
81	LV	1	Total	Mg	0
			1	1	
81	Lg	1	Total	Mg	0
			1	1	
81	Lj	1	Total	Mg	0
			1	1	
81	S2	14	Total	Mg	0
			14	14	
81	L5	191	Total	Mg	0
			191	191	

- Molecule 82 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
82	L8	1	Total K 1 1	0
82	LA	2	Total K 2 2	0
82	LI	1	Total K 1 1	0
82	Lf	1	Total K 1 1	0
82	SL	1	Total K 1 1	0
82	SO	1	Total K 1 1	0
82	S2	2	Total K 2 2	0
82	L5	42	Total K 42 42	0

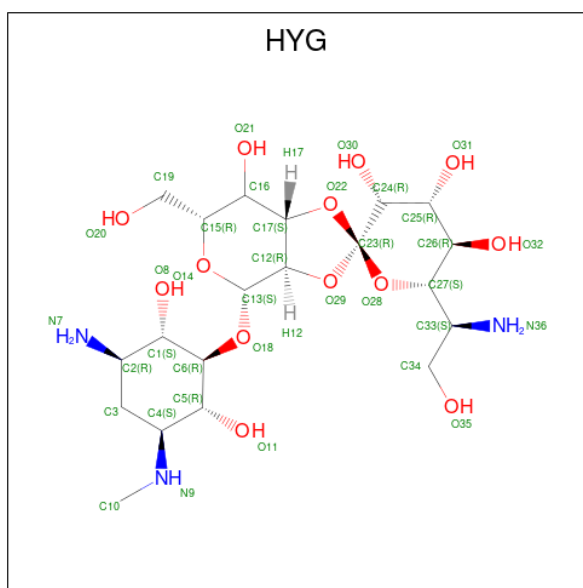
- Molecule 83 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
83	LS	1	Total Na 1 1	0
83	Le	1	Total Na 1 1	0
83	S2	4	Total Na 4 4	0
83	L5	2	Total Na 2 2	0

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

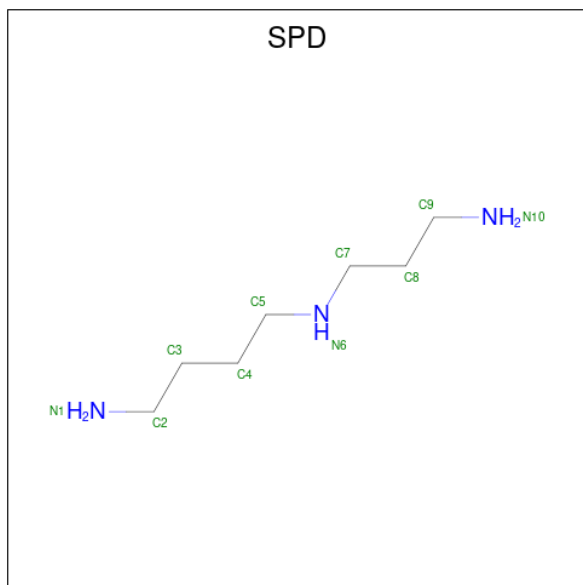
Mol	Chain	Residues	Atoms	AltConf
84	Lg	1	Total Zn 1 1	0
84	Lj	1	Total Zn 1 1	0
84	Lm	1	Total Zn 1 1	0
84	Lo	1	Total Zn 1 1	0
84	Lp	1	Total Zn 1 1	0
84	Sd	1	Total Zn 1 1	0

- Molecule 85 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



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

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

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

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	L7	18	Total	O	0
			18	18	
87	L8	52	Total	O	0
			52	52	
87	LA	41	Total	O	0
			41	41	
87	LB	33	Total	O	0
			33	33	
87	LC	39	Total	O	0
			39	39	
87	LD	5	Total	O	0
			5	5	
87	LE	2	Total	O	0
			2	2	
87	LF	22	Total	O	0
			22	22	
87	LG	2	Total	O	0
			2	2	
87	LH	3	Total	O	0
			3	3	
87	LI	6	Total	O	0
			6	6	
87	LJ	4	Total	O	0
			4	4	
87	LL	21	Total	O	0
			21	21	
87	LM	4	Total	O	0
			4	4	
87	LN	34	Total	O	0
			34	34	
87	LO	6	Total	O	0
			6	6	
87	LP	12	Total	O	0
			12	12	
87	LQ	32	Total	O	0
			32	32	

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Mol	Chain	Residues	Atoms		AltConf
87	LR	31	Total 31	O 31	0
87	LS	8	Total 8	O 8	0
87	LT	14	Total 14	O 14	0
87	LV	8	Total 8	O 8	0
87	LW	1	Total 1	O 1	0
87	LX	1	Total 1	O 1	0
87	LY	6	Total 6	O 6	0
87	La	25	Total 25	O 25	0
87	Lb	11	Total 11	O 11	0
87	Lc	10	Total 10	O 10	0
87	Ld	3	Total 3	O 3	0
87	Le	21	Total 21	O 21	0
87	Lf	11	Total 11	O 11	0
87	Lg	5	Total 5	O 5	0
87	Lh	4	Total 4	O 4	0
87	Lj	19	Total 19	O 19	0
87	Ll	6	Total 6	O 6	0
87	Ln	1	Total 1	O 1	0
87	Lo	9	Total 9	O 9	0
87	Lp	21	Total 21	O 21	0
87	Lr	11	Total 11	O 11	0

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Mol	Chain	Residues	Atoms		AltConf
87	Pt	6	Total 6	O 6	0
87	SB	6	Total 6	O 6	0
87	SC	2	Total 2	O 2	0
87	SF	1	Total 1	O 1	0
87	SI	5	Total 5	O 5	0
87	SE	1	Total 1	O 1	0
87	SL	1	Total 1	O 1	0
87	SN	10	Total 10	O 10	0
87	SO	3	Total 3	O 3	0
87	SS	7	Total 7	O 7	0
87	ST	1	Total 1	O 1	0
87	SW	1	Total 1	O 1	0
87	SX	3	Total 3	O 3	0
87	Sb	1	Total 1	O 1	0
87	S2	237	Total 237	O 237	0
87	L5	1979	Total 1979	O 1979	0
87	Sa	4	Total 4	O 4	0
87	S6	6	Total 6	O 6	0
87	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.

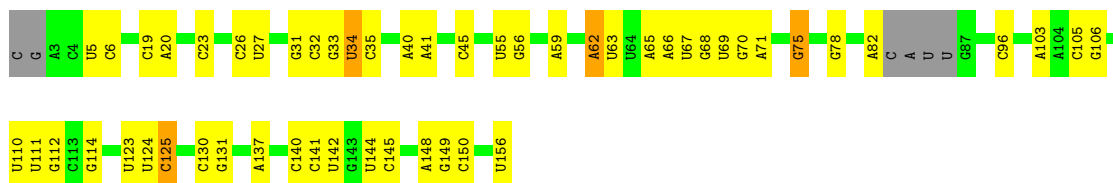
- Molecule 1: 5S rRNA

Chain L7: 




- Molecule 2: 5.8S rRNA

Chain L8: 




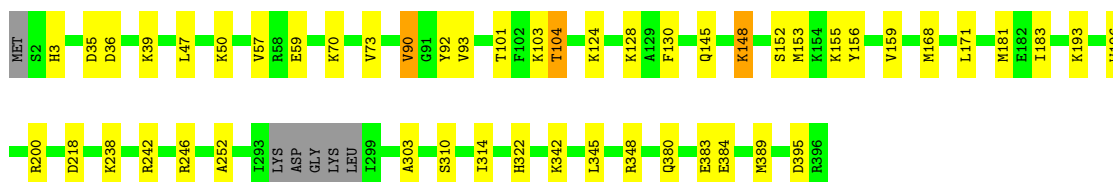
- Molecule 3: Large ribosomal subunit protein uL2

Chain LA: 




- Molecule 4: Large ribosomal subunit protein uL3

Chain LB: 



- Molecule 5: 60S ribosomal protein L4

Chain LC: 

- Molecule 11: Large ribosomal subunit protein uL16

- Molecule 12: 60S ribosomal protein L11

- Molecule 13: Large ribosomal subunit protein eL13

- Molecule 14: 60S ribosomal protein L14

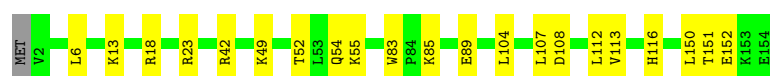
- Molecule 15: 60S ribosomal protein L15



- Molecule 16: 60S ribosomal protein L13a



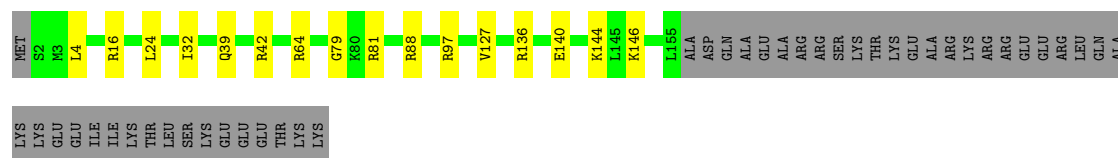
- Molecule 17: Large ribosomal subunit protein uL22



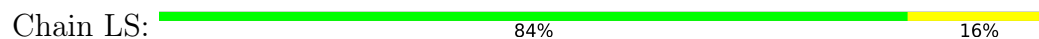
- Molecule 18: 60S ribosomal protein L18



- Molecule 19: 60S ribosomal protein L19



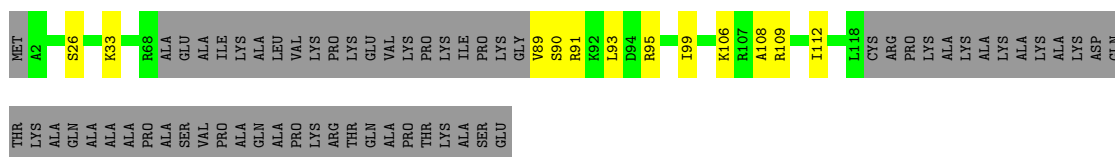
- Molecule 20: 60S ribosomal protein L18a



- Molecule 21: 60S ribosomal protein L21

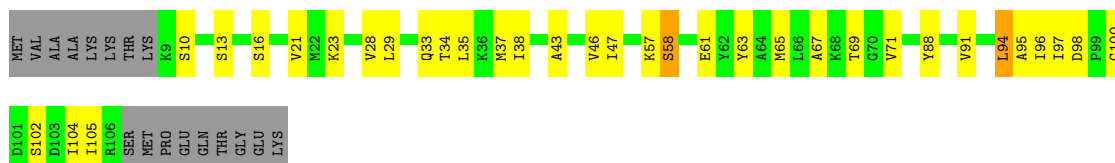


- Molecule 22: 60S ribosomal protein L23



- Molecule 29: 60S ribosomal protein L30

Chain Lc: 56% 28% 15%



- Molecule 30: 60S ribosomal protein L31

Chain Ld: 72% 11% 16%



- Molecule 31: Large ribosomal subunit protein eL32

Chain Le: 93% 6%



- Molecule 32: Large ribosomal subunit protein eL33

Chain Lf: 87% 12%



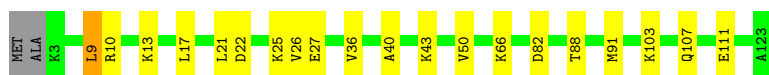
- Molecule 33: 60S ribosomal protein L34

Chain Lg: 80% 10% 9%




- Molecule 34: 60S ribosomal protein L35

Chain Lh: 82% 15% 2%



• Molecule 35: 60S ribosomal protein L36

Chain Li:  78% 13% 8%


• Molecule 36: Large ribosomal subunit protein eL37

Chain Lj:  94% 5%

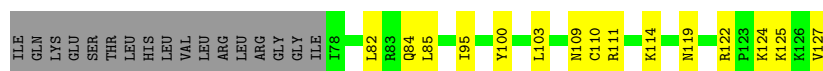
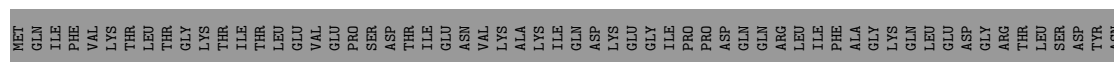
• Molecule 37: 60S ribosomal protein L38

Chain Lk:  94%

• Molecule 38: 60S ribosomal protein L39

Chain Ll:  76% 18% 6%


• Molecule 39: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  28% 12% 61%

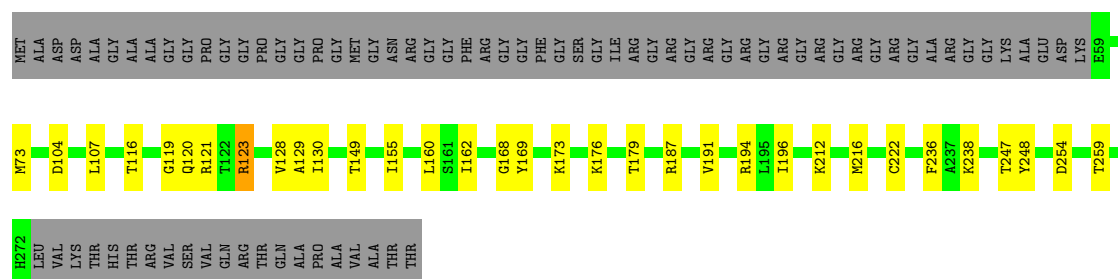
• Molecule 40: 60S ribosomal protein L41

Chain Ln:  88% 12%

• Molecule 41: Large ribosomal subunit protein eL42

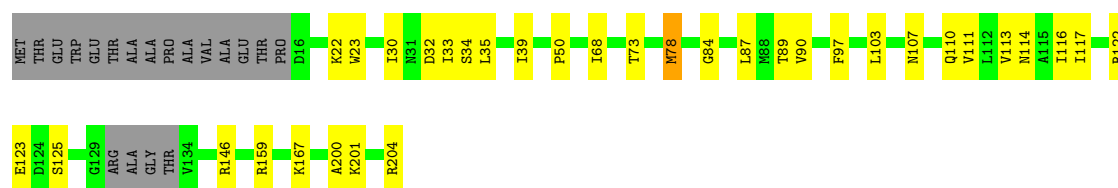
Chain Lo:  83% 10% 8%

Chain SC: 



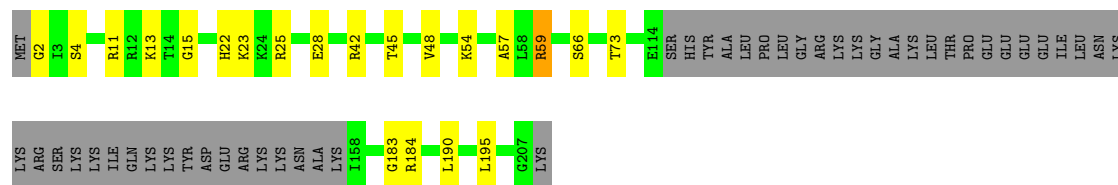
- Molecule 48: 40S ribosomal protein S5

Chain SF: 



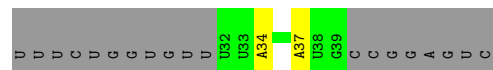
- Molecule 49: 40S ribosomal protein S8

Chain SI: 



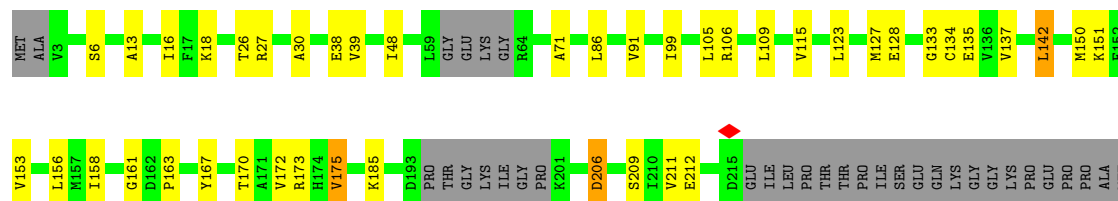
- Molecule 50: Histone H2B mRNA

Chain mR:  22% 7% 70%




- Molecule 51: 40S ribosomal protein S3

Chain SD: 



PRO
GLN
PRO
VAL
PRO
THR
ALA

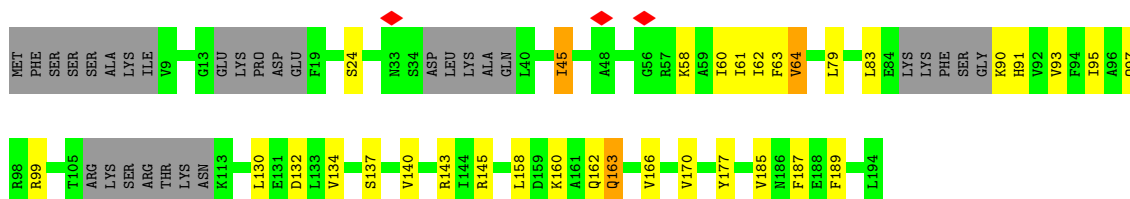
- Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE:  80% 17% ..



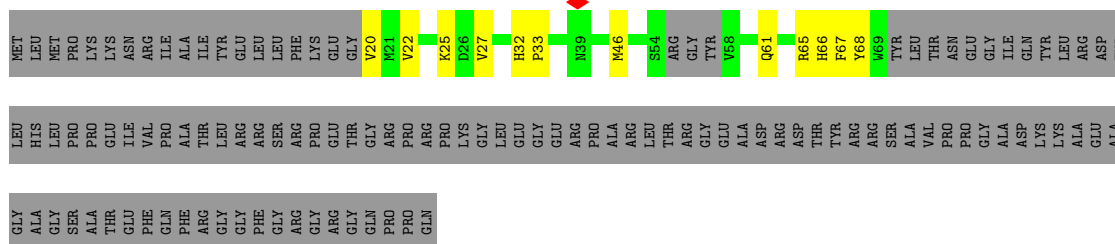
- Molecule 53: 40S ribosomal protein S7

Chain SH:  68% 15% 15%



- Molecule 54: 40S ribosomal protein S10

Chain SK:  21% 7% 72%




- Molecule 55: Small ribosomal subunit protein uS17

Chain SL:  73% 9% 18%



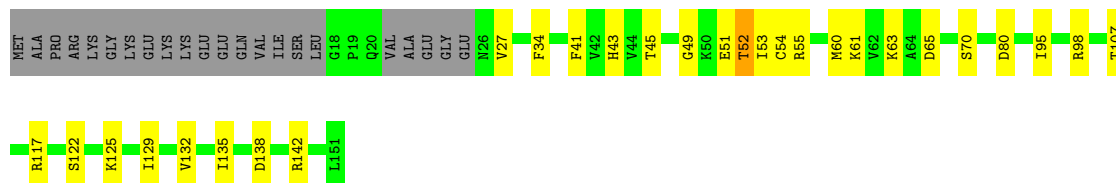
- Molecule 56: 40S ribosomal protein S13

Chain SN:  85% 15%




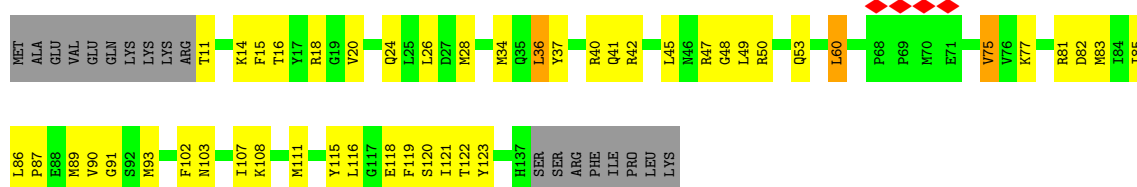
- Molecule 57: 40S ribosomal protein S14

Chain SO:  67% 18% 15%




- Molecule 58: 40S ribosomal protein S15

Chain SP:  55% 30% 12%




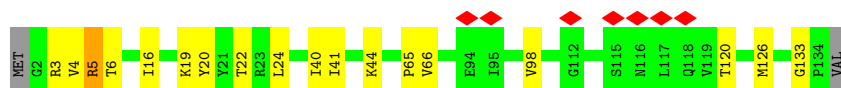
- Molecule 59: 40S ribosomal protein S16

Chain SQ:  78% 18% 2%



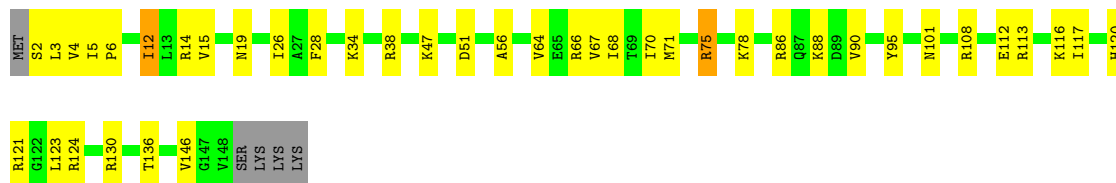
- Molecule 60: 40S ribosomal protein S17

Chain SR:  5% 85% 13%




- Molecule 61: 40S ribosomal protein S18

Chain SS:  70% 26% 2%

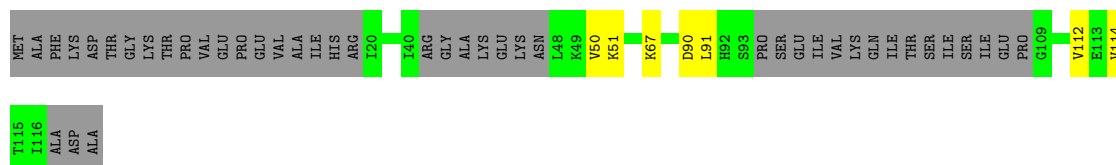


- Molecule 62: 40S ribosomal protein S19

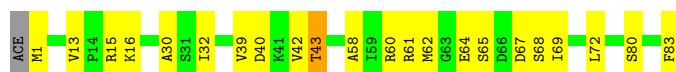
Chain ST:  79% 19% 2%



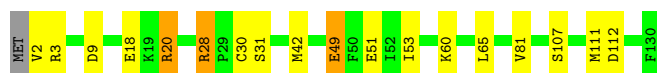
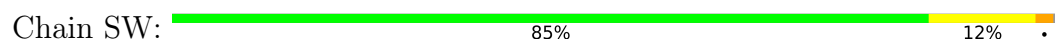
- Molecule 63: 40S ribosomal protein S20



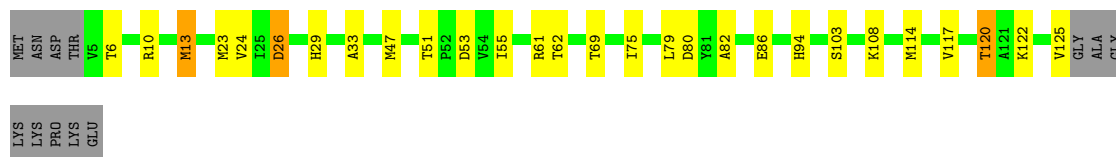
- Molecule 64: Small ribosomal subunit protein eS21



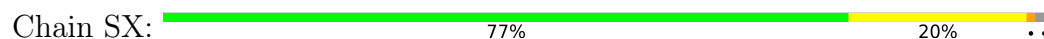
- Molecule 65: 40S ribosomal protein S15a



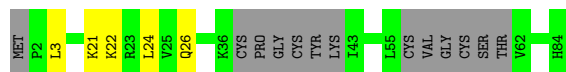
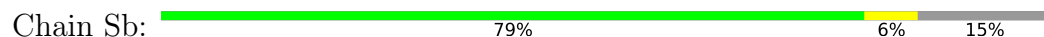
- Molecule 66: 40S ribosomal protein S24



- Molecule 67: 40S ribosomal protein S23



- Molecule 68: 40S ribosomal protein S27



- [illegible]

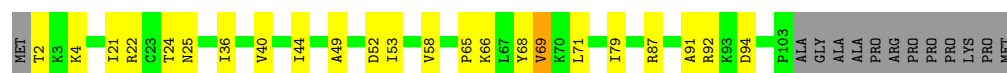
U1494	C1417	G1324	C1262	G1176	U1073	G949	G	U799	A668	U551	C503	A392	C310
G1495	C	U1333	A1285	U1177	C1074	G952	G	C903	A669	C552	G504	U993	C311
G1496	G	C1266	G1179	U1178	C1074	C953	U	U804	A670	C553	G507	A398	G312
U1498	A	C1267	C1180	A1083	U1088	U954	C	U805	A671	C554	G508	C399	A313
U1499	G	G1338	A1181	A1084	C1085	G956	U	A811	A672	G558	G509	C409	C315
U1504	C	U1342	G1270	G1187	G1086	A957	A	A812	C674	C559	A512	C409	G316
U	G	U1343	C1271	A1195	U1087	G958	U	A813	U675	G590	G413	A414	C317
A	U1426	A1344	C1272	A1196	U1088	G959	U	U814	U688	U591	G515	A414	A318
G	C1427	C1273	G1274	U1089	U1089	U960	U	U818	U689	C592	A516	A414	C319
U1508	G1428	U1346	A	C1090	G961	G961	G	A818	G690	C593	C517	A433	G
U1509	G1429	U1347	G	C1091	A962	U962	U	U822	G	A594	A520	G434	C
G1510	C1430	G1348	C	U1201	A963	U963	U	A825	G	U595	A521	G438	C
U1511	U1431	U1202	A	U1095	U965	U965	G	A826	A	U596	A521	G438	C
C1512	U1432	G1203	G	G1096	U966	U966	G	A827	C	A604	A525	C441	C
C1513	C1433	C1204	G	U1097	U968	U968	U	A830	C	A605	A526	C441	C
G1514	C1434	C1205	U	C1098	U968	U968	U	C941	C	G606	C527	C442	C
G1515	C1435	C1206	U	G1099	U968	U968	U	C942	C	U607	A445	A445	U
G1516	C1436	G1207	U	A1100	G971	G971	U	C943	C	C608	C532	A445	G
C1437	U1101	A1208	C	G1102	A972	A972	C	C934	A	U609	A	A448	G
A1438	G1212	G1212	G	C1109	A981	A981	G	A	G	G610	G	A449	C
A1448	G1212	G1212	G	C1109	A982	A982	G	A	G	G611	G	A449	C
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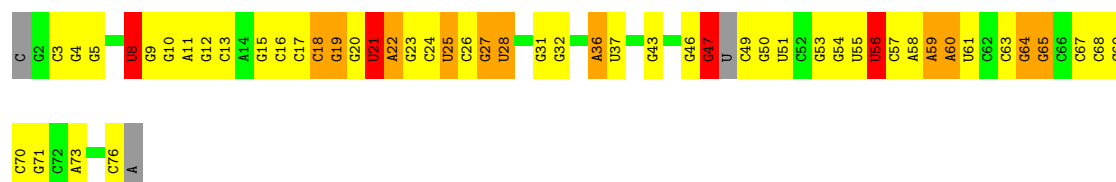
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C	U5053	C	C	G4827	C4727	C4727	U4416	A4323	C	C	A3934
C	U5054	C	C	G4828	C4728	C4728	U4417	A4324	C	C	A3935
C	U5055	C	C	G4829	C4729	C4729	U4418	A4325	C	C	A3936
C	U5056	C	C	G4830	C4730	C4730	U4419	A4326	C	C	A3937
C	U5057	C	C	G4831	C4731	C4731	U4420	A4327	C	C	A3938
C	U5058	C	C	G4832	C4732	C4732	U4421	A4328	C	C	A3939
C	U5059	C	C	G4833	C4733	C4733	U4422	A4329	C	C	A3940
C	U5060	C	C	G4834	C4734	C4734	U4423	A4330	C	C	A3941
C	U5061	C	C	G4835	C4735	C4735	U4424	A4331	C	C	A3942
C	U5062	C	C	G4836	C4736	C4736	U4425	A4332	C	C	A3943
C	U5063	C	C	G4837	C4737	C4737	U4426	A4333	C	C	A3944
C	U5064	C	C	G4838	C4738	C4738	U4427	A4334	C	C	A3945
C	U5065	C	C	G4839	C4739	C4739	U4428	A4335	C	C	A3946
C	U5066	C	C	G4840	C4740	C4740	U4429	A4336	C	C	A3947
C	U5067	C	C	G4841	C4741	C4741	U4430	A4337	C	C	A3948
C	U5068	C	C	G4842	C4742	C4742	U4431	A4338	C	C	A3949
C	U5069	C	C	G4843	C4743	C4743	U4432	A4339	C	C	A3950
C	U5070	C	C	G4844	C4744	C4744	U4433	A4340	C	C	A3951
C	U5071	C	C	G4845	C4745	C4745	U4434	A4341	C	C	A3952

Chain Sa:  69% 19% 11%




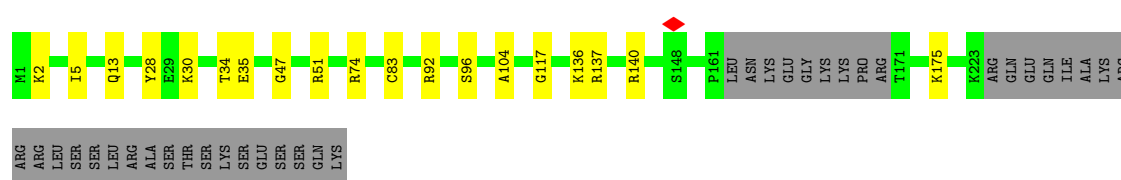
• Molecule 76: E site tRNA

Chain S6:  29% 48% 14% 5%



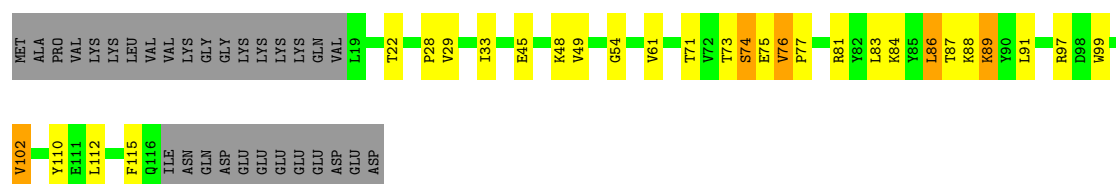
• Molecule 77: 40S ribosomal protein S6

Chain SG:  78% 8% 14%



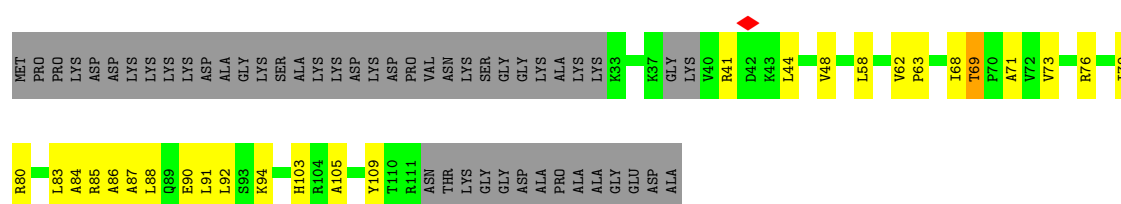
• Molecule 78: 60S ribosomal protein L22

Chain LU:  54% 19% 23%



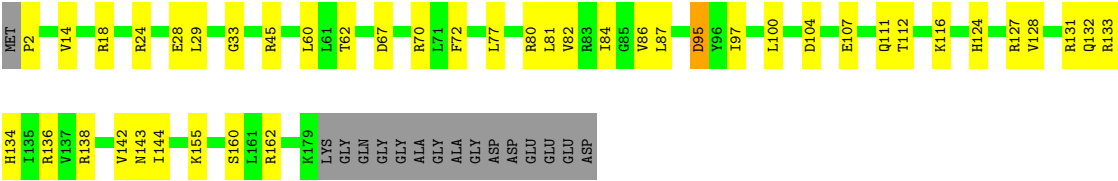
• Molecule 79: Small ribosomal subunit protein eS25

Chain SZ:  41% 20% 38%



• Molecule 80: 40S ribosomal protein S9

Chain SJ:  70% 22% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78814	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, ACE, MLZ, ZN, OMU, OMG, A2M, SPD, NA, 4SU, OMC, V5N, HYG, 5MC, G7M, K, UY1, MG, HIC, 1MA, PSU, 6MZ

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	L7	0.21	0/2840	0.32	0/4425
2	L8	0.24	0/3494	0.33	0/5441
3	LA	0.23	0/1913	0.44	0/2564
4	LB	0.20	0/3145	0.39	0/4220
5	LC	0.21	0/2883	0.38	0/3875
6	LD	0.14	0/1418	0.31	0/1971
7	LE	0.20	0/1591	0.40	0/2138
8	LF	0.21	0/1879	0.39	0/2507
9	LG	0.20	0/1628	0.40	0/2211
10	LH	0.19	0/1460	0.40	0/1974
11	LI	0.19	0/1661	0.35	0/2220
12	LJ	0.18	0/1261	0.43	0/1700
13	LL	0.19	0/1599	0.36	0/2150
14	LM	0.20	0/1102	0.39	0/1479
15	LN	0.23	0/1739	0.39	0/2331
16	LO	0.21	0/1666	0.37	0/2231
17	LP	0.21	0/1260	0.42	0/1692
18	LQ	0.21	0/1521	0.40	0/2036
19	LR	0.24	0/1267	0.38	0/1681
20	LS	0.21	0/1496	0.37	0/2009
21	LT	0.21	0/1321	0.35	0/1766
22	LV	0.20	0/987	0.42	0/1324
23	LW	0.19	0/530	0.40	0/709
24	LX	0.19	0/995	0.38	0/1338
25	LY	0.20	0/1101	0.37	0/1465
26	LZ	0.18	0/1056	0.37	0/1421
27	La	0.20	0/1171	0.37	0/1565
28	Lb	0.20	0/724	0.38	0/969
29	Lc	0.25	0/748	0.43	0/1009
30	Ld	0.24	0/869	0.38	0/1172
31	Le	0.21	0/1047	0.38	0/1403

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lf	0.22	0/894	0.39	0/1198
33	Lg	0.20	0/835	0.41	0/1115
34	Lh	0.18	0/1020	0.34	0/1350
35	Li	0.18	0/804	0.39	0/1065
36	Lj	0.21	0/731	0.41	0/967
37	Lk	0.17	0/453	0.32	0/615
38	Ll	0.20	0/427	0.38	0/566
39	Lm	0.17	0/406	0.36	0/541
40	Ln	0.22	0/225	0.33	0/288
41	Lo	0.19	0/803	0.40	0/1063
42	Lp	0.26	0/718	0.41	0/953
43	Lr	0.21	0/1000	0.39	0/1346
44	Pt	0.23	0/1697	0.41	0/2637
45	SA	0.18	0/1660	0.37	0/2259
46	SB	0.19	0/1749	0.35	0/2342
47	SC	0.20	0/1639	0.41	0/2222
48	SF	0.17	0/1382	0.35	0/1873
49	SI	0.19	0/1139	0.39	0/1535
50	mR	0.19	0/192	0.27	0/297
51	SD	0.18	0/1363	0.40	0/1847
52	SE	0.19	0/2071	0.38	0/2793
53	SH	0.17	0/1145	0.39	0/1551
54	SK	0.16	0/349	0.42	0/477
55	SL	0.18	0/1029	0.35	0/1385
56	SN	0.21	0/1184	0.35	0/1600
57	SO	0.21	0/968	0.41	0/1298
58	SP	0.18	0/981	0.38	0/1323
59	SQ	0.18	0/1116	0.36	0/1498
60	SR	0.16	0/876	0.40	0/1189
61	SS	0.19	0/1164	0.42	0/1568
62	ST	0.17	0/1061	0.36	0/1434
63	SU	0.14	0/380	0.36	0/525
64	SV	0.15	0/616	0.27	0/826
65	SW	0.21	0/1031	0.35	0/1382
66	SY	0.17	0/969	0.42	0/1296
67	SX	0.18	0/1098	0.35	0/1464
68	Sb	0.16	0/467	0.31	0/631
69	Sc	0.16	0/486	0.33	0/654
70	Sd	0.16	0/356	0.34	0/472
71	Se	0.16	0/373	0.32	0/493
72	Sg	0.13	0/1278	0.37	0/1766
73	S2	0.24	0/34705	0.37	0/54052
74	L5	0.26	3/73673 (0.0%)	0.37	1/114866 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sa	0.25	0/788	0.53	0/1061
76	S6	0.41	4/1695 (0.2%)	0.45	0/2639
77	SG	0.17	0/1160	0.41	0/1597
78	LU	0.19	0/679	0.48	0/921
79	SZ	0.19	0/546	0.47	0/744
80	SJ	0.20	0/1466	0.40	0/1967
All	All	0.23	7/200219 (0.0%)	0.37	1/294547 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S6	21	U	C5-C6	8.12	1.50	1.34
76	S6	21	U	C2-N3	5.79	1.49	1.37
76	S6	8	4SU	O3'-P	5.46	1.61	1.56
74	L5	3785	A2M	O3'-P	5.22	1.61	1.56
74	L5	1534	A2M	O3'-P	5.18	1.61	1.56
76	S6	21	U	N1-C2	5.07	1.48	1.38
74	L5	4523	A2M	O3'-P	5.03	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	417	G	O4'-C1'-N9	5.57	116.55	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L7	2542	0	1285	19	0
2	L8	3193	0	1621	29	0
3	LA	1888	0	1968	16	0
4	LB	3091	0	3148	32	0
5	LC	2829	0	2991	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	LD	1419	0	665	3	0
7	LE	1561	0	1663	29	0
8	LF	1845	0	1959	9	0
9	LG	1598	0	1574	12	0
10	LH	1441	0	1452	20	0
11	LI	1623	0	1665	19	0
12	LJ	1242	0	1190	27	0
13	LL	1570	0	1609	16	0
14	LM	1080	0	1103	18	0
15	LN	1694	0	1738	16	0
16	LO	1634	0	1768	17	0
17	LP	1234	0	1254	13	0
18	LQ	1497	0	1591	12	0
19	LR	1251	0	1351	12	0
20	LS	1456	0	1491	19	0
21	LT	1293	0	1355	11	0
22	LV	973	0	1034	9	0
23	LW	517	0	512	3	0
24	LX	977	0	1046	10	0
25	LY	1084	0	1170	14	0
26	LZ	1034	0	1041	20	0
27	La	1155	0	1184	10	0
28	Lb	723	0	703	9	0
29	Lc	738	0	745	19	0
30	Ld	854	0	897	8	0
31	Le	1029	0	1085	7	0
32	Lf	875	0	912	7	0
33	Lg	825	0	872	8	0
34	Lh	1012	0	1133	14	0
35	Li	793	0	865	10	0
36	Lj	712	0	744	2	0
37	Lk	450	0	385	2	0
38	Ll	417	0	442	8	0
39	Lm	400	0	410	12	0
40	Ln	224	0	260	2	0
41	Lo	786	0	834	6	0
42	Lp	708	0	756	12	0
43	Lr	988	0	1026	10	0
44	Pt	1605	0	824	21	0
45	SA	1624	0	1617	29	0
46	SB	1724	0	1750	36	0
47	SC	1605	0	1637	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	SF	1362	0	1331	22	0
49	SI	1123	0	989	12	0
50	mR	172	0	86	1	0
51	SD	1350	0	1218	22	0
52	SE	2029	0	2103	29	0
53	SH	1133	0	1031	18	0
54	SK	339	0	277	7	0
55	SL	1011	0	1001	9	0
56	SN	1160	0	1195	15	0
57	SO	956	0	979	18	0
58	SP	963	0	938	28	0
59	SQ	1099	0	1150	14	0
60	SR	867	0	729	12	0
61	SS	1146	0	1166	28	0
62	ST	1043	0	1005	18	0
63	SU	383	0	181	3	0
64	SV	610	0	598	16	0
65	SW	1014	0	1050	11	0
66	SY	952	0	973	21	0
67	SX	1082	0	1147	17	0
68	Sb	461	0	360	4	0
69	Sc	484	0	499	8	0
70	Sd	351	0	334	8	0
71	Se	371	0	382	5	0
72	Sg	1284	0	578	9	0
73	S2	31042	0	15693	336	0
74	L5	68538	0	34699	588	0
75	Sa	776	0	805	15	0
76	S6	1582	0	809	23	0
77	SG	1157	0	681	15	0
78	LU	671	0	592	18	0
79	SZ	540	0	507	19	0
80	SJ	1441	0	1520	26	0
81	L5	191	0	0	0	0
81	L7	3	0	0	0	0
81	L8	4	0	0	0	0
81	LA	1	0	0	0	0
81	LB	1	0	0	0	0
81	LH	2	0	0	0	0
81	LM	1	0	0	0	0
81	LN	2	0	0	0	0
81	LP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	LV	1	0	0	0	0
81	Lg	1	0	0	0	0
81	Lj	1	0	0	0	0
81	S2	14	0	0	0	0
82	L5	42	0	0	0	0
82	L8	1	0	0	0	0
82	LA	2	0	0	0	0
82	LI	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	2	0	0	0	0
82	SL	1	0	0	0	0
82	SO	1	0	0	0	0
83	L5	2	0	0	0	0
83	LS	1	0	0	0	0
83	Le	1	0	0	0	0
83	S2	4	0	0	0	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lo	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Sd	1	0	0	0	0
85	S2	36	0	37	0	0
86	L5	30	0	57	0	0
87	L5	1979	0	0	4	0
87	L7	18	0	0	0	0
87	L8	52	0	0	0	0
87	LA	41	0	0	0	0
87	LB	33	0	0	0	0
87	LC	39	0	0	0	0
87	LD	5	0	0	1	0
87	LE	2	0	0	0	0
87	LF	22	0	0	0	0
87	LG	2	0	0	0	0
87	LH	3	0	0	0	0
87	LI	6	0	0	1	0
87	LJ	4	0	0	0	0
87	LL	21	0	0	0	0
87	LM	4	0	0	0	0
87	LN	34	0	0	0	0
87	LO	6	0	0	0	0
87	LP	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LQ	32	0	0	0	0
87	LR	31	0	0	1	0
87	LS	8	0	0	0	0
87	LT	14	0	0	0	0
87	LV	8	0	0	0	0
87	LW	1	0	0	0	0
87	LX	1	0	0	0	0
87	LY	6	0	0	0	0
87	La	25	0	0	0	0
87	Lb	11	0	0	0	0
87	Lc	10	0	0	1	0
87	Ld	3	0	0	0	0
87	Le	21	0	0	0	0
87	Lf	11	0	0	0	0
87	Lg	5	0	0	0	0
87	Lh	4	0	0	0	0
87	Lj	19	0	0	1	0
87	Ll	6	0	0	0	0
87	Ln	1	0	0	0	0
87	Lo	9	0	0	0	0
87	Lp	21	0	0	0	0
87	Lr	11	0	0	0	0
87	Pt	6	0	0	1	0
87	S2	237	0	0	3	0
87	S6	6	0	0	0	0
87	SB	6	0	0	0	0
87	SC	2	0	0	0	0
87	SE	1	0	0	0	0
87	SF	1	0	0	0	0
87	SG	1	0	0	0	0
87	SI	5	0	0	0	0
87	SL	1	0	0	0	0
87	SN	10	0	0	0	0
87	SO	3	0	0	0	0
87	SS	7	0	0	1	0
87	ST	1	0	0	0	0
87	SW	1	0	0	0	0
87	SX	3	0	0	0	0
87	Sa	4	0	0	0	0
87	Sb	1	0	0	0	0
All	All	192496	0	135025	1750	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1750) 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)
76:S6:21:U:H2'	76:S6:22:A:H4'	1.58	0.86
53:SH:58:LYS:O	53:SH:90:LYS:HA	1.78	0.82
62:ST:43:LYS:NZ	73:S2:1540:G:OP2	2.16	0.79
10:LH:165:THR:HG21	10:LH:179:ILE:H	1.49	0.77
73:S2:1324:G:HO2'	73:S2:1510:G:HO2'	1.26	0.77
73:S2:1348:G:H1	73:S2:1381:G:H22	1.33	0.76
12:LJ:24:ILE:HD11	12:LJ:128:LEU:HD23	1.67	0.75
3:LA:137:ILE:HD11	3:LA:149:LYS:HB2	1.68	0.74
11:LI:36:LEU:HD11	11:LI:69:ARG:HH11	1.51	0.74
73:S2:1488:C:O2'	73:S2:1490:G:OP2	2.04	0.74
12:LJ:89:VAL:HG11	12:LJ:109:ILE:HD13	1.70	0.74
74:L5:2020:U:H2'	74:L5:2021:G:H8	1.51	0.73
74:L5:4421:C:N4	74:L5:4475:G:N2	2.37	0.73
73:S2:928:G:H1	73:S2:1013:U:H3	1.35	0.73
74:L5:4421:C:N4	74:L5:4475:G:H22	1.87	0.73
4:LB:3:HIS:ND1	74:L5:4515:G:N7	2.36	0.73
3:LA:215:ASN:ND2	74:L5:4546:A:N7	2.37	0.72
74:L5:4421:C:H42	74:L5:4475:G:N2	1.88	0.72
73:S2:170:A:OP2	77:SG:140:ARG:NH2	2.22	0.72
60:SR:3:ARG:HD2	73:S2:1454:A:H5''	1.72	0.72
1:L7:28:C:H1'	1:L7:54:A:H61	1.55	0.71
70:Sd:17:GLY:HA2	70:Sd:27:ARG:HH12	1.55	0.71
9:LG:43:GLN:O	74:L5:4124:G:N2	2.22	0.71
67:SX:134:TYR:O	71:Se:87:ARG:NH2	2.24	0.71
74:L5:2416:G:N2	74:L5:2427:G:N7	2.36	0.70
29:Lc:10:SER:H	29:Lc:13:SER:HB3	1.56	0.70
51:SD:27:ARG:HH22	73:S2:1497:G:H8	1.40	0.70
73:S2:1599:U:H3'	79:SZ:44:LEU:HD12	1.72	0.70
7:LE:154:THR:HG22	74:L5:4942:C:H4'	1.74	0.70
39:Lm:125:LYS:HG3	74:L5:4474:A:H5''	1.74	0.70
59:SQ:51:LEU:HD21	59:SQ:81:ILE:HD12	1.74	0.70
7:LE:183:ARG:NH1	74:L5:4936:G:N7	2.40	0.70
52:SE:104:ASP:HB3	52:SE:110:ALA:HB2	1.74	0.70
73:S2:1199:A:OP1	75:Sa:2:THR:OG1	2.08	0.70
73:S2:561:A:H61	73:S2:590:A:H2	1.38	0.69
73:S2:1536:G:H2'	73:S2:1537:A:H8	1.57	0.69
73:S2:818:A:OP1	80:SJ:80:ARG:NH2	2.24	0.69
46:SB:54:GLY:HA2	74:L5:3944:OMG:H4'	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SW:2:VAL:N	73:S2:1091:C:HO2'	1.90	0.69
5:LC:140:LYS:HE2	5:LC:245:HIS:HB2	1.75	0.69
38:L1:36:ARG:NH2	74:L5:413:G:OP2	2.26	0.69
72:Sg:236:ILE:HA	72:Sg:252:THR:HA	1.73	0.69
7:LE:282:TYR:HB2	7:LE:285:LYS:HG3	1.75	0.68
35:Li:84:LYS:NZ	74:L5:320:C:OP1	2.26	0.68
73:S2:1658:G:OP2	73:S2:1660:C:N4	2.25	0.68
21:LT:116:LYS:NZ	74:L5:1836:G:N7	2.42	0.68
74:L5:4745:G:H1	74:L5:4955:A:H61	1.40	0.68
25:LY:54:GLU:HB2	25:LY:108:ARG:HB3	1.74	0.68
73:S2:1589:A:N3	73:S2:1653:U:O2'	2.27	0.68
2:L8:71:A:OP1	25:LY:27:ARG:NH1	2.27	0.68
48:SF:34:SER:HA	69:Sc:55:VAL:HB	1.73	0.68
58:SP:42:ARG:NH2	73:S2:1613:G:OP1	2.26	0.67
66:SY:120:THR:OG1	73:S2:151:C:OP1	2.11	0.67
26:LZ:54:THR:H	26:LZ:57:MET:HE2	1.60	0.67
16:LO:106:ASP:O	74:L5:4910:G:N2	2.28	0.67
8:LF:35:LYS:HD3	8:LF:39:GLN:HE22	1.58	0.67
12:LJ:90:ARG:NH2	12:LJ:108:GLY:O	2.27	0.67
79:SZ:48:VAL:HG12	79:SZ:80:ARG:HD2	1.77	0.67
74:L5:3717:A:H2'	74:L5:3718:A2M:C8	2.25	0.67
2:L8:156:U:H3	74:L5:1:C:H42	1.42	0.67
12:LJ:113:ILE:HG21	61:SS:12:ILE:HD11	1.77	0.66
5:LC:143:ARG:NH1	74:L5:2300:A:N7	2.41	0.66
58:SP:18:ARG:NH1	61:SS:88:LYS:O	2.28	0.66
73:S2:957:A:H3'	73:S2:958:G:H21	1.61	0.66
74:L5:4993:G:H1	74:L5:5058:A:H61	1.42	0.66
73:S2:925:G:H1	73:S2:1017:U:H3	1.43	0.66
74:L5:1294:A:O4'	74:L5:1296:G:N2	2.28	0.66
74:L5:1480:C:O2'	74:L5:1482:G:OP2	2.14	0.66
4:LB:92:TYR:HB2	4:LB:159:VAL:HB	1.78	0.66
26:LZ:124:THR:HG22	26:LZ:126:LYS:H	1.60	0.66
51:SD:39:VAL:HG12	51:SD:48:ILE:HA	1.78	0.65
8:LF:182:TYR:HB3	8:LF:200:ARG:HG3	1.78	0.65
48:SF:201:LYS:HG2	48:SF:204:ARG:HH21	1.61	0.65
52:SE:108:ARG:NH2	73:S2:846:G:OP2	2.29	0.65
74:L5:505:G:H1	74:L5:653:U:H3	1.42	0.65
67:SX:68:LYS:HB3	67:SX:91:LEU:HD22	1.77	0.65
73:S2:318:A:H2	73:S2:333:G:H1	1.42	0.65
73:S2:566:U:H3	73:S2:584:G:H1	1.44	0.65
47:SC:123:ARG:NH2	73:S2:1358:U:OP1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SP:49:LEU:HD12	58:SP:53:GLN:HB2	1.79	0.65
58:SP:81:ARG:NH1	58:SP:120:SER:O	2.30	0.65
74:L5:4415:A:H62	74:L5:4427:G:H21	1.44	0.65
57:SO:52:THR:HG21	73:S2:952:G:H21	1.62	0.64
73:S2:153:G:N3	77:SG:13:GLN:NE2	2.44	0.64
74:L5:2573:A:H62	74:L5:2761:U:H3	1.42	0.64
46:SB:188:LEU:HD21	46:SB:215:VAL:HG21	1.78	0.64
31:Le:78:LEU:O	43:Lr:20:ARG:NH1	2.30	0.64
73:S2:1228:A:H2'	73:S2:1229:G:C8	2.32	0.64
16:LO:175:MET:HG2	74:L5:4873:G:C2	2.33	0.64
11:LI:207:ASP:OD1	11:LI:210:ARG:NH1	2.31	0.64
48:SF:23:TRP:HE1	48:SF:97:PHE:HB3	1.62	0.64
61:SS:2:SER:OG	61:SS:3:LEU:N	2.31	0.64
78:LU:76:VAL:HG22	78:LU:77:PRO:HD2	1.79	0.64
4:LB:242:ARG:NH2	74:L5:2856:C:O2	2.30	0.64
11:LI:193:ASP:OD2	74:L5:1750:G:N2	2.30	0.64
74:L5:450:G:N2	74:L5:1293:G:O2'	2.25	0.64
31:Le:128:ARG:NH1	74:L5:2306:G:OP1	2.31	0.64
59:SQ:113:ILE:HG13	59:SQ:120:LEU:HD12	1.80	0.64
73:S2:568:C:H42	73:S2:582:C:H42	1.44	0.64
18:LQ:37:ARG:NH2	74:L5:2088:A:OP2	2.30	0.63
33:Lg:28:ASN:ND2	74:L5:2637:U:OP1	2.30	0.63
5:LC:95:MET:HG3	74:L5:2351:OMC:HM22	1.80	0.63
7:LE:156:ARG:NH1	74:L5:4940:C:OP1	2.23	0.63
45:SA:84:GLN:HG2	45:SA:100:ALA:HB1	1.80	0.63
67:SX:63:ASN:OD1	73:S2:624:C:N4	2.32	0.63
75:Sa:87:ARG:NH1	75:Sa:91:ALA:O	2.32	0.63
4:LB:218:ASP:OD2	4:LB:348:ARG:NH2	2.26	0.63
39:Lm:100:TYR:O	74:L5:4472:G:O2'	2.16	0.63
44:Pt:15:G:OP2	44:Pt:16:C:N4	2.32	0.63
73:S2:1347:U:H2'	73:S2:1348:G:C8	2.34	0.63
74:L5:2520:C:O2	74:L5:2640:G:N2	2.32	0.63
74:L5:3715:PSU:OP1	76:S6:4:G:O2'	2.16	0.63
44:Pt:15:G:H5''	44:Pt:17:C:H42	1.64	0.62
74:L5:3732:A:H2'	74:L5:3733:A:H8	1.64	0.62
73:S2:870:A:N6	73:S2:916:A:O5'	2.31	0.62
74:L5:4594:U:H2'	74:L5:4595:G:H8	1.65	0.62
44:Pt:77:A:H2'	74:L5:4397:A:H1'	1.81	0.62
76:S6:55:U:O4	76:S6:59:A:N7	2.33	0.62
33:Lg:93:ARG:O	33:Lg:97:ILE:HG12	1.99	0.62
73:S2:1864:U:OP2	75:Sa:4:LYS:NZ	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LI:201:PRO:HB2	11:LI:203:ARG:HG3	1.80	0.62
52:SE:238:LEU:HB2	52:SE:242:LYS:HE3	1.81	0.62
72:Sg:109:LEU:H	72:Sg:124:SER:HA	1.64	0.62
74:L5:3946:G:N2	74:L5:4067:U:O2	2.27	0.62
76:S6:9:G:O4'	76:S6:47:G7M:H1'	2.00	0.62
73:S2:1428:G:H2'	73:S2:1429:G:C8	2.35	0.61
74:L5:1833:G:O2'	74:L5:1835:G:N2	2.33	0.61
74:L5:4750:G:H2'	74:L5:4751:G:C8	2.33	0.61
14:LM:69:HIS:ND1	74:L5:919:C:OP1	2.32	0.61
3:LA:70:LYS:NZ	74:L5:2503:G:O6	2.33	0.61
51:SD:163:PRO:O	51:SD:167:TYR:HB2	1.99	0.61
57:SO:34:PHE:HB3	57:SO:41:PHE:HB2	1.81	0.61
62:ST:41:LYS:NZ	73:S2:1569:A:OP1	2.32	0.61
73:S2:981:A:H2'	73:S2:982:G:C8	2.36	0.61
4:LB:103:LYS:HB3	4:LB:153:MET:HE2	1.82	0.61
21:LT:51:GLY:HA3	21:LT:92:ARG:HG3	1.83	0.61
73:S2:1743:G:H21	73:S2:1791:A:H62	1.47	0.61
74:L5:1399:G:H2'	74:L5:1400:G:H8	1.66	0.61
74:L5:2020:U:H2'	74:L5:2021:G:C8	2.34	0.61
55:SL:88:ILE:HD11	55:SL:109:MET:HE2	1.83	0.61
1:L7:28:C:O2'	1:L7:54:A:N1	2.34	0.61
75:Sa:24:THR:HG21	75:Sa:71:LEU:HD22	1.83	0.61
55:SL:127:THR:HB	55:SL:144:LYS:HB3	1.82	0.61
57:SO:117:ARG:HH22	69:Sc:62:GLU:HA	1.66	0.61
74:L5:1301:C:H5'	74:L5:1302:U:H5'	1.82	0.61
1:L7:51:G:N2	12:LJ:12:MET:SD	2.72	0.60
75:Sa:40:VAL:HB	75:Sa:69:VAL:HG13	1.82	0.60
16:LO:61:ARG:HA	16:LO:70:PRO:HD2	1.83	0.60
29:Lc:34:THR:HG23	29:Lc:95:ALA:HB2	1.83	0.60
29:Lc:38:ILE:HD11	29:Lc:46:VAL:HG21	1.84	0.60
59:SQ:142:GLN:NE2	73:S2:1527:C:OP1	2.34	0.60
66:SY:26:ASP:N	66:SY:26:ASP:OD1	2.34	0.60
73:S2:463:C:O2'	87:S2:2001:HOH:O	2.14	0.60
7:LE:202:ASP:O	7:LE:260:LYS:NZ	2.33	0.60
73:S2:1616:U:H3	73:S2:1620:A:H2	1.47	0.60
46:SB:150:ILE:HG12	73:S2:1124:C:H5''	1.83	0.60
49:SI:2:GLY:N	73:S2:441:C:OP2	2.34	0.60
66:SY:122:LYS:NZ	73:S2:85:A:OP1	2.31	0.60
58:SP:42:ARG:HH12	73:S2:1613:G:H5''	1.66	0.60
45:SA:50:ASN:HD22	45:SA:53:ARG:HD2	1.66	0.60
74:L5:1961:G:N2	74:L5:2025:A:H62	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Lo:6:LYS:HE3	41:Lo:93:LEU:HG	1.84	0.60
58:SP:18:ARG:HG3	58:SP:36:LEU:HG	1.84	0.60
74:L5:1961:G:N2	74:L5:2024:G:O2'	2.35	0.60
74:L5:4153:C:H2'	74:L5:4154:G:H8	1.66	0.60
76:S6:19:G:N1	76:S6:56:PSU:O2'	2.34	0.60
5:LC:189:MET:HE3	74:L5:2333:G:N7	2.17	0.60
74:L5:1762:C:H42	74:L5:1770:A:H61	1.49	0.60
12:LJ:144:LYS:O	12:LJ:148:THR:OG1	2.20	0.59
25:LY:66:GLN:H	25:LY:66:GLN:CD	2.10	0.59
30:Ld:29:ILE:HG13	30:Ld:84:ILE:HD12	1.84	0.59
44:Pt:15:G:H5''	44:Pt:17:C:N4	2.17	0.59
52:SE:59:ASP:OD1	52:SE:62:LYS:NZ	2.34	0.59
10:LH:30:PRO:HD2	10:LH:85:THR:HA	1.83	0.59
73:S2:466:G:O6	87:S2:2001:HOH:O	2.13	0.59
74:L5:3716:C:N4	74:L5:3735:G:O2'	2.35	0.59
38:Ll:3:SER:OG	74:L5:2783:A:OP2	2.20	0.59
16:LO:112:TYR:HA	16:LO:115:LYS:HG3	1.84	0.59
73:S2:116:U:H3	73:S2:347:G:H22	1.49	0.59
79:SZ:79:ILE:HD12	79:SZ:83:LEU:HG	1.85	0.59
4:LB:35:ASP:OD2	4:LB:193:LYS:NZ	2.34	0.59
73:S2:156:G:OP1	77:SG:2:LYS:NZ	2.36	0.59
74:L5:2024:G:O2'	74:L5:2025:A:N7	2.33	0.59
7:LE:219:LYS:NZ	74:L5:1291:G:OP1	2.35	0.59
73:S2:521:A:OP1	80:SJ:45:ARG:NH1	2.35	0.59
74:L5:1759:G:H1	74:L5:1773:U:H3	1.50	0.59
5:LC:149:GLU:OE2	43:Lr:71:ARG:NH2	2.34	0.59
73:S2:107:A:H2'	73:S2:108:G:C8	2.36	0.59
73:S2:1536:G:H2'	73:S2:1537:A:C8	2.37	0.59
78:LU:84:LYS:NZ	78:LU:102:VAL:O	2.35	0.59
76:S6:49:C:C2	76:S6:60:A:H1'	2.38	0.59
11:LI:170:LYS:HA	11:LI:177:ASN:HA	1.85	0.59
12:LJ:23:ASN:HB3	12:LJ:129:ASP:HB2	1.85	0.59
13:LL:222:ASN:O	74:L5:1378:C:N4	2.34	0.59
73:S2:583:C:OP2	80:SJ:162:ARG:NH2	2.36	0.59
74:L5:462:G:H2'	74:L5:463:A:C8	2.37	0.59
74:L5:752:G:O6	74:L5:911:U:O4	2.21	0.59
47:SC:104:ASP:HB3	47:SC:130:ILE:HD12	1.84	0.58
60:SR:41:ILE:H	60:SR:41:ILE:HD12	1.68	0.58
73:S2:1396:A:O2'	73:S2:1398:G:N7	2.36	0.58
74:L5:464:G:H2'	74:L5:465:G:H8	1.67	0.58
17:LP:13:LYS:NZ	17:LP:152:GLU:OE1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LZ:46:ILE:HG12	26:LZ:68:ILE:HD11	1.85	0.58
73:S2:1562:C:H2'	73:S2:1563:G:H8	1.68	0.58
74:L5:3946:G:H1	74:L5:4067:U:H3	1.52	0.58
7:LE:141:ARG:HB3	7:LE:144:ILE:HG13	1.85	0.58
10:LH:107:GLU:OE1	10:LH:127:ARG:NH1	2.36	0.58
12:LJ:99:PHE:O	12:LJ:159:LYS:NZ	2.37	0.58
15:LN:178:HIS:ND1	74:L5:68:U:OP1	2.28	0.58
74:L5:3717:A:H2'	74:L5:3718:A2M:H8	1.85	0.58
15:LN:60:VAL:HG22	15:LN:134:LEU:HB2	1.85	0.58
45:SA:77:ILE:HD12	45:SA:122:LEU:HD21	1.84	0.58
45:SA:94:THR:O	45:SA:186:ARG:NH2	2.35	0.58
9:LG:180:PRO:HG3	9:LG:223:ARG:HH21	1.68	0.58
74:L5:4274:A:H2'	74:L5:4275:G:C8	2.38	0.58
19:LR:16:ARG:NH2	74:L5:2699:C:OP1	2.37	0.58
61:SS:113:ARG:O	61:SS:117:ILE:HG22	2.03	0.58
73:S2:830:A:OP2	73:S2:846:G:N2	2.37	0.58
78:LU:91:LEU:HB2	78:LU:97:ARG:HG3	1.85	0.58
37:Lk:35:LYS:NZ	74:L5:2695:A:OP1	2.27	0.58
61:SS:112:GLU:OE1	74:L5:1767:A:H5'	2.04	0.58
73:S2:30:C:O2'	73:S2:596:U:OP1	2.18	0.58
73:S2:1348:G:H22	73:S2:1381:G:N2	2.02	0.58
9:LG:95:LEU:HD21	9:LG:156:VAL:HG21	1.86	0.58
39:Lm:114:LYS:NZ	74:L5:4485:C:O2'	2.34	0.58
10:LH:113:GLU:OE1	10:LH:113:GLU:N	2.37	0.58
66:SY:61:ARG:NH2	73:S2:572:U:O2'	2.37	0.58
73:S2:1606:G:H22	73:S2:1632:G:H2'	1.69	0.58
74:L5:3911:C:H4'	74:L5:4196:OMG:HM23	1.86	0.58
74:L5:4594:U:H2'	74:L5:4595:G:C8	2.39	0.58
45:SA:2:SER:HB3	45:SA:59:LEU:HD12	1.85	0.57
72:Sg:194:TYR:O	72:Sg:211:GLY:N	2.37	0.57
73:S2:857:U:H2'	73:S2:858:A:C8	2.39	0.57
74:L5:3663:A:N6	74:L5:4168:G:O2'	2.31	0.57
33:Lg:45:ALA:HB3	33:Lg:82:MET:HG2	1.86	0.57
74:L5:1961:G:H21	74:L5:2025:A:N6	2.02	0.57
35:Li:35:LYS:NZ	74:L5:275:C:OP2	2.37	0.57
69:Sc:44:ARG:NH2	69:Sc:60:GLU:O	2.38	0.57
74:L5:190:G:H2'	74:L5:191:G:C8	2.39	0.57
74:L5:1339:U:H2'	74:L5:1340:OMC:C6	2.38	0.57
79:SZ:79:ILE:HB	79:SZ:83:LEU:HD23	1.86	0.57
18:LQ:157:GLY:O	18:LQ:188:ASN:ND2	2.37	0.57
45:SA:10:MET:HG3	45:SA:55:TRP:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:3707:U:H2'	74:L5:3708:C:C6	2.40	0.57
47:SC:212:LYS:O	47:SC:216:MET:HG3	2.05	0.57
74:L5:2633:U:O4	78:LU:81:ARG:NH2	2.38	0.57
73:S2:118:C:H1'	73:S2:445:A:C5	2.40	0.57
74:L5:3718:A2M:H2	74:L5:3934:G:O4'	2.04	0.57
12:LJ:113:ILE:HD11	61:SS:14:ARG:HH11	1.70	0.57
13:LL:91:ALA:HB1	13:LL:96:ILE:HB	1.85	0.57
39:Lm:111:ARG:HH21	74:L5:4698:C:H3'	1.70	0.57
73:S2:928:G:H2'	73:S2:929:G:C8	2.40	0.57
7:LE:183:ARG:HD2	74:L5:4936:G:C5	2.40	0.57
34:Lh:103:LYS:HG2	34:Lh:107:GLN:HG2	1.87	0.57
74:L5:1406:G:H2'	74:L5:1407:C:C6	2.40	0.57
53:SH:170:VAL:HG13	53:SH:187:PHE:HB2	1.86	0.56
74:L5:394:G:N2	74:L5:397:G:OP2	2.33	0.56
2:L8:56:G:H21	2:L8:62:A:H5'	1.70	0.56
21:LT:140:PHE:HB3	21:LT:142:ARG:NH2	2.20	0.56
49:SI:13:LYS:HG3	55:SL:137:THR:HG21	1.88	0.56
56:SN:49:GLN:O	56:SN:53:ILE:HD12	2.05	0.56
73:S2:1428:G:H2'	73:S2:1429:G:H8	1.70	0.56
7:LE:279:ASN:ND2	74:L5:4755:G:N7	2.53	0.56
14:LM:114:LYS:HE3	74:L5:4929:C:H5''	1.86	0.56
44:Pt:24:C:OP2	87:Pt:101:HOH:O	2.17	0.56
49:SI:42:ARG:HB3	49:SI:59:ARG:HG2	1.87	0.56
51:SD:206:ASP:OD1	51:SD:206:ASP:N	2.27	0.56
56:SN:124:ARG:NH2	73:S2:1024:A:OP2	2.37	0.56
73:S2:640:A:H2'	73:S2:641:A:C8	2.41	0.56
20:LS:160:ARG:HB3	74:L5:1921:C:H1'	1.86	0.56
57:SO:125:LYS:HB3	75:Sa:58:VAL:HG13	1.88	0.56
74:L5:4967:A:H2'	74:L5:4968:A:C8	2.41	0.56
4:LB:252:ALA:HB3	74:L5:4457:PSU:H1'	1.87	0.56
11:LI:153:ARG:HA	11:LI:156:LYS:HD3	1.88	0.56
73:S2:1568:C:O2	73:S2:1627:C:O2'	2.23	0.56
73:S2:562:U:H2'	73:S2:563:G:C8	2.40	0.56
2:L8:65:A:O2'	34:Lh:10:ARG:NH2	2.38	0.56
4:LB:36:ASP:HB3	4:LB:39:LYS:HD2	1.87	0.56
46:SB:224:GLU:HG2	46:SB:227:LYS:HB2	1.87	0.56
61:SS:120:HIS:HA	61:SS:123:LEU:HD12	1.87	0.56
51:SD:99:ILE:HG23	51:SD:173:ARG:HH22	1.70	0.56
56:SN:127:ARG:O	56:SN:131:THR:HG23	2.06	0.56
80:SJ:131:ARG:NH1	80:SJ:143:ASN:O	2.39	0.56
10:LH:10:VAL:HG22	10:LH:55:LEU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LS:69:GLU:HG3	20:LS:101:THR:HA	1.88	0.56
42:Lp:69:TRP:CH2	74:L5:2739:C:H5'	2.41	0.56
47:SC:128:VAL:HG11	47:SC:155:ILE:HG13	1.88	0.56
61:SS:47:LYS:NZ	61:SS:78:LYS:O	2.39	0.56
65:SW:28:ARG:HB3	65:SW:60:LYS:HG2	1.88	0.56
18:LQ:173:LYS:NZ	74:L5:88:A:N7	2.53	0.55
63:SU:67:LYS:HA	70:Sd:44:ARG:HD2	1.88	0.55
46:SB:40:ASN:H	46:SB:75:GLN:HG2	1.71	0.55
73:S2:609:U:H2'	73:S2:610:G:H8	1.70	0.55
73:S2:1228:A:H2'	73:S2:1229:G:H8	1.71	0.55
11:LI:207:ASP:HA	11:LI:210:ARG:HD2	1.87	0.55
73:S2:940:U:H3	73:S2:1002:U:H3	1.55	0.55
74:L5:506:C:H2'	74:L5:507:G:C8	2.41	0.55
20:LS:128:LYS:NZ	20:LS:130:GLU:OE1	2.39	0.55
24:LX:83:THR:O	24:LX:87:MET:HG2	2.06	0.55
73:S2:1560:U:O2	73:S2:1575:G:O6	2.25	0.55
28:Lb:108:ALA:O	28:Lb:112:ILE:HG13	2.06	0.55
74:L5:1763:C:H2'	74:L5:1764:G:C8	2.41	0.55
9:LG:134:PRO:HB3	9:LG:206:GLN:HG3	1.88	0.55
25:LY:64:GLY:HA3	25:LY:66:GLN:HE22	1.72	0.55
49:SI:57:ALA:HB2	49:SI:183:GLY:HA2	1.86	0.55
73:S2:1101:U:H2'	73:S2:1102:G:C8	2.41	0.55
73:S2:1414:A:H62	73:S2:1429:G:H1	1.53	0.55
79:SZ:58:LEU:HD11	79:SZ:91:LEU:HD11	1.89	0.55
10:LH:12:ILE:HB	10:LH:53:LYS:HB3	1.88	0.55
19:LR:97:ARG:NH1	87:LR:202:HOH:O	2.40	0.55
58:SP:47:ARG:NH1	73:S2:1619:A:OP1	2.40	0.55
59:SQ:18:THR:HG21	73:S2:1546:G:H5'	1.89	0.55
73:S2:1660:C:O2'	73:S2:1662:U:OP2	2.24	0.55
45:SA:53:ARG:NH1	64:SV:83:PHE:O	2.39	0.54
74:L5:2573:A:N7	74:L5:2761:U:O4	2.40	0.54
74:L5:4745:G:H1	74:L5:4955:A:N6	2.04	0.54
24:LX:110:LYS:HG2	24:LX:114:LYS:HE2	1.88	0.54
73:S2:104:A:H62	73:S2:356:C:H5	1.55	0.54
73:S2:1744:G:H1'	73:S2:1790:A:H61	1.73	0.54
1:L7:3:C:H2'	1:L7:4:U:C6	2.43	0.54
9:LG:73:ARG:NE	74:L5:4076:G:OP1	2.31	0.54
26:LZ:4:PHE:HE1	29:Lc:67:ALA:HB2	1.71	0.54
28:Lb:90:SER:OG	74:L5:1266:G:N7	2.36	0.54
66:SY:114:MET:HG2	66:SY:122:LYS:HG2	1.89	0.54
73:S2:27:A:N1	73:S2:647:U:H5	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:3732:A:H2'	74:L5:3733:A:C8	2.42	0.54
80:SJ:107:GLU:HA	80:SJ:112:THR:HG21	1.88	0.54
46:SB:5:LYS:NZ	57:SO:65:ASP:OD2	2.40	0.54
46:SB:115:LYS:HZ1	73:S2:1869:A:H2'	1.72	0.54
51:SD:13:ALA:HA	51:SD:16:ILE:HG22	1.90	0.54
54:SK:65:ARG:NH2	70:Sd:21:CYS:O	2.40	0.54
74:L5:1961:G:H21	74:L5:2025:A:H62	1.56	0.54
51:SD:142:LEU:HD13	51:SD:150:MET:HE3	1.89	0.54
64:SV:58:ALA:O	64:SV:62:MET:HG3	2.07	0.54
20:LS:52:LYS:HB3	20:LS:54:MET:HE3	1.90	0.54
20:LS:138:ARG:HH21	20:LS:139:ARG:HH12	1.56	0.54
25:LY:43:ASN:OD1	25:LY:127:GLN:NE2	2.41	0.54
57:SO:122:SER:O	57:SO:122:SER:OG	2.23	0.54
73:S2:12:U:H2'	73:S2:13:C:C6	2.43	0.54
73:S2:515:G:O2'	73:S2:517:C:OP2	2.25	0.54
74:L5:2528:G:O6	87:L5:5401:HOH:O	2.18	0.54
38:LI:34:LYS:HE3	74:L5:361:C:H4'	1.90	0.54
45:SA:145:ILE:HG12	45:SA:159:ILE:HB	1.90	0.54
52:SE:192:ILE:HD13	52:SE:238:LEU:HD13	1.90	0.54
74:L5:3833:C:OP2	87:L5:5402:HOH:O	2.18	0.54
79:SZ:68:ILE:HB	79:SZ:109:TYR:HB2	1.90	0.54
74:L5:3770:PSU:H2'	74:L5:3771:C:C6	2.43	0.54
2:L8:148:A:H2'	2:L8:149:G:C8	2.43	0.53
4:LB:383:GLU:CD	4:LB:383:GLU:H	2.16	0.53
10:LH:76:HIS:O	10:LH:80:MET:HG3	2.08	0.53
11:LI:35:ASP:OD1	11:LI:86:HIS:NE2	2.41	0.53
16:LO:178:ARG:O	16:LO:182:GLU:HG2	2.09	0.53
53:SH:145:ARG:HA	65:SW:51:GLU:HG2	1.90	0.53
73:S2:223:C:H2'	73:S2:224:A:C8	2.43	0.53
73:S2:873:G:H2'	73:S2:874:G:C8	2.43	0.53
73:S2:1562:C:H2'	73:S2:1563:G:C8	2.43	0.53
74:L5:691:C:H2'	74:L5:692:A:C8	2.43	0.53
74:L5:3788:C:N4	74:L5:3812:C:OP2	2.39	0.53
15:LN:14:LYS:HE2	74:L5:280:G:H5''	1.89	0.53
60:SR:44:LYS:NZ	73:S2:1451:G:N7	2.55	0.53
73:S2:441:C:H2'	73:S2:442:C:C6	2.44	0.53
2:L8:96:C:H5''	34:Lh:66:LYS:HD3	1.90	0.53
39:Lm:111:ARG:NH2	74:L5:4699:U:OP2	2.41	0.53
44:Pt:16:C:H5'	44:Pt:60:A:C2	2.44	0.53
45:SA:6:ASP:HA	45:SA:9:GLN:HG2	1.89	0.53
45:SA:33:GLN:HB3	45:SA:154:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SW:3:ARG:NH1	65:SW:9:ASP:OD2	2.41	0.53
74:L5:1548:G:O2'	74:L5:2812:A:N3	2.34	0.53
74:L5:1577:G:O2'	74:L5:1612:G:H4'	2.08	0.53
74:L5:3917:A:H2'	74:L5:3918:G:H8	1.73	0.53
51:SD:212:GLU:HA	60:SR:19:LYS:HE2	1.91	0.53
73:S2:64:A:OP1	77:SG:136:LYS:NZ	2.42	0.53
73:S2:453:C:O2'	77:SG:92:ARG:O	2.18	0.53
74:L5:4967:A:H2'	74:L5:4968:A:H8	1.74	0.53
39:Lm:119:ASN:ND2	74:L5:1946:G:OP1	2.41	0.53
39:Lm:122:ARG:NH2	74:L5:4474:A:OP1	2.42	0.53
51:SD:172:VAL:HG22	51:SD:185:LYS:HG3	1.91	0.53
74:L5:1558:A:H2'	74:L5:1559:G:C8	2.43	0.53
26:LZ:69:LYS:NZ	74:L5:2577:C:OP2	2.42	0.53
29:Lc:58:SER:HB3	33:Lg:96:LEU:HD13	1.91	0.53
45:SA:33:GLN:NE2	64:SV:64:GLU:OE2	2.34	0.53
55:SL:133:PRO:O	73:S2:383:G:O2'	2.24	0.53
73:S2:491:C:O2'	73:S2:492:C:H5''	2.08	0.53
74:L5:1719:A:O2'	74:L5:1721:G:N7	2.35	0.53
66:SY:53:ASP:OD1	66:SY:53:ASP:N	2.41	0.53
73:S2:455:A:H2'	73:S2:456:C:C6	2.44	0.53
74:L5:673:C:H2'	74:L5:674:G:H8	1.73	0.53
15:LN:67:ARG:HD2	74:L5:2458:C:H5''	1.89	0.53
48:SF:123:GLU:HG2	48:SF:200:ALA:HB1	1.89	0.53
73:S2:1550:G:O2'	73:S2:1558:C:O2	2.25	0.53
74:L5:4741:C:H2'	74:L5:4950:U:C2	2.44	0.53
1:L7:47:G:OP1	6:LD:95:TYR:N	2.42	0.53
15:LN:172:ARG:NH1	74:L5:62:A:OP1	2.37	0.53
22:LV:34:ALA:HB2	22:LV:72:LEU:HD13	1.91	0.53
59:SQ:72:VAL:HG11	59:SQ:84:ILE:HD11	1.89	0.53
59:SQ:101:ASP:OD1	59:SQ:104:SER:N	2.30	0.53
73:S2:583:C:P	80:SJ:162:ARG:HH21	2.31	0.53
73:S2:1579:A:O2'	73:S2:1581:C:OP2	2.19	0.53
74:L5:1308:C:H2'	74:L5:1309:C:C6	2.44	0.53
2:L8:106:G:H4'	2:L8:137:A:H5'	1.91	0.53
31:Le:90:MET:HE3	43:Lr:113:ARG:HG3	1.90	0.53
36:Lj:13:ASN:ND2	74:L5:1618:G:OP1	2.41	0.53
52:SE:104:ASP:OD1	52:SE:108:ARG:N	2.35	0.53
62:ST:124:THR:OG1	62:ST:126:GLN:O	2.26	0.53
74:L5:1867:A:H2'	74:L5:1868:A:C8	2.44	0.53
74:L5:1956:A:H2'	74:L5:1957:U:C6	2.44	0.53
5:LC:328:LEU:HD22	8:LF:187:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LL:5:ARG:NH2	74:L5:1850:A:OP2	2.42	0.52
52:SE:27:PHE:O	73:S2:495:U:O2'	2.24	0.52
3:LA:101:VAL:HG22	3:LA:165:VAL:HG22	1.91	0.52
13:LL:92:ARG:NH1	74:L5:109:G:H5'	2.23	0.52
35:Li:51:ALA:HB3	35:Li:54:GLU:HG3	1.92	0.52
45:SA:3:GLY:H	45:SA:5:LEU:HD12	1.74	0.52
45:SA:89:LYS:HG3	45:SA:201:LEU:HD22	1.91	0.52
74:L5:2503:G:O4'	74:L5:4084:G:N2	2.42	0.52
74:L5:1307:A:H2'	74:L5:1308:C:C6	2.44	0.52
74:L5:4933:C:H2'	74:L5:4934:A:C8	2.44	0.52
8:LF:105:VAL:HG13	8:LF:136:VAL:HG12	1.91	0.52
72:Sg:251:ALA:HA	72:Sg:256:ILE:HA	1.92	0.52
73:S2:68:A:H62	73:S2:80:G:H1	1.56	0.52
73:S2:1588:A:O2'	73:S2:1589:A:OP2	2.24	0.52
73:S2:1693:G:N2	73:S2:1834:A:H8	2.07	0.52
74:L5:4415:A:H62	74:L5:4427:G:N2	2.06	0.52
67:SX:48:LYS:HE2	73:S2:483:C:H5''	1.91	0.52
69:Sc:18:LEU:HD12	69:Sc:29:GLN:HG2	1.92	0.52
74:L5:923:C:H2'	74:L5:924:C:C6	2.44	0.52
74:L5:1503:A:H4'	74:L5:1504:G:H5'	1.91	0.52
74:L5:1870:C:H2'	74:L5:1871:A2M:H8	1.89	0.52
74:L5:4239:A:H2'	74:L5:4240:G:C8	2.44	0.52
74:L5:4897:G:H2'	74:L5:4898:G:C8	2.44	0.52
78:LU:99:TRP:O	78:LU:115:PHE:N	2.36	0.52
7:LE:161:ARG:NH1	14:LM:106:ASP:OD1	2.41	0.52
12:LJ:17:ILE:HD11	12:LJ:20:LEU:HB2	1.92	0.52
27:La:115:GLY:O	27:La:136:LYS:NZ	2.40	0.52
53:SH:99:ARG:N	73:S2:913:A:N7	2.49	0.52
73:S2:317:C:H2'	73:S2:318:A:C8	2.44	0.52
73:S2:1609:C:H2'	73:S2:1610:G:H8	1.75	0.52
74:L5:1558:A:H2'	74:L5:1559:G:H8	1.74	0.52
74:L5:2090:U:H4'	74:L5:2091:C:H3'	1.92	0.52
75:Sa:87:ARG:HH12	75:Sa:94:ASP:HB3	1.74	0.52
8:LF:131:ASN:ND2	74:L5:1727:U:OP1	2.41	0.52
18:LQ:50:ARG:HA	18:LQ:53:MET:HG3	1.91	0.52
24:LX:47:ARG:NH1	74:L5:2504:C:OP2	2.42	0.52
74:L5:3723:A2M:H2'	74:L5:3724:A2M:H8	1.90	0.52
74:L5:4992:G:H2'	74:L5:4993:G:C8	2.45	0.52
78:LU:83:LEU:O	78:LU:87:THR:HG23	2.10	0.52
14:LM:11:ARG:HG2	14:LM:57:LEU:HD22	1.92	0.52
45:SA:8:LEU:HD11	64:SV:39:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SF:113:VAL:O	48:SF:117:ILE:HG12	2.10	0.52
52:SE:12:VAL:O	73:S2:812:A:O2'	2.26	0.52
52:SE:158:ASP:OD1	52:SE:175:PHE:N	2.41	0.52
53:SH:145:ARG:HE	65:SW:49:GLU:CD	2.18	0.52
56:SN:7:PRO:HD3	73:S2:996:A:H5''	1.90	0.52
73:S2:568:C:H2'	73:S2:569:A:C8	2.44	0.52
74:L5:2640:G:H2'	74:L5:2641:A:C8	2.45	0.52
74:L5:3603:G:N2	74:L5:3604:A:N1	2.57	0.52
74:L5:3770:PSU:H2'	74:L5:3771:C:H6	1.74	0.52
10:LH:44:GLU:OE2	14:LM:2:VAL:N	2.43	0.52
13:LL:257:ILE:O	13:LL:261:ARG:HG3	2.10	0.52
19:LR:136:ARG:O	19:LR:140:GLU:HG2	2.09	0.52
33:Lg:37:LYS:NZ	74:L5:2515:G:OP1	2.35	0.52
48:SF:110:GLN:NE2	48:SF:114:ASN:OD1	2.32	0.52
74:L5:506:C:H2'	74:L5:507:G:H8	1.75	0.52
74:L5:1759:G:N2	74:L5:1773:U:O2	2.42	0.52
4:LB:380:GLN:N	4:LB:384:GLU:OE1	2.41	0.52
20:LS:11:LYS:HD2	20:LS:29:ARG:HD2	1.91	0.52
29:Lc:38:ILE:HG21	29:Lc:63:TYR:HB3	1.92	0.52
70:Sd:17:GLY:N	73:S2:1262:C:O2	2.43	0.52
73:S2:520:A:O2'	73:S2:825:A:N3	2.42	0.52
73:S2:1114:U:O2'	73:S2:1116:C:OP2	2.20	0.52
24:LX:81:LEU:HG	24:LX:83:THR:HG23	1.92	0.51
73:S2:1405:A:H2'	73:S2:1406:G:O4'	2.10	0.51
74:L5:673:C:H2'	74:L5:674:G:C8	2.45	0.51
74:L5:3604:A:H2'	74:L5:3605:C:C6	2.44	0.51
74:L5:4274:A:H2'	74:L5:4275:G:H8	1.75	0.51
56:SN:87:ASP:OD1	56:SN:87:ASP:N	2.40	0.51
61:SS:67:VAL:O	61:SS:71:MET:HG3	2.11	0.51
1:L7:24:C:H2'	1:L7:25:G:O4'	2.09	0.51
46:SB:138:PHE:O	46:SB:213:ARG:N	2.43	0.51
48:SF:35:LEU:HD21	48:SF:146:ARG:HD3	1.92	0.51
73:S2:1470:C:H2'	73:S2:1471:C:H6	1.75	0.51
73:S2:1834:A:H2	73:S2:1837:G:N1	2.07	0.51
74:L5:2758:G:O2'	74:L5:2765:A:N3	2.35	0.51
74:L5:4227:OMU:HM21	74:L5:4336:A:H1'	1.92	0.51
13:LL:74:ARG:NH2	74:L5:109:G:OP2	2.42	0.51
26:LZ:48:ARG:NH2	74:L5:2575:U:OP1	2.43	0.51
59:SQ:44:PRO:HD3	59:SQ:77:HIS:HB3	1.93	0.51
59:SQ:58:LEU:HD11	59:SQ:112:LEU:HD11	1.92	0.51
73:S2:165:G:OP2	73:S2:165:G:N2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:S2:1144:A:H2'	73:S2:1145:A:C8	2.45	0.51
73:S2:1508:A:H2	73:S2:1510:G:H5'	1.74	0.51
74:L5:1942:A:H2'	74:L5:1943:A:C8	2.45	0.51
80:SJ:95:ASP:OD1	80:SJ:95:ASP:N	2.43	0.51
10:LH:151:ILE:O	10:LH:155:SER:OG	2.24	0.51
73:S2:398:A:H5''	73:S2:399:C:H3'	1.92	0.51
74:L5:93:G:H2'	74:L5:94:A:C8	2.46	0.51
74:L5:3910:C:H2'	74:L5:3911:C:C6	2.45	0.51
74:L5:4887:C:H42	74:L5:4932:U:H3	1.59	0.51
2:L8:45:C:H4'	38:L1:11:ARG:HD2	1.93	0.51
4:LB:246:ARG:NH2	74:L5:4525:C:OP1	2.42	0.51
7:LE:181:LEU:O	74:L5:4883:C:N4	2.39	0.51
73:S2:149:A:H3'	73:S2:150:A:H8	1.76	0.51
73:S2:1348:G:H22	73:S2:1381:G:H22	1.57	0.51
73:S2:1824:A:H2'	74:L5:3760:A:C6	2.46	0.51
74:L5:4504:C:H2'	74:L5:4505:C:C6	2.45	0.51
77:SG:136:LYS:NZ	77:SG:175:LYS:O	2.37	0.51
1:L7:3:C:H2'	1:L7:4:U:H6	1.76	0.51
23:LW:13:ILE:HG12	23:LW:32:LEU:HD13	1.93	0.51
26:LZ:68:ILE:O	26:LZ:115:LYS:NZ	2.32	0.51
74:L5:2411:C:H2'	74:L5:2412:A:C8	2.45	0.51
34:Lh:88:THR:OG1	34:Lh:91:MET:HG3	2.11	0.51
74:L5:1399:G:H2'	74:L5:1400:G:C8	2.45	0.51
74:L5:3783:A:OP2	74:L5:3808:OMC:N4	2.41	0.51
74:L5:4601:U:H2'	74:L5:4602:A:H8	1.76	0.51
79:SZ:103:HIS:HD1	79:SZ:105:ALA:H	1.59	0.51
5:LC:275:SER:OG	5:LC:276:ASN:N	2.43	0.51
14:LM:53:LYS:HD2	20:LS:160:ARG:NH2	2.26	0.51
46:SB:168:MET:O	46:SB:172:MET:HG3	2.11	0.51
53:SH:45:ILE:HG21	53:SH:62:ILE:HD11	1.93	0.51
73:S2:158:A:H2'	73:S2:159:A:O4'	2.10	0.51
73:S2:996:A:HO2'	73:S2:997:A:H8	1.59	0.51
73:S2:1533:A:H2	73:S2:1536:G:N3	2.09	0.51
11:LI:66:GLU:OE1	11:LI:69:ARG:NH2	2.44	0.50
42:Lp:36:LYS:HG2	42:Lp:48:LYS:HG3	1.92	0.50
57:SO:98:ARG:HB3	57:SO:132:VAL:HG23	1.92	0.50
73:S2:689:U:H5''	73:S2:690:G:H3'	1.92	0.50
4:LB:128:LYS:HG3	74:L5:4966:A:H5''	1.93	0.50
16:LO:4:VAL:HG12	16:LO:31:ARG:HH21	1.75	0.50
26:LZ:22:LYS:NZ	26:LZ:132:GLN:O	2.40	0.50
45:SA:32:PHE:CD1	73:S2:1097:G:H4'	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SC:259:THR:HG23	64:SV:16:LYS:HD3	1.92	0.50
73:S2:1244:U:H2'	73:S2:1245:G:H8	1.77	0.50
74:L5:1881:OMC:C2	74:L5:1881:OMC:HM23	2.47	0.50
79:SZ:86:ALA:O	79:SZ:90:GLU:HG3	2.10	0.50
18:LQ:42:THR:HA	18:LQ:45:GLN:HG3	1.94	0.50
58:SP:83:MET:HB3	58:SP:116:LEU:HD12	1.93	0.50
67:SX:53:GLU:HG2	67:SX:55:VAL:HG13	1.92	0.50
73:S2:1606:G:N2	73:S2:1632:G:H2'	2.27	0.50
74:L5:3727:A:H2'	74:L5:3728:A:C8	2.45	0.50
74:L5:4530:UR3:H2'	74:L5:4531:PSU:H2'	1.92	0.50
11:LI:133:GLN:NE2	74:L5:1785:C:OP1	2.39	0.50
34:Lh:9:LEU:HB3	34:Lh:17:LEU:HD21	1.94	0.50
73:S2:69:C:HO2'	73:S2:79:A:H61	1.58	0.50
74:L5:1833:G:N2	74:L5:1835:G:O4'	2.45	0.50
80:SJ:86:VAL:HG12	80:SJ:100:LEU:HD22	1.93	0.50
2:L8:67:U:H2'	2:L8:68:G:H8	1.77	0.50
53:SH:143:ARG:HD3	65:SW:53:ILE:HG12	1.93	0.50
57:SO:142:ARG:O	75:Sa:22:ARG:NH2	2.45	0.50
58:SP:122:THR:HG21	73:S2:1516:G:O3'	2.12	0.50
60:SR:126:MET:HG3	73:S2:1109:C:N3	2.27	0.50
61:SS:90:VAL:HG11	61:SS:113:ARG:HH12	1.77	0.50
74:L5:1332:C:H2'	74:L5:1333:A:H8	1.76	0.50
1:L7:110:G:H2'	1:L7:111:C:C6	2.47	0.50
20:LS:93:MET:SD	20:LS:95:ARG:NH1	2.85	0.50
74:L5:1771:U:H2'	74:L5:1772:C:H6	1.77	0.50
74:L5:3880:G:H2'	74:L5:3881:G:C8	2.47	0.50
2:L8:112:G:OP1	74:L5:2779:C:O2'	2.18	0.50
65:SW:18:GLU:HG2	65:SW:65:LEU:HD13	1.94	0.50
73:S2:113:G:N2	73:S2:293:C:O4'	2.45	0.50
73:S2:1457:U:H2'	73:S2:1458:G:H8	1.77	0.50
74:L5:25:A:H2'	74:L5:26:C:H6	1.77	0.50
74:L5:1326:A2M:OP2	74:L5:4445:U:O2'	2.28	0.50
74:L5:1756:U:H2'	74:L5:1757:U:H6	1.75	0.50
74:L5:4861:G:H2'	74:L5:4862:G:C8	2.47	0.50
27:La:47:LYS:NZ	74:L5:1684:A:OP1	2.45	0.50
30:Ld:61:ASP:OD2	30:Ld:63:ARG:NH1	2.45	0.50
43:Lr:92:SER:O	43:Lr:96:MET:HG3	2.11	0.50
60:SR:5:ARG:NH2	73:S2:1455:A:OP1	2.45	0.50
74:L5:717:U:H2'	74:L5:718:C:C6	2.47	0.50
74:L5:1475:G:H2'	74:L5:1476:C:C6	2.47	0.50
18:LQ:55:ARG:NH1	74:L5:1351:G:O6	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:4153:C:H2'	74:L5:4154:G:C8	2.45	0.50
46:SB:3:VAL:HG22	57:SO:63:LYS:HG2	1.93	0.49
76:S6:8:4SU:H6	76:S6:8:4SU:OP1	2.12	0.49
7:LE:153:LEU:HD21	7:LE:195:ILE:HD12	1.94	0.49
21:LT:17:ARG:HB2	21:LT:22:HIS:CE1	2.47	0.49
31:Le:104:SER:HB3	74:L5:2303:C:H5''	1.93	0.49
73:S2:873:G:H2'	73:S2:874:G:H8	1.76	0.49
74:L5:910:G:H2'	74:L5:911:U:C6	2.47	0.49
74:L5:910:G:H2'	74:L5:911:U:H6	1.76	0.49
39:Lm:124:LYS:HD2	74:L5:4474:A:P	2.52	0.49
74:L5:2671:C:H2'	74:L5:2672:C:C6	2.48	0.49
74:L5:4570:G:H2'	74:L5:4571:A2M:H8	1.92	0.49
76:S6:12:G:H2'	76:S6:13:C:H6	1.76	0.49
1:L7:58:A:H2'	1:L7:59:G:C8	2.48	0.49
20:LS:173:ASN:ND2	20:LS:175:PHE:O	2.46	0.49
58:SP:24:GLN:O	58:SP:28:MET:HB2	2.13	0.49
73:S2:1180:C:H2'	73:S2:1181:A:C8	2.47	0.49
73:S2:1232:U:H2'	73:S2:1233:G:C8	2.46	0.49
73:S2:1607:A:H61	73:S2:1632:G:H1'	1.77	0.49
10:LH:59:LYS:HE2	10:LH:66:GLU:HG3	1.94	0.49
17:LP:107:LEU:HD12	17:LP:152:GLU:CD	2.38	0.49
19:LR:4:LEU:HB2	74:L5:2386:U:H5'	1.93	0.49
21:LT:109:VAL:HG22	74:L5:1803:G:C6	2.46	0.49
73:S2:804:U:H2'	73:S2:805:U:C6	2.48	0.49
73:S2:1731:A:H2'	73:S2:1732:G:C8	2.48	0.49
74:L5:711:A:H2'	74:L5:712:C:C6	2.47	0.49
74:L5:1818:G:O2'	74:L5:1820:C:OP2	2.24	0.49
2:L8:140:C:H2'	2:L8:141:C:C6	2.48	0.49
7:LE:51:VAL:HG12	7:LE:54:ILE:HB	1.92	0.49
16:LO:191:LYS:O	16:LO:195:VAL:HG23	2.13	0.49
46:SB:114:VAL:O	73:S2:1869:A:N6	2.45	0.49
58:SP:108:LYS:HE2	58:SP:111:MET:HE3	1.94	0.49
73:S2:1822:A:H2'	73:S2:1823:A:C8	2.48	0.49
73:S2:1834:A:H2	73:S2:1837:G:H1	1.59	0.49
74:L5:3684:G:H2'	74:L5:3685:C:C6	2.47	0.49
74:L5:4861:G:H2'	74:L5:4862:G:H8	1.78	0.49
77:SG:35:GLU:OE2	77:SG:35:GLU:N	2.45	0.49
42:Lp:4:ARG:NH1	74:L5:1555:G:O6	2.40	0.49
46:SB:229:MET:SD	46:SB:229:MET:N	2.85	0.49
48:SF:123:GLU:OE2	69:Sc:63:ARG:NH2	2.41	0.49
57:SO:53:ILE:HG22	57:SO:54:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67: SX:129: SER: HB3	73: S2:29: G: H4'	1.95	0.49
73: S2:1272: C: H2'	73: S2:1273: C: H5''	1.94	0.49
1: L7:19: C: H2'	1: L7:20: U: C6	2.47	0.49
11: LI:38: ARG: HG2	11: LI:41: ALA: HB2	1.94	0.49
11: LI:59: GLN: NE2	87: LI:401: HOH: O	2.46	0.49
73: S2:1098: C: H2'	73: S2:1099: G: C8	2.48	0.49
73: S2:1414: A: N7	73: S2:1429: G: N2	2.56	0.49
73: S2:1550: G: H3'	73: S2:1579: A: H61	1.77	0.49
74: L5:1400: G: H2'	74: L5:1401: C: H6	1.78	0.49
74: L5:2588: C: OP1	74: L5:2768: C: O2'	2.27	0.49
74: L5:5030: U: H2'	74: L5:5031: G: H8	1.77	0.49
10: LH:89: ARG: HD3	10: LH:91: LYS: HE3	1.94	0.49
15: LN:10: LEU: HG	35: Li:44: ILE: HD12	1.93	0.49
56: SN:20: ARG: NE	73: S2:919: A: OP1	2.41	0.49
66: SY:10: ARG: N	66: SY:24: VAL: O	2.45	0.49
73: S2:15: U: H2'	73: S2:16: G: O4'	2.13	0.49
74: L5:919: C: H2'	74: L5:920: C: C6	2.48	0.49
74: L5:1662: C: H2'	74: L5:1663: C: C6	2.48	0.49
80: SJ:81: LEU: HD12	80: SJ:97: ILE: HG12	1.94	0.49
80: SJ:111: GLN: NE2	80: SJ:127: ARG: HB2	2.28	0.49
10: LH:93: ARG: NH1	10: LH:143: GLU: OE1	2.32	0.49
61: SS:38: ARG: HB3	62: ST:45: LEU: HD11	1.94	0.49
73: S2:145: G: H2'	73: S2:146: G: C8	2.48	0.49
73: S2:952: G: H2'	73: S2:953: C: C6	2.48	0.49
74: L5:3720: G: H1	74: L5:3733: A: H61	1.60	0.49
74: L5:3911: C: H2'	74: L5:3912: U: H6	1.78	0.49
4: LB:50: LYS: HB2	4: LB:345: LEU: HD11	1.95	0.48
53: SH:63: PHE: HA	53: SH:95: ILE: O	2.13	0.48
73: S2:218: U: H2'	73: S2:219: U: C6	2.48	0.48
73: S2:561: A: O2'	80: SJ:134: HIS: NE2	2.35	0.48
73: S2:1052: A: H4'	74: L5:3700: C: OP1	2.13	0.48
74: L5:4378: A: O2'	74: L5:4379: A: H2'	2.12	0.48
78: LU:87: THR: O	78: LU:91: LEU: HG	2.13	0.48
80: SJ:24: ARG: O	80: SJ:28: GLU: HG3	2.13	0.48
38: LI:10: LYS: NZ	74: L5:2782: U: OP2	2.44	0.48
72: Sg:215: GLN: HA	72: Sg:231: ASP: HA	1.96	0.48
73: S2:318: A: C2	73: S2:333: G: N1	2.67	0.48
74: L5:654: C: H2'	74: L5:655: C: C6	2.49	0.48
74: L5:3731: C: H2'	74: L5:3732: A: C8	2.48	0.48
6: LD:95: TYR: HA	87: LD:302: HOH: O	2.13	0.48
12: LJ:68: ILE: HD11	74: L5:4258: C: H5'	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LY:77:LYS:HB2	25:LY:79:VAL:HG22	1.94	0.48
44:Pt:24:C:H2'	44:Pt:25:U:C6	2.48	0.48
61:SS:121:ARG:NH1	73:S2:1610:G:OP1	2.45	0.48
62:ST:11:GLN:OE1	62:ST:62:ARG:NH1	2.40	0.48
65:SW:20:ARG:HD2	73:S2:1095:U:O3'	2.12	0.48
66:SY:55:ILE:O	66:SY:94:HIS:NE2	2.33	0.48
73:S2:1712:A:H2'	73:S2:1713:C:C6	2.48	0.48
74:L5:1414:C:H2'	74:L5:1415:G:H8	1.78	0.48
75:Sa:66:LYS:HB3	75:Sa:68:TYR:CE1	2.48	0.48
7:LE:74:SER:O	7:LE:74:SER:OG	2.28	0.48
11:LI:87:ILE:HG12	11:LI:138:ILE:HG12	1.95	0.48
15:LN:46:ASP:OD1	15:LN:50:ARG:NH2	2.46	0.48
53:SH:64:VAL:O	53:SH:97:GLN:N	2.37	0.48
55:SL:67:SER:OG	73:S2:114:G:OP2	2.31	0.48
58:SP:123:TYR:OH	61:SS:124:ARG:NH1	2.46	0.48
73:S2:566:U:O2	73:S2:584:G:N2	2.34	0.48
73:S2:929:G:H2'	73:S2:930:C:O4'	2.13	0.48
73:S2:1642:U:O2'	73:S2:1643:U:H5'	2.13	0.48
74:L5:752:G:O6	74:L5:911:U:C4	2.66	0.48
74:L5:2550:G:O2'	74:L5:2587:A:N1	2.45	0.48
74:L5:4188:U:H2'	74:L5:4189:U:C6	2.48	0.48
74:L5:4637:OMG:H2'	74:L5:4638:U:C6	2.48	0.48
74:L5:4887:C:N4	74:L5:4932:U:H3	2.11	0.48
12:LJ:141:ILE:HA	12:LJ:144:LYS:HG2	1.95	0.48
28:Lb:26:SER:O	74:L5:1805:A:N6	2.32	0.48
44:Pt:15:G:N2	44:Pt:49:C:O2	2.43	0.48
73:S2:942:G:H2'	73:S2:943:U:C6	2.48	0.48
73:S2:955:A:N1	73:S2:968:U:O2'	2.47	0.48
73:S2:1244:U:H2'	73:S2:1245:G:C8	2.49	0.48
73:S2:1845:A:H2'	73:S2:1846:G:C8	2.48	0.48
74:L5:2411:C:H2'	74:L5:2412:A:H8	1.78	0.48
76:S6:3:C:H2'	76:S6:4:G:C8	2.49	0.48
10:LH:92:MET:HB3	10:LH:179:ILE:HG22	1.95	0.48
47:SC:191:VAL:HG11	47:SC:236:PHE:HA	1.95	0.48
73:S2:1177:U:H2'	73:S2:1178:U:C6	2.49	0.48
73:S2:1839:U:H2'	73:S2:1840:U:C6	2.49	0.48
74:L5:2539:C:H2'	74:L5:2540:C:C6	2.48	0.48
74:L5:4258:C:H2'	74:L5:4259:C:C6	2.48	0.48
74:L5:5006:U:H4'	74:L5:5007:A:H5'	1.95	0.48
78:LU:48:LYS:HE2	78:LU:48:LYS:HB3	1.66	0.48
79:SZ:58:LEU:O	79:SZ:62:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LE:59:ARG:HD2	74:L5:1238:A:C8	2.49	0.48
13:LL:261:ARG:HA	13:LL:264:GLU:HB3	1.95	0.48
58:SP:48:GLY:O	58:SP:50:ARG:NH1	2.47	0.48
72:Sg:241:PHE:HA	72:Sg:248:LEU:HA	1.95	0.48
74:L5:911:U:H2'	74:L5:912:G:O4'	2.14	0.48
74:L5:2589:C:HO2'	74:L5:2767:U:HO2'	1.57	0.48
74:L5:4537:C:H2'	74:L5:4538:G:C8	2.48	0.48
57:SO:135:ILE:O	73:S2:943:U:O2'	2.32	0.48
73:S2:5:U:H2'	73:S2:6:G:H8	1.77	0.48
73:S2:1345:G:OP1	73:S2:1688:C:O2'	2.31	0.48
74:L5:2607:C:H2'	74:L5:2608:G:H8	1.78	0.48
7:LE:51:VAL:HG21	74:L5:947:C:H5''	1.96	0.48
12:LJ:32:ARG:HE	12:LJ:126:TYR:HE1	1.60	0.48
16:LO:125:LYS:HG3	16:LO:129:LEU:HD22	1.95	0.48
25:LY:10:ASP:HB3	25:LY:13:LYS:HB2	1.94	0.48
31:Le:90:MET:HG3	43:Lr:33:LYS:HA	1.96	0.48
61:SS:15:VAL:HG22	61:SS:68:ILE:HD11	1.96	0.48
73:S2:338:A:H2'	73:S2:339:A:C8	2.49	0.48
74:L5:1333:A:H2'	74:L5:1334:A:C8	2.49	0.48
74:L5:1846:G:H2'	74:L5:1847:C:C6	2.49	0.48
74:L5:2664:G:H4'	74:L5:2677:G:H4'	1.96	0.48
74:L5:4076:G:OP2	74:L5:4163:U:N3	2.44	0.48
74:L5:4427:G:O2'	74:L5:4428:A:OP2	2.28	0.48
1:L7:17:C:H2'	1:L7:18:C:C6	2.48	0.48
6:LD:11:ALA:HB1	74:L5:1743:A:H5'	1.95	0.48
16:LO:78:ARG:HD2	16:LO:78:ARG:HA	1.63	0.48
26:LZ:9:LYS:HB3	26:LZ:25:ILE:HD12	1.96	0.48
44:Pt:68:C:H2'	44:Pt:69:C:C6	2.49	0.48
61:SS:5:ILE:HG13	61:SS:6:PRO:HD2	1.94	0.48
64:SV:40:ASP:HB3	64:SV:43:THR:HG23	1.95	0.48
73:S2:113:G:N2	73:S2:293:C:O5'	2.46	0.48
74:L5:464:G:H2'	74:L5:465:G:C8	2.47	0.48
74:L5:1278:C:H2'	74:L5:1279:A:O4'	2.14	0.48
74:L5:4238:G:H2'	74:L5:4239:A:C8	2.49	0.48
74:L5:4934:A:H2'	74:L5:4935:C:H6	1.79	0.48
7:LE:188:ARG:NH2	74:L5:4941:G:OP2	2.41	0.47
14:LM:90:ARG:HH21	74:L5:4868:G:H4'	1.79	0.47
15:LN:104:GLU:HA	15:LN:160:GLU:HG3	1.96	0.47
18:LQ:65:ARG:NH1	74:L5:1459:A:OP1	2.44	0.47
45:SA:77:ILE:HG12	45:SA:99:ILE:HB	1.96	0.47
58:SP:115:TYR:OH	73:S2:1620:A:OP1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SS:51:ASP:OD1	61:SS:51:ASP:N	2.45	0.47
73:S2:338:A:H2'	73:S2:339:A:H8	1.79	0.47
73:S2:1061:U:OP1	87:S2:2002:HOH:O	2.20	0.47
73:S2:1457:U:H2'	73:S2:1458:G:C8	2.49	0.47
74:L5:3736:A:H2'	74:L5:3737:A:C8	2.48	0.47
2:L8:19:C:H2'	2:L8:20:A:C8	2.49	0.47
14:LM:53:LYS:HE2	74:L5:1923:A:H5''	1.96	0.47
47:SC:238:LYS:NZ	73:S2:1355:C:O3'	2.46	0.47
56:SN:130:LYS:NZ	56:SN:139:TRP:O	2.27	0.47
73:S2:1204:A:H2'	73:S2:1205:C:O4'	2.14	0.47
74:L5:704:C:O2'	74:L5:706:C:OP2	2.20	0.47
74:L5:4392:OMG:H2'	74:L5:4447:5MC:HM51	1.95	0.47
74:L5:4993:G:N2	74:L5:5058:A:N1	2.55	0.47
5:LC:182:LYS:HG2	5:LC:204:ARG:HD3	1.96	0.47
27:La:35:ALA:HB1	74:L5:39:A:H5''	1.96	0.47
47:SC:130:ILE:HG23	47:SC:162:ILE:HD11	1.96	0.47
64:SV:1:MET:HE2	64:SV:13:VAL:HG22	1.96	0.47
64:SV:68:SER:O	64:SV:72:LEU:HG	2.14	0.47
69:Sc:6:VAL:HG23	69:Sc:8:PRO:HD3	1.94	0.47
73:S2:1201:U:H2'	73:S2:1202:U:C6	2.48	0.47
80:SJ:136:ARG:HD3	80:SJ:160:SER:HA	1.96	0.47
2:L8:141:C:H2'	2:L8:142:U:C6	2.49	0.47
73:S2:1037:G:H4'	73:S2:1845:A:H4'	1.96	0.47
73:S2:1692:U:H2'	73:S2:1693:G:C8	2.50	0.47
74:L5:1733:G:N3	74:L5:4214:A:H2'	2.29	0.47
74:L5:4192:A:H2'	74:L5:4193:C:H6	1.78	0.47
74:L5:4737:G:N2	87:L5:5549:HOH:O	2.47	0.47
74:L5:4993:G:H1	74:L5:5058:A:N6	2.11	0.47
2:L8:26:C:O2'	5:LC:53:ALA:O	2.29	0.47
10:LH:93:ARG:HD2	10:LH:143:GLU:OE1	2.14	0.47
34:Lh:40:ALA:HB3	34:Lh:43:LYS:HE3	1.96	0.47
45:SA:40:LYS:HD3	45:SA:40:LYS:HA	1.66	0.47
52:SE:100:ARG:NH2	52:SE:121:TYR:O	2.44	0.47
53:SH:160:LYS:HA	53:SH:163:GLN:HG3	1.96	0.47
58:SP:118:GLU:O	61:SS:120:HIS:N	2.46	0.47
64:SV:30:ALA:O	64:SV:60:ARG:HD3	2.14	0.47
71:Se:109:ARG:NH2	73:S2:527:C:OP2	2.42	0.47
73:S2:388:U:H2'	73:S2:389:A:C8	2.50	0.47
73:S2:495:U:H2'	73:S2:496:C:O4'	2.14	0.47
73:S2:1171:G:O2'	73:S2:1187:G:O6	2.30	0.47
74:L5:5066:U:H2'	74:L5:5067:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LB:104:THR:OG1	74:L5:4724:A:O2'	2.21	0.47
17:LP:52:THR:HG23	17:LP:85:LYS:HG3	1.96	0.47
26:LZ:51:ARG:NH2	74:L5:2756:G:N7	2.63	0.47
55:SL:42:LEU:HD21	73:S2:292:A:OP2	2.15	0.47
58:SP:37:TYR:HB3	58:SP:41:GLN:HB2	1.95	0.47
66:SY:55:ILE:HG13	66:SY:75:ILE:HG23	1.95	0.47
73:S2:1232:U:H2'	73:S2:1233:G:H8	1.79	0.47
73:S2:1597:C:OP2	79:SZ:85:ARG:NH2	2.45	0.47
74:L5:4322:G:N2	74:L5:4325:A:OP2	2.43	0.47
74:L5:4638:U:H2'	74:L5:4639:G:N3	2.29	0.47
74:L5:4866:C:H2'	74:L5:4867:G:H8	1.80	0.47
79:SZ:84:ALA:O	79:SZ:88:LEU:HG	2.13	0.47
3:LA:37:ARG:NH2	74:L5:4088:C:OP1	2.38	0.47
4:LB:168:MET:HA	4:LB:171:LEU:HD12	1.97	0.47
5:LC:149:GLU:HG3	43:Lr:72:LYS:HG2	1.97	0.47
5:LC:298:ILE:O	5:LC:302:LEU:HG	2.14	0.47
5:LC:353:LYS:HB3	5:LC:353:LYS:HE2	1.62	0.47
10:LH:93:ARG:HG2	10:LH:182:SER:HB3	1.97	0.47
15:LN:178:HIS:HA	15:LN:181:HIS:NE2	2.29	0.47
26:LZ:104:PRO:HB2	26:LZ:108:ARG:NH2	2.29	0.47
46:SB:47:THR:OG1	46:SB:65:ARG:NH1	2.47	0.47
47:SC:116:THR:OG1	47:SC:119:GLY:O	2.26	0.47
51:SD:18:LYS:HE2	51:SD:39:VAL:HG22	1.97	0.47
73:S2:1007:C:H2'	73:S2:1008:A:C8	2.50	0.47
74:L5:1320:U:O2'	74:L5:1891:A:N1	2.35	0.47
74:L5:1468:C:H2'	74:L5:1469:C:C6	2.50	0.47
74:L5:2474:G:N2	74:L5:2502:G:H2'	2.29	0.47
74:L5:3923:A:H2'	74:L5:3924:C:C6	2.49	0.47
74:L5:4260:U:H2'	74:L5:4261:C:C6	2.49	0.47
74:L5:4600:G:O2'	74:L5:4609:G:O6	2.23	0.47
74:L5:4768:G:H2'	74:L5:4769:G:C8	2.50	0.47
80:SJ:116:LYS:HB3	80:SJ:116:LYS:HE2	1.82	0.47
49:SI:22:HIS:HB3	73:S2:433:A:H5''	1.96	0.47
73:S2:1025:U:H2'	73:S2:1026:C:O4'	2.15	0.47
74:L5:3911:C:H2'	74:L5:3912:U:C6	2.50	0.47
74:L5:5004:C:H2'	74:L5:5005:G:O4'	2.14	0.47
7:LE:258:LEU:HG	7:LE:262:LYS:HE3	1.95	0.47
15:LN:159:ARG:HB3	15:LN:164:LEU:HB2	1.96	0.47
17:LP:107:LEU:HD12	17:LP:152:GLU:OE1	2.15	0.47
32:Lf:83:MET:HE3	32:Lf:83:MET:HB3	1.85	0.47
42:Lp:69:TRP:HH2	74:L5:2739:C:H5''	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SI:23:LYS:HE2	49:SI:23:LYS:HB3	1.65	0.47
62:ST:42:HIS:HB3	62:ST:83:GLN:HB2	1.97	0.47
73:S2:1407:U:H2'	73:S2:1408:U:C6	2.50	0.47
74:L5:4905:C:H2'	74:L5:4906:C:C6	2.50	0.47
78:LU:102:VAL:HG12	78:LU:110:TYR:HB3	1.96	0.47
1:L7:92:C:H2'	1:L7:93:G:C8	2.50	0.47
7:LE:252:ALA:O	7:LE:256:GLN:NE2	2.37	0.47
16:LO:54:TYR:OH	16:LO:73:PHE:O	2.32	0.47
34:Lh:22:ASP:O	34:Lh:26:VAL:HG23	2.14	0.47
45:SA:122:LEU:HB3	45:SA:144:THR:HG22	1.96	0.47
47:SC:168:GLY:N	47:SC:179:THR:O	2.37	0.47
56:SN:132:LYS:HD3	56:SN:132:LYS:HA	1.72	0.47
67:SX:132:ALA:HB1	67:SX:138:LYS:HD3	1.96	0.47
74:L5:654:C:H2'	74:L5:655:C:H6	1.80	0.47
74:L5:1617:G:H1'	74:L5:2513:A:N6	2.30	0.47
74:L5:1764:G:O6	74:L5:1765:A:N6	2.48	0.47
74:L5:1806:G:H2'	74:L5:1807:C:C6	2.50	0.47
74:L5:1968:G:H2'	74:L5:1969:G:C8	2.50	0.47
17:LP:54:GLN:HA	17:LP:83:TRP:CD1	2.50	0.46
26:LZ:62:ILE:O	26:LZ:66:SER:OG	2.31	0.46
48:SF:78:MET:HE3	48:SF:78:MET:HB2	1.80	0.46
61:SS:14:ARG:HH12	61:SS:19:ASN:CG	2.23	0.46
67:SX:107:ARG:HB3	67:SX:110:HIS:HB3	1.98	0.46
73:S2:51:U:H2'	73:S2:52:G:C8	2.50	0.46
74:L5:3873:G:H2'	74:L5:3874:G:C8	2.50	0.46
3:LA:166:VAL:HG13	42:Lp:83:ILE:HD12	1.97	0.46
10:LH:95:VAL:HG22	39:Lm:82:LEU:HB3	1.97	0.46
12:LJ:20:LEU:HD13	12:LJ:132:VAL:HG22	1.97	0.46
21:LT:142:ARG:NH1	74:L5:1089:G:O3'	2.49	0.46
29:Lc:43:ALA:O	29:Lc:69:THR:OG1	2.26	0.46
47:SC:169:TYR:CD2	47:SC:173:LYS:HA	2.49	0.46
74:L5:4591:U:H2'	74:L5:4592:C:C6	2.50	0.46
75:Sa:49:ALA:O	75:Sa:53:ILE:HG12	2.15	0.46
16:LO:51:LYS:HA	16:LO:141:LEU:HD21	1.97	0.46
22:LV:109:LYS:HA	22:LV:109:LYS:HD2	1.68	0.46
46:SB:124:HIS:HA	46:SB:137:LEU:O	2.16	0.46
53:SH:162:GLN:O	53:SH:166:VAL:HG22	2.15	0.46
73:S2:656:G:H5'	73:S2:662:G:N2	2.30	0.46
73:S2:1693:G:H21	73:S2:1834:A:H8	1.62	0.46
74:L5:424:U:H2'	74:L5:425:U:C6	2.50	0.46
74:L5:1408:G:N2	74:L5:1409:C:N3	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:4174:U:H2'	74:L5:4175:G:H8	1.81	0.46
74:L5:4935:C:H2'	74:L5:4936:G:C8	2.50	0.46
78:LU:88:LYS:HG2	78:LU:97:ARG:NH1	2.31	0.46
16:LO:87:MET:HE2	74:L5:1912:G:N2	2.30	0.46
19:LR:136:ARG:NH2	74:L5:2895:A:O3'	2.49	0.46
24:LX:104:ALA:O	24:LX:134:LYS:NZ	2.43	0.46
46:SB:52:THR:HG23	46:SB:57:ILE:HA	1.98	0.46
52:SE:45:ILE:HG13	52:SE:61:VAL:HG21	1.96	0.46
58:SP:50:ARG:H	58:SP:53:GLN:HG3	1.80	0.46
59:SQ:58:LEU:HD21	59:SQ:108:ILE:HG23	1.97	0.46
73:S2:609:U:H2'	73:S2:610:G:C8	2.50	0.46
74:L5:410:A:OP2	87:L5:5403:HOH:O	2.21	0.46
44:Pt:45:A:H2'	44:Pt:46:G:C8	2.50	0.46
71:Se:100:LYS:HE2	73:S2:593:C:H4'	1.96	0.46
73:S2:5:U:H2'	73:S2:6:G:C8	2.50	0.46
74:L5:1332:C:H2'	74:L5:1333:A:C8	2.50	0.46
74:L5:2864:A:H2'	74:L5:2865:U:C6	2.50	0.46
46:SB:110:MET:HA	46:SB:113:MET:HE2	1.97	0.46
49:SI:184:ARG:NH2	73:S2:303:C:O2	2.28	0.46
51:SD:109:LEU:HD11	51:SD:115:VAL:HG22	1.97	0.46
57:SO:61:LYS:HA	57:SO:61:LYS:HD2	1.84	0.46
73:S2:1452:A:H5'	73:S2:1453:C:C6	2.50	0.46
73:S2:1727:G:H2'	73:S2:1728:U:C6	2.51	0.46
74:L5:1771:U:H2'	74:L5:1772:C:C6	2.50	0.46
74:L5:2538:U:H2'	74:L5:2539:C:C6	2.51	0.46
11:LI:22:PHE:CZ	74:L5:1788:A:H2'	2.50	0.46
13:LL:64:VAL:HG13	74:L5:71:C:H5'	1.98	0.46
42:Lp:51:ALA:HB3	42:Lp:54:ILE:HD12	1.97	0.46
64:SV:32:ILE:HG12	64:SV:60:ARG:HD2	1.97	0.46
73:S2:346:C:H2'	73:S2:347:G:O4'	2.16	0.46
74:L5:2079:G:H2'	74:L5:2080:U:C6	2.51	0.46
1:L7:54:A:H1'	12:LJ:13:ARG:HG2	1.98	0.46
13:LL:257:ILE:HD12	13:LL:260:LYS:HB3	1.98	0.46
48:SF:84:GLY:O	73:S2:1673:U:O2'	2.30	0.46
55:SL:136:LYS:HB2	73:S2:385:G:H3'	1.98	0.46
62:ST:123:LEU:HD21	62:ST:131:LEU:HD22	1.97	0.46
67:SX:45:SER:OG	67:SX:46:HIS:ND1	2.44	0.46
74:L5:2673:G:N3	74:L5:2673:G:H5'	2.31	0.46
74:L5:3848:U:H2'	74:L5:3849:A:C8	2.50	0.46
7:LE:276:ALA:HB1	32:Lf:3:GLY:HA3	1.98	0.46
17:LP:18:ARG:HG2	74:L5:399:G:H4'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LW:48:GLN:OE1	74:L5:3615:G:H5''	2.16	0.46
52:SE:88:ASP:HB2	52:SE:101:LEU:HD12	1.97	0.46
66:SY:82:ALA:O	66:SY:86:GLU:HB2	2.16	0.46
73:S2:69:C:O2'	73:S2:79:A:N6	2.36	0.46
73:S2:955:A:N3	73:S2:956:G:H1'	2.31	0.46
74:L5:1461:C:H2'	74:L5:1462:A:C8	2.51	0.46
74:L5:3917:A:H2'	74:L5:3918:G:C8	2.49	0.46
74:L5:4912:G:H5'	74:L5:4913:G:H5''	1.98	0.46
27:La:3:SER:HA	27:La:6:ARG:HG3	1.97	0.46
31:Le:82:VAL:O	31:Le:86:GLU:HG2	2.16	0.46
32:Lf:71:TRP:HB2	32:Lf:89:ARG:NH1	2.30	0.46
42:Lp:24:LYS:NZ	73:S2:1180:C:OP1	2.38	0.46
44:Pt:44:A:H2'	44:Pt:45:A:C8	2.51	0.46
51:SD:106:ARG:HD2	51:SD:175:VAL:HB	1.98	0.46
66:SY:62:THR:HA	66:SY:69:THR:HA	1.98	0.46
73:S2:1354:G:N2	73:S2:1357:A:OP2	2.39	0.46
74:L5:2685:C:H2'	74:L5:2686:G:O4'	2.16	0.46
74:L5:4522:G:O2'	74:L5:4525:C:OP2	2.27	0.46
77:SG:28:TYR:HE2	77:SG:104:ALA:HB2	1.81	0.46
2:L8:5:U:H2'	2:L8:6:C:H6	1.81	0.45
22:LV:107:ASN:OD1	22:LV:111:GLU:HG2	2.16	0.45
39:Lm:103:LEU:HD11	39:Lm:110:CYS:HA	1.98	0.45
45:SA:185:MET:HG3	45:SA:191:ARG:HH21	1.80	0.45
66:SY:33:ALA:HB2	73:S2:582:C:H1'	1.97	0.45
74:L5:62:A:N3	74:L5:77:U:O2'	2.39	0.45
74:L5:1298:C:H2'	74:L5:1299:G:H8	1.80	0.45
74:L5:2273:G:H2'	74:L5:2274:C:C6	2.52	0.45
74:L5:2461:G:H2'	74:L5:2462:C:C6	2.50	0.45
74:L5:3705:G:H2'	74:L5:3706:C:C6	2.51	0.45
74:L5:4345:C:H2'	74:L5:4346:U:C6	2.51	0.45
12:LJ:103:GLY:HA3	12:LJ:157:ILE:HG22	1.98	0.45
25:LY:31:SER:HA	25:LY:48:PRO:HA	1.98	0.45
28:Lb:95:ARG:HG3	74:L5:1266:G:C8	2.51	0.45
37:Lk:2:PRO:HD2	74:L5:2642:A:C2	2.51	0.45
39:Lm:109:ASN:HD22	74:L5:1947:U:H2'	1.81	0.45
44:Pt:8:4SU:H5''	44:Pt:50:G:OP2	2.16	0.45
47:SC:194:ARG:HD3	47:SC:196:ILE:HD11	1.98	0.45
58:SP:111:MET:HG2	58:SP:119:PHE:CZ	2.51	0.45
73:S2:1116:C:H2'	73:S2:1117:C:C6	2.52	0.45
74:L5:677:G:H2'	74:L5:678:C:C6	2.51	0.45
74:L5:1404:G:H2'	74:L5:1405:C:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:3848:U:H2'	74:L5:3849:A:H8	1.82	0.45
3:LA:204:MET:HG2	74:L5:1631:A:C2	2.51	0.45
7:LE:110:ARG:HH12	74:L5:2259:G:N2	2.14	0.45
12:LJ:13:ARG:O	12:LJ:136:ARG:NH1	2.44	0.45
16:LO:159:LYS:HB3	16:LO:159:LYS:HE2	1.72	0.45
66:SY:47:MET:HE3	66:SY:47:MET:HB2	1.82	0.45
72:Sg:254:PRO:HA	72:Sg:285:GLN:HA	1.98	0.45
74:L5:2547:G:H2'	74:L5:2548:C:C6	2.51	0.45
76:S6:53:G:N1	76:S6:64:G:O6	2.50	0.45
7:LE:161:ARG:O	7:LE:182:ASN:ND2	2.50	0.45
26:LZ:78:ASN:OD1	26:LZ:78:ASN:N	2.50	0.45
30:Ld:91:LYS:HG3	30:Ld:103:TYR:CE1	2.51	0.45
34:Lh:82:ASP:OD1	34:Lh:82:ASP:N	2.48	0.45
35:Li:38:LYS:HB3	35:Li:38:LYS:HE2	1.68	0.45
51:SD:161:GLY:HA3	73:S2:1388:A:H61	1.82	0.45
74:L5:2505:C:N4	74:L5:4084:G:H4'	2.31	0.45
74:L5:4738:C:H2'	74:L5:4739:C:H6	1.82	0.45
74:L5:5031:G:H2'	74:L5:5032:C:C6	2.51	0.45
80:SJ:18:ARG:O	80:SJ:24:ARG:NH1	2.49	0.45
14:LM:113:MET:HE3	74:L5:4881:U:C2	2.51	0.45
29:Lc:47:ILE:HB	29:Lc:94:LEU:HG	1.99	0.45
41:Lo:35:ALA:O	41:Lo:39:ARG:HG3	2.17	0.45
58:SP:34:MET:HE2	58:SP:45:LEU:HB3	1.99	0.45
74:L5:2424:OMG:HM22	74:L5:2426:U:C6	2.52	0.45
3:LA:108:PRO:HD3	42:Lp:90:LYS:HE2	1.99	0.45
5:LC:323:ARG:HB2	74:L5:1281:G:H5'	1.99	0.45
17:LP:6:LEU:HD12	17:LP:116:HIS:ND1	2.32	0.45
29:Lc:29:LEU:HD13	29:Lc:91:VAL:HG21	1.99	0.45
73:S2:581:U:OP1	80:SJ:133:ARG:NH2	2.49	0.45
74:L5:1414:C:H2'	74:L5:1415:G:C8	2.52	0.45
74:L5:3701:OMC:N4	74:L5:3745:U:H2'	2.31	0.45
74:L5:4263:C:H2'	74:L5:4264:G:O4'	2.16	0.45
16:LO:188:LYS:O	16:LO:191:LYS:NZ	2.49	0.45
44:Pt:19:G:H21	44:Pt:59:A:H5'	1.82	0.45
45:SA:143:PRO:HG3	64:SV:32:ILE:HB	1.98	0.45
51:SD:135:GLU:HG3	51:SD:153:VAL:HG22	1.99	0.45
52:SE:19:MET:SD	52:SE:108:ARG:HD2	2.57	0.45
52:SE:191:ARG:NH1	52:SE:245:ARG:HG2	2.31	0.45
73:S2:613:G:N2	73:S2:626:G:OP1	2.47	0.45
74:L5:693:C:H2'	74:L5:694:C:O4'	2.17	0.45
74:L5:4421:C:N3	74:L5:4475:G:N1	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LN:116:LEU:HD22	15:LN:135:ILE:HD11	1.98	0.45
17:LP:49:LYS:HB3	17:LP:49:LYS:HE2	1.78	0.45
42:Lp:38:THR:HA	42:Lp:45:THR:HA	1.98	0.45
46:SB:113:MET:HE3	46:SB:113:MET:HB2	1.81	0.45
47:SC:121:ARG:HG2	47:SC:123:ARG:NH1	2.32	0.45
61:SS:101:ASN:HB3	87:SS:204:HOH:O	2.17	0.45
62:ST:130:ASP:O	62:ST:134:ILE:HG12	2.17	0.45
73:S2:964:A:H2'	73:S2:965:U:H6	1.81	0.45
73:S2:1380:C:H2'	73:S2:1381:G:O4'	2.17	0.45
74:L5:1739:G:H2'	74:L5:1740:C:C6	2.52	0.45
74:L5:1786:A:H2'	74:L5:1789:C:C5	2.52	0.45
74:L5:4738:C:H2'	74:L5:4739:C:C6	2.52	0.45
76:S6:54:G:H2'	76:S6:55:U:C5	2.52	0.45
16:LO:175:MET:HG2	74:L5:4873:G:N3	2.32	0.45
30:Ld:44:ARG:HD3	30:Ld:44:ARG:HA	1.72	0.45
46:SB:222:LYS:HE3	46:SB:222:LYS:HB3	1.76	0.45
47:SC:187:ARG:HB3	47:SC:187:ARG:HH11	1.82	0.45
58:SP:87:PRO:HA	58:SP:90:VAL:HG23	1.99	0.45
73:S2:948:C:H2'	73:S2:949:G:H8	1.82	0.45
73:S2:1614:A:H2'	73:S2:1615:U:C6	2.52	0.45
74:L5:3932:U:H2'	74:L5:3933:G:C8	2.52	0.45
3:LA:24:LYS:HG3	3:LA:49:ILE:HD13	1.99	0.45
5:LC:83:GLY:HA3	74:L5:368:C:O4'	2.17	0.45
13:LL:241:ALA:N	27:La:134:GLU:OE2	2.43	0.45
20:LS:43:ARG:HA	20:LS:43:ARG:HD2	1.80	0.45
40:Ln:25:LYS:HG3	74:L5:2872:C:H5''	1.99	0.45
48:SF:73:THR:O	48:SF:89:THR:HG21	2.17	0.45
61:SS:75:ARG:HH21	61:SS:95:TYR:HB2	1.82	0.45
73:S2:674:C:H2'	73:S2:675:U:C6	2.52	0.45
73:S2:996:A:O2'	73:S2:997:A:H8	1.99	0.45
73:S2:1744:G:H1'	73:S2:1790:A:N6	2.32	0.45
74:L5:1400:G:H2'	74:L5:1401:C:C6	2.52	0.45
74:L5:2706:G:N2	74:L5:2708:U:H5''	2.32	0.45
74:L5:3726:A:H2'	74:L5:3727:A:C8	2.52	0.45
74:L5:4600:G:H1'	74:L5:4601:U:H5	1.82	0.45
78:LU:45:GLU:HA	78:LU:54:GLY:HA2	1.99	0.45
2:L8:66:A:H2'	2:L8:67:U:C6	2.52	0.44
28:Lb:89:VAL:N	28:Lb:91:ARG:HH12	2.15	0.44
28:Lb:106:LYS:HE2	28:Lb:106:LYS:HB2	1.76	0.44
46:SB:225:LEU:HD12	46:SB:229:MET:HE1	1.98	0.44
48:SF:122:ARG:NE	69:Sc:59:LEU:HD21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SH:158:LEU:HD21	53:SH:187:PHE:HD2	1.83	0.44
55:SL:126:VAL:HG12	55:SL:145:VAL:HG22	1.99	0.44
73:S2:290:U:O2'	73:S2:292:A:H8	2.00	0.44
74:L5:1577:G:H5'	74:L5:1578:U:H5''	1.99	0.44
79:SZ:90:GLU:O	79:SZ:94:LYS:HG2	2.17	0.44
2:L8:70:G:H5''	25:LY:27:ARG:CZ	2.48	0.44
13:LL:36:ARG:NH1	74:L5:1364:U:OP2	2.46	0.44
55:SL:75:GLY:HA3	55:SL:88:ILE:HD12	2.00	0.44
73:S2:1102:G:H1	73:S2:1130:G:H1	1.64	0.44
73:S2:1387:G:H2'	73:S2:1388:A:O4'	2.15	0.44
74:L5:23:C:H2'	74:L5:24:G:O4'	2.18	0.44
74:L5:106:A:H2'	74:L5:107:G:O4'	2.17	0.44
74:L5:508:G:O2'	74:L5:510:U:OP2	2.19	0.44
74:L5:4905:C:H2'	74:L5:4906:C:H6	1.82	0.44
74:L5:4929:C:H2'	74:L5:4930:C:C6	2.52	0.44
33:Lg:98:GLU:HA	33:Lg:98:GLU:OE2	2.17	0.44
38:Ll:2:SER:N	74:L5:2406:G:N7	2.65	0.44
46:SB:216:LYS:NZ	73:S2:943:U:OP2	2.49	0.44
51:SD:71:ALA:HB3	54:SK:20:VAL:HG11	1.99	0.44
52:SE:248:ILE:HD12	80:SJ:72:PHE:CG	2.52	0.44
53:SH:134:VAL:HG12	53:SH:137:SER:O	2.17	0.44
63:SU:50:VAL:HA	63:SU:91:LEU:HA	1.98	0.44
74:L5:4699:U:H1'	74:L5:4700:A:H5''	1.98	0.44
8:LF:162:ILE:HD12	8:LF:167:ILE:HB	1.98	0.44
9:LG:88:ASP:OD1	9:LG:88:ASP:N	2.50	0.44
13:LL:115:GLN:O	13:LL:119:GLU:HG3	2.17	0.44
46:SB:152:LYS:HD3	60:SR:133:GLY:HA2	1.99	0.44
54:SK:32:HIS:HA	54:SK:33:PRO:HD3	1.86	0.44
58:SP:75:VAL:HA	58:SP:93:MET:O	2.17	0.44
62:ST:51:ASN:HB3	62:ST:54:TYR:CD2	2.52	0.44
68:Sb:22:LYS:NZ	73:S2:1129:G:H5''	2.32	0.44
73:S2:1139:C:H5	73:S2:1149:A:H62	1.65	0.44
73:S2:1223:A:H2'	73:S2:1224:G:O4'	2.18	0.44
73:S2:1493:C:O2'	73:S2:1499:U:O4	2.32	0.44
73:S2:1588:A:O2'	73:S2:1589:A:C8	2.71	0.44
74:L5:2520:C:H2'	74:L5:2521:G:C8	2.53	0.44
74:L5:3910:C:H2'	74:L5:3911:C:H6	1.83	0.44
2:L8:67:U:H2'	2:L8:68:G:C8	2.52	0.44
19:LR:24:LEU:HB3	19:LR:32:ILE:HD13	2.00	0.44
24:LX:39:LYS:HB3	24:LX:40:ILE:H	1.64	0.44
42:Lp:46:LYS:HB3	42:Lp:46:LYS:HE3	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SD:123:LEU:HD12	51:SD:134:CYS:SG	2.58	0.44
54:SK:66:HIS:HB2	54:SK:68:TYR:CE1	2.52	0.44
62:ST:36:THR:O	62:ST:36:THR:OG1	2.34	0.44
66:SY:108:LYS:NZ	73:S2:507:G:OP1	2.31	0.44
67:SX:46:HIS:CD2	67:SX:103:ALA:HB2	2.52	0.44
74:L5:1967:A:H2'	74:L5:1968:G:C8	2.52	0.44
74:L5:4951:G:H2'	74:L5:4952:G:H8	1.81	0.44
4:LB:124:LYS:NZ	74:L5:5063:G:O6	2.40	0.44
16:LO:61:ARG:NH1	74:L5:4587:G:OP1	2.51	0.44
21:LT:11:THR:HG22	21:LT:14:MET:HE3	1.98	0.44
46:SB:68:GLU:OE1	46:SB:83:LYS:HD2	2.18	0.44
46:SB:83:LYS:HE3	46:SB:83:LYS:HB2	1.82	0.44
47:SC:259:THR:HG21	64:SV:16:LYS:H	1.82	0.44
52:SE:31:PRO:HB3	52:SE:43:PRO:HG3	2.00	0.44
53:SH:79:LEU:O	53:SH:83:LEU:N	2.49	0.44
73:S2:391:C:H2'	73:S2:392:A:H8	1.83	0.44
73:S2:1792:G:H2'	73:S2:1793:A:H8	1.83	0.44
74:L5:1384:C:O2'	74:L5:1505:C:OP1	2.33	0.44
74:L5:1417:C:H2'	74:L5:1418:C:O4'	2.18	0.44
74:L5:2581:A:N3	74:L5:2654:C:O2'	2.47	0.44
74:L5:4273:A:H2'	74:L5:4274:A:C8	2.53	0.44
74:L5:4659:G:H2'	74:L5:4660:G:C8	2.53	0.44
76:S6:54:G:H2'	76:S6:55:U:C6	2.52	0.44
76:S6:65:G:H8	76:S6:65:G:O5'	2.01	0.44
5:LC:179:ASP:O	5:LC:183:VAL:HG23	2.18	0.44
7:LE:149:ILE:HD12	7:LE:271:LEU:HD21	2.00	0.44
10:LH:177:ASP:OD2	10:LH:177:ASP:N	2.50	0.44
17:LP:108:ASP:N	17:LP:152:GLU:OE2	2.38	0.44
25:LY:15:ARG:NH1	74:L5:230:G:OP1	2.49	0.44
27:La:76:ASP:HB3	27:La:115:GLY:HA3	1.99	0.44
28:Lb:93:LEU:HD23	28:Lb:93:LEU:HA	1.89	0.44
29:Lc:88:TYR:CE1	56:SN:145:THR:HG23	2.53	0.44
43:Lr:32:LEU:HD23	43:Lr:113:ARG:HD3	1.98	0.44
46:SB:3:VAL:HG12	57:SO:60:MET:HA	1.99	0.44
46:SB:115:LYS:HZ3	46:SB:115:LYS:HG2	1.61	0.44
49:SI:48:VAL:HG11	49:SI:54:LYS:HD2	2.00	0.44
56:SN:16:LEU:HD22	73:S2:919:A:H5'	1.98	0.44
66:SY:23:MET:HE2	66:SY:23:MET:HB2	1.68	0.44
66:SY:117:VAL:HG23	66:SY:122:LYS:HG3	1.99	0.44
73:S2:318:A:N1	73:S2:333:G:O6	2.50	0.44
73:S2:848:U:H2'	73:S2:849:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:S2:1217:A:H2'	73:S2:1218:C:C6	2.52	0.44
74:L5:2848:G:O2'	74:L5:3838:U:O4	2.27	0.44
74:L5:3705:G:H2'	74:L5:3706:C:H6	1.83	0.44
74:L5:4524:G:OP2	74:L5:4524:G:H4'	2.18	0.44
77:SG:74:ARG:HA	77:SG:96:SER:HA	1.99	0.44
10:LH:117:PHE:O	10:LH:120:GLU:HB2	2.18	0.44
12:LJ:113:ILE:CG1	61:SS:14:ARG:HD2	2.48	0.44
30:Ld:64:ILE:O	74:L5:2374:A:H5'	2.17	0.44
34:Lh:10:ARG:HA	34:Lh:10:ARG:HD3	1.72	0.44
43:Lr:32:LEU:HD22	43:Lr:110:ALA:HA	2.00	0.44
66:SY:23:MET:HE1	66:SY:75:ILE:HG13	1.99	0.44
73:S2:156:G:H2'	73:S2:157:U:C6	2.52	0.44
73:S2:1448:A:H2'	73:S2:1449:G:O4'	2.17	0.44
74:L5:3871:A:H2'	74:L5:3872:A:C8	2.52	0.44
2:L8:75:OMG:OP2	25:LY:74:TYR:OH	2.34	0.44
10:LH:90:TYR:CE2	10:LH:184:LYS:HG2	2.53	0.44
12:LJ:87:LEU:HB3	12:LJ:92:TYR:CD2	2.53	0.44
20:LS:44:PHE:CZ	20:LS:48:VAL:HG21	2.53	0.44
35:Li:50:PHE:O	35:Li:55:ARG:NH1	2.51	0.44
70:Sd:34:TYR:OH	73:S2:1549:U:OP1	2.33	0.44
73:S2:1560:U:H2'	73:S2:1561:A:H8	1.83	0.44
74:L5:2475:G:H4'	74:L5:2476:G:H5''	2.00	0.44
74:L5:3865:A:H2'	74:L5:3866:C:C6	2.53	0.44
2:L8:144:U:H2'	2:L8:145:C:C6	2.53	0.43
3:LA:68:ARG:HH11	3:LA:68:ARG:HG3	1.83	0.43
4:LB:93:VAL:HG22	4:LB:156:TYR:O	2.18	0.43
5:LC:14:LYS:HA	5:LC:173:LYS:HG2	1.99	0.43
12:LJ:27:GLY:HA2	12:LJ:68:ILE:HB	1.99	0.43
26:LZ:25:ILE:HA	26:LZ:43:VAL:HG12	1.99	0.43
51:SD:127:MET:HE1	51:SD:133:GLY:HA2	1.99	0.43
67:SX:52:LEU:HD11	67:SX:73:GLN:HB2	1.99	0.43
73:S2:96:C:H2'	73:S2:97:U:C6	2.53	0.43
73:S2:414:A:OP1	73:S2:814:U:O2'	2.31	0.43
74:L5:1309:C:H2'	74:L5:1310:C:C6	2.52	0.43
74:L5:1565:A:C5	74:L5:1566:C:H1'	2.52	0.43
74:L5:1809:C:H2'	74:L5:1810:G:C8	2.53	0.43
74:L5:1857:C:H2'	74:L5:1858:A:H8	1.82	0.43
74:L5:2715:G:H2'	74:L5:2716:C:C6	2.53	0.43
74:L5:3751:G:O2'	74:L5:3775:A:N1	2.51	0.43
74:L5:4637:OMG:HM23	74:L5:4637:OMG:H1'	1.62	0.43
74:L5:4934:A:H2'	74:L5:4935:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SZ:87:ALA:O	79:SZ:91:LEU:HD12	2.18	0.43
9:LG:35:ARG:NH1	74:L5:4128:A:O2'	2.51	0.43
18:LQ:108:ARG:HH22	74:L5:1355:G:P	2.40	0.43
19:LR:79:GLY:O	74:L5:3619:G:H4'	2.18	0.43
27:La:125:LYS:HB3	27:La:125:LYS:HE3	1.90	0.43
29:Lc:102:SER:O	87:Lc:201:HOH:O	2.21	0.43
45:SA:89:LYS:HA	45:SA:89:LYS:HD3	1.72	0.43
73:S2:102:A:H4'	73:S2:104:A:C8	2.53	0.43
73:S2:1010:G:H2'	73:S2:1011:A:C8	2.53	0.43
73:S2:1240:A:N3	73:S2:1267:C:O2'	2.44	0.43
74:L5:1345:A:H2'	74:L5:1346:C:C6	2.53	0.43
74:L5:1662:C:H2'	74:L5:1663:C:H6	1.83	0.43
74:L5:2814:C:H5'	74:L5:2815:A2M:OP2	2.19	0.43
74:L5:3893:C:O2'	74:L5:4979:A:N1	2.48	0.43
78:LU:74:SER:OG	78:LU:75:GLU:N	2.50	0.43
4:LB:145:GLN:O	4:LB:148:LYS:HG3	2.18	0.43
4:LB:322:HIS:O	4:LB:342:LYS:HE2	2.18	0.43
20:LS:54:MET:HE2	20:LS:54:MET:HB3	1.84	0.43
29:Lc:28:VAL:HB	29:Lc:33:GLN:HB3	2.00	0.43
64:SV:61:ARG:NH1	64:SV:61:ARG:HB2	2.33	0.43
73:S2:803:C:H2'	73:S2:804:U:C6	2.54	0.43
73:S2:803:C:H2'	73:S2:804:U:H6	1.83	0.43
74:L5:2803:U:H2'	74:L5:2804:OMC:H6	1.83	0.43
74:L5:3928:A:H2'	74:L5:3929:G:O4'	2.19	0.43
74:L5:4345:C:H2'	74:L5:4346:U:H6	1.83	0.43
76:S6:24:C:H2'	76:S6:25:U:C6	2.53	0.43
79:SZ:69:THR:HG22	79:SZ:71:ALA:H	1.82	0.43
4:LB:389:MET:HE2	74:L5:5041:G:C5	2.53	0.43
14:LM:36:ALA:HB2	14:LM:52:PHE:CE1	2.54	0.43
18:LQ:128:LEU:HD23	18:LQ:128:LEU:HA	1.89	0.43
26:LZ:36:ARG:HH22	74:L5:2580:U:P	2.41	0.43
44:Pt:10:G:H2'	44:Pt:11:A:C8	2.54	0.43
45:SA:11:LYS:O	45:SA:15:VAL:HG23	2.18	0.43
45:SA:185:MET:HG3	45:SA:191:ARG:NH2	2.33	0.43
62:ST:90:SER:OG	73:S2:1654:G:OP1	2.36	0.43
68:Sb:21:LYS:NZ	68:Sb:26:GLN:OE1	2.32	0.43
74:L5:2045:G:O6	74:L5:3870:C:O2'	2.35	0.43
74:L5:2351:OMC:HM23	74:L5:2351:OMC:H1'	1.71	0.43
74:L5:2476:G:C6	74:L5:2502:G:C2	3.07	0.43
74:L5:4498:OMU:O5'	74:L5:4498:OMU:H6	2.17	0.43
1:L7:92:C:H2'	1:L7:93:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LA:133:TYR:HB3	3:LA:168:VAL:HG12	2.00	0.43
11:LI:88:ARG:HB2	11:LI:173:PHE:CE2	2.53	0.43
22:LV:48:ARG:HH21	22:LV:49:LEU:HB3	1.83	0.43
38:LI:2:SER:OG	38:LI:4:HIS:O	2.35	0.43
44:PT:33:OMC:HM22	44:PT:34:U:H5'	2.01	0.43
66:SY:55:ILE:HG23	66:SY:75:ILE:HG12	2.00	0.43
73:S2:1533:A:N7	73:S2:1604:G:H1'	2.34	0.43
74:L5:119:G:H3'	74:L5:120:A:H5''	2.01	0.43
74:L5:478:G:H2'	74:L5:479:G:H8	1.84	0.43
74:L5:732:A:H2'	74:L5:733:A:O4'	2.18	0.43
74:L5:2264:C:H2'	74:L5:2265:G:O4'	2.19	0.43
74:L5:2616:C:H2'	74:L5:2617:G:C8	2.54	0.43
74:L5:2699:C:H2'	74:L5:2700:G:H8	1.83	0.43
74:L5:4951:G:H2'	74:L5:4952:G:C8	2.54	0.43
76:S6:15:G:H21	76:S6:21:U:H3	1.66	0.43
78:LU:88:LYS:HG2	78:LU:97:ARG:HH11	1.84	0.43
9:LG:53:ARG:NH2	74:L5:4163:U:OP2	2.51	0.43
20:LS:71:SER:O	20:LS:76:LYS:NZ	2.51	0.43
22:LV:42:VAL:HB	22:LV:45:ILE:HG13	2.00	0.43
49:SI:190:LEU:HB3	49:SI:195:LEU:HB2	2.01	0.43
52:SE:134:LYS:HA	52:SE:134:LYS:HD3	1.69	0.43
62:ST:6:VAL:HB	62:ST:65:TYR:CE1	2.53	0.43
74:L5:1535:C:H2'	74:L5:1536:PSU:O4'	2.18	0.43
74:L5:1965:G:H4'	74:L5:4695:C:O2'	2.19	0.43
74:L5:3603:G:H2'	74:L5:3604:A:C8	2.54	0.43
74:L5:3920:PSU:H2'	74:L5:3921:U:C6	2.54	0.43
79:SZ:68:ILE:HG22	79:SZ:88:LEU:HD13	2.00	0.43
2:L8:31:G:H2'	2:L8:32:C:O4'	2.18	0.43
3:LA:83:HIS:ND1	3:LA:84:THR:O	2.45	0.43
5:LC:100:ARG:NH2	74:L5:1521:C:OP1	2.42	0.43
26:LZ:5:MET:O	26:LZ:28:ASN:ND2	2.52	0.43
59:SQ:44:PRO:HG2	59:SQ:47:LEU:HD12	2.00	0.43
61:SS:66:ARG:O	61:SS:70:ILE:HG13	2.19	0.43
61:SS:86:ARG:HA	61:SS:86:ARG:HD3	1.85	0.43
73:S2:491:C:HO2'	73:S2:492:C:H5''	1.83	0.43
73:S2:1533:A:C8	73:S2:1604:G:H1'	2.54	0.43
74:L5:1472:C:H2'	74:L5:1473:U:C6	2.54	0.43
74:L5:1490:G:H2'	74:L5:1491:A:H8	1.82	0.43
74:L5:1534:A2M:HM'3	74:L5:1637:A:C4	2.54	0.43
74:L5:2765:A:H2'	74:L5:2766:A:C8	2.54	0.43
74:L5:3619:G:H22	74:L5:3624:A:H1'	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:4088:C:H2'	74:L5:4089:G:C8	2.53	0.43
74:L5:4459:U:H2'	74:L5:4460:U:C6	2.53	0.43
74:L5:4685:U:H2'	74:L5:4686:G:C8	2.53	0.43
74:L5:4873:G:H4'	74:L5:4874:A:OP2	2.18	0.43
7:LE:110:ARG:HH12	74:L5:2259:G:H21	1.67	0.43
8:LF:83:VAL:HG22	20:LS:62:VAL:HA	2.01	0.43
10:LH:102:ASN:N	10:LH:102:ASN:OD1	2.51	0.43
19:LR:81:ARG:HG2	19:LR:88:ARG:CZ	2.48	0.43
22:LV:90:ARG:NE	22:LV:124:GLU:OE2	2.50	0.43
54:SK:22:VAL:HG22	54:SK:68:TYR:HD2	1.83	0.43
67:SX:36:LEU:HD12	67:SX:36:LEU:HA	1.87	0.43
70:Sd:22:ARG:HG2	70:Sd:37:ASN:O	2.19	0.43
73:S2:113:G:C2	73:S2:292:A:H1'	2.53	0.43
73:S2:1370:A:N3	73:S2:1372:U:H5'	2.33	0.43
73:S2:1434:C:H2'	73:S2:1435:C:C6	2.53	0.43
74:L5:1298:C:H2'	74:L5:1299:G:C8	2.54	0.43
74:L5:1779:PSU:H2'	74:L5:1780:A:C8	2.54	0.43
74:L5:2554:U:H1'	74:L5:2574:G:N2	2.34	0.43
74:L5:2591:A:H2'	74:L5:2592:U:H6	1.84	0.43
74:L5:3769:C:H2'	74:L5:3770:PSU:C6	2.54	0.43
78:LU:28:PRO:O	78:LU:33:ILE:N	2.29	0.43
1:L7:4:U:H2'	1:L7:5:A:H8	1.84	0.43
7:LE:154:THR:CG2	74:L5:4942:C:H4'	2.47	0.43
12:LJ:78:LYS:HD2	12:LJ:78:LYS:HA	1.91	0.43
13:LL:235:GLU:CD	13:LL:235:GLU:H	2.27	0.43
13:LL:250:ALA:HB2	74:L5:1487:G:H5'	2.01	0.43
19:LR:144:LYS:HB2	19:LR:144:LYS:HE2	1.87	0.43
26:LZ:9:LYS:HD2	26:LZ:83:THR:O	2.19	0.43
44:Pt:62:C:H2'	44:Pt:63:C:H6	1.82	0.43
45:SA:36:GLN:NE2	64:SV:67:ASP:OD1	2.52	0.43
48:SF:39:ILE:HG23	48:SF:68:ILE:HD13	2.01	0.43
48:SF:50:PRO:HG2	48:SF:90:VAL:HG23	2.01	0.43
52:SE:106:LYS:HD2	52:SE:108:ARG:HH21	1.84	0.43
58:SP:121:ILE:HG13	61:SS:120:HIS:HD2	1.83	0.43
73:S2:1088:U:H4'	73:S2:1089:G:OP2	2.18	0.43
73:S2:1474:A:H2'	73:S2:1475:G:C8	2.54	0.43
74:L5:4392:OMG:N2	74:L5:4395:U:O2	2.47	0.43
76:S6:70:C:N4	76:S6:71:G:O6	2.52	0.43
78:LU:89:LYS:HE3	78:LU:89:LYS:HB2	1.78	0.43
3:LA:206:PRO:HG3	3:LA:213:GLY:HA3	2.01	0.43
3:LA:223:SER:HG	74:L5:3748:A:HO2'	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LB:238:LYS:HB2	4:LB:238:LYS:HE2	1.91	0.43
12:LJ:20:LEU:HD11	12:LJ:130:PHE:HD2	1.84	0.43
14:LM:114:LYS:HD2	14:LM:114:LYS:HA	1.77	0.43
24:LX:151:ASN:ND2	24:LX:156:ILE:O	2.51	0.43
35:Li:68:ARG:HH12	35:Li:71:LYS:HD2	1.83	0.43
48:SF:78:MET:HB3	48:SF:159:ARG:CZ	2.48	0.43
52:SE:90:ILE:HD11	52:SE:101:LEU:HD11	2.00	0.43
59:SQ:98:LYS:HD3	59:SQ:99:TYR:CE2	2.54	0.43
62:ST:124:THR:C	62:ST:126:GLN:H	2.27	0.43
67:SX:81:ILE:HD11	67:SX:102:VAL:HG21	2.00	0.43
73:S2:1531:A:H2'	73:S2:1532:C:C6	2.54	0.43
74:L5:1300:G:H2'	74:L5:1301:C:C6	2.53	0.43
74:L5:2703:G:H2'	74:L5:2704:C:C6	2.54	0.43
74:L5:3762:PSU:H2'	74:L5:3763:A:O4'	2.19	0.43
74:L5:4196:OMG:HM22	74:L5:4197:G:H5'	2.01	0.43
74:L5:4481:U:H2'	74:L5:4482:U:C6	2.54	0.43
2:L8:124:U:H5'	2:L8:125:C:H5	1.83	0.42
5:LC:60:HIS:HA	5:LC:92:PHE:HE1	1.84	0.42
5:LC:193:LYS:O	5:LC:197:ARG:HG3	2.19	0.42
15:LN:140:LYS:HE3	15:LN:144:ARG:HH21	1.83	0.42
20:LS:160:ARG:HH12	74:L5:1923:A:P	2.42	0.42
28:Lb:99:ILE:O	28:Lb:109:ARG:NH1	2.52	0.42
34:Lh:21:LEU:HG	34:Lh:25:LYS:HD2	1.99	0.42
52:SE:62:LYS:HE3	73:S2:503:C:OP1	2.18	0.42
63:SU:51:LYS:N	63:SU:90:ASP:O	2.49	0.42
67:SX:54:LYS:HD2	67:SX:91:LEU:HD11	2.00	0.42
73:S2:115:U:H2'	73:S2:116:U:C6	2.54	0.42
73:S2:367:U:H4'	73:S2:371:A:C8	2.54	0.42
73:S2:945:U:H2'	73:S2:946:U:C6	2.54	0.42
73:S2:960:U:O2'	73:S2:962:A:N7	2.36	0.42
73:S2:1337:C:H2'	73:S2:1338:G:H8	1.83	0.42
74:L5:450:G:H1	74:L5:1296:G:H1	1.67	0.42
74:L5:2786:C:H5''	74:L5:2787:A:H5'	2.01	0.42
74:L5:4192:A:H2'	74:L5:4193:C:C6	2.54	0.42
74:L5:4601:U:H2'	74:L5:4602:A:C8	2.54	0.42
4:LB:181:MET:HE2	4:LB:183:ILE:HG12	2.02	0.42
20:LS:30:MET:HE2	20:LS:30:MET:HB3	1.85	0.42
46:SB:224:GLU:HB3	46:SB:227:LYS:HE2	1.99	0.42
52:SE:45:ILE:HA	52:SE:61:VAL:HG11	2.01	0.42
73:S2:51:U:H2'	73:S2:52:G:H8	1.84	0.42
74:L5:2591:A:H2'	74:L5:2592:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:3916:G:H2'	74:L5:3917:A:C8	2.53	0.42
74:L5:4390:A:H2'	74:L5:4391:G:O4'	2.19	0.42
74:L5:4710:C:H2'	74:L5:4711:C:C6	2.53	0.42
80:SJ:60:LEU:HD23	80:SJ:60:LEU:HA	1.86	0.42
2:L8:75:OMG:HM23	2:L8:75:OMG:H1'	1.69	0.42
4:LB:57:VAL:HG22	4:LB:73:VAL:HG22	2.01	0.42
4:LB:252:ALA:HB1	74:L5:4524:G:N3	2.34	0.42
5:LC:293:LEU:HD22	18:LQ:34:PHE:CD2	2.55	0.42
11:LI:202:SER:O	11:LI:202:SER:OG	2.25	0.42
12:LJ:19:LYS:HB2	12:LJ:75:ARG:NH1	2.35	0.42
18:LQ:89:ASP:HB3	18:LQ:92:VAL:HG23	2.00	0.42
21:LT:108:ARG:O	21:LT:112:ASN:ND2	2.42	0.42
22:LV:48:ARG:HD2	74:L5:4621:C:OP1	2.18	0.42
46:SB:28:LYS:NZ	57:SO:51:GLU:OE2	2.49	0.42
57:SO:45:THR:OG1	57:SO:49:GLY:HA2	2.18	0.42
61:SS:28:PHE:HE2	61:SS:38:ARG:HE	1.67	0.42
71:Se:112:TYR:CG	80:SJ:33:GLY:HA3	2.53	0.42
73:S2:218:U:H2'	73:S2:219:U:H6	1.84	0.42
73:S2:1435:C:OP1	73:S2:1436:C:N4	2.53	0.42
73:S2:1733:U:H2'	73:S2:1734:G:O4'	2.19	0.42
74:L5:2716:C:H2'	74:L5:2717:G:O4'	2.19	0.42
74:L5:2845:A:H62	74:L5:3843:C:H42	1.65	0.42
74:L5:4605:A:H8	74:L5:4605:A:OP1	2.01	0.42
74:L5:4653:C:H2'	74:L5:4654:C:C6	2.54	0.42
74:L5:4866:C:H2'	74:L5:4867:G:C8	2.53	0.42
74:L5:4977:A:O2'	74:L5:4982:A:N1	2.48	0.42
74:L5:5010:PSU:H2'	74:L5:5011:A:C8	2.54	0.42
3:LA:102:LEU:HB2	3:LA:107:MET:HE3	2.02	0.42
4:LB:47:LEU:HD23	4:LB:47:LEU:HA	1.89	0.42
5:LC:284:MET:HE2	5:LC:287:THR:HA	2.02	0.42
9:LG:138:ALA:HB1	9:LG:199:CYS:SG	2.59	0.42
11:LI:74:LYS:HD3	74:L5:4415:A:H4'	2.01	0.42
13:LL:226:LYS:NZ	74:L5:509:A:O3'	2.53	0.42
19:LR:42:ARG:NH2	74:L5:2525:U:OP2	2.44	0.42
29:Lc:35:LEU:HD23	29:Lc:35:LEU:HA	1.82	0.42
64:SV:64:GLU:HG3	68:Sb:3:LEU:HG	2.00	0.42
73:S2:57:U:OP1	73:S2:504:G:O2'	2.38	0.42
74:L5:1604:G:H2'	74:L5:1605:G:C8	2.54	0.42
74:L5:1933:G:H2'	74:L5:1934:A:C8	2.55	0.42
74:L5:1953:U:H2'	74:L5:1954:U:C6	2.55	0.42
74:L5:2362:U:H2'	74:L5:2363:A2M:H8	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:3865:A:H2'	74:L5:3866:C:H6	1.84	0.42
74:L5:5001:PSU:H2'	74:L5:5002:U:O4'	2.20	0.42
80:SJ:142:VAL:HG12	80:SJ:144:ILE:H	1.83	0.42
4:LB:90:VAL:HB	4:LB:104:THR:HG23	2.01	0.42
17:LP:112:LEU:HD13	17:LP:150:LEU:HD23	2.00	0.42
51:SD:209:SER:HB2	60:SR:40:ILE:HG12	2.01	0.42
66:SY:13:MET:HE3	66:SY:13:MET:HB3	1.65	0.42
73:S2:525:A:H2'	73:S2:526:A:H8	1.85	0.42
73:S2:1712:A:H2'	73:S2:1713:C:H6	1.84	0.42
74:L5:1764:G:C6	74:L5:1765:A:N7	2.87	0.42
74:L5:2745:A:H2'	74:L5:2746:A:C8	2.55	0.42
74:L5:5003:U:H2'	74:L5:5004:C:C6	2.55	0.42
19:LR:64:ARG:NH2	74:L5:2633:U:OP1	2.52	0.42
20:LS:53:LYS:HZ2	20:LS:53:LYS:HG3	1.62	0.42
26:LZ:57:MET:HB2	26:LZ:61:LYS:HD2	2.01	0.42
52:SE:122:LYS:HB2	52:SE:122:LYS:HE3	1.89	0.42
57:SO:129:ILE:O	75:Sa:65:PRO:HG3	2.20	0.42
60:SR:98:VAL:O	60:SR:120:THR:N	2.40	0.42
73:S2:874:G:H2'	73:S2:875:A:C8	2.54	0.42
73:S2:1374:C:O2'	73:S2:1464:C:O2	2.35	0.42
73:S2:1681:U:H2'	73:S2:1682:C:C6	2.54	0.42
74:L5:1086:C:H2'	74:L5:1087:A:H8	1.84	0.42
74:L5:4344:U:H2'	74:L5:4345:C:C6	2.54	0.42
74:L5:4917:C:H2'	74:L5:4918:C:C6	2.54	0.42
78:LU:86:LEU:HD13	78:LU:86:LEU:HA	1.88	0.42
1:L7:36:C:H2'	1:L7:37:G:C8	2.54	0.42
2:L8:20:A:O2'	74:L5:2333:G:OP1	2.33	0.42
5:LC:347:HIS:HB2	74:L5:724:C:H5'	2.02	0.42
9:LG:89:ARG:O	9:LG:93:THR:HG23	2.20	0.42
27:La:27:LYS:HA	27:La:27:LYS:HD2	1.82	0.42
28:Lb:33:LYS:HE2	28:Lb:33:LYS:HB3	1.68	0.42
32:Lf:42:TYR:HA	32:Lf:45:LYS:HG3	2.01	0.42
36:Lj:20:ARG:NH2	36:Lj:39:TYR:OH	2.52	0.42
45:SA:34:MET:HE3	45:SA:34:MET:HB3	1.80	0.42
50:mR:34:A:N6	76:S6:36:A:H61	2.17	0.42
53:SH:61:ILE:HA	53:SH:93:VAL:HG23	2.01	0.42
73:S2:460:A:H2'	73:S2:461:U:H5''	2.02	0.42
73:S2:1337:C:H2'	73:S2:1338:G:C8	2.55	0.42
73:S2:1390:U:H2'	73:S2:1391:C:C6	2.54	0.42
74:L5:28:C:H4'	74:L5:61:A:H4'	2.02	0.42
74:L5:3944:OMG:HM23	74:L5:3944:OMG:H1'	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LM:69:HIS:HB2	14:LM:72:TYR:CE2	2.54	0.42
33:Lg:60:ARG:HA	33:Lg:60:ARG:HD2	1.79	0.42
46:SB:121:ILE:HD13	46:SB:164:ILE:HG21	2.02	0.42
51:SD:137:VAL:HG13	51:SD:151:LYS:HG2	2.01	0.42
56:SN:96:VAL:HG21	56:SN:147:SER:HA	2.01	0.42
73:S2:1181:A:OP2	73:S2:1181:A:H8	2.02	0.42
73:S2:1468:C:H2'	73:S2:1469:A:C8	2.55	0.42
73:S2:1469:A:H2'	73:S2:1470:C:C6	2.55	0.42
74:L5:319:A:H1'	74:L5:3726:A:N3	2.34	0.42
74:L5:698:G:H2'	74:L5:699:C:C6	2.55	0.42
74:L5:751:G:C2	74:L5:752:G:H1'	2.55	0.42
74:L5:1564:A:H2'	74:L5:1565:A:C8	2.54	0.42
74:L5:1672:U:H2'	74:L5:1673:U:C6	2.55	0.42
74:L5:1769:G:H2'	74:L5:1770:A:H8	1.85	0.42
74:L5:2415:OMU:HM23	74:L5:2415:OMU:H1'	1.76	0.42
74:L5:2554:U:H1'	74:L5:2574:G:H21	1.85	0.42
74:L5:4208:U:OP1	74:L5:4334:U:O2'	2.33	0.42
74:L5:4619:U:H2'	74:L5:4620:OMU:H6	2.02	0.42
74:L5:4768:G:H2'	74:L5:4769:G:H8	1.84	0.42
74:L5:5013:C:N4	74:L5:5028:G:H5'	2.35	0.42
1:L7:16:A:H2'	1:L7:17:C:C6	2.55	0.42
5:LC:345:ARG:O	5:LC:349:LEU:HG	2.19	0.42
7:LE:270:TYR:OH	14:LM:106:ASP:HB3	2.19	0.42
12:LJ:151:ILE:HD12	12:LJ:156:ARG:HG2	2.01	0.42
14:LM:82:ILE:H	14:LM:82:ILE:HG12	1.71	0.42
20:LS:174:THR:OG1	74:L5:4763:U:O2'	2.30	0.42
27:La:123:ILE:HD13	27:La:143:ALA:HB3	2.02	0.42
29:Lc:98:ASP:OD1	29:Lc:100:GLY:N	2.42	0.42
35:Li:59:GLU:OE2	74:L5:4065:G:O2'	2.28	0.42
39:Lm:95:ILE:HD11	39:Lm:124:LYS:HD3	2.02	0.42
41:Lo:33:LEU:HD12	41:Lo:38:LYS:HE3	2.01	0.42
46:SB:228:LEU:HD12	46:SB:228:LEU:HA	1.80	0.42
69:Sc:52:GLU:H	69:Sc:52:GLU:HG3	1.63	0.42
73:S2:1227:G:C2	73:S2:1228:A:C8	3.08	0.42
73:S2:1348:G:H1	73:S2:1381:G:N2	2.10	0.42
74:L5:2756:G:H2'	74:L5:2757:A:C8	2.55	0.42
74:L5:3786:U:O2	74:L5:3814:U:H4'	2.20	0.42
74:L5:4750:G:H2'	74:L5:4751:G:H8	1.82	0.42
74:L5:4988:U:C5	74:L5:5060:A:H2'	2.55	0.42
77:SG:30:LYS:HD3	77:SG:34:THR:HG21	2.01	0.42
8:LF:174:LEU:HD23	8:LF:177:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Li:43:MET:HE2	35:Li:43:MET:HA	2.02	0.42
47:SC:169:TYR:CG	47:SC:173:LYS:HA	2.55	0.42
52:SE:10:LYS:HD3	52:SE:10:LYS:HA	1.90	0.42
53:SH:140:VAL:HG12	56:SN:19:ARG:HD3	2.01	0.42
58:SP:40:ARG:HA	58:SP:40:ARG:HD3	1.87	0.42
62:ST:22:LEU:HD23	62:ST:54:TYR:HD1	1.85	0.42
65:SW:30:CYS:SG	65:SW:31:SER:N	2.93	0.42
66:SY:122:LYS:HD3	73:S2:84:A:H5''	2.00	0.42
67:SX:130:LEU:HD23	67:SX:130:LEU:HA	1.96	0.42
73:S2:455:A:H2'	73:S2:456:C:H6	1.82	0.42
73:S2:488:U:H6	73:S2:488:U:H2'	1.60	0.42
73:S2:1139:C:H2'	73:S2:1140:G:O4'	2.20	0.42
73:S2:1414:A:H2'	73:S2:1415:C:O4'	2.19	0.42
73:S2:1828:C:H2'	73:S2:1829:G:O4'	2.20	0.42
74:L5:1483:C:H4'	74:L5:1484:G:O4'	2.19	0.42
74:L5:1629:G:H2'	74:L5:1631:A:N7	2.34	0.42
77:SG:35:GLU:HA	77:SG:51:ARG:HA	2.02	0.42
80:SJ:82:VAL:HG23	80:SJ:87:LEU:HD23	2.02	0.42
2:L8:5:U:H2'	2:L8:6:C:C6	2.55	0.41
4:LB:130:PHE:H	74:L5:4727:A:H5'	1.85	0.41
29:Lc:65:MET:HE3	29:Lc:65:MET:HB3	1.79	0.41
32:Lf:79:GLY:HA2	74:L5:2066:C:O2'	2.20	0.41
34:Lh:107:GLN:O	34:Lh:111:GLU:HG3	2.20	0.41
38:Ll:27:ILE:HD12	38:Ll:30:LYS:HD2	2.02	0.41
44:Pt:10:G:H2'	44:Pt:11:A:H8	1.85	0.41
49:SI:25:ARG:HB2	49:SI:28:GLU:OE1	2.20	0.41
49:SI:66:SER:HA	49:SI:73:THR:HA	2.02	0.41
52:SE:44:LEU:HD21	52:SE:70:ILE:HG21	2.02	0.41
52:SE:56:LEU:N	52:SE:60:GLU:OE1	2.36	0.41
56:SN:22:VAL:HG23	56:SN:66:VAL:HG22	2.02	0.41
60:SR:16:ILE:HG22	60:SR:24:LEU:HD11	2.02	0.41
73:S2:16:G:H2'	73:S2:17:C:C6	2.54	0.41
73:S2:1599:U:O2'	79:SZ:41:ARG:NH1	2.53	0.41
73:S2:1798:C:H2'	73:S2:1799:G:O4'	2.20	0.41
74:L5:223:G:H4'	74:L5:225:G:C8	2.55	0.41
74:L5:1590:C:H5''	74:L5:1591:U:O5'	2.20	0.41
74:L5:1956:A:H2'	74:L5:1957:U:H6	1.85	0.41
74:L5:3783:A:O5'	74:L5:3784:A:H5'	2.19	0.41
74:L5:3893:C:H2'	74:L5:3894:A:C8	2.55	0.41
74:L5:4536:OMC:HM22	74:L5:4537:C:O4'	2.20	0.41
2:L8:130:C:H2'	2:L8:131:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LJ:77:ALA:O	12:LJ:80:GLU:HG2	2.20	0.41
29:Lc:23:LYS:HE2	29:Lc:23:LYS:HB2	1.79	0.41
30:Ld:22:THR:OG1	30:Ld:122:VAL:HG23	2.20	0.41
52:SE:143:ASP:OD1	52:SE:143:ASP:N	2.53	0.41
53:SH:130:LEU:HG	53:SH:177:TYR:CE1	2.55	0.41
65:SW:111:MET:HE2	65:SW:111:MET:HB3	1.89	0.41
68:Sb:24:LEU:HD12	68:Sb:24:LEU:HA	1.86	0.41
73:S2:983:A:OP1	73:S2:1073:U:O2'	2.30	0.41
74:L5:223:G:H4'	74:L5:225:G:N7	2.34	0.41
74:L5:1490:G:H2'	74:L5:1491:A:C8	2.54	0.41
74:L5:4625:C:O2'	74:L5:4626:A:H5'	2.20	0.41
24:LX:143:ASP:OD1	24:LX:143:ASP:N	2.52	0.41
30:Ld:59:THR:HA	30:Ld:60:PRO:HD3	1.94	0.41
72:Sg:164:ILE:HA	72:Sg:178:ASN:HA	2.02	0.41
73:S2:1690:U:H2'	73:S2:1691:U:C6	2.55	0.41
74:L5:434:A:H2'	74:L5:435:A:O4'	2.20	0.41
74:L5:1504:G:H2'	74:L5:1505:C:C6	2.55	0.41
77:SG:137:ARG:HB3	77:SG:140:ARG:HD3	2.02	0.41
80:SJ:60:LEU:HD22	80:SJ:70:ARG:HA	2.01	0.41
1:L7:46:C:H2'	1:L7:47:G:C8	2.55	0.41
4:LB:196:TRP:O	4:LB:200:ARG:HG2	2.20	0.41
9:LG:101:LYS:H	9:LG:101:LYS:HG3	1.62	0.41
17:LP:104:LEU:HD23	17:LP:104:LEU:HA	1.94	0.41
30:Ld:23:ARG:NH1	74:L5:5058:A:H5'	2.36	0.41
31:Le:19:LYS:HE2	31:Le:19:LYS:HB3	1.91	0.41
41:Lo:36:GLN:HG2	74:L5:4363:A:H5''	2.03	0.41
43:Lr:66:ARG:NH1	74:L5:478:G:OP1	2.53	0.41
48:SF:159:ARG:NE	73:S2:1535:U:O4	2.50	0.41
53:SH:163:GLN:HG2	53:SH:189:PHE:CD1	2.55	0.41
61:SS:116:LYS:HA	74:L5:1766:A:H3'	2.01	0.41
73:S2:501:C:H2'	73:S2:502:C:H5''	2.03	0.41
73:S2:1792:G:H2'	73:S2:1793:A:C8	2.56	0.41
74:L5:158:A:H5''	74:L5:159:C:H2'	2.02	0.41
74:L5:474:C:H2'	74:L5:475:G:C8	2.55	0.41
74:L5:1535:C:O2'	74:L5:3642:A:N1	2.50	0.41
74:L5:1811:G:H2'	74:L5:1812:C:C6	2.55	0.41
74:L5:1963:C:H2'	74:L5:1964:A:O4'	2.19	0.41
74:L5:2607:C:H2'	74:L5:2608:G:C8	2.55	0.41
74:L5:2701:U:H2'	74:L5:2702:C:C6	2.56	0.41
74:L5:3785:A2M:H8	74:L5:3785:A2M:H2'	1.61	0.41
74:L5:5008:C:H2'	74:L5:5009:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Sa:44:ILE:HD12	75:Sa:65:PRO:HG2	2.01	0.41
4:LB:252:ALA:HB1	74:L5:4524:G:C2	2.56	0.41
21:LT:105:PHE:CD1	74:L5:1802:A:H4'	2.56	0.41
22:LV:72:LEU:HD21	22:LV:113:LYS:HE2	2.03	0.41
25:LY:121:ARG:HD3	74:L5:194:C:O2'	2.21	0.41
26:LZ:9:LYS:HA	26:LZ:9:LYS:HD3	1.77	0.41
47:SC:107:LEU:HD11	47:SC:129:ALA:HB2	2.02	0.41
47:SC:123:ARG:HE	47:SC:123:ARG:HB2	1.70	0.41
48:SF:30:ILE:HG22	48:SF:32:ASP:H	1.84	0.41
54:SK:25:LYS:HG3	54:SK:67:PHE:CE1	2.56	0.41
73:S2:639:C:H2'	73:S2:640:A:C8	2.55	0.41
73:S2:1395:C:O2'	73:S2:1396:A:OP1	2.32	0.41
73:S2:1544:C:H2'	73:S2:1545:A:H5''	2.02	0.41
74:L5:2744:A:H2'	74:L5:2745:A:C8	2.56	0.41
74:L5:4437:U:C2	74:L5:4515:G:H4'	2.55	0.41
74:L5:4859:C:H3'	74:L5:4860:G:H8	1.85	0.41
74:L5:5029:C:H2'	74:L5:5030:U:C6	2.56	0.41
77:SG:5:ILE:O	77:SG:13:GLN:HA	2.20	0.41
80:SJ:155:LYS:H	80:SJ:155:LYS:HG2	1.59	0.41
5:LC:347:HIS:ND1	74:L5:723:A:O3'	2.52	0.41
7:LE:68:MET:N	7:LE:68:MET:SD	2.92	0.41
14:LM:51:PRO:HB2	14:LM:53:LYS:HG2	2.02	0.41
27:La:72:THR:HG22	27:La:110:LYS:HB3	2.03	0.41
29:Lc:21:VAL:HG11	29:Lc:96:ILE:HG12	2.02	0.41
43:Lr:26:SER:OG	43:Lr:28:GLU:OE1	2.29	0.41
52:SE:162:ILE:HD13	52:SE:162:ILE:HA	1.85	0.41
62:ST:97:LYS:HE3	62:ST:97:LYS:HB2	1.84	0.41
73:S2:29:G:H2'	73:S2:30:C:C6	2.54	0.41
73:S2:508:A:H2'	73:S2:509:G:O4'	2.21	0.41
73:S2:1238:U:O2	73:S2:1242:U:H5	2.03	0.41
73:S2:1365:G:H2'	73:S2:1366:G:C8	2.55	0.41
73:S2:1456:G:H2'	73:S2:1457:U:C6	2.55	0.41
73:S2:1491:G:H2'	73:S2:1492:U:C6	2.56	0.41
73:S2:1863:A:H8	75:Sa:79:ILE:HG21	1.86	0.41
74:L5:697:G:P	74:L5:697:G:H8	2.44	0.41
74:L5:1633:G:H5'	74:L5:1634:A:OP1	2.20	0.41
74:L5:2616:C:H2'	74:L5:2617:G:H8	1.86	0.41
80:SJ:67:ASP:OD1	80:SJ:70:ARG:N	2.41	0.41
3:LA:200:ARG:NH2	74:L5:3650:C:OP1	2.51	0.41
7:LE:285:LYS:HE3	7:LE:285:LYS:HB3	1.86	0.41
16:LO:9:LEU:HD23	16:LO:118:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Lg:76:ARG:NH1	74:L5:2583:C:OP2	2.53	0.41
34:Lh:27:GLU:HG2	34:Lh:50:VAL:HG21	2.02	0.41
44:Pt:11:A:H2'	44:Pt:12:G:C8	2.55	0.41
44:Pt:62:C:H2'	44:Pt:63:C:C6	2.56	0.41
45:SA:42:LYS:HG2	45:SA:46:ILE:O	2.20	0.41
48:SF:107:ASN:O	48:SF:111:VAL:HG23	2.21	0.41
51:SD:99:ILE:HG23	51:SD:173:ARG:HH12	1.86	0.41
57:SO:95:ILE:HB	57:SO:129:ILE:HA	2.02	0.41
58:SP:91:GLY:H	58:SP:107:ILE:HB	1.86	0.41
59:SQ:45:ARG:HG2	59:SQ:48:GLN:NE2	2.35	0.41
66:SY:29:HIS:NE2	66:SY:69:THR:OG1	2.53	0.41
73:S2:550:C:H2'	73:S2:551:U:C6	2.56	0.41
73:S2:1174:U:H2'	73:S2:1175:G:H8	1.86	0.41
73:S2:1865:C:O2	75:Sa:92:ARG:HB3	2.20	0.41
74:L5:4068:U:H2'	74:L5:4069:U:C6	2.56	0.41
74:L5:4244:A:H2'	74:L5:4245:G:O4'	2.20	0.41
74:L5:4734:A:H2'	74:L5:4735:G:H8	1.83	0.41
76:S6:3:C:H2'	76:S6:4:G:H8	1.84	0.41
76:S6:17:C:H3'	76:S6:18:C:H2'	2.02	0.41
14:LM:46:ARG:HG2	74:L5:935:A:C5	2.55	0.41
24:LX:79:PHE:CD1	34:Lh:36:VAL:HG11	2.55	0.41
46:SB:81:PHE:CD2	46:SB:109:LYS:HD3	2.56	0.41
61:SS:136:THR:OG1	73:S2:1521:C:OP2	2.35	0.41
73:S2:1177:U:H2'	73:S2:1178:U:H6	1.85	0.41
73:S2:1617:G:N1	73:S2:1620:A:OP2	2.54	0.41
74:L5:919:C:H2'	74:L5:920:C:H6	1.85	0.41
74:L5:1770:A:H2'	74:L5:1771:U:O4'	2.20	0.41
74:L5:2448:G:H2'	74:L5:2449:A:C8	2.55	0.41
74:L5:4089:G:H2'	74:L5:4090:G:C8	2.55	0.41
74:L5:4300:U:H2'	74:L5:4301:U:C6	2.56	0.41
74:L5:4584:A:H2'	74:L5:4585:U:O4'	2.20	0.41
79:SZ:73:VAL:HG21	79:SZ:88:LEU:HD21	2.03	0.41
1:L7:22:A:H2'	1:L7:23:A:C8	2.56	0.41
4:LB:155:LYS:HE3	4:LB:155:LYS:HB2	1.83	0.41
8:LF:228:VAL:HA	20:LS:39:VAL:HG22	2.02	0.41
9:LG:77:PRO:HA	9:LG:78:PRO:HD3	1.96	0.41
22:LV:27:ASN:ND2	22:LV:100:ASP:OD2	2.48	0.41
29:Lc:37:MET:HG3	29:Lc:97:ILE:HD11	2.01	0.41
45:SA:10:MET:CE	45:SA:15:VAL:HG22	2.51	0.41
46:SB:46:LYS:HB2	46:SB:46:LYS:HE2	1.90	0.41
46:SB:199:LYS:HA	46:SB:199:LYS:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SB:199:LYS:O	46:SB:199:LYS:NZ	2.43	0.41
47:SC:259:THR:HG21	64:SV:15:ARG:HA	2.02	0.41
56:SN:84:LEU:HD23	56:SN:84:LEU:HA	1.93	0.41
58:SP:14:LYS:HD3	58:SP:15:PHE:H	1.86	0.41
58:SP:60:LEU:HD23	58:SP:89:MET:HG3	2.01	0.41
60:SR:4:VAL:HG22	73:S2:1466:G:H4'	2.03	0.41
62:ST:77:LYS:HE2	62:ST:94:ARG:NH2	2.36	0.41
72:Sg:17:TRP:O	72:Sg:36:ARG:N	2.53	0.41
73:S2:667:U:O2'	75:Sa:2:THR:OG1	2.29	0.41
73:S2:1617:G:N2	73:S2:1619:A:H3'	2.36	0.41
73:S2:1667:U:H2'	73:S2:1668:U:C6	2.56	0.41
73:S2:1718:G:O2'	73:S2:1815:A:N6	2.51	0.41
74:L5:424:U:H2'	74:L5:425:U:H6	1.86	0.41
74:L5:1754:U:O2'	74:L5:1755:C:O5'	2.38	0.41
74:L5:2859:G:H2'	74:L5:2860:C:H6	1.86	0.41
74:L5:3765:G:OP1	74:L5:3810:C:N4	2.50	0.41
74:L5:4537:C:H2'	74:L5:4538:G:H8	1.85	0.41
78:LU:112:LEU:HD13	78:LU:112:LEU:HA	1.93	0.41
4:LB:59:GLU:OE2	4:LB:70:LYS:N	2.54	0.41
4:LB:303:ALA:HB2	4:LB:314:ILE:HA	2.03	0.41
5:LC:152:LEU:HD23	5:LC:251:ILE:HG12	2.03	0.41
12:LJ:20:LEU:HD11	12:LJ:130:PHE:CD2	2.56	0.41
15:LN:138:PHE:CD2	74:L5:18:C:H4'	2.55	0.41
24:LX:90:ILE:HG12	24:LX:96:LEU:HD13	2.02	0.41
35:Li:16:LYS:HD3	35:Li:16:LYS:HA	1.85	0.41
40:Ln:2:ARG:HB3	40:Ln:5:TRP:CD1	2.56	0.41
44:Pt:25:U:H2'	44:Pt:26:C:C6	2.55	0.41
45:SA:76:VAL:HG12	45:SA:123:VAL:HB	2.03	0.41
46:SB:38:MET:HE3	46:SB:182:LYS:HA	2.03	0.41
51:SD:26:THR:O	51:SD:30:ALA:HB2	2.21	0.41
54:SK:27:VAL:HG12	54:SK:46:MET:SD	2.61	0.41
58:SP:16:THR:HB	58:SP:20:VAL:N	2.36	0.41
58:SP:77:LYS:HB3	58:SP:102:PHE:CD2	2.56	0.41
65:SW:42:MET:HE2	65:SW:42:MET:HB3	1.87	0.41
73:S2:948:C:H2'	73:S2:949:G:C8	2.56	0.41
73:S2:1220:A:H2'	73:S2:1221:G:O4'	2.20	0.41
74:L5:325:U:H2'	74:L5:326:C:C6	2.55	0.41
74:L5:398:A2M:H1'	74:L5:398:A2M:HM'3	1.83	0.41
74:L5:1664:U:H2'	74:L5:1665:C:C6	2.56	0.41
74:L5:1866:U:H2'	74:L5:1867:A:O4'	2.21	0.41
74:L5:2412:A:H2'	74:L5:2413:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:L5:2864:A:H2'	74:L5:2865:U:H6	1.86	0.41
74:L5:3925:OMU:H1'	74:L5:3925:OMU:HM23	1.68	0.41
74:L5:4174:U:H2'	74:L5:4175:G:C8	2.56	0.41
74:L5:4303:C:O2'	74:L5:4304:A:H2'	2.21	0.41
74:L5:5068:G:N2	74:L5:5069:U:O4	2.41	0.41
77:SG:47:GLY:O	77:SG:117:GLY:HA2	2.20	0.41
78:LU:61:VAL:HA	78:LU:74:SER:HA	2.03	0.41
2:L8:33:G:H5''	2:L8:34:U:OP1	2.20	0.40
5:LC:205:ARG:HG2	74:L5:2297:G:H5'	2.03	0.40
11:LI:91:LEU:HD23	11:LI:91:LEU:HA	1.91	0.40
12:LJ:26:VAL:HB	12:LJ:32:ARG:HG2	2.04	0.40
13:LL:226:LYS:HE3	13:LL:226:LYS:HB2	1.93	0.40
14:LM:90:ARG:NH2	74:L5:4868:G:H4'	2.36	0.40
26:LZ:53:VAL:HG11	26:LZ:62:ILE:HG23	2.03	0.40
29:Lc:57:LYS:O	29:Lc:61:GLU:HG3	2.21	0.40
87:Lj:203:HOH:O	74:L5:1534:A2M:H2	2.20	0.40
42:Lp:4:ARG:NH2	74:L5:1555:G:N7	2.56	0.40
56:SN:119:GLU:HG2	56:SN:141:TYR:CE2	2.56	0.40
59:SQ:13:PHE:O	59:SQ:90:LYS:HE3	2.22	0.40
61:SS:26:ILE:HA	61:SS:56:ALA:HB2	2.02	0.40
70:Sd:14:PHE:CZ	73:S2:1617:G:H4'	2.56	0.40
73:S2:1408:U:H2'	73:S2:1409:A:O4'	2.21	0.40
73:S2:1844:U:H2'	73:S2:1845:A:C8	2.56	0.40
74:L5:675:C:H2'	74:L5:676:C:O4'	2.21	0.40
74:L5:1431:C:H2'	74:L5:1432:G:O4'	2.21	0.40
74:L5:1765:A:H62	74:L5:1768:C:H42	1.69	0.40
74:L5:2018:C:N3	74:L5:2019:C:N4	2.69	0.40
74:L5:2529:A:H4'	74:L5:2531:C:C5	2.56	0.40
74:L5:4159:C:H2'	74:L5:4160:C:C6	2.55	0.40
74:L5:4961:G:H2'	74:L5:4962:C:C6	2.55	0.40
76:S6:25:U:H2'	76:S6:26:C:C6	2.55	0.40
79:SZ:62:VAL:HG23	79:SZ:63:PRO:HD3	2.03	0.40
80:SJ:84:ILE:HG13	80:SJ:86:VAL:HG23	2.01	0.40
2:L8:26:C:H2'	2:L8:27:U:C6	2.55	0.40
2:L8:40:A:H2'	2:L8:41:A:C8	2.57	0.40
5:LC:5:ARG:HB3	5:LC:24:LEU:HB3	2.03	0.40
14:LM:38:VAL:O	14:LM:47:ARG:HA	2.21	0.40
18:LQ:154:LYS:HA	18:LQ:154:LYS:HD2	1.73	0.40
25:LY:3:PHE:HD2	74:L5:243:A:H5''	1.87	0.40
44:Pt:46:G:H8	44:Pt:46:G:O5'	2.04	0.40
51:SD:211:VAL:O	60:SR:20:TYR:OH	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:S2:311:C:H2'	73:S2:312:G:O4'	2.21	0.40
73:S2:318:A:N1	73:S2:333:G:C6	2.89	0.40
73:S2:588:G:H1'	73:S2:590:A:OP2	2.21	0.40
74:L5:106:A:H1'	74:L5:336:A:N3	2.37	0.40
74:L5:1777:C:H2'	74:L5:1778:C:C6	2.56	0.40
74:L5:1789:C:H2'	74:L5:1790:U:C6	2.56	0.40
74:L5:1954:U:H2'	74:L5:1955:G:C8	2.56	0.40
74:L5:3724:A2M:H1'	74:L5:3724:A2M:HM'3	1.88	0.40
74:L5:3765:G:O2'	74:L5:3767:C:N4	2.54	0.40
74:L5:4066:U:H2'	74:L5:4067:U:O4'	2.21	0.40
74:L5:4236:G:H4'	74:L5:4328:G:O2'	2.21	0.40
74:L5:4620:OMU:H6	74:L5:4620:OMU:O5'	2.22	0.40
5:LC:322:LEU:O	5:LC:326:LEU:HG	2.22	0.40
15:LN:5:LYS:HE2	15:LN:9:GLU:HG2	2.03	0.40
15:LN:77:LYS:NZ	74:L5:1626:G:OP2	2.46	0.40
15:LN:150:TRP:CH2	15:LN:151:ILE:HD12	2.56	0.40
17:LP:85:LYS:HE2	17:LP:89:GLU:OE2	2.22	0.40
32:Lf:24:HIS:O	32:Lf:87:LYS:HE2	2.20	0.40
32:Lf:51:TYR:CZ	32:Lf:68:ARG:HB2	2.56	0.40
45:SA:10:MET:HG3	45:SA:55:TRP:CG	2.55	0.40
49:SI:11:ARG:NH1	49:SI:15:GLY:O	2.45	0.40
62:ST:87:VAL:CG2	73:S2:1229:G:H21	2.34	0.40
67:SX:88:ASP:HA	73:S2:617:G:H4'	2.04	0.40
71:Se:109:ARG:HG3	80:SJ:124:HIS:CE1	2.57	0.40
73:S2:388:U:H2'	73:S2:389:A:H8	1.84	0.40
73:S2:1221:G:H2'	73:S2:1222:G:C8	2.56	0.40
74:L5:679:C:H2'	74:L5:680:G:C8	2.55	0.40
74:L5:978:G:H2'	74:L5:979:C:C6	2.55	0.40
74:L5:1392:A:H2'	74:L5:1393:G:C8	2.57	0.40
74:L5:2694:G:H5'	74:L5:2695:A:C2	2.56	0.40
74:L5:2699:C:H2'	74:L5:2700:G:C8	2.56	0.40
74:L5:4727:A:H2'	74:L5:4728:U:O4'	2.21	0.40
74:L5:4918:C:H2'	74:L5:4919:G:C8	2.56	0.40
74:L5:5010:PSU:H2'	74:L5:5011:A:H8	1.86	0.40
76:S6:4:G:H2'	76:S6:5:G:C8	2.56	0.40
5:LC:181:LYS:HZ3	74:L5:218:A:H3'	1.87	0.40
7:LE:123:ARG:HG2	74:L5:959:G:C8	2.57	0.40
21:LT:136:ARG:HH11	21:LT:136:ARG:HB3	1.86	0.40
34:Lh:13:LYS:HD3	34:Lh:13:LYS:HA	1.89	0.40
41:Lo:18:HIS:ND1	74:L5:4318:C:O2'	2.46	0.40
46:SB:162:ARG:HH22	73:S2:1005:G:P	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SF:68:ILE:HD11	48:SF:116:ILE:HD13	2.01	0.40
48:SF:87:LEU:HD21	59:SQ:47:LEU:HD11	2.03	0.40
48:SF:122:ARG:HE	48:SF:122:ARG:HB2	1.59	0.40
52:SE:211:LYS:NZ	52:SE:215:GLY:O	2.55	0.40
57:SO:43:HIS:ND1	57:SO:55:ARG:HD3	2.35	0.40
67:SX:88:ASP:OD1	73:S2:616:A:O2'	2.38	0.40
73:S2:163:U:O3'	77:SG:83:CYS:HA	2.21	0.40
73:S2:555:A:O2'	73:S2:556:U:H5'	2.21	0.40
73:S2:926:A:H2'	73:S2:927:C:O4'	2.21	0.40
73:S2:1073:U:H2'	73:S2:1074:C:C6	2.56	0.40
73:S2:1743:G:N2	73:S2:1791:A:H62	2.16	0.40
76:S6:12:G:H2'	76:S6:13:C:C6	2.55	0.40
76:S6:27:G:C6	76:S6:28:U:C4	3.10	0.40
11:LI:56:GLU:HG3	11:LI:162:ARG:H	1.85	0.40
17:LP:42:ARG:HD3	17:LP:42:ARG:HA	1.87	0.40
19:LR:4:LEU:HD12	74:L5:2386:U:H4'	2.04	0.40
21:LT:136:ARG:HB3	21:LT:136:ARG:NH1	2.37	0.40
23:LW:54:LEU:HD23	23:LW:54:LEU:HA	1.97	0.40
25:LY:43:ASN:HD22	25:LY:43:ASN:HA	1.76	0.40
42:Lp:49:ARG:NH2	74:L5:2739:C:OP2	2.52	0.40
46:SB:120:MET:HG3	46:SB:142:PHE:CE2	2.57	0.40
48:SF:167:LYS:HA	79:SZ:71:ALA:HB1	2.04	0.40
52:SE:170:THR:OG1	52:SE:171:ASP:N	2.55	0.40
62:ST:47:PRO:HB3	73:S2:1540:G:H5'	2.02	0.40
70:Sd:54:LYS:HA	70:Sd:54:LYS:HD3	1.97	0.40
73:S2:164:A:H2'	73:S2:165:G:N3	2.37	0.40
73:S2:1797:U:H2'	73:S2:1798:C:C6	2.57	0.40
74:L5:652:G:H2'	74:L5:653:U:C6	2.57	0.40
74:L5:1905:U:H2'	74:L5:1906:U:O4'	2.21	0.40
74:L5:4369:A:H2'	74:L5:4370:OMG:C8	2.57	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	
3	LA	244/254 (96%)	232 (95%)	12 (5%)	0	100	100
4	LB	385/396 (97%)	378 (98%)	7 (2%)	0	100	100
5	LC	355/427 (83%)	347 (98%)	8 (2%)	0	100	100
6	LD	282/297 (95%)	261 (93%)	21 (7%)	0	100	100
7	LE	190/288 (66%)	180 (95%)	10 (5%)	0	100	100
8	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
9	LG	207/266 (78%)	201 (97%)	6 (3%)	0	100	100
10	LH	187/189 (99%)	178 (95%)	9 (5%)	0	100	100
11	LI	197/213 (92%)	191 (97%)	6 (3%)	0	100	100
12	LJ	166/178 (93%)	158 (95%)	8 (5%)	0	100	100
13	LL	199/211 (94%)	193 (97%)	6 (3%)	0	100	100
14	LM	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
15	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
16	LO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
17	LP	151/154 (98%)	147 (97%)	4 (3%)	0	100	100
18	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
19	LR	152/196 (78%)	151 (99%)	1 (1%)	0	100	100
20	LS	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
21	LT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
22	LV	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
23	LW	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
24	LX	117/156 (75%)	115 (98%)	2 (2%)	0	100	100
25	LY	128/145 (88%)	128 (100%)	0	0	100	100
26	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
27	La	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
28	Lb	92/159 (58%)	89 (97%)	3 (3%)	0	100	100
29	Lc	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
30	Ld	103/125 (82%)	102 (99%)	1 (1%)	0	100	100
31	Le	126/129 (98%)	126 (100%)	0	0	100	100
32	Lf	107/110 (97%)	106 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Lg	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
34	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
35	Li	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
36	Lj	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
37	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
38	Ll	46/51 (90%)	44 (96%)	2 (4%)	0	100	100
39	Lm	48/127 (38%)	46 (96%)	2 (4%)	0	100	100
40	Ln	23/25 (92%)	23 (100%)	0	0	100	100
41	Lo	96/105 (91%)	94 (98%)	2 (2%)	0	100	100
42	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
43	Lr	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
45	SA	207/295 (70%)	196 (95%)	11 (5%)	0	100	100
46	SB	215/264 (81%)	210 (98%)	5 (2%)	0	100	100
47	SC	212/293 (72%)	206 (97%)	6 (3%)	0	100	100
48	SF	181/204 (89%)	169 (93%)	12 (7%)	0	100	100
49	SI	159/208 (76%)	154 (97%)	5 (3%)	0	100	100
51	SD	196/243 (81%)	181 (92%)	15 (8%)	0	100	100
52	SE	256/263 (97%)	240 (94%)	16 (6%)	0	100	100
53	SH	154/194 (79%)	144 (94%)	10 (6%)	0	100	100
54	SK	43/165 (26%)	35 (81%)	8 (19%)	0	100	100
55	SL	126/158 (80%)	121 (96%)	5 (4%)	0	100	100
56	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
57	SO	125/151 (83%)	118 (94%)	7 (6%)	0	100	100
58	SP	125/145 (86%)	120 (96%)	5 (4%)	0	100	100
59	SQ	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
60	SR	131/135 (97%)	122 (93%)	7 (5%)	2 (2%)	8	16
61	SS	145/152 (95%)	133 (92%)	12 (8%)	0	100	100
62	ST	142/145 (98%)	134 (94%)	8 (6%)	0	100	100
63	SU	69/119 (58%)	67 (97%)	2 (3%)	0	100	100
64	SV	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
65	SW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	SY	119/133 (90%)	103 (87%)	15 (13%)	1 (1%)	16	31
67	SX	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
68	Sb	65/84 (77%)	63 (97%)	2 (3%)	0	100	100
69	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
70	Sd	43/56 (77%)	42 (98%)	1 (2%)	0	100	100
71	Se	45/133 (34%)	42 (93%)	3 (7%)	0	100	100
72	Sg	249/317 (78%)	210 (84%)	39 (16%)	0	100	100
75	Sa	100/115 (87%)	94 (94%)	6 (6%)	0	100	100
77	SG	210/249 (84%)	198 (94%)	12 (6%)	0	100	100
78	LU	96/128 (75%)	81 (84%)	15 (16%)	0	100	100
79	SZ	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
80	SJ	176/194 (91%)	174 (99%)	1 (1%)	1 (1%)	21	38
All	All	10475/12413 (84%)	10040 (96%)	431 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	SR	65	PRO
60	SR	66	VAL
66	SY	103	SER
80	SJ	138	ARG

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	
3	LA	187/195 (96%)	185 (99%)	2 (1%)	65	84
4	LB	325/344 (94%)	318 (98%)	7 (2%)	45	73
5	LC	294/348 (84%)	291 (99%)	3 (1%)	68	86
6	LD	1/250 (0%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LE	168/252 (67%)	159 (95%)	9 (5%)	20	41
8	LF	189/215 (88%)	186 (98%)	3 (2%)	55	79
9	LG	152/223 (68%)	146 (96%)	6 (4%)	28	55
10	LH	150/169 (89%)	136 (91%)	14 (9%)	8	18
11	LI	169/180 (94%)	160 (95%)	9 (5%)	20	42
12	LJ	117/149 (78%)	99 (85%)	18 (15%)	2	5
13	LL	152/177 (86%)	146 (96%)	6 (4%)	28	55
14	LM	106/161 (66%)	102 (96%)	4 (4%)	29	56
15	LN	170/172 (99%)	167 (98%)	3 (2%)	51	77
16	LO	170/174 (98%)	167 (98%)	3 (2%)	51	77
17	LP	132/135 (98%)	128 (97%)	4 (3%)	36	64
18	LQ	160/165 (97%)	159 (99%)	1 (1%)	78	91
19	LR	127/175 (73%)	124 (98%)	3 (2%)	43	70
20	LS	156/157 (99%)	153 (98%)	3 (2%)	50	76
21	LT	138/140 (99%)	129 (94%)	9 (6%)	15	32
22	LV	100/107 (94%)	96 (96%)	4 (4%)	28	54
23	LW	52/126 (41%)	52 (100%)	0	100	100
24	LX	107/133 (80%)	105 (98%)	2 (2%)	50	76
25	LY	121/135 (90%)	118 (98%)	3 (2%)	42	69
26	LZ	98/118 (83%)	93 (95%)	5 (5%)	21	43
27	La	117/120 (98%)	112 (96%)	5 (4%)	26	51
28	Lb	62/125 (50%)	62 (100%)	0	100	100
29	Lc	76/97 (78%)	70 (92%)	6 (8%)	11	24
30	Ld	91/110 (83%)	88 (97%)	3 (3%)	33	61
31	Le	108/115 (94%)	107 (99%)	1 (1%)	70	87
32	Lf	88/89 (99%)	86 (98%)	2 (2%)	44	72
33	Lg	85/100 (85%)	83 (98%)	2 (2%)	43	70
34	Lh	108/110 (98%)	107 (99%)	1 (1%)	70	87
35	Li	83/89 (93%)	80 (96%)	3 (4%)	31	58
36	Lj	74/74 (100%)	73 (99%)	1 (1%)	59	81
37	Lk	31/65 (48%)	30 (97%)	1 (3%)	34	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Ll	43/48 (90%)	43 (100%)	0	100	100
39	Lm	43/115 (37%)	40 (93%)	3 (7%)	14	29
40	Ln	21/24 (88%)	21 (100%)	0	100	100
41	Lo	83/93 (89%)	82 (99%)	1 (1%)	63	83
42	Lp	74/75 (99%)	70 (95%)	4 (5%)	20	41
43	Lr	104/120 (87%)	102 (98%)	2 (2%)	50	76
45	SA	168/242 (69%)	158 (94%)	10 (6%)	17	36
46	SB	183/231 (79%)	173 (94%)	10 (6%)	19	40
47	SC	165/225 (73%)	155 (94%)	10 (6%)	17	35
48	SF	128/170 (75%)	123 (96%)	5 (4%)	28	55
49	SI	79/180 (44%)	76 (96%)	3 (4%)	29	56
51	SD	108/202 (54%)	96 (89%)	12 (11%)	6	12
52	SE	216/225 (96%)	205 (95%)	11 (5%)	21	43
53	SH	97/174 (56%)	89 (92%)	8 (8%)	10	23
54	SK	28/136 (21%)	27 (96%)	1 (4%)	31	58
55	SL	102/142 (72%)	100 (98%)	2 (2%)	48	75
56	SN	116/131 (88%)	115 (99%)	1 (1%)	70	87
57	SO	98/119 (82%)	92 (94%)	6 (6%)	17	35
58	SP	94/130 (72%)	85 (90%)	9 (10%)	8	17
59	SQ	110/121 (91%)	104 (94%)	6 (6%)	19	40
60	SR	59/122 (48%)	56 (95%)	3 (5%)	21	43
61	SS	112/132 (85%)	104 (93%)	8 (7%)	13	29
62	ST	93/115 (81%)	86 (92%)	7 (8%)	12	26
63	SU	5/107 (5%)	3 (60%)	2 (40%)	0	0
64	SV	60/67 (90%)	55 (92%)	5 (8%)	10	22
65	SW	107/113 (95%)	101 (94%)	6 (6%)	19	39
66	SY	95/115 (83%)	87 (92%)	8 (8%)	10	22
67	SX	111/115 (96%)	103 (93%)	8 (7%)	13	28
68	Sb	30/76 (40%)	30 (100%)	0	100	100
69	Sc	53/62 (86%)	49 (92%)	4 (8%)	12	26
70	Sd	35/49 (71%)	31 (89%)	4 (11%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	Se	34/104 (33%)	28 (82%)	6 (18%)	2	3
72	Sg	1/275 (0%)	0	1 (100%)	0	0
75	Sa	78/98 (80%)	73 (94%)	5 (6%)	16	33
77	SG	28/218 (13%)	28 (100%)	0	100	100
78	LU	55/115 (48%)	45 (82%)	10 (18%)	2	3
79	SZ	45/103 (44%)	42 (93%)	3 (7%)	15	31
80	SJ	148/168 (88%)	139 (94%)	9 (6%)	17	35
All	All	7673/10551 (73%)	7334 (96%)	339 (4%)	27	50

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LA	138	SER
3	LA	208	GLU
4	LB	90	VAL
4	LB	101	THR
4	LB	104	THR
4	LB	148	LYS
4	LB	152	SER
4	LB	310	SER
4	LB	395	ASP
5	LC	20	LYS
5	LC	173	LYS
5	LC	335	MET
7	LE	121	VAL
7	LE	143	SER
7	LE	201	ILE
7	LE	206	VAL
7	LE	210	LYS
7	LE	213	THR
7	LE	243	THR
7	LE	247	LYS
7	LE	255	SER
8	LF	39	GLN
8	LF	52	GLU
8	LF	127	LYS
9	LG	33	GLU
9	LG	85	GLN
9	LG	91	THR
9	LG	100	HIS

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Mol	Chain	Res	Type
9	LG	108	GLN
9	LG	159	HIS
10	LH	16	VAL
10	LH	23	ARG
10	LH	27	VAL
10	LH	33	THR
10	LH	35	ARG
10	LH	48	LEU
10	LH	53	LYS
10	LH	74	CYS
10	LH	111	LEU
10	LH	112	VAL
10	LH	115	ARG
10	LH	173	ARG
10	LH	177	ASP
10	LH	179	ILE
11	LI	33	ILE
11	LI	79	SER
11	LI	82	LYS
11	LI	113	THR
11	LI	136	MET
11	LI	148	VAL
11	LI	185	VAL
11	LI	187	GLU
11	LI	189	ARG
12	LJ	22	LEU
12	LJ	25	CYS
12	LJ	32	ARG
12	LJ	33	LEU
12	LJ	44	THR
12	LJ	47	THR
12	LJ	72	CYS
12	LJ	73	THR
12	LJ	74	VAL
12	LJ	82	ILE
12	LJ	87	LEU
12	LJ	88	LYS
12	LJ	96	LYS
12	LJ	109	ILE
12	LJ	112	HIS
12	LJ	122	SER
12	LJ	151	ILE

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Mol	Chain	Res	Type
12	LJ	161	GLU
13	LL	52	SER
13	LL	92	ARG
13	LL	106	SER
13	LL	111	GLN
13	LL	223	VAL
13	LL	226	LYS
14	LM	42	CYS
14	LM	61	ILE
14	LM	118	MET
14	LM	135	LEU
15	LN	5	LYS
15	LN	56	LYS
15	LN	60	VAL
16	LO	174	LEU
16	LO	179	LYS
16	LO	187	LYS
17	LP	23	ARG
17	LP	55	LYS
17	LP	113	VAL
17	LP	151	THR
18	LQ	77	ASN
19	LR	39	GLN
19	LR	127	VAL
19	LR	146	LYS
20	LS	2	LYS
20	LS	19	THR
20	LS	148	SER
21	LT	27	LEU
21	LT	36	LYS
21	LT	76	VAL
21	LT	108	ARG
21	LT	115	LYS
21	LT	124	THR
21	LT	126	VAL
21	LT	143	THR
21	LT	150	LEU
22	LV	13	LYS
22	LV	67	LYS
22	LV	128	LEU
22	LV	134	SER
24	LX	118	ASP

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Mol	Chain	Res	Type
24	LX	119	ILE
25	LY	14	ASN
25	LY	63	LYS
25	LY	124	LYS
26	LZ	53	VAL
26	LZ	78	ASN
26	LZ	107	LYS
26	LZ	124	THR
26	LZ	132	GLN
27	La	56	VAL
27	La	63	LEU
27	La	80	THR
27	La	85	GLN
27	La	88	VAL
29	Lc	16	SER
29	Lc	58	SER
29	Lc	71	VAL
29	Lc	94	LEU
29	Lc	104	ILE
29	Lc	105	ILE
30	Ld	55	LYS
30	Ld	63	ARG
30	Ld	87	ARG
31	Le	33	ARG
32	Lf	7	SER
32	Lf	31	GLU
33	Lg	48	VAL
33	Lg	65	MET
34	Lh	9	LEU
35	Li	12	ASN
35	Li	34	THR
35	Li	43	MET
36	Lj	55	ARG
37	Lk	69	LEU
39	Lm	84	GLN
39	Lm	85	LEU
39	Lm	127	VAL
41	Lo	32	SER
42	Lp	45	THR
42	Lp	72	ASN
42	Lp	89	LEU
42	Lp	90	LYS

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Mol	Chain	Res	Type
43	Lr	37	SER
43	Lr	63	VAL
45	SA	13	GLU
45	SA	16	LEU
45	SA	28	THR
45	SA	104	THR
45	SA	113	GLN
45	SA	123	VAL
45	SA	157	VAL
45	SA	177	MET
45	SA	189	ILE
45	SA	191	ARG
46	SB	3	VAL
46	SB	57	ILE
46	SB	75	GLN
46	SB	79	VAL
46	SB	89	GLU
46	SB	108	ASP
46	SB	112	SER
46	SB	130	THR
46	SB	195	LYS
46	SB	224	GLU
47	SC	73	MET
47	SC	120	GLN
47	SC	123	ARG
47	SC	149	THR
47	SC	160	LEU
47	SC	176	LYS
47	SC	222	CYS
47	SC	247	THR
47	SC	248	TYR
47	SC	254	ASP
48	SF	22	LYS
48	SF	33	ILE
48	SF	78	MET
48	SF	103	LEU
48	SF	125	SER
49	SI	4	SER
49	SI	45	THR
49	SI	59	ARG
51	SD	6	SER
51	SD	38	GLU

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Mol	Chain	Res	Type
51	SD	86	LEU
51	SD	91	VAL
51	SD	105	LEU
51	SD	128	GLU
51	SD	142	LEU
51	SD	156	LEU
51	SD	158	ILE
51	SD	170	THR
51	SD	175	VAL
51	SD	206	ASP
52	SE	12	VAL
52	SE	78	THR
52	SE	105	THR
52	SE	115	THR
52	SE	133	THR
52	SE	134	LYS
52	SE	136	ILE
52	SE	146	THR
52	SE	173	ILE
52	SE	199	GLU
52	SE	220	THR
53	SH	24	SER
53	SH	45	ILE
53	SH	60	ILE
53	SH	64	VAL
53	SH	91	HIS
53	SH	132	ASP
53	SH	163	GLN
53	SH	185	VAL
54	SK	61	GLN
55	SL	18	GLN
55	SL	78	THR
56	SN	76	LYS
57	SO	27	VAL
57	SO	52	THR
57	SO	70	SER
57	SO	80	ASP
57	SO	107	THR
57	SO	138	ASP
58	SP	11	THR
58	SP	26	LEU
58	SP	36	LEU

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Mol	Chain	Res	Type
58	SP	60	LEU
58	SP	75	VAL
58	SP	82	ASP
58	SP	85	ILE
58	SP	86	LEU
58	SP	103	ASN
59	SQ	18	THR
59	SQ	41	MET
59	SQ	62	ARG
59	SQ	67	ASP
59	SQ	110	ASP
59	SQ	146	ARG
60	SR	5	ARG
60	SR	6	THR
60	SR	22	THR
61	SS	4	VAL
61	SS	12	ILE
61	SS	34	LYS
61	SS	64	VAL
61	SS	75	ARG
61	SS	108	ARG
61	SS	130	ARG
61	SS	146	VAL
62	ST	5	THR
62	ST	15	VAL
62	ST	22	LEU
62	ST	34	VAL
62	ST	74	SER
62	ST	76	THR
62	ST	87	VAL
63	SU	112	VAL
63	SU	114	VAL
64	SV	42	VAL
64	SV	43	THR
64	SV	65	SER
64	SV	69	ILE
64	SV	80	SER
65	SW	20	ARG
65	SW	28	ARG
65	SW	49	GLU
65	SW	81	VAL
65	SW	107	SER

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Mol	Chain	Res	Type
65	SW	112	ASP
66	SY	6	THR
66	SY	13	MET
66	SY	26	ASP
66	SY	51	THR
66	SY	79	LEU
66	SY	80	ASP
66	SY	120	THR
66	SY	125	VAL
67	SX	26	GLN
67	SX	71	ARG
67	SX	72	VAL
67	SX	82	THR
67	SX	94	ILE
67	SX	105	PHE
67	SX	123	VAL
67	SX	129	SER
69	Sc	21	THR
69	Sc	23	SER
69	Sc	52	GLU
69	Sc	58	LEU
70	Sd	27	ARG
70	Sd	38	MET
70	Sd	53	ILE
70	Sd	54	LYS
71	Se	87	ARG
71	Se	95	LYS
71	Se	100	LYS
71	Se	115	ARG
71	Se	118	ASN
71	Se	132	ASN
72	Sg	309	VAL
75	Sa	21	ILE
75	Sa	25	ASN
75	Sa	36	ILE
75	Sa	52	ASP
75	Sa	69	VAL
78	LU	22	THR
78	LU	29	VAL
78	LU	49	VAL
78	LU	71	THR
78	LU	73	THR

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Mol	Chain	Res	Type
78	LU	74	SER
78	LU	76	VAL
78	LU	86	LEU
78	LU	89	LYS
78	LU	102	VAL
79	SZ	69	THR
79	SZ	76	ARG
79	SZ	92	LEU
80	SJ	2	PRO
80	SJ	14	VAL
80	SJ	29	LEU
80	SJ	62	THR
80	SJ	77	LEU
80	SJ	95	ASP
80	SJ	104	ASP
80	SJ	128	VAL
80	SJ	132	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
4	LB	208	ASN
5	LC	43	ASN
5	LC	89	GLN
5	LC	187	GLN
5	LC	203	GLN
7	LE	128	HIS
7	LE	135	GLN
7	LE	157	HIS
7	LE	266	GLN
8	LF	39	GLN
9	LG	82	GLN
10	LH	163	GLN
10	LH	169	ASN
11	LI	73	ASN
11	LI	144	ASN
11	LI	147	HIS
11	LI	177	ASN
12	LJ	42	GLN
14	LM	34	ASN
15	LN	29	GLN
15	LN	109	HIS

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Mol	Chain	Res	Type
16	LO	50	ASN
17	LP	97	ASN
17	LP	133	HIS
18	LQ	57	ASN
18	LQ	160	HIS
24	LX	69	ASN
24	LX	107	HIS
24	LX	111	GLN
25	LY	18	HIS
25	LY	40	GLN
25	LY	66	GLN
25	LY	86	GLN
27	La	93	ASN
29	Lc	15	ASN
34	Lh	20	GLN
35	Li	20	ASN
38	Ll	17	GLN
39	Lm	117	HIS
42	Lp	72	ASN
43	Lr	4	HIS
45	SA	29	ASN
45	SA	50	ASN
45	SA	131	HIS
45	SA	132	GLN
47	SC	115	GLN
48	SF	79	HIS
48	SF	95	HIS
52	SE	142	HIS
52	SE	157	ASN
52	SE	188	ASN
52	SE	201	HIS
53	SH	91	HIS
53	SH	97	GLN
53	SH	114	GLN
53	SH	165	ASN
55	SL	18	GLN
56	SN	62	GLN
58	SP	41	GLN
59	SQ	35	ASN
59	SQ	48	GLN
64	SV	49	GLN
65	SW	82	GLN

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Mol	Chain	Res	Type
66	SY	112	ASN
67	SX	23	HIS
67	SX	92	ASN
70	Sd	28	HIS
71	Se	89	GLN
71	Se	118	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L7	118/120 (98%)	13 (11%)	0
2	L8	148/156 (94%)	16 (10%)	0
44	Pt	72/77 (93%)	15 (20%)	0
50	mR	7/27 (25%)	1 (14%)	0
73	S2	1436/1869 (76%)	284 (19%)	8 (0%)
74	L5	3152/5069 (62%)	472 (14%)	9 (0%)
76	S6	72/77 (93%)	36 (50%)	0
All	All	5005/7395 (67%)	837 (16%)	17 (0%)

All (837) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L7	7	G
1	L7	24	C
1	L7	33	U
1	L7	41	G
1	L7	49	A
1	L7	54	A
1	L7	61	G
1	L7	63	C
1	L7	64	G
1	L7	70	G
1	L7	97	G
1	L7	100	A
1	L7	110	G
2	L8	23	C
2	L8	34	U
2	L8	35	C
2	L8	59	A
2	L8	62	A
2	L8	63	U

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Mol	Chain	Res	Type
2	L8	78	G
2	L8	82	A
2	L8	103	A
2	L8	105	C
2	L8	110	U
2	L8	111	U
2	L8	114	G
2	L8	123	U
2	L8	125	C
2	L8	150	C
44	Pt	6	G
44	Pt	8	4SU
44	Pt	9	G
44	Pt	16	C
44	Pt	19	G
44	Pt	20	G
44	Pt	26	C
44	Pt	47	G7M
44	Pt	53	G
44	Pt	58	A
44	Pt	64	G
44	Pt	65	G
44	Pt	69	C
44	Pt	70	C
44	Pt	71	G
50	mR	37	A
73	S2	17	C
73	S2	33	G
73	S2	41	G
73	S2	44	U
73	S2	46	A
73	S2	56	G
73	S2	59	U
73	S2	64	A
73	S2	65	C
73	S2	66	G
73	S2	69	C
73	S2	82	G
73	S2	83	A
73	S2	85	A
73	S2	103	A
73	S2	113	G

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Mol	Chain	Res	Type
73	S2	114	G
73	S2	115	U
73	S2	147	A
73	S2	155	G
73	S2	157	U
73	S2	162	C
73	S2	163	U
73	S2	170	A
73	S2	218	U
73	S2	291	G
73	S2	292	A
73	S2	293	C
73	S2	302	A
73	S2	311	C
73	S2	312	G
73	S2	313	A
73	S2	315	C
73	S2	316	G
73	S2	317	C
73	S2	335	G
73	S2	351	G
73	S2	360	A
73	S2	362	C
73	S2	363	A
73	S2	364	A
73	S2	368	U
73	S2	369	C
73	S2	370	G
73	S2	381	C
73	S2	385	G
73	S2	386	C
73	S2	393	U
73	S2	398	A
73	S2	409	C
73	S2	413	G
73	S2	434	G
73	S2	438	G
73	S2	441	C
73	S2	448	A
73	S2	449	A
73	S2	450	C
73	S2	452	G

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Mol	Chain	Res	Type
73	S2	461	U
73	S2	464	A
73	S2	465	A
73	S2	466	G
73	S2	471	G
73	S2	472	C
73	S2	473	A
73	S2	474	G
73	S2	482	G
73	S2	487	U
73	S2	488	U
73	S2	489	A
73	S2	490	C
73	S2	492	C
73	S2	500	A
73	S2	509	G
73	S2	512	A
73	S2	525	A
73	S2	527	C
73	S2	532	C
73	S2	550	C
73	S2	552	G
73	S2	553	U
73	S2	556	U
73	S2	557	U
73	S2	559	G
73	S2	563	G
73	S2	570	C
73	S2	583	C
73	S2	588	G
73	S2	589	G
73	S2	590	A
73	S2	591	U
73	S2	592	C
73	S2	595	U
73	S2	596	U
73	S2	604	A
73	S2	605	A
73	S2	606	G
73	S2	607	U
73	S2	608	C
73	S2	614	C

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Mol	Chain	Res	Type
73	S2	617	G
73	S2	618	C
73	S2	628	A
73	S2	629	A
73	S2	631	U
73	S2	632	C
73	S2	634	A
73	S2	643	A
73	S2	644	G
73	S2	655	A
73	S2	660	C
73	S2	668	A
73	S2	669	A
73	S2	671	A
73	S2	672	A
73	S2	673	G
73	S2	688	U
73	S2	689	U
73	S2	690	G
73	S2	811	A
73	S2	822	U
73	S2	827	A
73	S2	830	A
73	S2	842	C
73	S2	847	A
73	S2	859	G
73	S2	861	A
73	S2	866	U
73	S2	869	A
73	S2	870	A
73	S2	871	U
73	S2	872	A
73	S2	874	G
73	S2	913	A
73	S2	919	A
73	S2	920	A
73	S2	922	A
73	S2	930	C
73	S2	933	G
73	S2	971	G
73	S2	972	A
73	S2	990	A

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Mol	Chain	Res	Type
73	S2	992	A
73	S2	996	A
73	S2	999	G
73	S2	1002	U
73	S2	1017	U
73	S2	1023	A
73	S2	1027	A
73	S2	1083	A
73	S2	1084	A
73	S2	1085	C
73	S2	1087	A
73	S2	1109	C
73	S2	1114	U
73	S2	1115	U
73	S2	1116	C
73	S2	1117	C
73	S2	1119	A
73	S2	1121	G
73	S2	1132	C
73	S2	1133	A
73	S2	1139	C
73	S2	1153	C
73	S2	1154	U
73	S2	1155	U
73	S2	1157	G
73	S2	1181	A
73	S2	1195	A
73	S2	1207	G
73	S2	1208	A
73	S2	1212	G
73	S2	1215	C
73	S2	1221	G
73	S2	1224	G
73	S2	1242	U
73	S2	1243	U
73	S2	1251	A
73	S2	1253	A
73	S2	1256	G
73	S2	1257	G
73	S2	1259	A
73	S2	1265	A
73	S2	1270	G

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Mol	Chain	Res	Type
73	S2	1274	G
73	S2	1333	U
73	S2	1342	U
73	S2	1343	U
73	S2	1348	G
73	S2	1363	C
73	S2	1364	U
73	S2	1371	U
73	S2	1372	U
73	S2	1373	C
73	S2	1378	A
73	S2	1396	A
73	S2	1397	U
73	S2	1402	A
73	S2	1403	C
73	S2	1409	A
73	S2	1431	G
73	S2	1432	U
73	S2	1436	C
73	S2	1437	C
73	S2	1438	A
73	S2	1454	A
73	S2	1462	U
73	S2	1463	U
73	S2	1464	C
73	S2	1475	G
73	S2	1478	U
73	S2	1480	A
73	S2	1487	A
73	S2	1489	A
73	S2	1490	G
73	S2	1494	U
73	S2	1495	G
73	S2	1497	G
73	S2	1498	A
73	S2	1509	U
73	S2	1510	G
73	S2	1511	U
73	S2	1512	C
73	S2	1513	C
73	S2	1514	G
73	S2	1516	G

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Mol	Chain	Res	Type
73	S2	1520	G
73	S2	1521	C
73	S2	1522	A
73	S2	1533	A
73	S2	1544	C
73	S2	1546	G
73	S2	1548	G
73	S2	1551	U
73	S2	1567	G
73	S2	1569	A
73	S2	1574	C
73	S2	1576	G
73	S2	1580	A
73	S2	1588	A
73	S2	1589	A
73	S2	1599	U
73	S2	1600	G
73	S2	1604	G
73	S2	1621	U
73	S2	1623	A
73	S2	1643	U
73	S2	1644	C
73	S2	1648	G
73	S2	1654	G
73	S2	1662	U
73	S2	1663	A
73	S2	1664	A
73	S2	1665	G
73	S2	1671	G
73	S2	1675	A
73	S2	1683	C
73	S2	1695	A
73	S2	1698	C
73	S2	1701	C
73	S2	1721	U
73	S2	1722	G
73	S2	1727	G
73	S2	1730	U
73	S2	1731	A
73	S2	1732	G
73	S2	1734	G
73	S2	1745	A

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Mol	Chain	Res	Type
73	S2	1793	A
73	S2	1798	C
73	S2	1820	G
73	S2	1822	A
73	S2	1823	A
73	S2	1829	G
73	S2	1831	A
73	S2	1838	U
73	S2	1849	G
73	S2	1850	A
73	S2	1851	A
73	S2	1861	G
73	S2	1862	G
73	S2	1863	A
73	S2	1865	C
73	S2	1869	A
74	L5	2	G
74	L5	3	C
74	L5	13	U
74	L5	15	A
74	L5	39	A
74	L5	42	A
74	L5	48	G
74	L5	59	A
74	L5	64	A
74	L5	65	A
74	L5	72	C
74	L5	73	A
74	L5	85	G
74	L5	91	G
74	L5	98	A
74	L5	108	A
74	L5	109	G
74	L5	110	C
74	L5	119	G
74	L5	120	A
74	L5	122	U
74	L5	159	C
74	L5	195	C
74	L5	200	U
74	L5	210	C
74	L5	218	A

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Mol	Chain	Res	Type
74	L5	233	U
74	L5	234	G
74	L5	274	C
74	L5	277	G
74	L5	280	G
74	L5	306	A
74	L5	315	G
74	L5	316	U
74	L5	340	C
74	L5	387	G
74	L5	409	G
74	L5	410	A
74	L5	412	G
74	L5	413	G
74	L5	414	C
74	L5	432	U
74	L5	449	C
74	L5	462	G
74	L5	467	U
74	L5	468	U
74	L5	469	C
74	L5	473	C
74	L5	477	C
74	L5	485	C
74	L5	489	C
74	L5	499	G
74	L5	509	A
74	L5	510	U
74	L5	652	G
74	L5	654	C
74	L5	683	C
74	L5	685	C
74	L5	686	A
74	L5	687	U
74	L5	694	C
74	L5	695	G
74	L5	704	C
74	L5	706	C
74	L5	729	G
74	L5	730	G
74	L5	731	G
74	L5	752	G

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Mol	Chain	Res	Type
74	L5	760	G
74	L5	915	A
74	L5	917	A
74	L5	926	G
74	L5	932	A
74	L5	933	G
74	L5	936	C
74	L5	937	U
74	L5	941	C
74	L5	944	A
74	L5	945	U
74	L5	946	C
74	L5	956	A
74	L5	959	G
74	L5	960	A
74	L5	961	G
74	L5	976	G
74	L5	1210	C
74	L5	1267	C
74	L5	1279	A
74	L5	1280	C
74	L5	1284	G
74	L5	1285	U
74	L5	1287	G
74	L5	1294	A
74	L5	1297	U
74	L5	1302	U
74	L5	1303	A
74	L5	1304	C
74	L5	1313	C
74	L5	1326	A2M
74	L5	1337	A
74	L5	1354	A
74	L5	1359	G
74	L5	1365	C
74	L5	1366	G
74	L5	1377	G
74	L5	1378	C
74	L5	1379	C
74	L5	1387	A
74	L5	1397	A
74	L5	1398	A

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Mol	Chain	Res	Type
74	L5	1399	G
74	L5	1403	G
74	L5	1407	C
74	L5	1410	U
74	L5	1411	C
74	L5	1415	G
74	L5	1420	A
74	L5	1450	C
74	L5	1457	G
74	L5	1476	C
74	L5	1477	C
74	L5	1498	G
74	L5	1502	G
74	L5	1534	A2M
74	L5	1547	A
74	L5	1566	C
74	L5	1578	U
74	L5	1591	U
74	L5	1596	U
74	L5	1614	C
74	L5	1624	G
74	L5	1625	OMG
74	L5	1626	G
74	L5	1631	A
74	L5	1633	G
74	L5	1634	A
74	L5	1638	A
74	L5	1640	C
74	L5	1641	G
74	L5	1654	G
74	L5	1661	C
74	L5	1676	C
74	L5	1677	PSU
74	L5	1691	G
74	L5	1694	C
74	L5	1720	C
74	L5	1721	G
74	L5	1724	G
74	L5	1734	G
74	L5	1741	G
74	L5	1750	G
74	L5	1755	C

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Mol	Chain	Res	Type
74	L5	1756	U
74	L5	1759	G
74	L5	1761	G
74	L5	1765	A
74	L5	1766	A
74	L5	1767	A
74	L5	1768	C
74	L5	1785	C
74	L5	1787	A
74	L5	1789	C
74	L5	1803	G
74	L5	1804	A
74	L5	1819	G
74	L5	1821	G
74	L5	1822	U
74	L5	1836	G
74	L5	1837	A
74	L5	1842	G
74	L5	1855	G
74	L5	1869	G
74	L5	1897	A
74	L5	1906	U
74	L5	1918	U
74	L5	1919	G
74	L5	1920	C
74	L5	1921	C
74	L5	1922	G
74	L5	1925	G
74	L5	1931	C
74	L5	1932	A
74	L5	1945	G
74	L5	1948	G
74	L5	1959	U
74	L5	1961	G
74	L5	1966	C
74	L5	1967	A
74	L5	1968	G
74	L5	1969	G
74	L5	2018	C
74	L5	2019	C
74	L5	2022	C
74	L5	2025	A

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Mol	Chain	Res	Type
74	L5	2026	A
74	L5	2042	A
74	L5	2046	G
74	L5	2048	U
74	L5	2055	G
74	L5	2056	G
74	L5	2069	A
74	L5	2092	G
74	L5	2257	C
74	L5	2289	C
74	L5	2300	A
74	L5	2301	G
74	L5	2313	A
74	L5	2314	G
74	L5	2316	G
74	L5	2333	G
74	L5	2348	G
74	L5	2351	OMC
74	L5	2360	A
74	L5	2395	A
74	L5	2397	G
74	L5	2398	U
74	L5	2421	G
74	L5	2434	G
74	L5	2450	G
74	L5	2469	C
74	L5	2470	C
74	L5	2474	G
74	L5	2475	G
74	L5	2476	G
74	L5	2503	G
74	L5	2504	C
74	L5	2505	C
74	L5	2506	G
74	L5	2513	A
74	L5	2519	U
74	L5	2520	C
74	L5	2554	U
74	L5	2583	C
74	L5	2587	A
74	L5	2589	C
74	L5	2601	A

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Mol	Chain	Res	Type
74	L5	2638	G
74	L5	2653	C
74	L5	2660	A
74	L5	2662	G
74	L5	2669	C
74	L5	2687	U
74	L5	2694	G
74	L5	2695	A
74	L5	2696	A
74	L5	2706	G
74	L5	2708	U
74	L5	2709	C
74	L5	2710	C
74	L5	2711	G
74	L5	2721	G
74	L5	2725	A
74	L5	2728	U
74	L5	2735	G
74	L5	2739	C
74	L5	2743	A
74	L5	2754	G
74	L5	2760	G
74	L5	2761	U
74	L5	2763	U
74	L5	2764	A
74	L5	2770	C
74	L5	2787	A
74	L5	2788	U
74	L5	2790	U
74	L5	2798	A
74	L5	2814	C
74	L5	2815	A2M
74	L5	2826	U
74	L5	2827	G
74	L5	2855	G
74	L5	2856	C
74	L5	2877	G
74	L5	3605	C
74	L5	3615	G
74	L5	3616	U
74	L5	3618	C
74	L5	3626	G

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Mol	Chain	Res	Type
74	L5	3635	A
74	L5	3644	U
74	L5	3662	A
74	L5	3664	G
74	L5	3673	C
74	L5	3710	G
74	L5	3711	A
74	L5	3712	A
74	L5	3714	G
74	L5	3748	A
74	L5	3753	G
74	L5	3754	G
74	L5	3760	A
74	L5	3776	G
74	L5	3777	G
74	L5	3780	G
74	L5	3783	A
74	L5	3784	A
74	L5	3785	A2M
74	L5	3788	C
74	L5	3811	G
74	L5	3812	C
74	L5	3814	U
74	L5	3817	A
74	L5	3819	G
74	L5	3838	U
74	L5	3840	U
74	L5	3876	A
74	L5	3877	A
74	L5	3878	C
74	L5	3879	G
74	L5	3897	G
74	L5	3901	A
74	L5	3906	A
74	L5	3907	G
74	L5	3915	U
74	L5	3944	OMG
74	L5	3946	G
74	L5	4066	U
74	L5	4070	U
74	L5	4076	G
74	L5	4084	G

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Mol	Chain	Res	Type
74	L5	4091	G
74	L5	4092	G
74	L5	4119	C
74	L5	4121	G
74	L5	4122	G
74	L5	4127	A
74	L5	4158	C
74	L5	4162	C
74	L5	4163	U
74	L5	4164	C
74	L5	4170	A
74	L5	4183	G
74	L5	4184	G
74	L5	4191	G
74	L5	4203	A
74	L5	4214	A
74	L5	4222	G
74	L5	4228	OMG
74	L5	4229	U
74	L5	4233	A
74	L5	4250	G
74	L5	4251	A
74	L5	4253	A
74	L5	4254	G
74	L5	4255	A
74	L5	4256	A
74	L5	4261	C
74	L5	4266	G
74	L5	4268	A
74	L5	4273	A
74	L5	4281	A
74	L5	4291	G
74	L5	4305	G
74	L5	4314	C
74	L5	4329	G
74	L5	4330	G
74	L5	4332	C
74	L5	4373	G
74	L5	4376	A
74	L5	4377	G
74	L5	4378	A
74	L5	4379	A

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Mol	Chain	Res	Type
74	L5	4380	A
74	L5	4387	C
74	L5	4391	G
74	L5	4394	A
74	L5	4405	G
74	L5	4410	G
74	L5	4421	C
74	L5	4422	A
74	L5	4426	C
74	L5	4427	G
74	L5	4433	G
74	L5	4440	G
74	L5	4444	C
74	L5	4448	G
74	L5	4464	A
74	L5	4465	U
74	L5	4500	PSU
74	L5	4512	U
74	L5	4513	A
74	L5	4515	G
74	L5	4519	C
74	L5	4524	G
74	L5	4548	A
74	L5	4557	U
74	L5	4560	C
74	L5	4567	G
74	L5	4573	G
74	L5	4574	U
74	L5	4575	G
74	L5	4584	A
74	L5	4590	A2M
74	L5	4600	G
74	L5	4601	U
74	L5	4636	PSU
74	L5	4637	OMG
74	L5	4652	G
74	L5	4656	A
74	L5	4657	U
74	L5	4670	C
74	L5	4672	A
74	L5	4687	A
74	L5	4693	C

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Mol	Chain	Res	Type
74	L5	4694	G
74	L5	4695	C
74	L5	4700	A
74	L5	4708	A
74	L5	4709	U
74	L5	4719	G
74	L5	4722	G
74	L5	4730	C
74	L5	4731	G
74	L5	4732	G
74	L5	4733	C
74	L5	4734	A
74	L5	4740	G
74	L5	4741	C
74	L5	4742	G
74	L5	4743	G
74	L5	4745	G
74	L5	4750	G
74	L5	4754	G
74	L5	4757	C
74	L5	4759	C
74	L5	4761	G
74	L5	4765	G
74	L5	4770	U
74	L5	4771	C
74	L5	4775	C
74	L5	4860	G
74	L5	4861	G
74	L5	4862	G
74	L5	4870	G
74	L5	4871	C
74	L5	4875	G
74	L5	4876	U
74	L5	4882	U
74	L5	4883	C
74	L5	4885	U
74	L5	4889	G
74	L5	4895	C
74	L5	4896	G
74	L5	4899	G
74	L5	4900	C
74	L5	4907	G

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Mol	Chain	Res	Type
74	L5	4908	G
74	L5	4910	G
74	L5	4912	G
74	L5	4913	G
74	L5	4914	C
74	L5	4917	C
74	L5	4921	C
74	L5	4922	C
74	L5	4925	U
74	L5	4934	A
74	L5	4937	C
74	L5	4943	A
74	L5	4951	G
74	L5	4952	G
74	L5	4953	G
74	L5	4956	A
74	L5	4976	U
74	L5	4994	G
74	L5	5007	A
74	L5	5017	G
74	L5	5041	G
74	L5	5050	C
74	L5	5054	C
74	L5	5055	G
74	L5	5058	A
74	L5	5069	U
76	S6	8	4SU
76	S6	10	G
76	S6	11	A
76	S6	16	C
76	S6	18	C
76	S6	19	G
76	S6	20	G
76	S6	21	U
76	S6	22	A
76	S6	23	G
76	S6	25	U
76	S6	27	G
76	S6	28	U
76	S6	31	G
76	S6	32	G
76	S6	36	A

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Mol	Chain	Res	Type
76	S6	37	U
76	S6	43	G
76	S6	46	G
76	S6	47	G7M
76	S6	50	G
76	S6	51	U
76	S6	56	PSU
76	S6	57	C
76	S6	58	A
76	S6	59	A
76	S6	60	A
76	S6	61	U
76	S6	63	C
76	S6	64	G
76	S6	65	G
76	S6	67	C
76	S6	68	C
76	S6	69	C
76	S6	73	A
76	S6	76	C

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
73	S2	146	G
73	S2	156	G
73	S2	604	A
73	S2	671	A
73	S2	868	G
73	S2	912	C
73	S2	1342	U
73	S2	1395	C
74	L5	955	G
74	L5	1590	C
74	L5	1625	OMG
74	L5	1633	G
74	L5	1754	U
74	L5	2055	G
74	L5	3876	A
74	L5	4378	A
74	L5	4699	U

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

140 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$
74	UR3	L5	4530	74	19,22,23	2.72	8 (42%)	26,32,35	1.36	3 (11%)
74	PSU	L5	4493	74,82	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	L5	4312	74	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
74	PSU	L5	1782	74	18,21,22	1.01	1 (5%)	22,30,33	1.74	3 (13%)
74	PSU	L5	1792	74	18,21,22	1.01	1 (5%)	22,30,33	1.71	4 (18%)
74	PSU	L5	3884	74	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
74	OMG	L5	3899	74,81	23,26,27	2.41	8 (34%)	33,38,41	2.19	10 (30%)
74	PSU	L5	4471	74	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)
74	OMU	L5	4620	74	19,22,23	2.83	8 (42%)	26,31,34	1.56	5 (19%)
74	OMG	L5	2424	74	23,26,27	2.42	8 (34%)	33,38,41	2.21	9 (27%)
74	5MC	L5	4447	74,82	18,22,23	3.45	7 (38%)	26,32,35	1.11	1 (3%)
74	OMC	L5	3701	74,82	19,22,23	2.90	8 (42%)	26,31,34	0.90	0
74	OMU	L5	4498	74	19,22,23	2.93	8 (42%)	26,31,34	1.71	5 (19%)
74	OMG	L5	4494	74	23,26,27	2.41	8 (34%)	33,38,41	2.23	10 (30%)
74	OMG	L5	2364	74	23,26,27	2.37	8 (34%)	33,38,41	2.15	8 (24%)
74	A2M	L5	3718	74	22,25,26	3.89	10 (45%)	31,36,39	3.59	14 (45%)
74	OMG	L5	1316	74	23,26,27	2.43	8 (34%)	33,38,41	2.25	10 (30%)
74	PSU	L5	4403	74	18,21,22	1.02	1 (5%)	22,30,33	1.77	5 (22%)
74	OMG	L5	4623	74	23,26,27	2.44	8 (34%)	33,38,41	2.28	10 (30%)
74	A2M	L5	1524	74	22,25,26	3.95	9 (40%)	31,36,39	3.81	12 (38%)
74	A2M	L5	3723	74	22,25,26	3.96	11 (50%)	31,36,39	3.72	14 (45%)
74	PSU	L5	4532	74	18,21,22	1.12	1 (5%)	22,30,33	1.66	4 (18%)
74	A2M	L5	2815	74	22,25,26	3.92	10 (45%)	31,36,39	3.65	14 (45%)
76	G7M	S6	47	76	23,26,27	2.78	8 (34%)	35,39,42	2.24	10 (28%)
74	OMC	L5	2824	74	19,22,23	2.96	8 (42%)	26,31,34	0.79	0
74	PSU	L5	5010	74	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	A2M	L5	400	74	22,25,26	3.94	11 (50%)	31,36,39	3.67	13 (41%)
74	1MA	L5	1322	74,81	21,25,26	2.78	6 (28%)	31,37,40	1.64	5 (16%)
74	PSU	L5	4353	74	18,21,22	1.03	1 (5%)	22,30,33	1.88	4 (18%)
74	OMC	L5	2861	74	19,22,23	2.98	8 (42%)	26,31,34	0.89	1 (3%)
74	PSU	L5	4457	74	18,21,22	1.09	1 (5%)	22,30,33	1.60	4 (18%)
74	PSU	L5	1860	74	18,21,22	1.00	1 (5%)	22,30,33	1.82	4 (18%)
74	PSU	L5	3853	74,81	18,21,22	1.03	1 (5%)	22,30,33	1.66	3 (13%)
74	PSU	L5	1781	74	18,21,22	1.02	1 (5%)	22,30,33	1.69	4 (18%)
44	PSU	Pt	56	44	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
74	PSU	L5	3758	74	18,21,22	1.01	1 (5%)	22,30,33	1.65	3 (13%)
74	OMU	L5	3925	74	19,22,23	2.96	8 (42%)	26,31,34	1.76	5 (19%)
74	OMG	L5	1522	74	23,26,27	2.44	8 (34%)	33,38,41	2.29	11 (33%)
74	PSU	L5	4431	74,81	18,21,22	1.08	1 (5%)	22,30,33	1.79	3 (13%)
74	OMG	L5	4618	74	23,26,27	2.42	8 (34%)	33,38,41	2.30	10 (30%)
74	A2M	L5	1871	74,82	22,25,26	3.87	12 (54%)	31,36,39	3.63	15 (48%)
74	PSU	L5	4689	74	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
74	PSU	L5	4673	74,81	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
74	OMG	L5	3627	74	23,26,27	2.42	8 (34%)	33,38,41	2.26	10 (30%)
74	OMC	L5	1340	74	19,22,23	2.86	8 (42%)	26,31,34	0.66	0
74	OMC	L5	2351	74	19,22,23	2.96	8 (42%)	26,31,34	0.80	1 (3%)
74	PSU	L5	3768	74	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
74	OMG	L5	4370	74	23,26,27	2.41	8 (34%)	33,38,41	2.23	9 (27%)
74	PSU	L5	4442	74	18,21,22	1.08	1 (5%)	22,30,33	1.81	6 (27%)
74	OMC	L5	4456	74	19,22,23	2.89	8 (42%)	26,31,34	0.77	0
74	PSU	L5	1683	74,82	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
74	PSU	L5	4531	74	18,21,22	1.11	1 (5%)	22,30,33	1.86	5 (22%)
74	OMC	L5	4536	74	19,22,23	2.95	8 (42%)	26,31,34	0.74	0
74	A2M	L5	4571	74	22,25,26	3.97	10 (45%)	31,36,39	3.61	15 (48%)
74	OMG	L5	3944	74	23,26,27	2.43	8 (34%)	33,38,41	2.19	9 (27%)
28	MLZ	Lb	5	28	8,9,10	0.80	0	4,9,11	0.58	0
74	PSU	L5	3770	74	18,21,22	1.01	1 (5%)	22,30,33	1.70	4 (18%)
74	6MZ	L5	4220	74	22,25,26	2.72	3 (13%)	30,36,39	3.50	11 (36%)
76	PSU	S6	56	76	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
74	A2M	L5	4590	74	22,25,26	3.94	11 (50%)	31,36,39	3.69	15 (48%)
74	OMC	L5	3887	74	19,22,23	2.94	8 (42%)	26,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OMC	L5	3808	74	19,22,23	2.98	8 (42%)	26,31,34	0.81	1 (3%)
74	PSU	L5	4576	74	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
74	PSU	L5	5001	74	18,21,22	1.03	1 (5%)	22,30,33	1.71	3 (13%)
4	HIC	LB	245	4	10,11,12	0.58	0	8,14,16	0.35	0
74	OMU	L5	2415	74	19,22,23	2.99	8 (42%)	26,31,34	1.74	4 (15%)
74	PSU	L5	3695	74	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
74	A2M	L5	2363	74,81	22,25,26	3.95	12 (54%)	31,36,39	3.56	13 (41%)
27	V5N	La	39	27	9,11,12	2.77	2 (22%)	9,14,16	1.40	2 (22%)
74	PSU	L5	4552	74	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
74	PSU	L5	4420	74	18,21,22	1.03	1 (5%)	22,30,33	1.61	4 (18%)
2	OMG	L8	75	2	23,26,27	2.43	8 (34%)	33,38,41	2.18	10 (30%)
74	A2M	L5	1326	74	22,25,26	3.93	11 (50%)	31,36,39	3.56	14 (45%)
74	PSU	L5	1677	74,81	18,21,22	1.13	1 (5%)	22,30,33	1.81	4 (18%)
74	PSU	L5	3637	74,81	18,21,22	1.08	1 (5%)	22,30,33	1.75	2 (9%)
74	PSU	L5	4299	74	18,21,22	1.05	1 (5%)	22,30,33	1.72	2 (9%)
74	PSU	L5	4579	74	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
74	OMG	L5	4637	74,82	23,26,27	2.41	7 (30%)	33,38,41	2.22	9 (27%)
74	PSU	L5	4423	74	18,21,22	1.07	1 (5%)	22,30,33	1.68	4 (18%)
76	4SU	S6	8	76	18,21,22	3.81	8 (44%)	26,30,33	2.33	6 (23%)
74	5MC	L5	3782	74,81	18,22,23	3.42	7 (38%)	26,32,35	1.10	2 (7%)
74	A2M	L5	3825	74	22,25,26	3.88	10 (45%)	31,36,39	3.47	14 (45%)
74	PSU	L5	1744	74,82	18,21,22	1.12	1 (5%)	22,30,33	1.83	4 (18%)
2	PSU	L8	69	2	18,21,22	1.03	1 (5%)	22,30,33	1.68	5 (22%)
74	PSU	L5	1779	74	18,21,22	1.11	1 (5%)	22,30,33	1.80	5 (22%)
74	PSU	L5	4500	74	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
74	PSU	L5	4293	74	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
74	OMG	L5	3792	74	23,26,27	2.40	8 (34%)	33,38,41	2.16	10 (30%)
74	PSU	L5	4569	74	18,21,22	1.17	1 (5%)	22,30,33	1.68	3 (13%)
74	A2M	L5	3830	74	22,25,26	3.91	11 (50%)	31,36,39	3.66	14 (45%)
74	PSU	L5	4636	74	18,21,22	1.17	1 (5%)	22,30,33	1.70	4 (18%)
74	OMU	L5	4306	74	19,22,23	2.95	8 (42%)	26,31,34	1.68	5 (19%)
74	PSU	L5	4972	74	18,21,22	1.00	1 (5%)	22,30,33	1.74	4 (18%)
74	PSU	L5	3762	74	18,21,22	1.08	1 (5%)	22,30,33	1.67	4 (18%)
74	OMG	L5	4499	74	23,26,27	2.43	9 (39%)	33,38,41	2.28	9 (27%)
74	OMG	L5	1625	74,82	23,26,27	2.44	8 (34%)	33,38,41	2.18	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	PSU	L5	2508	74	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
74	OMG	L5	4196	74	23,26,27	2.44	8 (34%)	33,38,41	2.27	10 (30%)
74	OMG	L5	4392	74	23,26,27	2.43	8 (34%)	33,38,41	2.23	10 (30%)
74	PSU	L5	4361	74	18,21,22	1.03	1 (5%)	22,30,33	1.74	3 (13%)
44	G7M	Pt	47	44	23,26,27	2.74	8 (34%)	35,39,42	2.32	10 (28%)
74	PSU	L5	2843	74	18,21,22	1.04	1 (5%)	22,30,33	1.70	3 (13%)
74	PSU	L5	1862	74	18,21,22	1.13	1 (5%)	22,30,33	1.78	2 (9%)
74	UY1	L5	3818	74,81,82	19,22,23	4.12	9 (47%)	22,31,34	2.09	5 (22%)
74	OMC	L5	3869	74	19,22,23	2.96	8 (42%)	26,31,34	0.76	0
74	PSU	L5	3734	74	18,21,22	0.94	1 (5%)	22,30,33	1.79	4 (18%)
74	OMU	L5	2837	74	19,22,23	2.95	8 (42%)	26,31,34	1.78	5 (19%)
3	V5N	LA	216	3	9,11,12	2.78	2 (22%)	9,14,16	1.33	1 (11%)
44	OMC	Pt	33	44	19,22,23	3.01	8 (42%)	26,31,34	1.00	1 (3%)
74	PSU	L5	3851	74	18,21,22	1.09	1 (5%)	22,30,33	1.68	3 (13%)
74	A2M	L5	1534	74,81	22,25,26	3.91	11 (50%)	31,36,39	3.69	16 (51%)
74	PSU	L5	3764	74	18,21,22	0.96	1 (5%)	22,30,33	1.80	4 (18%)
74	A2M	L5	4523	74,81	22,25,26	3.88	10 (45%)	31,36,39	3.52	15 (48%)
74	PSU	L5	1582	74	18,21,22	1.06	1 (5%)	22,30,33	1.63	3 (13%)
74	OMG	L5	3744	74	23,26,27	2.44	7 (30%)	33,38,41	2.25	10 (30%)
74	A2M	L5	3867	74	22,25,26	3.93	11 (50%)	31,36,39	3.64	12 (38%)
74	A2M	L5	2401	74	22,25,26	3.90	11 (50%)	31,36,39	3.67	15 (48%)
74	PSU	L5	4521	74,81,82	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
74	PSU	L5	2632	74	18,21,22	1.06	1 (5%)	22,30,33	1.84	5 (22%)
44	4SU	Pt	8	44	18,21,22	3.77	8 (44%)	26,30,33	2.18	4 (15%)
74	PSU	L5	1536	74	18,21,22	1.09	1 (5%)	22,30,33	1.99	5 (22%)
74	A2M	L5	398	74	22,25,26	3.87	10 (45%)	31,36,39	3.79	15 (48%)
74	A2M	L5	3724	74	22,25,26	3.95	10 (45%)	31,36,39	3.67	15 (48%)
74	PSU	L5	3920	74,81	18,21,22	1.12	1 (5%)	22,30,33	1.85	4 (18%)
74	PSU	L5	3844	74	18,21,22	1.12	1 (5%)	22,30,33	1.74	4 (18%)
74	OMC	L5	3841	74	19,22,23	2.94	8 (42%)	26,31,34	0.68	0
2	PSU	L8	55	2	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
74	OMG	L5	4228	74	23,26,27	2.43	8 (34%)	33,38,41	2.32	10 (30%)
74	OMC	L5	2365	74	19,22,23	2.98	8 (42%)	26,31,34	0.83	0
74	PSU	L5	3639	74	18,21,22	1.08	1 (5%)	22,30,33	1.91	4 (18%)
74	A2M	L5	3785	74	22,25,26	3.91	11 (50%)	31,36,39	3.66	15 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	OMC	L5	1881	74,81	19,22,23	2.87	8 (42%)	26,31,34	0.79	0
74	PSU	L5	2839	74	18,21,22	1.15	1 (5%)	22,30,33	1.76	4 (18%)
74	PSU	L5	4628	74	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
74	OMC	L5	2804	74	19,22,23	2.94	8 (42%)	26,31,34	0.65	0
74	PSU	L5	3729	74	18,21,22	1.10	1 (5%)	22,30,33	1.75	4 (18%)
74	PSU	L5	3715	74,81	18,21,22	0.99	1 (5%)	22,30,33	1.57	3 (13%)
74	OMC	L5	2422	74,81	19,22,23	2.87	8 (42%)	26,31,34	0.68	0
74	OMU	L5	4227	74	19,22,23	3.02	8 (42%)	26,31,34	1.75	4 (15%)
74	PSU	L5	4296	74	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)

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
74	UR3	L5	4530	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4493	74,82	-	0/7/25/26	0/2/2/2
74	PSU	L5	4312	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	1782	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	1792	74	-	2/7/25/26	0/2/2/2
74	PSU	L5	3884	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	3899	74,81	-	0/9/27/28	0/3/3/3
74	PSU	L5	4471	74	-	0/7/25/26	0/2/2/2
74	OMU	L5	4620	74	-	0/9/27/28	0/2/2/2
74	OMG	L5	2424	74	-	0/9/27/28	0/3/3/3
74	5MC	L5	4447	74,82	-	4/7/25/26	0/2/2/2
74	OMC	L5	3701	74,82	-	4/9/27/28	0/2/2/2
74	OMU	L5	4498	74	-	0/9/27/28	0/2/2/2
74	OMG	L5	4494	74	-	1/9/27/28	0/3/3/3
74	OMG	L5	2364	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	3718	74	-	1/9/27/28	0/3/3/3
74	OMG	L5	1316	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4403	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	4623	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	1524	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	3723	74	-	3/9/27/28	0/3/3/3
74	PSU	L5	4532	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	2815	74	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	G7M	S6	47	76	-	2/7/25/26	0/3/3/3
74	OMC	L5	2824	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	5010	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	400	74	-	0/9/27/28	0/3/3/3
74	1MA	L5	1322	74,81	-	2/7/25/26	0/3/3/3
74	PSU	L5	4353	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	2861	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4457	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	1860	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3853	74,81	-	0/7/25/26	0/2/2/2
74	PSU	L5	1781	74	-	2/7/25/26	0/2/2/2
44	PSU	Pt	56	44	-	1/7/25/26	0/2/2/2
74	PSU	L5	3758	74	-	2/7/25/26	0/2/2/2
74	OMU	L5	3925	74	-	1/9/27/28	0/2/2/2
74	OMG	L5	1522	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4431	74,81	-	0/7/25/26	0/2/2/2
74	OMG	L5	4618	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	1871	74,82	-	0/9/27/28	0/3/3/3
74	PSU	L5	4689	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4673	74,81	-	0/7/25/26	0/2/2/2
74	OMG	L5	3627	74	-	0/9/27/28	0/3/3/3
74	OMC	L5	1340	74	-	0/9/27/28	0/2/2/2
74	OMC	L5	2351	74	-	2/9/27/28	0/2/2/2
74	PSU	L5	3768	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	4370	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4442	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	4456	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	1683	74,82	-	0/7/25/26	0/2/2/2
74	PSU	L5	4531	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	4536	74	-	0/9/27/28	0/2/2/2
74	A2M	L5	4571	74	-	2/9/27/28	0/3/3/3
74	OMG	L5	3944	74	-	3/9/27/28	0/3/3/3
28	MLZ	Lb	5	28	-	1/7/8/10	-
74	PSU	L5	3770	74	-	0/7/25/26	0/2/2/2
74	6MZ	L5	4220	74	-	0/9/27/28	0/3/3/3
76	PSU	S6	56	76	-	2/7/25/26	0/2/2/2
74	A2M	L5	4590	74	-	2/9/27/28	0/3/3/3
74	OMC	L5	3887	74	-	0/9/27/28	0/2/2/2
74	OMC	L5	3808	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4576	74	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	PSU	L5	5001	74	-	0/7/25/26	0/2/2/2
4	HIC	LB	245	4	-	1/5/6/8	0/1/1/1
74	OMU	L5	2415	74	-	1/9/27/28	0/2/2/2
74	PSU	L5	3695	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	2363	74,81	-	0/9/27/28	0/3/3/3
27	V5N	La	39	27	-	1/9/10/12	0/1/1/1
74	PSU	L5	4552	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4420	74	-	1/7/25/26	0/2/2/2
2	OMG	L8	75	2	-	1/9/27/28	0/3/3/3
74	A2M	L5	1326	74	-	1/9/27/28	0/3/3/3
74	PSU	L5	1677	74,81	-	1/7/25/26	0/2/2/2
74	PSU	L5	3637	74,81	-	0/7/25/26	0/2/2/2
74	PSU	L5	4299	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4579	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	4637	74,82	-	1/9/27/28	0/3/3/3
74	PSU	L5	4423	74	-	0/7/25/26	0/2/2/2
76	4SU	S6	8	76	-	3/7/25/26	0/2/2/2
74	5MC	L5	3782	74,81	-	0/7/25/26	0/2/2/2
74	A2M	L5	3825	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	1744	74,82	-	0/7/25/26	0/2/2/2
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
74	PSU	L5	1779	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4500	74	-	1/7/25/26	0/2/2/2
74	PSU	L5	4293	74	-	1/7/25/26	0/2/2/2
74	OMG	L5	3792	74	-	2/9/27/28	0/3/3/3
74	PSU	L5	4569	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	3830	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4636	74	-	2/7/25/26	0/2/2/2
74	OMU	L5	4306	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4972	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	3762	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	4499	74	-	0/9/27/28	0/3/3/3
74	OMG	L5	1625	74,82	-	1/9/27/28	0/3/3/3
74	PSU	L5	2508	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	4196	74	-	0/9/27/28	0/3/3/3
74	OMG	L5	4392	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4361	74	-	0/7/25/26	0/2/2/2
44	G7M	Pt	47	44	-	0/7/25/26	0/3/3/3
74	PSU	L5	2843	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	1862	74	-	0/7/25/26	0/2/2/2
74	UY1	L5	3818	74,81,82	-	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	OMC	L5	3869	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	3734	74	-	1/7/25/26	0/2/2/2
74	OMU	L5	2837	74	-	0/9/27/28	0/2/2/2
3	V5N	LA	216	3	-	1/9/10/12	0/1/1/1
44	OMC	Pt	33	44	-	0/9/27/28	0/2/2/2
74	PSU	L5	3851	74	-	1/7/25/26	0/2/2/2
74	A2M	L5	1534	74,81	-	2/9/27/28	0/3/3/3
74	PSU	L5	3764	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	4523	74,81	-	1/9/27/28	0/3/3/3
74	PSU	L5	1582	74	-	0/7/25/26	0/2/2/2
74	OMG	L5	3744	74	-	0/9/27/28	0/3/3/3
74	A2M	L5	3867	74	-	2/9/27/28	0/3/3/3
74	A2M	L5	2401	74	-	0/9/27/28	0/3/3/3
74	PSU	L5	4521	74,81,82	-	0/7/25/26	0/2/2/2
74	PSU	L5	2632	74	-	0/7/25/26	0/2/2/2
44	4SU	Pt	8	44	-	0/7/25/26	0/2/2/2
74	PSU	L5	1536	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	398	74	-	3/9/27/28	0/3/3/3
74	A2M	L5	3724	74	-	1/9/27/28	0/3/3/3
74	PSU	L5	3920	74,81	-	0/7/25/26	0/2/2/2
74	PSU	L5	3844	74	-	1/7/25/26	0/2/2/2
74	OMC	L5	3841	74	-	1/9/27/28	0/2/2/2
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
74	OMG	L5	4228	74	-	2/9/27/28	0/3/3/3
74	OMC	L5	2365	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	3639	74	-	0/7/25/26	0/2/2/2
74	A2M	L5	3785	74	-	2/9/27/28	0/3/3/3
74	OMC	L5	1881	74,81	-	0/9/27/28	0/2/2/2
74	PSU	L5	2839	74	-	0/7/25/26	0/2/2/2
74	PSU	L5	4628	74	-	0/7/25/26	0/2/2/2
74	OMC	L5	2804	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	3729	74	-	1/7/25/26	0/2/2/2
74	PSU	L5	3715	74,81	-	0/7/25/26	0/2/2/2
74	OMC	L5	2422	74,81	-	2/9/27/28	0/2/2/2
74	OMU	L5	4227	74	-	0/9/27/28	0/2/2/2
74	PSU	L5	4296	74	-	0/7/25/26	0/2/2/2

All (685) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	3867	A2M	C3'-C2'	-12.77	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2363	A2M	C3'-C2'	-12.73	1.24	1.52
74	L5	400	A2M	C3'-C2'	-12.73	1.24	1.52
74	L5	1326	A2M	C3'-C2'	-12.71	1.24	1.52
74	L5	3723	A2M	C3'-C2'	-12.70	1.24	1.52
74	L5	4590	A2M	C3'-C2'	-12.66	1.24	1.52
74	L5	3724	A2M	C3'-C2'	-12.56	1.24	1.52
74	L5	4571	A2M	C3'-C2'	-12.54	1.25	1.52
74	L5	2401	A2M	C3'-C2'	-12.53	1.25	1.52
74	L5	2815	A2M	C3'-C2'	-12.51	1.25	1.52
74	L5	3830	A2M	C3'-C2'	-12.48	1.25	1.52
74	L5	3718	A2M	C3'-C2'	-12.48	1.25	1.52
74	L5	1524	A2M	C3'-C2'	-12.42	1.25	1.52
74	L5	398	A2M	C3'-C2'	-12.41	1.25	1.52
74	L5	3785	A2M	C3'-C2'	-12.41	1.25	1.52
74	L5	4523	A2M	C3'-C2'	-12.40	1.25	1.52
74	L5	3825	A2M	C3'-C2'	-12.38	1.25	1.52
74	L5	1534	A2M	C3'-C2'	-12.31	1.25	1.52
74	L5	1871	A2M	C3'-C2'	-12.29	1.25	1.52
74	L5	4220	6MZ	C6-N6	11.40	1.46	1.34
74	L5	3818	UY1	C6-C5	10.97	1.48	1.35
74	L5	3818	UY1	C2-N1	9.33	1.49	1.36
74	L5	4447	5MC	C6-C5	9.14	1.49	1.34
74	L5	3782	5MC	C6-C5	8.75	1.49	1.34
76	S6	8	4SU	C4-N3	8.31	1.46	1.37
74	L5	1322	1MA	C2-N3	8.24	1.45	1.30
44	Pt	8	4SU	C4-N3	8.19	1.46	1.37
76	S6	8	4SU	C2-N3	7.40	1.51	1.38
74	L5	4227	OMU	C2-N1	7.35	1.50	1.38
76	S6	8	4SU	C2-N1	7.13	1.49	1.38
74	L5	4530	UR3	C2-N1	7.05	1.48	1.38
74	L5	3818	UY1	C2-N3	7.02	1.49	1.37
74	L5	2415	OMU	C2-N1	6.91	1.49	1.38
3	LA	216	V5N	CG-ND1	-6.91	1.31	1.37
74	L5	2837	OMU	C2-N1	6.82	1.49	1.38
74	L5	4571	A2M	O4'-C4'	-6.82	1.29	1.45
74	L5	4306	OMU	C2-N1	6.81	1.49	1.38
44	Pt	8	4SU	C2-N3	6.81	1.50	1.38
74	L5	3925	OMU	C2-N1	6.80	1.49	1.38
44	Pt	8	4SU	C2-N1	6.79	1.49	1.38
74	L5	1524	A2M	O4'-C4'	-6.78	1.29	1.45
27	La	39	V5N	CG-ND1	-6.77	1.31	1.37
74	L5	4498	OMU	C2-N1	6.73	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2415	OMU	C2-N3	6.66	1.49	1.38
76	S6	47	G7M	C4-N3	6.63	1.50	1.34
74	L5	2837	OMU	C2-N3	6.61	1.49	1.38
74	L5	3723	A2M	O4'-C4'	-6.59	1.30	1.45
74	L5	2363	A2M	O4'-C4'	-6.59	1.30	1.45
74	L5	4498	OMU	C2-N3	6.58	1.49	1.38
74	L5	2815	A2M	O4'-C4'	-6.53	1.30	1.45
74	L5	400	A2M	O4'-C4'	-6.53	1.30	1.45
74	L5	1522	OMG	C4-N3	6.52	1.49	1.34
74	L5	1534	A2M	O4'-C4'	-6.49	1.30	1.45
74	L5	1871	A2M	O4'-C4'	-6.48	1.30	1.45
74	L5	3744	OMG	C4-N3	6.48	1.49	1.34
74	L5	3925	OMU	C2-N3	6.47	1.49	1.38
74	L5	2861	OMC	C2-N3	6.47	1.49	1.36
74	L5	3724	A2M	O4'-C4'	-6.46	1.30	1.45
44	Pt	47	G7M	C4-N3	6.45	1.49	1.34
2	L8	75	OMG	C4-N3	6.44	1.49	1.34
74	L5	3867	A2M	O4'-C4'	-6.44	1.30	1.45
44	Pt	33	OMC	C2-N3	6.43	1.49	1.36
74	L5	4306	OMU	C2-N3	6.43	1.49	1.38
74	L5	4227	OMU	C2-N3	6.42	1.49	1.38
74	L5	4590	A2M	O4'-C4'	-6.41	1.30	1.45
74	L5	3785	A2M	O4'-C4'	-6.41	1.30	1.45
74	L5	4392	OMG	C4-N3	6.40	1.49	1.34
74	L5	1326	A2M	O4'-C4'	-6.40	1.30	1.45
74	L5	3825	A2M	O4'-C4'	-6.40	1.30	1.45
74	L5	3944	OMG	C4-N3	6.39	1.49	1.34
74	L5	1322	1MA	C4-N3	6.37	1.48	1.35
74	L5	4228	OMG	C4-N3	6.37	1.49	1.34
74	L5	3808	OMC	C2-N3	6.36	1.49	1.36
74	L5	1625	OMG	C4-N3	6.34	1.49	1.34
74	L5	3627	OMG	C4-N3	6.33	1.49	1.34
74	L5	2365	OMC	C2-N3	6.33	1.49	1.36
74	L5	3718	A2M	O4'-C4'	-6.33	1.30	1.45
74	L5	4623	OMG	C4-N3	6.31	1.49	1.34
74	L5	4370	OMG	C4-N3	6.31	1.49	1.34
74	L5	4620	OMU	C2-N1	6.30	1.48	1.38
74	L5	2401	A2M	O4'-C4'	-6.29	1.30	1.45
74	L5	1316	OMG	C4-N3	6.29	1.49	1.34
74	L5	4618	OMG	C4-N3	6.29	1.49	1.34
74	L5	4637	OMG	C4-N3	6.28	1.49	1.34
74	L5	3792	OMG	C4-N3	6.28	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	3830	A2M	O4'-C4'	-6.28	1.31	1.45
74	L5	4523	A2M	O4'-C4'	-6.27	1.31	1.45
74	L5	398	A2M	O4'-C4'	-6.27	1.31	1.45
74	L5	3899	OMG	C4-N3	6.27	1.49	1.34
74	L5	2364	OMG	C4-N3	6.23	1.49	1.34
74	L5	4620	OMU	C2-N3	6.23	1.49	1.38
74	L5	4499	OMG	C4-N3	6.22	1.49	1.34
74	L5	2424	OMG	C4-N3	6.22	1.49	1.34
74	L5	4196	OMG	C4-N3	6.22	1.49	1.34
74	L5	3782	5MC	C4-N3	6.21	1.44	1.34
74	L5	4494	OMG	C4-N3	6.20	1.49	1.34
74	L5	3869	OMC	C2-N3	6.17	1.48	1.36
74	L5	1340	OMC	C2-N3	6.15	1.48	1.36
74	L5	3887	OMC	C2-N3	6.13	1.48	1.36
74	L5	2804	OMC	C2-N3	6.12	1.48	1.36
74	L5	3701	OMC	C2-N3	6.12	1.48	1.36
74	L5	2824	OMC	C2-N3	6.11	1.48	1.36
74	L5	2351	OMC	C6-C5	6.07	1.49	1.35
74	L5	3841	OMC	C2-N3	6.05	1.48	1.36
74	L5	3869	OMC	C6-C5	6.02	1.49	1.35
74	L5	4536	OMC	C6-C5	6.02	1.49	1.35
74	L5	2422	OMC	C2-N3	5.99	1.48	1.36
74	L5	3782	5MC	C2-N3	5.99	1.48	1.36
74	L5	2804	OMC	C6-C5	5.98	1.48	1.35
74	L5	3701	OMC	C6-C5	5.97	1.48	1.35
74	L5	2824	OMC	C6-C5	5.97	1.48	1.35
74	L5	2365	OMC	C6-C5	5.95	1.48	1.35
74	L5	4456	OMC	C2-N3	5.95	1.48	1.36
74	L5	3887	OMC	C6-C5	5.95	1.48	1.35
74	L5	4530	UR3	C6-C5	5.93	1.48	1.35
74	L5	4536	OMC	C2-N3	5.92	1.48	1.36
74	L5	2351	OMC	C2-N3	5.92	1.48	1.36
74	L5	3808	OMC	C6-C5	5.92	1.48	1.35
44	Pt	33	OMC	C6-C5	5.92	1.48	1.35
74	L5	2422	OMC	C6-C5	5.92	1.48	1.35
74	L5	4456	OMC	C6-C5	5.89	1.48	1.35
74	L5	3841	OMC	C6-C5	5.86	1.48	1.35
76	S6	47	G7M	C2-N2	5.86	1.48	1.34
44	Pt	8	4SU	C6-C5	5.86	1.48	1.35
74	L5	4447	5MC	C4-N3	5.84	1.44	1.34
74	L5	1881	OMC	C6-C5	5.82	1.48	1.35
74	L5	1881	OMC	C2-N3	5.78	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	3785	A2M	C3'-C4'	5.77	1.67	1.53
74	L5	2861	OMC	C6-C5	5.74	1.48	1.35
74	L5	4227	OMU	C6-C5	5.72	1.48	1.35
74	L5	4623	OMG	C2-N3	5.68	1.46	1.33
74	L5	1340	OMC	C6-C5	5.68	1.48	1.35
44	Pt	47	G7M	C2-N2	5.66	1.47	1.34
74	L5	3744	OMG	C2-N3	5.66	1.46	1.33
74	L5	2415	OMU	C6-C5	5.64	1.48	1.35
74	L5	4392	OMG	C2-N3	5.63	1.46	1.33
74	L5	4447	5MC	C2-N3	5.63	1.47	1.36
74	L5	1625	OMG	C2-N3	5.60	1.46	1.33
74	L5	4306	OMU	C6-C5	5.59	1.48	1.35
76	S6	8	4SU	C6-C5	5.57	1.48	1.35
74	L5	2424	OMG	C2-N3	5.57	1.46	1.33
2	L8	75	OMG	C2-N3	5.56	1.46	1.33
74	L5	3925	OMU	C6-C5	5.55	1.47	1.35
44	Pt	47	G7M	C2-N3	5.52	1.46	1.33
76	S6	47	G7M	C2-N3	5.51	1.46	1.33
74	L5	4620	OMU	C6-C5	5.50	1.47	1.35
74	L5	1534	A2M	C6-N6	5.48	1.47	1.34
74	L5	3792	OMG	C2-N3	5.46	1.46	1.33
74	L5	3944	OMG	C2-N3	5.46	1.46	1.33
74	L5	4196	OMG	C2-N3	5.46	1.46	1.33
74	L5	1522	OMG	C2-N3	5.45	1.46	1.33
74	L5	4228	OMG	C2-N3	5.45	1.46	1.33
74	L5	2837	OMU	C6-C5	5.44	1.47	1.35
74	L5	3899	OMG	C2-N3	5.44	1.46	1.33
74	L5	4637	OMG	C2-N3	5.43	1.46	1.33
74	L5	3724	A2M	C6-N6	5.43	1.47	1.34
74	L5	4498	OMU	C6-C5	5.42	1.47	1.35
74	L5	3627	OMG	C2-N3	5.41	1.46	1.33
74	L5	4499	OMG	C2-N3	5.40	1.46	1.33
74	L5	4618	OMG	C2-N3	5.39	1.46	1.33
74	L5	1524	A2M	C6-N6	5.38	1.47	1.34
74	L5	4571	A2M	C6-N6	5.37	1.47	1.34
74	L5	3724	A2M	C3'-C4'	5.37	1.66	1.53
74	L5	3723	A2M	C6-N6	5.35	1.47	1.34
74	L5	4494	OMG	C2-N3	5.35	1.46	1.33
74	L5	400	A2M	C6-N6	5.34	1.47	1.34
74	L5	4571	A2M	C3'-C4'	5.34	1.66	1.53
74	L5	1316	OMG	C2-N3	5.33	1.46	1.33
74	L5	3718	A2M	C3'-C4'	5.33	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4523	A2M	C3'-C4'	5.32	1.66	1.53
74	L5	2364	OMG	C2-N3	5.32	1.46	1.33
74	L5	4370	OMG	C2-N3	5.31	1.46	1.33
74	L5	3867	A2M	C6-N6	5.27	1.47	1.34
74	L5	3830	A2M	C3'-C4'	5.27	1.66	1.53
74	L5	398	A2M	C6-N6	5.25	1.47	1.34
74	L5	2815	A2M	C3'-C4'	5.24	1.66	1.53
74	L5	3723	A2M	C3'-C4'	5.21	1.66	1.53
74	L5	2363	A2M	C3'-C4'	5.21	1.66	1.53
74	L5	2815	A2M	C6-N6	5.21	1.47	1.34
74	L5	4523	A2M	C6-N6	5.21	1.47	1.34
74	L5	3825	A2M	C6-N6	5.20	1.47	1.34
74	L5	4590	A2M	C6-N6	5.17	1.47	1.34
74	L5	3718	A2M	C6-N6	5.17	1.47	1.34
74	L5	1524	A2M	C1'-N9	-5.15	1.31	1.46
74	L5	1326	A2M	C6-N6	5.15	1.47	1.34
74	L5	3830	A2M	C6-N6	5.15	1.47	1.34
74	L5	3825	A2M	C3'-C4'	5.14	1.66	1.53
74	L5	1871	A2M	C6-N6	5.14	1.47	1.34
74	L5	1534	A2M	C3'-C4'	5.12	1.66	1.53
74	L5	2363	A2M	C6-N6	5.11	1.47	1.34
74	L5	1326	A2M	C3'-C4'	5.11	1.66	1.53
74	L5	2401	A2M	C6-N6	5.10	1.46	1.34
74	L5	4590	A2M	C3'-C4'	5.08	1.66	1.53
74	L5	3785	A2M	C6-N6	5.06	1.46	1.34
74	L5	398	A2M	C3'-C4'	5.05	1.65	1.53
74	L5	2401	A2M	C3'-C4'	5.05	1.65	1.53
74	L5	400	A2M	C3'-C4'	5.02	1.65	1.53
74	L5	2861	OMC	C4-N3	5.02	1.44	1.34
74	L5	2824	OMC	C4-N3	5.02	1.44	1.34
44	Pt	33	OMC	C4-N3	5.00	1.44	1.34
74	L5	1871	A2M	C3'-C4'	4.99	1.65	1.53
74	L5	3867	A2M	C3'-C4'	4.95	1.65	1.53
74	L5	3818	UY1	C6-N1	4.94	1.44	1.36
74	L5	2365	OMC	C4-N3	4.94	1.44	1.34
44	Pt	33	OMC	C4-N4	4.94	1.45	1.33
74	L5	2804	OMC	C4-N3	4.92	1.44	1.34
74	L5	3841	OMC	C4-N3	4.92	1.44	1.34
74	L5	3701	OMC	C4-N3	4.90	1.44	1.34
44	Pt	8	4SU	C4-S4	-4.89	1.59	1.68
74	L5	3887	OMC	C4-N3	4.88	1.44	1.34
74	L5	4530	UR3	C2-N3	4.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4536	OMC	C4-N3	4.86	1.44	1.34
74	L5	3808	OMC	C4-N3	4.84	1.44	1.34
74	L5	2351	OMC	C4-N4	4.83	1.45	1.33
74	L5	3869	OMC	C4-N4	4.83	1.45	1.33
74	L5	1881	OMC	C4-N3	4.83	1.44	1.34
74	L5	4499	OMG	C2-N2	4.82	1.45	1.34
74	L5	2804	OMC	C4-N4	4.82	1.45	1.33
44	Pt	33	OMC	C2-N1	4.78	1.50	1.40
74	L5	1524	A2M	C3'-C4'	4.78	1.65	1.53
74	L5	2365	OMC	C4-N4	4.77	1.45	1.33
74	L5	2824	OMC	C4-N4	4.77	1.45	1.33
74	L5	3887	OMC	C4-N4	4.76	1.45	1.33
74	L5	3841	OMC	C4-N4	4.76	1.45	1.33
44	Pt	8	4SU	C5-C4	4.75	1.48	1.42
74	L5	3869	OMC	C4-N3	4.74	1.44	1.34
74	L5	2861	OMC	C4-N4	4.73	1.45	1.33
74	L5	4536	OMC	C4-N4	4.73	1.45	1.33
74	L5	1340	OMC	C4-N3	4.71	1.44	1.34
74	L5	3701	OMC	C4-N4	4.71	1.45	1.33
74	L5	4456	OMC	C4-N4	4.71	1.45	1.33
74	L5	3808	OMC	C4-N4	4.71	1.45	1.33
74	L5	4456	OMC	C4-N3	4.71	1.44	1.34
74	L5	2351	OMC	C4-N3	4.70	1.44	1.34
76	S6	8	4SU	C4-S4	-4.69	1.59	1.68
74	L5	4590	A2M	C1'-N9	-4.69	1.33	1.46
74	L5	4196	OMG	C2-N2	4.68	1.45	1.34
74	L5	1881	OMC	C4-N4	4.67	1.44	1.33
74	L5	1534	A2M	C1'-N9	-4.64	1.33	1.46
74	L5	3944	OMG	C2-N2	4.64	1.45	1.34
74	L5	3792	OMG	C2-N2	4.64	1.45	1.34
74	L5	2424	OMG	C2-N2	4.63	1.45	1.34
74	L5	1340	OMC	C4-N4	4.61	1.44	1.33
74	L5	2861	OMC	C2-N1	4.60	1.50	1.40
74	L5	3627	OMG	C2-N2	4.60	1.45	1.34
2	L8	75	OMG	C2-N2	4.60	1.45	1.34
74	L5	4571	A2M	C1'-N9	-4.60	1.33	1.46
74	L5	4370	OMG	C2-N2	4.60	1.45	1.34
74	L5	2422	OMC	C4-N3	4.59	1.43	1.34
74	L5	3744	OMG	C2-N2	4.59	1.45	1.34
74	L5	2422	OMC	C4-N4	4.58	1.44	1.33
74	L5	4228	OMG	C2-N2	4.58	1.45	1.34
74	L5	1316	OMG	C2-N2	4.58	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4494	OMG	C2-N2	4.58	1.45	1.34
74	L5	1522	OMG	C2-N2	4.57	1.45	1.34
74	L5	2364	OMG	C2-N2	4.57	1.45	1.34
74	L5	1625	OMG	C2-N2	4.56	1.45	1.34
74	L5	4623	OMG	C2-N2	4.54	1.45	1.34
74	L5	4637	OMG	C2-N2	4.53	1.45	1.34
74	L5	4618	OMG	C2-N2	4.52	1.44	1.34
74	L5	3785	A2M	C1'-N9	-4.51	1.33	1.46
74	L5	3808	OMC	C2-N1	4.50	1.49	1.40
74	L5	3724	A2M	C1'-N9	-4.50	1.33	1.46
74	L5	3718	A2M	O4'-C1'	4.49	1.52	1.42
74	L5	2824	OMC	C2-N1	4.48	1.49	1.40
74	L5	2815	A2M	C1'-N9	-4.48	1.33	1.46
74	L5	1326	A2M	C1'-N9	-4.47	1.33	1.46
74	L5	4447	5MC	C6-N1	4.47	1.45	1.38
74	L5	3830	A2M	C1'-N9	-4.47	1.33	1.46
74	L5	398	A2M	O4'-C1'	4.46	1.52	1.42
74	L5	4392	OMG	C2-N2	4.46	1.44	1.34
74	L5	2401	A2M	O4'-C1'	4.45	1.52	1.42
74	L5	3899	OMG	C2-N2	4.44	1.44	1.34
74	L5	2401	A2M	C1'-N9	-4.44	1.33	1.46
74	L5	2351	OMC	C2-N1	4.43	1.49	1.40
74	L5	3830	A2M	O4'-C1'	4.42	1.52	1.42
74	L5	3825	A2M	C1'-N9	-4.42	1.33	1.46
74	L5	1871	A2M	C1'-N9	-4.41	1.33	1.46
74	L5	3867	A2M	C1'-N9	-4.39	1.33	1.46
74	L5	4456	OMC	C2-N1	4.39	1.49	1.40
74	L5	3724	A2M	O4'-C1'	4.39	1.52	1.42
74	L5	2363	A2M	O4'-C1'	4.37	1.52	1.42
74	L5	2815	A2M	O4'-C1'	4.37	1.52	1.42
74	L5	3867	A2M	O4'-C1'	4.37	1.52	1.42
74	L5	3841	OMC	C2-N1	4.36	1.49	1.40
74	L5	3723	A2M	C1'-N9	-4.35	1.34	1.46
74	L5	400	A2M	O4'-C1'	4.35	1.52	1.42
74	L5	2365	OMC	C2-N1	4.35	1.49	1.40
76	S6	8	4SU	C5-C4	4.35	1.48	1.42
74	L5	2363	A2M	C1'-N9	-4.33	1.34	1.46
74	L5	4590	A2M	O4'-C1'	4.33	1.52	1.42
74	L5	1871	A2M	O4'-C1'	4.32	1.52	1.42
74	L5	1322	1MA	C2-N1	4.32	1.43	1.35
74	L5	4523	A2M	O4'-C1'	4.31	1.52	1.42
74	L5	4536	OMC	C2-N1	4.30	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4571	A2M	O4'-C1'	4.28	1.52	1.42
74	L5	3825	A2M	O4'-C1'	4.28	1.52	1.42
74	L5	3723	A2M	O4'-C1'	4.27	1.52	1.42
74	L5	4523	A2M	C1'-N9	-4.26	1.34	1.46
74	L5	1534	A2M	O4'-C1'	4.24	1.52	1.42
74	L5	3869	OMC	C2-N1	4.24	1.49	1.40
74	L5	4447	5MC	C4-N4	4.24	1.45	1.34
74	L5	3887	OMC	C2-N1	4.23	1.49	1.40
74	L5	398	A2M	C1'-N9	-4.20	1.34	1.46
74	L5	400	A2M	C1'-N9	-4.19	1.34	1.46
74	L5	2422	OMC	C2-N1	4.18	1.49	1.40
74	L5	1326	A2M	O4'-C1'	4.17	1.51	1.42
76	S6	47	G7M	C5-C6	4.17	1.55	1.43
74	L5	3782	5MC	C4-N4	4.12	1.44	1.34
74	L5	2804	OMC	C2-N1	4.12	1.48	1.40
74	L5	1340	OMC	C2-N1	4.11	1.48	1.40
44	Pt	47	G7M	C5-C6	4.10	1.54	1.43
3	LA	216	V5N	CD2-NE2	-4.06	1.31	1.37
74	L5	3782	5MC	C6-N1	4.05	1.45	1.38
74	L5	3701	OMC	C2-N1	4.03	1.48	1.40
74	L5	1524	A2M	O4'-C1'	4.02	1.51	1.42
27	La	39	V5N	CD2-NE2	-4.01	1.31	1.37
74	L5	1881	OMC	C2-N1	4.00	1.48	1.40
74	L5	3718	A2M	C1'-N9	-3.99	1.35	1.46
74	L5	4498	OMU	C4-N3	3.92	1.45	1.38
74	L5	4636	PSU	C6-C5	3.91	1.39	1.35
44	Pt	47	G7M	C5-N7	-3.89	1.34	1.39
74	L5	3782	5MC	C2-N1	3.88	1.48	1.40
74	L5	2415	OMU	C4-N3	3.88	1.45	1.38
74	L5	4306	OMU	C4-N3	3.88	1.45	1.38
74	L5	3925	OMU	C4-N3	3.81	1.45	1.38
74	L5	4532	PSU	C6-C5	3.76	1.39	1.35
74	L5	4227	OMU	C4-N3	3.76	1.45	1.38
74	L5	4569	PSU	C6-C5	3.75	1.39	1.35
74	L5	3844	PSU	C6-C5	3.69	1.39	1.35
74	L5	3818	UY1	C4-N3	3.69	1.45	1.38
74	L5	4447	5MC	C2-N1	3.69	1.48	1.40
76	S6	47	G7M	C5-N7	-3.68	1.34	1.39
74	L5	1862	PSU	C6-C5	3.68	1.39	1.35
74	L5	2839	PSU	C6-C5	3.65	1.39	1.35
74	L5	2837	OMU	C4-N3	3.64	1.45	1.38
74	L5	3762	PSU	C6-C5	3.61	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	1779	PSU	C6-C5	3.59	1.39	1.35
74	L5	1744	PSU	C6-C5	3.59	1.39	1.35
74	L5	4293	PSU	C6-C5	3.59	1.39	1.35
74	L5	4620	OMU	C4-N3	3.57	1.45	1.38
74	L5	1322	1MA	C5-C6	3.57	1.53	1.43
74	L5	4531	PSU	C6-C5	3.56	1.39	1.35
74	L5	4423	PSU	C6-C5	3.56	1.39	1.35
74	L5	4420	PSU	C6-C5	3.55	1.39	1.35
74	L5	3637	PSU	C6-C5	3.55	1.39	1.35
44	Pt	47	G7M	C2-N1	3.53	1.46	1.37
74	L5	4500	PSU	C6-C5	3.53	1.39	1.35
74	L5	3744	OMG	C5-N7	-3.53	1.32	1.39
74	L5	3899	OMG	C5-N7	-3.53	1.32	1.39
74	L5	4392	OMG	C5-N7	-3.52	1.32	1.39
74	L5	2424	OMG	C5-N7	-3.52	1.32	1.39
74	L5	4196	OMG	C5-N7	-3.51	1.32	1.39
74	L5	3851	PSU	C6-C5	3.50	1.39	1.35
2	L8	55	PSU	C6-C5	3.49	1.39	1.35
74	L5	1677	PSU	C6-C5	3.49	1.39	1.35
74	L5	2632	PSU	C6-C5	3.48	1.39	1.35
74	L5	3785	A2M	O4'-C1'	3.48	1.50	1.42
76	S6	47	G7M	C2-N1	3.48	1.46	1.37
74	L5	4431	PSU	C6-C5	3.47	1.39	1.35
74	L5	4521	PSU	C6-C5	3.47	1.39	1.35
74	L5	4296	PSU	C6-C5	3.45	1.39	1.35
74	L5	1625	OMG	C5-N7	-3.44	1.32	1.39
74	L5	1316	OMG	C5-N7	-3.44	1.32	1.39
74	L5	3729	PSU	C6-C5	3.43	1.39	1.35
74	L5	4471	PSU	C6-C5	3.42	1.39	1.35
74	L5	3920	PSU	C6-C5	3.42	1.39	1.35
74	L5	3627	OMG	C5-N7	-3.42	1.32	1.39
44	Pt	56	PSU	C6-C5	3.42	1.39	1.35
74	L5	4552	PSU	C6-C5	3.41	1.39	1.35
74	L5	4370	OMG	C5-N7	-3.41	1.32	1.39
74	L5	4457	PSU	C6-C5	3.40	1.39	1.35
74	L5	4637	OMG	C5-N7	-3.38	1.32	1.39
74	L5	2351	OMC	C6-N1	3.37	1.46	1.38
74	L5	4536	OMC	C6-N1	3.36	1.46	1.38
74	L5	4673	PSU	C6-C5	3.36	1.39	1.35
74	L5	2837	OMU	O4-C4	-3.36	1.18	1.24
74	L5	3792	OMG	C5-N7	-3.35	1.32	1.39
74	L5	4494	OMG	C5-N7	-3.35	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4618	OMG	C5-N7	-3.35	1.32	1.39
74	L5	3768	PSU	C6-C5	3.34	1.39	1.35
74	L5	4623	OMG	C5-N7	-3.33	1.32	1.39
74	L5	4442	PSU	C6-C5	3.32	1.39	1.35
74	L5	4628	PSU	C6-C5	3.32	1.39	1.35
74	L5	4312	PSU	C6-C5	3.31	1.39	1.35
74	L5	1781	PSU	C6-C5	3.31	1.39	1.35
76	S6	56	PSU	C6-C5	3.31	1.39	1.35
74	L5	3639	PSU	C6-C5	3.30	1.39	1.35
74	L5	4361	PSU	C6-C5	3.30	1.39	1.35
74	L5	4689	PSU	C6-C5	3.27	1.39	1.35
44	Pt	8	4SU	C6-N1	3.26	1.45	1.38
74	L5	3808	OMC	C6-N1	3.26	1.45	1.38
74	L5	3884	PSU	C6-C5	3.26	1.39	1.35
74	L5	1792	PSU	C6-C5	3.25	1.39	1.35
74	L5	1322	1MA	C5-N7	-3.25	1.32	1.39
74	L5	3758	PSU	C6-C5	3.25	1.39	1.35
74	L5	1881	OMC	C6-N1	3.25	1.45	1.38
74	L5	2843	PSU	C6-C5	3.24	1.39	1.35
74	L5	3869	OMC	O2-C2	-3.24	1.17	1.23
74	L5	1683	PSU	C6-C5	3.23	1.39	1.35
74	L5	2508	PSU	C6-C5	3.23	1.39	1.35
74	L5	4499	OMG	C5-N7	-3.21	1.32	1.39
74	L5	3887	OMC	C6-N1	3.21	1.45	1.38
74	L5	4353	PSU	C6-C5	3.21	1.39	1.35
74	L5	3853	PSU	C6-C5	3.20	1.39	1.35
74	L5	4493	PSU	C6-C5	3.20	1.39	1.35
74	L5	5001	PSU	C6-C5	3.20	1.39	1.35
2	L8	75	OMG	C5-N7	-3.19	1.32	1.39
74	L5	1536	PSU	C6-C5	3.19	1.39	1.35
74	L5	4972	PSU	C6-C5	3.19	1.39	1.35
74	L5	4498	OMU	O4-C4	-3.19	1.18	1.24
74	L5	3925	OMU	O4-C4	-3.18	1.18	1.24
76	S6	47	G7M	O6-C6	-3.18	1.17	1.23
74	L5	4299	PSU	C6-C5	3.17	1.39	1.35
74	L5	4228	OMG	C5-N7	-3.16	1.33	1.39
74	L5	2422	OMC	C6-N1	3.16	1.45	1.38
74	L5	1782	PSU	C6-C5	3.16	1.39	1.35
74	L5	5010	PSU	C6-C5	3.15	1.39	1.35
74	L5	2415	OMU	O4-C4	-3.15	1.18	1.24
74	L5	3841	OMC	O2-C2	-3.15	1.17	1.23
74	L5	1522	OMG	C5-N7	-3.14	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2365	OMC	O2-C2	-3.14	1.17	1.23
74	L5	1860	PSU	C6-C5	3.14	1.39	1.35
74	L5	4576	PSU	C6-C5	3.14	1.39	1.35
74	L5	3869	OMC	C6-N1	3.13	1.45	1.38
74	L5	2365	OMC	C6-N1	3.13	1.45	1.38
74	L5	2804	OMC	C6-N1	3.13	1.45	1.38
74	L5	4620	OMU	O4-C4	-3.13	1.18	1.24
74	L5	2861	OMC	C6-N1	3.10	1.45	1.38
44	Pt	33	OMC	C6-N1	3.10	1.45	1.38
74	L5	4403	PSU	C6-C5	3.09	1.38	1.35
74	L5	3944	OMG	C5-N7	-3.09	1.33	1.39
2	L8	69	PSU	C6-C5	3.08	1.38	1.35
74	L5	4196	OMG	O6-C6	-3.08	1.17	1.23
74	L5	3841	OMC	C6-N1	3.07	1.45	1.38
74	L5	4306	OMU	O4-C4	-3.07	1.18	1.24
74	L5	1582	PSU	C6-C5	3.07	1.38	1.35
74	L5	2351	OMC	O2-C2	-3.05	1.18	1.23
74	L5	3770	PSU	C6-C5	3.05	1.38	1.35
74	L5	4456	OMC	C6-N1	3.05	1.45	1.38
74	L5	4536	OMC	O2-C2	-3.04	1.18	1.23
74	L5	1340	OMC	C6-N1	3.04	1.45	1.38
74	L5	3701	OMC	C6-N1	3.04	1.45	1.38
74	L5	4447	5MC	O2-C2	-3.04	1.18	1.23
74	L5	1881	OMC	O2-C2	-3.04	1.18	1.23
74	L5	4227	OMU	O4-C4	-3.03	1.18	1.24
74	L5	4530	UR3	C6-N1	3.03	1.45	1.38
74	L5	2824	OMC	C6-N1	3.02	1.45	1.38
74	L5	3830	A2M	O2'-C2'	3.02	1.50	1.42
74	L5	4579	PSU	C6-C5	3.02	1.38	1.35
74	L5	1524	A2M	O2'-C2'	3.02	1.50	1.42
74	L5	1326	A2M	O2'-C2'	3.02	1.50	1.42
74	L5	2363	A2M	O2'-C2'	3.00	1.50	1.42
74	L5	2364	OMG	C5-N7	-3.00	1.33	1.39
74	L5	3723	A2M	O2'-C2'	3.00	1.50	1.42
74	L5	1316	OMG	O6-C6	-2.99	1.17	1.23
74	L5	3734	PSU	C6-C5	2.99	1.38	1.35
74	L5	2824	OMC	O2-C2	-2.99	1.18	1.23
74	L5	1340	OMC	O2-C2	-2.99	1.18	1.23
74	L5	2804	OMC	O2-C2	-2.99	1.18	1.23
74	L5	3715	PSU	C6-C5	2.99	1.38	1.35
74	L5	3724	A2M	O2'-C2'	2.97	1.50	1.42
74	L5	3695	PSU	C6-C5	2.97	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4618	OMG	O6-C6	-2.97	1.17	1.23
74	L5	1534	A2M	O2'-C2'	2.96	1.50	1.42
74	L5	4571	A2M	O2'-C2'	2.95	1.50	1.42
74	L5	3808	OMC	O2-C2	-2.94	1.18	1.23
74	L5	2401	A2M	C2'-C1'	2.94	1.60	1.53
74	L5	400	A2M	O2'-C2'	2.94	1.50	1.42
74	L5	2422	OMC	O2-C2	-2.94	1.18	1.23
74	L5	3718	A2M	O2'-C2'	2.93	1.50	1.42
74	L5	4637	OMG	O6-C6	-2.92	1.18	1.23
74	L5	1871	A2M	C5-C4	-2.92	1.33	1.39
74	L5	4523	A2M	O2'-C2'	2.92	1.50	1.42
44	Pt	47	G7M	O6-C6	-2.92	1.18	1.23
74	L5	4623	OMG	O6-C6	-2.91	1.18	1.23
74	L5	3825	A2M	O2'-C2'	2.91	1.50	1.42
74	L5	2815	A2M	O2'-C2'	2.91	1.50	1.42
74	L5	1522	OMG	O6-C6	-2.91	1.18	1.23
76	S6	8	4SU	C6-N1	2.91	1.45	1.38
74	L5	2401	A2M	O2'-C2'	2.91	1.50	1.42
74	L5	1524	A2M	C2'-C1'	2.90	1.60	1.53
74	L5	3887	OMC	O2-C2	-2.89	1.18	1.23
74	L5	3764	PSU	C6-C5	2.88	1.38	1.35
74	L5	4227	OMU	C6-N1	2.88	1.44	1.38
74	L5	1871	A2M	O2'-C2'	2.87	1.50	1.42
74	L5	2861	OMC	O2-C2	-2.87	1.18	1.23
74	L5	398	A2M	C2'-C1'	2.86	1.60	1.53
74	L5	4523	A2M	C2'-C1'	2.86	1.60	1.53
74	L5	3782	5MC	O2-C2	-2.85	1.18	1.23
74	L5	4456	OMC	O2-C2	-2.85	1.18	1.23
74	L5	4220	6MZ	C5-C4	-2.85	1.33	1.39
74	L5	4590	A2M	C5-C4	-2.85	1.33	1.39
74	L5	3925	OMU	C6-N1	2.84	1.44	1.38
74	L5	3867	A2M	O2'-C2'	2.84	1.49	1.42
74	L5	398	A2M	O2'-C2'	2.83	1.49	1.42
74	L5	400	A2M	C2'-C1'	2.83	1.60	1.53
74	L5	4590	A2M	O2'-C2'	2.82	1.49	1.42
74	L5	4392	OMG	O6-C6	-2.82	1.18	1.23
74	L5	3830	A2M	C2'-C1'	2.82	1.60	1.53
74	L5	3785	A2M	O2'-C2'	2.81	1.49	1.42
74	L5	3792	OMG	O6-C6	-2.81	1.18	1.23
74	L5	2415	OMU	C6-N1	2.81	1.44	1.38
74	L5	3785	A2M	C2'-C1'	2.80	1.60	1.53
74	L5	4370	OMG	O6-C6	-2.80	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4220	6MZ	C5-N7	-2.79	1.33	1.39
74	L5	1326	A2M	C2'-C1'	2.78	1.60	1.53
74	L5	3744	OMG	O6-C6	-2.78	1.18	1.23
74	L5	4499	OMG	O6-C6	-2.78	1.18	1.23
74	L5	3718	A2M	C2'-C1'	2.77	1.60	1.53
74	L5	3723	A2M	C2'-C1'	2.77	1.60	1.53
74	L5	1326	A2M	C5-C4	-2.77	1.33	1.39
44	Pt	47	G7M	C6-N1	2.75	1.43	1.38
74	L5	3818	UY1	O4-C4	-2.75	1.18	1.23
74	L5	2815	A2M	C2'-C1'	2.74	1.60	1.53
74	L5	1625	OMG	O6-C6	-2.74	1.18	1.23
74	L5	2364	OMG	O6-C6	-2.73	1.18	1.23
74	L5	3627	OMG	O6-C6	-2.72	1.18	1.23
74	L5	3785	A2M	C5-C4	-2.72	1.33	1.39
74	L5	3724	A2M	C2'-C1'	2.72	1.60	1.53
74	L5	3825	A2M	C2'-C1'	2.72	1.60	1.53
74	L5	3701	OMC	O2-C2	-2.71	1.18	1.23
74	L5	3724	A2M	C5-C4	-2.70	1.34	1.39
74	L5	3925	OMU	O2-C2	-2.70	1.18	1.23
74	L5	3830	A2M	C5-C4	-2.70	1.34	1.39
74	L5	4620	OMU	C6-N1	2.70	1.44	1.38
74	L5	4571	A2M	C5-C4	-2.70	1.34	1.39
74	L5	4228	OMG	O6-C6	-2.69	1.18	1.23
74	L5	4494	OMG	O6-C6	-2.69	1.18	1.23
74	L5	3944	OMG	C2-N1	2.69	1.44	1.37
74	L5	3867	A2M	C5-C4	-2.69	1.34	1.39
74	L5	2815	A2M	C5-C4	-2.69	1.34	1.39
74	L5	1524	A2M	C5-C4	-2.69	1.34	1.39
74	L5	1871	A2M	C2'-C1'	2.67	1.60	1.53
74	L5	2837	OMU	C6-N1	2.67	1.44	1.38
74	L5	4306	OMU	C6-N1	2.67	1.44	1.38
74	L5	2401	A2M	C5-C4	-2.67	1.34	1.39
44	Pt	33	OMC	O2-C2	-2.66	1.18	1.23
74	L5	3899	OMG	O6-C6	-2.66	1.18	1.23
2	L8	75	OMG	O6-C6	-2.65	1.18	1.23
74	L5	4498	OMU	C6-N1	2.63	1.44	1.38
74	L5	2364	OMG	C5-C6	2.63	1.54	1.44
74	L5	4228	OMG	C2-N1	2.62	1.44	1.37
74	L5	4523	A2M	C5-C4	-2.60	1.34	1.39
74	L5	398	A2M	C5-C4	-2.60	1.34	1.39
76	S6	47	G7M	C6-N1	2.60	1.43	1.38
74	L5	2363	A2M	C5-C4	-2.60	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	1534	A2M	C5-C4	-2.60	1.34	1.39
74	L5	1625	OMG	C2-N1	2.60	1.44	1.37
74	L5	1316	OMG	C2-N1	2.59	1.44	1.37
74	L5	3825	A2M	C5-C4	-2.59	1.34	1.39
74	L5	2424	OMG	O6-C6	-2.59	1.18	1.23
74	L5	4494	OMG	C5-C6	2.59	1.54	1.44
74	L5	3627	OMG	C2-N1	2.58	1.44	1.37
74	L5	4494	OMG	C2-N1	2.58	1.44	1.37
74	L5	2363	A2M	C2'-C1'	2.58	1.59	1.53
74	L5	2424	OMG	C2-N1	2.57	1.44	1.37
74	L5	4499	OMG	C2-N1	2.56	1.44	1.37
74	L5	400	A2M	C5-C4	-2.55	1.34	1.39
74	L5	4536	OMC	C5-C4	2.55	1.48	1.42
74	L5	3723	A2M	C5-C4	-2.54	1.34	1.39
2	L8	75	OMG	C2-N1	2.54	1.44	1.37
74	L5	4370	OMG	C2-N1	2.54	1.44	1.37
74	L5	3718	A2M	C5-C4	-2.53	1.34	1.39
74	L5	4498	OMU	O2-C2	-2.52	1.18	1.23
74	L5	3701	OMC	C5-C4	2.52	1.48	1.42
74	L5	2415	OMU	O2-C2	-2.51	1.18	1.23
74	L5	2837	OMU	O2-C2	-2.51	1.18	1.23
74	L5	3867	A2M	C2'-C1'	2.51	1.59	1.53
74	L5	4228	OMG	C5-C6	2.51	1.53	1.44
74	L5	3792	OMG	C2-N1	2.50	1.43	1.37
74	L5	3899	OMG	C2-N1	2.50	1.43	1.37
74	L5	4637	OMG	C2-N1	2.50	1.43	1.37
74	L5	4590	A2M	C2'-C1'	2.50	1.59	1.53
74	L5	4392	OMG	C5-C6	2.50	1.53	1.44
74	L5	4306	OMU	C5-C4	2.50	1.49	1.43
2	L8	75	OMG	C5-C6	2.49	1.53	1.44
74	L5	3944	OMG	C5-C6	2.48	1.53	1.44
74	L5	4618	OMG	C2-N1	2.48	1.43	1.37
74	L5	4620	OMU	O2-C2	-2.47	1.18	1.23
74	L5	1881	OMC	C5-C4	2.47	1.48	1.42
74	L5	4571	A2M	C2'-C1'	2.47	1.59	1.53
74	L5	2351	OMC	C5-C4	2.47	1.48	1.42
74	L5	4370	OMG	C5-C6	2.46	1.53	1.44
74	L5	1522	OMG	C2-N1	2.46	1.43	1.37
74	L5	1522	OMG	C6-N1	2.46	1.43	1.38
74	L5	2424	OMG	C5-C6	2.45	1.53	1.44
74	L5	3718	A2M	C5-N7	-2.45	1.34	1.39
74	L5	4530	UR3	O4-C4	-2.45	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2364	OMG	C2-N1	2.45	1.43	1.37
74	L5	4196	OMG	C5-C6	2.45	1.53	1.44
74	L5	3808	OMC	C5-C4	2.45	1.48	1.42
74	L5	4623	OMG	C2-N1	2.44	1.43	1.37
74	L5	1534	A2M	C2'-C1'	2.44	1.59	1.53
74	L5	3944	OMG	C6-N1	2.44	1.43	1.38
74	L5	4227	OMU	C5-C4	2.44	1.49	1.43
74	L5	1522	OMG	C5-C6	2.44	1.53	1.44
74	L5	3744	OMG	C2-N1	2.44	1.43	1.37
74	L5	4306	OMU	O2-C2	-2.43	1.18	1.23
74	L5	3869	OMC	C5-C4	2.43	1.48	1.42
74	L5	4499	OMG	C5-C6	2.43	1.53	1.44
74	L5	2804	OMC	C5-C4	2.43	1.48	1.42
74	L5	3627	OMG	C5-C6	2.41	1.53	1.44
74	L5	4618	OMG	C5-C6	2.41	1.53	1.44
74	L5	3944	OMG	O6-C6	-2.41	1.19	1.23
74	L5	4392	OMG	C2-N1	2.41	1.43	1.37
74	L5	4456	OMC	C5-C4	2.41	1.48	1.42
74	L5	1625	OMG	C5-C6	2.41	1.53	1.44
74	L5	3792	OMG	C5-C6	2.40	1.53	1.44
74	L5	4623	OMG	C5-C6	2.39	1.53	1.44
74	L5	3818	UY1	O2-C2	-2.38	1.18	1.23
74	L5	3887	OMC	C5-C4	2.38	1.48	1.42
74	L5	3841	OMC	C5-C4	2.37	1.48	1.42
74	L5	2365	OMC	C5-C4	2.37	1.48	1.42
74	L5	3818	UY1	C1'-C5	2.36	1.55	1.50
74	L5	3899	OMG	C5-C6	2.35	1.53	1.44
74	L5	3825	A2M	C5-N7	-2.35	1.34	1.39
74	L5	4637	OMG	C5-C6	2.35	1.53	1.44
74	L5	1316	OMG	C5-C6	2.35	1.53	1.44
74	L5	3925	OMU	C5-C4	2.33	1.48	1.43
74	L5	3744	OMG	C5-C6	2.33	1.53	1.44
74	L5	4227	OMU	O2-C2	-2.33	1.18	1.23
74	L5	2837	OMU	C5-C4	2.32	1.48	1.43
74	L5	4196	OMG	C2-N1	2.32	1.43	1.37
74	L5	400	A2M	C5-N7	-2.32	1.34	1.39
74	L5	4228	OMG	C6-N1	2.31	1.43	1.38
74	L5	2861	OMC	C5-C4	2.30	1.48	1.42
74	L5	2415	OMU	C5-C4	2.30	1.48	1.43
74	L5	4494	OMG	C6-N1	2.29	1.43	1.38
74	L5	4530	UR3	O2-C2	-2.29	1.18	1.22
74	L5	2363	A2M	C5-N7	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	2824	OMC	C5-C4	2.28	1.48	1.42
74	L5	4620	OMU	C5-C4	2.26	1.48	1.43
74	L5	3867	A2M	C5-N7	-2.25	1.34	1.39
74	L5	1625	OMG	C6-N1	2.24	1.43	1.38
74	L5	4499	OMG	C6-N1	2.23	1.43	1.38
74	L5	4618	OMG	C6-N1	2.23	1.43	1.38
44	Pt	33	OMC	C5-C4	2.22	1.48	1.42
74	L5	3785	A2M	O5'-C5'	-2.22	1.39	1.44
74	L5	3627	OMG	C6-N1	2.21	1.42	1.38
74	L5	4530	UR3	C4-N3	2.21	1.45	1.40
74	L5	398	A2M	C5-N7	-2.21	1.34	1.39
74	L5	1534	A2M	O3'-C3'	2.20	1.48	1.43
74	L5	2422	OMC	C5-C4	2.20	1.48	1.42
74	L5	1316	OMG	C6-N1	2.19	1.42	1.38
74	L5	4523	A2M	C5-N7	-2.19	1.34	1.39
74	L5	1340	OMC	C5-C4	2.18	1.47	1.42
74	L5	4499	OMG	C4-N9	-2.18	1.32	1.38
74	L5	3785	A2M	O3'-C3'	2.18	1.48	1.43
74	L5	3792	OMG	C6-N1	2.17	1.42	1.38
74	L5	4623	OMG	C6-N1	2.16	1.42	1.38
74	L5	1322	1MA	C4-N9	-2.15	1.32	1.38
74	L5	4571	A2M	C5-N7	-2.15	1.35	1.39
74	L5	3830	A2M	C5-N7	-2.14	1.35	1.39
74	L5	4498	OMU	C5-C4	2.14	1.48	1.43
74	L5	4590	A2M	C5-N7	-2.14	1.35	1.39
2	L8	75	OMG	C6-N1	2.14	1.42	1.38
74	L5	2401	A2M	C5-N7	-2.13	1.35	1.39
74	L5	1871	A2M	C5-N7	-2.13	1.35	1.39
76	S6	8	4SU	O2-C2	-2.12	1.19	1.23
74	L5	3723	A2M	C5-N7	-2.12	1.35	1.39
74	L5	3867	A2M	O5'-C5'	-2.11	1.39	1.44
74	L5	3899	OMG	C6-N1	2.10	1.42	1.38
74	L5	4370	OMG	C6-N1	2.10	1.42	1.38
74	L5	4196	OMG	C6-N1	2.10	1.42	1.38
44	Pt	8	4SU	O2-C2	-2.09	1.19	1.23
74	L5	1326	A2M	C5-N7	-2.09	1.35	1.39
74	L5	2815	A2M	O3'-C3'	2.08	1.47	1.43
74	L5	400	A2M	O5'-C5'	-2.07	1.39	1.44
74	L5	2424	OMG	C6-N1	2.07	1.42	1.38
74	L5	3830	A2M	O3'-C3'	2.06	1.47	1.43
74	L5	3724	A2M	C5-N7	-2.06	1.35	1.39
74	L5	3723	A2M	O5'-C5'	-2.05	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	L5	4392	OMG	C6-N1	2.05	1.42	1.38
74	L5	3818	UY1	O4'-C1'	-2.05	1.41	1.43
74	L5	2401	A2M	O5'-C5'	-2.04	1.39	1.44
74	L5	2364	OMG	C6-N1	2.04	1.42	1.38
74	L5	2363	A2M	O3'-C3'	2.03	1.47	1.43
74	L5	1326	A2M	O5'-C5'	-2.03	1.39	1.44
74	L5	2363	A2M	O5'-C5'	-2.03	1.39	1.44
74	L5	1534	A2M	C5-N7	-2.02	1.35	1.39
74	L5	1871	A2M	O5'-C5'	-2.02	1.39	1.44
74	L5	1871	A2M	O3'-C3'	2.01	1.47	1.43
74	L5	4530	UR3	C5-C4	2.00	1.49	1.43
74	L5	4590	A2M	C4-N9	-2.00	1.33	1.37

All (808) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	1524	A2M	C1'-N9-C8	-12.20	99.58	127.14
74	L5	3723	A2M	C1'-N9-C8	-11.06	102.16	127.14
74	L5	3867	A2M	C1'-N9-C8	-11.04	102.20	127.14
74	L5	400	A2M	C1'-N9-C8	-11.00	102.29	127.14
74	L5	398	A2M	C1'-N9-C8	-10.80	102.75	127.14
74	L5	1534	A2M	C1'-N9-C8	-10.74	102.89	127.14
74	L5	3724	A2M	C1'-N9-C8	-10.64	103.11	127.14
74	L5	4571	A2M	C1'-N9-C8	-10.58	103.24	127.14
74	L5	2815	A2M	C1'-N9-C8	-10.57	103.27	127.14
74	L5	4220	6MZ	C1'-N9-C8	-10.54	103.33	127.14
74	L5	3718	A2M	C1'-N9-C8	-10.49	103.45	127.14
74	L5	2401	A2M	C1'-N9-C8	-10.46	103.53	127.14
74	L5	3785	A2M	C1'-N9-C8	-10.44	103.56	127.14
74	L5	2363	A2M	C1'-N9-C8	-10.43	103.58	127.14
74	L5	1326	A2M	C1'-N9-C8	-10.33	103.81	127.14
74	L5	4590	A2M	C1'-N9-C8	-10.29	103.89	127.14
74	L5	1524	A2M	C4-N9-C1'	10.21	150.91	126.59
74	L5	3830	A2M	C1'-N9-C8	-10.06	104.43	127.14
74	L5	400	A2M	C4-N9-C1'	10.04	150.51	126.59
74	L5	3718	A2M	C4-N9-C1'	10.01	150.43	126.59
74	L5	1871	A2M	C1'-N9-C8	-9.90	104.78	127.14
74	L5	3867	A2M	C4-N9-C1'	9.82	150.00	126.59
74	L5	3825	A2M	C1'-N9-C8	-9.77	105.08	127.14
74	L5	398	A2M	C4-N9-C1'	9.75	149.81	126.59
74	L5	3723	A2M	C4-N9-C1'	9.72	149.76	126.59
74	L5	4220	6MZ	C4-N9-C1'	9.64	149.55	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4523	A2M	C1'-N9-C8	-9.62	105.41	127.14
74	L5	2815	A2M	C4-N9-C1'	9.38	148.94	126.59
74	L5	3724	A2M	C4-N9-C1'	9.36	148.89	126.59
74	L5	1534	A2M	C4-N9-C1'	9.31	148.78	126.59
74	L5	2363	A2M	C4-N9-C1'	9.30	148.76	126.59
74	L5	2401	A2M	C4-N9-C1'	9.26	148.65	126.59
74	L5	4571	A2M	C4-N9-C1'	9.25	148.63	126.59
74	L5	1326	A2M	C4-N9-C1'	9.16	148.42	126.59
74	L5	3785	A2M	C4-N9-C1'	9.00	148.04	126.59
74	L5	3825	A2M	C4-N9-C1'	8.94	147.88	126.59
74	L5	4590	A2M	C4-N9-C1'	8.87	147.73	126.59
74	L5	3830	A2M	C4-N9-C1'	8.85	147.68	126.59
74	L5	4523	A2M	C4-N9-C1'	8.73	147.38	126.59
74	L5	1871	A2M	C4-N9-C1'	8.72	147.37	126.59
44	Pt	8	4SU	C4-N3-C2	-7.38	120.17	127.34
76	S6	8	4SU	C4-N3-C2	-7.06	120.48	127.34
74	L5	4590	A2M	N6-C6-N1	-6.46	104.20	118.35
74	L5	1534	A2M	N6-C6-N1	-6.39	104.36	118.35
74	L5	3744	OMG	C5-C4-N3	-6.26	118.30	128.46
74	L5	1871	A2M	N6-C6-N1	-6.25	104.66	118.35
74	L5	398	A2M	N6-C6-N1	-6.22	104.73	118.35
74	L5	3718	A2M	N6-C6-N1	-6.21	104.76	118.35
44	Pt	8	4SU	C5-C4-N3	6.19	120.43	114.69
74	L5	2815	A2M	N6-C6-N1	-6.17	104.83	118.35
74	L5	3724	A2M	N6-C6-N1	-6.14	104.91	118.35
74	L5	4392	OMG	C5-C4-N3	-6.12	118.54	128.46
74	L5	2401	A2M	N6-C6-N1	-6.11	104.98	118.35
74	L5	4196	OMG	C5-C4-N3	-6.10	118.56	128.46
74	L5	4228	OMG	C1'-N9-C4	-6.09	108.41	126.50
76	S6	47	G7M	CN7-N7-C5	6.08	134.32	126.77
74	L5	3830	A2M	N6-C6-N1	-6.05	105.10	118.35
74	L5	4523	A2M	N6-C6-N1	-6.04	105.13	118.35
44	Pt	47	G7M	CN7-N7-C5	6.01	134.24	126.77
74	L5	1326	A2M	N6-C6-N1	-6.01	105.18	118.35
74	L5	1871	A2M	N3-C2-N1	-6.01	119.21	128.60
74	L5	3792	OMG	C5-C4-N3	-5.97	118.77	128.46
74	L5	4590	A2M	N3-C2-N1	-5.94	119.32	128.60
74	L5	3785	A2M	N6-C6-N1	-5.89	105.44	118.35
74	L5	2363	A2M	N6-C6-N1	-5.87	105.48	118.35
74	L5	3825	A2M	N6-C6-N1	-5.86	105.51	118.35
74	L5	4590	A2M	C5-C6-N6	5.84	136.14	123.43
74	L5	2424	OMG	C5-C4-N3	-5.82	119.02	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	3723	A2M	N3-C2-N1	-5.81	119.51	128.60
74	L5	4228	OMG	C1'-N9-C8	5.81	143.22	126.70
74	L5	3723	A2M	N6-C6-N1	-5.79	105.67	118.35
74	L5	3830	A2M	N3-C2-N1	-5.77	119.58	128.60
74	L5	1326	A2M	N3-C2-N1	-5.77	119.58	128.60
74	L5	4499	OMG	C1'-N9-C4	-5.76	109.40	126.50
74	L5	4637	OMG	C5-C4-N3	-5.74	119.15	128.46
74	L5	1534	A2M	C5-C6-N6	5.73	135.90	123.43
74	L5	400	A2M	N6-C6-N1	-5.72	105.82	118.35
74	L5	1625	OMG	C5-C4-N3	-5.69	119.24	128.46
74	L5	1524	A2M	N3-C2-N1	-5.65	119.76	128.60
74	L5	1524	A2M	N6-C6-N1	-5.64	105.99	118.35
74	L5	1871	A2M	C5-C6-N6	5.64	135.70	123.43
74	L5	4618	OMG	C5-C4-N3	-5.63	119.32	128.46
74	L5	2815	A2M	N3-C2-N1	-5.63	119.79	128.60
74	L5	4571	A2M	N3-C2-N1	-5.63	119.80	128.60
74	L5	4220	6MZ	N1-C2-N3	-5.62	119.81	128.60
74	L5	4370	OMG	C5-C4-N3	-5.62	119.35	128.46
74	L5	3724	A2M	C5-C6-N6	5.58	135.58	123.43
74	L5	2401	A2M	N3-C2-N1	-5.58	119.88	128.60
74	L5	4571	A2M	N6-C6-N1	-5.58	106.14	118.35
74	L5	1522	OMG	C1'-N9-C4	-5.57	109.95	126.50
74	L5	3627	OMG	C5-C4-N3	-5.57	119.42	128.46
74	L5	400	A2M	N3-C2-N1	-5.57	119.89	128.60
74	L5	398	A2M	N3-C2-N1	-5.56	119.91	128.60
74	L5	3724	A2M	N3-C2-N1	-5.55	119.92	128.60
74	L5	4494	OMG	C5-C4-N3	-5.54	119.47	128.46
74	L5	3867	A2M	N6-C6-N1	-5.54	106.22	118.35
74	L5	4220	6MZ	C9-N6-C6	5.54	127.64	122.87
2	L8	75	OMG	C5-C4-N3	-5.53	119.48	128.46
74	L5	2363	A2M	N3-C2-N1	-5.53	119.95	128.60
74	L5	3785	A2M	N3-C2-N1	-5.53	119.95	128.60
74	L5	3899	OMG	C5-C4-N3	-5.52	119.50	128.46
74	L5	1316	OMG	C5-C4-N3	-5.51	119.52	128.46
74	L5	4499	OMG	C1'-N9-C8	5.49	142.34	126.70
74	L5	2401	A2M	C5-C6-N6	5.49	135.37	123.43
74	L5	3944	OMG	C1'-N9-C4	-5.48	110.23	126.50
74	L5	3718	A2M	C5-C6-N6	5.47	135.33	123.43
74	L5	4523	A2M	C5-C6-N6	5.46	135.32	123.43
74	L5	2415	OMU	C4-N3-C2	-5.45	119.39	126.58
74	L5	398	A2M	C5-C6-N6	5.44	135.28	123.43
74	L5	4227	OMU	C4-N3-C2	-5.42	119.43	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4623	OMG	C5-C4-N3	-5.42	119.67	128.46
74	L5	4623	OMG	C1'-N9-C4	-5.42	110.41	126.50
74	L5	4523	A2M	N3-C2-N1	-5.40	120.15	128.60
74	L5	398	A2M	C5-C4-N3	-5.39	119.72	126.75
74	L5	3825	A2M	N3-C2-N1	-5.37	120.20	128.60
74	L5	2815	A2M	C5-C6-N6	5.36	135.10	123.43
74	L5	3867	A2M	N3-C2-N1	-5.35	120.24	128.60
74	L5	3925	OMU	C4-N3-C2	-5.33	119.55	126.58
74	L5	2364	OMG	C5-C4-N3	-5.32	119.83	128.46
74	L5	1522	OMG	C1'-N9-C8	5.31	141.81	126.70
74	L5	3830	A2M	C5-C6-N6	5.31	134.98	123.43
74	L5	3718	A2M	C5-C4-N3	-5.30	119.84	126.75
74	L5	4498	OMU	C4-N3-C2	-5.29	119.61	126.58
74	L5	4618	OMG	C1'-N9-C4	-5.29	110.80	126.50
74	L5	3825	A2M	C5-C6-N6	5.28	134.93	123.43
74	L5	1534	A2M	N3-C2-N1	-5.28	120.34	128.60
74	L5	1536	PSU	C4-N3-C2	-5.24	118.79	126.34
74	L5	2837	OMU	C4-N3-C2	-5.23	119.68	126.58
74	L5	1522	OMG	C5-C4-N3	-5.21	120.01	128.46
74	L5	4623	OMG	C1'-N9-C8	5.20	141.49	126.70
76	S6	8	4SU	C5-C4-N3	5.19	119.51	114.69
74	L5	1326	A2M	C5-C6-N6	5.19	134.73	123.43
74	L5	3944	OMG	C1'-N9-C8	5.19	141.48	126.70
74	L5	2363	A2M	C5-C6-N6	5.16	134.65	123.43
74	L5	4306	OMU	C4-N3-C2	-5.14	119.80	126.58
74	L5	400	A2M	C5-C4-N3	-5.14	120.05	126.75
74	L5	4499	OMG	C5-C4-N3	-5.13	120.14	128.46
74	L5	3639	PSU	N1-C2-N3	5.12	120.93	115.13
74	L5	3627	OMG	C1'-N9-C4	-5.11	111.32	126.50
74	L5	1536	PSU	N1-C2-N3	5.11	120.92	115.13
74	L5	4370	OMG	C1'-N9-C4	-5.11	111.34	126.50
74	L5	4494	OMG	C1'-N9-C4	-5.10	111.34	126.50
74	L5	3944	OMG	C5-C4-N3	-5.09	120.20	128.46
74	L5	3723	A2M	C5-C6-N6	5.08	134.48	123.43
74	L5	400	A2M	C5-C6-N6	5.07	134.46	123.43
74	L5	4494	OMG	C1'-N9-C8	5.05	141.08	126.70
74	L5	2364	OMG	C1'-N9-C4	-5.05	111.50	126.50
74	L5	3627	OMG	C1'-N9-C8	5.04	141.05	126.70
74	L5	1524	A2M	C5-C6-N6	5.04	134.39	123.43
74	L5	4618	OMG	C1'-N9-C8	5.03	141.01	126.70
74	L5	4228	OMG	C5-C4-N3	-5.01	120.34	128.46
74	L5	4370	OMG	C1'-N9-C8	4.99	140.89	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	3785	A2M	C5-C6-N6	4.97	134.25	123.43
74	L5	4523	A2M	O4'-C1'-N9	4.97	117.85	108.06
74	L5	3867	A2M	C5-C4-N3	-4.97	120.27	126.75
74	L5	2364	OMG	C1'-N9-C8	4.96	140.83	126.70
74	L5	4353	PSU	N1-C2-N3	4.95	120.73	115.13
74	L5	4571	A2M	C5-C6-N6	4.94	134.19	123.43
74	L5	3723	A2M	C5-C4-N3	-4.94	120.31	126.75
74	L5	4353	PSU	C4-N3-C2	-4.94	119.22	126.34
2	L8	75	OMG	C1'-N9-C4	-4.94	111.84	126.50
74	L5	3818	UY1	C4-N3-C2	-4.93	119.24	126.34
74	L5	3920	PSU	C4-N3-C2	-4.92	119.24	126.34
74	L5	4637	OMG	C1'-N9-C4	-4.90	111.94	126.50
74	L5	4196	OMG	C2-N3-C4	4.90	121.02	112.30
74	L5	4531	PSU	N1-C2-N3	4.87	120.64	115.13
74	L5	4312	PSU	N1-C2-N3	4.86	120.64	115.13
74	L5	3818	UY1	N1-C2-N3	4.84	120.62	115.13
74	L5	1677	PSU	C4-N3-C2	-4.84	119.36	126.34
74	L5	3639	PSU	C4-N3-C2	-4.84	119.36	126.34
74	L5	4531	PSU	C4-N3-C2	-4.83	119.38	126.34
74	L5	1524	A2M	N9-C8-N7	-4.83	107.31	113.91
74	L5	1322	1MA	N1-C2-N3	-4.82	120.27	126.00
74	L5	2424	OMG	C1'-N9-C8	4.82	140.42	126.70
74	L5	2424	OMG	C1'-N9-C4	-4.81	112.21	126.50
74	L5	3899	OMG	C1'-N9-C4	-4.81	112.22	126.50
74	L5	1744	PSU	N1-C2-N3	4.81	120.58	115.13
74	L5	3920	PSU	N1-C2-N3	4.80	120.57	115.13
74	L5	3695	PSU	C4-N3-C2	-4.80	119.42	126.34
74	L5	1871	A2M	O4'-C1'-N9	4.80	117.52	108.06
74	L5	1860	PSU	N1-C2-N3	4.80	120.56	115.13
74	L5	3867	A2M	C5-C6-N6	4.79	133.86	123.43
74	L5	2363	A2M	C5-C4-N3	-4.79	120.50	126.75
74	L5	1744	PSU	C4-N3-C2	-4.79	119.44	126.34
74	L5	2632	PSU	N1-C2-N3	4.77	120.54	115.13
74	L5	4220	6MZ	C4-C5-C6	4.77	120.50	116.81
74	L5	4220	6MZ	C5-C4-N3	-4.75	120.55	126.75
74	L5	3844	PSU	N1-C2-N3	4.74	120.50	115.13
74	L5	4431	PSU	C4-N3-C2	-4.73	119.52	126.34
74	L5	4628	PSU	N1-C2-N3	4.73	120.49	115.13
74	L5	4500	PSU	N1-C2-N3	4.73	120.48	115.13
74	L5	2401	A2M	C5-C4-N3	-4.72	120.59	126.75
74	L5	4618	OMG	C2-N3-C4	4.72	120.72	112.30
74	L5	4361	PSU	C4-N3-C2	-4.72	119.54	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	1683	PSU	N1-C2-N3	4.72	120.47	115.13
74	L5	1316	OMG	C1'-N9-C4	-4.72	112.49	126.50
74	L5	1779	PSU	N1-C2-N3	4.71	120.47	115.13
74	L5	4431	PSU	N1-C2-N3	4.71	120.47	115.13
74	L5	3830	A2M	O4'-C1'-N9	4.71	117.34	108.06
74	L5	1316	OMG	C2-N3-C4	4.71	120.68	112.30
74	L5	4972	PSU	N1-C2-N3	4.70	120.46	115.13
74	L5	3792	OMG	C2-N3-C4	4.70	120.68	112.30
74	L5	4521	PSU	C4-N3-C2	-4.70	119.57	126.34
74	L5	4576	PSU	C4-N3-C2	-4.69	119.58	126.34
74	L5	3764	PSU	N1-C2-N3	4.69	120.45	115.13
74	L5	3734	PSU	N1-C2-N3	4.69	120.44	115.13
44	Pt	47	G7M	CN7-N7-C8	-4.68	117.61	124.84
74	L5	2815	A2M	C5-C4-N3	-4.68	120.64	126.75
74	L5	4637	OMG	C1'-N9-C8	4.68	140.01	126.70
74	L5	3744	OMG	C2-N3-C4	4.67	120.63	112.30
74	L5	1860	PSU	C4-N3-C2	-4.67	119.60	126.34
74	L5	4299	PSU	C4-N3-C2	-4.67	119.61	126.34
74	L5	4493	PSU	N1-C2-N3	4.67	120.42	115.13
74	L5	1862	PSU	N1-C2-N3	4.67	120.42	115.13
74	L5	3785	A2M	C5-C4-N3	-4.66	120.67	126.75
74	L5	3637	PSU	N1-C2-N3	4.65	120.40	115.13
74	L5	4571	A2M	C5-C4-N3	-4.65	120.69	126.75
74	L5	4442	PSU	N1-C2-N3	4.65	120.39	115.13
74	L5	3637	PSU	C4-N3-C2	-4.64	119.65	126.34
74	L5	3825	A2M	C5-C4-N3	-4.63	120.71	126.75
74	L5	3830	A2M	C5-C4-N3	-4.63	120.71	126.75
74	L5	4523	A2M	C5-C4-N3	-4.63	120.71	126.75
74	L5	1683	PSU	C4-N3-C2	-4.63	119.67	126.34
2	L8	75	OMG	C1'-N9-C8	4.62	139.86	126.70
74	L5	3734	PSU	C4-N3-C2	-4.62	119.69	126.34
74	L5	4521	PSU	N1-C2-N3	4.62	120.36	115.13
74	L5	3884	PSU	C4-N3-C2	-4.62	119.69	126.34
74	L5	1326	A2M	C5-C4-N3	-4.62	120.73	126.75
74	L5	3724	A2M	C5-C4-N3	-4.61	120.73	126.75
74	L5	5001	PSU	C4-N3-C2	-4.61	119.70	126.34
74	L5	1862	PSU	C4-N3-C2	-4.60	119.70	126.34
74	L5	3758	PSU	C4-N3-C2	-4.60	119.70	126.34
74	L5	4590	A2M	N9-C8-N7	-4.60	107.62	113.91
74	L5	4530	UR3	C4-N3-C2	-4.60	120.23	124.56
74	L5	3764	PSU	C4-N3-C2	-4.60	119.72	126.34
74	L5	3695	PSU	N1-C2-N3	4.60	120.34	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S6	8	4SU	C5-C4-S4	-4.59	118.55	124.47
74	L5	1625	OMG	C1'-N9-C4	-4.59	112.86	126.50
74	L5	2632	PSU	C4-N3-C2	-4.59	119.72	126.34
74	L5	4296	PSU	C4-N3-C2	-4.59	119.72	126.34
74	L5	4628	PSU	C4-N3-C2	-4.59	119.73	126.34
76	S6	47	G7M	CN7-N7-C8	-4.59	117.76	124.84
74	L5	4370	OMG	C2-N3-C4	4.58	120.46	112.30
74	L5	4493	PSU	C4-N3-C2	-4.58	119.75	126.34
74	L5	1522	OMG	C2-N3-C4	4.58	120.45	112.30
74	L5	2839	PSU	C4-N3-C2	-4.57	119.75	126.34
74	L5	2839	PSU	N1-C2-N3	4.57	120.31	115.13
74	L5	4494	OMG	C2-N3-C4	4.57	120.44	112.30
74	L5	4293	PSU	C4-N3-C2	-4.57	119.76	126.34
74	L5	398	A2M	O4'-C1'-N9	4.56	117.05	108.06
74	L5	2843	PSU	C4-N3-C2	-4.56	119.77	126.34
74	L5	4579	PSU	C4-N3-C2	-4.55	119.78	126.34
74	L5	1625	OMG	C1'-N9-C8	4.55	139.65	126.70
74	L5	1625	OMG	C2-N3-C4	4.55	120.40	112.30
74	L5	4637	OMG	C2-N3-C4	4.55	120.40	112.30
74	L5	4392	OMG	C2-N3-C4	4.54	120.39	112.30
74	L5	4442	PSU	C4-N3-C2	-4.54	119.80	126.34
74	L5	4471	PSU	N1-C2-N3	4.54	120.27	115.13
74	L5	4392	OMG	C1'-N9-C4	-4.54	113.03	126.50
74	L5	3899	OMG	C1'-N9-C8	4.54	139.61	126.70
74	L5	4293	PSU	N1-C2-N3	4.53	120.26	115.13
74	L5	4576	PSU	N1-C2-N3	4.53	120.26	115.13
74	L5	3851	PSU	N1-C2-N3	4.53	120.26	115.13
74	L5	4296	PSU	N1-C2-N3	4.53	120.26	115.13
74	L5	1782	PSU	C4-N3-C2	-4.53	119.82	126.34
76	S6	56	PSU	C4-N3-C2	-4.51	119.84	126.34
74	L5	4673	PSU	N1-C2-N3	4.51	120.24	115.13
74	L5	4403	PSU	N1-C2-N3	4.51	120.24	115.13
74	L5	4636	PSU	N1-C2-N3	4.51	120.23	115.13
74	L5	5010	PSU	N1-C2-N3	4.49	120.21	115.13
2	L8	75	OMG	C2-N3-C4	4.48	120.29	112.30
74	L5	4361	PSU	N1-C2-N3	4.48	120.21	115.13
74	L5	3627	OMG	C2-N3-C4	4.48	120.28	112.30
74	L5	1792	PSU	N1-C2-N3	4.48	120.20	115.13
74	L5	2424	OMG	C2-N3-C4	4.47	120.27	112.30
74	L5	4623	OMG	C2-N3-C4	4.47	120.26	112.30
74	L5	1534	A2M	C5-C4-N3	-4.47	120.92	126.75
74	L5	4620	OMU	C4-N3-C2	-4.47	120.69	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L8	55	PSU	C4-N3-C2	-4.47	119.90	126.34
74	L5	4403	PSU	C4-N3-C2	-4.47	119.91	126.34
44	Pt	47	G7M	C2-N3-C4	4.46	120.25	112.30
74	L5	4312	PSU	C4-N3-C2	-4.46	119.91	126.34
74	L5	5001	PSU	N1-C2-N3	4.46	120.18	115.13
74	L5	4500	PSU	C4-N3-C2	-4.46	119.92	126.34
74	L5	1534	A2M	N9-C8-N7	-4.46	107.82	113.91
74	L5	4569	PSU	N1-C2-N3	4.46	120.18	115.13
74	L5	4196	OMG	C1'-N9-C4	-4.45	113.28	126.50
74	L5	3718	A2M	N3-C2-N1	-4.45	121.65	128.60
74	L5	4579	PSU	N1-C2-N3	4.44	120.17	115.13
74	L5	1316	OMG	C1'-N9-C8	4.44	139.34	126.70
74	L5	2364	OMG	C2-N3-C4	4.44	120.21	112.30
74	L5	1524	A2M	C5-C4-N3	-4.44	120.96	126.75
74	L5	1677	PSU	N1-C2-N3	4.44	120.16	115.13
74	L5	5010	PSU	C4-N3-C2	-4.43	119.95	126.34
74	L5	3884	PSU	N1-C2-N3	4.43	120.15	115.13
74	L5	2508	PSU	N1-C2-N3	4.42	120.14	115.13
74	L5	4299	PSU	N1-C2-N3	4.41	120.13	115.13
76	S6	56	PSU	N1-C2-N3	4.41	120.13	115.13
74	L5	3768	PSU	C4-N3-C2	-4.41	119.98	126.34
74	L5	3853	PSU	N1-C2-N3	4.41	120.13	115.13
2	L8	55	PSU	N1-C2-N3	4.41	120.13	115.13
74	L5	4689	PSU	N1-C2-N3	4.41	120.12	115.13
74	L5	4471	PSU	C4-N3-C2	-4.41	119.99	126.34
74	L5	1782	PSU	N1-C2-N3	4.41	120.12	115.13
74	L5	1792	PSU	C4-N3-C2	-4.40	120.00	126.34
74	L5	2508	PSU	C4-N3-C2	-4.40	120.00	126.34
74	L5	1582	PSU	N1-C2-N3	4.39	120.11	115.13
74	L5	3785	A2M	N9-C8-N7	-4.39	107.90	113.91
74	L5	3844	PSU	C4-N3-C2	-4.38	120.02	126.34
74	L5	3768	PSU	N1-C2-N3	4.38	120.10	115.13
74	L5	4590	A2M	O4'-C1'-N9	4.38	116.70	108.06
74	L5	1781	PSU	C4-N3-C2	-4.38	120.03	126.34
74	L5	3729	PSU	N1-C2-N3	4.38	120.09	115.13
74	L5	3825	A2M	O4'-C1'-N9	4.38	116.69	108.06
74	L5	3899	OMG	C2-N3-C4	4.37	120.09	112.30
74	L5	1781	PSU	N1-C2-N3	4.37	120.08	115.13
74	L5	4499	OMG	C2-N3-C4	4.37	120.09	112.30
74	L5	4689	PSU	C4-N3-C2	-4.37	120.05	126.34
74	L5	1779	PSU	C4-N3-C2	-4.36	120.06	126.34
74	L5	3944	OMG	C2-N3-C4	4.35	120.06	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4392	OMG	C1'-N9-C8	4.35	139.08	126.70
74	L5	3830	A2M	C2'-C1'-N9	-4.35	106.21	113.53
74	L5	3770	PSU	C4-N3-C2	-4.34	120.08	126.34
74	L5	3724	A2M	N9-C8-N7	-4.34	107.97	113.91
74	L5	3744	OMG	C1'-N9-C4	-4.34	113.61	126.50
74	L5	4972	PSU	C4-N3-C2	-4.34	120.09	126.34
74	L5	4532	PSU	C4-N3-C2	-4.34	120.09	126.34
74	L5	2843	PSU	N1-C2-N3	4.33	120.04	115.13
74	L5	4552	PSU	N1-C2-N3	4.32	120.03	115.13
74	L5	3770	PSU	N1-C2-N3	4.32	120.03	115.13
74	L5	4552	PSU	C4-N3-C2	-4.32	120.11	126.34
74	L5	4423	PSU	C4-N3-C2	-4.32	120.12	126.34
74	L5	1871	A2M	C5-C4-N3	-4.32	121.12	126.75
74	L5	4532	PSU	N1-C2-N3	4.32	120.02	115.13
74	L5	4673	PSU	C4-N3-C2	-4.31	120.12	126.34
74	L5	1322	1MA	C5-C4-N3	-4.31	120.83	127.26
74	L5	3762	PSU	N1-C2-N3	4.31	120.01	115.13
44	Pt	56	PSU	N1-C2-N3	4.31	120.01	115.13
74	L5	3762	PSU	C4-N3-C2	-4.30	120.14	126.34
74	L5	3851	PSU	C4-N3-C2	-4.30	120.14	126.34
74	L5	4228	OMG	C2-N3-C4	4.30	119.96	112.30
74	L5	4196	OMG	C1'-N9-C8	4.30	138.93	126.70
74	L5	1582	PSU	C4-N3-C2	-4.28	120.17	126.34
74	L5	3715	PSU	C4-N3-C2	-4.28	120.18	126.34
2	L8	69	PSU	N1-C2-N3	4.28	119.97	115.13
74	L5	4423	PSU	N1-C2-N3	4.27	119.97	115.13
74	L5	3830	A2M	N9-C8-N7	-4.27	108.07	113.91
74	L5	3785	A2M	O4'-C1'-N9	4.26	116.45	108.06
76	S6	47	G7M	C2-N3-C4	4.25	119.87	112.30
74	L5	3744	OMG	N9-C4-N3	4.24	134.46	125.94
74	L5	4569	PSU	C4-N3-C2	-4.24	120.23	126.34
74	L5	3853	PSU	C4-N3-C2	-4.23	120.24	126.34
74	L5	3818	UY1	C6-C5-C4	4.23	121.16	118.20
74	L5	3729	PSU	C4-N3-C2	-4.22	120.25	126.34
44	Pt	56	PSU	C4-N3-C2	-4.22	120.26	126.34
74	L5	3744	OMG	C1'-N9-C8	4.22	138.71	126.70
74	L5	1871	A2M	N9-C8-N7	-4.21	108.15	113.91
74	L5	4571	A2M	N9-C8-N7	-4.21	108.15	113.91
74	L5	2401	A2M	N9-C8-N7	-4.21	108.15	113.91
74	L5	2363	A2M	O4'-C1'-N9	4.20	116.34	108.06
74	L5	4457	PSU	C4-N3-C2	-4.18	120.31	126.34
74	L5	3792	OMG	C1'-N9-C4	-4.17	114.12	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L8	69	PSU	C4-N3-C2	-4.17	120.33	126.34
74	L5	3723	A2M	N9-C8-N7	-4.16	108.22	113.91
74	L5	3792	OMG	C1'-N9-C8	4.14	138.48	126.70
74	L5	2401	A2M	O4'-C1'-N9	4.14	116.21	108.06
74	L5	4227	OMU	N3-C2-N1	4.14	120.38	114.89
74	L5	2815	A2M	N9-C8-N7	-4.12	108.28	113.91
74	L5	3724	A2M	O4'-C1'-N9	4.12	116.18	108.06
44	Pt	47	G7M	C5-C4-N3	-4.12	120.26	128.15
74	L5	4590	A2M	C5-C4-N3	-4.09	121.42	126.75
74	L5	4420	PSU	N1-C2-N3	4.08	119.76	115.13
74	L5	4636	PSU	C4-N3-C2	-4.08	120.46	126.34
74	L5	4571	A2M	O4'-C1'-N9	4.07	116.09	108.06
74	L5	3718	A2M	O4'-C1'-N9	4.07	116.08	108.06
74	L5	3723	A2M	O4'-C1'-N9	4.05	116.05	108.06
74	L5	3867	A2M	N9-C8-N7	-4.05	108.37	113.91
74	L5	2415	OMU	N3-C2-N1	4.04	120.25	114.89
74	L5	4392	OMG	N9-C4-N3	4.03	134.03	125.94
74	L5	1326	A2M	N9-C8-N7	-4.03	108.40	113.91
74	L5	2363	A2M	N9-C8-N7	-4.01	108.44	113.91
74	L5	4447	5MC	C5-C6-N1	-3.96	119.27	123.34
76	S6	47	G7M	C5-C6-N1	3.95	120.04	111.79
74	L5	398	A2M	N9-C8-N7	-3.94	108.52	113.91
74	L5	4306	OMU	N3-C2-N1	3.93	120.11	114.89
74	L5	3758	PSU	N1-C2-N3	3.92	119.58	115.13
74	L5	3925	OMU	N3-C2-N1	3.90	120.07	114.89
74	L5	3785	A2M	C4'-O4'-C1'	-3.90	100.86	109.47
74	L5	4457	PSU	N1-C2-N3	3.90	119.55	115.13
44	Pt	47	G7M	C5-C6-N1	3.89	119.92	111.79
74	L5	4196	OMG	N9-C4-N3	3.89	133.75	125.94
74	L5	4420	PSU	C4-N3-C2	-3.87	120.76	126.34
74	L5	1326	A2M	O4'-C1'-N9	3.86	115.67	108.06
44	Pt	47	G7M	C1'-N9-C8	-3.84	113.78	126.74
74	L5	3715	PSU	N1-C2-N3	3.82	119.46	115.13
74	L5	2815	A2M	O4'-C1'-N9	3.82	115.59	108.06
44	Pt	47	G7M	C1'-N9-C4	3.82	137.84	126.50
74	L5	3792	OMG	N9-C4-N3	3.79	133.55	125.94
76	S6	47	G7M	C5-C4-N3	-3.79	120.88	128.15
74	L5	4523	A2M	N9-C8-N7	-3.79	108.73	113.91
74	L5	2837	OMU	N3-C2-N1	3.76	119.89	114.89
74	L5	1322	1MA	C2-N3-C4	3.74	119.77	112.41
76	S6	47	G7M	C1'-N9-C8	-3.74	114.10	126.74
76	S6	8	4SU	N3-C2-N1	3.73	119.83	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4637	OMG	N9-C4-N3	3.71	133.39	125.94
74	L5	4498	OMU	N3-C2-N1	3.68	119.78	114.89
2	L8	75	OMG	N9-C4-N3	3.68	133.32	125.94
74	L5	3899	OMG	N9-C4-N3	3.67	133.30	125.94
74	L5	1316	OMG	N9-C4-N3	3.66	133.29	125.94
74	L5	3723	A2M	C2-N3-C4	3.66	120.39	111.75
44	Pt	47	G7M	O6-C6-C5	-3.66	119.81	128.06
74	L5	1625	OMG	N9-C4-N3	3.66	133.28	125.94
74	L5	398	A2M	C2-N3-C4	3.64	120.36	111.75
74	L5	3867	A2M	O4'-C1'-N9	3.64	115.23	108.06
74	L5	4220	6MZ	N9-C8-N7	-3.63	108.94	113.91
44	Pt	8	4SU	C5-C4-S4	-3.62	119.80	124.47
74	L5	400	A2M	N9-C8-N7	-3.61	108.97	113.91
74	L5	2424	OMG	N9-C4-N3	3.61	133.18	125.94
74	L5	4618	OMG	N9-C4-N3	3.59	133.16	125.94
74	L5	2415	OMU	C5-C4-N3	3.58	120.20	114.84
76	S6	47	G7M	C1'-N9-C4	3.58	137.13	126.50
76	S6	47	G7M	O6-C6-C5	-3.56	120.04	128.06
74	L5	400	A2M	C2-N3-C4	3.55	120.14	111.75
74	L5	4590	A2M	C2'-C1'-N9	-3.54	107.56	113.53
74	L5	1326	A2M	C2-N3-C4	3.54	120.12	111.75
74	L5	2815	A2M	C2-N3-C4	3.54	120.11	111.75
74	L5	4620	OMU	N3-C2-N1	3.53	119.58	114.89
74	L5	3782	5MC	C5-C6-N1	-3.53	119.71	123.34
74	L5	3825	A2M	N9-C8-N7	-3.53	109.09	113.91
74	L5	3830	A2M	C2-N3-C4	3.53	120.08	111.75
74	L5	3925	OMU	C5-C4-N3	3.52	120.11	114.84
74	L5	2363	A2M	C2-N3-C4	3.48	119.97	111.75
74	L5	1534	A2M	C2'-C1'-N9	3.48	119.39	113.53
74	L5	2401	A2M	C2-N3-C4	3.47	119.95	111.75
74	L5	4370	OMG	N9-C4-N3	3.47	132.91	125.94
74	L5	1524	A2M	C4-N9-C8	3.47	109.48	105.73
74	L5	1871	A2M	C2-N3-C4	3.46	119.92	111.75
74	L5	3867	A2M	C2-N3-C4	3.46	119.92	111.75
74	L5	4623	OMG	N9-C4-N3	3.44	132.85	125.94
74	L5	2424	OMG	C2-N1-C6	-3.42	118.87	125.10
74	L5	3627	OMG	N9-C4-N3	3.41	132.79	125.94
74	L5	3785	A2M	C2-N3-C4	3.41	119.81	111.75
74	L5	4498	OMU	C5-C4-N3	3.41	119.94	114.84
74	L5	4523	A2M	C2-N3-C4	3.40	119.78	111.75
74	L5	2837	OMU	C5-C4-N3	3.40	119.93	114.84
74	L5	4196	OMG	C2-N1-C6	-3.40	118.91	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4227	OMU	C5-C4-N3	3.39	119.92	114.84
74	L5	3724	A2M	C2-N3-C4	3.39	119.76	111.75
74	L5	4571	A2M	C2-N3-C4	3.39	119.76	111.75
74	L5	1871	A2M	C2'-C1'-N9	-3.38	107.83	113.53
74	L5	3825	A2M	C2-N3-C4	3.38	119.74	111.75
74	L5	4392	OMG	C2-N1-C6	-3.38	118.94	125.10
74	L5	400	A2M	O4'-C1'-N9	3.37	114.69	108.06
74	L5	4590	A2M	C2-N3-C4	3.35	119.67	111.75
76	S6	8	4SU	C1'-N1-C2	3.32	123.58	117.57
74	L5	1524	A2M	C2-N3-C4	3.31	119.58	111.75
74	L5	1522	OMG	N9-C4-N3	3.31	132.58	125.94
74	L5	3729	PSU	O2-C2-N1	-3.30	119.15	122.79
74	L5	4220	6MZ	C2-N3-C4	3.30	119.56	111.75
74	L5	4494	OMG	N9-C4-N3	3.29	132.54	125.94
74	L5	3744	OMG	C2-N1-C6	-3.28	119.11	125.10
74	L5	4637	OMG	C2-N1-C6	-3.28	119.12	125.10
74	L5	3792	OMG	C2-N1-C6	-3.28	119.12	125.10
74	L5	1534	A2M	C2-N3-C4	3.26	119.45	111.75
74	L5	1316	OMG	C2-N1-C6	-3.24	119.20	125.10
44	Pt	47	G7M	C2-N1-C6	-3.21	119.24	125.10
74	L5	3627	OMG	C2-N1-C6	-3.20	119.26	125.10
74	L5	4494	OMG	C2-N1-C6	-3.20	119.27	125.10
74	L5	3718	A2M	C2-N3-C4	3.19	119.29	111.75
44	Pt	56	PSU	O2-C2-N1	-3.17	119.30	122.79
74	L5	4618	OMG	C2-N1-C6	-3.17	119.32	125.10
74	L5	1534	A2M	C5-N7-C8	3.17	108.01	103.51
74	L5	4623	OMG	C2-N1-C6	-3.15	119.36	125.10
74	L5	4370	OMG	C2-N1-C6	-3.13	119.39	125.10
74	L5	3944	OMG	N9-C4-N3	3.13	132.23	125.94
74	L5	2632	PSU	O2-C2-N1	-3.12	119.36	122.79
44	Pt	8	4SU	N3-C2-N1	3.10	119.01	114.89
74	L5	3899	OMG	C2-N1-C6	-3.10	119.45	125.10
74	L5	3695	PSU	O2-C2-N1	-3.08	119.40	122.79
74	L5	4499	OMG	C2-N1-C6	-3.07	119.50	125.10
74	L5	2364	OMG	N9-C4-N3	3.06	132.09	125.94
74	L5	4306	OMU	C5-C4-N3	3.05	119.40	114.84
74	L5	4620	OMU	C5-C4-N3	3.05	119.40	114.84
74	L5	4499	OMG	N9-C4-N3	3.04	132.04	125.94
74	L5	4590	A2M	C5-N7-C8	3.04	107.83	103.51
74	L5	3724	A2M	C5-N7-C8	3.04	107.82	103.51
74	L5	398	A2M	C5-N7-C8	3.02	107.80	103.51
74	L5	1625	OMG	C2-N1-C6	-3.02	119.59	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	3818	UY1	C6-N1-C2	-3.02	119.60	122.68
74	L5	2401	A2M	C5-N7-C8	3.02	107.80	103.51
76	S6	47	G7M	C2-N1-C6	-3.01	119.61	125.10
74	L5	3830	A2M	C5-N7-C8	3.01	107.78	103.51
74	L5	2401	A2M	C2'-C1'-N9	-2.99	108.50	113.53
74	L5	3925	OMU	O4-C4-C5	-2.98	119.92	125.16
74	L5	4498	OMU	O4-C4-C5	-2.98	119.92	125.16
74	L5	3770	PSU	O2-C2-N1	-2.97	119.52	122.79
74	L5	1524	A2M	N3-C4-N9	2.97	131.98	127.08
74	L5	1524	A2M	C5-N7-C8	2.97	107.72	103.51
74	L5	4228	OMG	N9-C4-N3	2.96	131.88	125.94
74	L5	398	A2M	N3-C4-N9	2.96	131.95	127.08
74	L5	4228	OMG	C2-N1-C6	-2.93	119.76	125.10
74	L5	2815	A2M	C2'-C1'-N9	-2.92	108.61	113.53
2	L8	75	OMG	C2-N1-C6	-2.92	119.78	125.10
74	L5	4636	PSU	C6-N1-C2	-2.91	119.71	122.68
74	L5	1322	1MA	N9-C8-N7	-2.91	107.92	113.39
74	L5	4228	OMG	N9-C8-N7	-2.91	107.92	113.39
74	L5	4420	PSU	O2-C2-N1	-2.90	119.60	122.79
74	L5	2837	OMU	O4-C4-C5	-2.90	120.07	125.16
74	L5	4689	PSU	O2-C2-N1	-2.89	119.61	122.79
74	L5	4618	OMG	N9-C8-N7	-2.89	107.95	113.39
74	L5	3724	A2M	C4'-O4'-C1'	-2.89	103.10	109.47
74	L5	3723	A2M	C5-N7-C8	2.89	107.61	103.51
74	L5	3944	OMG	C2-N1-C6	-2.87	119.86	125.10
74	L5	2364	OMG	C2-N1-C6	-2.87	119.87	125.10
74	L5	1316	OMG	C5-C6-N1	2.87	120.47	113.19
74	L5	4499	OMG	N9-C8-N7	-2.86	108.00	113.39
74	L5	3785	A2M	C5-N7-C8	2.86	107.58	103.51
74	L5	3764	PSU	O2-C2-N1	-2.86	119.65	122.79
74	L5	4312	PSU	O2-C2-N1	-2.85	119.65	122.79
74	L5	3867	A2M	N3-C4-N9	2.85	131.78	127.08
74	L5	4623	OMG	C5-C6-N1	2.84	120.40	113.19
74	L5	3867	A2M	C5-N7-C8	2.84	107.54	103.51
74	L5	2815	A2M	C5-N7-C8	2.84	107.54	103.51
74	L5	4571	A2M	C5-N7-C8	2.83	107.53	103.51
74	L5	4196	OMG	C5-C6-N1	2.82	120.35	113.19
74	L5	4403	PSU	O2-C2-N1	-2.82	119.69	122.79
74	L5	4576	PSU	O2-C2-N1	-2.82	119.69	122.79
44	Pt	47	G7M	N9-C4-N3	2.82	131.59	125.94
74	L5	4530	UR3	C1'-N1-C2	2.81	121.74	116.99
74	L5	1522	OMG	N9-C8-N7	-2.80	108.12	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	400	A2M	N3-C4-N9	2.79	131.69	127.08
74	L5	1522	OMG	C2-N1-C6	-2.79	120.02	125.10
74	L5	3718	A2M	C5-C4-N9	2.78	109.02	105.78
74	L5	4392	OMG	N9-C8-N7	-2.78	108.15	113.39
74	L5	1316	OMG	N9-C8-N7	-2.78	108.15	113.39
74	L5	1871	A2M	C5-N7-C8	2.78	107.46	103.51
74	L5	3744	OMG	O6-C6-C5	-2.78	119.23	126.60
74	L5	1536	PSU	O2-C2-N1	-2.78	119.73	122.79
74	L5	3723	A2M	N3-C4-N9	2.77	131.65	127.08
74	L5	4623	OMG	N9-C8-N7	-2.77	108.18	113.39
74	L5	4637	OMG	C5-C6-N1	2.76	120.21	113.19
74	L5	1781	PSU	O2-C2-N1	-2.76	119.75	122.79
74	L5	4531	PSU	O2-C2-N1	-2.76	119.75	122.79
74	L5	3718	A2M	N9-C8-N7	-2.76	110.14	113.91
74	L5	4353	PSU	O2-C2-N1	-2.75	119.76	122.79
74	L5	4618	OMG	C5-C6-N1	2.75	120.18	113.19
74	L5	3899	OMG	N9-C8-N7	-2.75	108.21	113.39
74	L5	4628	PSU	O2-C2-N1	-2.75	119.77	122.79
2	L8	75	OMG	N9-C8-N7	-2.74	108.23	113.39
74	L5	400	A2M	C5-N7-C8	2.74	107.40	103.51
74	L5	4552	PSU	O2-C2-N1	-2.73	119.78	122.79
74	L5	4361	PSU	O2-C2-N1	-2.73	119.79	122.79
74	L5	2363	A2M	C5-N7-C8	2.73	107.38	103.51
74	L5	4532	PSU	O2-C2-N1	-2.72	119.79	122.79
74	L5	1779	PSU	C6-N1-C2	-2.72	119.90	122.68
74	L5	3729	PSU	C6-N1-C2	-2.72	119.90	122.68
74	L5	3744	OMG	C5-C6-N1	2.72	120.10	113.19
74	L5	3944	OMG	N9-C8-N7	-2.72	108.26	113.39
74	L5	1522	OMG	C5-C6-N1	2.72	120.10	113.19
74	L5	3785	A2M	O4'-C1'-C2'	-2.72	101.80	106.57
74	L5	3792	OMG	C5-C6-N1	2.72	120.09	113.19
74	L5	1326	A2M	C5-N7-C8	2.72	107.37	103.51
74	L5	1316	OMG	O6-C6-C5	-2.72	119.40	126.60
74	L5	2424	OMG	C5-C6-N1	2.70	120.05	113.19
74	L5	4499	OMG	C5-C6-N1	2.70	120.05	113.19
74	L5	3627	OMG	C5-C6-N1	2.69	120.03	113.19
74	L5	4392	OMG	C5-C6-N1	2.68	120.01	113.19
74	L5	4220	6MZ	C5-N7-C8	2.68	107.32	103.51
74	L5	4370	OMG	C5-C6-N1	2.67	119.98	113.19
74	L5	4370	OMG	N9-C8-N7	-2.67	108.36	113.39
74	L5	3734	PSU	O2-C2-N1	-2.67	119.86	122.79
74	L5	4523	A2M	C5-N7-C8	2.66	107.29	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4196	OMG	N9-C8-N7	-2.65	108.40	113.39
74	L5	4312	PSU	C6-N1-C2	-2.64	119.98	122.68
74	L5	4228	OMG	O6-C6-C5	-2.64	119.61	126.60
74	L5	4623	OMG	O6-C6-C5	-2.64	119.61	126.60
74	L5	3944	OMG	C5-C6-N1	2.63	119.88	113.19
74	L5	4637	OMG	N9-C8-N7	-2.63	108.43	113.39
74	L5	2837	OMU	O2-C2-N1	-2.63	119.29	122.79
74	L5	4228	OMG	C5-C6-N1	2.63	119.87	113.19
76	S6	47	G7M	N9-C4-N3	2.63	131.22	125.94
2	L8	75	OMG	C5-C6-N1	2.62	119.86	113.19
76	S6	8	4SU	C6-N1-C2	-2.62	117.64	120.99
74	L5	3899	OMG	C5-C6-N1	2.62	119.84	113.19
74	L5	3627	OMG	N9-C8-N7	-2.61	108.47	113.39
74	L5	4423	PSU	O2-C2-N1	-2.61	119.92	122.79
74	L5	3825	A2M	C5-N7-C8	2.61	107.21	103.51
74	L5	2415	OMU	O4-C4-C5	-2.60	120.58	125.16
74	L5	1782	PSU	O2-C2-N1	-2.60	119.93	122.79
74	L5	1625	OMG	O6-C6-C5	-2.60	119.70	126.60
74	L5	4494	OMG	C5-C6-N1	2.60	119.79	113.19
74	L5	2839	PSU	O2-C2-N1	-2.60	119.93	122.79
74	L5	1534	A2M	C4-C5-N7	-2.60	107.45	110.62
74	L5	4590	A2M	C4'-O4'-C1'	-2.59	103.75	109.47
74	L5	1625	OMG	C5-C6-N1	2.59	119.77	113.19
74	L5	3639	PSU	O2-C2-N1	-2.59	119.94	122.79
74	L5	4457	PSU	O2-C2-N1	-2.59	119.94	122.79
74	L5	1683	PSU	O2-C2-N1	-2.58	119.94	122.79
74	L5	4370	OMG	O6-C6-C5	-2.58	119.74	126.60
74	L5	3627	OMG	O6-C6-C5	-2.58	119.75	126.60
74	L5	4494	OMG	N9-C8-N7	-2.58	108.54	113.39
74	L5	3844	PSU	C6-N1-C2	-2.57	120.05	122.68
74	L5	3818	UY1	O2-C2-N1	-2.57	119.96	122.79
74	L5	3899	OMG	O6-C6-C5	-2.57	119.79	126.60
74	L5	1860	PSU	O2-C2-N1	-2.56	119.97	122.79
44	Pt	56	PSU	C6-N1-C2	-2.56	120.06	122.68
74	L5	4431	PSU	O2-C2-N1	-2.56	119.97	122.79
74	L5	3844	PSU	O2-C2-N1	-2.55	119.98	122.79
74	L5	1683	PSU	C6-N1-C2	-2.55	120.07	122.68
74	L5	4673	PSU	C6-N1-C2	-2.55	120.08	122.68
74	L5	2363	A2M	N3-C4-N9	2.55	131.28	127.08
74	L5	4471	PSU	O2-C2-N1	-2.54	119.99	122.79
74	L5	2364	OMG	C5-C6-N1	2.54	119.65	113.19
74	L5	3785	A2M	N3-C4-N9	2.54	131.27	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4972	PSU	O2-C2-N1	-2.54	119.99	122.79
74	L5	1779	PSU	O2-C2-N1	-2.54	119.99	122.79
74	L5	1522	OMG	O6-C6-C5	-2.54	119.86	126.60
74	L5	4493	PSU	O2-C2-N1	-2.54	120.00	122.79
74	L5	4571	A2M	N3-C4-N9	2.54	131.26	127.08
74	L5	4523	A2M	C5-C4-N9	2.53	108.72	105.78
74	L5	4637	OMG	O6-C6-C5	-2.53	119.89	126.60
74	L5	2424	OMG	O6-C6-C5	-2.52	119.91	126.60
74	L5	3639	PSU	C6-N1-C2	-2.52	120.11	122.68
74	L5	4618	OMG	O6-C6-C5	-2.51	119.94	126.60
74	L5	3782	5MC	CM5-C5-C6	-2.51	119.50	122.85
74	L5	3920	PSU	O2-C2-N1	-2.51	120.03	122.79
74	L5	3762	PSU	O2-C2-N1	-2.50	120.03	122.79
74	L5	1677	PSU	O2-C2-N1	-2.50	120.04	122.79
74	L5	3792	OMG	O6-C6-C5	-2.50	119.97	126.60
74	L5	2364	OMG	N9-C8-N7	-2.49	108.70	113.39
74	L5	4579	PSU	O2-C2-N1	-2.49	120.05	122.79
74	L5	4521	PSU	O2-C2-N1	-2.49	120.05	122.79
44	Pt	33	OMC	O2-C2-N3	-2.49	118.28	122.33
74	L5	3768	PSU	O2-C2-N1	-2.48	120.06	122.79
74	L5	4972	PSU	C6-N1-C2	-2.48	120.15	122.68
74	L5	3758	PSU	O2-C2-N1	-2.47	120.07	122.79
74	L5	4569	PSU	C6-N1-C2	-2.47	120.16	122.68
74	L5	4499	OMG	O6-C6-C5	-2.46	120.06	126.60
74	L5	3718	A2M	N3-C4-N9	2.46	131.14	127.08
74	L5	3744	OMG	N9-C8-N7	-2.46	108.75	113.39
74	L5	4493	PSU	C6-N1-C2	-2.46	120.17	122.68
74	L5	1744	PSU	C6-N1-C2	-2.45	120.18	122.68
74	L5	4590	A2M	C4-N9-C8	2.44	108.38	105.73
74	L5	3825	A2M	C5-C4-N9	2.44	108.62	105.78
74	L5	4628	PSU	C6-N1-C2	-2.43	120.19	122.68
74	L5	2424	OMG	N9-C8-N7	-2.43	108.81	113.39
74	L5	1625	OMG	N9-C8-N7	-2.43	108.82	113.39
76	S6	56	PSU	O2-C2-N1	-2.43	120.12	122.79
74	L5	3785	A2M	C4-N9-C8	2.42	108.35	105.73
74	L5	4220	6MZ	N3-C4-N9	2.42	131.07	127.08
74	L5	4523	A2M	C4'-O4'-C1'	-2.42	104.14	109.47
74	L5	1582	PSU	C6-N1-C2	-2.41	120.21	122.68
74	L5	4306	OMU	O2-C2-N1	-2.41	119.59	122.79
74	L5	3944	OMG	O6-C6-C5	-2.40	120.22	126.60
74	L5	3792	OMG	N9-C8-N7	-2.40	108.86	113.39
74	L5	3770	PSU	C6-N1-C2	-2.40	120.23	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4552	PSU	C6-N1-C2	-2.40	120.23	122.68
74	L5	4423	PSU	C6-N1-C2	-2.39	120.23	122.68
74	L5	4306	OMU	O4-C4-C5	-2.39	120.95	125.16
74	L5	2508	PSU	O2-C2-N1	-2.39	120.16	122.79
74	L5	4196	OMG	O6-C6-C5	-2.39	120.26	126.60
74	L5	1792	PSU	O2-C2-N1	-2.39	120.16	122.79
74	L5	4471	PSU	C6-N1-C2	-2.39	120.24	122.68
74	L5	4571	A2M	C2'-C1'-N9	-2.38	109.52	113.53
74	L5	4673	PSU	O2-C2-N1	-2.37	120.18	122.79
3	LA	216	V5N	O-C-CA	-2.37	118.56	124.78
74	L5	4530	UR3	C6-N1-C2	-2.37	119.67	121.79
74	L5	4620	OMU	O4-C4-C5	-2.37	121.00	125.16
74	L5	2401	A2M	N3-C4-N9	2.36	130.98	127.08
74	L5	1326	A2M	N3-C4-N9	2.36	130.97	127.08
74	L5	1534	A2M	C5-C4-N9	2.36	108.53	105.78
74	L5	2815	A2M	C5-C4-N9	2.36	108.53	105.78
74	L5	1860	PSU	C6-N1-C2	-2.36	120.27	122.68
74	L5	4494	OMG	O6-C6-C5	-2.35	120.36	126.60
74	L5	4227	OMU	O4-C4-C5	-2.35	121.03	125.16
2	L8	75	OMG	O6-C6-C5	-2.34	120.39	126.60
76	S6	56	PSU	C6-N1-C2	-2.34	120.29	122.68
74	L5	3851	PSU	C6-N1-C2	-2.34	120.29	122.68
74	L5	2401	A2M	C4'-O4'-C1'	-2.34	104.32	109.47
2	L8	69	PSU	C6-N1-C2	-2.33	120.31	122.68
74	L5	4392	OMG	O6-C6-C5	-2.32	120.44	126.60
74	L5	2401	A2M	C4-C5-N7	-2.32	107.79	110.62
74	L5	3724	A2M	N3-C4-N9	2.32	130.90	127.08
74	L5	4590	A2M	C4-C5-N7	-2.31	107.80	110.62
74	L5	4457	PSU	C6-N1-C2	-2.31	120.32	122.68
74	L5	4392	OMG	C8-N7-C5	2.31	108.42	104.24
74	L5	3867	A2M	C4'-O4'-C1'	-2.31	104.38	109.47
74	L5	4442	PSU	C6-C5-C4	2.31	119.81	118.20
74	L5	3718	A2M	C5-N7-C8	2.31	106.79	103.51
74	L5	3925	OMU	O2-C2-N1	-2.31	119.72	122.79
74	L5	1326	A2M	C2'-C1'-N9	-2.30	109.65	113.53
74	L5	3695	PSU	C6-N1-C2	-2.30	120.33	122.68
74	L5	3830	A2M	N3-C4-N9	2.30	130.87	127.08
2	L8	55	PSU	C6-N1-C2	-2.30	120.33	122.68
74	L5	4579	PSU	C6-N1-C2	-2.30	120.33	122.68
74	L5	4531	PSU	C6-C5-C4	2.29	119.80	118.20
74	L5	4442	PSU	O2-C2-N1	-2.29	120.27	122.79
74	L5	1534	A2M	C3'-C2'-C1'	-2.29	98.58	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	4296	PSU	C6-N1-C2	-2.29	120.34	122.68
74	L5	3724	A2M	C4-C5-N7	-2.29	107.83	110.62
74	L5	4296	PSU	O2-C2-N1	-2.28	120.28	122.79
74	L5	2401	A2M	C5-C4-N9	2.28	108.43	105.78
74	L5	2815	A2M	N3-C4-N9	2.27	130.83	127.08
74	L5	3830	A2M	C4-C5-N7	-2.27	107.85	110.62
74	L5	4620	OMU	O2-C2-N1	-2.27	119.77	122.79
74	L5	3884	PSU	C6-N1-C2	-2.27	120.36	122.68
74	L5	1534	A2M	C4-N9-C8	2.27	108.19	105.73
74	L5	3853	PSU	C6-N1-C2	-2.27	120.36	122.68
74	L5	3830	A2M	C5-C4-N9	2.27	108.42	105.78
2	L8	55	PSU	O2-C2-N1	-2.26	120.31	122.79
74	L5	3718	A2M	C6-C5-C4	2.26	120.22	117.18
74	L5	2815	A2M	C4-C5-N7	-2.25	107.87	110.62
74	L5	3723	A2M	C4'-O4'-C1'	-2.25	104.50	109.47
2	L8	69	PSU	O4'-C1'-C2'	2.25	108.31	105.14
74	L5	398	A2M	C2'-C1'-N9	-2.25	109.75	113.53
27	La	39	V5N	O-C-CA	-2.25	118.89	124.78
74	L5	1871	A2M	C5-C4-N9	2.24	108.39	105.78
74	L5	3884	PSU	O2-C2-N1	-2.24	120.32	122.79
74	L5	4220	6MZ	C5-C4-N9	2.23	108.38	105.78
74	L5	4590	A2M	C5-C4-N9	2.23	108.38	105.78
74	L5	3762	PSU	C6-N1-C2	-2.23	120.40	122.68
74	L5	4420	PSU	C6-N1-C2	-2.23	120.40	122.68
74	L5	5001	PSU	O2-C2-N1	-2.22	120.34	122.79
74	L5	398	A2M	C4-C5-N7	-2.22	107.91	110.62
74	L5	3724	A2M	C5-C4-N9	2.22	108.37	105.78
74	L5	4636	PSU	O4'-C1'-C2'	2.22	108.27	105.14
74	L5	4571	A2M	C4-N9-C8	2.21	108.13	105.73
74	L5	4498	OMU	O2-C2-N1	-2.21	119.84	122.79
74	L5	4442	PSU	C6-N1-C2	-2.21	120.43	122.68
74	L5	2843	PSU	O2-C2-N1	-2.21	120.36	122.79
74	L5	4531	PSU	C6-N1-C2	-2.21	120.43	122.68
27	La	39	V5N	O2-CB-CA	2.20	111.93	107.28
74	L5	4196	OMG	C8-N7-C5	2.20	108.23	104.24
74	L5	2508	PSU	C6-N1-C2	-2.20	120.44	122.68
74	L5	4618	OMG	C8-N7-C5	2.20	108.22	104.24
74	L5	2861	OMC	C1'-N1-C2	2.19	123.32	118.42
74	L5	3718	A2M	C4-C5-N7	-2.19	107.95	110.62
74	L5	3734	PSU	C6-N1-C2	-2.19	120.44	122.68
74	L5	4523	A2M	C2'-C1'-N9	-2.19	109.84	113.53
74	L5	1792	PSU	C6-N1-C2	-2.19	120.44	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	1536	PSU	C6-N1-C2	-2.19	120.45	122.68
74	L5	398	A2M	C5-C4-N9	2.19	108.33	105.78
74	L5	4500	PSU	C6-N1-C2	-2.18	120.45	122.68
74	L5	4576	PSU	C6-N1-C2	-2.18	120.45	122.68
74	L5	1677	PSU	O4'-C1'-C2'	2.18	108.22	105.14
74	L5	3825	A2M	N3-C4-N9	2.18	130.67	127.08
74	L5	1524	A2M	C4'-O4'-C1'	-2.17	104.69	109.47
74	L5	4689	PSU	C6-N1-C2	-2.17	120.47	122.68
74	L5	1326	A2M	C5-C4-N9	2.16	108.30	105.78
74	L5	5010	PSU	C6-C5-C4	2.16	119.71	118.20
74	L5	2632	PSU	C6-N1-C2	-2.16	120.48	122.68
74	L5	3764	PSU	C6-N1-C2	-2.15	120.48	122.68
74	L5	3723	A2M	C4-N9-C8	2.15	108.06	105.73
74	L5	4532	PSU	C6-N1-C2	-2.15	120.48	122.68
74	L5	1534	A2M	O4'-C1'-C2'	-2.15	102.80	106.57
2	L8	69	PSU	O2-C2-N1	-2.14	120.43	122.79
74	L5	3825	A2M	C2'-C1'-N9	-2.14	109.93	113.53
74	L5	4228	OMG	C8-N7-C5	2.13	108.10	104.24
74	L5	400	A2M	C5-C4-N9	2.13	108.26	105.78
74	L5	2363	A2M	C4'-O4'-C1'	-2.13	104.78	109.47
74	L5	5010	PSU	C6-N1-C2	-2.12	120.51	122.68
74	L5	4293	PSU	O2-C2-N1	-2.12	120.46	122.79
74	L5	1779	PSU	C6-C5-C4	2.12	119.68	118.20
74	L5	3825	A2M	C4-C5-N7	-2.12	108.04	110.62
74	L5	3899	OMG	C8-N7-C5	2.11	108.07	104.24
74	L5	4523	A2M	N3-C4-N9	2.11	130.56	127.08
74	L5	4353	PSU	C6-N1-C2	-2.11	120.53	122.68
74	L5	1534	A2M	N3-C4-N9	2.11	130.56	127.08
74	L5	400	A2M	C4'-O4'-C1'	-2.11	104.82	109.47
74	L5	3768	PSU	C6-N1-C2	-2.10	120.53	122.68
74	L5	3723	A2M	C4-C5-N7	-2.10	108.06	110.62
74	L5	3724	A2M	C4-N9-C8	2.10	108.00	105.73
74	L5	1781	PSU	C6-N1-C2	-2.10	120.54	122.68
74	L5	4523	A2M	C4-C5-N7	-2.10	108.06	110.62
74	L5	4403	PSU	O4'-C1'-C2'	2.09	108.09	105.14
74	L5	2363	A2M	C5-C4-N9	2.09	108.22	105.78
74	L5	4442	PSU	O4'-C1'-C2'	2.09	108.09	105.14
74	L5	4494	OMG	C8-N7-C5	2.09	108.02	104.24
74	L5	2632	PSU	C6-C5-C4	2.09	119.66	118.20
74	L5	4403	PSU	C6-N1-C2	-2.08	120.56	122.68
74	L5	1522	OMG	C8-N7-C5	2.08	108.00	104.24
74	L5	3715	PSU	O2-C2-N1	-2.08	120.51	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L5	2839	PSU	C6-N1-C2	-2.07	120.56	122.68
74	L5	1522	OMG	C2'-C1'-N9	-2.07	110.20	114.22
74	L5	1625	OMG	C8-N7-C5	2.07	107.98	104.24
74	L5	1871	A2M	N3-C4-N9	2.07	130.49	127.08
74	L5	4500	PSU	C6-C5-C4	2.06	119.64	118.20
74	L5	3785	A2M	C4-C5-N7	-2.06	108.11	110.62
74	L5	1744	PSU	O2-C2-N1	-2.06	120.52	122.79
74	L5	1316	OMG	C8-N7-C5	2.06	107.96	104.24
74	L5	4293	PSU	C6-N1-C2	-2.06	120.58	122.68
2	L8	75	OMG	C8-N7-C5	2.05	107.96	104.24
74	L5	3627	OMG	C8-N7-C5	2.05	107.94	104.24
74	L5	2351	OMC	O2-C2-N3	-2.04	119.01	122.33
74	L5	4571	A2M	C4-C5-N7	-2.04	108.14	110.62
74	L5	3920	PSU	C6-N1-C2	-2.03	120.61	122.68
74	L5	4623	OMG	C8-N7-C5	2.03	107.92	104.24
74	L5	1871	A2M	C4'-O4'-C1'	-2.02	105.00	109.47
74	L5	1322	1MA	C8-N7-C5	2.02	107.90	104.24
74	L5	3808	OMC	O2-C2-N3	-2.02	119.05	122.33
74	L5	4521	PSU	C6-N1-C2	-2.02	120.62	122.68
74	L5	1326	A2M	C4-C5-N7	-2.02	108.16	110.62
74	L5	1871	A2M	C4-C5-N7	-2.02	108.16	110.62
74	L5	3792	OMG	C8-N7-C5	2.02	107.89	104.24
74	L5	3744	OMG	C8-N7-C5	2.01	107.89	104.24
74	L5	4571	A2M	C4'-O4'-C1'	-2.01	105.03	109.47
74	L5	1536	PSU	C6-C5-C4	2.01	119.60	118.20
74	L5	398	A2M	C6-C5-C4	2.00	119.88	117.18

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	LA	216	V5N	O-C-CA-CB
4	LB	245	HIC	O-C-CA-CB
76	S6	8	4SU	C3'-C4'-C5'-O5'
76	S6	47	G7M	O4'-C4'-C5'-O5'
76	S6	47	G7M	C3'-C4'-C5'-O5'
2	L8	75	OMG	C1'-C2'-O2'-CM2
74	L5	398	A2M	C1'-C2'-O2'-CM'
74	L5	2351	OMC	C1'-C2'-O2'-CM2
74	L5	2415	OMU	C1'-C2'-O2'-CM2
74	L5	2815	A2M	O4'-C4'-C5'-O5'
74	L5	2815	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
74	L5	3701	OMC	C2'-C1'-N1-C2
74	L5	3701	OMC	C2'-C1'-N1-C6
74	L5	3718	A2M	C1'-C2'-O2'-CM'
74	L5	3723	A2M	C1'-C2'-O2'-CM'
74	L5	3724	A2M	C1'-C2'-O2'-CM'
74	L5	3785	A2M	O4'-C4'-C5'-O5'
74	L5	3841	OMC	C1'-C2'-O2'-CM2
74	L5	3925	OMU	C1'-C2'-O2'-CM2
74	L5	3944	OMG	C3'-C4'-C5'-O5'
74	L5	3944	OMG	C1'-C2'-O2'-CM2
74	L5	4420	PSU	C2'-C1'-C5-C4
74	L5	4523	A2M	C1'-C2'-O2'-CM'
74	L5	4571	A2M	C1'-C2'-O2'-CM'
74	L5	4590	A2M	C4'-C5'-O5'-P
74	L5	4636	PSU	C3'-C4'-C5'-O5'
74	L5	4637	OMG	C1'-C2'-O2'-CM2
76	S6	8	4SU	O4'-C4'-C5'-O5'
76	S6	56	PSU	O4'-C4'-C5'-O5'
74	L5	398	A2M	O4'-C4'-C5'-O5'
74	L5	3723	A2M	O4'-C4'-C5'-O5'
74	L5	3758	PSU	O4'-C4'-C5'-O5'
74	L5	3785	A2M	C3'-C4'-C5'-O5'
74	L5	4636	PSU	O4'-C4'-C5'-O5'
28	Lb	5	MLZ	CA-CB-CG-CD
76	S6	56	PSU	C3'-C4'-C5'-O5'
74	L5	4447	5MC	C2'-C1'-N1-C6
74	L5	1781	PSU	C3'-C4'-C5'-O5'
74	L5	3758	PSU	C3'-C4'-C5'-O5'
74	L5	2422	OMC	C3'-C4'-C5'-O5'
74	L5	2422	OMC	O4'-C4'-C5'-O5'
74	L5	4228	OMG	O4'-C4'-C5'-O5'
74	L5	3944	OMG	O4'-C4'-C5'-O5'
74	L5	4500	PSU	C4'-C5'-O5'-P
74	L5	1792	PSU	O4'-C4'-C5'-O5'
74	L5	3792	OMG	O4'-C4'-C5'-O5'
74	L5	4228	OMG	C3'-C4'-C5'-O5'
74	L5	4590	A2M	C1'-C2'-O2'-CM'
74	L5	3867	A2M	C3'-C4'-C5'-O5'
74	L5	4447	5MC	C2'-C1'-N1-C2
74	L5	4447	5MC	O4'-C1'-N1-C6
74	L5	3818	UY1	C4'-C5'-O5'-P
74	L5	1781	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
74	L5	1326	A2M	C4'-C5'-O5'-P
74	L5	1534	A2M	C4'-C5'-O5'-P
74	L5	4447	5MC	O4'-C1'-N1-C2
74	L5	3844	PSU	C4'-C5'-O5'-P
74	L5	3701	OMC	O4'-C1'-N1-C6
27	La	39	V5N	O2-CB-CG-CD2
74	L5	3867	A2M	O4'-C4'-C5'-O5'
74	L5	3723	A2M	C3'-C4'-C5'-O5'
74	L5	3792	OMG	C3'-C4'-C5'-O5'
74	L5	3851	PSU	C3'-C4'-C5'-O5'
74	L5	3818	UY1	O4'-C1'-C5-C4
74	L5	4494	OMG	C3'-C2'-O2'-CM2
74	L5	1322	1MA	C2'-C1'-N9-C4
74	L5	1322	1MA	C2'-C1'-N9-C8
74	L5	4571	A2M	O4'-C4'-C5'-O5'
74	L5	398	A2M	C3'-C4'-C5'-O5'
74	L5	3729	PSU	O4'-C4'-C5'-O5'
74	L5	1792	PSU	C3'-C4'-C5'-O5'
74	L5	3734	PSU	O4'-C4'-C5'-O5'
74	L5	1677	PSU	O4'-C1'-C5-C6
74	L5	3818	UY1	O4'-C1'-C5-C6
74	L5	3701	OMC	O4'-C1'-N1-C2
74	L5	1534	A2M	O4'-C4'-C5'-O5'
74	L5	2351	OMC	O4'-C4'-C5'-O5'
74	L5	4293	PSU	O4'-C4'-C5'-O5'
44	Pt	56	PSU	O4'-C4'-C5'-O5'
74	L5	1625	OMG	C3'-C4'-C5'-O5'
76	S6	8	4SU	C4'-C5'-O5'-P

There are no ring outliers.

47 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
74	L5	4530	UR3	1	0
74	L5	4620	OMU	2	0
74	L5	2424	OMG	1	0
74	L5	4447	5MC	1	0
74	L5	3701	OMC	1	0
74	L5	4498	OMU	1	0
74	L5	3718	A2M	3	0
74	L5	3723	A2M	1	0
74	L5	2815	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	S6	47	G7M	1	0
74	L5	5010	PSU	2	0
74	L5	4457	PSU	1	0
74	L5	3925	OMU	1	0
74	L5	1871	A2M	1	0
74	L5	1340	OMC	1	0
74	L5	2351	OMC	2	0
74	L5	4370	OMG	1	0
74	L5	4531	PSU	1	0
74	L5	4536	OMC	1	0
74	L5	4571	A2M	1	0
74	L5	3944	OMG	2	0
74	L5	3770	PSU	3	0
76	S6	56	PSU	1	0
74	L5	3808	OMC	1	0
74	L5	5001	PSU	1	0
74	L5	2415	OMU	1	0
74	L5	2363	A2M	1	0
2	L8	75	OMG	2	0
74	L5	1326	A2M	1	0
74	L5	4637	OMG	2	0
76	S6	8	4SU	1	0
74	L5	1779	PSU	1	0
74	L5	3762	PSU	1	0
74	L5	4196	OMG	2	0
74	L5	4392	OMG	2	0
44	Pt	33	OMC	1	0
74	L5	1534	A2M	2	0
44	Pt	8	4SU	1	0
74	L5	1536	PSU	1	0
74	L5	398	A2M	1	0
74	L5	3724	A2M	2	0
74	L5	3920	PSU	1	0
74	L5	3785	A2M	1	0
74	L5	1881	OMC	1	0
74	L5	2804	OMC	1	0
74	L5	3715	PSU	1	0
74	L5	4227	OMU	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 292 ligands modelled in this entry, 288 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
85	HYG	S2	1901	-	35,39,39	3.07	11 (31%)	43,60,60	1.59	10 (23%)
86	SPD	L5	5102	-	9,9,9	0.28	0	8,8,8	0.35	0
86	SPD	L5	5101	-	9,9,9	0.28	0	8,8,8	0.42	0
86	SPD	L5	5103	-	9,9,9	0.28	0	8,8,8	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	HYG	S2	1901	-	-	6/12/87/87	0/4/4/4
86	SPD	L5	5102	-	-	3/7/7/7	-
86	SPD	L5	5101	-	-	0/7/7/7	-
86	SPD	L5	5103	-	-	1/7/7/7	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	S2	1901	HYG	O29-C12	10.97	1.61	1.43
85	S2	1901	HYG	O22-C17	6.54	1.53	1.43
85	S2	1901	HYG	O14-C13	6.47	1.58	1.41
85	S2	1901	HYG	O28-C23	5.90	1.47	1.40
85	S2	1901	HYG	C16-C15	4.34	1.62	1.53
85	S2	1901	HYG	C17-C12	-4.27	1.43	1.53
85	S2	1901	HYG	O28-C27	3.06	1.48	1.44
85	S2	1901	HYG	O18-C13	-2.72	1.34	1.41
85	S2	1901	HYG	O30-C24	2.38	1.47	1.42
85	S2	1901	HYG	C25-C24	-2.16	1.49	1.53
85	S2	1901	HYG	O31-C25	2.15	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	1901	HYG	O29-C12-C13	5.06	124.13	110.86
85	S2	1901	HYG	O22-C17-C16	4.38	121.87	111.22
85	S2	1901	HYG	O22-C17-C12	2.88	108.18	103.58
85	S2	1901	HYG	O28-C27-C26	2.48	112.05	108.52
85	S2	1901	HYG	C13-O18-C6	-2.29	112.29	117.96
85	S2	1901	HYG	C3-C4-C5	2.21	114.52	109.72
85	S2	1901	HYG	O14-C15-C16	2.20	113.69	109.69
85	S2	1901	HYG	O29-C12-C17	2.16	107.03	103.58
85	S2	1901	HYG	C26-C25-C24	2.07	114.15	111.30
85	S2	1901	HYG	C3-C4-N9	-2.06	107.59	112.17

There are no chirality outliers.

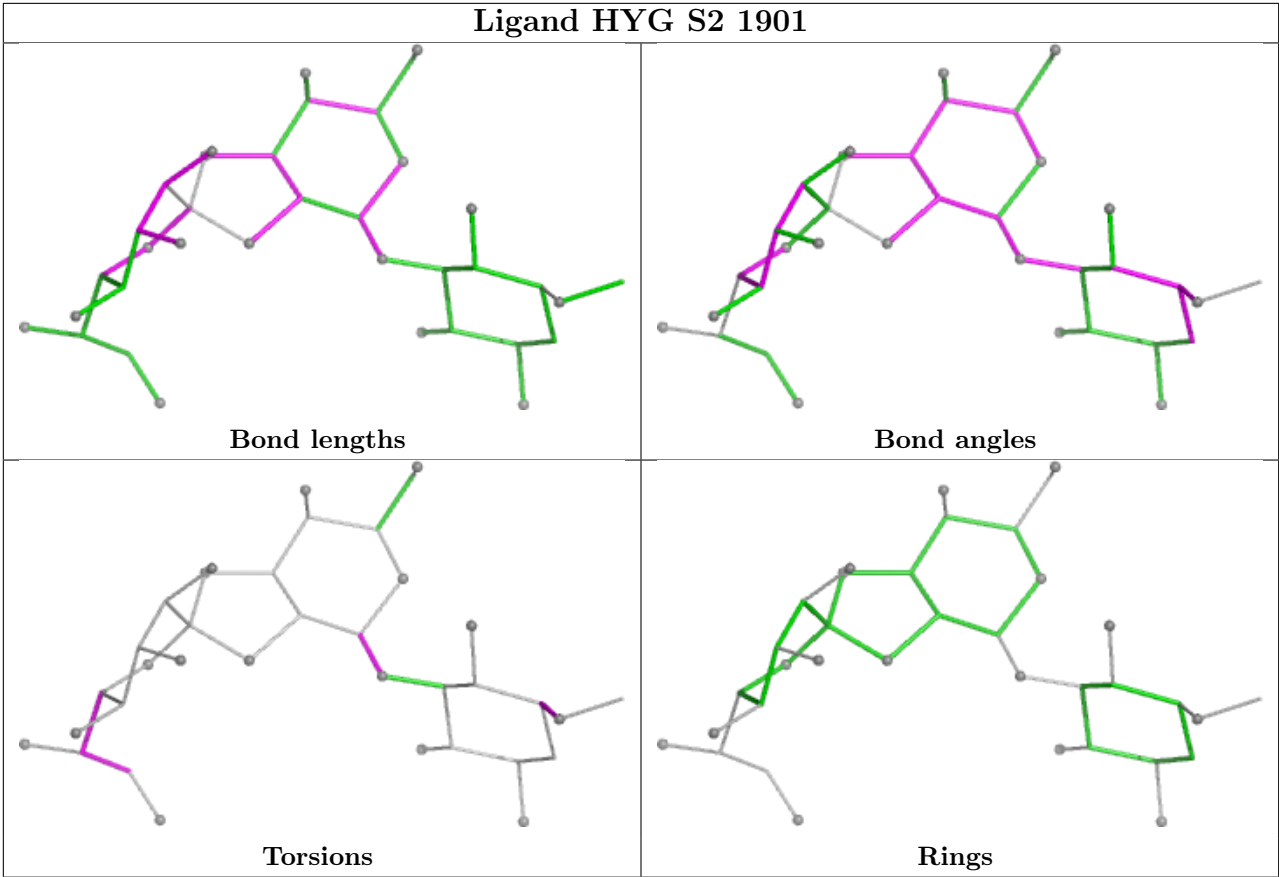
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	S2	1901	HYG	C26-C27-C33-C34
85	S2	1901	HYG	O28-C27-C33-C34
85	S2	1901	HYG	C27-C33-C34-O35
85	S2	1901	HYG	N36-C33-C34-O35
85	S2	1901	HYG	O14-C13-O18-C6
86	L5	5102	SPD	C4-C5-N6-C7
86	L5	5103	SPD	C2-C3-C4-C5
85	S2	1901	HYG	C5-C4-N9-C10
86	L5	5102	SPD	C8-C7-N6-C5
86	L5	5102	SPD	N6-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
74	L5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	1268:G	O3'	1274:A	P	24.24

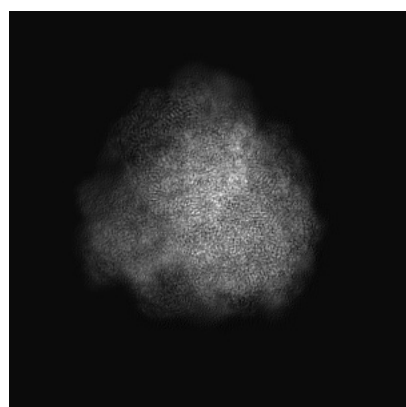
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54269. These allow visual inspection of the internal detail of the map and identification of artifacts.

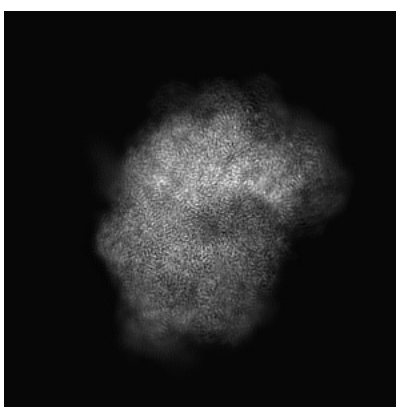
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

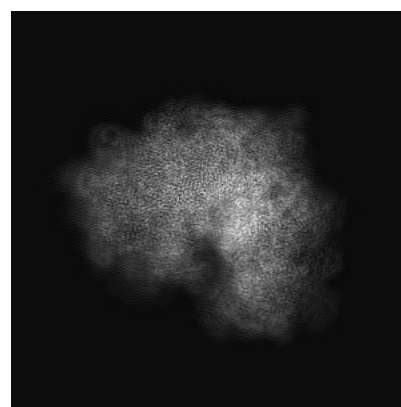
6.1.1 Primary map



X



Y

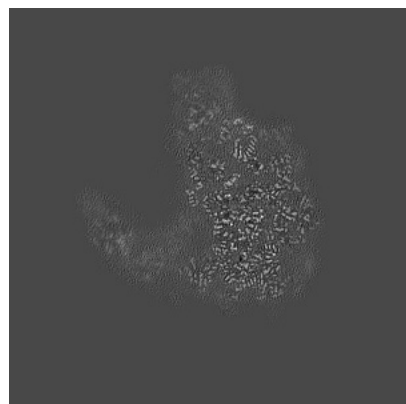


Z

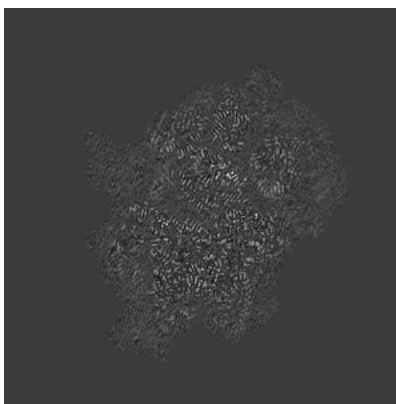
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

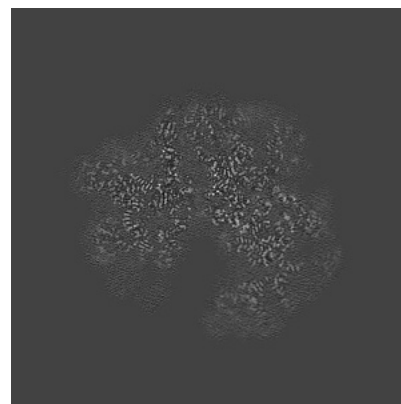
6.2.1 Primary map



X Index: 240



Y Index: 240

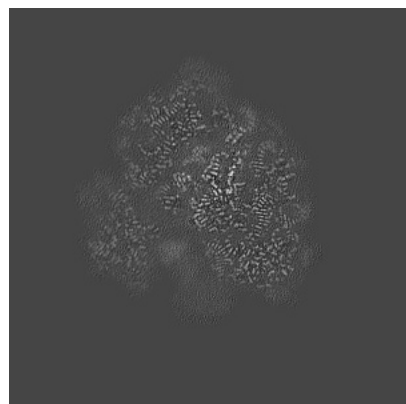


Z Index: 240

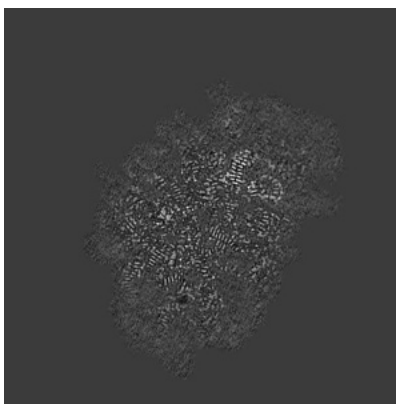
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

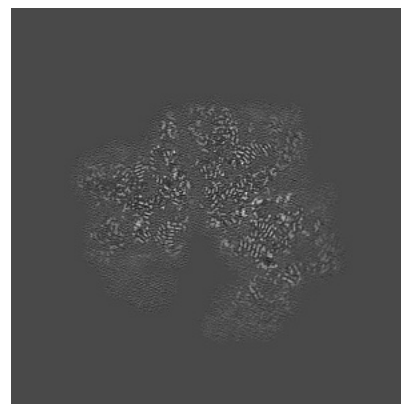
6.3.1 Primary map



X Index: 273



Y Index: 266

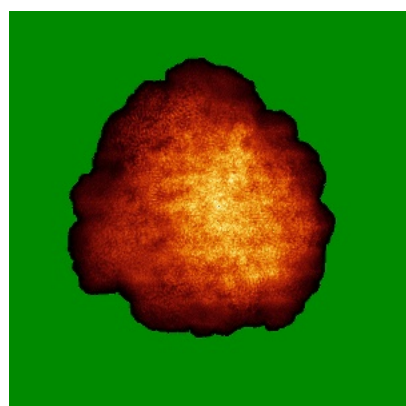


Z Index: 248

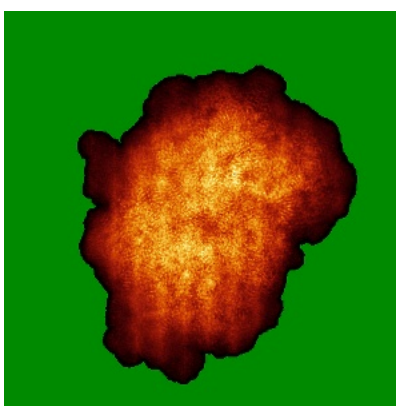
The images above show the largest variance slices of the map in three orthogonal directions.

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

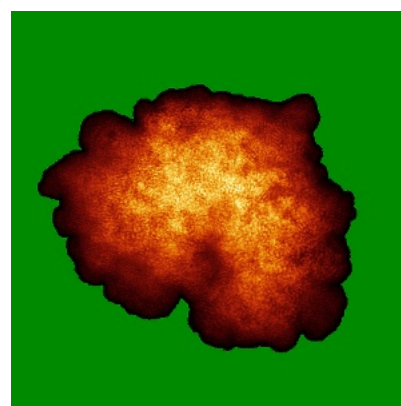
6.4.1 Primary map



X



Y

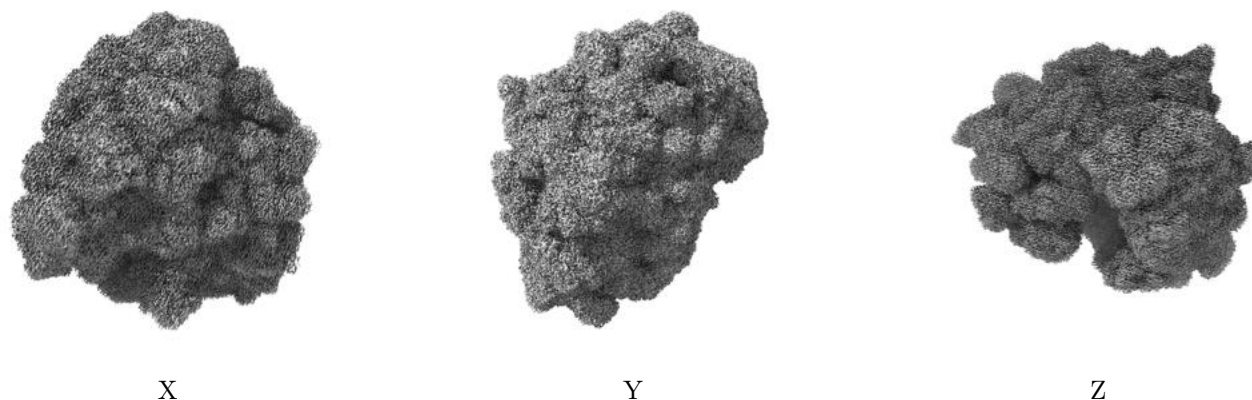


Z

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.

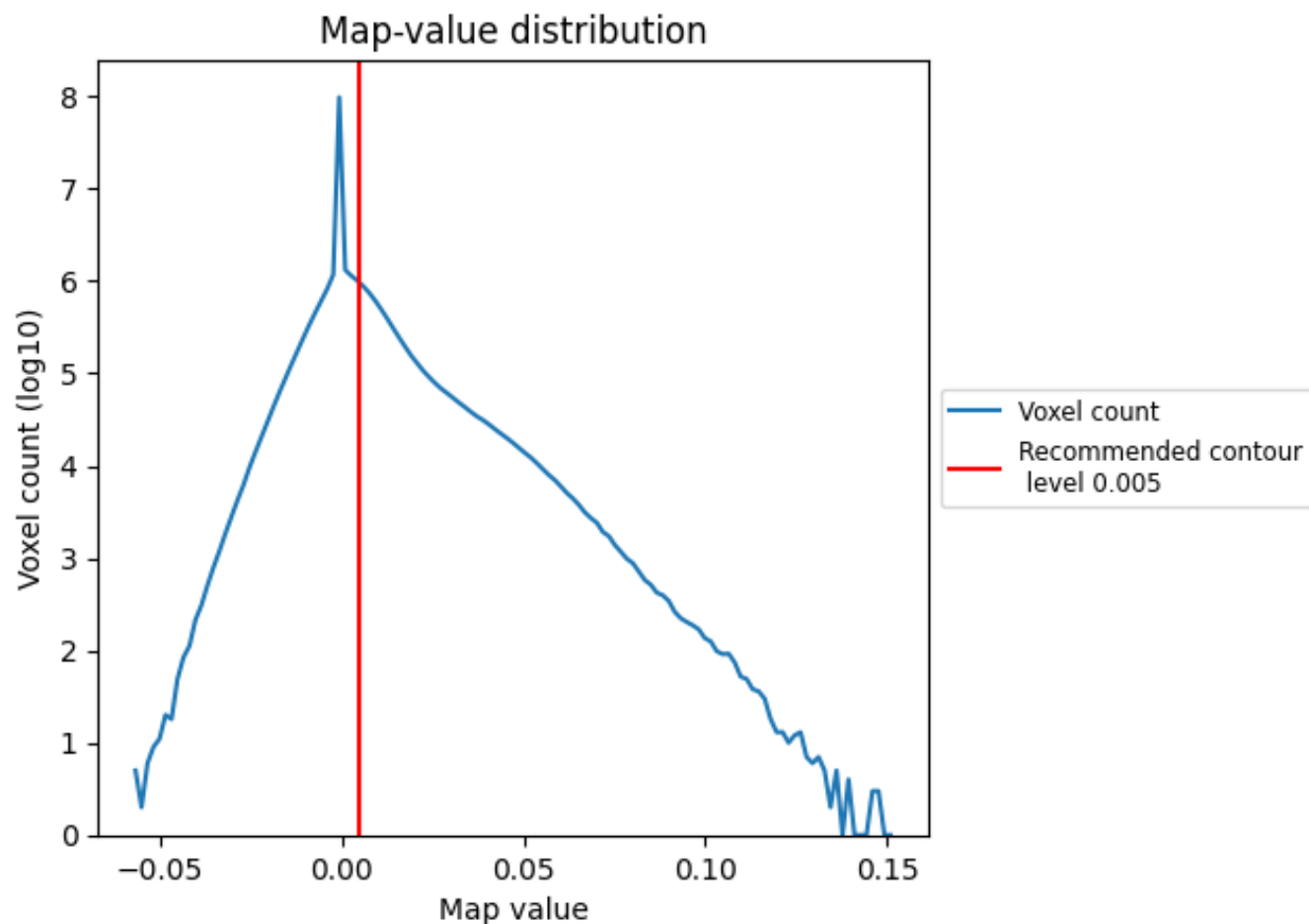
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

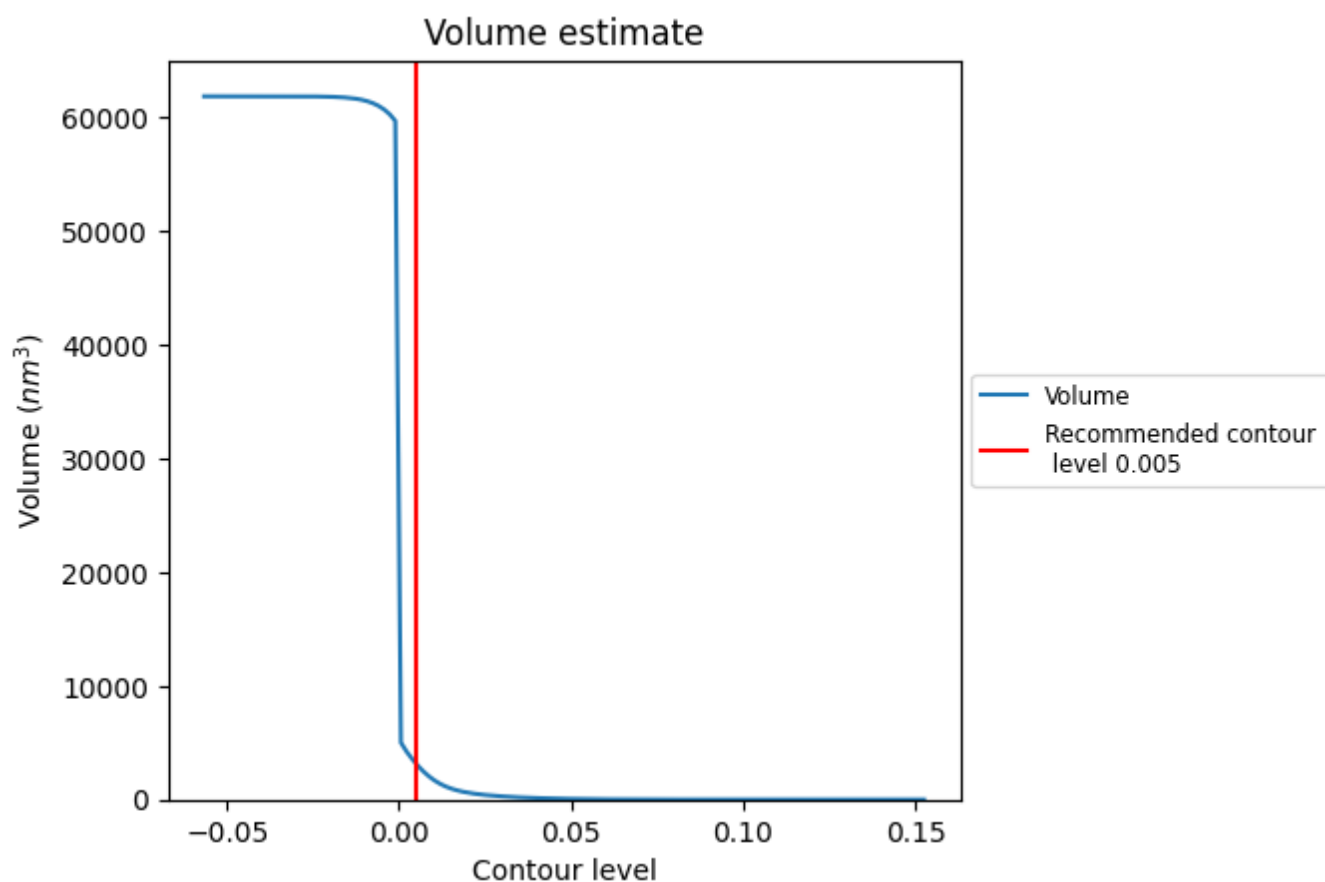
This section contains the results of statistical analysis of the map.

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.

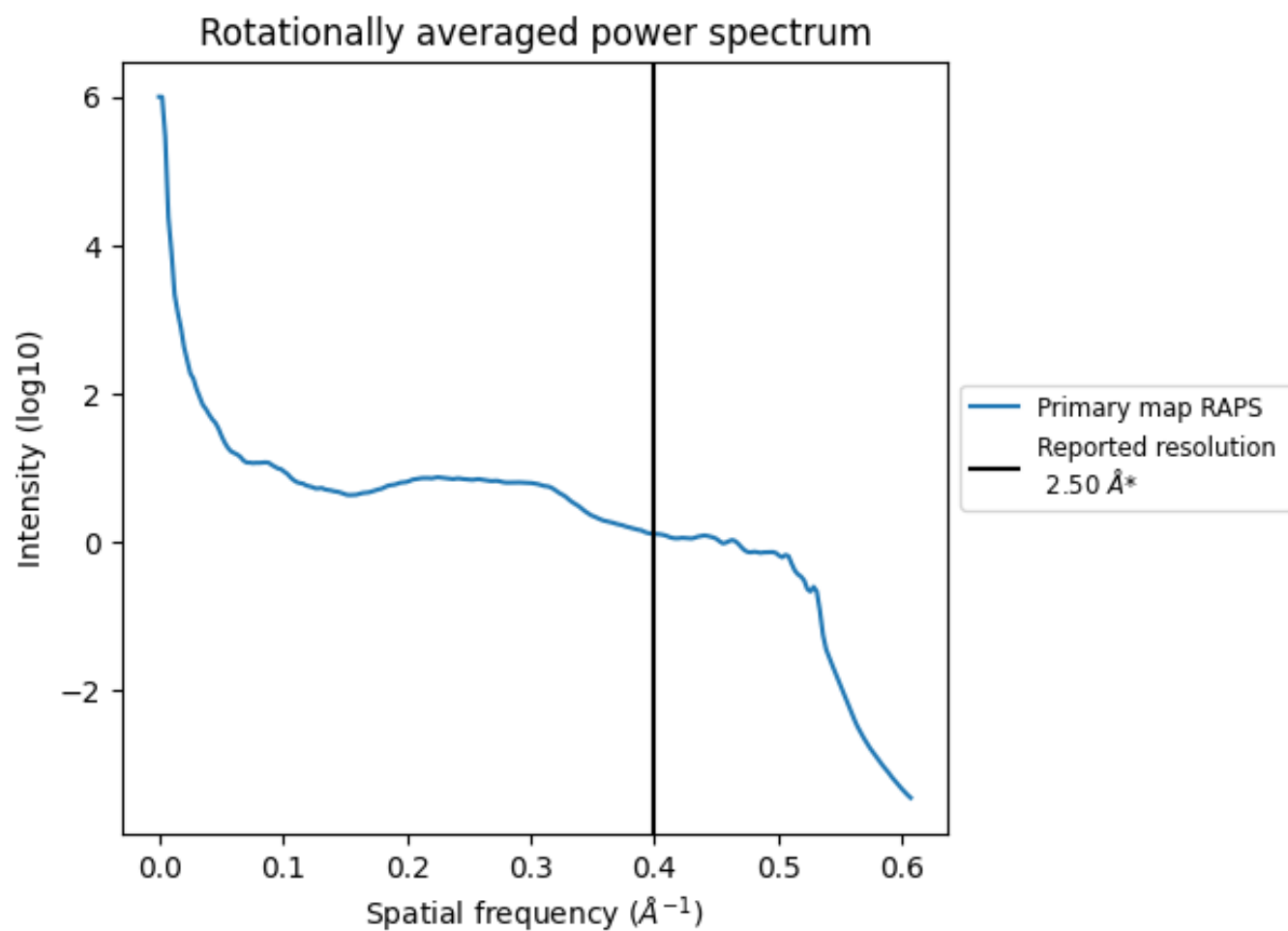
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3149 nm^3 ; this corresponds to an approximate mass of 2845 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

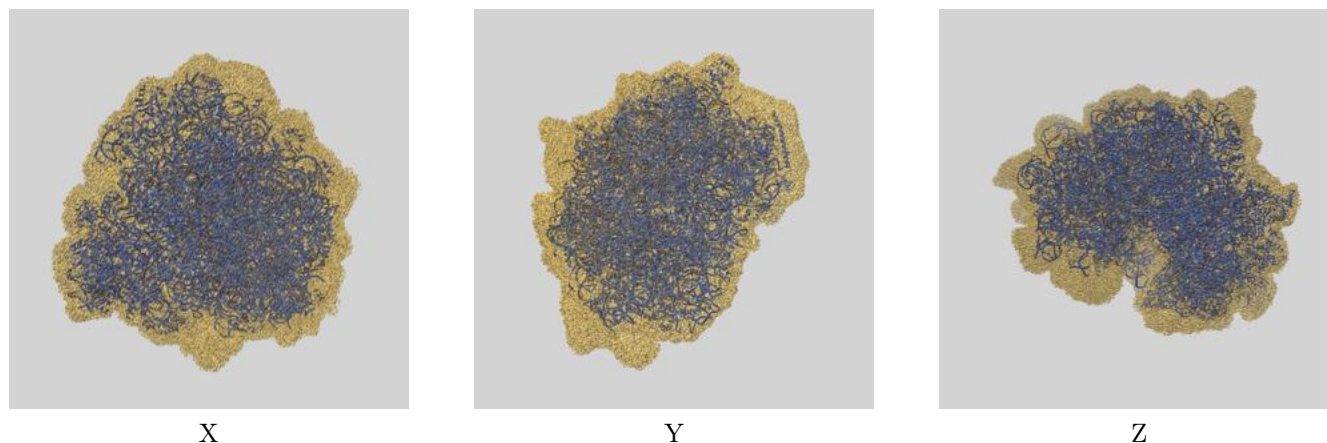
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

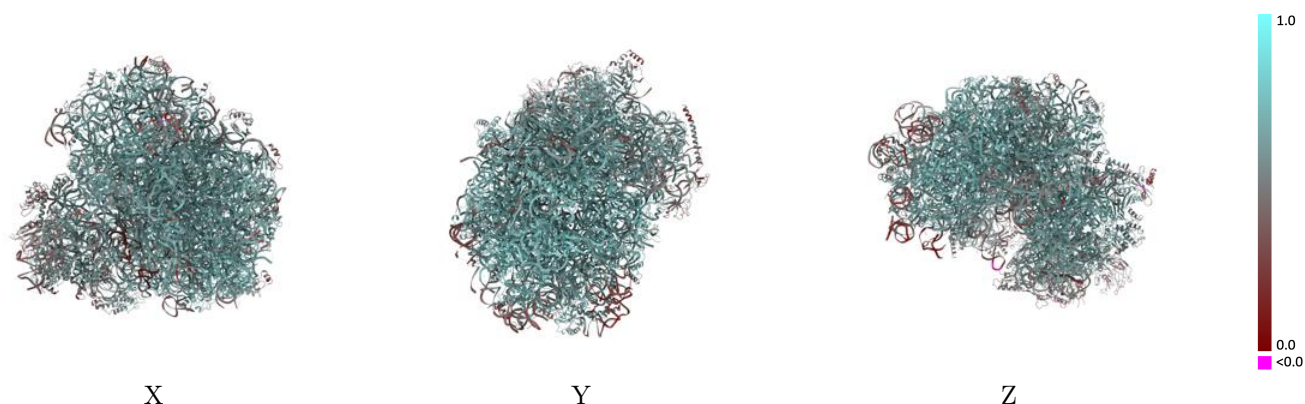
This section contains information regarding the fit between EMDB map EMD-54269 and PDB model 9RUC. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



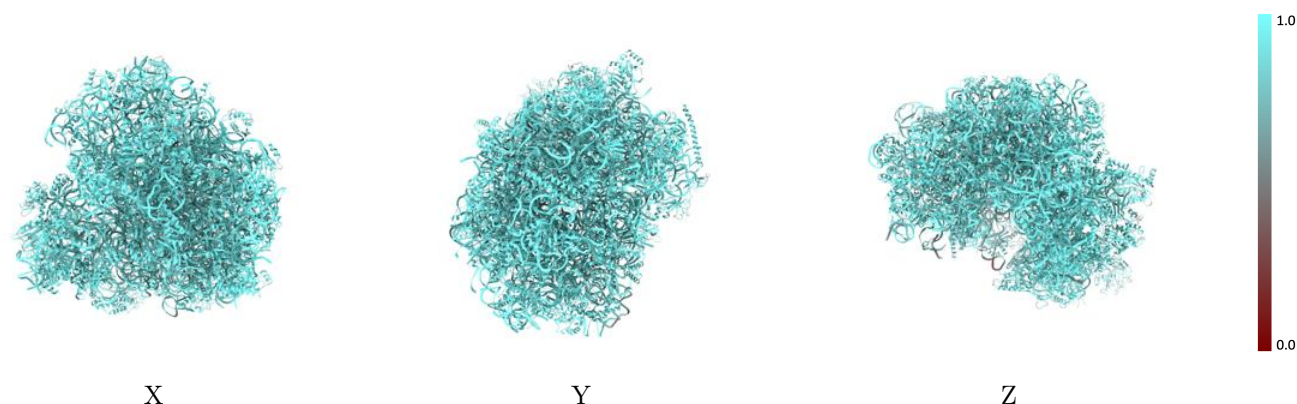
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



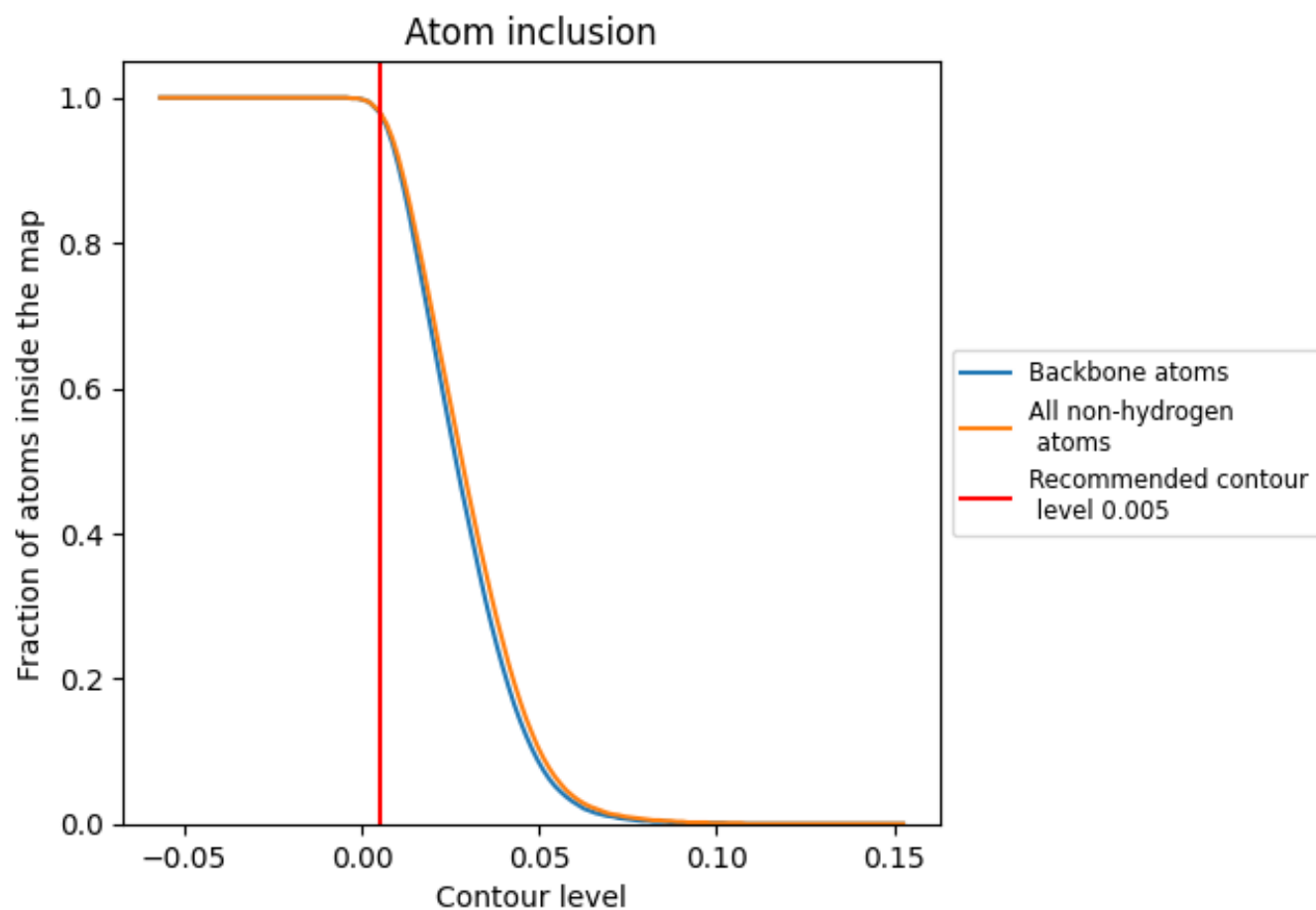
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 98% of all backbone atoms, 98% 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	 0.9820	 0.6330
L5	 0.9800	 0.6440
L7	 0.9950	 0.6230
L8	 0.9940	 0.6690
LA	 1.0000	 0.7360
LB	 0.9970	 0.7120
LC	 0.9970	 0.7210
LD	 0.9840	 0.5580
LE	 0.9930	 0.6320
LF	 0.9960	 0.7200
LG	 0.9880	 0.6360
LH	 0.9860	 0.6000
LI	 0.9920	 0.6610
LJ	 0.9600	 0.4630
LL	 0.9920	 0.6860
LM	 0.9940	 0.6480
LN	 1.0000	 0.7480
LO	 0.9940	 0.7070
LP	 0.9980	 0.7290
LQ	 0.9990	 0.7370
LR	 0.9980	 0.6850
LS	 0.9940	 0.6980
LT	 0.9950	 0.6850
LU	 0.9380	 0.4800
LV	 0.9980	 0.7140
LW	 0.9940	 0.6820
LX	 0.9950	 0.6820
LY	 0.9950	 0.6970
LZ	 0.9870	 0.6030
La	 0.9950	 0.7220
Lb	 0.9890	 0.6340
Lc	 0.9960	 0.6350
Ld	 0.9890	 0.6710
Le	 0.9990	 0.7330
Lf	 0.9980	 0.7370











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Chain	Atom inclusion	Q-score
Lg	 0.9960	 0.6920
Lh	 0.9930	 0.6760
Li	 0.9880	 0.6430
Lj	 0.9990	 0.7400
Lk	 0.9620	 0.5490
Ll	 0.9980	 0.7080
Lm	 0.9690	 0.6060
Ln	 1.0000	 0.6670
Lo	 0.9960	 0.6950
Lp	 0.9990	 0.6980
Lr	 0.9970	 0.7050
Pt	 0.9030	 0.3980
S2	 0.9870	 0.6170
S6	 0.9050	 0.2730
SA	 0.9790	 0.6050
SB	 0.9940	 0.6290
SC	 0.9860	 0.6490
SD	 0.9520	 0.5300
SE	 0.9850	 0.6300
SF	 0.9930	 0.6000
SG	 0.9410	 0.4700
SH	 0.9240	 0.5100
SI	 0.9940	 0.6360
SJ	 0.9850	 0.6050
SK	 0.8650	 0.3870
SL	 0.9980	 0.6700
SN	 0.9980	 0.6600
SO	 0.9960	 0.6630
SP	 0.9330	 0.4810
SQ	 0.9850	 0.5900
SR	 0.9150	 0.5160
SS	 0.9710	 0.5250
ST	 0.9740	 0.5690
SU	 0.9450	 0.5190
SV	 0.9650	 0.6150
SW	 1.0000	 0.6880
SX	 0.9920	 0.6530
SY	 0.9820	 0.5770
SZ	 0.9370	 0.4510
Sa	 0.9920	 0.6450
Sb	 0.9910	 0.6290
Sc	 0.9600	 0.5800

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Chain	Atom inclusion	Q-score
Sd	 0.9850	 0.6020
Se	 0.9640	 0.5600
Sg	 0.8540	 0.4230
mR	 0.9590	 0.5440