



Full wwPDB EM Validation Report ⓘ

May 28, 2026 – 11:32 am BST

PDB ID : 9RUA / pdb_00009rua
EMDB ID : EMD-54268
Title : RPS26dC HEK mutant 80S ribosome bound to TISU mRNA (RPS26dC-TISU)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 2.90 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:

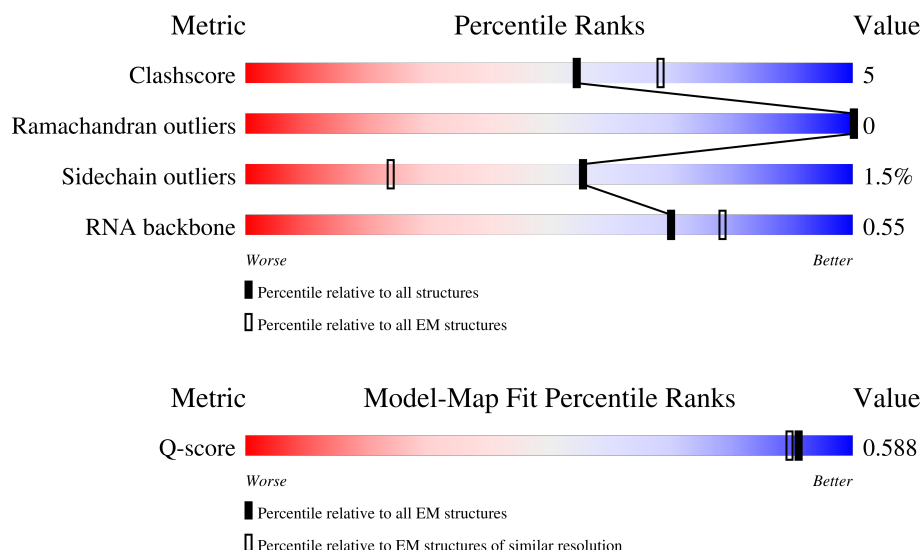
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.90 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.















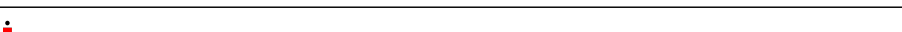

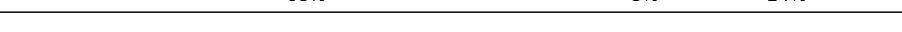

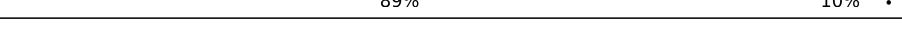








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	Lm	128	 38% 60%
2	Ll	51	 86% 12%
3	Lo	106	 89% 10%


























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Mol	Chain	Length	Quality of chain
4	SY	133	
5	SX	143	
6	SW	130	
7	SV	83	
8	SU	119	
9	SR	135	
10	SQ	146	
11	SO	151	
12	SN	151	
13	SL	158	
14	SK	165	
15	SJ	194	
16	SH	194	
17	Sg	317	
18	SF	204	
19	SE	263	
20	Se	133	
21	SD	243	
22	Sd	56	
23	SC	293	
24	Sc	69	
25	SB	264	
26	Sb	84	
27	SA	295	
28	mR	27	

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Mol	Chain	Length	Quality of chain
29	LZ	136	 78%21%..
30	LY	145	 74%17%8%
31	LX	156	 72%.24%
32	LW	157	 34%5%61%
33	LV	140	 84%9%6%
34	LU	128	 58%19%.23%
35	LT	160	 88%11%..
36	LS	176	 86%14%
37	LR	196	 .80%12%8%
38	Lr	138	 79%10%.10%
39	LQ	188	 86%13%..
40	LP	154	 88%12%.
41	Lp	92	 82%15%..
42	LO	203	 89%9%.
43	LN	204	 88%11%
44	Ln	25	 72%24%.
45	LM	215	 58%6%37%
46	LL	211	 .90%9%
47	Lk	70	 86%13%.
48	LJ	178	 80%15%5%
49	Lj	97	 77%11%11%
50	LI	214	 79%16%5%
51	Li	105	 90%7%..
52	LH	192	 86%12%..
53	Lh	123	 84%15%.

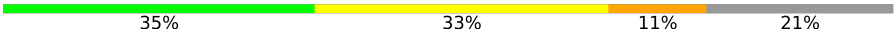

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Mol	Chain	Length	Quality of chain
54	LG	266	
55	Lg	112	
56	LF	248	
57	Lf	111	
58	LE	288	
59	Le	129	
60	LD	297	
61	Ld	125	
62	LC	427	
63	Lc	115	
64	LB	397	
65	Lb	159	
66	LA	257	
67	La	148	
68	L7	120	
69	Pt	77	
70	Sa	115	
71	L8	156	
72	L5	5069	
73	SZ	125	
74	ST	145	
75	SP	145	
76	S2	1869	
77	SG	249	
78	SI	208	

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Mol	Chain	Length	Quality of chain
79	S6	75	 35% 33% 11% 21%
80	SS	152	 78% 12% 9%

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 201456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Lm	51	Total	C	N	O	S	0	0
			407	251	87	63	6		

- Molecule 2 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ll	50	Total	C	N	O	S	0	0
			434	275	94	64	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ll	34	ILE	LYS	conflict	UNP P62891

- Molecule 3 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Lo	105	Total	C	N	O	S	0	0
			822	516	166	134	6		

- Molecule 4 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SY	123	Total	C	N	O	S	0	0
			894	561	180	150	3		

- Molecule 5 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SX	141	Total	C	N	O	S	0	0
			1060	669	214	174	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	62	HIS	PRO	conflict	UNP P62266

- Molecule 6 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SW	129	Total	C	N	O	S	0	0
			1023	653	192	172	6		

- Molecule 7 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SV	83	Total	C	N	O	S	0	0
			623	388	117	113	5		

- Molecule 8 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SU	60	Total	C	N	O	S	0	0
			428	262	90	73	3		

- Molecule 9 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SR	132	Total	C	N	O	S	0	0
			936	591	173	169	3		

- Molecule 10 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SQ	139	Total	C	N	O	S	0	0
			912	567	178	166	1		

- Molecule 11 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SO	134	Total	C	N	O	S	1	0
			981	602	199	174	6		

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SN	150	Total	C	N	O	S	0	0
			1186	761	221	203	1		

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SL	142	Total	C	N	O	S	0	0
			1158	737	218	197	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SK	74	Total	C	N	O	S	0	0
			470	304	86	79	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SK	68	PHE	TYR	conflict	UNP P46783

- Molecule 15 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SJ	178	Total	C	N	O	S	0	0
			1430	915	285	228	2		

- Molecule 16 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SH	189	Total	C	N	O		0	0
			1389	891	263	235			

- Molecule 17 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Sg	241	Total	C	N	O		0	0
			1259	757	255	247			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sg	155	PHE	ARG	conflict	UNP P63244

- Molecule 18 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SF	185	Total	C	N	O	S	0	0
			1324	834	250	237	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SF	15	LYS	PRO	conflict	UNP P46782

- Molecule 19 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SE	260	Total	C	N	O	S	0	0
			2037	1304	383	342	8		

- Molecule 20 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Se	51	Total	C	N	O	S	0	0
			395	240	89	65	1		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SD	175	Total	C	N	O	S	0	0
			1082	680	201	198	3		

- Molecule 22 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Sd	55	Total	C	N	O	S	0	0
			430	270	87	68	5		

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SC	220	Total	C	N	O	S	0	0
			1681	1090	291	290	10		

- Molecule 24 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sc	61	Total	C	N	O	S	0	0
			434	264	87	81	2		

- Molecule 25 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SB	212	Total	C	N	O	S	1	0
			1698	1080	306	297	15		

- Molecule 26 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Sb	82	Total	C	N	O	S	0	0
			613	383	113	110	7		

- Molecule 27 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SA	215	Total	C	N	O	S	0	0
			1669	1062	296	303	8		

- Molecule 28 is a RNA chain called TISU mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	mR	8	Total	C	N	O	P	0	0
			172	77	33	54	8		

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LZ	135	Total	C	N	O	S	0	0
			1095	709	207	176	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LY	133	Total	C	N	O	S	0	0
			1085	680	220	182	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LY	52	LYS	ASP	conflict	UNP P61254

- Molecule 31 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 32 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LW	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 33 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LV	131	Total	C	N	O	S	1	0
			987	623	187	172	5		

- Molecule 34 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LU	99	Total	C	N	O	S	0	0
			800	513	140	145	2		

- Molecule 35 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

- Molecule 36 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LS	176	Total	C	N	O	S	0	0
			1454	925	283	235	11		

- Molecule 37 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LR	181	Total	C	N	O	S	0	0
			1462	906	313	234	9		

- Molecule 38 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lr	124	Total	C	N	O	S	0	0
			990	614	205	167	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	1	MET	-	initiating methionine	UNP P46779
Lr	2	ACE	-	expression tag	UNP P46779

- Molecule 39 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LQ	187	Total	C	N	O	S	0	0
			1505	940	312	248	5		

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 41 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lp	90	Total	C	N	O	S	0	0
			695	439	134	115	7		

- Molecule 42 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LO	199	Total	C	N	O	S	0	0
			1620	1044	318	253	5		

- Molecule 43 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 44 is a protein called Ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ln	24	Total	C	N	O	S	0	0
			235	142	65	25	3		

- Molecule 45 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LM	136	Total	C	N	O	S	0	0
			1116	716	214	179	7		

- Molecule 46 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LL	210	Total	C	N	O	S	0	0
			1693	1059	351	279	4		

- Molecule 47 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lk	69	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 48 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LJ	169	Total	C	N	O	S	0	0
			1329	843	246	234	6		

- Molecule 49 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lj	86	Total	C	N	O	S	0	0
			701	432	154	110	5		

- Molecule 50 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LI	203	Total	C	N	O	S	0	0
			1632	1038	314	267	13		

- Molecule 51 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Li	102	Total	C	N	O	S	0	0
			812	509	171	127	5		

- Molecule 52 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LH	190	Total	C	N	O	S	0	0
			1499	946	281	266	6		

- Molecule 53 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lh	122	Total	C	N	O	S	0	0
			1010	638	204	167	1		

- Molecule 54 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LG	228	Total	C	N	O	S	0	0
			1791	1142	346	299	4		

- Molecule 55 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lg	110	Total	C	N	O	S	1	0
			872	544	182	140	6		

- Molecule 56 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LF	225	Total	C	N	O	S	0	0
			1835	1178	350	298	9		

- Molecule 57 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lf	109	Total	C	N	O	S	0	0
			868	549	173	143	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lf	111	LYS	-	expression tag	UNP P18077

- Molecule 58 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LE	219	Total	C	N	O	S	1	0
			1742	1123	330	285	4		

- Molecule 59 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Le	128	Total	C	N	O	S	0	0
			1053	666	217	165	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Le	129	LYS	-	expression tag	UNP P62910

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LD	292	Total	C	N	O	S	0	0
			2354	1487	429	424	14		

- Molecule 61 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ld	106	Total	C	N	O	S	0	0
			840	534	165	139	2		

- Molecule 62 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LC	359	Total	C	N	O	S	0	0
			2862	1802	572	475	13		

- Molecule 63 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lc	98	Total	C	N	O	S	0	0
			760	482	134	138	6		

- Molecule 64 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LB	396	Total	C	N	O	S	0	0
			3177	2024	597	542	14		

- Molecule 65 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Lb	101	Total	C	N	O	S	0	0
			815	506	178	127	4		

- Molecule 66 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LA	248	Total	C	N	O	S	1	0
			1905	1193	392	314	6		

- Molecule 67 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 68 is a RNA chain called 5S rRNA.

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

- Molecule 69 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 70 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sa	98	Total	C	N	O	S	0	0
			770	481	158	127	4		

- Molecule 71 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	L8	153	Total	C	N	O	P	0	0
			3256	1453	574	1076	153		

- Molecule 72 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	L5	3453	Total	C	N	O	P	1	0
			74115	33043	13558	24060	3454		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	483	C	G	conflict	GB 86475748

- Molecule 73 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	SZ	63	Total	C	N	O	0	0
			383	245	69	69		

- Molecule 74 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	ST	129	Total	C	N	O	S	0	0
			837	529	163	143	2		

- Molecule 75 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SP	126	Total	C	N	O	S	0	0
			800	498	155	144	3		

- Molecule 76 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	S2	1575	Total	C	N	O	P	0	0
			33681	15059	6058	10989	1575		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SG	220	Total	C	N	O	S	0	0
			1679	1051	337	284	7		

- Molecule 78 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SI	206	Total	C	N	O	S	0	0
			1648	1035	326	282	5		

- Molecule 79 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	S6	59	Total	C	N	O	P	0	0
			1263	565	238	402	58		

- Molecule 80 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
80	SS	138	Total	C	N	O	0	0
			903	565	178	160		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SS	115	ILE	LYS	conflict	UNP P62269
SS	117	ALA	ILE	conflict	UNP P62269
SS	119	PHE	ALA	conflict	UNP P62269

- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	Lm	1	Total	Zn	0
			1	1	
81	Lo	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
81	Sd	1	Total 1	Zn 1	0
81	Lp	1	Total 1	Zn 1	0
81	Lg	1	Total 1	Zn 1	0

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

Mol	Chain	Residues	Atoms		AltConf
82	SQ	1	Total 1	K 1	0
82	Lf	1	Total 1	K 1	0
82	L8	1	Total 1	K 1	0
82	L5	61	Total 61	K 61	0
82	S2	12	Total 12	K 12	0

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
83	Sd	2	Total 2	Mg 2	0
83	mR	1	Total 1	Mg 1	0
83	LV	1	Total 1	Mg 1	0
83	LS	1	Total 1	Mg 1	0
83	LP	1	Total 1	Mg 1	0
83	LI	1	Total 1	Mg 1	0
83	Le	1	Total 1	Mg 1	0
83	LB	1	Total 1	Mg 1	0
83	L7	5	Total 5	Mg 5	0

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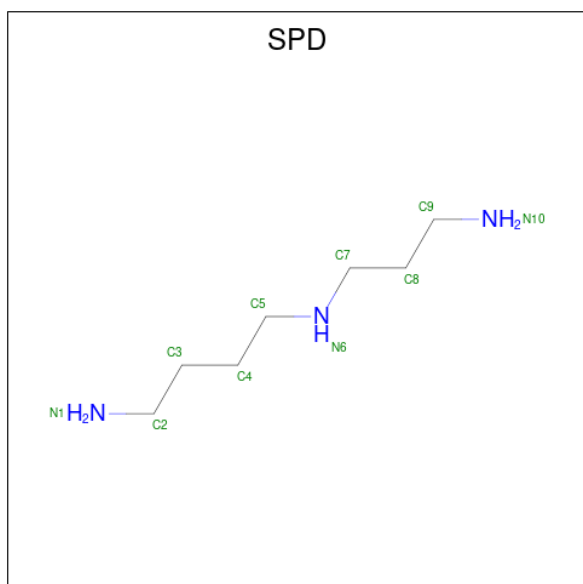
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Mol	Chain	Residues	Atoms		AltConf
83	Pt	1	Total	Mg	0
			1	1	
83	L8	5	Total	Mg	0
			5	5	
83	L5	80	Total	Mg	0
			80	80	
83	S2	19	Total	Mg	0
			19	19	
83	S6	1	Total	Mg	0
			1	1	

- Molecule 84 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
84	LN	1	Total	Na	0
			1	1	
84	L5	47	Total	Na	0
			47	47	
84	S2	11	Total	Na	0
			11	11	

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

- Molecule 86 is water.

Mol	Chain	Residues	Atoms	AltConf
86	Ll	2	Total O 2 2	0
86	Lo	1	Total O 1 1	0
86	SN	4	Total O 4 4	0
86	SL	1	Total O 1 1	0
86	SF	1	Total O 1 1	0
86	LY	1	Total O 1 1	0
86	LW	1	Total O 1 1	0
86	LV	2	Total O 2 2	0
86	LT	4	Total O 4 4	0
86	LR	5	Total O 5 5	0
86	LQ	2	Total O 2 2	0
86	LP	2	Total O 2 2	0
86	LN	4	Total O 4 4	0
86	Ln	1	Total O 1 1	0
86	LL	5	Total O 5 5	0
86	LJ	1	Total O 1 1	0
86	Lj	1	Total O 1 1	0
86	LI	1	Total O 1 1	0
86	LH	1	Total O 1 1	0
86	Lh	1	Total O 1 1	0
86	LG	1	Total O 1 1	0

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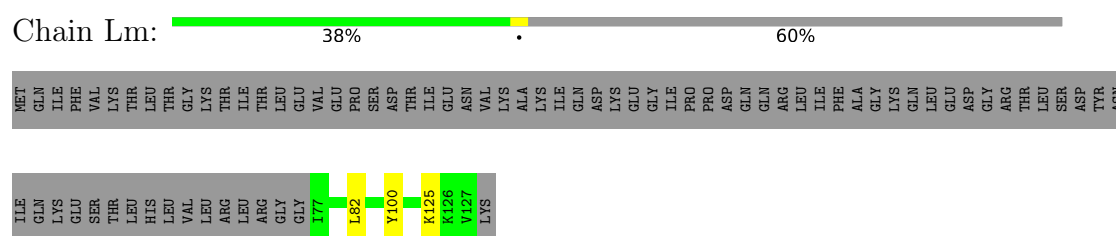
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Mol	Chain	Residues	Atoms		AltConf
86	Lg	4	Total 4	O 4	0
86	LF	2	Total 2	O 2	0
86	Le	2	Total 2	O 2	0
86	LD	1	Total 1	O 1	0
86	LC	3	Total 3	O 3	0
86	Lc	2	Total 2	O 2	0
86	LB	5	Total 5	O 5	0
86	Lb	4	Total 4	O 4	0
86	LA	6	Total 6	O 6	0
86	La	4	Total 4	O 4	0
86	L7	9	Total 9	O 9	0
86	Sa	1	Total 1	O 1	0
86	L8	16	Total 16	O 16	0
86	L5	467	Total 467	O 467	0
86	S2	105	Total 105	O 105	0
86	SI	3	Total 3	O 3	0
86	S6	1	Total 1	O 1	0

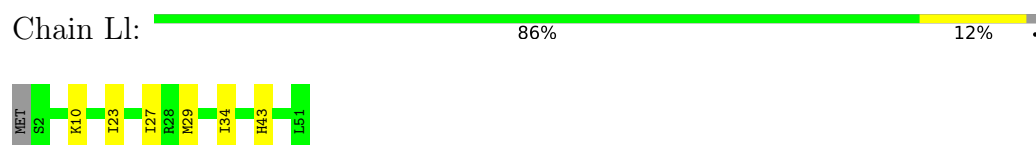
3 Residue-property plots

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.

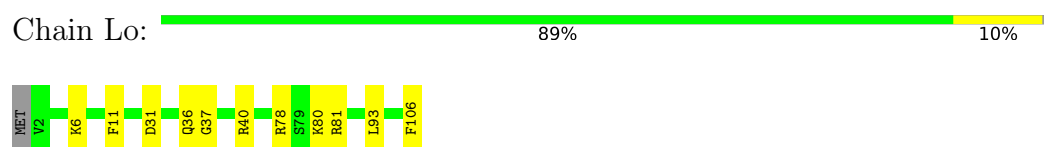
- Molecule 1: Ubiquitin-60S ribosomal protein L40



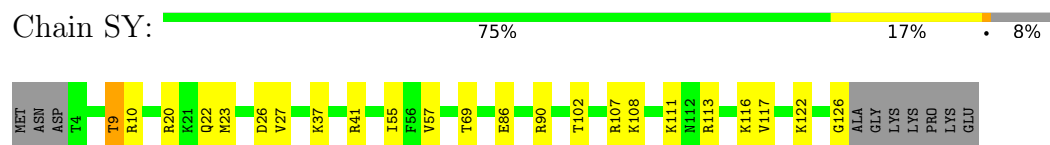
- Molecule 2: Large ribosomal subunit protein eL39



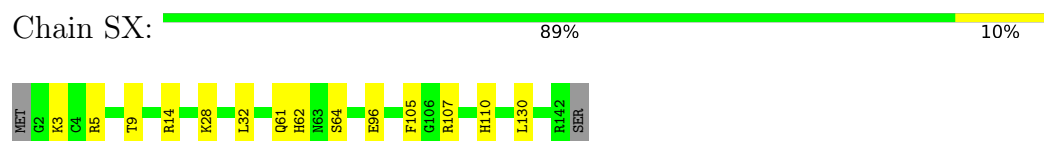
- Molecule 3: Large ribosomal subunit protein eL42




- Molecule 4: 40S ribosomal protein S24



- Molecule 5: Small ribosomal subunit protein uS12



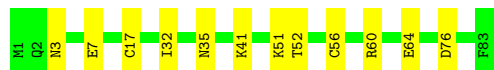
- Molecule 6: 40S ribosomal protein S15a

Chain SW:  88% 10% ..



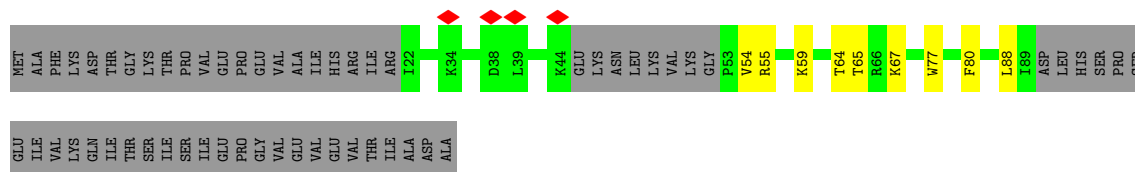
- Molecule 7: 40S ribosomal protein S21

Chain SV:  86% 14%



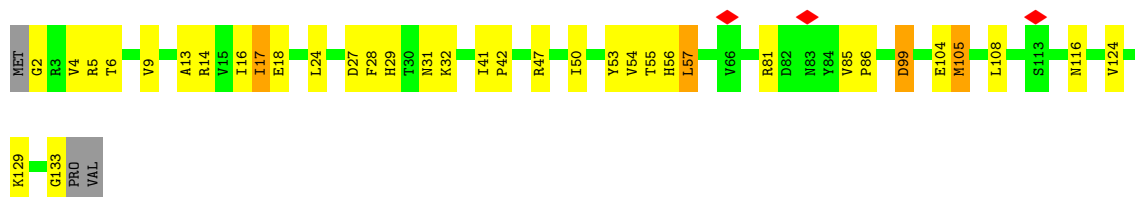
- Molecule 8: 40S ribosomal protein S20

Chain SU:  43% 8% 50%




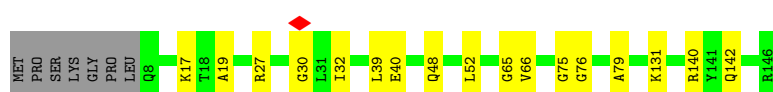
- Molecule 9: 40S ribosomal protein S17

Chain SR:  71% 24% ..



- Molecule 10: 40S ribosomal protein S16

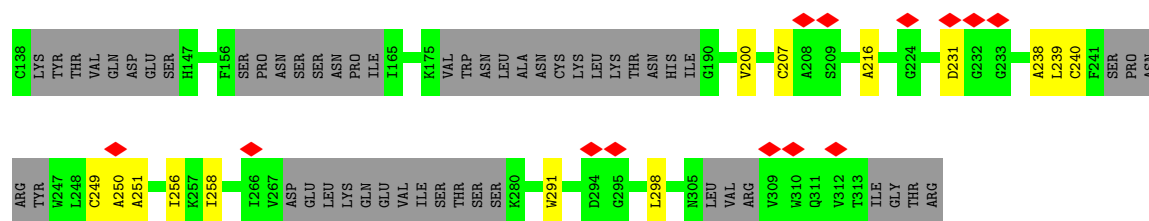
Chain SQ:  84% 12% 5%



- Molecule 11: 40S ribosomal protein S14

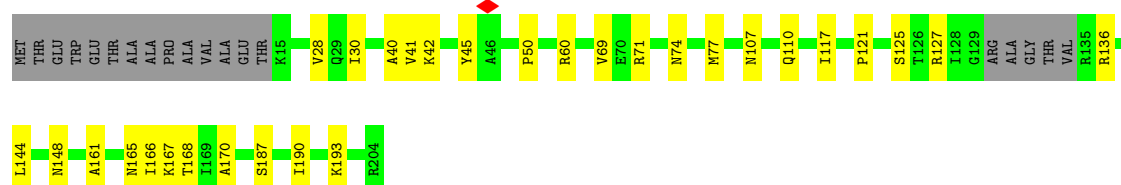
Chain SO:  74% 15% 11%





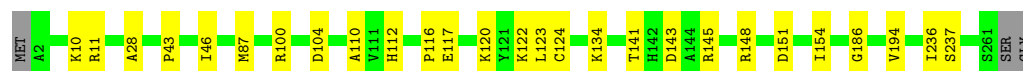
- Molecule 18: Small ribosomal subunit protein uS7

Chain SF: 76% 15% 9%



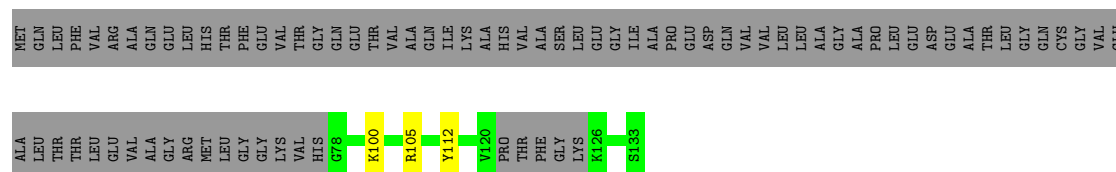
- Molecule 19: Small ribosomal subunit protein eS4, X isoform

Chain SE: 89% 10%



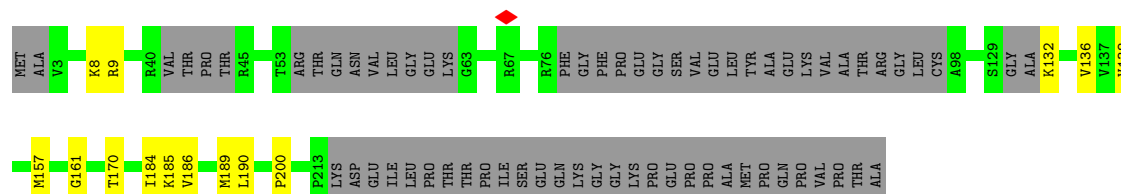
- Molecule 20: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se: 36% 62%



- Molecule 21: 40S ribosomal protein S3

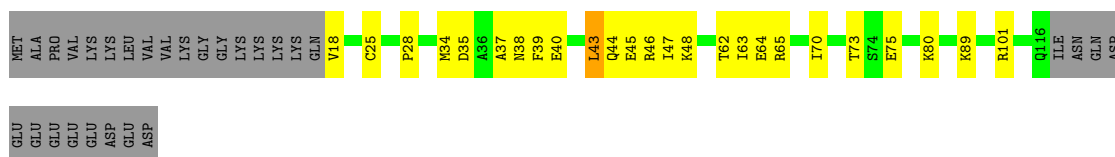
Chain SD: 66% 6% 28%



- Molecule 22: 40S ribosomal protein S29

Chain Sd: 77% 21%

Chain LU: 58% 19% 0% 23%



- Molecule 35: 60S ribosomal protein L21

Chain LT: 88% 11% ..



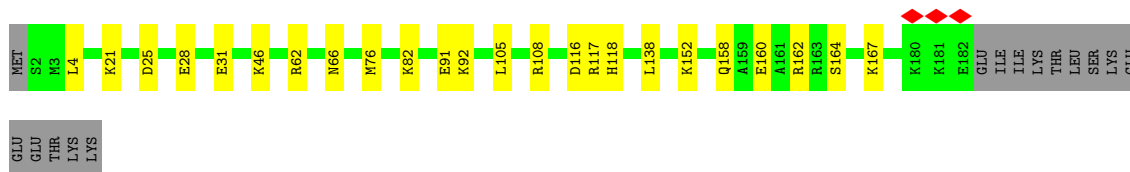
- Molecule 36: 60S ribosomal protein L18a

Chain LS: 86% 14%



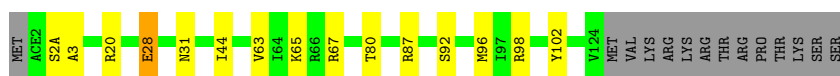
- Molecule 37: 60S ribosomal protein L19

Chain LR: 80% 12% 8%



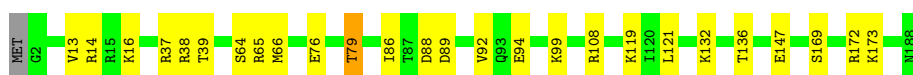
- Molecule 38: Large ribosomal subunit protein eL28

Chain Lr: 79% 10% 10%



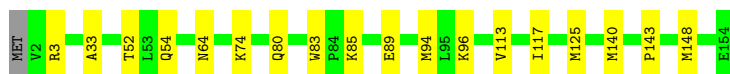
- Molecule 39: 60S ribosomal protein L18

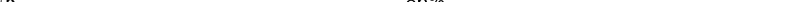
Chain LQ: 86% 13% ..



- Molecule 40: Large ribosomal subunit protein uL22

Chain LP: 88% 12%



- Chain Lk:  86% 13%



- Molecule 48: 60S ribosomal protein L11

Chain LJ: 80% 15% 5%



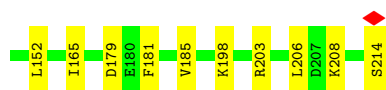
- Molecule 49: Large ribosomal subunit protein eL37

Chain Lj: 77% 11% 11%



- Molecule 50: 60S ribosomal protein L10

Chain LI: 79% 16% 5%



- Molecule 51: 60S ribosomal protein L36

Chain Li: 90% 7% ..



- Molecule 52: 60S ribosomal protein L9

Chain LH: 86% 12% ..

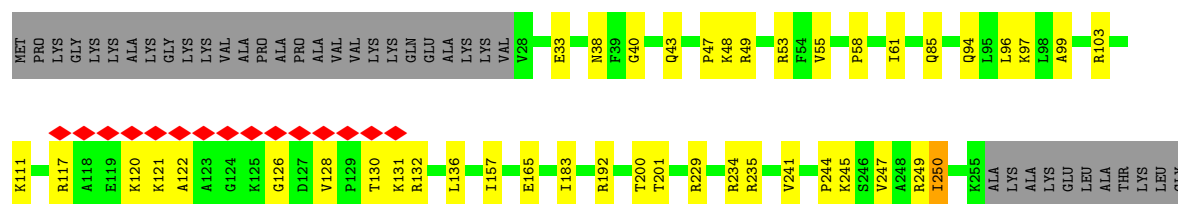
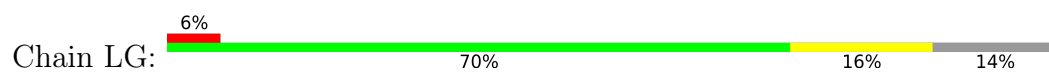


- Molecule 53: 60S ribosomal protein L35

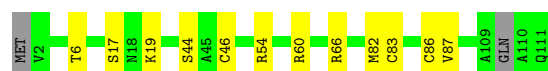
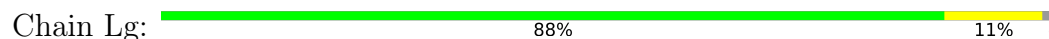
Chain Lh: 84% 15% .



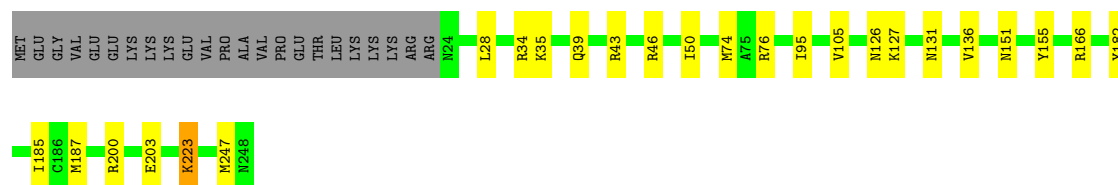
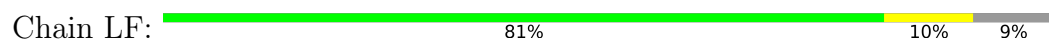
- Molecule 54: 60S ribosomal protein L7a



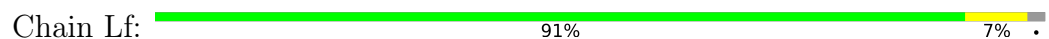
- Molecule 55: Large ribosomal subunit protein eL34



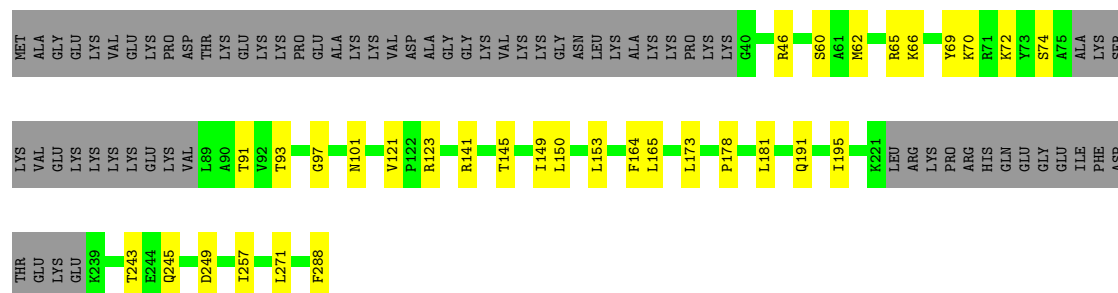
- Molecule 56: Large ribosomal subunit protein uL30



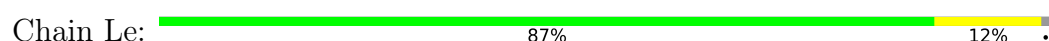
- Molecule 57: Large ribosomal subunit protein eL33

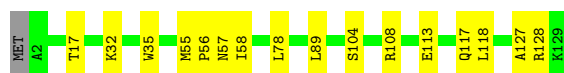


- Molecule 58: Large ribosomal subunit protein eL6



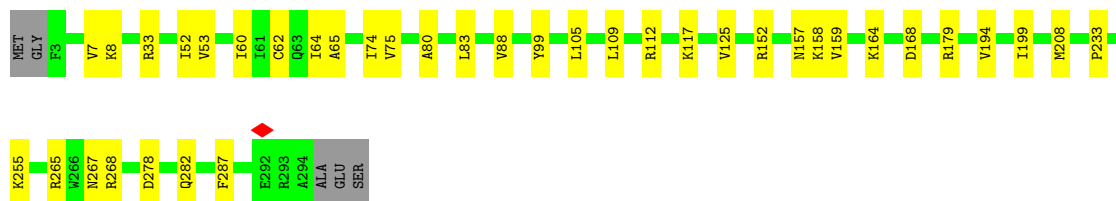
- Molecule 59: Large ribosomal subunit protein eL32





- Molecule 60: 60S ribosomal protein L5

Chain LD: 86% 13%



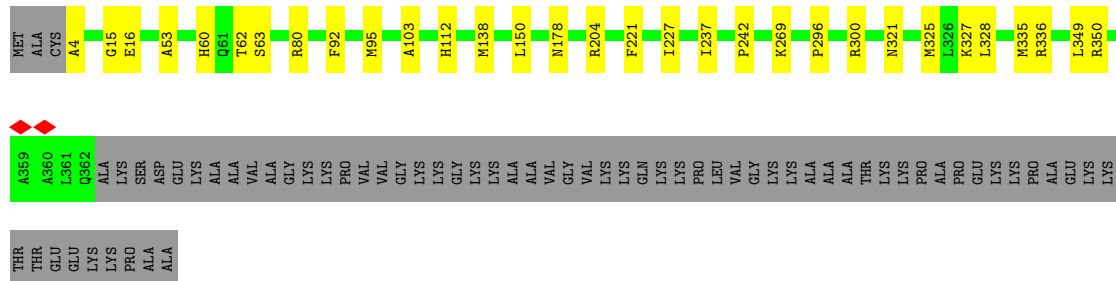
- Molecule 61: 60S ribosomal protein L31

Chain Ld: 77% 7% 15%



- Molecule 62: 60S ribosomal protein L4

Chain LC: 77% 7% 16%



- Molecule 63: 60S ribosomal protein L30

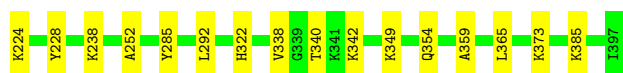
Chain Lc: 67% 17% 15%



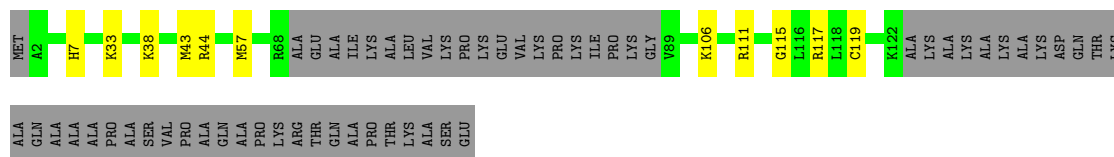
- Molecule 64: Large ribosomal subunit protein uL3

Chain LB: 88% 12%

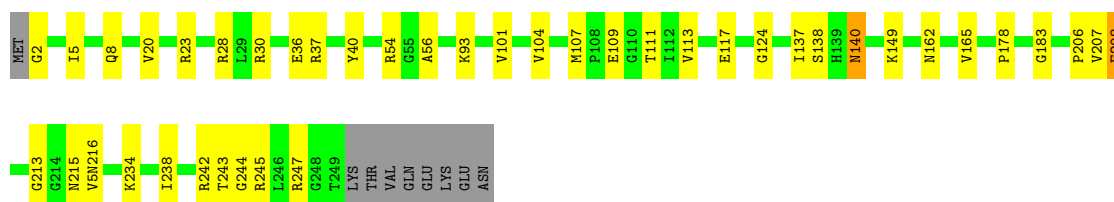
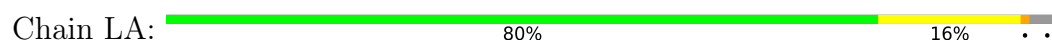




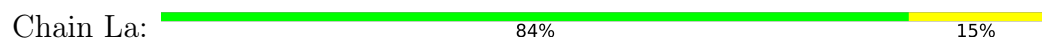
- Molecule 65: Large ribosomal subunit protein eL29



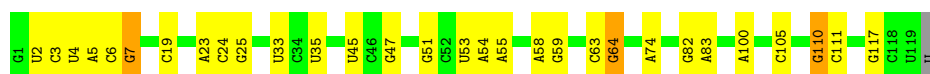
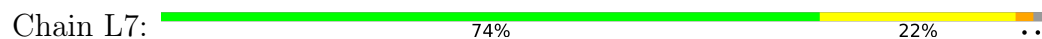
- Molecule 66: Large ribosomal subunit protein uL2



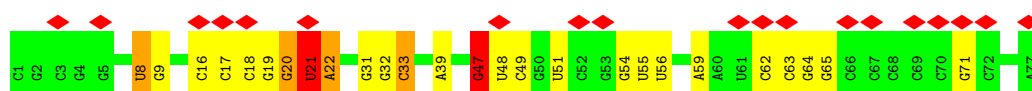
- Molecule 67: Large ribosomal subunit protein uL15



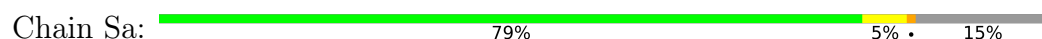
- Molecule 68: 5S rRNA

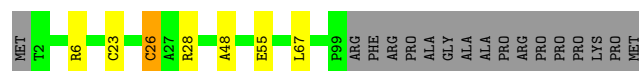


- Molecule 69: P site tRNA



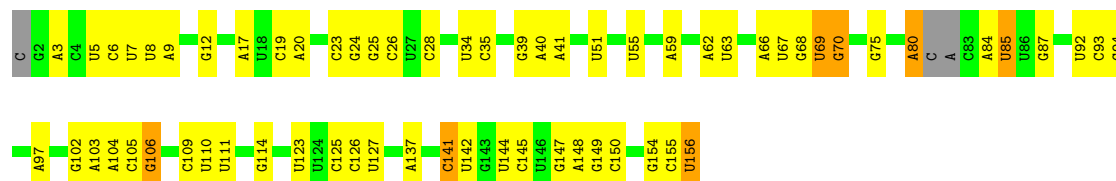
- Molecule 70: 40S ribosomal protein S26





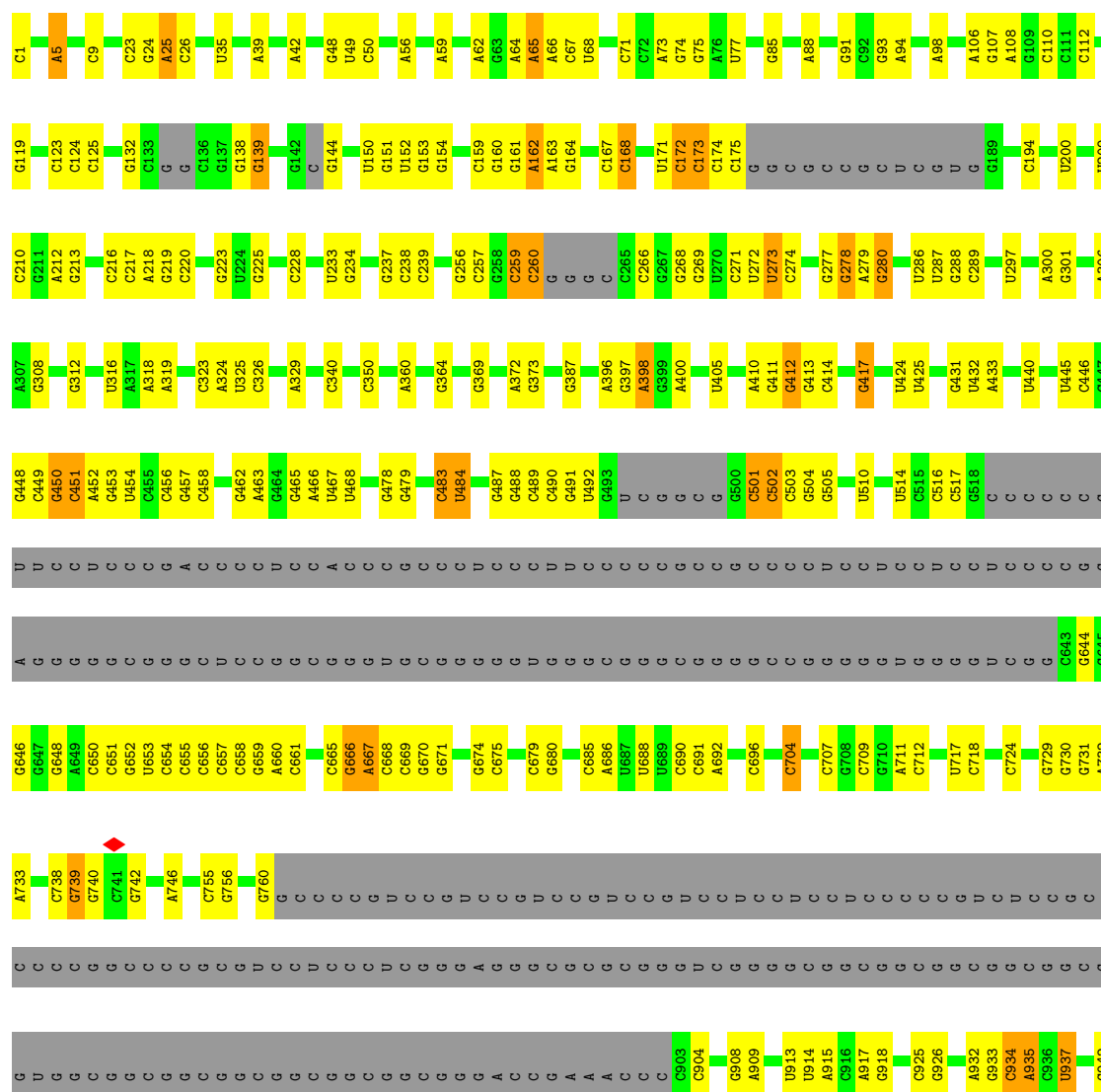
- Molecule 71: 5.8S rRNA

Chain L8: 57% 37%



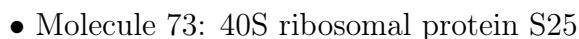
- Molecule 72: 28S rRNA

Chain L5: 43% 22% 32%





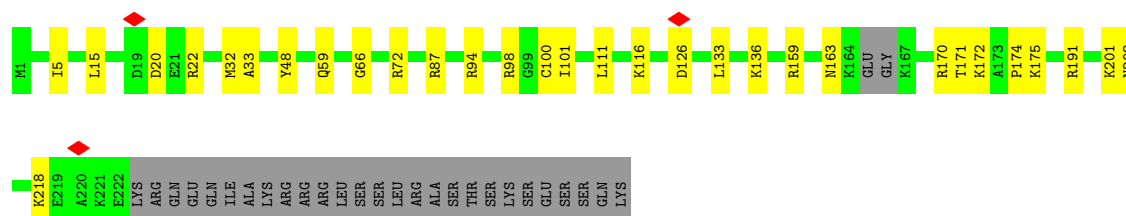
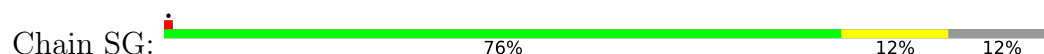




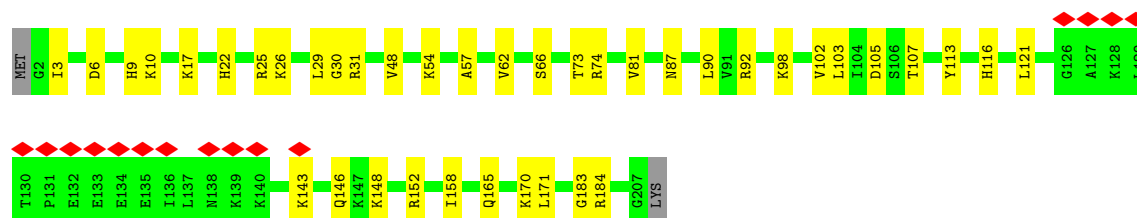
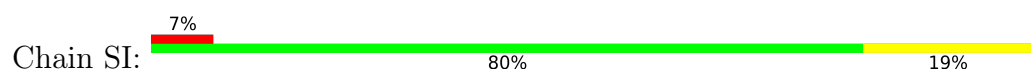




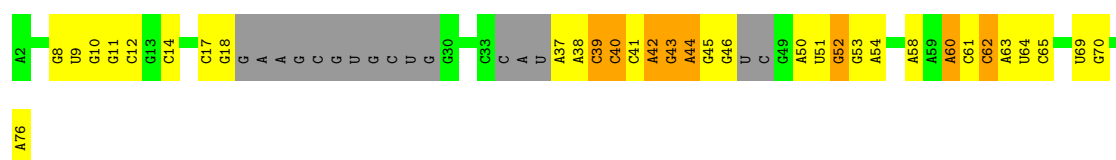
- Molecule 77: 40S ribosomal protein S6



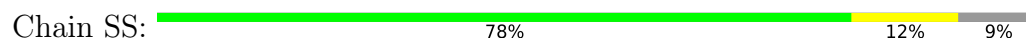
- Molecule 78: 40S ribosomal protein S8



- Molecule 79: E site tRNA



- Molecule 80: Small ribosomal subunit protein uS13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50884	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	0.062	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	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: 4AC, V5N, 5MC, OMC, A2M, 4SU, G7M, PSU, NA, ACE, SPD, MG, UR3, 6MZ, OMG, 1MA, ZN, B8N, OMU, K, MLZ, MA6, H2U

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	Lm	0.15	0/413	0.33	0/549
2	Ll	0.16	0/444	0.30	0/588
3	Lo	0.14	0/823	0.26	0/1088
4	SY	0.11	0/911	0.28	0/1227
5	SX	0.12	0/1077	0.30	0/1441
6	SW	0.13	0/1040	0.28	0/1393
7	SV	0.11	0/630	0.26	0/843
8	SU	0.11	0/433	0.27	0/582
9	SR	0.13	0/950	0.36	0/1291
10	SQ	0.09	0/921	0.28	0/1251
11	SO	0.12	0/994	0.28	0/1336
12	SN	0.13	0/1210	0.27	0/1633
13	SL	0.12	0/1178	0.26	0/1578
14	SK	0.08	0/484	0.23	0/667
15	SJ	0.11	0/1455	0.25	0/1954
16	SH	0.12	0/1409	0.30	0/1903
17	Sg	0.11	0/1259	0.37	1/1730 (0.1%)
18	SF	0.09	0/1342	0.25	0/1823
19	SE	0.12	0/2079	0.29	0/2801
20	Se	0.12	0/397	0.35	0/520
21	SD	0.13	0/1090	0.30	0/1487
22	Sd	0.12	0/441	0.32	0/589
23	SC	0.14	0/1718	0.32	0/2326
24	Sc	0.09	0/435	0.22	0/587
25	SB	0.12	0/1725	0.28	0/2309
26	Sb	0.14	0/625	0.30	0/842
27	SA	0.13	0/1706	0.28	0/2322
28	mR	0.15	0/192	0.39	0/297
29	LZ	0.12	0/1118	0.23	0/1494
30	LY	0.13	0/1102	0.27	0/1469
31	LX	0.13	0/993	0.26	0/1334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LW	0.13	0/532	0.27	0/708
33	LV	0.13	0/1004	0.27	0/1346
34	LU	0.17	0/814	0.41	0/1094
35	LT	0.13	0/1325	0.25	0/1770
36	LS	0.14	0/1493	0.27	0/2004
37	LR	0.12	0/1478	0.28	0/1961
38	Lr	0.14	0/1002	0.29	0/1343
39	LQ	0.14	0/1529	0.28	0/2044
40	LP	0.15	0/1260	0.29	0/1692
41	Lp	0.15	0/705	0.34	0/937
42	LO	0.14	0/1652	0.28	0/2211
43	LN	0.14	0/1745	0.26	0/2338
44	Ln	0.12	0/236	0.25	0/300
45	LM	0.13	0/1138	0.25	0/1523
46	LL	0.13	0/1724	0.25	0/2306
47	Lk	0.14	0/563	0.31	0/748
48	LJ	0.14	0/1352	0.34	0/1812
49	Lj	0.14	0/716	0.28	0/947
50	LI	0.14	0/1670	0.29	0/2230
51	Li	0.10	0/823	0.23	0/1092
52	LH	0.13	0/1518	0.25	0/2043
53	Lh	0.13	0/1018	0.30	0/1347
54	LG	0.15	0/1824	0.31	0/2465
55	Lg	0.14	0/885	0.29	0/1180
56	LF	0.15	0/1869	0.29	0/2498
57	Lf	0.15	0/887	0.33	0/1190
58	LE	0.14	0/1779	0.32	0/2388
59	Le	0.15	0/1071	0.28	0/1427
60	LD	0.12	0/2400	0.24	0/3220
61	Ld	0.14	0/854	0.27	0/1153
62	LC	0.14	0/2916	0.28	0/3917
63	Lc	0.13	0/770	0.31	0/1034
64	LB	0.14	0/3245	0.28	0/4346
65	Lb	0.13	0/817	0.29	0/1080
66	LA	0.16	0/1933	0.32	0/2589
67	La	0.15	0/1179	0.29	0/1573
68	L7	0.15	0/2840	0.24	0/4425
69	Pt	0.20	0/1721	0.27	0/2679
70	Sa	0.14	0/783	0.32	0/1052
71	L8	0.16	0/3564	0.29	0/5550
72	L5	0.18	1/79977 (0.0%)	0.29	0/124726
73	SZ	0.11	0/385	0.28	0/530
74	ST	0.09	0/851	0.26	0/1157

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SP	0.14	0/807	0.41	0/1100
76	S2	0.17	0/35874	0.28	0/55878
77	SG	0.13	0/1699	0.31	0/2280
78	SI	0.13	0/1677	0.30	0/2243
79	S6	0.11	0/1411	0.26	0/2192
80	SS	0.11	0/916	0.33	0/1256
All	All	0.16	1/210825 (0.0%)	0.29	1/310178 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	4523	A2M	O3'-P	5.06	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Sg	92	LEU	CB-CA-C	-5.12	110.27	117.23

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	Lm	407	0	423	3	0
2	Ll	434	0	461	5	0
3	Lo	822	0	856	8	0
4	SY	894	0	815	14	0
5	SX	1060	0	1087	10	0
6	SW	1023	0	1063	11	0
7	SV	623	0	627	7	0
8	SU	428	0	394	8	0
9	SR	936	0	866	22	0
10	SQ	912	0	793	10	0
11	SO	981	0	993	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	SN	1186	0	1247	8	0
13	SL	1158	0	1214	6	0
14	SK	470	0	323	3	0
15	SJ	1430	0	1498	15	0
16	SH	1389	0	1384	18	0
17	Sg	1259	0	646	13	0
18	SF	1324	0	1247	20	0
19	SE	2037	0	2131	17	0
20	Se	395	0	422	3	0
21	SD	1082	0	894	9	0
22	Sd	430	0	397	12	0
23	SC	1681	0	1747	14	0
24	Sc	434	0	419	0	0
25	SB	1698	0	1748	20	0
26	Sb	613	0	614	8	0
27	SA	1669	0	1655	19	0
28	mR	172	0	88	3	0
29	LZ	1095	0	1164	18	0
30	LY	1085	0	1144	16	0
31	LX	976	0	1053	6	0
32	LW	519	0	533	7	0
33	LV	987	0	1052	9	0
34	LU	800	0	816	18	0
35	LT	1297	0	1366	15	0
36	LS	1454	0	1485	16	0
37	LR	1462	0	1566	20	0
38	Lr	990	0	1053	8	0
39	LQ	1505	0	1613	17	0
40	LP	1234	0	1254	14	0
41	Lp	695	0	746	10	0
42	LO	1620	0	1753	14	0
43	LN	1700	0	1749	19	0
44	Ln	235	0	284	4	0
45	LM	1116	0	1176	10	0
46	LL	1693	0	1803	15	0
47	Lk	557	0	611	4	0
48	LJ	1329	0	1346	21	0
49	Lj	701	0	735	10	0
50	LI	1632	0	1675	20	0
51	Li	812	0	870	6	0
52	LH	1499	0	1572	15	0
53	Lh	1010	0	1137	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	LG	1791	0	1883	32	0
55	Lg	872	0	950	7	0
56	LF	1835	0	1926	20	0
57	Lf	868	0	891	5	0
58	LE	1742	0	1878	21	0
59	Le	1053	0	1145	13	0
60	LD	2354	0	2345	22	0
61	Ld	840	0	859	4	0
62	LC	2862	0	3036	24	0
63	Lc	760	0	793	12	0
64	LB	3177	0	3301	29	0
65	Lb	815	0	869	12	0
66	LA	1905	0	1994	34	0
67	La	1163	0	1206	15	0
68	L7	2542	0	1284	21	0
69	Pt	1645	0	843	11	0
70	Sa	770	0	811	7	0
71	L8	3256	0	1652	36	0
72	L5	74115	0	37553	617	0
73	SZ	383	0	313	5	0
74	ST	837	0	694	12	0
75	SP	800	0	645	11	0
76	S2	33681	0	17055	379	0
77	SG	1679	0	1731	26	0
78	SI	1648	0	1700	26	0
79	S6	1263	0	647	17	0
80	SS	903	0	728	14	0
81	Lg	1	0	0	0	0
81	Lm	1	0	0	0	0
81	Lo	1	0	0	0	0
81	Lp	1	0	0	0	0
81	Sd	1	0	0	0	0
82	L5	61	0	0	0	0
82	L8	1	0	0	0	0
82	Lf	1	0	0	0	0
82	S2	12	0	0	0	0
82	SQ	1	0	0	0	0
83	L5	80	0	0	0	0
83	L7	5	0	0	0	0
83	L8	5	0	0	0	0
83	LB	1	0	0	0	0
83	LI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	LP	1	0	0	0	0
83	LS	1	0	0	0	0
83	LV	1	0	0	0	0
83	Le	1	0	0	0	0
83	Pt	1	0	0	0	0
83	S2	19	0	0	0	0
83	S6	1	0	0	0	0
83	Sd	2	0	0	0	0
83	mR	1	0	0	0	0
84	L5	47	0	0	0	0
84	LN	1	0	0	0	0
84	S2	11	0	0	0	0
85	L5	10	0	19	0	0
86	L5	467	0	0	1	0
86	L7	9	0	0	0	0
86	L8	16	0	0	0	0
86	LA	6	0	0	0	0
86	LB	5	0	0	0	0
86	LC	3	0	0	0	0
86	LD	1	0	0	0	0
86	LF	2	0	0	1	0
86	LG	1	0	0	0	0
86	LH	1	0	0	0	0
86	LI	1	0	0	0	0
86	LJ	1	0	0	0	0
86	LL	5	0	0	0	0
86	LN	4	0	0	0	0
86	LP	2	0	0	0	0
86	LQ	2	0	0	0	0
86	LR	5	0	0	1	0
86	LT	4	0	0	0	0
86	LV	2	0	0	0	0
86	LW	1	0	0	0	0
86	LY	1	0	0	0	0
86	La	4	0	0	0	0
86	Lb	4	0	0	0	0
86	Lc	2	0	0	0	0
86	Le	2	0	0	0	0
86	Lg	4	0	0	0	0
86	Lh	1	0	0	0	0
86	Lj	1	0	0	0	0
86	Ll	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Ln	1	0	0	0	0
86	Lo	1	0	0	0	0
86	S2	105	0	0	1	0
86	S6	1	0	0	0	0
86	SF	1	0	0	0	0
86	SI	3	0	0	0	0
86	SL	1	0	0	0	0
86	SN	4	0	0	0	0
86	Sa	1	0	0	1	0
All	All	201456	0	144359	1710	0

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

All (1710) 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:S2:880:G:H1	76:S2:906:U:H3	1.26	0.79
72:L5:4095:G:H1	72:L5:4113:U:H3	1.32	0.78
22:Sd:16:GLN:O	22:Sd:27:ARG:NH2	2.18	0.77
72:L5:2611:A:H5'	72:L5:2688:G:H4'	1.66	0.77
72:L5:3717:A:H2'	72:L5:3718:A2M:H8	1.66	0.77
76:S2:885:U:H3	76:S2:901:G:H1	1.32	0.75
72:L5:3723:A:H2'	72:L5:3724:A2M:H8	1.68	0.75
41:Lp:5:THR:HG21	41:Lp:9:GLY:H	1.53	0.73
36:LS:99:ASP:OD2	36:LS:108:GLN:NE2	2.22	0.72
66:LA:104:VAL:HA	66:LA:107:MET:HE2	1.72	0.71
76:S2:798:G:N2	76:S2:798:G:OP2	2.24	0.71
1:Lm:125:LYS:HG3	72:L5:4474:A:H5''	1.72	0.71
76:S2:878:G:O6	76:S2:908:A:N7	2.25	0.70
5:SX:107:ARG:HB3	5:SX:110:HIS:HB3	1.74	0.70
76:S2:1742:C:H5	76:S2:1792:G:H1	1.37	0.69
16:SH:76:GLN:HE21	16:SH:94:PHE:HB2	1.57	0.69
11:SO:34:PHE:HB3	11:SO:41:PHE:HB2	1.74	0.69
56:LF:43:ARG:NH1	72:L5:1704:C:OP1	2.25	0.69
72:L5:2478:C:H2'	72:L5:2479:G:H8	1.57	0.69
17:Sg:249:CYS:HA	17:Sg:258:ILE:HA	1.75	0.69
27:SA:184:ARG:HD3	27:SA:191:ARG:HG2	1.75	0.68
72:L5:3634:G:H1	72:L5:3826:C:H5	1.39	0.68
25:SB:131:ASP:OD1	25:SB:131:ASP:N	2.27	0.68
32:LW:9:SER:HA	32:LW:52:THR:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:3765:G:O2'	72:L5:3767:C:N4	2.27	0.68
79:S6:37:A:H3'	79:S6:38:A:H2'	1.77	0.67
76:S2:925:G:H1	76:S2:1017:U:H3	1.41	0.67
17:Sg:291:TRP:HA	17:Sg:298:LEU:HA	1.76	0.67
50:LI:87:ILE:HG12	50:LI:138:ILE:HG12	1.76	0.67
72:L5:1804:A:H4'	72:L5:1805:A:H5''	1.77	0.67
42:LO:106:ASP:O	72:L5:4910:G:N2	2.27	0.67
56:LF:203:GLU:N	56:LF:203:GLU:OE2	2.27	0.67
72:L5:2582:A:H8	72:L5:2681:G:H21	1.41	0.67
5:SX:61:GLN:O	5:SX:62:HIS:ND1	2.28	0.67
23:SC:62:PRO:HD2	23:SC:68:ARG:HH21	1.59	0.67
76:S2:210:U:H2'	76:S2:211:G:H8	1.60	0.66
72:L5:2866:C:O2'	72:L5:2867:C:O5'	2.14	0.66
76:S2:880:G:N2	76:S2:906:U:O2	2.23	0.66
8:SU:55:ARG:HD2	76:S2:1446:A:H1'	1.77	0.66
48:LJ:164:ARG:NH1	48:LJ:167:GLN:OE1	2.29	0.66
42:LO:188:LYS:HD2	72:L5:4892:A:H5''	1.78	0.66
1:Lm:100:TYR:O	72:L5:4472:G:O2'	2.13	0.66
76:S2:1726:G:H1	76:S2:1808:U:H3	1.42	0.66
41:Lp:4:ARG:NH1	72:L5:1555:G:O6	2.29	0.66
76:S2:1228:A:H2'	76:S2:1229:G:C8	2.31	0.66
22:Sd:10:HIS:NE2	76:S2:1261:C:O2	2.29	0.65
76:S2:534:G:H1	76:S2:552:G:H22	1.44	0.65
13:SL:126:VAL:HG12	13:SL:145:VAL:HG22	1.78	0.65
72:L5:1961:G:N2	72:L5:2024:G:O2'	2.29	0.65
75:SP:135:ALA:HA	76:S2:1235:G:H21	1.61	0.65
76:S2:1536:G:H2'	76:S2:1537:A:H8	1.60	0.65
48:LJ:99:PHE:HB2	48:LJ:159:LYS:HZ3	1.61	0.65
19:SE:117:GLU:N	19:SE:117:GLU:OE2	2.29	0.65
66:LA:215:ASN:ND2	72:L5:4546:A:N7	2.44	0.65
76:S2:1550:G:H3'	76:S2:1579:A:H61	1.62	0.65
52:LH:71:ARG:HG2	72:L5:4691:A:H4'	1.79	0.64
58:LE:243:THR:HG22	58:LE:245:GLN:H	1.62	0.64
72:L5:4541:G:N2	72:L5:4544:A:OP2	2.29	0.64
76:S2:420:G:O2'	76:S2:660:C:N3	2.28	0.64
66:LA:245:ARG:NH2	72:L5:3698:G:OP2	2.30	0.64
76:S2:851:C:H5''	76:S2:852:G:H5'	1.79	0.64
71:L8:156:U:H3	72:L5:1:C:H42	1.46	0.64
54:LG:58:PRO:HD2	54:LG:61:ILE:HD12	1.80	0.64
76:S2:218:PSU:O4	78:SI:184:ARG:NH2	2.30	0.64
54:LG:38:ASN:OD1	54:LG:43:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LE:65:ARG:NH2	72:L5:1070:G:OP2	2.30	0.64
38:Lr:3:ALA:HB3	38:Lr:44:ILE:HB	1.79	0.64
45:LM:40:GLY:HA3	45:LM:45:VAL:HB	1.80	0.64
76:S2:312:G:H1	76:S2:337:C:H5	1.46	0.64
8:SU:65:THR:HG22	8:SU:67:LYS:H	1.62	0.63
54:LG:85:GLN:OE1	54:LG:229:ARG:NH2	2.31	0.63
72:L5:2579:G:N2	72:L5:2582:A:OP2	2.24	0.63
75:SP:43:ARG:NH1	76:S2:1617:G:O6	2.29	0.63
76:S2:67:C:H41	77:SG:163:ASN:HA	1.63	0.63
76:S2:1410:C:H2'	76:S2:1411:G:H8	1.64	0.63
75:SP:60:LEU:HD21	75:SP:89:MET:HB3	1.80	0.63
76:S2:433:A:H5''	78:SI:22:HIS:HB3	1.81	0.63
76:S2:885:U:O2	76:S2:901:G:N2	2.29	0.63
76:S2:1735:A:O2'	76:S2:1736:G:O4'	2.16	0.63
10:SQ:142:GLN:NE2	76:S2:1527:C:OP1	2.30	0.63
29:LZ:112:ARG:NH2	72:L5:2572:C:O2'	2.32	0.63
76:S2:1114:U:H3	76:S2:1119:A:H61	1.46	0.63
18:SF:144:LEU:O	18:SF:148:ASN:ND2	2.31	0.63
26:Sb:40:CYS:SG	26:Sb:41:TYR:N	2.71	0.63
53:Lh:112:ARG:NH2	72:L5:173:C:O2	2.31	0.63
58:LE:165:LEU:HD21	58:LE:257:ILE:HD11	1.81	0.63
72:L5:3663:A:N6	72:L5:4168:G:O2'	2.29	0.63
72:L5:4570:G:H2'	72:L5:4571:A2M:H8	1.81	0.63
58:LE:149:ILE:HD13	58:LE:271:LEU:HD21	1.79	0.62
72:L5:2555:G:H2'	72:L5:2556:G:C8	2.34	0.62
72:L5:3689:G:O2'	72:L5:3818:U:OP2	2.16	0.62
72:L5:1870:C:H2'	72:L5:1871:A2M:H8	1.79	0.62
76:S2:306:C:O2	76:S2:308:G:N1	2.30	0.62
18:SF:71:ARG:NH2	18:SF:148:ASN:OD1	2.31	0.62
72:L5:1332:C:H2'	72:L5:1333:A:H8	1.63	0.62
76:S2:1677:U:H2'	76:S2:1678:A2M:H8	1.81	0.62
76:S2:1746:U:H5''	77:SG:33:ALA:HB3	1.81	0.62
8:SU:88:LEU:HD13	76:S2:1403:C:H41	1.64	0.62
50:LI:30:LYS:HG3	50:LI:63:GLU:HG3	1.81	0.62
61:Ld:87:ARG:HB3	61:Ld:107:THR:HG22	1.81	0.62
76:S2:882:U:N3	76:S2:905:C:O2	2.32	0.62
77:SG:98:ARG:NH2	77:SG:101:ILE:O	2.32	0.62
16:SH:73:GLN:HA	16:SH:76:GLN:HB2	1.81	0.62
72:L5:3641:U:OP2	72:L5:3646:A:N6	2.31	0.62
76:S2:928:G:H2'	76:S2:929:G:C8	2.35	0.62
9:SR:27:ASP:O	9:SR:31:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SO:135:ILE:O	76:S2:943:U:O2'	2.18	0.62
37:LR:117:ARG:NH2	72:L5:2660:A:OP1	2.31	0.62
72:L5:4274:A:H2'	72:L5:4275:G:C8	2.35	0.62
72:L5:2091:C:O2	72:L5:2094:G:O2'	2.18	0.62
30:LY:50:ARG:NH2	71:L8:85:U:O4	2.33	0.62
65:Lb:111:ARG:NH2	72:L5:1268:G:N7	2.48	0.62
78:SI:165:GLN:HB3	78:SI:171:LEU:HD23	1.81	0.62
19:SE:87:MET:HE1	19:SE:236:ILE:HG21	1.81	0.62
27:SA:108:PHE:HB2	27:SA:136:GLU:HG2	1.82	0.61
4:SY:108:LYS:NZ	76:S2:506:G:OP1	2.32	0.61
35:LT:68:THR:HG21	72:L5:4314:C:H4'	1.81	0.61
74:ST:12:GLN:NE2	76:S2:1593:C:O2	2.33	0.61
18:SF:161:ALA:O	18:SF:165:ASN:ND2	2.33	0.61
56:LF:105:VAL:HG13	56:LF:136:VAL:HG12	1.83	0.61
60:LD:208:MET:HB2	60:LD:233:PRO:HG3	1.83	0.61
64:LB:168:MET:HA	64:LB:171:LEU:HD12	1.81	0.61
29:LZ:94:THR:O	29:LZ:97:ASN:ND2	2.33	0.61
65:Lb:57:MET:HE1	72:L5:1828:C:H1'	1.83	0.61
58:LE:46:ARG:O	58:LE:65:ARG:NH1	2.34	0.61
75:SP:40:ARG:NH2	76:S2:1616:U:O4	2.33	0.61
76:S2:981:A:H2'	76:S2:982:G:C8	2.35	0.60
56:LF:35:LYS:NZ	72:L5:2097:U:OP1	2.32	0.60
76:S2:320:C:H42	76:S2:331:C:H42	1.49	0.60
26:Sb:72:ARG:NH2	76:S2:1119:A:O3'	2.34	0.60
72:L5:704:C:N4	72:L5:707:C:OP2	2.34	0.60
13:SL:49:GLU:HG3	13:SL:116:CYS:HA	1.83	0.60
23:SC:254:ASP:N	23:SC:254:ASP:OD1	2.35	0.60
45:LM:46:ARG:NH1	72:L5:935:A:O2'	2.35	0.60
46:LL:116:ARG:NH2	46:LL:155:MET:O	2.34	0.60
54:LG:249:ARG:NH2	72:L5:4075:U:OP1	2.34	0.60
31:LX:47:ARG:NH1	72:L5:2473:A:OP1	2.35	0.60
37:LR:158:GLN:HB3	37:LR:162:ARG:HH21	1.66	0.60
3:Lo:11:PHE:O	3:Lo:81:ARG:NH2	2.35	0.60
64:LB:176:LYS:HG3	72:L5:4986:G:H5''	1.82	0.60
3:Lo:36:GLN:OE1	3:Lo:40:ARG:NH2	2.34	0.60
16:SH:42:GLU:N	16:SH:42:GLU:OE2	2.32	0.60
54:LG:53:ARG:NH1	72:L5:4163:U:OP2	2.34	0.60
16:SH:17:ASP:N	16:SH:20:GLU:OE1	2.34	0.60
60:LD:33:ARG:NH1	68:L7:7:G:OP1	2.35	0.60
9:SR:41:ILE:HG12	9:SR:47:ARG:HB2	1.83	0.60
72:L5:4620:OMU:OP2	72:L5:4670:C:N4	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S2:1401:A:H2'	76:S2:1402:A:C8	2.37	0.60
76:S2:1546:G:N2	76:S2:1670:C:O2	2.35	0.60
6:SW:2:VAL:N	76:S2:1091:C:HO2'	1.99	0.59
48:LJ:164:ARG:HH21	48:LJ:168:GLN:HG3	1.67	0.59
11:SO:117:ARG:NH2	70:Sa:48:ALA:O	2.35	0.59
36:LS:147:ASP:HB3	36:LS:150:ILE:HB	1.84	0.59
72:L5:4734:A:H2'	72:L5:4735:G:C8	2.38	0.59
35:LT:130:ARG:NH1	72:L5:1837:A:OP2	2.35	0.59
43:LN:14:LYS:HE2	72:L5:280:G:H5''	1.85	0.59
60:LD:62:CYS:HB3	60:LD:105:LEU:HD22	1.84	0.59
76:S2:1736:G:H2'	76:S2:1737:G:H8	1.67	0.59
15:SJ:45:ARG:NH2	76:S2:522:A:OP2	2.33	0.59
18:SF:125:SER:O	18:SF:136:ARG:NH2	2.35	0.59
54:LG:43:GLN:HE21	72:L5:4116:C:HO2'	1.48	0.59
72:L5:1833:G:O2'	72:L5:1835:G:N2	2.34	0.59
76:S2:1562:C:H2'	76:S2:1563:G:H8	1.67	0.59
21:SD:161:GLY:HA3	76:S2:1388:A:H61	1.66	0.59
72:L5:2555:G:H2'	72:L5:2556:G:H8	1.65	0.59
72:L5:4274:A:H2'	72:L5:4275:G:H8	1.68	0.59
76:S2:1354:G:N2	76:S2:1357:A:OP2	2.29	0.59
76:S2:1536:G:H2'	76:S2:1537:A:C8	2.37	0.59
76:S2:1658:G:OP2	76:S2:1660:C:N4	2.36	0.59
34:LU:45:GLU:N	34:LU:45:GLU:OE2	2.35	0.59
63:Lc:34:THR:HG23	63:Lc:95:ALA:HB2	1.85	0.59
76:S2:28:U:H2'	76:S2:29:G:H8	1.68	0.59
76:S2:880:G:N1	76:S2:906:U:N3	2.39	0.59
52:LH:37:ASP:OD1	52:LH:39:ASN:ND2	2.29	0.58
72:L5:3663:A:H61	72:L5:4168:G:HO2'	1.50	0.58
39:LQ:38:ARG:NH1	72:L5:2088:A:OP1	2.35	0.58
48:LJ:146:ARG:HG2	48:LJ:147:ARG:HG3	1.84	0.58
64:LB:92:TYR:HB2	64:LB:159:VAL:HB	1.85	0.58
72:L5:4537:C:H2'	72:L5:4538:G:H8	1.67	0.58
72:L5:3664:G:H2'	72:L5:3665:G:H8	1.68	0.58
72:L5:4992:G:H2'	72:L5:4993:G:C8	2.38	0.58
27:SA:85:ARG:NH1	27:SA:203:PHE:O	2.36	0.58
54:LG:200:THR:OG1	72:L5:150:U:OP2	2.22	0.58
69:Pt:21:H2U:H3'	69:Pt:21:H2U:OP2	2.04	0.58
15:SJ:127:ARG:HD3	20:Se:105:ARG:HD3	1.86	0.58
44:Ln:1:MET:HE3	44:Ln:6:ARG:HD2	1.86	0.58
66:LA:30:ARG:NH1	66:LA:36:GLU:OE1	2.36	0.58
72:L5:956:A:H1'	72:L5:2076:G:H5''	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:1942:A:H2'	72:L5:1943:A:C8	2.39	0.58
76:S2:1610:G:O2'	76:S2:1611:G:O5'	2.21	0.58
15:SJ:58:ARG:HD3	23:SC:199:PRO:HG2	1.86	0.58
34:LU:65:ARG:HG3	34:LU:70:ILE:HG13	1.85	0.58
72:L5:67:C:OP2	72:L5:312:G:N2	2.37	0.58
76:S2:381:C:OP2	78:SI:31:ARG:NH2	2.36	0.58
72:L5:2351:OMC:HM22	72:L5:2352:U:H5'	1.86	0.57
45:LM:2:VAL:N	52:LH:44:GLU:OE2	2.36	0.57
56:LF:182:TYR:HB3	56:LF:200:ARG:HG3	1.85	0.57
72:L5:300:A:H2'	72:L5:301:G:H8	1.69	0.57
74:ST:41:LYS:NZ	76:S2:1627:C:OP1	2.36	0.57
10:SQ:40:GLU:O	10:SQ:48:GLN:NE2	2.38	0.57
22:Sd:53:ILE:HG22	22:Sd:55:LEU:HB2	1.86	0.57
38:Lr:67:ARG:NH2	72:L5:666:G:OP2	2.38	0.57
48:LJ:97:ASN:ND2	72:L5:4250:G:OP1	2.37	0.57
77:SG:59:GLN:OE1	77:SG:72:ARG:NH2	2.37	0.57
17:Sg:18:VAL:HG11	17:Sg:21:ILE:HG23	1.86	0.57
2:Ll:43:HIS:HE2	72:L5:2429:A:H5''	1.69	0.57
9:SR:81:ARG:O	27:SA:85:ARG:NH2	2.38	0.57
14:SK:3:MET:HG3	14:SK:44:HIS:HB3	1.84	0.57
31:LX:41:ARG:HD3	54:LG:55:VAL:HG21	1.87	0.57
47:Lk:30:ASP:OD1	47:Lk:30:ASP:N	2.37	0.57
72:L5:2745:A:H2'	72:L5:2746:A:H8	1.70	0.57
72:L5:4563:U:H2'	72:L5:4564:A:H8	1.68	0.57
4:SY:37:LYS:HD2	4:SY:57:VAL:HG23	1.86	0.57
66:LA:93:LYS:NZ	72:L5:4115:G:OP1	2.36	0.57
76:S2:1513:C:H2'	76:S2:1514:G:H8	1.70	0.57
51:Li:46:GLU:OE2	54:LG:234:ARG:NH1	2.38	0.57
21:SD:132:LYS:N	21:SD:189:MET:O	2.37	0.57
60:LD:152:ARG:O	60:LD:157:ASN:ND2	2.37	0.57
76:S2:183:G:N7	76:S2:184:G:O2'	2.38	0.57
76:S2:640:A:H2'	76:S2:641:A:C8	2.40	0.57
76:S2:948:C:H2'	76:S2:949:G:H8	1.68	0.57
76:S2:1617:G:N1	76:S2:1620:A:OP2	2.37	0.57
30:LY:30:MET:HB3	30:LY:101:PRO:HG2	1.87	0.57
72:L5:5053:U:H3'	72:L5:5054:C:H5''	1.87	0.57
76:S2:65:C:OP1	77:SG:136:LYS:NZ	2.38	0.57
19:SE:11:ARG:HA	19:SE:28:ALA:HB2	1.87	0.56
28:mR:32:C:H3'	28:mR:33:C:H4'	1.86	0.56
30:LY:53:ASP:OD2	30:LY:115:ARG:NH2	2.38	0.56
72:L5:1188:C:H2'	72:L5:1189:G:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:2745:A:H2'	72:L5:2746:A:C8	2.40	0.56
79:S6:40:C:H2'	79:S6:41:C:C6	2.39	0.56
52:LH:64:ARG:NH1	72:L5:4693:C:OP1	2.38	0.56
72:L5:4537:C:H2'	72:L5:4538:G:C8	2.40	0.56
76:S2:322:C:H2'	76:S2:323:U:H4'	1.86	0.56
80:SS:86:ARG:NH1	80:SS:89:ASP:OD1	2.39	0.56
9:SR:2:GLY:N	76:S2:1368:U:O3'	2.38	0.56
25:SB:25:PHE:HA	25:SB:28:LYS:HG3	1.87	0.56
43:LN:113:LEU:HD11	71:L8:141:C:H5''	1.86	0.56
63:Lc:101:ASP:OD1	63:Lc:101:ASP:N	2.37	0.56
64:LB:107:ALA:HB2	64:LB:201:LEU:HD22	1.87	0.56
66:LA:37[A]:ARG:NH1	72:L5:4088:C:OP1	2.38	0.56
67:La:72:THR:HG22	67:La:110:LYS:HB3	1.87	0.56
72:L5:982:U:H2'	72:L5:983:C:C6	2.40	0.56
72:L5:2520:C:H2'	72:L5:2521:G:H8	1.71	0.56
76:S2:857:U:H2'	76:S2:858:A:C8	2.40	0.56
76:S2:1130:G:OP2	76:S2:1130:G:N2	2.36	0.56
76:S2:1737:G:OP1	77:SG:94:ARG:NH2	2.35	0.56
79:S6:53:G:H2'	79:S6:54:A:H8	1.71	0.56
39:LQ:88:ASP:OD1	39:LQ:89:ASP:N	2.38	0.56
45:LM:46:ARG:NH1	72:L5:937:U:OP1	2.39	0.56
66:LA:208:GLU:HG2	72:L5:1629:G:H1	1.71	0.56
76:S2:562:U:H2'	76:S2:563:G:C8	2.40	0.56
76:S2:1745:A:H1'	77:SG:66:GLY:HA2	1.88	0.56
59:Le:89:LEU:HD13	59:Le:118:LEU:HD22	1.87	0.56
72:L5:162:A:H2'	72:L5:163:A:H8	1.69	0.56
72:L5:1447:C:H2'	72:L5:1448:G:H8	1.71	0.56
72:L5:2411:C:H2'	72:L5:2412:A:H8	1.71	0.56
72:L5:4750:G:H2'	72:L5:4751:G:C8	2.41	0.56
76:S2:145:G:H2'	76:S2:146:G:C8	2.41	0.56
54:LG:130:THR:OG1	54:LG:131:LYS:N	2.38	0.56
66:LA:117:GLU:HG2	66:LA:124:GLY:H	1.70	0.56
72:L5:1332:C:H2'	72:L5:1333:A:C8	2.41	0.56
9:SR:28:PHE:HA	9:SR:55:THR:HG21	1.88	0.56
72:L5:1097:C:H2'	72:L5:1098:G:H8	1.71	0.56
4:SY:10:ARG:NH2	4:SY:26:ASP:OD1	2.38	0.56
15:SJ:107:GLU:O	15:SJ:113:GLN:NE2	2.37	0.56
50:LI:101:LYS:HB2	50:LI:121:LYS:HZ1	1.70	0.56
66:LA:20:VAL:HA	66:LA:23:ARG:HG3	1.88	0.56
69:Pt:22:A:N6	69:Pt:47:G7M:O2'	2.38	0.56
76:S2:190:G:OP2	78:SI:148:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S2:528:A:H2'	76:S2:529:A:C8	2.41	0.56
17:Sg:238:ALA:HB3	17:Sg:251:ALA:HB3	1.87	0.55
64:LB:210:VAL:O	64:LB:349:LYS:NZ	2.37	0.55
72:L5:478:G:H2'	72:L5:479:G:H8	1.71	0.55
72:L5:1538:U:H2'	72:L5:1539:G:H8	1.71	0.55
72:L5:2724:G:O2'	72:L5:2726:G:OP2	2.24	0.55
76:S2:553:U:H2'	76:S2:554:A:C8	2.40	0.55
76:S2:1407:U:H2'	76:S2:1408:U:C6	2.41	0.55
76:S2:1528:G:O2'	76:S2:1666:C:OP1	2.22	0.55
23:SC:65:LYS:HD2	23:SC:273:LEU:HD13	1.87	0.55
30:LY:27:ARG:CZ	71:L8:70:G:H5''	2.37	0.55
43:LN:49:ARG:NH2	72:L5:152:U:OP2	2.32	0.55
72:L5:62:A:N3	72:L5:77:U:O2'	2.32	0.55
72:L5:163:A:H2'	72:L5:164:G:H8	1.70	0.55
11:SO:142:ARG:NH1	70:Sa:23:CYS:O	2.39	0.55
29:LZ:50:PRO:HD3	29:LZ:68:ILE:HG12	1.88	0.55
59:Le:113:GLU:OE1	59:Le:117:GLN:NE2	2.39	0.55
76:S2:1492:U:O2'	76:S2:1495:G:OP1	2.24	0.55
16:SH:183:LYS:NZ	76:S2:689:U:O2	2.39	0.55
59:Le:108:ARG:NH2	72:L5:2326:G:OP1	2.38	0.55
72:L5:308:G:OP2	72:L5:308:G:N2	2.31	0.55
76:S2:534:G:H22	76:S2:552:G:H22	1.53	0.55
78:SI:116:HIS:O	78:SI:152:ARG:NH1	2.39	0.55
65:Lb:33:LYS:NZ	72:L5:4299:PSU:OP1	2.36	0.55
76:S2:1226:G:N1	76:S2:1639:G7M:OP2	2.36	0.55
76:S2:1532:C:O2'	76:S2:1601:A:N1	2.40	0.55
4:SY:113:ARG:NH1	4:SY:126:GLY:O	2.40	0.55
46:LL:129:ARG:NH2	72:L5:173:C:O5'	2.39	0.55
25:SB:136:ARG:HB2	25:SB:218:LEU:HD11	1.89	0.55
28:mR:39:G:OP1	76:S2:1704:C:N4	2.33	0.55
58:LE:91:THR:OG1	72:L5:2258:C:O2	2.21	0.55
72:L5:3717:A:H2'	72:L5:3718:A2M:C8	2.35	0.55
35:LT:107:LYS:NZ	35:LT:111:GLU:OE2	2.39	0.55
69:Pt:31:G:OP1	76:S2:1524:G:O2'	2.23	0.55
76:S2:1101:U:H2'	76:S2:1102:G:H8	1.71	0.55
72:L5:1396:G:HO2'	72:L5:1468:C:HO2'	1.55	0.55
72:L5:4736:C:H2'	72:L5:4737:G:H8	1.72	0.55
18:SF:30:ILE:HG13	18:SF:117:ILE:HD11	1.90	0.54
26:Sb:30:SER:OG	76:S2:1016:U:OP1	2.18	0.54
30:LY:14:ASN:ND2	72:L5:228:C:O2'	2.39	0.54
65:Lb:38:LYS:NZ	72:L5:1816:C:O3'	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:3598:C:H2'	72:L5:3599:A:H8	1.72	0.54
72:L5:3654:G:O2'	72:L5:3693:U:OP1	2.19	0.54
72:L5:3736:A:H2'	72:L5:3737:A:C8	2.42	0.54
72:L5:4967:A:H2'	72:L5:4968:A:H8	1.72	0.54
73:SZ:102:LYS:HG3	73:SZ:107:VAL:HG13	1.89	0.54
75:SP:40:ARG:NH1	76:S2:1615:U:O4	2.40	0.54
76:S2:107:A:H2'	76:S2:108:G:C8	2.42	0.54
56:LF:46:ARG:NH1	72:L5:1704:C:O3'	2.40	0.54
72:L5:4260:U:H2'	72:L5:4261:C:C6	2.42	0.54
72:L5:138:G:H2'	72:L5:139:G:H8	1.71	0.54
72:L5:967:C:H5'	72:L5:968:C:H5	1.72	0.54
19:SE:87:MET:HE2	19:SE:123:LEU:HB2	1.88	0.54
27:SA:198:MET:HE3	27:SA:200:ASP:HB2	1.90	0.54
43:LN:116:LEU:HD22	43:LN:135:ILE:HD11	1.88	0.54
58:LE:123:ARG:HG2	72:L5:959:G:C8	2.42	0.54
72:L5:1326:A2M:OP2	72:L5:4445:U:O2'	2.25	0.54
72:L5:3868:G:H22	72:L5:3900:G:H1'	1.72	0.54
48:LJ:112:HIS:HD2	48:LJ:117:ILE:HD11	1.73	0.54
71:L8:102:G:OP2	71:L8:104:A:O2'	2.25	0.54
27:SA:190:SER:OG	27:SA:192:GLU:OE1	2.22	0.54
38:Lr:20:ARG:NH1	59:Le:78:LEU:O	2.39	0.54
54:LG:47:PRO:HG2	54:LG:49:ARG:HD3	1.90	0.54
64:LB:92:TYR:HB3	64:LB:99:LEU:HD22	1.88	0.54
72:L5:4090:G:H1	72:L5:4159:C:H5	1.54	0.54
76:S2:857:U:H2'	76:S2:858:A:H8	1.72	0.54
76:S2:1726:G:H2'	76:S2:1727:G:H8	1.72	0.54
25:SB:150:ILE:HG12	76:S2:1124:C:H5''	1.89	0.54
41:Lp:84:ARG:HG2	41:Lp:84:ARG:HH11	1.72	0.54
51:Li:59:GLU:OE2	51:Li:62:LYS:NZ	2.36	0.54
62:LC:204:ARG:HH21	72:L5:2298:U:H5''	1.72	0.54
63:Lc:23:LYS:HE2	63:Lc:24:SER:HB3	1.90	0.54
63:Lc:38:ILE:HG21	63:Lc:63:TYR:HB3	1.89	0.54
72:L5:3917:A:H2'	72:L5:3918:G:H8	1.72	0.54
9:SR:4:VAL:HG23	76:S2:1370:A:H62	1.73	0.54
42:LO:61:ARG:HD2	42:LO:66:PRO:HB3	1.89	0.54
76:S2:385:G:O2'	78:SI:10:LYS:NZ	2.41	0.54
12:SN:87:ASP:OD1	12:SN:87:ASP:N	2.38	0.54
72:L5:3663:A:N6	72:L5:4168:G:HO2'	2.06	0.54
72:L5:4594:U:H2'	72:L5:4595:G:H8	1.72	0.54
76:S2:1228:A:H2'	76:S2:1229:G:H8	1.73	0.54
76:S2:1705:C:H2'	76:S2:1706:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SD:185:LYS:NZ	76:S2:1336:C:OP2	2.41	0.54
48:LJ:141:ILE:HA	48:LJ:144:LYS:HD3	1.90	0.54
54:LG:49:ARG:NH2	72:L5:4158:C:OP1	2.41	0.54
72:L5:3700:C:O2'	72:L5:3774:A:N3	2.39	0.54
76:S2:78:C:H1'	77:SG:175:LYS:HG3	1.89	0.54
76:S2:1568:C:H2'	76:S2:1569:A:C8	2.42	0.54
46:LL:63:THR:HG21	67:La:66:ASN:HB3	1.91	0.53
72:L5:1077:C:OP1	72:L5:1215:C:O2'	2.25	0.53
72:L5:4239:A:H2'	72:L5:4240:G:C8	2.43	0.53
4:SY:111:LYS:NZ	76:S2:56:G:OP1	2.41	0.53
29:LZ:51:ARG:NH1	72:L5:2755:A:OP2	2.40	0.53
34:LU:101:ARG:NH1	72:L5:2623:A:OP1	2.41	0.53
76:S2:96:C:H2'	76:S2:97:U:C6	2.43	0.53
76:S2:1144:A:H5'	76:S2:1355:C:H41	1.72	0.53
76:S2:1259:A:N6	76:S2:1519:U:OP1	2.38	0.53
18:SF:28:VAL:HG11	18:SF:41:VAL:HG11	1.90	0.53
76:S2:1430:C:N4	76:S2:1431:G:O6	2.41	0.53
12:SN:64:ARG:NH2	76:S2:919:A:OP2	2.38	0.53
72:L5:1273:G:H2'	72:L5:1274:A:C8	2.43	0.53
76:S2:1726:G:N2	76:S2:1808:U:O2	2.31	0.53
17:Sg:239:LEU:HA	17:Sg:250:ALA:HA	1.90	0.53
25:SB:37:ALA:HA	25:SB:42:ARG:HE	1.73	0.53
40:LP:52:THR:HG23	40:LP:85:LYS:HG3	1.90	0.53
46:LL:178:ALA:N	67:La:134:GLU:OE2	2.42	0.53
47:Lk:14:THR:HA	47:Lk:17:ARG:HD3	1.89	0.53
58:LE:72:LYS:HD3	65:Lb:119:CYS:HB2	1.91	0.53
64:LB:165:HIS:HB3	64:LB:180:LEU:HD12	1.91	0.53
72:L5:162:A:H2'	72:L5:163:A:C8	2.43	0.53
72:L5:1339:U:H2'	72:L5:1340:OMC:C6	2.43	0.53
76:S2:67:C:OP2	77:SG:172:LYS:NZ	2.30	0.53
36:LS:95:ARG:NH2	36:LS:112:ASP:OD2	2.40	0.53
72:L5:755:C:H2'	72:L5:756:G:H8	1.73	0.53
72:L5:4954:G:H2'	72:L5:4955:A:C8	2.44	0.53
7:SV:64:GLU:OE2	27:SA:33:GLN:NE2	2.41	0.53
62:LC:221:PHE:HB3	62:LC:227:ILE:HG21	1.91	0.53
67:La:93:ASN:ND2	67:La:97:ALA:HB3	2.24	0.53
13:SL:111:VAL:HG12	13:SL:140:PHE:HB2	1.91	0.53
34:LU:64:GLU:N	34:LU:64:GLU:OE2	2.41	0.53
72:L5:163:A:H2'	72:L5:164:G:C8	2.43	0.53
72:L5:2520:C:H2'	72:L5:2521:G:C8	2.44	0.53
72:L5:3799:A:N3	72:L5:4506:C:O2'	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S2:1221:G:O2'	76:S2:1676:U:O2	2.26	0.53
56:LF:34:ARG:NH1	72:L5:1439:C:H5'	2.24	0.53
72:L5:483:C:H4'	72:L5:484:U:H5'	1.91	0.53
11:SO:147:ARG:HA	70:Sa:28:ARG:HH11	1.74	0.53
42:LO:163:LYS:NZ	72:L5:4909:A:OP1	2.41	0.53
66:LA:137:ILE:HD11	66:LA:149:LYS:HB2	1.90	0.53
76:S2:1013:U:OP1	76:S2:1129:G:O2'	2.27	0.53
15:SJ:158:ASP:OD1	15:SJ:158:ASP:N	2.41	0.52
50:LI:214:SER:HB3	60:LD:287:PHE:HZ	1.74	0.52
72:L5:3718:A2M:H2	72:L5:3934:G:O4'	2.09	0.52
76:S2:1101:U:H2'	76:S2:1102:G:C8	2.44	0.52
79:S6:43:G:C2	79:S6:44:A:H1'	2.44	0.52
6:SW:71:LYS:NZ	76:S2:1153:C:OP2	2.34	0.52
35:LT:5:LYS:HD2	72:L5:4302:U:H4'	1.91	0.52
37:LR:46:LYS:NZ	72:L5:2705:G:O6	2.39	0.52
53:Lh:45:SER:OG	71:L8:80:A:N6	2.42	0.52
56:LF:131:ASN:ND2	72:L5:1727:U:OP1	2.42	0.52
66:LA:107:MET:HE1	66:LA:113:VAL:HG11	1.91	0.52
72:L5:167:C:HO2'	72:L5:168:C:H6	1.57	0.52
76:S2:558:G:H2'	76:S2:559:G:C8	2.45	0.52
25:SB:164:ILE:O	25:SB:168:MET:HG3	2.10	0.52
72:L5:4188:U:H2'	72:L5:4189:U:C6	2.45	0.52
72:L5:4862:G:H2'	72:L5:4863:G:C8	2.45	0.52
42:LO:54:TYR:OH	42:LO:73:PHE:O	2.26	0.52
43:LN:67:ARG:HD2	72:L5:2458:C:H5'	1.91	0.52
58:LE:74:SER:HA	65:Lb:117:ARG:HG3	1.91	0.52
62:LC:60:HIS:HA	62:LC:92:PHE:HE1	1.73	0.52
71:L8:148:A:H2'	71:L8:149:G:C8	2.44	0.52
72:L5:670:G:H2'	72:L5:671:G:H8	1.74	0.52
72:L5:1202:C:H2'	72:L5:1203:G:H8	1.74	0.52
77:SG:32:MET:HG3	77:SG:100:CYS:HB2	1.91	0.52
79:S6:69:U:H2'	79:S6:70:G:C8	2.44	0.52
36:LS:74:ARG:O	36:LS:76:LYS:NZ	2.39	0.52
48:LJ:68:ILE:HD11	72:L5:4258:C:H5'	1.92	0.52
49:Lj:55:ARG:NH2	72:L5:364:G:O6	2.41	0.52
56:LF:187:MET:HE2	62:LC:328:LEU:HD13	1.90	0.52
64:LB:153:MET:HB3	64:LB:194:LEU:HD11	1.90	0.52
71:L8:17:A:H61	72:L5:417:G:H1'	1.73	0.52
72:L5:2744:A:H2'	72:L5:2745:A:C8	2.44	0.52
76:S2:170:A:P	77:SG:136:LYS:H	2.33	0.52
76:S2:1545:A:H2'	76:S2:1546:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LZ:78:ASN:OD1	63:Lc:39:ARG:NH2	2.43	0.52
72:L5:501:C:H42	72:L5:656:C:H42	1.57	0.52
72:L5:1294:A:H1'	72:L5:1295:C:H5	1.75	0.52
72:L5:1308:C:H2'	72:L5:1309:C:C6	2.45	0.52
72:L5:1377:G:H21	72:L5:1380:G:H5'	1.74	0.52
72:L5:5027:C:H1'	72:L5:5028:G:C8	2.44	0.52
75:SP:89:MET:SD	75:SP:89:MET:N	2.77	0.52
17:Sg:17:TRP:O	17:Sg:36:ARG:N	2.41	0.52
21:SD:9:ARG:NH2	76:S2:1551:U:OP1	2.43	0.52
39:LQ:147:GLU:N	72:L5:1504:G:OP1	2.43	0.52
76:S2:833:C:H2'	76:S2:834:C:C6	2.45	0.52
76:S2:1736:G:H2'	76:S2:1737:G:C8	2.44	0.52
1:Lm:82:LEU:HD13	52:LH:95:VAL:HG12	1.92	0.52
72:L5:2557:G:H1	72:L5:2570:U:H3	1.58	0.52
17:Sg:251:ALA:HA	17:Sg:256:ILE:HA	1.92	0.52
39:LQ:173:LYS:NZ	72:L5:88:A:N7	2.58	0.52
43:LN:96:ARG:NH2	43:LN:100:SER:OG	2.42	0.52
76:S2:184:G:H5'	76:S2:185:G:C8	2.45	0.52
3:Lo:31:ASP:OD1	72:L5:4343:U:O2'	2.28	0.52
32:LW:1:MET:HE1	33:LV:92:ASP:HB2	1.92	0.52
32:LW:52:THR:HG22	32:LW:54:LEU:H	1.75	0.52
57:Lf:89:ARG:NH2	72:L5:709:C:OP1	2.43	0.52
67:La:95:THR:OG1	67:La:96:GLY:N	2.43	0.52
72:L5:2640:G:H2'	72:L5:2641:A:C8	2.45	0.52
72:L5:2758:G:O2'	72:L5:2765:A:N3	2.36	0.52
76:S2:535:G:H22	76:S2:551:U:H3	1.58	0.52
76:S2:1411:G:H2'	76:S2:1412:C:C6	2.45	0.52
9:SR:5:ARG:NH2	76:S2:1455:A:OP1	2.42	0.51
17:Sg:216:ALA:H	17:Sg:231:ASP:HA	1.75	0.51
29:LZ:79:HIS:ND1	72:L5:2580:U:O2'	2.42	0.51
37:LR:46:LYS:NZ	72:L5:2712:G:O6	2.43	0.51
66:LA:5:ILE:HG12	66:LA:8:GLN:HG3	1.92	0.51
72:L5:1086:C:H2'	72:L5:1087:A:H8	1.75	0.51
72:L5:2318:G:N2	72:L5:2321:G:OP2	2.31	0.51
15:SJ:172:ARG:NH2	76:S2:587:A:OP2	2.42	0.51
40:LP:3:ARG:NH1	71:L8:12:G:OP1	2.43	0.51
42:LO:176:ARG:HD3	72:L5:4769:G:H5''	1.92	0.51
69:Pt:19:G:N2	69:Pt:59:A:O5'	2.44	0.51
76:S2:1719:A:N6	76:S2:1814:G:O2'	2.43	0.51
76:S2:1750:C:N4	76:S2:1784:G:N7	2.52	0.51
9:SR:29:HIS:HA	9:SR:32:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LI:7:ARG:NH2	72:L5:4405:G:OP2	2.42	0.51
66:LA:140:ASN:ND2	66:LA:140:ASN:C	2.66	0.51
76:S2:649:PSU:H2'	76:S2:650:A:H8	1.74	0.51
76:S2:980:A:H2'	76:S2:981:A:C8	2.45	0.51
21:SD:136:VAL:HG22	21:SD:186:VAL:HG22	1.93	0.51
66:LA:207:VAL:HG13	66:LA:208:GLU:HG3	1.92	0.51
72:L5:4238:G:H2'	72:L5:4239:A:H8	1.75	0.51
4:SY:41:ARG:HG2	4:SY:55:ILE:HG22	1.91	0.51
51:LI:50:PHE:O	51:LI:55:ARG:NH1	2.44	0.51
62:LC:4:ALA:HB3	72:L5:667:A:H1'	1.92	0.51
72:L5:1563:A:N6	76:S2:1028:A:N1	2.58	0.51
76:S2:106:C:H2'	76:S2:107:A:H8	1.75	0.51
76:S2:1461:G:N1	76:S2:1464:C:OP2	2.44	0.51
19:SE:10:LYS:NZ	76:S2:95:G:OP1	2.38	0.51
22:SD:2:GLY:N	76:S2:1301:A:OP2	2.43	0.51
37:LR:164:SER:HA	37:LR:167:LYS:NZ	2.25	0.51
72:L5:4174:U:H2'	72:L5:4175:G:H8	1.75	0.51
76:S2:948:C:H2'	76:S2:949:G:C8	2.46	0.51
79:S6:51:U:H2'	79:S6:52:G:C8	2.46	0.51
35:LT:102:ARG:HD2	72:L5:1801:A:H4'	1.93	0.51
37:LR:62:ARG:O	37:LR:66:ASN:ND2	2.37	0.51
50:LI:52:MET:HB2	50:LI:152:LEU:HD22	1.93	0.51
72:L5:1775:A:H3'	72:L5:1776:A:H8	1.76	0.51
76:S2:12:U:H2'	76:S2:13:C:C6	2.45	0.51
76:S2:559:G:O2'	76:S2:560:A:O5'	2.27	0.51
34:LU:37:ALA:HA	34:LU:40:GLU:HG3	1.92	0.51
54:LG:94:GLN:HA	54:LG:97:LYS:HE2	1.92	0.51
76:S2:534:G:H22	76:S2:552:G:N2	2.08	0.51
4:SY:20:ARG:HE	4:SY:22:GLN:HE21	1.58	0.51
72:L5:1548:G:O2'	72:L5:2812:A:N3	2.37	0.51
72:L5:1604:G:H2'	72:L5:1605:G:C8	2.45	0.51
72:L5:1933:G:H2'	72:L5:1934:A:C8	2.46	0.51
76:S2:96:C:H2'	76:S2:97:U:H6	1.76	0.51
9:SR:56:HIS:NE2	76:S2:1465:A:OP1	2.43	0.51
15:SJ:160:SER:O	15:SJ:163:SER:OG	2.29	0.51
29:LZ:54:THR:H	29:LZ:57:MET:HG3	1.76	0.51
34:LU:40:GLU:O	34:LU:43:LEU:N	2.41	0.51
38:Lr:28:GLU:OE2	38:Lr:31:ASN:ND2	2.37	0.51
58:LE:173:LEU:HD21	58:LE:191:GLN:HB3	1.93	0.51
76:S2:391:C:H2'	76:S2:392:A:H8	1.75	0.51
33:LV:43:LYS:HG3	33:LV:60:MET:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:LQ:37:ARG:NH2	72:L5:2088:A:OP2	2.44	0.50
72:L5:268:G:H2'	72:L5:269:G:H8	1.76	0.50
72:L5:505:G:H1	72:L5:653:U:H3	1.59	0.50
10:SQ:131:LYS:HB2	10:SQ:140:ARG:HH22	1.76	0.50
54:LG:235:ARG:N	54:LG:235:ARG:HD2	2.26	0.50
76:S2:1140:G:HO2'	76:S2:1151:G:HO2'	1.58	0.50
6:SW:4:MET:SD	76:S2:682:U:O2'	2.66	0.50
11:SO:55:ARG:NH1	76:S2:973:C:N3	2.57	0.50
72:L5:4741:C:O2'	72:L5:4742:G:OP1	2.28	0.50
76:S2:656:G:N2	76:S2:663:C:H5''	2.26	0.50
76:S2:1630:A:H5'	80:SS:37:GLY:N	2.27	0.50
5:SX:96:GLU:N	5:SX:96:GLU:OE2	2.45	0.50
11:SO:134:PRO:HB3	76:S2:944:A:H5''	1.93	0.50
14:SK:64:TRP:CD2	22:Sd:23:VAL:HG12	2.46	0.50
16:SH:36:LEU:HG	16:SH:78:ARG:HH21	1.77	0.50
39:LQ:119:LYS:HE3	39:LQ:121:LEU:HD21	1.93	0.50
42:LO:176:ARG:NH1	72:L5:4769:G:OP1	2.40	0.50
43:LN:4:TYR:OH	72:L5:151:G:OP2	2.22	0.50
46:LL:59:VAL:HB	72:L5:74:G:H5'	1.92	0.50
72:L5:4260:U:H2'	72:L5:4261:C:H6	1.76	0.50
76:S2:801:PSU:H2'	76:S2:802:A:H8	1.77	0.50
5:SX:5:ARG:NH2	76:S2:1158:G:OP1	2.45	0.50
19:SE:104:ASP:HB3	19:SE:110:ALA:HB2	1.93	0.50
66:LA:247:ARG:HH21	76:S2:1070:A:H5'	1.75	0.50
72:L5:4740:G:H2'	72:L5:4742:G:H5''	1.94	0.50
77:SG:5:ILE:HD13	77:SG:111:LEU:HB2	1.93	0.50
6:SW:30:CYS:HB2	6:SW:61:ILE:HG13	1.93	0.50
19:SE:151:ASP:HB3	19:SE:154:ILE:HG13	1.94	0.50
52:LH:114:ILE:HB	52:LH:124:ARG:HB2	1.94	0.50
53:Lh:88:THR:HB	53:Lh:91:MET:HB2	1.93	0.50
62:LC:95:MET:HG3	72:L5:2351:OMC:HM23	1.93	0.50
72:L5:49:U:H2'	72:L5:50:C:H6	1.77	0.50
72:L5:478:G:H2'	72:L5:479:G:C8	2.47	0.50
72:L5:1426:G:N1	72:L5:1458:C:OP2	2.37	0.50
72:L5:1514:U:H2'	72:L5:1515:A:C8	2.47	0.50
72:L5:4761:G:H2'	72:L5:4762:A:H8	1.76	0.50
76:S2:940:U:H2'	76:S2:941:C:C6	2.47	0.50
76:S2:1410:C:H2'	76:S2:1411:G:C8	2.43	0.50
76:S2:1726:G:H2'	76:S2:1727:G:C8	2.46	0.50
76:S2:1845:A:H2'	76:S2:1846:G:C8	2.47	0.50
45:LM:67:SER:O	45:LM:67:SER:OG	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:LL:58:ILE:HG12	46:LL:157:VAL:HG13	1.94	0.50
52:LH:107:GLU:O	52:LH:110:SER:OG	2.30	0.50
59:Le:57:ASN:OD1	72:L5:1899:G:O2'	2.30	0.50
72:L5:1333:A:H2'	72:L5:1334:A:C8	2.46	0.50
72:L5:1683:PSU:H2'	72:L5:1684:A:C8	2.47	0.50
76:S2:1562:C:H2'	76:S2:1563:G:C8	2.47	0.50
76:S2:1809:A:H2'	76:S2:1810:U:C6	2.47	0.50
3:Lo:78:ARG:O	3:Lo:80:LYS:NZ	2.45	0.50
23:SC:167:ARG:HB3	23:SC:177:PRO:HB2	1.93	0.50
37:LR:92:LYS:NZ	72:L5:1574:G:OP2	2.40	0.50
66:LA:40:TYR:OH	72:L5:4117:U:O2'	2.27	0.50
71:L8:67:U:H2'	71:L8:68:G:H8	1.77	0.50
71:L8:144:U:H2'	71:L8:145:C:C6	2.47	0.50
79:S6:69:U:H2'	79:S6:70:G:H8	1.77	0.50
80:SS:121:ARG:HG2	80:SS:131:VAL:HB	1.92	0.50
30:LY:46:SER:OG	72:L5:239:C:OP1	2.29	0.50
38:Lr:87:ARG:NH1	72:L5:690:C:OP1	2.43	0.50
50:LI:66:GLU:OE1	50:LI:69:ARG:NH1	2.45	0.50
72:L5:2701:U:H2'	72:L5:2702:C:C6	2.46	0.50
72:L5:3636:C:H4'	72:L5:3825:A2M:H2	1.93	0.50
72:L5:4699:U:H1'	72:L5:4700:A:H5''	1.94	0.50
76:S2:367:U:H4'	76:S2:371:A:C8	2.47	0.50
76:S2:1221:G:H2'	76:S2:1222:G:C8	2.47	0.50
4:SY:27:VAL:HB	4:SY:69:THR:HB	1.93	0.49
10:SQ:19:ALA:HB2	10:SQ:75:GLY:HA3	1.94	0.49
35:LT:133:ALA:HB3	56:LF:127:LYS:HB2	1.94	0.49
42:LO:61:ARG:HA	42:LO:70:PRO:HD2	1.94	0.49
70:Sa:6:ARG:NH1	76:S2:1147:C:OP1	2.43	0.49
72:L5:1479:G:H2'	72:L5:1480:C:C6	2.47	0.49
76:S2:72:C:H42	77:SG:170:ARG:HD3	1.77	0.49
76:S2:928:G:H1	76:S2:1013:U:H3	1.60	0.49
76:S2:1692:PSU:H2'	76:S2:1693:G:C8	2.47	0.49
76:S2:1801:A:H2'	76:S2:1802:C:C6	2.47	0.49
60:LD:278:ASP:OD2	60:LD:282:GLN:NE2	2.45	0.49
72:L5:4239:A:H2'	72:L5:4240:G:H8	1.76	0.49
72:L5:4459:U:H2'	72:L5:4460:U:C6	2.47	0.49
75:SP:58:LYS:HA	75:SP:58:LYS:HE3	1.94	0.49
76:S2:588:G:OP2	76:S2:588:G:N2	2.35	0.49
8:SU:54:VAL:HG22	8:SU:88:LEU:HB2	1.94	0.49
18:SF:121:PRO:HA	18:SF:193:LYS:HE3	1.95	0.49
23:SC:252:THR:HG22	23:SC:254:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:LI:146:GLU:OE2	50:LI:146:GLU:N	2.36	0.49
78:SI:6:ASP:OD2	78:SI:9:HIS:ND1	2.38	0.49
79:S6:51:U:H2'	79:S6:52:G:H8	1.77	0.49
18:SF:127:ARG:HG2	18:SF:136:ARG:HG2	1.94	0.49
65:Lb:44:ARG:NH2	72:L5:1466:G:OP2	2.45	0.49
72:L5:679:C:H2'	72:L5:680:G:H8	1.77	0.49
72:L5:1097:C:H2'	72:L5:1098:G:C8	2.47	0.49
72:L5:1577:G:O2'	72:L5:1612:G:H4'	2.13	0.49
72:L5:2539:C:H2'	72:L5:2540:C:C6	2.47	0.49
76:S2:165:G:OP2	76:S2:165:G:N2	2.35	0.49
76:S2:312:G:C8	77:SG:191:ARG:HD3	2.45	0.49
76:S2:942:G:H2'	76:S2:943:U:C6	2.48	0.49
30:LY:121:ARG:NH2	72:L5:194:C:O2	2.45	0.49
60:LD:125:VAL:HG11	60:LD:199:ILE:HG21	1.94	0.49
72:L5:5006:U:H4'	72:L5:5007:A:H5'	1.94	0.49
76:S2:512:A2M:H4'	76:S2:576:A2M:H2	1.95	0.49
76:S2:910:G:OP2	76:S2:910:G:N2	2.35	0.49
79:S6:41:C:H2'	79:S6:42:A:C8	2.48	0.49
16:SH:95:ILE:HD13	16:SH:129:ILE:HG23	1.95	0.49
72:L5:956:A:H8	72:L5:957:G:C8	2.31	0.49
72:L5:2884:G:H2'	72:L5:2885:A:H8	1.76	0.49
76:S2:484:A2M:H8	76:S2:484:A2M:O5'	2.12	0.49
30:LY:45:ARG:NH2	72:L5:238:C:OP2	2.44	0.49
59:Le:104:SER:HB3	72:L5:2303:C:H5''	1.93	0.49
72:L5:1846:G:H2'	72:L5:1847:C:C6	2.48	0.49
72:L5:4238:G:H2'	72:L5:4239:A:C8	2.47	0.49
72:L5:4591:U:H2'	72:L5:4592:C:C6	2.47	0.49
76:S2:1144:A:H2'	76:S2:1145:A:C8	2.48	0.49
79:S6:53:G:H2'	79:S6:54:A:C8	2.48	0.49
37:LR:82:LYS:NZ	86:LR:201:HOH:O	2.44	0.49
55:Lg:44:SER:OG	55:Lg:46:CYS:SG	2.71	0.49
72:L5:1890:G:OP2	72:L5:1890:G:N2	2.43	0.49
72:L5:1942:A:H2'	72:L5:1943:A:H8	1.75	0.49
76:S2:455:A:H2'	76:S2:456:C:H6	1.77	0.49
76:S2:874:G:H2'	76:S2:875:A:H8	1.78	0.49
76:S2:1797:U:H2'	76:S2:1798:C:C6	2.48	0.49
11:SO:45:THR:HG22	11:SO:52:THR:HA	1.94	0.49
39:LQ:79:THR:HB	39:LQ:99:LYS:HD3	1.94	0.49
46:LL:106:SER:OG	72:L5:73:A:OP1	2.25	0.49
58:LE:123:ARG:HD3	72:L5:970:G:C2	2.48	0.49
72:L5:4761:G:H2'	72:L5:4762:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:5057:C:H2'	72:L5:5058:A:C8	2.48	0.49
73:SZ:79:ILE:HB	73:SZ:83:LEU:HD23	1.93	0.49
76:S2:1588:A:H2'	76:S2:1589:A:C8	2.48	0.49
29:LZ:83:THR:HG23	29:LZ:85:TYR:HD1	1.78	0.49
31:LX:38:LYS:HB2	72:L5:1:C:H5''	1.95	0.49
59:Le:17:THR:HB	72:L5:1302:U:H5'	1.94	0.49
67:La:114:LYS:HG3	72:L5:1397:A:H8	1.78	0.49
70:Sa:26:CYS:SG	86:Sa:201:HOH:O	2.60	0.49
72:L5:450:G:H2'	72:L5:451:C:C6	2.48	0.49
72:L5:908:G:H2'	72:L5:909:A:H8	1.78	0.49
72:L5:1662:C:H2'	72:L5:1663:C:C6	2.48	0.49
72:L5:2848:G:O2'	72:L5:3838:U:O4	2.23	0.49
76:S2:527:C:H2'	76:S2:528:A:H8	1.78	0.49
36:LS:69:GLU:OE2	36:LS:102:THR:N	2.40	0.48
37:LR:160:GLU:O	37:LR:164:SER:OG	2.24	0.48
72:L5:4594:U:H2'	72:L5:4595:G:C8	2.48	0.48
27:SA:76:VAL:HG12	27:SA:123:VAL:HB	1.94	0.48
34:LU:44:GLN:HG3	34:LU:63:ILE:HD13	1.95	0.48
41:Lp:76:ALA:HA	41:Lp:79:VAL:HG12	1.95	0.48
66:LA:140:ASN:C	66:LA:140:ASN:HD22	2.19	0.48
66:LA:242:ARG:NH2	66:LA:244:GLY:O	2.47	0.48
72:L5:657:C:H2'	72:L5:658:C:C6	2.48	0.48
72:L5:2411:C:H2'	72:L5:2412:A:C8	2.47	0.48
72:L5:5027:C:H4'	72:L5:5028:G:H5'	1.95	0.48
2:Ll:23:ILE:HD12	2:Ll:27:ILE:HD11	1.96	0.48
4:SY:102:THR:O	4:SY:107:ARG:NH1	2.46	0.48
11:SO:147:ARG:HB3	11:SO:150:ARG:HD3	1.95	0.48
50:LI:19:LYS:HD2	50:LI:26:VAL:HB	1.95	0.48
53:Lh:15:GLU:CD	53:Lh:15:GLU:H	2.22	0.48
63:Lc:57:LYS:O	63:Lc:61:GLU:HG3	2.13	0.48
72:L5:1320:U:O2'	72:L5:1891:A:N1	2.42	0.48
72:L5:2658:G:O2'	72:L5:2675:G:N2	2.47	0.48
72:L5:4967:A:H2'	72:L5:4968:A:C8	2.47	0.48
76:S2:1098:C:H2'	76:S2:1099:G:C8	2.47	0.48
61:Ld:64:ILE:HG23	61:Ld:68:LEU:HD23	1.95	0.48
66:LA:234:LYS:HG2	66:LA:238:ILE:HG12	1.94	0.48
72:L5:325:U:H2'	72:L5:326:C:C6	2.48	0.48
72:L5:1576:G:O2'	72:L5:1578:U:O2	2.32	0.48
72:L5:3910:C:H2'	72:L5:3911:C:H6	1.78	0.48
76:S2:17:C:O2'	76:S2:1194:A:N1	2.43	0.48
76:S2:1712:A:H2'	76:S2:1713:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SV:32:ILE:HG12	7:SV:60:ARG:HD2	1.96	0.48
53:Lh:10:ARG:NH2	53:Lh:63:GLN:OE1	2.46	0.48
39:LQ:64:SER:OG	39:LQ:89:ASP:OD2	2.30	0.48
64:LB:122:TRP:O	64:LB:127:LYS:NZ	2.46	0.48
67:La:79:TRP:HH2	67:La:99:PRO:HG2	1.78	0.48
71:L8:17:A:N6	72:L5:417:G:H1'	2.28	0.48
72:L5:755:C:H2'	72:L5:756:G:C8	2.48	0.48
72:L5:1198:G:O2'	72:L5:1200:G:OP1	2.32	0.48
72:L5:1879:C:O2'	72:L5:1891:A:N3	2.42	0.48
72:L5:2651:C:O2'	72:L5:2653:C:OP1	2.26	0.48
75:SP:40:ARG:NH1	76:S2:1624:U:O4	2.44	0.48
76:S2:17:C:H2'	76:S2:18:C:C6	2.49	0.48
76:S2:28:U:H2'	76:S2:29:G:C8	2.48	0.48
76:S2:51:U:H2'	76:S2:52:G:C8	2.48	0.48
9:SR:105:MET:HE3	27:SA:50:ASN:HA	1.94	0.48
63:Lc:21:VAL:HG11	63:Lc:96:ILE:HG12	1.96	0.48
64:LB:373:LYS:HE3	72:L5:4627:U:H4'	1.96	0.48
72:L5:1262:G:H2'	72:L5:1263:A:H8	1.79	0.48
72:L5:3598:C:H2'	72:L5:3599:A:C8	2.48	0.48
72:L5:3633:C:H2'	72:L5:3634:G:C8	2.48	0.48
76:S2:448:A:H5''	78:SI:25:ARG:HA	1.95	0.48
76:S2:1007:C:H2'	76:S2:1008:A:C8	2.48	0.48
76:S2:1217:A:H2'	76:S2:1218:C:C6	2.48	0.48
72:L5:2480:G:H2'	72:L5:2481:G:C8	2.49	0.48
72:L5:3873:G:H2'	72:L5:3874:G:C8	2.47	0.48
72:L5:4750:G:H2'	72:L5:4751:G:H8	1.77	0.48
72:L5:5030:U:H2'	72:L5:5031:G:H8	1.78	0.48
9:SR:133:GLY:HA2	25:SB:152:LYS:HD3	1.95	0.48
39:LQ:66:MET:HE1	39:LQ:86:ILE:HD13	1.95	0.48
41:Lp:74:THR:O	41:Lp:78:THR:HG23	2.14	0.48
43:LN:12:ARG:HG2	72:L5:279:A:C4	2.48	0.48
52:LH:59:LYS:HE2	52:LH:66:GLU:HB3	1.96	0.48
52:LH:94:SER:HB2	52:LH:142:ASP:HB3	1.96	0.48
68:L7:82:G:H2'	68:L7:83:A:C8	2.49	0.48
72:L5:3870:C:H2'	72:L5:3871:A:H8	1.79	0.48
74:ST:22:LEU:HD21	74:ST:28:LEU:HG	1.95	0.48
6:SW:12:LYS:HD3	6:SW:12:LYS:HA	1.68	0.48
8:SU:59:LYS:HD3	21:SD:8:LYS:HZ2	1.79	0.48
14:SK:28:HIS:CG	22:Sd:8:TRP:HE1	2.32	0.48
21:SD:138:VAL:HG22	21:SD:184:ILE:HG13	1.95	0.48
36:LS:116:ARG:NH1	72:L5:1950:U:O2'	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LE:97:GLY:HA3	58:LE:101:ASN:HB2	1.95	0.48
63:Lc:48:LEU:HD21	63:Lc:60:ILE:HD13	1.95	0.48
72:L5:1306:C:H2'	72:L5:1307:A:H8	1.79	0.48
76:S2:656:G:H5'	76:S2:662:G:N2	2.29	0.48
6:SW:107:SER:HB2	76:S2:860:G:H21	1.79	0.47
44:Ln:15:ARG:O	44:Ln:19:LYS:HG3	2.14	0.47
48:LJ:90:ARG:NH2	48:LJ:110:GLN:OE1	2.38	0.47
53:Lh:66:LYS:NZ	71:L8:97:A:OP2	2.39	0.47
72:L5:1190:C:H2'	72:L5:1191:C:C6	2.49	0.47
72:L5:3726:A:H2'	72:L5:3727:A:C8	2.49	0.47
72:L5:3925:OMU:HM23	72:L5:3925:OMU:H1'	1.57	0.47
76:S2:5:U:H2'	76:S2:6:G:H8	1.79	0.47
76:S2:528:A:H2'	76:S2:529:A:H8	1.79	0.47
76:S2:1189:A:H2'	76:S2:1190:A:C8	2.49	0.47
76:S2:1809:A:N6	86:S2:2016:HOH:O	2.46	0.47
23:SC:64:THR:OG1	23:SC:90:GLU:OE1	2.27	0.47
26:Sb:67:THR:HG22	26:Sb:69:GLY:H	1.79	0.47
29:LZ:72:VAL:HG22	29:LZ:111:ARG:HG3	1.95	0.47
39:LQ:13:VAL:HG12	72:L5:1691:G:H5''	1.97	0.47
40:LP:94:MET:HG2	40:LP:148:MET:SD	2.54	0.47
66:LA:101:VAL:HG22	66:LA:165:VAL:HG22	1.95	0.47
72:L5:3910:C:H2'	72:L5:3911:C:C6	2.48	0.47
11:SO:85:CYS:HB3	11:SO:90:ILE:HB	1.95	0.47
15:SJ:152:ASP:OD1	15:SJ:152:ASP:N	2.42	0.47
19:SE:116:PRO:O	19:SE:120:LYS:NZ	2.43	0.47
34:LU:39:PHE:O	34:LU:43:LEU:HD23	2.14	0.47
57:Lf:20:ASN:ND2	72:L5:1885:G:OP1	2.42	0.47
64:LB:252:ALA:HB3	72:L5:4457:PSU:H1'	1.95	0.47
66:LA:247:ARG:NH2	76:S2:1070:A:H5'	2.30	0.47
68:L7:24:C:O2	68:L7:117:G:N2	2.40	0.47
72:L5:1398:A:H62	72:L5:1419:G:H2'	1.78	0.47
72:L5:4680:G:H2'	72:L5:4681:A:C8	2.49	0.47
76:S2:1787:G:H2'	76:S2:1788:A:C8	2.50	0.47
16:SH:46:THR:HG21	16:SH:97:GLN:HG2	1.95	0.47
71:L8:19:C:H2'	71:L8:20:A:C8	2.48	0.47
76:S2:1084:A:OP1	76:S2:1858:G:O2'	2.28	0.47
76:S2:1630:A:OP1	80:SS:40:TYR:N	2.36	0.47
9:SR:129:LYS:HE2	76:S2:1125:C:OP1	2.15	0.47
34:LU:48:LYS:NZ	72:L5:2630:U:OP1	2.48	0.47
54:LG:117:ARG:NE	54:LG:128:VAL:O	2.48	0.47
64:LB:238:LYS:HE2	64:LB:238:LYS:HB2	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:LA:247:ARG:HB3	76:S2:1069:U:H4'	1.96	0.47
69:Pt:51:U:H3	69:Pt:65:G:H1	1.61	0.47
72:L5:417:G:OP1	72:L5:2329:U:O2'	2.30	0.47
72:L5:424:U:H2'	72:L5:425:U:H6	1.79	0.47
72:L5:3599:A:H2'	72:L5:3600:G:C8	2.50	0.47
72:L5:3770:PSU:H2'	72:L5:3771:C:C6	2.49	0.47
72:L5:3808:OMC:HM23	72:L5:3808:OMC:H1'	1.75	0.47
72:L5:4093:G:O2'	72:L5:4094:G:H8	1.98	0.47
76:S2:1277:C:H2'	76:S2:1278:A:H8	1.80	0.47
76:S2:1317:C:H2'	76:S2:1318:G:H8	1.79	0.47
18:SF:40:ALA:HB1	18:SF:45:TYR:CG	2.49	0.47
72:L5:1733:G:N3	72:L5:4214:A:H2'	2.29	0.47
72:L5:3656:A:H2'	72:L5:3657:U:H6	1.80	0.47
72:L5:3722:G:HO2'	72:L5:3723:A:H8	1.62	0.47
76:S2:185:G:H2'	76:S2:186:C:O4'	2.15	0.47
76:S2:1533:A:H2	76:S2:1536:G:N3	2.13	0.47
76:S2:1609:C:H3'	80:SS:132:ARG:HH12	1.79	0.47
10:SQ:32:ILE:HG21	10:SQ:39:LEU:HD22	1.97	0.47
21:SD:157:MET:O	76:S2:1384:C:H5''	2.15	0.47
72:L5:93:G:H2'	72:L5:94:A:C8	2.50	0.47
72:L5:653:U:H2'	72:L5:654:C:C6	2.49	0.47
72:L5:1563:A:H2'	72:L5:1564:A:C8	2.50	0.47
72:L5:1662:C:H2'	72:L5:1663:C:H6	1.79	0.47
72:L5:3736:A:H2'	72:L5:3737:A:H8	1.78	0.47
72:L5:3923:A:H2'	72:L5:3924:C:C6	2.50	0.47
76:S2:51:U:H2'	76:S2:52:G:H8	1.78	0.47
76:S2:996:A:H2'	76:S2:997:A:C8	2.49	0.47
76:S2:1201:U:H2'	76:S2:1202:U:C6	2.50	0.47
76:S2:1798:C:H2'	76:S2:1799:G:O4'	2.15	0.47
77:SG:159:ARG:NH1	77:SG:171:THR:O	2.46	0.47
6:SW:42:MET:HE1	16:SH:146:VAL:HG12	1.97	0.47
54:LG:121:LYS:O	54:LG:126:GLY:N	2.48	0.47
72:L5:153:G:H2'	72:L5:154:G:H8	1.80	0.47
72:L5:1307:A:H2'	72:L5:1308:C:C6	2.48	0.47
72:L5:5053:U:O2'	72:L5:5054:C:OP1	2.33	0.47
73:SZ:69:THR:H	73:SZ:72:VAL:HG22	1.80	0.47
74:ST:60:THR:O	74:ST:64:LEU:HD22	2.15	0.47
35:LT:142:ARG:NH1	72:L5:1090:G:OP1	2.43	0.47
54:LG:33:GLU:O	72:L5:4128:A:O2'	2.28	0.47
66:LA:37[B]:ARG:CZ	72:L5:4088:C:H5''	2.44	0.47
72:L5:1399:G:O2'	72:L5:1400:G:OP1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:2407:G:OP2	72:L5:2407:G:N2	2.45	0.47
74:ST:56:ARG:O	74:ST:60:THR:OG1	2.31	0.47
76:S2:952:G:H2'	76:S2:953:C:C6	2.50	0.47
76:S2:1735:A:H2'	76:S2:1736:G:C8	2.49	0.47
78:SI:113:TYR:CD1	78:SI:121:LEU:HD12	2.49	0.47
12:SN:31:ASP:O	12:SN:35:GLU:HG2	2.14	0.47
48:LJ:12:MET:CE	68:L7:51:G:H21	2.28	0.47
60:LD:65:ALA:HB2	60:LD:74:ILE:HD13	1.97	0.47
72:L5:516:C:H2'	72:L5:517:C:C6	2.50	0.47
72:L5:3893:C:O2'	72:L5:4979:A:N1	2.47	0.47
72:L5:4088:C:H2'	72:L5:4089:G:H8	1.79	0.47
72:L5:4088:C:H2'	72:L5:4089:G:C8	2.50	0.47
72:L5:4619:U:H2'	72:L5:4620:OMU:H6	1.96	0.47
76:S2:97:U:H2'	76:S2:98:C:C6	2.50	0.47
76:S2:1521:C:N4	80:SS:137:LYS:HE2	2.29	0.47
78:SI:143:LYS:HA	78:SI:146:GLN:HB2	1.96	0.47
8:SU:80:PHE:HB3	22:Sd:52:PHE:HB3	1.97	0.46
36:LS:157:ARG:NH2	45:LM:55:MET:O	2.46	0.46
72:L5:651:C:H2'	72:L5:652:G:H8	1.79	0.46
72:L5:659:G:H2'	72:L5:660:A:C8	2.49	0.46
72:L5:1906:U:H2'	72:L5:1907:A:H8	1.80	0.46
72:L5:2029:A:H2'	72:L5:2030:A:C8	2.50	0.46
72:L5:3684:G:H2'	72:L5:3685:C:C6	2.50	0.46
72:L5:3893:C:H2'	72:L5:3894:A:C8	2.50	0.46
76:S2:1189:A:H2'	76:S2:1190:A:H8	1.80	0.46
76:S2:1393:G:H2'	76:S2:1394:G:C8	2.50	0.46
37:LR:25:ASP:HB3	37:LR:28:GLU:HB2	1.96	0.46
56:LF:50:ILE:HD11	56:LF:185:ILE:HG13	1.97	0.46
72:L5:106:A:H2'	72:L5:107:G:O4'	2.15	0.46
72:L5:256:G:H2'	72:L5:257:C:C6	2.50	0.46
76:S2:1030:A:H2'	76:S2:1031:A2M:H8	1.98	0.46
76:S2:1808:U:H2'	76:S2:1809:A:C8	2.50	0.46
78:SI:87:ASN:HB3	78:SI:90:LEU:HG	1.97	0.46
17:Sg:200:VAL:HA	17:Sg:207:CYS:HA	1.98	0.46
29:LZ:29:ILE:HG22	29:LZ:32:GLY:H	1.81	0.46
36:LS:113:MET:HE3	36:LS:113:MET:HB3	1.79	0.46
50:LI:203:ARG:NH2	68:L7:105:C:OP2	2.39	0.46
56:LF:200:ARG:NH1	56:LF:203:GLU:OE1	2.45	0.46
60:LD:75:VAL:O	60:LD:112:ARG:NH1	2.47	0.46
63:Lc:78:ASN:OD1	63:Lc:78:ASN:N	2.49	0.46
64:LB:223:THR:HG22	64:LB:338:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:1591:U:N3	72:L5:4555:U:OP1	2.37	0.46
72:L5:1669:A:H4'	72:L5:1685:G:N2	2.30	0.46
72:L5:4458:C:H2'	72:L5:4459:U:C6	2.50	0.46
72:L5:4922:C:H2'	72:L5:4923:C:C6	2.50	0.46
74:ST:47:PRO:HB3	76:S2:1540:G:H5'	1.98	0.46
76:S2:349:A:H2'	76:S2:350:C:C6	2.50	0.46
78:SI:57:ALA:HB2	78:SI:183:GLY:HA2	1.96	0.46
16:SH:78:ARG:NH1	16:SH:82:GLU:OE1	2.42	0.46
23:SC:60:TRP:O	23:SC:71:LYS:NZ	2.40	0.46
26:Sb:19:HIS:HB3	26:Sb:22:LYS:HG3	1.97	0.46
30:LY:59:ARG:HG3	30:LY:103:LYS:HD2	1.97	0.46
31:LX:93:ASN:OD1	72:L5:2532:C:O2'	2.33	0.46
62:LC:103:ALA:HA	72:L5:1517:G:H22	1.80	0.46
64:LB:354:GLN:HB3	64:LB:359:ALA:HB1	1.97	0.46
72:L5:2809:G:O2'	72:L5:4644:G:OP1	2.28	0.46
72:L5:4523:A2M:H5''	72:L5:4524:G:H5'	1.98	0.46
76:S2:377:G:H5'	78:SI:98:LYS:HB3	1.96	0.46
76:S2:553:U:H2'	76:S2:554:A:H8	1.78	0.46
76:S2:1204:A:O2'	76:S2:1700:C:OP2	2.31	0.46
11:SO:31:CYS:HB2	11:SO:93:LEU:HD13	1.96	0.46
18:SF:107:ASN:OD1	18:SF:110:GLN:N	2.46	0.46
23:SC:207:ALA:HB2	76:S2:4:C:H4'	1.97	0.46
46:LL:63:THR:HG22	46:LL:65:ARG:H	1.81	0.46
55:Lg:60:ARG:HD2	55:Lg:60:ARG:HA	1.67	0.46
62:LC:242:PRO:HB2	72:L5:2297:G:H4'	1.98	0.46
64:LB:195:ASP:O	64:LB:199:GLU:HG2	2.15	0.46
66:LA:245:ARG:HG2	72:L5:3747:A:C8	2.50	0.46
72:L5:171:U:H4'	72:L5:172:C:H5'	1.97	0.46
72:L5:1195:G:H2'	72:L5:1196:G:C8	2.51	0.46
72:L5:1195:G:H2'	72:L5:1196:G:H8	1.79	0.46
72:L5:2894:A:H2'	72:L5:2895:A:C8	2.50	0.46
72:L5:5017:G:H4'	78:SI:92:ARG:HD3	1.98	0.46
22:Sd:27:ARG:CZ	22:Sd:27:ARG:HB3	2.45	0.46
29:LZ:88:ASP:OD1	29:LZ:121:ARG:NH1	2.43	0.46
35:LT:137:GLU:N	35:LT:137:GLU:OE2	2.46	0.46
40:LP:140:MET:HE3	40:LP:140:MET:HB3	1.88	0.46
43:LN:178:HIS:ND1	72:L5:68:U:OP1	2.36	0.46
54:LG:192:ARG:HH21	72:L5:5:A:H1'	1.80	0.46
56:LF:155:TYR:CE1	62:LC:325:MET:HE1	2.51	0.46
72:L5:1564:A:H2'	72:L5:1565:A:C8	2.50	0.46
72:L5:1704:C:O2'	72:L5:1706:A:OP2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:2884:G:H2'	72:L5:2885:A:C8	2.50	0.46
72:L5:3805:U:H2'	72:L5:3806:G:H8	1.81	0.46
76:S2:116:OMU:O5'	76:S2:116:OMU:H6	2.15	0.46
19:SE:43:PRO:HD2	19:SE:46:ILE:HD12	1.97	0.46
27:SA:44:ASP:OD1	27:SA:44:ASP:N	2.49	0.46
37:LR:4:LEU:HB2	72:L5:2386:U:H5'	1.97	0.46
37:LR:76:MET:HE2	37:LR:76:MET:HB3	1.79	0.46
58:LE:178:PRO:HD2	58:LE:181:LEU:HD12	1.97	0.46
60:LD:179:ARG:HA	60:LD:179:ARG:HD3	1.73	0.46
64:LB:90:VAL:HB	64:LB:104:THR:HG23	1.98	0.46
68:L7:4:U:H2'	68:L7:5:A:H8	1.81	0.46
72:L5:1446:C:H2'	72:L5:1447:C:O4'	2.16	0.46
72:L5:3707:U:H2'	72:L5:3708:C:C6	2.50	0.46
72:L5:3727:A:H2'	72:L5:3728:A:C8	2.51	0.46
72:L5:3785:A2M:H8	72:L5:3785:A2M:H2'	1.58	0.46
76:S2:1230:C:OP1	80:SS:130:ARG:NH2	2.49	0.46
60:LD:265:ARG:NE	60:LD:267:ASN:O	2.48	0.46
70:Sa:55:GLU:N	70:Sa:55:GLU:OE2	2.48	0.46
72:L5:980:U:H2'	72:L5:981:C:C6	2.51	0.46
72:L5:1514:U:H2'	72:L5:1515:A:H8	1.81	0.46
72:L5:2765:A:H2'	72:L5:2766:A:C8	2.50	0.46
72:L5:3710:G:O2'	72:L5:3713:U:O4	2.33	0.46
72:L5:4353:PSU:H5'	72:L5:4354:U:H5'	1.97	0.46
72:L5:4934:A:H2'	72:L5:4935:C:C6	2.50	0.46
76:S2:182:C:H2'	76:S2:183:G:C8	2.51	0.46
76:S2:880:G:O6	76:S2:906:U:O4	2.34	0.46
78:SI:103:LEU:HD13	78:SI:170:LYS:HD3	1.97	0.46
16:SH:106:ARG:O	76:S2:798:G:O2'	2.34	0.46
55:Lg:82:MET:HG2	55:Lg:87:VAL:HG23	1.98	0.46
72:L5:259:C:H1'	72:L5:260:C:H5	1.80	0.46
72:L5:2498:C:H2'	72:L5:2499:C:H6	1.81	0.46
72:L5:4237:C:H2'	72:L5:4238:G:H8	1.81	0.46
76:S2:1203:G:H2'	76:S2:1204:A:C8	2.51	0.46
39:LQ:79:THR:HG23	39:LQ:136:THR:HG22	1.97	0.46
42:LO:168:TYR:OH	72:L5:4768:G:OP1	2.26	0.46
76:S2:1395:C:H1'	76:S2:1474:A:C4	2.52	0.46
29:LZ:11:VAL:HG12	29:LZ:82:PRO:HA	1.98	0.45
33:LV:92:ASP:OD1	33:LV:92:ASP:N	2.34	0.45
43:LN:24:ARG:NH1	72:L5:3938:G:H5''	2.31	0.45
62:LC:269:LYS:HB3	62:LC:269:LYS:HE3	1.77	0.45
66:LA:107:MET:HB3	66:LA:111:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:985:C:H2'	72:L5:986:C:H6	1.81	0.45
72:L5:2434:G:O2'	72:L5:2527:A:N1	2.49	0.45
72:L5:2556:G:H2'	72:L5:2557:G:H8	1.81	0.45
76:S2:321:U:H5	76:S2:330:G:H1	1.62	0.45
76:S2:1037:G:H4'	76:S2:1845:A:H4'	1.97	0.45
15:SJ:33:GLY:HA3	20:Se:112:TYR:CG	2.51	0.45
35:LT:153:PRO:HB2	36:LS:127:MET:HG2	1.97	0.45
42:LO:81:TRP:HB2	42:LO:104:VAL:HG21	1.98	0.45
49:Lj:22:CYS:SG	49:Lj:24:SER:OG	2.63	0.45
62:LC:53:ALA:O	71:L8:26:C:O2'	2.32	0.45
72:L5:456:C:H2'	72:L5:457:G:H8	1.81	0.45
72:L5:659:G:O2'	72:L5:660:A:O4'	2.19	0.45
72:L5:1333:A:H2'	72:L5:1334:A:H8	1.81	0.45
72:L5:3916:G:H2'	72:L5:3917:A:C8	2.51	0.45
72:L5:4934:A:H2'	72:L5:4935:C:H6	1.81	0.45
76:S2:455:A:H2'	76:S2:456:C:C6	2.50	0.45
80:SS:89:ASP:HB3	80:SS:93:GLY:HA2	1.98	0.45
4:SY:86:GLU:OE1	4:SY:90:ARG:NH1	2.44	0.45
17:Sg:67:SER:H	17:Sg:82:SER:HA	1.81	0.45
19:SE:112:HIS:NE2	19:SE:237:SER:O	2.47	0.45
19:SE:124:CYS:HB3	19:SE:141:THR:HB	1.98	0.45
33:LV:91:LYS:HA	33:LV:91:LYS:HD2	1.70	0.45
34:LU:18:VAL:HG12	34:LU:75:GLU:HA	1.97	0.45
34:LU:80:LYS:NZ	72:L5:2621:A:OP1	2.42	0.45
48:LJ:155:HIS:HB2	68:L7:55:A:H4'	1.98	0.45
50:LI:114:GLY:HA2	72:L5:4441:A:H5''	1.98	0.45
56:LF:247:MET:HE2	56:LF:247:MET:HB3	1.81	0.45
72:L5:2362:U:H2'	72:L5:2363:A2M:H8	1.98	0.45
72:L5:3848:U:H2'	72:L5:3849:A:H8	1.81	0.45
76:S2:115:U:H2'	76:S2:116:OMU:C6	2.46	0.45
76:S2:797:C:H2'	76:S2:798:G:C4	2.50	0.45
76:S2:1337:4AC:H2'	76:S2:1338:G:C8	2.52	0.45
76:S2:1845:A:H2'	76:S2:1846:G:H8	1.81	0.45
10:SQ:17:LYS:HE3	76:S2:1648:G:N7	2.31	0.45
16:SH:20:GLU:H	16:SH:20:GLU:CD	2.23	0.45
23:SC:169:TYR:CG	23:SC:173:LYS:HA	2.51	0.45
29:LZ:95:VAL:HG23	29:LZ:96:VAL:HG23	1.98	0.45
49:Lj:27:TYR:HA	49:Lj:34:CYS:HA	1.99	0.45
53:Lh:117:ARG:HD2	53:Lh:117:ARG:HA	1.74	0.45
55:Lg:17:SER:OG	72:L5:2514:G:OP1	2.31	0.45
64:LB:56:ILE:HD13	64:LB:365:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Pt:33:OMC:HM23	69:Pt:33:OMC:H1'	1.80	0.45
76:S2:29:G:H2'	76:S2:30:C:C6	2.52	0.45
76:S2:1457:U:H3	76:S2:1469:A:H62	1.63	0.45
30:LY:10:ASP:HB3	30:LY:13:LYS:HB2	1.98	0.45
40:LP:74:LYS:NZ	72:L5:4982:A:OP1	2.38	0.45
46:LL:207:VAL:HG13	46:LL:210:LYS:HZ1	1.81	0.45
50:LI:38:ARG:NH1	50:LI:45:GLU:OE1	2.44	0.45
64:LB:213:GLN:NE2	64:LB:285:TYR:O	2.38	0.45
72:L5:2412:A:H2'	72:L5:2413:U:C6	2.52	0.45
76:S2:1317:C:H2'	76:S2:1318:G:C8	2.51	0.45
76:S2:1521:C:H2'	80:SS:136:THR:HG22	1.99	0.45
43:LN:144:ARG:NH2	72:L5:125:C:OP2	2.49	0.45
50:LI:152:LEU:HB3	50:LI:165:ILE:HD12	1.97	0.45
67:La:79:TRP:CE3	67:La:87:ARG:HG3	2.51	0.45
72:L5:1705:G:H2'	72:L5:1706:A:C8	2.52	0.45
72:L5:1927:U:OP1	72:L5:1949:U:O2'	2.33	0.45
72:L5:4258:C:H2'	72:L5:4259:C:H6	1.81	0.45
76:S2:382:C:H2'	76:S2:383:G:H8	1.81	0.45
78:SI:26:LYS:HG3	78:SI:29:LEU:HD23	1.99	0.45
6:SW:83:LEU:HD23	6:SW:83:LEU:HA	1.85	0.45
30:LY:54:GLU:HG3	30:LY:108:ARG:HB3	1.99	0.45
33:LV:41:SER:HG	72:L5:4507:A:HO2'	1.60	0.45
34:LU:35:ASP:OD1	34:LU:38:ASN:N	2.32	0.45
60:LD:7:VAL:HG23	60:LD:8:LYS:HG3	1.99	0.45
65:Lb:57:MET:CE	72:L5:1811:G:H21	2.30	0.45
68:L7:110:G:H2'	68:L7:111:C:C6	2.52	0.45
72:L5:457:G:H2'	72:L5:458:C:H6	1.82	0.45
72:L5:1086:C:H2'	72:L5:1087:A:C8	2.51	0.45
72:L5:1278:C:H2'	72:L5:1279:A:O4'	2.17	0.45
72:L5:1345:A:H2'	72:L5:1346:C:C6	2.51	0.45
72:L5:2582:A:C8	72:L5:2654:C:H1'	2.52	0.45
72:L5:3880:G:H2'	72:L5:3881:G:C8	2.52	0.45
75:SP:33:LEU:HD13	75:SP:86:LEU:HD12	1.99	0.45
76:S2:454:U:H2'	76:S2:455:A:H8	1.82	0.45
3:Lo:36:GLN:HG2	72:L5:4363:A:H5''	1.99	0.45
18:SF:168:THR:HG22	18:SF:170:ALA:H	1.81	0.45
34:LU:46:ARG:HH22	34:LU:89:LYS:HE2	1.81	0.45
37:LR:164:SER:HA	37:LR:167:LYS:HZ1	1.81	0.45
40:LP:64:ASN:ND2	40:LP:80:GLN:OE1	2.48	0.45
49:Lj:73:ARG:NH2	53:Lh:87:LYS:O	2.50	0.45
50:LI:133:GLN:NE2	72:L5:1785:C:OP1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:LG:245:LYS:NZ	72:L5:4165:C:OP1	2.50	0.45
63:Lc:32:LYS:HG3	72:L5:2675:G:N7	2.32	0.45
64:LB:322:HIS:O	64:LB:342:LYS:HE3	2.17	0.45
72:L5:691:C:H2'	72:L5:692:A:C8	2.52	0.45
72:L5:3917:A:H2'	72:L5:3918:G:C8	2.50	0.45
72:L5:4065:G:H2'	72:L5:4066:U:C6	2.52	0.45
72:L5:4090:G:H22	72:L5:4159:C:H5	1.63	0.45
76:S2:1628:C:H2'	76:S2:1629:C:C6	2.51	0.45
15:SJ:137:VAL:HG12	15:SJ:138:ARG:HG3	1.98	0.45
30:LY:74:TYR:OH	71:L8:75:OMG:OP2	2.34	0.45
40:LP:125:MET:HE3	40:LP:143:PRO:HG3	1.97	0.45
56:LF:35:LYS:NZ	72:L5:2099:G:OP2	2.32	0.45
58:LE:150:LEU:HD11	58:LE:164:PHE:HB2	1.99	0.45
72:L5:318:A:H2'	72:L5:319:A:H8	1.82	0.45
72:L5:424:U:H2'	72:L5:425:U:C6	2.52	0.45
72:L5:963:G:N2	86:L5:5366:HOH:O	2.50	0.45
72:L5:4584:A:H2'	72:L5:4585:U:O4'	2.17	0.45
9:SR:104:GLU:O	9:SR:108:LEU:HD12	2.16	0.45
12:SN:53:ILE:HD13	12:SN:53:ILE:HA	1.84	0.45
16:SH:20:GLU:HB3	16:SH:48:ALA:HB3	1.99	0.45
19:SE:134:LYS:N	76:S2:298:G:OP1	2.37	0.45
25:SB:114:VAL:O	76:S2:1869:A:N6	2.50	0.45
34:LU:40:GLU:OE2	34:LU:65:ARG:HB2	2.17	0.45
42:LO:87:MET:SD	72:L5:1912:G:N2	2.90	0.45
43:LN:202:ARG:HG2	62:LC:112:HIS:CE1	2.52	0.45
66:LA:109:GLU:HG2	66:LA:138:SER:HA	1.99	0.45
72:L5:1262:G:H2'	72:L5:1263:A:C8	2.51	0.45
76:S2:1033:G:N1	76:S2:1080:A:O2'	2.31	0.45
76:S2:1272:C:H2'	76:S2:1273:C:C6	2.52	0.45
76:S2:1528:G:H2'	76:S2:1529:C:C6	2.52	0.45
19:SE:122:LYS:NZ	19:SE:143:ASP:OD2	2.45	0.44
38:Lr:92:SER:O	38:Lr:96:MET:HG3	2.17	0.44
48:LJ:52:LYS:HA	48:LJ:67:LYS:HA	1.98	0.44
56:LF:151:ASN:ND2	72:L5:943:A:N7	2.61	0.44
64:LB:69:LYS:HA	64:LB:69:LYS:HD3	1.72	0.44
71:L8:17:A:N6	72:L5:417:G:O2'	2.50	0.44
72:L5:1317:U:H2'	72:L5:1318:C:C6	2.51	0.44
72:L5:4389:C:H2'	72:L5:4390:A:C8	2.52	0.44
76:S2:535:G:H2'	76:S2:536:A:H8	1.82	0.44
76:S2:964:A:H2'	76:S2:965:U:H6	1.82	0.44
76:S2:1171:G:O2'	76:S2:1187:G:O6	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S2:1623:A:H62	80:SS:132:ARG:HE	1.65	0.44
44:Ln:10:MET:HE2	76:S2:1172:U:H4'	1.98	0.44
47:Lk:9:LYS:O	47:Lk:13:LEU:HG	2.16	0.44
71:L8:147:G:H2'	71:L8:148:A:H8	1.82	0.44
72:L5:220:C:H5	72:L5:237:G:H1	1.64	0.44
72:L5:1460:C:H2'	72:L5:1461:C:H6	1.83	0.44
72:L5:3855:C:H2'	72:L5:3856:A:H8	1.82	0.44
76:S2:1567:G:H2'	76:S2:1568:C:C6	2.52	0.44
79:S6:63:A:H2'	79:S6:64:U:C6	2.52	0.44
3:Lo:37:GLY:HA3	72:L5:4342:C:O3'	2.17	0.44
12:SN:53:ILE:HD13	26:Sb:52:THR:HG21	2.00	0.44
15:SJ:88:ASP:OD1	15:SJ:89:GLU:N	2.50	0.44
22:Sd:34:TYR:OH	76:S2:1549:U:OP1	2.28	0.44
25:SB:168:MET:O	25:SB:172:MET:HG3	2.18	0.44
31:LX:114:LYS:HE3	31:LX:114:LYS:HB3	1.70	0.44
37:LR:31:GLU:H	37:LR:31:GLU:CD	2.26	0.44
37:LR:108:ARG:NH2	72:L5:2899:C:OP1	2.50	0.44
49:Lj:67:LEU:HD23	49:Lj:67:LEU:HA	1.88	0.44
53:Lh:103:LYS:HG2	53:Lh:107:GLN:HG2	1.98	0.44
56:LF:76:ARG:NE	72:L5:730:G:OP2	2.44	0.44
58:LE:153:LEU:HD21	58:LE:195:ILE:HD12	1.99	0.44
59:Le:128:ARG:NH1	72:L5:2306:G:OP1	2.51	0.44
72:L5:300:A:H2'	72:L5:301:G:C8	2.52	0.44
72:L5:711:A:H2'	72:L5:712:C:C6	2.53	0.44
72:L5:1100:U:H2'	72:L5:1101:C:C6	2.53	0.44
72:L5:1749:A:H2'	72:L5:1750:G:C8	2.52	0.44
72:L5:4862:G:H2'	72:L5:4863:G:H8	1.81	0.44
72:L5:4959:U:H2'	72:L5:4960:G:C8	2.52	0.44
73:SZ:85:ARG:HH22	76:S2:1596:U:H3'	1.82	0.44
76:S2:1265:A:O2'	76:S2:1327:G:OP2	2.22	0.44
76:S2:1523:C:H2'	76:S2:1524:G:H8	1.82	0.44
79:S6:39:C:N3	79:S6:40:C:N4	2.66	0.44
15:SJ:149:VAL:HG11	15:SJ:157:ILE:HD11	1.99	0.44
27:SA:122:LEU:HD23	27:SA:144:THR:HG22	1.99	0.44
29:LZ:30:ASP:O	29:LZ:39:SER:OG	2.27	0.44
36:LS:53:LYS:NZ	68:L7:74:A:O2'	2.39	0.44
48:LJ:164:ARG:NH2	48:LJ:168:GLN:HG3	2.31	0.44
62:LC:15:GLY:O	62:LC:16:GLU:HG2	2.18	0.44
66:LA:54:ARG:HG2	66:LA:56:ALA:H	1.82	0.44
69:Pt:54:G:H2'	69:Pt:55:U:C6	2.53	0.44
71:L8:5:U:H2'	71:L8:6:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:942:G:H21	72:L5:945:U:H5''	1.82	0.44
72:L5:1244:G:H2'	72:L5:1245:C:H6	1.82	0.44
72:L5:1483:C:H4'	72:L5:1484:G:O5'	2.17	0.44
72:L5:2476:G:H2'	72:L5:2477:A:C8	2.52	0.44
72:L5:2543:A:H2	72:L5:2773:G:H22	1.66	0.44
74:ST:40:ALA:HB3	74:ST:43:LYS:HG2	2.00	0.44
80:SS:125:HIS:ND1	80:SS:131:VAL:HG11	2.32	0.44
16:SH:69:LEU:HD22	16:SH:96:ALA:HB2	1.98	0.44
31:LX:64:SER:OG	53:Lh:82:ASP:OD2	2.26	0.44
43:LN:124:ASP:OD2	43:LN:126:THR:N	2.47	0.44
72:L5:1472:C:H2'	72:L5:1473:U:C6	2.53	0.44
72:L5:4273:A:H2'	72:L5:4274:A:C8	2.53	0.44
76:S2:1004:PSU:H2'	76:S2:1005:G:H8	1.82	0.44
77:SG:218:LYS:HB2	77:SG:218:LYS:HE2	1.65	0.44
35:LT:39:ILE:HG22	35:LT:99:SER:HB3	2.00	0.44
36:LS:71:SER:O	36:LS:76:LYS:NZ	2.50	0.44
64:LB:128:LYS:O	64:LB:131:THR:OG1	2.33	0.44
72:L5:433:A:C2	72:L5:3867:A2M:H4'	2.53	0.44
76:S2:563:G:O2'	76:S2:564:A:H8	2.00	0.44
76:S2:1670:C:H2'	76:S2:1671:G:C8	2.53	0.44
77:SG:201:LYS:HB3	77:SG:201:LYS:HE3	1.73	0.44
80:SS:85:ASN:N	80:SS:97:GLN:OE1	2.42	0.44
80:SS:106:LYS:HD3	80:SS:106:LYS:HA	1.86	0.44
7:SV:17:CYS:HB2	7:SV:56:CYS:HB3	1.99	0.44
29:LZ:54:THR:HG23	29:LZ:57:MET:HE3	1.99	0.44
62:LC:178:ASN:OD1	72:L5:2300:A:N6	2.50	0.44
67:La:27:LYS:HB3	67:La:27:LYS:HE2	1.78	0.44
72:L5:138:G:H2'	72:L5:139:G:C8	2.52	0.44
72:L5:1088:C:H2'	72:L5:1089:G:H8	1.83	0.44
72:L5:1340:OMC:HM23	72:L5:1340:OMC:H1'	1.84	0.44
72:L5:1367:C:O2'	72:L5:1369:C:OP2	2.35	0.44
72:L5:1399:G:H2'	72:L5:1400:G:C8	2.52	0.44
72:L5:4467:A:O2'	72:L5:4510:A:N3	2.44	0.44
23:SC:102:LEU:HD23	23:SC:102:LEU:HA	1.87	0.44
41:Lp:7:LYS:O	41:Lp:27:LYS:NZ	2.51	0.44
46:LL:164:GLU:HB3	67:La:100:ILE:HD13	2.00	0.44
62:LC:80:ARG:NH2	72:L5:1645:C:OP1	2.50	0.44
72:L5:4174:U:H2'	72:L5:4175:G:C8	2.51	0.44
72:L5:4692:A:H62	72:L5:4696:C:H5	1.65	0.44
76:S2:1113:A:H2'	76:S2:1114:U:C6	2.52	0.44
9:SR:86:PRO:O	27:SA:198:MET:HE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LY:87:ARG:NH2	72:L5:405:U:OP1	2.50	0.44
37:LR:105:LEU:HD23	37:LR:138:LEU:HD23	1.99	0.44
49:Lj:20:ARG:NH2	71:L8:109:C:O2'	2.50	0.44
72:L5:650:C:H2'	72:L5:651:C:H6	1.83	0.44
72:L5:717:U:H2'	72:L5:718:C:C6	2.52	0.44
72:L5:2094:G:H2'	72:L5:2095:A:C8	2.53	0.44
74:ST:93:SER:OG	74:ST:94:ARG:N	2.51	0.44
76:S2:1118:C:H2'	76:S2:1119:A:C8	2.53	0.44
9:SR:50:ILE:O	9:SR:54:VAL:HG23	2.17	0.43
21:SD:190:LEU:HB2	21:SD:200:PRO:HD3	2.00	0.43
27:SA:37:TYR:OH	27:SA:57:LYS:NZ	2.51	0.43
34:LU:62:THR:OG1	34:LU:73:THR:OG1	2.36	0.43
60:LD:53:VAL:HG11	60:LD:159:VAL:HA	2.00	0.43
72:L5:4237:C:H2'	72:L5:4238:G:C8	2.53	0.43
76:S2:106:C:H2'	76:S2:107:A:C8	2.52	0.43
76:S2:203:G:OP2	78:SI:143:LYS:NZ	2.43	0.43
76:S2:1277:C:H2'	76:S2:1278:A:C8	2.52	0.43
77:SG:48:TYR:OH	77:SG:116:LYS:NZ	2.51	0.43
7:SV:3:ASN:HD21	7:SV:7:GLU:HB2	1.84	0.43
20:Se:100:LYS:NZ	76:S2:591:U:OP1	2.29	0.43
27:SA:77:ILE:HG12	27:SA:99:ILE:HB	2.00	0.43
41:Lp:26:VAL:HG13	66:LA:178:PRO:HG2	2.00	0.43
48:LJ:128:LEU:HD23	48:LJ:128:LEU:HA	1.85	0.43
52:LH:177:ASP:OD1	52:LH:177:ASP:N	2.51	0.43
72:L5:501:C:O2'	72:L5:502:C:O2	2.28	0.43
72:L5:2517:A:N3	72:L5:2539:C:O2'	2.50	0.43
72:L5:4389:C:H2'	72:L5:4390:A:H8	1.83	0.43
72:L5:4978:G:H2'	72:L5:4979:A:H5''	2.00	0.43
76:S2:1025:U:OP1	76:S2:1090:C:O2'	2.36	0.43
76:S2:1714:U:H2'	76:S2:1715:A:C8	2.53	0.43
78:SI:3:ILE:O	78:SI:30:GLY:N	2.40	0.43
79:S6:10:G:H1'	79:S6:45:G:H2'	2.00	0.43
5:SX:130:LEU:HD23	5:SX:130:LEU:HA	1.87	0.43
10:SQ:76:GLY:H	10:SQ:79:ALA:HB3	1.83	0.43
18:SF:60:ARG:HH11	76:S2:1679:A:H2'	1.83	0.43
22:Sd:27:ARG:HH11	76:S2:1263:U:H4'	1.83	0.43
29:LZ:112:ARG:NH1	72:L5:2573:A:O2'	2.51	0.43
50:LI:86:HIS:HB3	50:LI:139:ARG:HG2	2.00	0.43
55:Lg:66:ARG:HD2	72:L5:2539:C:H5''	1.99	0.43
72:L5:220:C:H5	72:L5:237:G:H22	1.65	0.43
72:L5:318:A:H2'	72:L5:319:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:3823:G:OP2	72:L5:3823:G:N2	2.33	0.43
72:L5:3948:C:H2'	72:L5:3949:A:H8	1.83	0.43
72:L5:4746:C:H2'	72:L5:4747:C:H6	1.83	0.43
76:S2:102:A:H4'	76:S2:104:A:C8	2.53	0.43
76:S2:1199:A:H2'	76:S2:1200:A:C8	2.53	0.43
76:S2:1446:A:O2'	76:S2:1447:OMG:O5'	2.35	0.43
76:S2:1740:C:H2'	76:S2:1741:U:C6	2.54	0.43
18:SF:190:ILE:HD12	18:SF:193:LYS:HD3	2.01	0.43
33:LV:19:GLY:O	72:L5:2846:G:O2'	2.27	0.43
38:Lr:98:ARG:NH2	72:L5:2262:G:OP2	2.34	0.43
54:LG:157:ILE:HB	54:LG:183:ILE:HD13	1.99	0.43
58:LE:66:LYS:HD3	72:L5:979:C:OP2	2.19	0.43
60:LD:117:LYS:HB2	60:LD:117:LYS:HE3	1.75	0.43
72:L5:1346:C:H2'	72:L5:1347:G:H8	1.84	0.43
72:L5:1811:G:H2'	72:L5:1812:C:C6	2.53	0.43
72:L5:3861:A:H2'	72:L5:3862:A:H8	1.83	0.43
76:S2:65:C:H4'	77:SG:172:LYS:HE3	2.00	0.43
76:S2:212:C:H2'	76:S2:213:G:C8	2.53	0.43
76:S2:1010:G:H2'	76:S2:1011:A:C8	2.53	0.43
76:S2:1245:G:O2'	76:S2:1492:U:OP1	2.29	0.43
76:S2:1375:G:H2'	76:S2:1376:A:C8	2.54	0.43
15:SJ:131:ARG:HA	15:SJ:131:ARG:HD2	1.80	0.43
17:Sg:56:GLN:HG3	17:Sg:57:ARG:H	1.83	0.43
18:SF:50:PRO:HB3	18:SF:69:VAL:HG12	1.99	0.43
72:L5:4344:U:H2'	72:L5:4345:C:C6	2.54	0.43
72:L5:4589:A:N1	72:L5:4621:C:O2'	2.43	0.43
76:S2:118:C:H1'	76:S2:445:A:C5	2.52	0.43
76:S2:168:C:O2'	77:SG:133:LEU:O	2.35	0.43
76:S2:1217:A:H2'	76:S2:1218:C:H6	1.83	0.43
76:S2:1244:PSU:H2'	76:S2:1245:G:C8	2.53	0.43
79:S6:58:A:O2'	79:S6:60:A:OP2	2.26	0.43
30:LY:31:SER:HA	30:LY:48:PRO:HA	2.00	0.43
32:LW:54:LEU:HD23	32:LW:54:LEU:HA	1.86	0.43
35:LT:100:LYS:HB3	35:LT:100:LYS:HE2	1.87	0.43
42:LO:170:LYS:HE3	42:LO:170:LYS:HB3	1.79	0.43
47:Lk:33:LYS:HG2	47:Lk:46:VAL:HG22	2.01	0.43
49:Lj:24:SER:H	49:Lj:24:SER:HG	1.60	0.43
50:LI:198:LYS:HB2	50:LI:198:LYS:HE3	1.89	0.43
56:LF:166:ARG:NH2	86:LF:301:HOH:O	2.51	0.43
62:LC:327:LYS:NZ	72:L5:974:C:O2	2.51	0.43
71:L8:66:A:H2'	71:L8:67:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:1494:U:H2'	72:L5:1495:G:H8	1.84	0.43
72:L5:4208:U:OP1	72:L5:4334:U:O2'	2.32	0.43
72:L5:4578:G:H2'	72:L5:4579:PSU:H6	1.82	0.43
75:SP:78:THR:HA	76:S2:1298:G:H4'	2.01	0.43
76:S2:436:OMG:OP2	76:S2:471:G:O2'	2.35	0.43
25:SB:139:CYS:SG	25:SB:168:MET:HE2	2.58	0.43
27:SA:41:ARG:HD3	27:SA:47:TYR:CZ	2.54	0.43
36:LS:154:LEU:HB3	36:LS:157:ARG:HD3	2.00	0.43
40:LP:96:LYS:HE3	40:LP:96:LYS:HB2	1.87	0.43
46:LL:18:TRP:NE1	72:L5:1516:G:O2'	2.40	0.43
48:LJ:164:ARG:O	48:LJ:164:ARG:NE	2.51	0.43
50:LI:181:PHE:O	50:LI:185:VAL:HG23	2.18	0.43
67:La:36:GLY:HA3	67:La:40:HIS:CE1	2.54	0.43
71:L8:8:U:H2'	71:L8:9:A:C8	2.53	0.43
76:S2:1230:C:H2'	76:S2:1231:C:C6	2.54	0.43
76:S2:1620:A:H4'	76:S2:1621:U:H5	1.84	0.43
78:SI:105:ASP:CG	78:SI:107:THR:HG1	2.26	0.43
16:SH:66:VAL:HG22	16:SH:96:ALA:HB1	2.00	0.43
40:LP:85:LYS:HB2	40:LP:85:LYS:HE3	1.78	0.43
42:LO:125:LYS:HE2	42:LO:125:LYS:HB3	1.85	0.43
43:LN:20:ARG:HH21	43:LN:24:ARG:NH2	2.17	0.43
51:Li:76:ARG:HD3	51:Li:76:ARG:HA	1.78	0.43
54:LG:99:ALA:HB1	54:LG:136:LEU:HD11	2.01	0.43
62:LC:150:LEU:HD23	62:LC:150:LEU:HA	1.89	0.43
71:L8:106:G:H4'	71:L8:137:A:H5'	2.01	0.43
72:L5:268:G:H2'	72:L5:269:G:C8	2.53	0.43
72:L5:674:G:H2'	72:L5:675:C:C6	2.54	0.43
72:L5:1244:G:H2'	72:L5:1245:C:C6	2.53	0.43
72:L5:2865:U:O2'	72:L5:2866:C:H5'	2.18	0.43
76:S2:902:G:H2'	76:S2:903:A:C8	2.53	0.43
76:S2:1374:C:H2'	76:S2:1375:G:O4'	2.18	0.43
77:SG:20:ASP:OD1	77:SG:22:ARG:HG2	2.19	0.43
78:SI:74:ARG:HA	78:SI:74:ARG:HD3	1.76	0.43
78:SI:121:LEU:HD21	78:SI:158:ILE:HD11	2.00	0.43
15:SJ:67:ASP:HB3	15:SJ:70:ARG:HB3	2.01	0.43
17:Sg:240:CYS:O	17:Sg:249:CYS:N	2.49	0.43
23:SC:66:LEU:HD11	23:SC:81:ILE:HG12	2.00	0.43
48:LJ:154:LYS:NZ	68:L7:19:C:OP2	2.42	0.43
72:L5:4392:OMG:N3	72:L5:4447:5MC:HM52	2.33	0.43
72:L5:4734:A:H2'	72:L5:4735:G:H8	1.83	0.43
79:S6:64:U:H2'	79:S6:65:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SV:51:LYS:HD2	7:SV:76:ASP:OD2	2.19	0.43
35:LT:132:PRO:HB2	56:LF:126:ASN:HB2	2.01	0.43
40:LP:148:MET:HE2	40:LP:148:MET:HB3	1.83	0.43
45:LM:127:VAL:O	45:LM:131:GLN:HG3	2.19	0.43
48:LJ:147:ARG:HE	48:LJ:147:ARG:HB3	1.68	0.43
61:Ld:57:MET:HG2	61:Ld:88:LEU:HD23	2.01	0.43
66:LA:183:GLY:HA2	72:L5:1613:A:H5'	2.01	0.43
72:L5:456:C:H2'	72:L5:457:G:C8	2.54	0.43
72:L5:468:U:O2'	72:L5:686:A:N1	2.43	0.43
72:L5:1802:A:H5''	72:L5:1803:G:H5'	1.99	0.43
72:L5:2582:A:C2	72:L5:2583:C:H1'	2.54	0.43
72:L5:3823:G:H2'	72:L5:3824:A:C8	2.54	0.43
72:L5:4578:G:H2'	72:L5:4579:PSU:C6	2.54	0.43
72:L5:4935:C:H2'	72:L5:4936:G:C8	2.54	0.43
76:S2:1315:U:H2'	76:S2:1316:C:C6	2.54	0.43
76:S2:1417:C:H2'	76:S2:1418:C:C6	2.54	0.43
34:LU:28:PRO:HB2	34:LU:34:MET:HG2	1.99	0.42
57:Lf:50:VAL:HG22	57:Lf:69:VAL:HG22	2.00	0.42
66:LA:206:PRO:HG3	66:LA:213:GLY:HA3	2.01	0.42
72:L5:23:C:H2'	72:L5:24:G:O4'	2.19	0.42
72:L5:1316:OMG:HM23	72:L5:1316:OMG:H1'	1.90	0.42
72:L5:1472:C:H2'	72:L5:1473:U:H6	1.83	0.42
72:L5:1590:C:H4'	72:L5:2857:A:H5'	2.01	0.42
72:L5:2079:G:H2'	72:L5:2080:U:C6	2.54	0.42
72:L5:2765:A:H2'	72:L5:2766:A:H8	1.84	0.42
72:L5:2844:A:O2'	72:L5:4631:G:H4'	2.19	0.42
72:L5:4188:U:H2'	72:L5:4189:U:H6	1.84	0.42
76:S2:15:U:H2'	76:S2:16:G:O4'	2.19	0.42
76:S2:1673:U:H2'	76:S2:1674:G:O4'	2.19	0.42
76:S2:1740:C:H41	76:S2:1794:C:N4	2.17	0.42
4:SY:116:LYS:HG2	76:S2:161:U:H5'	2.01	0.42
12:SN:33:VAL:HG21	12:SN:66:VAL:HG11	2.01	0.42
18:SF:42:LYS:HA	18:SF:42:LYS:HD3	1.79	0.42
32:LW:44:ARG:NH2	72:L5:3615:G:O2'	2.52	0.42
36:LS:23:HIS:CD2	36:LS:23:HIS:N	2.87	0.42
37:LR:91:GLU:H	37:LR:91:GLU:HG3	1.66	0.42
53:Lh:4:ILE:HD13	53:Lh:4:ILE:HA	1.85	0.42
56:LF:95:ILE:O	56:LF:223:LYS:HE2	2.19	0.42
58:LE:245:GLN:NE2	58:LE:249:ASP:OD2	2.51	0.42
68:L7:63:C:H5'	68:L7:64:G:H5''	2.00	0.42
72:L5:223:G:H4'	72:L5:225:G:N7	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:323:C:H2'	72:L5:324:A:H8	1.84	0.42
72:L5:1617:G:H1'	72:L5:2513:A:N6	2.34	0.42
72:L5:2448:G:H2'	72:L5:2449:A:C8	2.54	0.42
72:L5:3664:G:H2'	72:L5:3665:G:C8	2.52	0.42
72:L5:3672:G:OP2	72:L5:3672:G:N2	2.47	0.42
72:L5:4536:OMC:HM22	72:L5:4537:C:O4'	2.18	0.42
76:S2:867:OMG:H1'	76:S2:867:OMG:HM23	1.75	0.42
76:S2:1731:A:H2'	76:S2:1732:G:C8	2.53	0.42
10:SQ:48:GLN:O	10:SQ:52:LEU:HD12	2.19	0.42
19:SE:100:ARG:HH12	19:SE:122:LYS:HA	1.84	0.42
46:LL:210:LYS:HB3	46:LL:210:LYS:HE3	1.73	0.42
64:LB:385:LYS:NZ	72:L5:5002:U:OP2	2.50	0.42
66:LA:117:GLU:O	66:LA:162:ASN:ND2	2.52	0.42
72:L5:490:C:H2'	72:L5:491:G:C8	2.54	0.42
72:L5:1245:C:H2'	72:L5:1246:G:H8	1.84	0.42
72:L5:4601:U:H2'	72:L5:4602:A:H8	1.83	0.42
76:S2:1248:B8N:O36	76:S2:1701:C:N4	2.44	0.42
76:S2:1616:U:O2'	76:S2:1661:A:N3	2.44	0.42
76:S2:1801:A:H2'	76:S2:1802:C:H6	1.84	0.42
78:SI:113:TYR:CG	78:SI:121:LEU:HD12	2.54	0.42
25:SB:214:LYS:HD3	25:SB:216:LYS:HD2	2.01	0.42
54:LG:122:ALA:HA	54:LG:126:GLY:HA2	2.00	0.42
54:LG:157:ILE:HA	54:LG:201:THR:HG22	2.02	0.42
62:LC:296:PRO:O	62:LC:300:ARG:HG3	2.19	0.42
68:L7:35:U:O2	68:L7:45:U:O2'	2.32	0.42
71:L8:154:G:H2'	71:L8:155:C:C6	2.54	0.42
72:L5:445:U:H2'	72:L5:446:C:O4'	2.20	0.42
72:L5:1471:U:H5	72:L5:1493:G:H1	1.67	0.42
72:L5:1677:PSU:H4'	72:L5:1680:G:C2	2.55	0.42
72:L5:3648:A:H1'	72:L5:3785:A2M:N6	2.33	0.42
76:S2:432:G:H2'	76:S2:433:A:C8	2.55	0.42
76:S2:639:C:H2'	76:S2:640:A:H8	1.84	0.42
76:S2:848:U:H2'	76:S2:849:A:H8	1.84	0.42
76:S2:1533:A:N7	76:S2:1604:G:H1'	2.33	0.42
4:SY:117:VAL:HG23	4:SY:122:LYS:HG2	2.00	0.42
16:SH:170:VAL:HG13	16:SH:187:PHE:HB2	2.00	0.42
17:Sg:67:SER:N	17:Sg:81:GLY:O	2.52	0.42
19:SE:143:ASP:HB3	19:SE:145:ARG:HG3	2.01	0.42
25:SB:181:LEU:HD12	25:SB:181:LEU:HA	1.93	0.42
45:LM:50:MET:HB2	45:LM:50:MET:HE3	1.82	0.42
52:LH:50:LYS:HD2	52:LH:50:LYS:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:LC:138:MET:HE3	62:LC:138:MET:HB3	1.83	0.42
62:LC:350:ARG:HD2	72:L5:724:C:OP1	2.20	0.42
69:Pt:63:C:H2'	69:Pt:64:G:H8	1.84	0.42
71:L8:19:C:H2'	71:L8:20:A:H8	1.85	0.42
72:L5:457:G:H2'	72:L5:458:C:C6	2.54	0.42
72:L5:651:C:H2'	72:L5:652:G:C8	2.54	0.42
72:L5:670:G:H2'	72:L5:671:G:C8	2.54	0.42
76:S2:659:G:O2'	76:S2:662:G:O2'	2.33	0.42
76:S2:1606:G:N2	76:S2:1632:G:H1'	2.34	0.42
76:S2:1856:C:H2'	76:S2:1857:G:C8	2.55	0.42
30:LY:32:SER:OG	30:LY:101:PRO:O	2.30	0.42
35:LT:87:LYS:HE3	35:LT:87:LYS:HB3	1.92	0.42
37:LR:21:LYS:NZ	72:L5:2822:G:OP2	2.53	0.42
46:LL:36:ARG:NH1	72:L5:1364:U:OP2	2.37	0.42
48:LJ:90:ARG:HD3	48:LJ:90:ARG:HA	1.89	0.42
48:LJ:109:ILE:HB	48:LJ:128:LEU:HB2	2.01	0.42
54:LG:249:ARG:HG3	54:LG:250:ILE:N	2.33	0.42
59:Le:127:ALA:HB2	72:L5:2326:G:H5''	2.01	0.42
66:LA:2:GLY:HA2	66:LA:207:VAL:HG23	2.02	0.42
66:LA:243:THR:HB	72:L5:3748:A:H5''	2.02	0.42
72:L5:411:G:H4'	72:L5:412:G:H5''	2.01	0.42
72:L5:934:C:H4'	72:L5:935:A:O5'	2.18	0.42
72:L5:2521:G:H2'	72:L5:2522:G:H8	1.84	0.42
72:L5:5003:U:H2'	72:L5:5004:C:C6	2.54	0.42
76:S2:65:C:C2	77:SG:133:LEU:HD22	2.55	0.42
76:S2:441:C:H2'	76:S2:442:C:C6	2.54	0.42
76:S2:644:OMG:H1'	76:S2:644:OMG:HM23	1.78	0.42
76:S2:796:G:H2'	76:S2:797:C:C6	2.54	0.42
76:S2:1445:PSU:O2	76:S2:1446:A:N6	2.52	0.42
4:SY:9:THR:HG23	4:SY:23:MET:HB2	2.01	0.42
5:SX:28:LYS:HE2	5:SX:32:LEU:HD22	2.00	0.42
7:SV:41:LYS:HE3	27:SA:5:LEU:HD22	2.02	0.42
9:SR:41:ILE:HD12	9:SR:42:PRO:HD2	2.00	0.42
25:SB:107:ARG:HA	25:SB:110[B]:MET:HE2	2.02	0.42
49:Lj:64:MET:HB3	49:Lj:64:MET:HE3	1.81	0.42
58:LE:46:ARG:HB2	58:LE:62:MET:HE1	2.00	0.42
62:LC:349:LEU:HD23	62:LC:349:LEU:HA	1.81	0.42
64:LB:54:THR:OG1	64:LB:55:HIS:N	2.53	0.42
68:L7:58:A:H2'	68:L7:59:G:H8	1.84	0.42
72:L5:123:C:H2'	72:L5:124:C:H6	1.85	0.42
72:L5:1248:C:H2'	72:L5:1249:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:2784:C:H2'	72:L5:2785:C:H6	1.85	0.42
72:L5:4651:A:H2'	72:L5:4652:G:O4'	2.19	0.42
76:S2:26:U:H2'	76:S2:27:A2M:H8	2.01	0.42
76:S2:85:A:H2'	76:S2:86:C:H6	1.84	0.42
76:S2:495:U:H2'	76:S2:496:C:O4'	2.19	0.42
76:S2:1390:U:H2'	76:S2:1391:OMC:C6	2.54	0.42
76:S2:1550:G:O2'	76:S2:1558:C:O2	2.24	0.42
22:Sd:26:ASN:HB3	22:Sd:39:CYS:SG	2.60	0.42
25:SB:57:ILE:HG22	25:SB:59:SER:H	1.84	0.42
25:SB:88:THR:HA	25:SB:98:THR:HA	2.02	0.42
50:LI:54:SER:HB2	50:LI:135:ILE:HD11	2.00	0.42
52:LH:4:ILE:HG12	52:LH:61:TRP:CH2	2.54	0.42
63:Lc:22:MET:HG3	63:Lc:85:CYS:O	2.20	0.42
68:L7:58:A:H2'	68:L7:59:G:C8	2.55	0.42
72:L5:278:G:H5'	72:L5:329:A:N6	2.34	0.42
72:L5:2376:A:H2'	72:L5:2377:C:C6	2.54	0.42
72:L5:3933:G:H2'	72:L5:3934:G:H8	1.85	0.42
76:S2:804:U:H2'	76:S2:805:U:C6	2.55	0.42
3:Lo:106:PHE:HA	69:Pt:20:G:C4	2.54	0.42
25:SB:144:LYS:HG3	25:SB:208:HIS:HB3	2.02	0.42
46:LL:130:LYS:HG2	46:LL:133:ALA:H	1.84	0.42
48:LJ:99:PHE:HB2	48:LJ:159:LYS:NZ	2.32	0.42
51:Li:16:LYS:HD3	51:Li:16:LYS:HA	1.89	0.42
54:LG:48:LYS:HA	54:LG:48:LYS:HD3	1.89	0.42
57:Lf:106:TYR:HB2	57:Lf:107:PRO:HD3	2.02	0.42
64:LB:21:ARG:NH2	72:L5:4981:G:O6	2.53	0.42
72:L5:369:G:N2	72:L5:372:A:OP2	2.45	0.42
72:L5:2094:G:N2	72:L5:2095:A:O2'	2.53	0.42
72:L5:2588:C:H5''	72:L5:2589:C:H5''	2.01	0.42
72:L5:2621:A:H2'	72:L5:2622:G:C8	2.54	0.42
72:L5:2743:A:H2'	72:L5:2744:A:C8	2.55	0.42
72:L5:3783:A:O5'	72:L5:3784:A:H5'	2.19	0.42
76:S2:527:C:H2'	76:S2:528:A:C8	2.54	0.42
76:S2:1240:A:N3	76:S2:1267:C:O2'	2.45	0.42
35:LT:148:PRO:HB2	36:LS:29:ARG:HB2	2.02	0.42
36:LS:69:GLU:OE1	36:LS:76:LYS:HE3	2.20	0.42
50:LI:208:LYS:HE3	50:LI:208:LYS:HB3	1.82	0.42
53:Lh:52:LYS:HA	53:Lh:52:LYS:HD3	1.68	0.42
53:Lh:109:ARG:HE	53:Lh:109:ARG:HB3	1.73	0.42
58:LE:69:TYR:CD1	58:LE:70:LYS:HG3	2.54	0.42
71:L8:6:C:H2'	71:L8:7:U:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:L8:144:U:H2'	71:L8:145:C:H6	1.84	0.42
72:L5:1177:U:H2'	72:L5:1178:G:C8	2.54	0.42
72:L5:3816:A:O2'	72:L5:3819:G:N3	2.50	0.42
72:L5:4519:C:H5''	72:L5:4520:G:H5''	2.02	0.42
72:L5:4593:C:H2'	72:L5:4594:U:H6	1.83	0.42
72:L5:4704:C:H2'	72:L5:4705:A:C8	2.55	0.42
75:SP:94:VAL:HG11	75:SP:116:LEU:HD11	2.01	0.42
76:S2:668:A2M:H8	76:S2:668:A2M:H2'	1.71	0.42
76:S2:1407:U:H1'	76:S2:1442:U:H3	1.85	0.42
6:SW:88:LYS:NZ	76:S2:420:G:OP1	2.53	0.41
11:SO:19:PRO:HG3	11:SO:27:VAL:HG11	2.02	0.41
32:LW:2:LYS:HD2	32:LW:2:LYS:HA	1.74	0.41
32:LW:8:PHE:HZ	32:LW:49:ILE:HG13	1.84	0.41
40:LP:83:TRP:O	72:L5:3856:A:H5''	2.20	0.41
54:LG:244:PRO:HA	54:LG:247:VAL:HG22	2.02	0.41
55:Lg:83:CYS:SG	55:Lg:86:CYS:HB2	2.61	0.41
60:LD:52:ILE:HD13	68:L7:6:C:H4'	2.01	0.41
61:Ld:92:ARG:HA	61:Ld:102:LEU:HD23	2.01	0.41
68:L7:2:U:H2'	68:L7:3:C:C6	2.55	0.41
72:L5:396:A:H2'	72:L5:397:G:C8	2.55	0.41
72:L5:2335:C:H2'	72:L5:2336:G:H8	1.85	0.41
72:L5:3711:A:H5'	72:L5:3712:A:N7	2.35	0.41
72:L5:4406:U:C2	72:L5:4407:G:C8	3.08	0.41
76:S2:1633:A:H2'	76:S2:1634:A:H8	1.85	0.41
76:S2:1713:C:H2'	76:S2:1714:U:C6	2.55	0.41
79:S6:63:A:H2'	79:S6:64:U:H6	1.84	0.41
2:Ll:29:MET:HE3	2:Ll:29:MET:HB3	1.98	0.41
9:SR:14:ARG:O	9:SR:18:GLU:HG3	2.19	0.41
10:SQ:27:ARG:HA	10:SQ:66:VAL:HG22	2.02	0.41
13:SL:136:LYS:HB2	76:S2:385:G:H3'	2.03	0.41
33:LV:87:SER:HA	33:LV:97:TYR:HB3	2.02	0.41
41:Lp:36:LYS:HD3	41:Lp:48:LYS:HB3	2.02	0.41
72:L5:490:C:H2'	72:L5:491:G:H8	1.85	0.41
72:L5:1088:C:H2'	72:L5:1089:G:C8	2.55	0.41
72:L5:1741:G:N3	72:L5:1781:PSU:H5''	2.35	0.41
72:L5:1847:C:H2'	72:L5:1848:C:C6	2.54	0.41
72:L5:2424:OMG:H1'	72:L5:2424:OMG:HM23	1.86	0.41
72:L5:3672:G:H2'	72:L5:3673:C:C6	2.55	0.41
72:L5:4138:C:H2'	72:L5:4139:G:C8	2.56	0.41
72:L5:4458:C:H2'	72:L5:4459:U:H6	1.85	0.41
72:L5:4951:G:H3'	72:L5:4952:G:H21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S2:155:G:H4'	77:SG:15:LEU:HD13	2.00	0.41
78:SI:66:SER:HA	78:SI:73:THR:HA	2.02	0.41
9:SR:99:ASP:OD1	9:SR:99:ASP:N	2.53	0.41
16:SH:143:ARG:HB2	16:SH:155:LYS:HB2	2.03	0.41
23:SC:142:LYS:HB2	23:SC:157:LEU:HD12	2.02	0.41
39:LQ:14:ARG:HG3	39:LQ:16:LYS:HE3	2.02	0.41
41:Lp:84:ARG:HG2	41:Lp:84:ARG:NH1	2.35	0.41
44:Ln:1:MET:HE1	44:Ln:9:ARG:CZ	2.51	0.41
49:Lj:49:TRP:O	72:L5:1646:A:O2'	2.35	0.41
59:Le:56:PRO:HB3	72:L5:2319:C:O2'	2.20	0.41
72:L5:272:U:H2'	72:L5:273:U:C6	2.55	0.41
72:L5:655:C:H2'	72:L5:656:C:C6	2.55	0.41
72:L5:2824:OMC:H1'	72:L5:2824:OMC:HM23	1.68	0.41
72:L5:3944:G:H2'	72:L5:3945:A:C8	2.55	0.41
76:S2:468:A2M:H1'	76:S2:468:A2M:HM'3	1.90	0.41
76:S2:534:G:H1	76:S2:552:G:H1	1.67	0.41
76:S2:1810:U:H2'	76:S2:1811:C:C6	2.55	0.41
18:SF:144:LEU:HG	18:SF:148:ASN:HD21	1.85	0.41
33:LV:21:PRO:HA	33:LV:54:ALA:HA	2.01	0.41
33:LV:107:ASN:ND2	33:LV:111:GLU:OE1	2.52	0.41
41:Lp:84:ARG:O	41:Lp:88:GLU:HG2	2.20	0.41
43:LN:26:ARG:NH2	54:LG:165:GLU:OE1	2.33	0.41
52:LH:129:ARG:NE	52:LH:156:ASN:OD1	2.49	0.41
55:Lg:19:LYS:HD3	55:Lg:19:LYS:HA	1.79	0.41
57:Lf:43:LEU:O	57:Lf:109:ARG:NH1	2.53	0.41
60:LD:255:LYS:HE3	60:LD:255:LYS:HB3	1.92	0.41
64:LB:224:LYS:HG2	64:LB:340:THR:HG22	2.02	0.41
64:LB:228:TYR:O	72:L5:2835:A:O2'	2.35	0.41
65:Lb:43:MET:HE2	72:L5:1826:G:H4'	2.02	0.41
67:La:76:ASP:OD1	67:La:76:ASP:N	2.37	0.41
69:Pt:39:A:O2'	76:S2:1058:A:OP1	2.34	0.41
71:L8:6:C:H2'	71:L8:7:U:H6	1.85	0.41
71:L8:28:C:O2'	72:L5:1371:A:N1	2.49	0.41
72:L5:653:U:H2'	72:L5:654:C:H6	1.84	0.41
72:L5:1399:G:OP2	72:L5:1399:G:H8	2.03	0.41
76:S2:943:U:C2	76:S2:944:A:C8	3.08	0.41
76:S2:1093:A:H2'	76:S2:1094:C:C6	2.56	0.41
76:S2:1539:U:H2'	76:S2:1540:G:C8	2.56	0.41
2:Ll:10:LYS:NZ	72:L5:2782:U:OP2	2.48	0.41
6:SW:80:ASP:OD1	6:SW:124:LYS:NZ	2.39	0.41
8:SU:59:LYS:HZ3	8:SU:59:LYS:HG3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SB:155:TYR:OH	76:S2:989:C:OP2	2.28	0.41
29:LZ:73:LYS:HD3	29:LZ:75:TYR:CZ	2.55	0.41
34:LU:89:LYS:HB3	34:LU:89:LYS:HE3	1.88	0.41
42:LO:78:ARG:HA	42:LO:78:ARG:HD2	1.91	0.41
43:LN:56:LYS:NZ	72:L5:153:G:OP1	2.53	0.41
58:LE:60:SER:HB2	72:L5:1239:C:H5	1.85	0.41
60:LD:158:LYS:NZ	68:L7:47:G:OP2	2.49	0.41
72:L5:667:A:H2'	72:L5:668:C:C6	2.55	0.41
72:L5:739:G:H2'	72:L5:740:G:C8	2.55	0.41
72:L5:1186:U:H2'	72:L5:1187:G:N3	2.36	0.41
72:L5:1252:C:O2'	72:L5:1254:A:N6	2.52	0.41
72:L5:2610:G:H2'	72:L5:2611:A:C8	2.55	0.41
72:L5:2864:A:H2'	72:L5:2865:U:H6	1.84	0.41
74:ST:91:HIS:NE2	76:S2:1665:G:OP1	2.52	0.41
76:S2:27:A2M:HM'3	76:S2:27:A2M:H1'	1.87	0.41
76:S2:96:C:O2	76:S2:473:A:O2'	2.36	0.41
76:S2:1579:A:O2'	76:S2:1581:C:OP2	2.33	0.41
76:S2:1633:A:H2'	76:S2:1634:A:C8	2.55	0.41
5:SX:64:SER:OG	76:S2:615:C:OP2	2.32	0.41
27:SA:89:LYS:HD3	27:SA:89:LYS:HA	1.91	0.41
40:LP:94:MET:HE3	40:LP:94:MET:HB2	1.76	0.41
59:Le:32:LYS:HB2	59:Le:32:LYS:HE2	1.69	0.41
60:LD:60:ILE:HB	60:LD:80:ALA:HB2	2.02	0.41
63:Lc:103:ASP:OD1	63:Lc:103:ASP:N	2.52	0.41
64:LB:43:LEU:HD12	64:LB:205:VAL:HG11	2.02	0.41
65:Lb:106:LYS:HB3	65:Lb:106:LYS:HE3	1.75	0.41
72:L5:35:U:H4'	72:L5:1525:A:C2	2.56	0.41
72:L5:167:C:O2'	72:L5:168:C:H5'	2.21	0.41
72:L5:1645:C:H2'	72:L5:1646:A:C8	2.55	0.41
72:L5:4522:G:O2'	72:L5:4525:C:OP2	2.24	0.41
74:ST:88:MET:HE1	76:S2:1665:G:C5	2.55	0.41
76:S2:509:OMG:HM23	76:S2:509:OMG:H1'	1.87	0.41
76:S2:639:C:H2'	76:S2:640:A:C8	2.56	0.41
7:SV:35:ASN:ND2	7:SV:52:THR:HG23	2.36	0.41
15:SJ:107:GLU:HA	15:SJ:112:THR:HG21	2.03	0.41
16:SH:37:LYS:O	16:SH:41:ARG:HG2	2.20	0.41
36:LS:161:ARG:HG2	36:LS:164:LYS:HB3	2.02	0.41
39:LQ:39:THR:HG21	39:LQ:132:LYS:HG2	2.01	0.41
39:LQ:108:ARG:NH2	72:L5:1355:G:OP1	2.49	0.41
40:LP:33:ALA:HB1	40:LP:117:ILE:HG12	2.02	0.41
48:LJ:48:PRO:HB3	48:LJ:72:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:LG:111:LYS:HE2	54:LG:111:LYS:HB3	1.82	0.41
68:L7:23:A:H2'	68:L7:24:C:C6	2.56	0.41
71:L8:92:U:H2'	71:L8:93:C:O4'	2.21	0.41
72:L5:979:C:H2'	72:L5:980:U:O2	2.21	0.41
72:L5:3911:C:H2'	72:L5:3912:U:H6	1.85	0.41
72:L5:4563:U:H2'	72:L5:4564:A:C8	2.51	0.41
76:S2:162:C:H5''	77:SG:87:ARG:HH22	1.85	0.41
76:S2:1004:PSU:H2'	76:S2:1005:G:C8	2.56	0.41
76:S2:1223:A:H2'	76:S2:1224:G:O4'	2.20	0.41
76:S2:1324:G:O2'	76:S2:1510:G:O2'	2.32	0.41
76:S2:1383:A2M:H1'	76:S2:1383:A2M:HM'3	1.87	0.41
76:S2:1408:U:H2'	76:S2:1409:A:H8	1.84	0.41
76:S2:1560:U:O2'	76:S2:1583:C:O2'	2.31	0.41
76:S2:1727:G:H2'	76:S2:1728:U:C6	2.54	0.41
2:L1:34:ILE:HD12	2:L1:34:ILE:HA	1.97	0.41
9:SR:53:TYR:O	9:SR:57:LEU:HD12	2.20	0.41
22:Sd:53:ILE:HD13	22:Sd:53:ILE:HA	1.91	0.41
23:SC:196:ILE:HB	23:SC:223:TYR:HB2	2.03	0.41
25:SB:120:MET:HE1	76:S2:987:A:C6	2.56	0.41
27:SA:132:GLN:NE2	27:SA:136:GLU:OE1	2.50	0.41
39:LQ:76:GLU:CD	39:LQ:76:GLU:H	2.29	0.41
43:LN:125:SER:HB3	72:L5:3937:C:H1'	2.02	0.41
43:LN:203:TYR:HB2	72:L5:1359:G:H4'	2.01	0.41
45:LM:108:ASP:OD1	45:LM:108:ASP:N	2.53	0.41
50:LI:206:LEU:HD23	50:LI:206:LEU:HA	1.82	0.41
54:LG:43:GLN:NE2	72:L5:4116:C:O2'	2.38	0.41
60:LD:99:TYR:HE2	60:LD:164:LYS:HG3	1.85	0.41
68:L7:4:U:H2'	68:L7:5:A:C8	2.56	0.41
69:Pt:21:H2U:OP2	69:Pt:21:H2U:H61	2.21	0.41
71:L8:67:U:H2'	71:L8:68:G:C8	2.56	0.41
72:L5:288:G:H2'	72:L5:289:C:C6	2.56	0.41
72:L5:732:A:H2'	72:L5:733:A:O4'	2.21	0.41
72:L5:1866:U:H2'	72:L5:1867:A:O4'	2.21	0.41
76:S2:535:G:H2'	76:S2:536:A:C8	2.55	0.41
76:S2:949:G:H2'	76:S2:950:C:C6	2.55	0.41
76:S2:1278:A:H2'	76:S2:1279:C:C6	2.56	0.41
76:S2:1365:G:H2'	76:S2:1366:G:H8	1.85	0.41
76:S2:1598:G:OP1	80:SS:55:ARG:NH2	2.51	0.41
4:SY:108:LYS:HZ2	4:SY:108:LYS:HG2	1.78	0.41
18:SF:74:ASN:HA	18:SF:77:MET:HE2	2.03	0.41
19:SE:148:ARG:NH2	77:SG:202:ASN:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:SE:186:GLY:HA3	76:S2:809:A:OP1	2.21	0.41
26:Sb:69:GLY:HA3	76:S2:1105:G:O3'	2.21	0.41
27:SA:94:THR:O	27:SA:186:ARG:NH2	2.49	0.41
28:mR:35:A:H1'	76:S2:1063:C:O2	2.21	0.41
37:LR:116:ASP:OD2	37:LR:118:HIS:ND1	2.48	0.41
37:LR:152:LYS:HD3	37:LR:152:LYS:HA	1.79	0.41
46:LL:181:SER:HB3	51:Li:7:MET:HE1	2.02	0.41
54:LG:131:LYS:HD3	54:LG:132:ARG:O	2.21	0.41
58:LE:141:ARG:NH1	58:LE:191:GLN:O	2.53	0.41
60:LD:83:LEU:HB3	60:LD:88:VAL:HB	2.02	0.41
67:La:13:GLY:HA2	72:L5:1660:U:H3'	2.01	0.41
67:La:26:ARG:NH1	72:L5:1655:C:OP2	2.51	0.41
71:L8:75:OMG:HM23	71:L8:75:OMG:H1'	1.73	0.41
72:L5:1075:G:H2'	72:L5:1076:C:C6	2.56	0.41
72:L5:2529:A:O2'	72:L5:2531:C:OP2	2.39	0.41
72:L5:2610:G:H2'	72:L5:2611:A:H8	1.86	0.41
72:L5:4115:G:H5''	72:L5:4116:C:C5	2.55	0.41
76:S2:191:A:H62	76:S2:208:G:H21	1.69	0.41
76:S2:388:U:H2'	76:S2:389:A:C8	2.56	0.41
76:S2:433:A:H2'	76:S2:434:G:C8	2.56	0.41
76:S2:1025:U:H2'	76:S2:1026:C:O4'	2.20	0.41
29:LZ:10:VAL:HG23	29:LZ:86:SER:HA	2.03	0.41
35:LT:83:LYS:HE3	35:LT:83:LYS:HB2	1.88	0.41
38:Lr:65:LYS:O	38:Lr:102:TYR:OH	2.34	0.41
49:Lj:59:THR:HG23	71:L8:41:A:H4'	2.03	0.41
53:Lh:14:LYS:HE3	53:Lh:61:ILE:HG23	2.02	0.41
59:Le:35:TRP:CH2	59:Le:55:MET:HG2	2.56	0.41
72:L5:465:G:H2'	72:L5:466:A:C8	2.56	0.41
72:L5:650:C:H2'	72:L5:651:C:C6	2.55	0.41
72:L5:1500:A:H5''	72:L5:1501:C:H5'	2.02	0.41
72:L5:1867:A:H2'	72:L5:1868:A:C8	2.56	0.41
72:L5:2295:C:H2'	72:L5:2296:G:H8	1.86	0.41
72:L5:3944:G:H2'	72:L5:3945:A:H8	1.85	0.41
72:L5:5004:C:H2'	72:L5:5005:G:O4'	2.21	0.41
76:S2:300:U:H2'	76:S2:301:A:C8	2.56	0.41
76:S2:454:U:H2'	76:S2:455:A:C8	2.56	0.41
76:S2:799:U:H2'	76:S2:800:U:C6	2.56	0.41
76:S2:1398:G:H22	76:S2:1448:A:H2	1.69	0.41
5:SX:9:THR:HG22	76:S2:681:PSU:H4'	2.02	0.40
5:SX:14:ARG:HG3	13:SL:99:TYR:HE2	1.86	0.40
6:SW:51:GLU:HG2	26:Sb:8:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SQ:30:GLY:HA3	10:SQ:65:GLY:H	1.86	0.40
12:SN:54:LEU:HB3	12:SN:60:VAL:HG13	2.03	0.40
12:SN:124:ARG:NH2	76:S2:1024:A:OP2	2.45	0.40
13:SL:75:GLY:HA3	13:SL:88:ILE:HD12	2.03	0.40
25:SB:134:LEU:HG	25:SB:218:LEU:HD12	2.03	0.40
39:LQ:172:ARG:NH1	67:La:56:VAL:O	2.49	0.40
43:LN:178:HIS:HA	43:LN:181:HIS:NE2	2.36	0.40
54:LG:120:LYS:HB2	54:LG:120:LYS:HE2	1.91	0.40
66:LA:244:GLY:HA3	72:L5:3746:A:H5''	2.03	0.40
68:L7:24:C:H2'	68:L7:25:G:O4'	2.20	0.40
71:L8:40:A:H2'	71:L8:41:A:C8	2.56	0.40
72:L5:1100:U:H2'	72:L5:1101:C:H6	1.86	0.40
72:L5:3861:A:H2'	72:L5:3862:A:C8	2.55	0.40
72:L5:4439:U:H2'	72:L5:4440:G:O4'	2.21	0.40
72:L5:4605:A:H2'	72:L5:4606:G:O4'	2.21	0.40
76:S2:65:C:C6	77:SG:174:PRO:HB3	2.56	0.40
76:S2:1204:A:H2'	76:S2:1205:C:C6	2.56	0.40
3:Lo:6:LYS:NZ	3:Lo:93:LEU:O	2.55	0.40
5:SX:3:LYS:NZ	76:S2:663:C:OP2	2.48	0.40
9:SR:13:ALA:O	9:SR:17:ILE:HG13	2.22	0.40
18:SF:166:ILE:HG13	76:S2:1599:U:C5	2.56	0.40
39:LQ:65:ARG:NH1	72:L5:1459:A:OP1	2.54	0.40
40:LP:54:GLN:HA	40:LP:83:TRP:CD1	2.56	0.40
52:LH:140:GLN:OE1	52:LH:141:LYS:N	2.54	0.40
60:LD:99:TYR:OH	60:LD:168:ASP:OD2	2.37	0.40
64:LB:128:LYS:HG3	72:L5:4966:A:H5''	2.02	0.40
68:L7:3:C:H2'	68:L7:4:U:C6	2.56	0.40
72:L5:488:G:H8	72:L5:488:G:O5'	2.04	0.40
72:L5:1173:G:H2'	72:L5:1174:G:C8	2.56	0.40
72:L5:3848:U:H2'	72:L5:3849:A:C8	2.56	0.40
72:L5:4478:G:O2'	72:L5:4602:A:N1	2.48	0.40
76:S2:300:U:H2'	76:S2:301:A:H8	1.85	0.40
76:S2:909:G:H3'	76:S2:910:G:N2	2.36	0.40
76:S2:1511:U:H2'	76:S2:1512:C:C6	2.57	0.40
79:S6:62:C:H2'	79:S6:63:A:H8	1.86	0.40
8:SU:64:THR:HG22	8:SU:77:TRP:HE3	1.87	0.40
9:SR:16:ILE:HG22	9:SR:24:LEU:HD11	2.02	0.40
9:SR:116:ASN:OD1	9:SR:116:ASN:N	2.52	0.40
11:SO:55:ARG:HE	11:SO:55:ARG:HB3	1.67	0.40
18:SF:60:ARG:HH12	76:S2:1679:A:P	2.43	0.40
18:SF:167:LYS:HA	73:SZ:71:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LY:85:VAL:HG12	30:LY:97:VAL:HB	2.03	0.40
53:Lh:87:LYS:HA	53:Lh:87:LYS:HD2	1.90	0.40
54:LG:40:GLY:HA3	72:L5:4116:C:H1'	2.03	0.40
62:LC:237:ILE:HD12	62:LC:237:ILE:HA	1.96	0.40
62:LC:321:ASN:OD1	72:L5:1280:C:O2'	2.29	0.40
65:Lb:7:HIS:HB3	72:L5:4219:A:H5''	2.03	0.40
72:L5:462:G:H2'	72:L5:463:A:C8	2.56	0.40
72:L5:1857:C:H2'	72:L5:1858:A:C8	2.56	0.40
72:L5:1963:C:C2	72:L5:1964:A:C8	3.09	0.40
72:L5:1967:A:H2'	72:L5:1968:G:O4'	2.21	0.40
72:L5:2079:G:H2'	72:L5:2080:U:H6	1.86	0.40
72:L5:4192:A:H2'	72:L5:4193:C:H6	1.85	0.40
72:L5:4538:G:H2'	72:L5:4539:U:C6	2.56	0.40
72:L5:5030:U:H2'	72:L5:5031:G:C8	2.57	0.40
76:S2:5:U:H2'	76:S2:6:G:C8	2.56	0.40
76:S2:352:U:H2'	76:S2:353:C:C6	2.57	0.40
11:SO:147:ARG:HA	70:Sa:28:ARG:NH1	2.36	0.40
25:SB:86:LEU:HB3	25:SB:98:THR:HB	2.03	0.40
45:LM:121:ARG:HE	45:LM:121:ARG:HB2	1.78	0.40
52:LH:142:ASP:N	52:LH:142:ASP:OD1	2.54	0.40
62:LC:63:SER:O	62:LC:63:SER:OG	2.39	0.40
64:LB:338:VAL:HA	72:L5:4625:C:H5'	2.03	0.40
65:Lb:115:GLY:HA2	72:L5:1241:C:C6	2.57	0.40
71:L8:24:G:H1'	72:L5:360:A:C4	2.57	0.40
71:L8:126:C:N4	72:L5:2543:A:O3'	2.44	0.40
72:L5:2292:C:H2'	72:L5:2293:U:C6	2.56	0.40
72:L5:2570:U:H2'	72:L5:2571:C:C6	2.57	0.40
72:L5:2890:C:H2'	72:L5:2891:U:C6	2.56	0.40
72:L5:4670:C:O2'	72:L5:4672:A:OP2	2.31	0.40
76:S2:1365:G:H2'	76:S2:1366:G:C8	2.56	0.40
78:SI:48:VAL:HG11	78:SI:54:LYS:HD2	2.03	0.40
78:SI:81:VAL:HG22	78:SI:102:VAL:HG12	2.04	0.40
34:LU:43:LEU:O	34:LU:47:ILE:HG13	2.22	0.40
59:Le:58:ILE:HD12	59:Le:58:ILE:HA	1.93	0.40
60:LD:64:ILE:HG13	60:LD:109:LEU:HD22	2.02	0.40
72:L5:25:A:H2'	72:L5:26:C:H6	1.86	0.40
72:L5:65:A:N6	72:L5:75:G:H1'	2.37	0.40
72:L5:212:A:H2'	72:L5:213:G:H8	1.86	0.40
72:L5:286:U:H2'	72:L5:287:U:C6	2.56	0.40
72:L5:1205:G:H2'	72:L5:1206:C:H6	1.87	0.40
72:L5:1447:C:H2'	72:L5:1448:G:C8	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:L5:3867:A2M:H1'	72:L5:3867:A2M:HM'3	1.90	0.40
72:L5:4620:OMU:H1'	72:L5:4620:OMU:HM23	1.81	0.40
72:L5:4887:C:H2'	72:L5:4888:U:O4'	2.21	0.40
74:ST:72:VAL:HG11	74:ST:101:ARG:HG3	2.02	0.40
74:ST:101:ARG:NH2	76:S2:1566:G:N7	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Lm	49/128 (38%)	49 (100%)	0	0	100	100
2	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
3	Lo	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
4	SY	121/133 (91%)	117 (97%)	4 (3%)	0	100	100
5	SX	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
6	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
7	SV	81/83 (98%)	81 (100%)	0	0	100	100
8	SU	56/119 (47%)	52 (93%)	4 (7%)	0	100	100
9	SR	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
10	SQ	137/146 (94%)	127 (93%)	10 (7%)	0	100	100
11	SO	133/151 (88%)	125 (94%)	8 (6%)	0	100	100
12	SN	148/151 (98%)	148 (100%)	0	0	100	100
13	SL	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
14	SK	70/165 (42%)	66 (94%)	4 (6%)	0	100	100
15	SJ	176/194 (91%)	174 (99%)	2 (1%)	0	100	100
16	SH	187/194 (96%)	180 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Sg	221/317 (70%)	181 (82%)	40 (18%)	0	100	100
18	SF	181/204 (89%)	173 (96%)	8 (4%)	0	100	100
19	SE	258/263 (98%)	254 (98%)	4 (2%)	0	100	100
20	Se	47/133 (35%)	46 (98%)	1 (2%)	0	100	100
21	SD	165/243 (68%)	159 (96%)	6 (4%)	0	100	100
22	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
23	SC	218/293 (74%)	213 (98%)	5 (2%)	0	100	100
24	Sc	59/69 (86%)	56 (95%)	3 (5%)	0	100	100
25	SB	211/264 (80%)	209 (99%)	2 (1%)	0	100	100
26	Sb	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
27	SA	213/295 (72%)	208 (98%)	5 (2%)	0	100	100
29	LZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
30	LY	131/145 (90%)	128 (98%)	3 (2%)	0	100	100
31	LX	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
32	LW	60/157 (38%)	60 (100%)	0	0	100	100
33	LV	130/140 (93%)	129 (99%)	1 (1%)	0	100	100
34	LU	97/128 (76%)	93 (96%)	4 (4%)	0	100	100
35	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
36	LS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
37	LR	179/196 (91%)	178 (99%)	1 (1%)	0	100	100
38	Lr	120/138 (87%)	118 (98%)	2 (2%)	0	100	100
39	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
40	LP	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
41	Lp	88/92 (96%)	84 (96%)	4 (4%)	0	100	100
42	LO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
43	LN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
44	Ln	22/25 (88%)	22 (100%)	0	0	100	100
45	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
46	LL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
47	Lk	67/70 (96%)	67 (100%)	0	0	100	100
48	LJ	167/178 (94%)	164 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Lj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
50	LI	199/214 (93%)	196 (98%)	3 (2%)	0	100	100
51	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
52	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
53	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
54	LG	226/266 (85%)	219 (97%)	7 (3%)	0	100	100
55	Lg	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
56	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
57	Lf	107/111 (96%)	106 (99%)	1 (1%)	0	100	100
58	LE	214/288 (74%)	201 (94%)	13 (6%)	0	100	100
59	Le	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
60	LD	290/297 (98%)	284 (98%)	6 (2%)	0	100	100
61	Ld	104/125 (83%)	101 (97%)	3 (3%)	0	100	100
62	LC	357/427 (84%)	348 (98%)	9 (2%)	0	100	100
63	Lc	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
64	LB	394/397 (99%)	391 (99%)	3 (1%)	0	100	100
65	Lb	96/159 (60%)	91 (95%)	5 (5%)	0	100	100
66	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
67	La	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
70	Sa	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
73	SZ	61/125 (49%)	59 (97%)	2 (3%)	0	100	100
74	ST	125/145 (86%)	122 (98%)	3 (2%)	0	100	100
75	SP	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
77	SG	216/249 (87%)	209 (97%)	7 (3%)	0	100	100
78	SI	204/208 (98%)	202 (99%)	2 (1%)	0	100	100
80	SS	136/152 (90%)	128 (94%)	8 (6%)	0	100	100
All	All	10651/12429 (86%)	10356 (97%)	295 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Lm	43/116 (37%)	43 (100%)	0	100	100
2	Ll	45/48 (94%)	45 (100%)	0	100	100
3	Lo	82/93 (88%)	82 (100%)	0	100	100
4	SY	73/115 (64%)	72 (99%)	1 (1%)	59	85
5	SX	101/115 (88%)	100 (99%)	1 (1%)	68	89
6	SW	109/113 (96%)	107 (98%)	2 (2%)	51	80
7	SV	63/67 (94%)	63 (100%)	0	100	100
8	SU	37/107 (35%)	37 (100%)	0	100	100
9	SR	83/122 (68%)	75 (90%)	8 (10%)	8	26
10	SQ	65/121 (54%)	65 (100%)	0	100	100
11	SO	96/119 (81%)	89 (93%)	7 (7%)	13	38
12	SN	125/131 (95%)	124 (99%)	1 (1%)	73	90
13	SL	127/142 (89%)	127 (100%)	0	100	100
14	SK	25/136 (18%)	25 (100%)	0	100	100
15	SJ	145/168 (86%)	145 (100%)	0	100	100
16	SH	131/174 (75%)	130 (99%)	1 (1%)	73	90
17	Sg	17/275 (6%)	17 (100%)	0	100	100
18	SF	116/170 (68%)	115 (99%)	1 (1%)	70	90
19	SE	215/225 (96%)	214 (100%)	1 (0%)	81	93
20	Se	38/104 (36%)	38 (100%)	0	100	100
21	SD	71/202 (35%)	70 (99%)	1 (1%)	59	85
22	Sd	41/49 (84%)	41 (100%)	0	100	100
23	SC	178/225 (79%)	176 (99%)	2 (1%)	65	88
24	Sc	42/62 (68%)	39 (93%)	3 (7%)	13	40
25	SB	184/231 (80%)	179 (97%)	5 (3%)	39	73
26	Sb	68/76 (90%)	67 (98%)	1 (2%)	57	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	SA	172/243 (71%)	168 (98%)	4 (2%)	44	76
29	LZ	113/118 (96%)	111 (98%)	2 (2%)	51	80
30	LY	117/135 (87%)	115 (98%)	2 (2%)	53	82
31	LX	107/133 (80%)	106 (99%)	1 (1%)	70	90
32	LW	54/126 (43%)	54 (100%)	0	100	100
33	LV	102/107 (95%)	101 (99%)	1 (1%)	68	89
34	LU	87/115 (76%)	85 (98%)	2 (2%)	44	76
35	LT	139/140 (99%)	137 (99%)	2 (1%)	59	85
36	LS	155/157 (99%)	151 (97%)	4 (3%)	40	73
37	LR	148/175 (85%)	148 (100%)	0	100	100
38	Lr	107/121 (88%)	103 (96%)	4 (4%)	30	64
39	LQ	162/165 (98%)	158 (98%)	4 (2%)	42	74
40	LP	132/135 (98%)	130 (98%)	2 (2%)	57	84
41	Lp	72/75 (96%)	70 (97%)	2 (3%)	38	72
42	LO	167/174 (96%)	165 (99%)	2 (1%)	63	86
43	LN	171/172 (99%)	170 (99%)	1 (1%)	78	93
44	Ln	23/24 (96%)	23 (100%)	0	100	100
45	LM	115/161 (71%)	114 (99%)	1 (1%)	70	90
46	LL	174/177 (98%)	170 (98%)	4 (2%)	44	76
47	Lk	61/65 (94%)	59 (97%)	2 (3%)	33	67
48	LJ	136/149 (91%)	134 (98%)	2 (2%)	57	84
49	Lj	72/80 (90%)	72 (100%)	0	100	100
50	LI	170/181 (94%)	165 (97%)	5 (3%)	37	71
51	Li	80/89 (90%)	79 (99%)	1 (1%)	61	86
52	LH	164/171 (96%)	161 (98%)	3 (2%)	51	80
53	Lh	108/110 (98%)	107 (99%)	1 (1%)	70	90
54	LG	184/223 (82%)	180 (98%)	4 (2%)	45	77
55	Lg	92/96 (96%)	89 (97%)	3 (3%)	33	67
56	LF	186/215 (86%)	182 (98%)	4 (2%)	45	77
57	Lf	86/90 (96%)	86 (100%)	0	100	100
58	LE	188/252 (75%)	184 (98%)	4 (2%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	Le	114/115 (99%)	114 (100%)	0	100	100
60	LD	239/250 (96%)	237 (99%)	2 (1%)	73	90
61	Ld	85/110 (77%)	82 (96%)	3 (4%)	32	66
62	LC	299/348 (86%)	296 (99%)	3 (1%)	68	89
63	Lc	82/97 (84%)	78 (95%)	4 (5%)	22	54
64	LB	340/346 (98%)	339 (100%)	1 (0%)	86	96
65	Lb	81/125 (65%)	81 (100%)	0	100	100
66	LA	189/198 (96%)	186 (98%)	3 (2%)	55	83
67	La	119/120 (99%)	118 (99%)	1 (1%)	73	90
70	Sa	82/98 (84%)	80 (98%)	2 (2%)	43	75
73	SZ	22/103 (21%)	20 (91%)	2 (9%)	9	28
74	ST	52/115 (45%)	52 (100%)	0	100	100
75	SP	50/130 (38%)	50 (100%)	0	100	100
77	SG	166/218 (76%)	165 (99%)	1 (1%)	78	93
78	SI	168/180 (93%)	166 (99%)	2 (1%)	63	86
80	SS	59/132 (45%)	56 (95%)	3 (5%)	21	53
All	All	8311/10565 (79%)	8182 (98%)	129 (2%)	55	83

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SY	9	THR
5	SX	105	PHE
6	SW	28	ARG
6	SW	30	CYS
9	SR	6	THR
9	SR	9	VAL
9	SR	17	ILE
9	SR	57	LEU
9	SR	85	VAL
9	SR	99	ASP
9	SR	105	MET
9	SR	124	VAL
11	SO	40	THR
11	SO	88	LEU
11	SO	103	ASN

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Mol	Chain	Res	Type
11	SO	116	LEU
11	SO	121[A]	ARG
11	SO	121[B]	ARG
11	SO	130	GLU
12	SN	60	VAL
16	SH	92	VAL
18	SF	187	SER
19	SE	194	VAL
21	SD	170	THR
23	SC	113	GLN
23	SC	270	THR
24	Sc	29	GLN
24	Sc	36	ASP
24	Sc	55	VAL
25	SB	88	THR
25	SB	110[A]	MET
25	SB	110[B]	MET
25	SB	127	VAL
25	SB	131	ASP
26	Sb	44	THR
27	SA	34	MET
27	SA	76	VAL
27	SA	104	THR
27	SA	190	SER
29	LZ	83	THR
29	LZ	132	GLN
30	LY	42	TYR
30	LY	93	THR
31	LX	57	GLN
33	LV	16	ILE
34	LU	25	CYS
34	LU	43	LEU
35	LT	68	THR
35	LT	154	ILE
36	LS	2	LYS
36	LS	125	GLN
36	LS	158	VAL
36	LS	174	THR
38	Lr	2(A)	SER
38	Lr	28	GLU
38	Lr	63	VAL
38	Lr	80	THR

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Mol	Chain	Res	Type
39	LQ	79	THR
39	LQ	92	VAL
39	LQ	94	GLU
39	LQ	169	SER
40	LP	89	GLU
40	LP	113	VAL
41	Lp	5	THR
41	Lp	89	LEU
42	LO	58	LEU
42	LO	145	VAL
43	LN	182	HIS
45	LM	105	THR
46	LL	63	THR
46	LL	70	VAL
46	LL	93	THR
46	LL	160	VAL
47	Lk	36	VAL
47	Lk	68	GLU
48	LJ	47	THR
48	LJ	59	SER
50	LI	44	ASP
50	LI	56	GLU
50	LI	79	SER
50	LI	123	GLN
50	LI	179	ASP
51	Li	59	GLU
52	LH	9	THR
52	LH	46	SER
52	LH	142	ASP
53	Lh	16	GLU
54	LG	96	LEU
54	LG	103	ARG
54	LG	241	VAL
54	LG	250	ILE
55	Lg	6	THR
55	Lg	54[A]	ARG
55	Lg	54[B]	ARG
56	LF	28	LEU
56	LF	39	GLN
56	LF	74	MET
56	LF	223	LYS
58	LE	93	THR

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Mol	Chain	Res	Type
58	LE	121	VAL
58	LE	145	THR
58	LE	288	PHE
60	LD	194	VAL
60	LD	268	ARG
61	Ld	46	LEU
61	Ld	107	THR
61	Ld	122	VAL
62	LC	62	THR
62	LC	335	MET
62	LC	336	ARG
63	Lc	28	VAL
63	Lc	60	ILE
63	Lc	94	LEU
63	Lc	101	ASP
64	LB	292	LEU
66	LA	28	ARG
66	LA	140	ASN
66	LA	208	GLU
67	La	15	VAL
70	Sa	26	CYS
70	Sa	67	LEU
73	SZ	72	VAL
73	SZ	77	LEU
77	SG	126	ASP
78	SI	17	LYS
78	SI	62	VAL
80	SS	18	THR
80	SS	134	GLN
80	SS	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	Lm	117	HIS
3	Lo	51	GLN
4	SY	22	GLN
5	SX	16	HIS
5	SX	31	HIS
5	SX	73	GLN
6	SW	120	HIS
7	SV	35	ASN

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Mol	Chain	Res	Type
8	SU	28	ASN
9	SR	29	HIS
10	SQ	77	HIS
10	SQ	86	GLN
13	SL	11	GLN
13	SL	19	ASN
13	SL	94	HIS
15	SJ	27	GLN
15	SJ	132	GLN
16	SH	76	GLN
16	SH	165	ASN
18	SF	165	ASN
18	SF	203	ASN
21	SD	145	GLN
22	Sd	26	ASN
22	Sd	37	ASN
23	SC	120	GLN
23	SC	134	ASN
26	Sb	51	GLN
27	SA	36	GLN
29	LZ	132	GLN
30	LY	61	HIS
36	LS	173	ASN
39	LQ	57	ASN
40	LP	93	HIS
43	LN	29	GLN
45	LM	34	ASN
45	LM	66	HIS
45	LM	131	GLN
46	LL	19	GLN
46	LL	40	GLN
46	LL	67	HIS
46	LL	175	ASN
48	LJ	65	ASN
48	LJ	97	ASN
51	Li	15	HIS
51	Li	36	HIS
51	Li	80	HIS
52	LH	98	HIS
54	LG	38	ASN
54	LG	43	GLN
54	LG	195	HIS

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Mol	Chain	Res	Type
55	Lg	3	GLN
59	Le	52	GLN
60	LD	45	ASN
60	LD	111	ASN
60	LD	282	GLN
61	Ld	121	ASN
62	LC	21	ASN
62	LC	38	ASN
62	LC	212	ASN
62	LC	329	ASN
64	LB	123	HIS
64	LB	138	GLN
64	LB	167	GLN
64	LB	184	GLN
64	LB	376	HIS
65	Lb	61	ASN
66	LA	8	GLN
66	LA	97	ASN
67	La	60	HIS
70	Sa	8	ASN
73	SZ	89	GLN
74	ST	11	GLN
77	SG	65	GLN
78	SI	52	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	mR	7/27 (25%)	2 (28%)	0
68	L7	118/120 (98%)	7 (5%)	0
69	Pt	76/77 (98%)	14 (18%)	0
71	L8	151/156 (96%)	30 (19%)	0
72	L5	3424/5069 (67%)	553 (16%)	15 (0%)
76	S2	1556/1869 (83%)	291 (18%)	6 (0%)
79	S6	55/75 (73%)	18 (32%)	1 (1%)
All	All	5387/7393 (72%)	915 (16%)	22 (0%)

All (915) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	mR	33	C

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Mol	Chain	Res	Type
28	mR	37	A
68	L7	7	G
68	L7	33	U
68	L7	53	U
68	L7	54	A
68	L7	64	G
68	L7	100	A
68	L7	110	G
69	Pt	8	4SU
69	Pt	9	G
69	Pt	16	C
69	Pt	17	C
69	Pt	18	C
69	Pt	20	G
69	Pt	21	H2U
69	Pt	22	A
69	Pt	32	G
69	Pt	47	G7M
69	Pt	48	U
69	Pt	49	C
69	Pt	62	C
69	Pt	71	G
71	L8	3	A
71	L8	23	C
71	L8	25	G
71	L8	34	U
71	L8	35	C
71	L8	39	G
71	L8	51	U
71	L8	59	A
71	L8	62	A
71	L8	63	U
71	L8	69	PSU
71	L8	70	G
71	L8	80	A
71	L8	84	A
71	L8	85	U
71	L8	87	G
71	L8	94	G
71	L8	103	A
71	L8	105	C
71	L8	106	G

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Mol	Chain	Res	Type
71	L8	110	U
71	L8	111	U
71	L8	114	G
71	L8	123	U
71	L8	125	C
71	L8	127	U
71	L8	141	C
71	L8	142	U
71	L8	150	C
71	L8	156	U
72	L5	5	A
72	L5	9	C
72	L5	25	A
72	L5	39	A
72	L5	42	A
72	L5	48	G
72	L5	56	A
72	L5	59	A
72	L5	64	A
72	L5	65	A
72	L5	66	A
72	L5	71	C
72	L5	85	G
72	L5	91	G
72	L5	98	A
72	L5	108	A
72	L5	110	C
72	L5	112	C
72	L5	119	G
72	L5	132	G
72	L5	139	G
72	L5	144	G
72	L5	159	C
72	L5	160	G
72	L5	161	G
72	L5	162	A
72	L5	168	C
72	L5	172	C
72	L5	173	C
72	L5	174	C
72	L5	175	C
72	L5	200	U

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Mol	Chain	Res	Type
72	L5	209	U
72	L5	210	C
72	L5	216	C
72	L5	217	C
72	L5	218	A
72	L5	219	G
72	L5	233	U
72	L5	234	G
72	L5	259	C
72	L5	260	C
72	L5	266	C
72	L5	271	C
72	L5	273	U
72	L5	274	C
72	L5	277	G
72	L5	278	G
72	L5	280	G
72	L5	297	U
72	L5	306	A
72	L5	316	U
72	L5	340	C
72	L5	350	C
72	L5	373	G
72	L5	387	G
72	L5	398	A2M
72	L5	410	A
72	L5	412	G
72	L5	413	G
72	L5	414	C
72	L5	417	G
72	L5	431	G
72	L5	432	U
72	L5	440	U
72	L5	448	G
72	L5	449	C
72	L5	450	G
72	L5	451	C
72	L5	452	A
72	L5	453	G
72	L5	454	U
72	L5	467	U
72	L5	483	C

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Mol	Chain	Res	Type
72	L5	484	U
72	L5	487	G
72	L5	489	C
72	L5	492	U
72	L5	501	C
72	L5	502	C
72	L5	503	C
72	L5	504	G
72	L5	510	U
72	L5	514	U
72	L5	644	G
72	L5	646	G
72	L5	648	G
72	L5	661	C
72	L5	665	C
72	L5	666	G
72	L5	667	A
72	L5	669	C
72	L5	685	C
72	L5	688	U
72	L5	696	C
72	L5	704	C
72	L5	729	G
72	L5	731	G
72	L5	738	C
72	L5	739	G
72	L5	742	G
72	L5	746	A
72	L5	760	G
72	L5	904	C
72	L5	913	U
72	L5	914	U
72	L5	915	A
72	L5	917	A
72	L5	918	G
72	L5	925	C
72	L5	926	G
72	L5	932	A
72	L5	933	G
72	L5	935	A
72	L5	937	U
72	L5	945	U

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Mol	Chain	Res	Type
72	L5	959	G
72	L5	960	A
72	L5	962	C
72	L5	965	G
72	L5	966	A
72	L5	967	C
72	L5	968	C
72	L5	969	C
72	L5	970	G
72	L5	977	C
72	L5	982	U
72	L5	1072	C
72	L5	1168	G
72	L5	1181	C
72	L5	1182	C
72	L5	1183	C
72	L5	1199	G
72	L5	1200	G
72	L5	1210	C
72	L5	1211	G
72	L5	1214	C
72	L5	1215	C
72	L5	1216	C
72	L5	1220	G
72	L5	1241	C
72	L5	1254	A
72	L5	1255	A
72	L5	1266	G
72	L5	1270	A
72	L5	1271	G
72	L5	1272	C
72	L5	1273	G
72	L5	1277	G
72	L5	1284	G
72	L5	1285	U
72	L5	1287	G
72	L5	1293	G
72	L5	1294	A
72	L5	1296	G
72	L5	1302	U
72	L5	1303	A
72	L5	1304	C

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Mol	Chain	Res	Type
72	L5	1313	C
72	L5	1326	A2M
72	L5	1337	A
72	L5	1354	A
72	L5	1359	G
72	L5	1365	C
72	L5	1387	A
72	L5	1391	A
72	L5	1397	A
72	L5	1398	A
72	L5	1400	G
72	L5	1402	C
72	L5	1418	C
72	L5	1427	A
72	L5	1438	U
72	L5	1439	C
72	L5	1443	A
72	L5	1452	A
72	L5	1454	G
72	L5	1476	C
72	L5	1477	C
72	L5	1478	C
72	L5	1479	G
72	L5	1481	C
72	L5	1482	G
72	L5	1483	C
72	L5	1484	G
72	L5	1485	C
72	L5	1498	G
72	L5	1502	G
72	L5	1504	G
72	L5	1523	A
72	L5	1534	A2M
72	L5	1547	A
72	L5	1553	A
72	L5	1564	A
72	L5	1578	U
72	L5	1591	U
72	L5	1596	U
72	L5	1612	G
72	L5	1613	A
72	L5	1624	G

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Mol	Chain	Res	Type
72	L5	1625	OMG
72	L5	1631	A
72	L5	1633	G
72	L5	1634	A
72	L5	1638	A
72	L5	1640	C
72	L5	1641	G
72	L5	1642	A
72	L5	1654	G
72	L5	1661	C
72	L5	1676	C
72	L5	1677	PSU
72	L5	1678	C
72	L5	1691	G
72	L5	1697	G
72	L5	1698	C
72	L5	1702	C
72	L5	1703	C
72	L5	1704	C
72	L5	1719	A
72	L5	1720	C
72	L5	1721	G
72	L5	1734	G
72	L5	1741	G
72	L5	1755	C
72	L5	1757	U
72	L5	1758	G
72	L5	1759	G
72	L5	1773	U
72	L5	1774	C
72	L5	1776	A
72	L5	1777	C
72	L5	1787	A
72	L5	1794	A
72	L5	1804	A
72	L5	1805	A
72	L5	1806	G
72	L5	1815	G
72	L5	1821	G
72	L5	1836	G
72	L5	1837	A
72	L5	1842	G

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Mol	Chain	Res	Type
72	L5	1855	G
72	L5	1869	G
72	L5	1882	U
72	L5	1891	A
72	L5	1892	A
72	L5	1897	A
72	L5	1918	U
72	L5	1919	G
72	L5	1921	C
72	L5	1922	G
72	L5	1925	G
72	L5	1931	C
72	L5	1932	A
72	L5	1940	G
72	L5	1948	G
72	L5	1951	G
72	L5	1959	U
72	L5	1960	A
72	L5	1961	G
72	L5	1962	A
72	L5	1969	G
72	L5	2025	A
72	L5	2026	A
72	L5	2034	G
72	L5	2046	G
72	L5	2048	U
72	L5	2055	G
72	L5	2056	G
72	L5	2069	A
72	L5	2084	C
72	L5	2085	G
72	L5	2088	A
72	L5	2092	G
72	L5	2093	A
72	L5	2095	A
72	L5	2097	U
72	L5	2098	G
72	L5	2099	G
72	L5	2100	A
72	L5	2111	G
72	L5	2258	C
72	L5	2279	A

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Mol	Chain	Res	Type
72	L5	2289	C
72	L5	2300	A
72	L5	2301	G
72	L5	2306	G
72	L5	2313	A
72	L5	2322	G
72	L5	2348	G
72	L5	2351	OMC
72	L5	2357	G
72	L5	2360	A
72	L5	2395	A
72	L5	2397	G
72	L5	2417	A
72	L5	2421	G
72	L5	2425	U
72	L5	2447	U
72	L5	2450	G
72	L5	2453	A
72	L5	2469	C
72	L5	2471	G
72	L5	2474	G
72	L5	2483	G
72	L5	2503	G
72	L5	2513	A
72	L5	2519	U
72	L5	2529	A
72	L5	2542	G
72	L5	2554	U
72	L5	2558	C
72	L5	2570	U
72	L5	2571	C
72	L5	2573	A
72	L5	2583	C
72	L5	2587	A
72	L5	2589	C
72	L5	2601	A
72	L5	2602	G
72	L5	2627	C
72	L5	2630	U
72	L5	2653	C
72	L5	2657	G
72	L5	2658	G

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Mol	Chain	Res	Type
72	L5	2659	A
72	L5	2669	C
72	L5	2681	G
72	L5	2687	U
72	L5	2694	G
72	L5	2695	A
72	L5	2696	A
72	L5	2711	G
72	L5	2712	G
72	L5	2714	G
72	L5	2724	G
72	L5	2726	G
72	L5	2743	A
72	L5	2754	G
72	L5	2759	G
72	L5	2760	G
72	L5	2788	U
72	L5	2790	U
72	L5	2798	A
72	L5	2814	C
72	L5	2826	U
72	L5	2827	G
72	L5	2829	U
72	L5	2855	G
72	L5	2866	C
72	L5	2867	C
72	L5	2870	A
72	L5	3604	A
72	L5	3614	G
72	L5	3615	G
72	L5	3618	C
72	L5	3626	G
72	L5	3635	A
72	L5	3644	U
72	L5	3646	A
72	L5	3648	A
72	L5	3662	A
72	L5	3664	G
72	L5	3672	G
72	L5	3674	G
72	L5	3712	A
72	L5	3723	A

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Mol	Chain	Res	Type
72	L5	3726	A
72	L5	3727	A
72	L5	3729	PSU
72	L5	3732	A
72	L5	3733	A
72	L5	3748	A
72	L5	3750	G
72	L5	3753	G
72	L5	3759	A
72	L5	3776	G
72	L5	3777	G
72	L5	3783	A
72	L5	3784	A
72	L5	3785	A2M
72	L5	3786	U
72	L5	3787	G
72	L5	3810	C
72	L5	3811	G
72	L5	3812	C
72	L5	3814	U
72	L5	3816	A
72	L5	3817	A
72	L5	3818	U
72	L5	3819	G
72	L5	3824	A
72	L5	3838	U
72	L5	3839	G
72	L5	3840	U
72	L5	3844	PSU
72	L5	3877	A
72	L5	3878	C
72	L5	3879	G
72	L5	3897	G
72	L5	3901	A
72	L5	3905	A
72	L5	3906	A
72	L5	3907	G
72	L5	3908	A
72	L5	3915	U
72	L5	3948	C
72	L5	3951	G
72	L5	3952	A

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Mol	Chain	Res	Type
72	L5	4072	C
72	L5	4073	A
72	L5	4076	G
72	L5	4084	G
72	L5	4094	G
72	L5	4095	G
72	L5	4096	C
72	L5	4097	G
72	L5	4115	G
72	L5	4116	C
72	L5	4117	U
72	L5	4118	U
72	L5	4119	C
72	L5	4122	G
72	L5	4127	A
72	L5	4150	G
72	L5	4161	G
72	L5	4162	C
72	L5	4163	U
72	L5	4170	A
72	L5	4183	G
72	L5	4184	G
72	L5	4191	G
72	L5	4203	A
72	L5	4219	A
72	L5	4220	6MZ
72	L5	4229	U
72	L5	4233	A
72	L5	4251	A
72	L5	4254	G
72	L5	4266	G
72	L5	4268	A
72	L5	4273	A
72	L5	4280	A
72	L5	4281	A
72	L5	4282	A
72	L5	4287	G
72	L5	4291	G
72	L5	4304	A
72	L5	4305	G
72	L5	4306	U
72	L5	4314	C

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Mol	Chain	Res	Type
72	L5	4329	G
72	L5	4330	G
72	L5	4332	C
72	L5	4349	C
72	L5	4350	C
72	L5	4354	U
72	L5	4373	G
72	L5	4376	A
72	L5	4377	G
72	L5	4378	A
72	L5	4379	A
72	L5	4387	C
72	L5	4391	G
72	L5	4394	A
72	L5	4420	PSU
72	L5	4440	G
72	L5	4448	G
72	L5	4449	A
72	L5	4453	C
72	L5	4464	A
72	L5	4465	U
72	L5	4475	G
72	L5	4512	U
72	L5	4513	A
72	L5	4519	C
72	L5	4524	G
72	L5	4528	G
72	L5	4548	A
72	L5	4560	C
72	L5	4567	G
72	L5	4575	G
72	L5	4584	A
72	L5	4590	A2M
72	L5	4600	G
72	L5	4610	A
72	L5	4627	U
72	L5	4636	PSU
72	L5	4637	OMG
72	L5	4656	A
72	L5	4670	C
72	L5	4672	A
72	L5	4700	A

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Mol	Chain	Res	Type
72	L5	4703	U
72	L5	4708	A
72	L5	4709	U
72	L5	4721	G
72	L5	4739	C
72	L5	4740	G
72	L5	4741	C
72	L5	4742	G
72	L5	4750	G
72	L5	4754	G
72	L5	4757	C
72	L5	4759	C
72	L5	4761	G
72	L5	4765	G
72	L5	4771	C
72	L5	4772	C
72	L5	4773	C
72	L5	4775	C
72	L5	4776	G
72	L5	4860	G
72	L5	4863	G
72	L5	4864	U
72	L5	4870	G
72	L5	4871	C
72	L5	4882	U
72	L5	4883	C
72	L5	4895	C
72	L5	4900	C
72	L5	4901	G
72	L5	4910	G
72	L5	4911	A
72	L5	4912	G
72	L5	4913	G
72	L5	4931	G
72	L5	4934	A
72	L5	4937	C
72	L5	4943	A
72	L5	4961	G
72	L5	4967	A
72	L5	4976	U
72	L5	4988	U
72	L5	4989	U

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Mol	Chain	Res	Type
72	L5	4990	C
72	L5	4991	U
72	L5	4993	G
72	L5	4994	G
72	L5	5006	U
72	L5	5007	A
72	L5	5013	C
72	L5	5014	A
72	L5	5017	G
72	L5	5034	A
72	L5	5041	G
72	L5	5050	C
72	L5	5054	C
72	L5	5055	G
72	L5	5061	A
72	L5	5062	G
72	L5	5066	U
76	S2	17	C
76	S2	33	G
76	S2	44	U
76	S2	46	A
76	S2	56	G
76	S2	58	C
76	S2	62	G
76	S2	65	C
76	S2	67	C
76	S2	68	A
76	S2	71	G
76	S2	97	U
76	S2	99	A2M
76	S2	103	A
76	S2	113	G
76	S2	115	U
76	S2	126	G
76	S2	127	C
76	S2	142	C
76	S2	143	U
76	S2	148	U
76	S2	158	A
76	S2	161	U
76	S2	162	C
76	S2	163	U

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Mol	Chain	Res	Type
76	S2	170	A
76	S2	183	G
76	S2	184	G
76	S2	185	G
76	S2	187	G
76	S2	190	G
76	S2	191	A
76	S2	192	C
76	S2	214	U
76	S2	292	A
76	S2	294	U
76	S2	295	C
76	S2	298	G
76	S2	302	A
76	S2	306	C
76	S2	307	G
76	S2	308	G
76	S2	309	G
76	S2	312	G
76	S2	319	C
76	S2	320	C
76	S2	321	U
76	S2	323	U
76	S2	332	G
76	S2	333	G
76	S2	339	A
76	S2	340	C
76	S2	347	G
76	S2	362	C
76	S2	364	A
76	S2	370	G
76	S2	385	G
76	S2	386	C
76	S2	407	G
76	S2	409	C
76	S2	421	G
76	S2	438	G
76	S2	448	A
76	S2	449	A
76	S2	450	C
76	S2	452	G
76	S2	464	A

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Mol	Chain	Res	Type
76	S2	466	G
76	S2	467	G
76	S2	471	G
76	S2	472	C
76	S2	473	A
76	S2	474	G
76	S2	476	A
76	S2	482	G
76	S2	487	U
76	S2	488	U
76	S2	492	C
76	S2	493	A
76	S2	496	C
76	S2	502	C
76	S2	508	A
76	S2	509	OMG
76	S2	512	A2M
76	S2	516	A
76	S2	525	A
76	S2	531	A
76	S2	533	A
76	S2	534	G
76	S2	535	G
76	S2	551	U
76	S2	552	G
76	S2	554	A
76	S2	556	U
76	S2	560	A
76	S2	563	G
76	S2	564	A
76	S2	568	C
76	S2	574	A
76	S2	576	A2M
76	S2	587	A
76	S2	589	G
76	S2	590	A2M
76	S2	591	U
76	S2	604	A
76	S2	606	G
76	S2	607	U
76	S2	614	C
76	S2	617	G

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Mol	Chain	Res	Type
76	S2	626	G
76	S2	627	OMU
76	S2	628	A
76	S2	643	A
76	S2	644	OMG
76	S2	655	A
76	S2	660	C
76	S2	663	C
76	S2	668	A2M
76	S2	669	A
76	S2	671	A
76	S2	672	A
76	S2	673	G
76	S2	683	OMG
76	S2	688	U
76	S2	797	C
76	S2	799	U
76	S2	821	G
76	S2	822	PSU
76	S2	845	G
76	S2	847	A
76	S2	869	A
76	S2	870	A
76	S2	876	C
76	S2	877	C
76	S2	878	G
76	S2	879	C
76	S2	881	G
76	S2	901	G
76	S2	904	A
76	S2	908	A
76	S2	912	C
76	S2	913	A
76	S2	914	U
76	S2	920	A
76	S2	922	A
76	S2	933	G
76	S2	943	U
76	S2	955	A
76	S2	971	G
76	S2	990	A
76	S2	992	A

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Mol	Chain	Res	Type
76	S2	999	G
76	S2	1017	U
76	S2	1023	A
76	S2	1026	C
76	S2	1027	A
76	S2	1045	U
76	S2	1049	A
76	S2	1061	U
76	S2	1062	A
76	S2	1083	A
76	S2	1085	C
76	S2	1096	G
76	S2	1109	C
76	S2	1119	A
76	S2	1121	G
76	S2	1133	A
76	S2	1138	C
76	S2	1153	C
76	S2	1154	U
76	S2	1157	G
76	S2	1171	G
76	S2	1188	A
76	S2	1195	A
76	S2	1203	G
76	S2	1207	G
76	S2	1208	A
76	S2	1215	C
76	S2	1216	C
76	S2	1224	G
76	S2	1242	U
76	S2	1243	PSU
76	S2	1245	G
76	S2	1247	C
76	S2	1251	A
76	S2	1253	A
76	S2	1256	G
76	S2	1257	G
76	S2	1258	A
76	S2	1259	A
76	S2	1264	C
76	S2	1271	C
76	S2	1274	G

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Mol	Chain	Res	Type
76	S2	1275	G
76	S2	1278	A
76	S2	1301	A
76	S2	1302	G
76	S2	1303	C
76	S2	1325	G
76	S2	1326	U
76	S2	1327	G
76	S2	1330	G
76	S2	1342	U
76	S2	1358	U
76	S2	1371	U
76	S2	1372	U
76	S2	1378	A
76	S2	1397	U
76	S2	1403	C
76	S2	1404	U
76	S2	1405	A
76	S2	1407	U
76	S2	1408	U
76	S2	1415	C
76	S2	1438	A
76	S2	1439	A
76	S2	1440	C
76	S2	1441	U
76	S2	1442	U
76	S2	1447	OMG
76	S2	1449	G
76	S2	1454	A
76	S2	1462	U
76	S2	1463	U
76	S2	1464	C
76	S2	1466	G
76	S2	1477	U
76	S2	1489	A
76	S2	1490	OMG
76	S2	1498	A
76	S2	1508	A
76	S2	1509	U
76	S2	1520	G
76	S2	1521	C
76	S2	1528	G

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Mol	Chain	Res	Type
76	S2	1531	A
76	S2	1533	A
76	S2	1536	G
76	S2	1560	U
76	S2	1570	G
76	S2	1579	A
76	S2	1580	A
76	S2	1585	U
76	S2	1586	U
76	S2	1587	G
76	S2	1588	A
76	S2	1598	G
76	S2	1599	U
76	S2	1601	A
76	S2	1603	G
76	S2	1604	G
76	S2	1606	G
76	S2	1610	G
76	S2	1611	G
76	S2	1612	G
76	S2	1614	A
76	S2	1622	U
76	S2	1623	A
76	S2	1636	G
76	S2	1637	A
76	S2	1638	G
76	S2	1639	G7M
76	S2	1646	C
76	S2	1648	G
76	S2	1661	A
76	S2	1665	G
76	S2	1671	G
76	S2	1699	A
76	S2	1721	U
76	S2	1722	G
76	S2	1735	A
76	S2	1736	G
76	S2	1744	G
76	S2	1750	C
76	S2	1785	C
76	S2	1805	G
76	S2	1823	A

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Mol	Chain	Res	Type
76	S2	1824	A
76	S2	1825	A
76	S2	1826	G
76	S2	1829	G
76	S2	1831	A
76	S2	1835	A
76	S2	1838	U
76	S2	1849	G
76	S2	1851	MA6
76	S2	1861	G
76	S2	1862	G
76	S2	1863	A
76	S2	1864	U
76	S2	1865	C
79	S6	8	G
79	S6	9	U
79	S6	11	G
79	S6	12	C
79	S6	14	C
79	S6	17	C
79	S6	18	G
79	S6	39	C
79	S6	40	C
79	S6	42	A
79	S6	43	G
79	S6	44	A
79	S6	46	G
79	S6	50	A
79	S6	52	G
79	S6	61	C
79	S6	62	C
79	S6	76	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
72	L5	172	C
72	L5	934	C
72	L5	1303	A
72	L5	1399	G
72	L5	1475	G
72	L5	1483	C

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Mol	Chain	Res	Type
72	L5	1563	A
72	L5	1633	G
72	L5	1757	U
72	L5	2098	G
72	L5	2541	G
72	L5	4096	C
72	L5	4281	A
72	L5	4699	U
72	L5	4741	C
76	S2	96	C
76	S2	169	U
76	S2	1244	PSU
76	S2	1508	A
76	S2	1598	G
76	S2	1825	A
79	S6	60	A

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

210 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$
76	PSU	S2	1347	76	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	2401	72	22,25,26	3.93	10 (45%)	31,36,39	3.71	15 (48%)
76	OMU	S2	116	76	19,22,23	3.00	8 (42%)	26,31,34	1.66	4 (15%)
72	OMG	L5	4637	72	23,26,27	0.52	0	33,38,41	0.49	0
76	PSU	S2	609	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
76	OMU	S2	627	76	19,22,23	3.03	8 (42%)	26,31,34	1.69	5 (19%)
72	PSU	L5	3853	72,84	18,21,22	1.04	1 (5%)	22,30,33	1.61	4 (18%)
72	PSU	L5	2843	72	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
72	OMC	L5	1340	72	19,22,23	0.57	0	26,31,34	0.81	1 (3%)
72	PSU	L5	3734	72	18,21,22	1.00	1 (5%)	22,30,33	1.66	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	OMC	L5	3841	72	19,22,23	0.53	0	26,31,34	0.68	0
76	A2M	S2	576	76	22,25,26	3.94	11 (50%)	31,36,39	3.72	16 (51%)
76	OMG	S2	1328	76	23,26,27	0.47	0	33,38,41	0.48	0
76	OMG	S2	1490	76	23,26,27	0.50	0	33,38,41	0.48	0
72	OMG	L5	4196	69,72	23,26,27	0.52	0	33,38,41	0.46	0
76	PSU	S2	815	76	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
72	OMG	L5	4228	72	23,26,27	0.51	0	33,38,41	0.57	0
76	PSU	S2	801	76	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
72	OMG	L5	1316	72	23,26,27	0.54	0	33,38,41	0.55	0
72	PSU	L5	4403	72	18,21,22	1.02	1 (5%)	22,30,33	1.78	4 (18%)
72	PSU	L5	3762	72	18,21,22	1.12	1 (5%)	22,30,33	1.71	4 (18%)
72	PSU	L5	4972	72	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
72	PSU	L5	4552	72	18,21,22	1.10	1 (5%)	22,30,33	1.76	4 (18%)
76	A2M	S2	1383	76	22,25,26	3.92	10 (45%)	31,36,39	3.69	14 (45%)
69	PSU	Pt	56	69	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
76	OMG	S2	509	76	23,26,27	0.51	0	33,38,41	0.50	0
76	PSU	S2	1445	76	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
76	A2M	S2	484	76	22,25,26	3.86	11 (50%)	31,36,39	3.68	14 (45%)
72	OMC	L5	2422	72,84	19,22,23	0.57	0	26,31,34	0.75	1 (3%)
72	PSU	L5	3770	72	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
76	OMG	S2	1447	76	23,26,27	0.48	0	33,38,41	0.55	0
72	6MZ	L5	4220	72	22,25,26	2.49	5 (22%)	30,36,39	2.18	10 (33%)
72	A2M	L5	398	72	22,25,26	3.90	10 (45%)	31,36,39	3.68	13 (41%)
72	A2M	L5	3867	72	22,25,26	3.95	10 (45%)	31,36,39	3.76	15 (48%)
72	A2M	L5	1871	72	22,25,26	3.92	10 (45%)	31,36,39	3.67	14 (45%)
72	PSU	L5	4353	72	18,21,22	1.04	1 (5%)	22,30,33	1.77	3 (13%)
72	OMC	L5	4536	72	19,22,23	0.58	0	26,31,34	0.72	0
76	PSU	S2	573	76	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
76	OMG	S2	436	76	23,26,27	0.51	0	33,38,41	0.50	0
76	PSU	S2	649	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
72	OMG	L5	2364	72	23,26,27	0.51	0	33,38,41	0.47	0
72	OMC	L5	2351	72	19,22,23	0.60	0	26,31,34	0.94	1 (3%)
72	OMU	L5	4227	72	19,22,23	2.99	8 (42%)	26,31,34	1.76	5 (19%)
69	H2U	Pt	21	69	18,21,22	0.54	0	21,30,33	1.14	1 (4%)
72	PSU	L5	4442	72	18,21,22	1.06	1 (5%)	22,30,33	1.79	5 (22%)
72	OMG	L5	3627	72	23,26,27	0.51	0	33,38,41	0.64	0
76	OMC	S2	517	76	19,22,23	0.56	0	26,31,34	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	OMG	L5	3899	72,83	23,26,27	0.56	0	33,38,41	0.55	0
76	A2M	S2	468	76	22,25,26	3.93	10 (45%)	31,36,39	3.67	14 (45%)
76	PSU	S2	572	76	18,21,22	1.04	1 (5%)	22,30,33	1.70	5 (22%)
72	OMU	L5	2837	72	19,22,23	3.00	8 (42%)	26,31,34	1.74	5 (19%)
72	A2M	L5	1326	72	22,25,26	3.93	10 (45%)	31,36,39	3.66	13 (41%)
76	A2M	S2	1678	76	22,25,26	3.94	10 (45%)	31,36,39	3.81	14 (45%)
72	A2M	L5	3785	72	22,25,26	3.93	11 (50%)	31,36,39	3.78	14 (45%)
76	PSU	S2	218	76	18,21,22	1.02	1 (5%)	22,30,33	1.64	5 (22%)
72	5MC	L5	4447	72	18,22,23	0.72	0	26,32,35	0.72	0
72	A2M	L5	3830	72	22,25,26	3.92	10 (45%)	31,36,39	3.70	14 (45%)
72	OMG	L5	4392	72	23,26,27	0.49	0	33,38,41	0.48	0
76	PSU	S2	1367	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
72	PSU	L5	3884	72	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
72	PSU	L5	4296	72	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
72	PSU	L5	1779	72	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
76	A2M	S2	512	76	22,25,26	3.94	10 (45%)	31,36,39	3.68	12 (38%)
76	PSU	S2	918	76	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
65	MLZ	Lb	5	65	8,9,10	0.78	0	4,9,11	0.63	0
72	A2M	L5	4590	72	22,25,26	3.95	10 (45%)	31,36,39	3.75	16 (51%)
76	PSU	S2	1232	76	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
72	OMC	L5	3887	72	19,22,23	0.59	0	26,31,34	0.72	0
72	OMG	L5	1522	72	23,26,27	0.52	0	33,38,41	0.58	0
72	PSU	L5	4312	72	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
76	OMC	S2	1703	76	19,22,23	0.54	0	26,31,34	0.66	0
66	V5N	LA	216	66	9,11,12	2.67	2 (22%)	9,14,16	1.22	0
72	PSU	L5	4521	72,83	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
72	OMG	L5	4623	72	23,26,27	0.52	0	33,38,41	0.54	0
76	PSU	S2	1136	76	18,21,22	1.06	1 (5%)	22,30,33	1.80	5 (22%)
76	PSU	S2	109	76	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
72	PSU	L5	1792	72	18,21,22	1.05	1 (5%)	22,30,33	1.64	4 (18%)
76	B8N	S2	1248	76	24,29,30	3.03	6 (25%)	29,42,45	1.79	6 (20%)
76	PSU	S2	119	76	18,21,22	1.01	1 (5%)	22,30,33	1.59	4 (18%)
76	PSU	S2	406	76	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
72	PSU	L5	1683	72	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
72	OMC	L5	2824	72	19,22,23	0.57	0	26,31,34	0.77	1 (3%)
72	OMU	L5	3925	72	19,22,23	2.99	8 (42%)	26,31,34	1.76	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	PSU	L5	4299	72	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
76	OMG	S2	683	76	23,26,27	0.54	0	33,38,41	0.48	0
72	OMC	L5	3701	82,72,84	19,22,23	0.55	0	26,31,34	0.56	0
71	PSU	L8	69	71	18,21,22	1.05	1 (5%)	22,30,33	1.69	5 (22%)
72	A2M	L5	4523	72,83	22,25,26	3.90	11 (50%)	31,36,39	3.65	14 (45%)
76	PSU	S2	36	76	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
76	PSU	S2	1625	76	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
72	PSU	L5	4576	72	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
72	A2M	L5	2363	72,83,84	22,25,26	3.92	10 (45%)	31,36,39	3.72	13 (41%)
72	PSU	L5	3639	72	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
72	PSU	L5	4293	72	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
76	OMU	S2	1804	76	19,22,23	3.03	8 (42%)	26,31,34	1.72	5 (19%)
72	5MC	L5	3782	72,83	18,22,23	0.59	0	26,32,35	0.65	0
72	PSU	L5	3844	72	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	1534	72,83	22,25,26	3.93	9 (40%)	31,36,39	3.83	15 (48%)
76	PSU	S2	1238	76	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
69	OMC	Pt	33	69	19,22,23	0.55	0	26,31,34	0.89	2 (7%)
72	PSU	L5	3758	72	18,21,22	1.06	1 (5%)	22,30,33	1.82	4 (18%)
72	OMU	L5	4498	72	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
72	PSU	L5	4579	72	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
72	PSU	L5	4500	72	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
72	PSU	L5	4493	72	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
72	PSU	L5	3637	72	18,21,22	1.05	1 (5%)	22,30,33	1.78	3 (13%)
72	PSU	L5	4673	72	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
72	1MA	L5	1322	72,84	21,25,26	0.53	0	31,37,40	0.76	1 (3%)
76	PSU	S2	1081	76	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
72	PSU	L5	4532	72	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
76	G7M	S2	1639	76,69	23,26,27	2.77	8 (34%)	35,39,42	2.32	10 (28%)
72	PSU	L5	4689	72	18,21,22	1.03	1 (5%)	22,30,33	1.83	4 (18%)
72	OMC	L5	4456	72	19,22,23	0.59	0	26,31,34	0.83	1 (3%)
72	PSU	L5	2508	72	18,21,22	1.06	1 (5%)	22,30,33	1.63	4 (18%)
72	PSU	L5	1860	72	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
76	PSU	S2	34	76	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
76	OMC	S2	1391	76	19,22,23	0.52	0	26,31,34	0.65	0
76	PSU	S2	1243	76	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	PSU	L8	55	71	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
72	A2M	L5	3760	72	22,25,26	3.95	10 (45%)	31,36,39	3.95	13 (41%)
76	PSU	S2	681	76	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
72	UR3	L5	4530	72	19,22,23	2.75	8 (42%)	26,32,35	1.30	2 (7%)
72	OMG	L5	4499	72	23,26,27	0.52	0	33,38,41	0.47	0
72	PSU	L5	4628	72	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
72	PSU	L5	3729	72	18,21,22	1.10	1 (5%)	22,30,33	1.69	4 (18%)
76	PSU	S2	93	76	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
76	PSU	S2	1643	76,83	18,21,22	1.08	1 (5%)	22,30,33	1.76	5 (22%)
72	PSU	L5	4423	72	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
76	MA6	S2	1851	76	23,26,27	1.45	3 (13%)	34,38,41	3.34	11 (32%)
72	PSU	L5	4420	72	18,21,22	1.05	1 (5%)	22,30,33	1.63	5 (22%)
71	OMG	L8	75	71	23,26,27	0.50	0	33,38,41	0.51	0
72	PSU	L5	2839	72	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
67	V5N	La	39	67	9,11,12	2.65	2 (22%)	9,14,16	1.22	1 (11%)
72	OMG	L5	3792	72	23,26,27	0.51	0	33,38,41	0.52	0
72	PSU	L5	1744	72	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	3724	72	22,25,26	3.92	10 (45%)	31,36,39	3.73	14 (45%)
72	PSU	L5	3764	72	18,21,22	1.00	1 (5%)	22,30,33	1.65	5 (22%)
76	PSU	S2	866	76	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
72	OMU	L5	4620	72	19,22,23	2.93	8 (42%)	26,31,34	1.59	4 (15%)
72	PSU	L5	1582	72	18,21,22	1.05	1 (5%)	22,30,33	1.60	4 (18%)
76	PSU	S2	686	76	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
76	PSU	S2	1692	76	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
76	A2M	S2	590	76	22,25,26	3.97	9 (40%)	31,36,39	3.97	14 (45%)
72	OMG	L5	2876	72	23,26,27	0.52	0	33,38,41	0.53	0
72	OMC	L5	2861	72	19,22,23	0.58	0	26,31,34	0.77	1 (3%)
3	MLZ	Lo	53	3	8,9,10	0.76	0	4,9,11	0.59	0
72	OMC	L5	1881	82,72	19,22,23	0.58	0	26,31,34	0.64	0
72	PSU	L5	2632	72	18,21,22	1.03	1 (5%)	22,30,33	1.65	4 (18%)
76	A2M	S2	99	76	22,25,26	3.92	10 (45%)	31,36,39	3.69	14 (45%)
72	A2M	L5	2815	72,84	22,25,26	3.93	11 (50%)	31,36,39	3.80	16 (51%)
76	PSU	S2	651	76	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
72	PSU	L5	3920	72,83	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
72	PSU	L5	3715	72	18,21,22	1.07	1 (5%)	22,30,33	1.77	5 (22%)
72	OMG	L5	3744	72	23,26,27	0.51	0	33,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	PSU	S2	296	76	18,21,22	1.03	1 (5%)	22,30,33	1.74	4 (18%)
72	OMC	L5	3869	72	19,22,23	0.56	0	26,31,34	0.68	0
72	A2M	L5	3825	72	22,25,26	3.92	10 (45%)	31,36,39	3.75	14 (45%)
72	PSU	L5	3851	72	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
72	A2M	L5	400	72	22,25,26	3.92	10 (45%)	31,36,39	3.71	14 (45%)
72	OMG	L5	2424	72	23,26,27	0.51	0	33,38,41	0.44	0
72	A2M	L5	3718	72	22,25,26	3.91	10 (45%)	31,36,39	3.70	15 (48%)
72	PSU	L5	5010	72	18,21,22	1.03	1 (5%)	22,30,33	1.74	4 (18%)
72	OMC	L5	2365	72,83	19,22,23	0.55	0	26,31,34	0.63	0
72	OMC	L5	2804	72	19,22,23	0.55	0	26,31,34	0.68	0
72	PSU	L5	4361	72	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
76	OMG	S2	867	76	23,26,27	0.50	0	33,38,41	0.49	0
76	PSU	S2	814	76	18,21,22	1.02	1 (5%)	22,30,33	1.69	4 (18%)
76	PSU	S2	1174	76	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	A2M	L5	1524	72	22,25,26	3.97	10 (45%)	31,36,39	3.95	13 (41%)
76	A2M	S2	1031	76	22,25,26	3.93	10 (45%)	31,36,39	3.67	14 (45%)
69	G7M	Pt	47	69	23,26,27	2.74	10 (43%)	35,39,42	2.13	11 (31%)
76	PSU	S2	863	76	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
72	OMG	L5	4618	72	23,26,27	0.50	0	33,38,41	0.52	0
76	A2M	S2	668	76,83	22,25,26	3.89	11 (50%)	31,36,39	3.62	15 (48%)
72	OMG	L5	4494	72	23,26,27	0.52	0	33,38,41	0.52	0
72	A2M	L5	4571	72	22,25,26	3.94	10 (45%)	31,36,39	3.75	15 (48%)
72	PSU	L5	1677	72	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
72	PSU	L5	5001	72	18,21,22	1.05	1 (5%)	22,30,33	1.68	4 (18%)
76	PSU	S2	1004	76	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
72	PSU	L5	4471	72	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
76	OMG	S2	644	76	23,26,27	0.49	0	33,38,41	0.51	0
69	4SU	Pt	8	69	18,21,22	3.80	8 (44%)	26,30,33	2.22	5 (19%)
76	PSU	S2	966	76	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
72	PSU	L5	1781	72	18,21,22	1.06	1 (5%)	22,30,33	1.68	4 (18%)
72	PSU	L5	3768	72	18,21,22	1.07	1 (5%)	22,30,33	1.69	4 (18%)
72	PSU	L5	4569	72	18,21,22	1.09	1 (5%)	22,30,33	1.67	4 (18%)
76	PSU	S2	1239	76	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
76	4AC	S2	1337	76	21,24,25	3.52	10 (47%)	29,34,37	1.08	3 (10%)
72	PSU	L5	4457	72	18,21,22	1.05	1 (5%)	22,30,33	1.75	5 (22%)
72	OMC	L5	3808	72	19,22,23	0.61	0	26,31,34	0.91	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	PSU	L5	1536	72	18,21,22	1.08	1 (5%)	22,30,33	1.80	4 (18%)
76	6MZ	S2	1832	76,83	22,25,26	2.63	3 (13%)	30,36,39	2.50	12 (40%)
72	PSU	L5	1862	72	18,21,22	1.03	1 (5%)	22,30,33	1.76	4 (18%)
76	4AC	S2	1842	76	21,24,25	3.43	10 (47%)	29,34,37	1.09	3 (10%)
76	OMU	S2	428	76	19,22,23	3.02	8 (42%)	26,31,34	1.74	5 (19%)
76	PSU	S2	105	76	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
76	PSU	S2	822	76	18,21,22	1.11	2 (11%)	22,30,33	1.83	5 (22%)
76	PSU	S2	1244	76	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
72	OMG	L5	1625	72	23,26,27	0.51	0	33,38,41	0.50	0
72	PSU	L5	3695	72	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
72	OMG	L5	4370	72	23,26,27	0.51	0	33,38,41	0.49	0
72	PSU	L5	1782	72	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
76	MA6	S2	1850	76	23,26,27	1.47	4 (17%)	34,38,41	3.31	12 (35%)
72	PSU	L5	4431	72	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
76	PSU	S2	1056	76	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
76	PSU	S2	1177	76	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
72	PSU	L5	4531	72	18,21,22	1.07	1 (5%)	22,30,33	1.80	5 (22%)
76	OMC	S2	462	76	19,22,23	0.54	0	26,31,34	0.71	0
72	PSU	L5	4636	72	18,21,22	1.07	1 (5%)	22,30,33	1.89	6 (27%)
76	A2M	S2	27	76,83	22,25,26	3.92	10 (45%)	31,36,39	3.68	13 (41%)

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
76	PSU	S2	1347	76	-	0/7/25/26	0/2/2/2
72	A2M	L5	2401	72	-	0/9/27/28	0/3/3/3
76	OMU	S2	116	76	-	1/9/27/28	0/2/2/2
72	OMG	L5	4637	72	-	3/9/27/28	0/3/3/3
76	PSU	S2	609	76	-	0/7/25/26	0/2/2/2
76	OMU	S2	627	76	-	4/9/27/28	0/2/2/2
72	PSU	L5	3853	72,84	-	0/7/25/26	0/2/2/2
72	PSU	L5	2843	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	1340	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	3734	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	3841	72	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	A2M	S2	576	76	-	3/9/27/28	0/3/3/3
76	OMG	S2	1328	76	-	0/9/27/28	0/3/3/3
76	OMG	S2	1490	76	-	1/9/27/28	0/3/3/3
72	OMG	L5	4196	69,72	-	1/9/27/28	0/3/3/3
76	PSU	S2	815	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	4228	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	801	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	1316	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4403	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3762	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4972	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4552	72	-	0/7/25/26	0/2/2/2
76	A2M	S2	1383	76	-	1/9/27/28	0/3/3/3
69	PSU	Pt	56	69	-	0/7/25/26	0/2/2/2
76	OMG	S2	509	76	-	1/9/27/28	0/3/3/3
76	PSU	S2	1445	76	-	0/7/25/26	0/2/2/2
76	A2M	S2	484	76	-	1/9/27/28	0/3/3/3
72	OMC	L5	2422	72,84	-	2/9/27/28	0/2/2/2
72	PSU	L5	3770	72	-	0/7/25/26	0/2/2/2
76	OMG	S2	1447	76	-	3/9/27/28	0/3/3/3
72	6MZ	L5	4220	72	-	0/9/27/28	0/3/3/3
72	A2M	L5	398	72	-	3/9/27/28	0/3/3/3
72	A2M	L5	3867	72	-	3/9/27/28	0/3/3/3
72	A2M	L5	1871	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4353	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	4536	72	-	0/9/27/28	0/2/2/2
76	PSU	S2	573	76	-	0/7/25/26	0/2/2/2
76	OMG	S2	436	76	-	0/9/27/28	0/3/3/3
76	PSU	S2	649	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	2364	72	-	2/9/27/28	0/3/3/3
72	OMC	L5	2351	72	-	2/9/27/28	0/2/2/2
72	OMU	L5	4227	72	-	0/9/27/28	0/2/2/2
69	H2U	Pt	21	69	-	4/7/38/39	0/2/2/2
72	PSU	L5	4442	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	3627	72	-	0/9/27/28	0/3/3/3
76	OMC	S2	517	76	-	0/9/27/28	0/2/2/2
72	OMG	L5	3899	72,83	-	0/9/27/28	0/3/3/3
76	A2M	S2	468	76	-	2/9/27/28	0/3/3/3
76	PSU	S2	572	76	-	0/7/25/26	0/2/2/2
72	OMU	L5	2837	72	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	A2M	L5	1326	72	-	1/9/27/28	0/3/3/3
76	A2M	S2	1678	76	-	1/9/27/28	0/3/3/3
72	A2M	L5	3785	72	-	3/9/27/28	0/3/3/3
76	PSU	S2	218	76	-	0/7/25/26	0/2/2/2
72	5MC	L5	4447	72	-	4/7/25/26	0/2/2/2
72	A2M	L5	3830	72	-	0/9/27/28	0/3/3/3
72	OMG	L5	4392	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	1367	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	3884	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4296	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	1779	72	-	0/7/25/26	0/2/2/2
76	A2M	S2	512	76	-	2/9/27/28	0/3/3/3
76	PSU	S2	918	76	-	2/7/25/26	0/2/2/2
65	MLZ	Lb	5	65	-	3/7/8/10	-
72	A2M	L5	4590	72	-	1/9/27/28	0/3/3/3
76	PSU	S2	1232	76	-	2/7/25/26	0/2/2/2
72	OMC	L5	3887	72	-	1/9/27/28	0/2/2/2
72	OMG	L5	1522	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4312	72	-	0/7/25/26	0/2/2/2
76	OMC	S2	1703	76	-	0/9/27/28	0/2/2/2
66	V5N	LA	216	66	-	1/9/10/12	0/1/1/1
72	PSU	L5	4521	72,83	-	0/7/25/26	0/2/2/2
72	OMG	L5	4623	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	1136	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	109	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	1792	72	-	0/7/25/26	0/2/2/2
76	B8N	S2	1248	76	-	4/16/34/35	0/2/2/2
76	PSU	S2	119	76	-	2/7/25/26	0/2/2/2
76	PSU	S2	406	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	1683	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	2824	72	-	1/9/27/28	0/2/2/2
72	OMU	L5	3925	72	-	1/9/27/28	0/2/2/2
72	PSU	L5	4299	72	-	0/7/25/26	0/2/2/2
76	OMG	S2	683	76	-	2/9/27/28	0/3/3/3
72	OMC	L5	3701	82,72,84	-	4/9/27/28	0/2/2/2
71	PSU	L8	69	71	-	2/7/25/26	0/2/2/2
72	A2M	L5	4523	72,83	-	1/9/27/28	0/3/3/3
76	PSU	S2	36	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1625	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4576	72	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	A2M	L5	2363	72,83,84	-	0/9/27/28	0/3/3/3
72	PSU	L5	3639	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4293	72	-	0/7/25/26	0/2/2/2
76	OMU	S2	1804	76	-	0/9/27/28	0/2/2/2
72	5MC	L5	3782	72,83	-	0/7/25/26	0/2/2/2
72	PSU	L5	3844	72	-	3/7/25/26	0/2/2/2
72	A2M	L5	1534	72,83	-	2/9/27/28	0/3/3/3
76	PSU	S2	1238	76	-	1/7/25/26	0/2/2/2
69	OMC	Pt	33	69	-	1/9/27/28	0/2/2/2
72	PSU	L5	3758	72	-	2/7/25/26	0/2/2/2
72	OMU	L5	4498	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	4579	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4500	72	-	1/7/25/26	0/2/2/2
72	PSU	L5	4493	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3637	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4673	72	-	0/7/25/26	0/2/2/2
72	1MA	L5	1322	72,84	-	2/7/25/26	0/3/3/3
76	PSU	S2	1081	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4532	72	-	0/7/25/26	0/2/2/2
76	G7M	S2	1639	76,69	-	2/7/25/26	0/3/3/3
72	PSU	L5	4689	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	4456	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	2508	72	-	2/7/25/26	0/2/2/2
72	PSU	L5	1860	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	34	76	-	0/7/25/26	0/2/2/2
76	OMC	S2	1391	76	-	0/9/27/28	0/2/2/2
76	PSU	S2	1243	76	-	2/7/25/26	0/2/2/2
71	PSU	L8	55	71	-	0/7/25/26	0/2/2/2
72	A2M	L5	3760	72	-	4/9/27/28	0/3/3/3
76	PSU	S2	681	76	-	0/7/25/26	0/2/2/2
72	UR3	L5	4530	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	4499	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	4628	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3729	72	-	2/7/25/26	0/2/2/2
76	PSU	S2	93	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1643	76,83	-	0/7/25/26	0/2/2/2
72	PSU	L5	4423	72	-	0/7/25/26	0/2/2/2
76	MA6	S2	1851	76	-	1/11/29/30	0/3/3/3
72	PSU	L5	4420	72	-	3/7/25/26	0/2/2/2
71	OMG	L8	75	71	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	PSU	L5	2839	72	-	0/7/25/26	0/2/2/2
67	V5N	La	39	67	-	0/9/10/12	0/1/1/1
72	OMG	L5	3792	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	1744	72	-	0/7/25/26	0/2/2/2
72	A2M	L5	3724	72	-	1/9/27/28	0/3/3/3
72	PSU	L5	3764	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	866	76	-	0/7/25/26	0/2/2/2
72	OMU	L5	4620	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	1582	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	686	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1692	76	-	0/7/25/26	0/2/2/2
76	A2M	S2	590	76	-	6/9/27/28	0/3/3/3
72	OMG	L5	2876	72	-	2/9/27/28	0/3/3/3
72	OMC	L5	2861	72	-	0/9/27/28	0/2/2/2
3	MLZ	Lo	53	3	-	3/7/8/10	-
72	OMC	L5	1881	82,72	-	0/9/27/28	0/2/2/2
72	PSU	L5	2632	72	-	0/7/25/26	0/2/2/2
76	A2M	S2	99	76	-	2/9/27/28	0/3/3/3
72	A2M	L5	2815	72,84	-	1/9/27/28	0/3/3/3
76	PSU	S2	651	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	3920	72,83	-	0/7/25/26	0/2/2/2
72	PSU	L5	3715	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	3744	72	-	0/9/27/28	0/3/3/3
76	PSU	S2	296	76	-	0/7/25/26	0/2/2/2
72	OMC	L5	3869	72	-	0/9/27/28	0/2/2/2
72	A2M	L5	3825	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	3851	72	-	0/7/25/26	0/2/2/2
72	A2M	L5	400	72	-	1/9/27/28	0/3/3/3
72	OMG	L5	2424	72	-	0/9/27/28	0/3/3/3
72	A2M	L5	3718	72	-	1/9/27/28	0/3/3/3
72	PSU	L5	5010	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	2365	72,83	-	0/9/27/28	0/2/2/2
72	OMC	L5	2804	72	-	0/9/27/28	0/2/2/2
72	PSU	L5	4361	72	-	1/7/25/26	0/2/2/2
76	OMG	S2	867	76	-	1/9/27/28	0/3/3/3
76	PSU	S2	814	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1174	76	-	0/7/25/26	0/2/2/2
72	A2M	L5	1524	72	-	0/9/27/28	0/3/3/3
76	A2M	S2	1031	76	-	0/9/27/28	0/3/3/3
69	G7M	Pt	47	69	-	1/7/25/26	0/3/3/3
76	PSU	S2	863	76	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	OMG	L5	4618	72	-	0/9/27/28	0/3/3/3
76	A2M	S2	668	76,83	-	3/9/27/28	0/3/3/3
72	OMG	L5	4494	72	-	0/9/27/28	0/3/3/3
72	A2M	L5	4571	72	-	0/9/27/28	0/3/3/3
72	PSU	L5	1677	72	-	3/7/25/26	0/2/2/2
72	PSU	L5	5001	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	1004	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4471	72	-	0/7/25/26	0/2/2/2
76	OMG	S2	644	76	-	4/9/27/28	0/3/3/3
69	4SU	Pt	8	69	-	0/7/25/26	0/2/2/2
76	PSU	S2	966	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	1781	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	3768	72	-	0/7/25/26	0/2/2/2
72	PSU	L5	4569	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	1239	76	-	1/7/25/26	0/2/2/2
76	4AC	S2	1337	76	-	0/11/29/30	0/2/2/2
72	PSU	L5	4457	72	-	0/7/25/26	0/2/2/2
72	OMC	L5	3808	72	-	1/9/27/28	0/2/2/2
72	PSU	L5	1536	72	-	0/7/25/26	0/2/2/2
76	6MZ	S2	1832	76,83	-	2/9/27/28	0/3/3/3
72	PSU	L5	1862	72	-	0/7/25/26	0/2/2/2
76	4AC	S2	1842	76	-	0/11/29/30	0/2/2/2
76	OMU	S2	428	76	-	5/9/27/28	0/2/2/2
76	PSU	S2	105	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	822	76	-	1/7/25/26	0/2/2/2
76	PSU	S2	1244	76	-	0/7/25/26	0/2/2/2
72	OMG	L5	1625	72	-	2/9/27/28	0/3/3/3
72	PSU	L5	3695	72	-	0/7/25/26	0/2/2/2
72	OMG	L5	4370	72	-	1/9/27/28	0/3/3/3
72	PSU	L5	1782	72	-	0/7/25/26	0/2/2/2
76	MA6	S2	1850	76	-	1/11/29/30	0/3/3/3
72	PSU	L5	4431	72	-	0/7/25/26	0/2/2/2
76	PSU	S2	1056	76	-	0/7/25/26	0/2/2/2
76	PSU	S2	1177	76	-	0/7/25/26	0/2/2/2
72	PSU	L5	4531	72	-	0/7/25/26	0/2/2/2
76	OMC	S2	462	76	-	0/9/27/28	0/2/2/2
72	PSU	L5	4636	72	-	4/7/25/26	0/2/2/2
76	A2M	S2	27	76,83	-	1/9/27/28	0/3/3/3

All (560) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	3867	A2M	C3'-C2'	-12.75	1.24	1.52
72	L5	1534	A2M	C3'-C2'	-12.70	1.24	1.52
72	L5	4590	A2M	C3'-C2'	-12.69	1.24	1.52
76	S2	590	A2M	C3'-C2'	-12.68	1.24	1.52
76	S2	1031	A2M	C3'-C2'	-12.66	1.24	1.52
76	S2	468	A2M	C3'-C2'	-12.63	1.24	1.52
76	S2	512	A2M	C3'-C2'	-12.62	1.24	1.52
72	L5	1326	A2M	C3'-C2'	-12.62	1.24	1.52
72	L5	3830	A2M	C3'-C2'	-12.61	1.24	1.52
72	L5	3760	A2M	C3'-C2'	-12.61	1.24	1.52
72	L5	4571	A2M	C3'-C2'	-12.61	1.24	1.52
72	L5	1524	A2M	C3'-C2'	-12.59	1.24	1.52
72	L5	2363	A2M	C3'-C2'	-12.59	1.24	1.52
76	S2	1678	A2M	C3'-C2'	-12.58	1.24	1.52
76	S2	1383	A2M	C3'-C2'	-12.58	1.24	1.52
72	L5	3825	A2M	C3'-C2'	-12.58	1.24	1.52
76	S2	99	A2M	C3'-C2'	-12.58	1.24	1.52
76	S2	27	A2M	C3'-C2'	-12.57	1.24	1.52
72	L5	2401	A2M	C3'-C2'	-12.57	1.24	1.52
72	L5	1871	A2M	C3'-C2'	-12.56	1.24	1.52
72	L5	400	A2M	C3'-C2'	-12.55	1.25	1.52
72	L5	3724	A2M	C3'-C2'	-12.53	1.25	1.52
76	S2	576	A2M	C3'-C2'	-12.53	1.25	1.52
72	L5	3718	A2M	C3'-C2'	-12.51	1.25	1.52
72	L5	2815	A2M	C3'-C2'	-12.51	1.25	1.52
72	L5	3785	A2M	C3'-C2'	-12.46	1.25	1.52
72	L5	398	A2M	C3'-C2'	-12.45	1.25	1.52
72	L5	4523	A2M	C3'-C2'	-12.45	1.25	1.52
76	S2	484	A2M	C3'-C2'	-12.19	1.25	1.52
76	S2	668	A2M	C3'-C2'	-12.08	1.26	1.52
76	S2	1832	6MZ	C6-N6	11.02	1.46	1.34
72	L5	4220	6MZ	C6-N6	10.09	1.45	1.34
69	Pt	8	4SU	C4-N3	8.18	1.46	1.37
76	S2	1248	B8N	C4-N3	-7.92	1.25	1.40
76	S2	1248	B8N	C6-N1	7.59	1.55	1.36
72	L5	4530	UR3	C2-N1	7.25	1.48	1.38
76	S2	1337	4AC	C4-N3	7.22	1.45	1.32
69	Pt	8	4SU	C2-N3	7.12	1.50	1.38
76	S2	1804	OMU	C2-N1	7.08	1.49	1.38
76	S2	1842	4AC	C4-N3	7.04	1.45	1.32
72	L5	3925	OMU	C2-N1	7.00	1.49	1.38
76	S2	627	OMU	C2-N1	7.00	1.49	1.38
72	L5	2837	OMU	C2-N1	6.99	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S2	116	OMU	C2-N1	6.98	1.49	1.38
72	L5	4498	OMU	C2-N1	6.97	1.49	1.38
72	L5	4227	OMU	C2-N1	6.94	1.49	1.38
76	S2	428	OMU	C2-N1	6.92	1.49	1.38
76	S2	668	A2M	O4'-C4'	-6.91	1.29	1.45
76	S2	627	OMU	C2-N3	6.86	1.50	1.38
76	S2	116	OMU	C2-N3	6.85	1.50	1.38
76	S2	1337	4AC	C2-N3	6.84	1.50	1.36
76	S2	428	OMU	C2-N3	6.81	1.50	1.38
69	Pt	8	4SU	C2-N1	6.80	1.49	1.38
76	S2	1804	OMU	C2-N3	6.79	1.50	1.38
72	L5	4620	OMU	C2-N1	6.72	1.49	1.38
72	L5	3925	OMU	C2-N3	6.72	1.49	1.38
72	L5	4498	OMU	C2-N3	6.69	1.49	1.38
72	L5	2837	OMU	C2-N3	6.69	1.49	1.38
72	L5	1524	A2M	O4'-C4'	-6.68	1.30	1.45
76	S2	1842	4AC	C2-N3	6.67	1.49	1.36
76	S2	1639	G7M	C4-N3	6.65	1.50	1.34
76	S2	590	A2M	O4'-C4'	-6.62	1.30	1.45
72	L5	3867	A2M	O4'-C4'	-6.62	1.30	1.45
76	S2	1678	A2M	O4'-C4'	-6.61	1.30	1.45
72	L5	4227	OMU	C2-N3	6.61	1.49	1.38
72	L5	4620	OMU	C2-N3	6.57	1.49	1.38
72	L5	1326	A2M	O4'-C4'	-6.56	1.30	1.45
72	L5	4571	A2M	O4'-C4'	-6.56	1.30	1.45
72	L5	4590	A2M	O4'-C4'	-6.53	1.30	1.45
72	L5	400	A2M	O4'-C4'	-6.53	1.30	1.45
72	L5	2815	A2M	O4'-C4'	-6.52	1.30	1.45
76	S2	512	A2M	O4'-C4'	-6.52	1.30	1.45
76	S2	484	A2M	O4'-C4'	-6.50	1.30	1.45
72	L5	3825	A2M	O4'-C4'	-6.50	1.30	1.45
76	S2	576	A2M	O4'-C4'	-6.50	1.30	1.45
72	L5	3724	A2M	O4'-C4'	-6.49	1.30	1.45
72	L5	2363	A2M	O4'-C4'	-6.48	1.30	1.45
66	LA	216	V5N	CG-ND1	-6.48	1.31	1.37
76	S2	1031	A2M	O4'-C4'	-6.47	1.30	1.45
72	L5	2401	A2M	O4'-C4'	-6.45	1.30	1.45
76	S2	27	A2M	O4'-C4'	-6.44	1.30	1.45
69	Pt	47	G7M	C4-N3	6.42	1.49	1.34
76	S2	468	A2M	O4'-C4'	-6.40	1.30	1.45
72	L5	3785	A2M	O4'-C4'	-6.40	1.30	1.45
67	La	39	V5N	CG-ND1	-6.39	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	398	A2M	O4'-C4'	-6.36	1.30	1.45
72	L5	3830	A2M	O4'-C4'	-6.36	1.30	1.45
72	L5	1871	A2M	O4'-C4'	-6.36	1.30	1.45
72	L5	4523	A2M	O4'-C4'	-6.35	1.30	1.45
76	S2	99	A2M	O4'-C4'	-6.34	1.30	1.45
76	S2	1383	A2M	O4'-C4'	-6.34	1.30	1.45
76	S2	1337	4AC	C6-C5	6.33	1.49	1.35
72	L5	3718	A2M	O4'-C4'	-6.33	1.30	1.45
72	L5	3760	A2M	O4'-C4'	-6.31	1.30	1.45
72	L5	1534	A2M	O4'-C4'	-6.28	1.31	1.45
76	S2	1842	4AC	C6-C5	6.21	1.49	1.35
72	L5	4530	UR3	C6-C5	6.06	1.49	1.35
69	Pt	8	4SU	C6-C5	5.92	1.48	1.35
76	S2	1248	B8N	C6-C5	5.92	1.43	1.34
76	S2	1639	G7M	C2-N2	5.89	1.48	1.34
76	S2	1248	B8N	C2-N1	5.88	1.56	1.39
72	L5	3785	A2M	C3'-C4'	5.87	1.68	1.53
76	S2	428	OMU	C6-C5	5.69	1.48	1.35
69	Pt	47	G7M	C2-N2	5.69	1.47	1.34
76	S2	627	OMU	C6-C5	5.68	1.48	1.35
72	L5	4227	OMU	C6-C5	5.67	1.48	1.35
76	S2	1804	OMU	C6-C5	5.64	1.48	1.35
72	L5	4498	OMU	C6-C5	5.63	1.48	1.35
72	L5	2837	OMU	C6-C5	5.62	1.48	1.35
72	L5	4620	OMU	C6-C5	5.57	1.48	1.35
72	L5	3925	OMU	C6-C5	5.57	1.48	1.35
76	S2	1337	4AC	C4-N4	5.56	1.47	1.39
76	S2	116	OMU	C6-C5	5.56	1.48	1.35
76	S2	1639	G7M	C2-N3	5.49	1.46	1.33
72	L5	3760	A2M	C3'-C4'	5.47	1.67	1.53
72	L5	3760	A2M	C6-N6	5.46	1.47	1.34
76	S2	1678	A2M	C6-N6	5.44	1.47	1.34
76	S2	512	A2M	C6-N6	5.42	1.47	1.34
76	S2	590	A2M	C6-N6	5.42	1.47	1.34
72	L5	4571	A2M	C6-N6	5.42	1.47	1.34
72	L5	3724	A2M	C6-N6	5.41	1.47	1.34
76	S2	1842	4AC	C4-N4	5.41	1.47	1.39
76	S2	1383	A2M	C6-N6	5.41	1.47	1.34
76	S2	576	A2M	C6-N6	5.40	1.47	1.34
72	L5	3718	A2M	C6-N6	5.40	1.47	1.34
76	S2	468	A2M	C6-N6	5.40	1.47	1.34
76	S2	484	A2M	C6-N6	5.40	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S2	27	A2M	C6-N6	5.39	1.47	1.34
72	L5	398	A2M	C6-N6	5.39	1.47	1.34
72	L5	1534	A2M	C3'-C4'	5.38	1.66	1.53
72	L5	1524	A2M	C6-N6	5.38	1.47	1.34
72	L5	1871	A2M	C6-N6	5.37	1.47	1.34
76	S2	1031	A2M	C6-N6	5.37	1.47	1.34
72	L5	400	A2M	C6-N6	5.37	1.47	1.34
72	L5	2401	A2M	C6-N6	5.36	1.47	1.34
76	S2	668	A2M	C6-N6	5.36	1.47	1.34
72	L5	1326	A2M	C6-N6	5.35	1.47	1.34
72	L5	2815	A2M	C6-N6	5.35	1.47	1.34
72	L5	3867	A2M	C6-N6	5.35	1.47	1.34
72	L5	4523	A2M	C6-N6	5.35	1.47	1.34
72	L5	4590	A2M	C6-N6	5.33	1.47	1.34
72	L5	2363	A2M	C6-N6	5.33	1.47	1.34
76	S2	99	A2M	C6-N6	5.33	1.47	1.34
72	L5	3825	A2M	C6-N6	5.32	1.47	1.34
72	L5	3830	A2M	C6-N6	5.30	1.47	1.34
72	L5	1534	A2M	C6-N6	5.26	1.47	1.34
76	S2	484	A2M	C3'-C4'	5.25	1.66	1.53
72	L5	4523	A2M	C3'-C4'	5.24	1.66	1.53
76	S2	1678	A2M	C3'-C4'	5.24	1.66	1.53
72	L5	2363	A2M	C3'-C4'	5.22	1.66	1.53
72	L5	3785	A2M	C6-N6	5.21	1.47	1.34
76	S2	27	A2M	C3'-C4'	5.21	1.66	1.53
76	S2	668	A2M	C3'-C4'	5.20	1.66	1.53
69	Pt	47	G7M	C2-N3	5.19	1.45	1.33
76	S2	1383	A2M	C3'-C4'	5.17	1.66	1.53
76	S2	99	A2M	C3'-C4'	5.17	1.66	1.53
72	L5	3718	A2M	C3'-C4'	5.17	1.66	1.53
76	S2	468	A2M	C3'-C4'	5.16	1.66	1.53
72	L5	398	A2M	C3'-C4'	5.16	1.66	1.53
72	L5	1326	A2M	C3'-C4'	5.15	1.66	1.53
72	L5	1871	A2M	C3'-C4'	5.15	1.66	1.53
76	S2	512	A2M	C3'-C4'	5.15	1.66	1.53
72	L5	3724	A2M	C3'-C4'	5.15	1.66	1.53
76	S2	590	A2M	C3'-C4'	5.14	1.66	1.53
72	L5	2815	A2M	C3'-C4'	5.13	1.66	1.53
72	L5	400	A2M	C3'-C4'	5.11	1.66	1.53
76	S2	1031	A2M	C3'-C4'	5.11	1.66	1.53
72	L5	1524	A2M	C3'-C4'	5.10	1.66	1.53
72	L5	3825	A2M	C3'-C4'	5.10	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	3830	A2M	C3'-C4'	5.09	1.66	1.53
72	L5	4590	A2M	C3'-C4'	5.09	1.66	1.53
76	S2	576	A2M	C3'-C4'	5.08	1.66	1.53
72	L5	3867	A2M	C3'-C4'	5.07	1.65	1.53
72	L5	4571	A2M	C3'-C4'	5.07	1.65	1.53
69	Pt	8	4SU	C5-C4	5.06	1.49	1.42
72	L5	2401	A2M	C3'-C4'	5.05	1.65	1.53
72	L5	1524	A2M	C1'-N9	-4.94	1.32	1.46
76	S2	590	A2M	C1'-N9	-4.89	1.32	1.46
72	L5	3760	A2M	C1'-N9	-4.87	1.32	1.46
72	L5	4530	UR3	C2-N3	4.85	1.48	1.39
76	S2	576	A2M	C1'-N9	-4.64	1.33	1.46
76	S2	1851	MA6	C6-N6	4.62	1.50	1.36
76	S2	1337	4AC	C5-C4	4.62	1.50	1.40
76	S2	1850	MA6	C6-N6	4.59	1.50	1.36
72	L5	4590	A2M	C1'-N9	-4.57	1.33	1.46
76	S2	1383	A2M	O4'-C1'	4.55	1.52	1.42
76	S2	1337	4AC	C2-N1	4.55	1.49	1.40
72	L5	1534	A2M	C1'-N9	-4.51	1.33	1.46
69	Pt	8	4SU	C4-S4	-4.50	1.59	1.68
76	S2	1678	A2M	O4'-C1'	4.48	1.52	1.42
72	L5	398	A2M	O4'-C1'	4.47	1.52	1.42
72	L5	3830	A2M	C1'-N9	-4.46	1.33	1.46
72	L5	1871	A2M	O4'-C1'	4.46	1.52	1.42
76	S2	512	A2M	C1'-N9	-4.46	1.33	1.46
72	L5	4590	A2M	O4'-C1'	4.45	1.52	1.42
76	S2	99	A2M	O4'-C1'	4.45	1.52	1.42
72	L5	2815	A2M	O4'-C1'	4.45	1.52	1.42
72	L5	2401	A2M	O4'-C1'	4.45	1.52	1.42
76	S2	1842	4AC	C5-C4	4.44	1.50	1.40
72	L5	3724	A2M	O4'-C1'	4.43	1.52	1.42
72	L5	2815	A2M	C1'-N9	-4.43	1.33	1.46
72	L5	3785	A2M	C1'-N9	-4.43	1.33	1.46
72	L5	3830	A2M	O4'-C1'	4.43	1.52	1.42
72	L5	3825	A2M	O4'-C1'	4.42	1.52	1.42
72	L5	4571	A2M	C1'-N9	-4.42	1.33	1.46
72	L5	2363	A2M	O4'-C1'	4.41	1.52	1.42
72	L5	2401	A2M	C1'-N9	-4.41	1.33	1.46
76	S2	576	A2M	O4'-C1'	4.41	1.52	1.42
72	L5	4571	A2M	O4'-C1'	4.41	1.52	1.42
72	L5	3718	A2M	O4'-C1'	4.41	1.52	1.42
76	S2	1031	A2M	O4'-C1'	4.40	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S2	468	A2M	O4'-C1'	4.40	1.52	1.42
72	L5	1871	A2M	C1'-N9	-4.39	1.33	1.46
72	L5	400	A2M	O4'-C1'	4.39	1.52	1.42
76	S2	512	A2M	O4'-C1'	4.39	1.52	1.42
72	L5	4523	A2M	O4'-C1'	4.36	1.52	1.42
72	L5	400	A2M	C1'-N9	-4.36	1.34	1.46
76	S2	468	A2M	C1'-N9	-4.35	1.34	1.46
76	S2	1031	A2M	C1'-N9	-4.35	1.34	1.46
76	S2	1842	4AC	C2-N1	4.34	1.49	1.40
76	S2	27	A2M	O4'-C1'	4.34	1.52	1.42
72	L5	3867	A2M	O4'-C1'	4.34	1.52	1.42
72	L5	1326	A2M	O4'-C1'	4.33	1.52	1.42
76	S2	1337	4AC	C7-N4	4.33	1.45	1.37
76	S2	27	A2M	C1'-N9	-4.33	1.34	1.46
72	L5	3724	A2M	C1'-N9	-4.33	1.34	1.46
72	L5	2363	A2M	C1'-N9	-4.32	1.34	1.46
76	S2	99	A2M	C1'-N9	-4.32	1.34	1.46
72	L5	1326	A2M	C1'-N9	-4.32	1.34	1.46
76	S2	668	A2M	C1'-N9	-4.30	1.34	1.46
72	L5	1534	A2M	O4'-C1'	4.30	1.52	1.42
72	L5	3867	A2M	C1'-N9	-4.30	1.34	1.46
76	S2	1678	A2M	C1'-N9	-4.30	1.34	1.46
72	L5	3825	A2M	C1'-N9	-4.28	1.34	1.46
72	L5	398	A2M	C1'-N9	-4.28	1.34	1.46
76	S2	1383	A2M	C1'-N9	-4.26	1.34	1.46
76	S2	1842	4AC	C7-N4	4.22	1.45	1.37
76	S2	484	A2M	O4'-C1'	4.22	1.52	1.42
72	L5	4523	A2M	C1'-N9	-4.22	1.34	1.46
76	S2	590	A2M	O4'-C1'	4.20	1.52	1.42
76	S2	627	OMU	C4-N3	4.19	1.46	1.38
76	S2	1804	OMU	C4-N3	4.19	1.46	1.38
72	L5	3718	A2M	C1'-N9	-4.19	1.34	1.46
72	L5	3760	A2M	O4'-C1'	4.16	1.51	1.42
76	S2	116	OMU	C4-N3	4.15	1.46	1.38
69	Pt	47	G7M	C5-C6	4.14	1.55	1.43
76	S2	428	OMU	C4-N3	4.10	1.45	1.38
76	S2	1639	G7M	C5-C6	4.10	1.54	1.43
76	S2	484	A2M	C1'-N9	-4.10	1.34	1.46
67	La	39	V5N	CD2-NE2	-4.09	1.31	1.37
72	L5	1524	A2M	O4'-C1'	4.08	1.51	1.42
66	LA	216	V5N	CD2-NE2	-4.08	1.31	1.37
72	L5	4498	OMU	C4-N3	4.01	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	2837	OMU	C4-N3	3.99	1.45	1.38
72	L5	3925	OMU	C4-N3	3.99	1.45	1.38
76	S2	668	A2M	O4'-C1'	3.91	1.51	1.42
76	S2	1639	G7M	C5-N7	-3.90	1.34	1.39
72	L5	4227	OMU	C4-N3	3.90	1.45	1.38
72	L5	4620	OMU	C4-N3	3.84	1.45	1.38
69	Pt	47	G7M	C5-N7	-3.75	1.34	1.39
72	L5	3785	A2M	O4'-C1'	3.73	1.50	1.42
76	S2	1337	4AC	C6-N1	3.67	1.46	1.38
72	L5	3762	PSU	C6-C5	3.67	1.39	1.35
76	S2	1232	PSU	C6-C5	3.66	1.39	1.35
69	Pt	56	PSU	C6-C5	3.62	1.39	1.35
76	S2	1239	PSU	C6-C5	3.58	1.39	1.35
76	S2	1244	PSU	C6-C5	3.58	1.39	1.35
76	S2	93	PSU	C6-C5	3.55	1.39	1.35
76	S2	1842	4AC	C6-N1	3.53	1.46	1.38
69	Pt	47	G7M	C2-N1	3.53	1.46	1.37
72	L5	4552	PSU	C6-C5	3.53	1.39	1.35
72	L5	4569	PSU	C6-C5	3.52	1.39	1.35
76	S2	1639	G7M	C2-N1	3.52	1.46	1.37
72	L5	4296	PSU	C6-C5	3.51	1.39	1.35
76	S2	1004	PSU	C6-C5	3.50	1.39	1.35
76	S2	801	PSU	C6-C5	3.50	1.39	1.35
76	S2	866	PSU	C6-C5	3.50	1.39	1.35
76	S2	1445	PSU	C6-C5	3.49	1.39	1.35
72	L5	4312	PSU	C6-C5	3.49	1.39	1.35
76	S2	609	PSU	C6-C5	3.48	1.39	1.35
72	L5	4420	PSU	C6-C5	3.48	1.39	1.35
76	S2	1238	PSU	C6-C5	3.47	1.39	1.35
76	S2	1243	PSU	C6-C5	3.47	1.39	1.35
72	L5	3729	PSU	C6-C5	3.46	1.39	1.35
76	S2	1367	PSU	C6-C5	3.46	1.39	1.35
76	S2	573	PSU	C6-C5	3.45	1.39	1.35
76	S2	1643	PSU	C6-C5	3.45	1.39	1.35
76	S2	649	PSU	C6-C5	3.45	1.39	1.35
72	L5	2508	PSU	C6-C5	3.44	1.39	1.35
76	S2	966	PSU	C6-C5	3.43	1.39	1.35
76	S2	863	PSU	C6-C5	3.43	1.39	1.35
76	S2	1177	PSU	C6-C5	3.43	1.39	1.35
72	L5	1744	PSU	C6-C5	3.42	1.39	1.35
76	S2	406	PSU	C6-C5	3.42	1.39	1.35
72	L5	1582	PSU	C6-C5	3.42	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	3637	PSU	C6-C5	3.42	1.39	1.35
72	L5	1792	PSU	C6-C5	3.42	1.39	1.35
72	L5	3768	PSU	C6-C5	3.42	1.39	1.35
72	L5	1781	PSU	C6-C5	3.42	1.39	1.35
72	L5	2632	PSU	C6-C5	3.41	1.39	1.35
72	L5	4531	PSU	C6-C5	3.41	1.39	1.35
72	L5	1782	PSU	C6-C5	3.41	1.39	1.35
72	L5	4431	PSU	C6-C5	3.41	1.39	1.35
76	S2	109	PSU	C6-C5	3.41	1.39	1.35
76	S2	1625	PSU	C6-C5	3.41	1.39	1.35
72	L5	5001	PSU	C6-C5	3.41	1.39	1.35
76	S2	1347	PSU	C6-C5	3.40	1.39	1.35
72	L5	4423	PSU	C6-C5	3.40	1.39	1.35
76	S2	822	PSU	C6-C5	3.40	1.39	1.35
76	S2	1692	PSU	C6-C5	3.40	1.39	1.35
72	L5	4299	PSU	C6-C5	3.39	1.39	1.35
72	L5	1779	PSU	C6-C5	3.39	1.39	1.35
76	S2	815	PSU	C6-C5	3.39	1.39	1.35
76	S2	1056	PSU	C6-C5	3.38	1.39	1.35
72	L5	3758	PSU	C6-C5	3.38	1.39	1.35
72	L5	4521	PSU	C6-C5	3.38	1.39	1.35
72	L5	1536	PSU	C6-C5	3.37	1.39	1.35
72	L5	4673	PSU	C6-C5	3.37	1.39	1.35
76	S2	651	PSU	C6-C5	3.37	1.39	1.35
76	S2	686	PSU	C6-C5	3.36	1.39	1.35
72	L5	2839	PSU	C6-C5	3.36	1.39	1.35
72	L5	3844	PSU	C6-C5	3.36	1.39	1.35
71	L8	69	PSU	C6-C5	3.36	1.39	1.35
76	S2	119	PSU	C6-C5	3.36	1.39	1.35
76	S2	1174	PSU	C6-C5	3.36	1.39	1.35
72	L5	1683	PSU	C6-C5	3.35	1.39	1.35
71	L8	55	PSU	C6-C5	3.35	1.39	1.35
72	L5	4532	PSU	C6-C5	3.35	1.39	1.35
72	L5	4972	PSU	C6-C5	3.35	1.39	1.35
72	L5	3853	PSU	C6-C5	3.34	1.39	1.35
72	L5	4493	PSU	C6-C5	3.34	1.39	1.35
76	S2	1136	PSU	C6-C5	3.34	1.39	1.35
72	L5	3695	PSU	C6-C5	3.34	1.39	1.35
72	L5	4628	PSU	C6-C5	3.34	1.39	1.35
72	L5	3920	PSU	C6-C5	3.34	1.39	1.35
76	S2	36	PSU	C6-C5	3.34	1.39	1.35
76	S2	918	PSU	C6-C5	3.33	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	3770	PSU	C6-C5	3.32	1.39	1.35
72	L5	4293	PSU	C6-C5	3.32	1.39	1.35
72	L5	1860	PSU	C6-C5	3.32	1.39	1.35
72	L5	4361	PSU	C6-C5	3.32	1.39	1.35
72	L5	4353	PSU	C6-C5	3.31	1.39	1.35
76	S2	572	PSU	C6-C5	3.31	1.39	1.35
76	S2	1081	PSU	C6-C5	3.31	1.39	1.35
72	L5	4471	PSU	C6-C5	3.31	1.39	1.35
76	S2	34	PSU	C6-C5	3.30	1.39	1.35
72	L5	2843	PSU	C6-C5	3.30	1.39	1.35
76	S2	218	PSU	C6-C5	3.30	1.39	1.35
72	L5	4576	PSU	C6-C5	3.30	1.39	1.35
72	L5	4442	PSU	C6-C5	3.30	1.39	1.35
72	L5	3715	PSU	C6-C5	3.29	1.39	1.35
76	S2	296	PSU	C6-C5	3.29	1.39	1.35
72	L5	1862	PSU	C6-C5	3.28	1.39	1.35
72	L5	5010	PSU	C6-C5	3.28	1.39	1.35
76	S2	814	PSU	C6-C5	3.28	1.39	1.35
72	L5	3639	PSU	C6-C5	3.28	1.39	1.35
72	L5	4500	PSU	C6-C5	3.28	1.39	1.35
72	L5	3884	PSU	C6-C5	3.27	1.39	1.35
72	L5	4636	PSU	C6-C5	3.26	1.39	1.35
76	S2	105	PSU	C6-C5	3.25	1.39	1.35
72	L5	3851	PSU	C6-C5	3.25	1.39	1.35
76	S2	681	PSU	C6-C5	3.22	1.39	1.35
72	L5	4457	PSU	C6-C5	3.21	1.39	1.35
72	L5	3764	PSU	C6-C5	3.20	1.39	1.35
72	L5	3734	PSU	C6-C5	3.18	1.39	1.35
76	S2	668	A2M	C2'-C1'	3.18	1.61	1.53
72	L5	4579	PSU	C6-C5	3.16	1.39	1.35
69	Pt	8	4SU	C6-N1	3.13	1.45	1.38
72	L5	4689	PSU	C6-C5	3.12	1.39	1.35
69	Pt	47	G7M	O6-C6	-3.10	1.17	1.23
72	L5	1677	PSU	C6-C5	3.09	1.38	1.35
72	L5	3760	A2M	O2'-C2'	3.09	1.50	1.42
72	L5	4530	UR3	C6-N1	3.09	1.45	1.38
72	L5	4403	PSU	C6-C5	3.08	1.38	1.35
72	L5	4498	OMU	O4-C4	-3.02	1.18	1.24
72	L5	4620	OMU	O4-C4	-3.00	1.18	1.24
76	S2	484	A2M	C2'-C1'	3.00	1.60	1.53
72	L5	2837	OMU	O4-C4	-3.00	1.18	1.24
72	L5	3925	OMU	O4-C4	-3.00	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S2	1639	G7M	O6-C6	-3.00	1.17	1.23
72	L5	4227	OMU	O4-C4	-2.99	1.18	1.24
72	L5	3724	A2M	O2'-C2'	2.98	1.50	1.42
76	S2	484	A2M	O2'-C2'	2.98	1.50	1.42
76	S2	1678	A2M	O2'-C2'	2.98	1.50	1.42
76	S2	590	A2M	O2'-C2'	2.98	1.50	1.42
72	L5	4571	A2M	O2'-C2'	2.97	1.50	1.42
72	L5	4523	A2M	C2'-C1'	2.97	1.60	1.53
72	L5	400	A2M	O2'-C2'	2.96	1.50	1.42
76	S2	1383	A2M	O2'-C2'	2.96	1.50	1.42
76	S2	468	A2M	O2'-C2'	2.96	1.50	1.42
72	L5	398	A2M	O2'-C2'	2.96	1.50	1.42
72	L5	1871	A2M	O2'-C2'	2.96	1.50	1.42
76	S2	428	OMU	O4-C4	-2.95	1.18	1.24
76	S2	116	OMU	O4-C4	-2.95	1.18	1.24
72	L5	4220	6MZ	C5-C4	-2.95	1.33	1.39
72	L5	1524	A2M	O2'-C2'	2.94	1.50	1.42
76	S2	668	A2M	O2'-C2'	2.94	1.50	1.42
72	L5	4590	A2M	O2'-C2'	2.94	1.50	1.42
76	S2	512	A2M	O2'-C2'	2.94	1.50	1.42
72	L5	1326	A2M	O2'-C2'	2.94	1.50	1.42
76	S2	576	A2M	O2'-C2'	2.94	1.50	1.42
76	S2	99	A2M	O2'-C2'	2.93	1.50	1.42
72	L5	2815	A2M	O2'-C2'	2.93	1.50	1.42
72	L5	3718	A2M	O2'-C2'	2.92	1.50	1.42
72	L5	2363	A2M	O2'-C2'	2.92	1.50	1.42
72	L5	3785	A2M	O2'-C2'	2.92	1.50	1.42
76	S2	27	A2M	O2'-C2'	2.91	1.50	1.42
72	L5	3830	A2M	O2'-C2'	2.91	1.50	1.42
72	L5	2401	A2M	O2'-C2'	2.90	1.50	1.42
72	L5	3867	A2M	O2'-C2'	2.90	1.50	1.42
72	L5	4523	A2M	O2'-C2'	2.89	1.50	1.42
76	S2	627	OMU	O4-C4	-2.89	1.18	1.24
72	L5	1534	A2M	O2'-C2'	2.89	1.50	1.42
72	L5	3785	A2M	C5-C4	-2.88	1.33	1.39
72	L5	3825	A2M	O2'-C2'	2.88	1.50	1.42
76	S2	1804	OMU	O4-C4	-2.87	1.18	1.24
72	L5	3718	A2M	C2'-C1'	2.87	1.60	1.53
72	L5	398	A2M	C2'-C1'	2.87	1.60	1.53
76	S2	627	OMU	C6-N1	2.86	1.44	1.38
76	S2	1832	6MZ	C5-C4	-2.86	1.33	1.39
76	S2	468	A2M	C2'-C1'	2.86	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S2	1031	A2M	O2'-C2'	2.86	1.49	1.42
72	L5	2815	A2M	C2'-C1'	2.86	1.60	1.53
72	L5	2401	A2M	C2'-C1'	2.85	1.60	1.53
76	S2	576	A2M	C2'-C1'	2.84	1.60	1.53
76	S2	1804	OMU	C6-N1	2.82	1.44	1.38
72	L5	3785	A2M	C2'-C1'	2.82	1.60	1.53
76	S2	1383	A2M	C2'-C1'	2.79	1.60	1.53
76	S2	428	OMU	C6-N1	2.79	1.44	1.38
76	S2	99	A2M	C2'-C1'	2.79	1.60	1.53
72	L5	4498	OMU	C6-N1	2.78	1.44	1.38
72	L5	4227	OMU	C6-N1	2.78	1.44	1.38
72	L5	2837	OMU	C6-N1	2.77	1.44	1.38
72	L5	3830	A2M	C2'-C1'	2.76	1.60	1.53
72	L5	1871	A2M	C2'-C1'	2.75	1.60	1.53
72	L5	1326	A2M	C2'-C1'	2.75	1.60	1.53
72	L5	400	A2M	C2'-C1'	2.74	1.60	1.53
76	S2	512	A2M	C2'-C1'	2.74	1.60	1.53
72	L5	1524	A2M	C2'-C1'	2.73	1.60	1.53
76	S2	1850	MA6	C5-C4	-2.73	1.33	1.39
76	S2	1031	A2M	C2'-C1'	2.73	1.60	1.53
69	Pt	47	G7M	C6-N1	2.73	1.43	1.38
72	L5	3724	A2M	C2'-C1'	2.72	1.60	1.53
72	L5	4571	A2M	C2'-C1'	2.71	1.60	1.53
76	S2	590	A2M	C2'-C1'	2.70	1.60	1.53
72	L5	3830	A2M	C5-C4	-2.70	1.34	1.39
76	S2	27	A2M	C2'-C1'	2.69	1.60	1.53
72	L5	4590	A2M	C5-C4	-2.69	1.34	1.39
72	L5	2815	A2M	C5-C4	-2.69	1.34	1.39
72	L5	4590	A2M	C2'-C1'	2.68	1.60	1.53
72	L5	3825	A2M	C5-C4	-2.68	1.34	1.39
76	S2	1031	A2M	C5-C4	-2.67	1.34	1.39
76	S2	576	A2M	C5-C4	-2.67	1.34	1.39
76	S2	1851	MA6	C5-C4	-2.67	1.34	1.39
76	S2	99	A2M	C5-C4	-2.67	1.34	1.39
72	L5	1524	A2M	C5-C4	-2.67	1.34	1.39
72	L5	3925	OMU	C6-N1	2.66	1.44	1.38
72	L5	4620	OMU	C6-N1	2.66	1.44	1.38
76	S2	668	A2M	C5-C4	-2.66	1.34	1.39
72	L5	1326	A2M	C5-C4	-2.66	1.34	1.39
72	L5	2401	A2M	C5-C4	-2.66	1.34	1.39
76	S2	116	OMU	C6-N1	2.66	1.44	1.38
72	L5	1534	A2M	C5-C4	-2.66	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	L5	3825	A2M	C2'-C1'	2.65	1.59	1.53
72	L5	1871	A2M	C5-C4	-2.65	1.34	1.39
72	L5	2363	A2M	C5-C4	-2.63	1.34	1.39
72	L5	4523	A2M	C5-C4	-2.63	1.34	1.39
76	S2	512	A2M	C5-C4	-2.63	1.34	1.39
72	L5	400	A2M	C5-C4	-2.63	1.34	1.39
76	S2	27	A2M	C5-C4	-2.63	1.34	1.39
72	L5	2363	A2M	C2'-C1'	2.62	1.59	1.53
72	L5	4220	6MZ	C5-N7	-2.61	1.34	1.39
76	S2	468	A2M	C5-C4	-2.61	1.34	1.39
76	S2	1383	A2M	C5-C4	-2.60	1.34	1.39
76	S2	590	A2M	C5-C4	-2.60	1.34	1.39
72	L5	3867	A2M	C2'-C1'	2.60	1.59	1.53
76	S2	1639	G7M	C6-N1	2.60	1.43	1.38
72	L5	3718	A2M	C5-C4	-2.59	1.34	1.39
76	S2	1678	A2M	C2'-C1'	2.59	1.59	1.53
72	L5	3867	A2M	C5-C4	-2.59	1.34	1.39
72	L5	3724	A2M	C5-C4	-2.59	1.34	1.39
72	L5	398	A2M	C5-C4	-2.58	1.34	1.39
72	L5	4571	A2M	C5-C4	-2.57	1.34	1.39
76	S2	1842	4AC	O2-C2	-2.56	1.19	1.23
72	L5	3760	A2M	C2'-C1'	2.52	1.59	1.53
76	S2	1678	A2M	C5-C4	-2.51	1.34	1.39
72	L5	1534	A2M	C2'-C1'	2.51	1.59	1.53
72	L5	3760	A2M	C5-C4	-2.50	1.34	1.39
76	S2	484	A2M	C5-C4	-2.49	1.34	1.39
76	S2	1337	4AC	O2-C2	-2.47	1.19	1.23
72	L5	4227	OMU	C5-C4	2.46	1.49	1.43
76	S2	627	OMU	C5-C4	2.42	1.49	1.43
76	S2	1804	OMU	C5-C4	2.42	1.49	1.43
72	L5	2837	OMU	C5-C4	2.41	1.49	1.43
76	S2	428	OMU	C5-C4	2.41	1.49	1.43
72	L5	4620	OMU	O2-C2	-2.36	1.18	1.23
72	L5	3925	OMU	O2-C2	-2.35	1.18	1.23
72	L5	4498	OMU	O2-C2	-2.35	1.18	1.23
76	S2	428	OMU	O2-C2	-2.32	1.18	1.23
72	L5	4498	OMU	C5-C4	2.32	1.48	1.43
72	L5	2837	OMU	O2-C2	-2.32	1.18	1.23
72	L5	4227	OMU	O2-C2	-2.31	1.18	1.23
72	L5	3925	OMU	C5-C4	2.30	1.48	1.43
72	L5	3718	A2M	C5-N7	-2.30	1.34	1.39
76	S2	116	OMU	O2-C2	-2.26	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S2	1851	MA6	C5-N7	-2.25	1.34	1.39
76	S2	1850	MA6	C5-N7	-2.25	1.34	1.39
72	L5	3867	A2M	C5-N7	-2.25	1.34	1.39
72	L5	4530	UR3	O2-C2	-2.24	1.18	1.22
76	S2	116	OMU	C5-C4	2.24	1.48	1.43
72	L5	3785	A2M	O3'-C3'	2.24	1.48	1.43
72	L5	4220	6MZ	C8-N9	-2.23	1.33	1.37
72	L5	4530	UR3	O4-C4	-2.22	1.18	1.23
72	L5	4530	UR3	C5-C4	2.22	1.49	1.43
72	L5	4620	OMU	C5-C4	2.21	1.48	1.43
72	L5	4523	A2M	C5-N7	-2.21	1.34	1.39
72	L5	3825	A2M	C5-N7	-2.20	1.34	1.39
76	S2	484	A2M	C5-N7	-2.19	1.34	1.39
72	L5	1326	A2M	C5-N7	-2.19	1.34	1.39
76	S2	1804	OMU	O2-C2	-2.18	1.19	1.23
72	L5	4530	UR3	C4-N3	2.17	1.45	1.40
72	L5	2363	A2M	C5-N7	-2.17	1.34	1.39
76	S2	1031	A2M	C5-N7	-2.17	1.34	1.39
76	S2	627	OMU	O2-C2	-2.17	1.19	1.23
76	S2	99	A2M	C5-N7	-2.16	1.34	1.39
69	Pt	47	G7M	C4-N9	-2.16	1.32	1.38
76	S2	1850	MA6	C8-N9	-2.16	1.33	1.37
76	S2	1842	4AC	O7-C7	-2.16	1.18	1.23
76	S2	512	A2M	C5-N7	-2.16	1.34	1.39
72	L5	1871	A2M	C5-N7	-2.16	1.34	1.39
72	L5	398	A2M	C5-N7	-2.16	1.34	1.39
72	L5	4571	A2M	C5-N7	-2.15	1.35	1.39
72	L5	3724	A2M	C5-N7	-2.14	1.35	1.39
76	S2	1248	B8N	O2-C2	-2.14	1.18	1.22
76	S2	1832	6MZ	C6-N1	-2.13	1.31	1.35
72	L5	2401	A2M	C5-N7	-2.12	1.35	1.39
76	S2	1337	4AC	O7-C7	-2.12	1.18	1.23
72	L5	400	A2M	C5-N7	-2.11	1.35	1.39
76	S2	468	A2M	C5-N7	-2.11	1.35	1.39
76	S2	1678	A2M	C5-N7	-2.11	1.35	1.39
76	S2	668	A2M	C5-N7	-2.11	1.35	1.39
72	L5	3785	A2M	C5-N7	-2.10	1.35	1.39
76	S2	484	A2M	O3'-C3'	2.10	1.47	1.43
72	L5	3830	A2M	C5-N7	-2.09	1.35	1.39
76	S2	27	A2M	C5-N7	-2.09	1.35	1.39
72	L5	2815	A2M	C5-N7	-2.09	1.35	1.39
69	Pt	8	4SU	O2-C2	-2.08	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	S2	668	A2M	O3'-C3'	2.07	1.47	1.43
76	S2	1383	A2M	C5-N7	-2.07	1.35	1.39
76	S2	822	PSU	O4'-C1'	-2.07	1.41	1.43
76	S2	576	A2M	C5-N7	-2.06	1.35	1.39
72	L5	4523	A2M	O3'-C3'	2.06	1.47	1.43
69	Pt	47	G7M	C8-N7	2.05	1.36	1.33
72	L5	4590	A2M	C5-N7	-2.04	1.35	1.39
76	S2	1248	B8N	C32-C31	2.04	1.56	1.52
72	L5	2815	A2M	O3'-C3'	2.04	1.47	1.43
72	L5	1524	A2M	C5-N7	-2.02	1.35	1.39
72	L5	4220	6MZ	C6-N1	-2.01	1.31	1.35
72	L5	3760	A2M	O3'-C3'	2.01	1.47	1.43
76	S2	576	A2M	O3'-C3'	2.00	1.47	1.43

All (997) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1851	MA6	N1-C6-N6	-13.30	102.54	117.08
76	S2	1850	MA6	N1-C6-N6	-13.06	102.80	117.08
72	L5	1524	A2M	C1'-N9-C8	-12.67	98.53	127.14
76	S2	590	A2M	C1'-N9-C8	-12.64	98.59	127.14
72	L5	3760	A2M	C1'-N9-C8	-12.51	98.88	127.14
76	S2	1678	A2M	C1'-N9-C8	-11.56	101.03	127.14
72	L5	1534	A2M	C1'-N9-C8	-11.46	101.25	127.14
72	L5	3867	A2M	C1'-N9-C8	-11.42	101.35	127.14
72	L5	4571	A2M	C1'-N9-C8	-11.33	101.56	127.14
72	L5	2815	A2M	C1'-N9-C8	-11.18	101.88	127.14
72	L5	3724	A2M	C1'-N9-C8	-11.11	102.05	127.14
72	L5	3825	A2M	C1'-N9-C8	-11.03	102.22	127.14
72	L5	400	A2M	C1'-N9-C8	-11.00	102.30	127.14
72	L5	2363	A2M	C1'-N9-C8	-11.00	102.31	127.14
72	L5	1326	A2M	C1'-N9-C8	-10.97	102.36	127.14
76	S2	576	A2M	C1'-N9-C8	-10.91	102.50	127.14
72	L5	1524	A2M	C4-N9-C1'	10.89	152.54	126.59
72	L5	2401	A2M	C1'-N9-C8	-10.88	102.57	127.14
76	S2	590	A2M	C4-N9-C1'	10.87	152.50	126.59
72	L5	4590	A2M	C1'-N9-C8	-10.85	102.63	127.14
76	S2	27	A2M	C1'-N9-C8	-10.84	102.65	127.14
76	S2	512	A2M	C1'-N9-C8	-10.84	102.67	127.14
72	L5	398	A2M	C1'-N9-C8	-10.81	102.72	127.14
72	L5	3718	A2M	C1'-N9-C8	-10.81	102.74	127.14
76	S2	484	A2M	C1'-N9-C8	-10.79	102.78	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1383	A2M	C1'-N9-C8	-10.77	102.82	127.14
72	L5	3785	A2M	C1'-N9-C8	-10.74	102.89	127.14
76	S2	99	A2M	C1'-N9-C8	-10.72	102.93	127.14
76	S2	1031	A2M	C1'-N9-C8	-10.71	102.96	127.14
72	L5	3760	A2M	C4-N9-C1'	10.69	152.07	126.59
76	S2	468	A2M	C1'-N9-C8	-10.69	102.99	127.14
72	L5	3830	A2M	C1'-N9-C8	-10.61	103.19	127.14
72	L5	4523	A2M	C1'-N9-C8	-10.55	103.30	127.14
76	S2	668	A2M	C1'-N9-C8	-10.45	103.53	127.14
72	L5	1871	A2M	C1'-N9-C8	-10.43	103.59	127.14
76	S2	1678	A2M	C4-N9-C1'	10.27	151.06	126.59
72	L5	3867	A2M	C4-N9-C1'	10.26	151.03	126.59
72	L5	4571	A2M	C4-N9-C1'	10.14	150.76	126.59
72	L5	1534	A2M	C4-N9-C1'	10.00	150.42	126.59
72	L5	3724	A2M	C4-N9-C1'	9.97	150.34	126.59
72	L5	3718	A2M	C4-N9-C1'	9.96	150.33	126.59
72	L5	3825	A2M	C4-N9-C1'	9.94	150.28	126.59
76	S2	484	A2M	C4-N9-C1'	9.90	150.19	126.59
72	L5	2815	A2M	C4-N9-C1'	9.90	150.18	126.59
72	L5	2363	A2M	C4-N9-C1'	9.86	150.09	126.59
72	L5	1326	A2M	C4-N9-C1'	9.85	150.06	126.59
72	L5	400	A2M	C4-N9-C1'	9.81	149.97	126.59
72	L5	398	A2M	C4-N9-C1'	9.73	149.77	126.59
72	L5	2401	A2M	C4-N9-C1'	9.70	149.70	126.59
76	S2	27	A2M	C4-N9-C1'	9.68	149.65	126.59
76	S2	512	A2M	C4-N9-C1'	9.64	149.56	126.59
76	S2	99	A2M	C4-N9-C1'	9.63	149.55	126.59
76	S2	1031	A2M	C4-N9-C1'	9.62	149.52	126.59
76	S2	1383	A2M	C4-N9-C1'	9.62	149.51	126.59
76	S2	576	A2M	C4-N9-C1'	9.62	149.51	126.59
76	S2	468	A2M	C4-N9-C1'	9.55	149.35	126.59
72	L5	4523	A2M	C4-N9-C1'	9.55	149.35	126.59
72	L5	4590	A2M	C4-N9-C1'	9.48	149.19	126.59
72	L5	3830	A2M	C4-N9-C1'	9.39	148.96	126.59
72	L5	3785	A2M	C4-N9-C1'	9.38	148.94	126.59
72	L5	1871	A2M	C4-N9-C1'	9.34	148.85	126.59
76	S2	668	A2M	C4-N9-C1'	9.32	148.79	126.59
69	Pt	8	4SU	C4-N3-C2	-7.82	119.75	127.34
76	S2	1832	6MZ	N1-C2-N3	-7.41	117.00	128.60
76	S2	1851	MA6	C5-C6-N6	7.12	137.70	125.30
76	S2	1850	MA6	C5-C6-N6	7.06	137.61	125.30
72	L5	1534	A2M	N6-C6-N1	-6.24	104.68	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1639	G7M	CN7-N7-C5	6.15	134.41	126.77
72	L5	4590	A2M	N6-C6-N1	-6.13	104.92	118.35
72	L5	3825	A2M	N6-C6-N1	-6.10	105.00	118.35
72	L5	2815	A2M	N6-C6-N1	-6.08	105.03	118.35
72	L5	1871	A2M	N6-C6-N1	-5.99	105.23	118.35
76	S2	1031	A2M	N6-C6-N1	-5.96	105.30	118.35
72	L5	3718	A2M	N6-C6-N1	-5.95	105.31	118.35
76	S2	668	A2M	N6-C6-N1	-5.94	105.34	118.35
72	L5	2401	A2M	N6-C6-N1	-5.94	105.34	118.35
72	L5	2363	A2M	N6-C6-N1	-5.93	105.36	118.35
76	S2	484	A2M	N6-C6-N1	-5.92	105.39	118.35
76	S2	590	A2M	N6-C6-N1	-5.88	105.47	118.35
72	L5	1524	A2M	N6-C6-N1	-5.88	105.47	118.35
72	L5	3830	A2M	N6-C6-N1	-5.88	105.48	118.35
76	S2	99	A2M	N6-C6-N1	-5.88	105.48	118.35
72	L5	400	A2M	N6-C6-N1	-5.87	105.49	118.35
76	S2	27	A2M	N6-C6-N1	-5.87	105.49	118.35
72	L5	398	A2M	N6-C6-N1	-5.87	105.50	118.35
72	L5	3867	A2M	N6-C6-N1	-5.87	105.50	118.35
76	S2	468	A2M	N6-C6-N1	-5.86	105.51	118.35
76	S2	576	A2M	N6-C6-N1	-5.86	105.52	118.35
76	S2	1383	A2M	N6-C6-N1	-5.85	105.53	118.35
72	L5	3724	A2M	N6-C6-N1	-5.84	105.56	118.35
72	L5	3760	A2M	N6-C6-N1	-5.83	105.57	118.35
72	L5	4571	A2M	N6-C6-N1	-5.81	105.63	118.35
72	L5	4220	6MZ	N1-C2-N3	-5.79	119.54	128.60
72	L5	1326	A2M	N6-C6-N1	-5.79	105.67	118.35
72	L5	4523	A2M	N6-C6-N1	-5.79	105.67	118.35
72	L5	3785	A2M	N6-C6-N1	-5.78	105.70	118.35
76	S2	512	A2M	N6-C6-N1	-5.77	105.71	118.35
76	S2	1678	A2M	N6-C6-N1	-5.77	105.72	118.35
76	S2	512	A2M	N3-C2-N1	-5.73	119.63	128.60
69	Pt	47	G7M	CN7-N7-C5	5.69	133.84	126.77
72	L5	1534	A2M	N3-C2-N1	-5.62	119.80	128.60
72	L5	1871	A2M	N3-C2-N1	-5.61	119.83	128.60
76	S2	1851	MA6	N1-C2-N3	-5.57	119.89	128.60
72	L5	3785	A2M	N3-C2-N1	-5.56	119.91	128.60
72	L5	3724	A2M	N3-C2-N1	-5.55	119.91	128.60
72	L5	3830	A2M	N3-C2-N1	-5.55	119.92	128.60
72	L5	2815	A2M	N3-C2-N1	-5.54	119.94	128.60
72	L5	4590	A2M	N3-C2-N1	-5.53	119.95	128.60
72	L5	1326	A2M	N3-C2-N1	-5.53	119.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	590	A2M	N3-C2-N1	-5.53	119.95	128.60
72	L5	4523	A2M	N3-C2-N1	-5.51	119.98	128.60
76	S2	27	A2M	N3-C2-N1	-5.51	119.99	128.60
72	L5	3760	A2M	N3-C2-N1	-5.51	119.99	128.60
72	L5	2363	A2M	N3-C2-N1	-5.49	120.02	128.60
76	S2	99	A2M	N3-C2-N1	-5.49	120.02	128.60
76	S2	1383	A2M	N3-C2-N1	-5.48	120.03	128.60
72	L5	4590	A2M	C5-C6-N6	5.47	135.34	123.43
72	L5	398	A2M	N3-C2-N1	-5.47	120.05	128.60
72	L5	2401	A2M	N3-C2-N1	-5.47	120.05	128.60
72	L5	4227	OMU	C4-N3-C2	-5.47	119.37	126.58
76	S2	1031	A2M	N3-C2-N1	-5.46	120.06	128.60
72	L5	400	A2M	N3-C2-N1	-5.46	120.06	128.60
76	S2	1850	MA6	N1-C2-N3	-5.45	120.08	128.60
72	L5	4571	A2M	N3-C2-N1	-5.43	120.10	128.60
69	Pt	8	4SU	C5-C4-N3	5.43	119.72	114.69
76	S2	468	A2M	N3-C2-N1	-5.43	120.11	128.60
72	L5	3925	OMU	C4-N3-C2	-5.42	119.43	126.58
76	S2	1678	A2M	N3-C2-N1	-5.42	120.13	128.60
76	S2	668	A2M	N3-C2-N1	-5.41	120.15	128.60
72	L5	3718	A2M	C5-C4-N3	-5.40	119.70	126.75
76	S2	428	OMU	C4-N3-C2	-5.40	119.46	126.58
76	S2	484	A2M	C5-C4-N3	-5.39	119.72	126.75
76	S2	484	A2M	N3-C2-N1	-5.37	120.19	128.60
72	L5	3867	A2M	C5-C4-N3	-5.37	119.75	126.75
72	L5	1534	A2M	C5-C6-N6	5.36	135.09	123.43
76	S2	1678	A2M	C5-C4-N3	-5.35	119.77	126.75
76	S2	576	A2M	N3-C2-N1	-5.34	120.26	128.60
76	S2	1248	B8N	C5-C4-N3	5.33	126.05	116.17
72	L5	2837	OMU	C4-N3-C2	-5.33	119.55	126.58
72	L5	3825	A2M	C5-C4-N3	-5.32	119.81	126.75
72	L5	1871	A2M	C5-C6-N6	5.32	135.01	123.43
76	S2	1804	OMU	C4-N3-C2	-5.31	119.58	126.58
72	L5	3825	A2M	C5-C6-N6	5.31	134.98	123.43
72	L5	4498	OMU	C4-N3-C2	-5.30	119.59	126.58
72	L5	2815	A2M	C5-C6-N6	5.28	134.91	123.43
76	S2	668	A2M	C5-C6-N6	5.25	134.85	123.43
72	L5	3718	A2M	C5-C6-N6	5.23	134.82	123.43
72	L5	3867	A2M	N3-C2-N1	-5.22	120.43	128.60
72	L5	2401	A2M	C5-C6-N6	5.21	134.77	123.43
72	L5	3825	A2M	N3-C2-N1	-5.21	120.46	128.60
76	S2	99	A2M	C5-C4-N3	-5.19	119.98	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	3724	A2M	C5-C6-N6	5.19	134.72	123.43
72	L5	1524	A2M	N3-C2-N1	-5.19	120.49	128.60
76	S2	1031	A2M	C5-C6-N6	5.18	134.71	123.43
72	L5	4571	A2M	C5-C4-N3	-5.18	119.99	126.75
76	S2	576	A2M	C5-C6-N6	5.18	134.70	123.43
72	L5	398	A2M	C5-C4-N3	-5.17	120.00	126.75
76	S2	512	A2M	C5-C6-N6	5.17	134.68	123.43
76	S2	627	OMU	C4-N3-C2	-5.17	119.77	126.58
72	L5	2363	A2M	C5-C6-N6	5.17	134.67	123.43
76	S2	484	A2M	C5-C6-N6	5.16	134.67	123.43
72	L5	2363	A2M	C5-C4-N3	-5.16	120.02	126.75
72	L5	3724	A2M	C5-C4-N3	-5.16	120.02	126.75
76	S2	1383	A2M	C5-C4-N3	-5.16	120.02	126.75
72	L5	2815	A2M	C5-C4-N3	-5.16	120.02	126.75
72	L5	4220	6MZ	C5-C4-N3	-5.15	120.03	126.75
72	L5	398	A2M	C5-C6-N6	5.15	134.65	123.43
76	S2	27	A2M	C5-C6-N6	5.14	134.62	123.43
72	L5	1524	A2M	C5-C6-N6	5.14	134.61	123.43
72	L5	400	A2M	C5-C6-N6	5.13	134.59	123.43
72	L5	4523	A2M	C5-C4-N3	-5.12	120.07	126.75
76	S2	468	A2M	C5-C6-N6	5.12	134.57	123.43
76	S2	1383	A2M	C5-C6-N6	5.11	134.54	123.43
72	L5	3867	A2M	C5-C6-N6	5.10	134.54	123.43
72	L5	3830	A2M	C5-C6-N6	5.09	134.51	123.43
76	S2	1031	A2M	C5-C4-N3	-5.09	120.11	126.75
76	S2	590	A2M	C5-C6-N6	5.09	134.51	123.43
72	L5	400	A2M	C5-C4-N3	-5.09	120.11	126.75
72	L5	1326	A2M	C5-C6-N6	5.08	134.49	123.43
76	S2	99	A2M	C5-C6-N6	5.08	134.49	123.43
72	L5	4571	A2M	C5-C6-N6	5.08	134.48	123.43
76	S2	1851	MA6	C5-C4-N3	-5.05	120.16	126.75
72	L5	2401	A2M	C5-C4-N3	-5.04	120.17	126.75
72	L5	1326	A2M	C5-C4-N3	-5.04	120.17	126.75
76	S2	27	A2M	C5-C4-N3	-5.04	120.17	126.75
72	L5	4523	A2M	C5-C6-N6	5.03	134.38	123.43
76	S2	468	A2M	C5-C4-N3	-5.03	120.19	126.75
72	L5	3760	A2M	C5-C6-N6	5.03	134.37	123.43
76	S2	1678	A2M	C5-C6-N6	5.02	134.35	123.43
72	L5	3760	A2M	C5-C4-N3	-5.01	120.22	126.75
72	L5	1534	A2M	C5-C4-N3	-5.00	120.23	126.75
72	L5	3785	A2M	C5-C4-N3	-5.00	120.23	126.75
72	L5	3718	A2M	N3-C2-N1	-4.98	120.81	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	3830	A2M	C5-C4-N3	-4.98	120.25	126.75
76	S2	590	A2M	C5-C4-N3	-4.98	120.25	126.75
76	S2	116	OMU	C4-N3-C2	-4.96	120.04	126.58
76	S2	1850	MA6	C5-C4-N3	-4.94	120.30	126.75
72	L5	3785	A2M	C4'-O4'-C1'	-4.93	98.59	109.47
76	S2	668	A2M	C5-C4-N3	-4.93	120.32	126.75
72	L5	1524	A2M	C5-C4-N3	-4.92	120.33	126.75
76	S2	512	A2M	C5-C4-N3	-4.89	120.37	126.75
72	L5	1871	A2M	C5-C4-N3	-4.89	120.38	126.75
72	L5	4636	PSU	C4-N3-C2	-4.88	119.31	126.34
72	L5	3785	A2M	C5-C6-N6	4.84	133.97	123.43
76	S2	576	A2M	C5-C4-N3	-4.82	120.46	126.75
72	L5	3760	A2M	N9-C8-N7	-4.80	107.35	113.91
72	L5	3637	PSU	N1-C2-N3	4.79	120.56	115.13
72	L5	1677	PSU	C4-N3-C2	-4.76	119.48	126.34
72	L5	4636	PSU	N1-C2-N3	4.74	120.50	115.13
72	L5	2843	PSU	C4-N3-C2	-4.73	119.52	126.34
72	L5	4689	PSU	N1-C2-N3	4.72	120.48	115.13
76	S2	1639	G7M	CN7-N7-C8	-4.72	117.56	124.84
72	L5	4628	PSU	C4-N3-C2	-4.72	119.55	126.34
76	S2	590	A2M	N9-C8-N7	-4.71	107.47	113.91
72	L5	4530	UR3	C4-N3-C2	-4.71	120.13	124.56
72	L5	1524	A2M	N9-C8-N7	-4.70	107.48	113.91
72	L5	4628	PSU	N1-C2-N3	4.69	120.45	115.13
72	L5	4590	A2M	C5-C4-N3	-4.69	120.63	126.75
72	L5	4353	PSU	C4-N3-C2	-4.67	119.61	126.34
72	L5	3758	PSU	N1-C2-N3	4.67	120.42	115.13
72	L5	4521	PSU	C4-N3-C2	-4.66	119.62	126.34
72	L5	4620	OMU	C4-N3-C2	-4.65	120.44	126.58
72	L5	3695	PSU	C4-N3-C2	-4.64	119.65	126.34
72	L5	4500	PSU	C4-N3-C2	-4.63	119.67	126.34
72	L5	4531	PSU	C4-N3-C2	-4.63	119.67	126.34
76	S2	1445	PSU	C4-N3-C2	-4.63	119.67	126.34
72	L5	1536	PSU	C4-N3-C2	-4.63	119.67	126.34
76	S2	686	PSU	C4-N3-C2	-4.62	119.68	126.34
72	L5	4293	PSU	C4-N3-C2	-4.61	119.69	126.34
72	L5	4403	PSU	C4-N3-C2	-4.61	119.69	126.34
76	S2	1136	PSU	C4-N3-C2	-4.61	119.69	126.34
72	L5	4500	PSU	N1-C2-N3	4.61	120.35	115.13
72	L5	3758	PSU	C4-N3-C2	-4.60	119.70	126.34
72	L5	4296	PSU	C4-N3-C2	-4.60	119.70	126.34
76	S2	801	PSU	C4-N3-C2	-4.60	119.71	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	109	PSU	C4-N3-C2	-4.60	119.71	126.34
76	S2	866	PSU	C4-N3-C2	-4.60	119.71	126.34
72	L5	1536	PSU	N1-C2-N3	4.60	120.34	115.13
72	L5	4689	PSU	C4-N3-C2	-4.60	119.71	126.34
72	L5	4471	PSU	N1-C2-N3	4.59	120.33	115.13
72	L5	3884	PSU	C4-N3-C2	-4.59	119.72	126.34
72	L5	1860	PSU	N1-C2-N3	4.59	120.33	115.13
72	L5	4531	PSU	N1-C2-N3	4.58	120.32	115.13
72	L5	4552	PSU	N1-C2-N3	4.58	120.32	115.13
72	L5	1862	PSU	C4-N3-C2	-4.58	119.74	126.34
76	S2	822	PSU	N1-C2-N3	4.58	120.32	115.13
72	L5	3639	PSU	N1-C2-N3	4.58	120.32	115.13
76	S2	34	PSU	C4-N3-C2	-4.58	119.74	126.34
72	L5	4442	PSU	C4-N3-C2	-4.57	119.76	126.34
76	S2	406	PSU	C4-N3-C2	-4.57	119.76	126.34
76	S2	815	PSU	C4-N3-C2	-4.57	119.76	126.34
76	S2	1056	PSU	C4-N3-C2	-4.57	119.76	126.34
72	L5	4457	PSU	C4-N3-C2	-4.57	119.76	126.34
72	L5	3920	PSU	C4-N3-C2	-4.57	119.76	126.34
76	S2	1445	PSU	N1-C2-N3	4.57	120.30	115.13
72	L5	4293	PSU	N1-C2-N3	4.56	120.30	115.13
69	Pt	56	PSU	C4-N3-C2	-4.56	119.76	126.34
76	S2	822	PSU	C4-N3-C2	-4.56	119.76	126.34
72	L5	1677	PSU	N1-C2-N3	4.56	120.30	115.13
76	S2	1850	MA6	N9-C8-N7	-4.56	107.68	113.91
72	L5	3695	PSU	N1-C2-N3	4.56	120.29	115.13
72	L5	3920	PSU	N1-C2-N3	4.56	120.29	115.13
72	L5	2839	PSU	C4-N3-C2	-4.55	119.78	126.34
72	L5	4521	PSU	N1-C2-N3	4.55	120.29	115.13
76	S2	573	PSU	C4-N3-C2	-4.54	119.79	126.34
76	S2	1832	6MZ	C5-C4-N3	-4.54	120.83	126.75
76	S2	1692	PSU	C4-N3-C2	-4.54	119.80	126.34
76	S2	966	PSU	C4-N3-C2	-4.53	119.81	126.34
72	L5	4299	PSU	C4-N3-C2	-4.53	119.81	126.34
72	L5	3639	PSU	C4-N3-C2	-4.53	119.81	126.34
76	S2	1238	PSU	C4-N3-C2	-4.53	119.82	126.34
72	L5	1779	PSU	C4-N3-C2	-4.53	119.82	126.34
72	L5	4312	PSU	C4-N3-C2	-4.53	119.82	126.34
72	L5	5010	PSU	C4-N3-C2	-4.52	119.82	126.34
76	S2	863	PSU	C4-N3-C2	-4.52	119.82	126.34
72	L5	2843	PSU	N1-C2-N3	4.52	120.26	115.13
72	L5	4442	PSU	N1-C2-N3	4.52	120.26	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	4431	PSU	C4-N3-C2	-4.52	119.82	126.34
76	S2	406	PSU	N1-C2-N3	4.52	120.25	115.13
76	S2	651	PSU	C4-N3-C2	-4.52	119.82	126.34
76	S2	1248	B8N	C4-N3-C2	-4.52	119.74	125.46
76	S2	36	PSU	C4-N3-C2	-4.52	119.82	126.34
72	L5	1862	PSU	N1-C2-N3	4.52	120.25	115.13
72	L5	4673	PSU	N1-C2-N3	4.52	120.25	115.13
76	S2	1239	PSU	C4-N3-C2	-4.52	119.83	126.34
76	S2	1174	PSU	C4-N3-C2	-4.52	119.83	126.34
72	L5	3884	PSU	N1-C2-N3	4.52	120.25	115.13
72	L5	3844	PSU	C4-N3-C2	-4.52	119.83	126.34
76	S2	1232	PSU	C4-N3-C2	-4.51	119.83	126.34
72	L5	3637	PSU	C4-N3-C2	-4.51	119.84	126.34
76	S2	1177	PSU	C4-N3-C2	-4.51	119.84	126.34
72	L5	1782	PSU	N1-C2-N3	4.51	120.24	115.13
76	S2	1625	PSU	N1-C2-N3	4.51	120.24	115.13
72	L5	3715	PSU	C4-N3-C2	-4.51	119.84	126.34
72	L5	3851	PSU	N1-C2-N3	4.51	120.24	115.13
72	L5	4296	PSU	N1-C2-N3	4.51	120.24	115.13
72	L5	4576	PSU	C4-N3-C2	-4.51	119.84	126.34
72	L5	3851	PSU	C4-N3-C2	-4.51	119.84	126.34
76	S2	296	PSU	C4-N3-C2	-4.51	119.84	126.34
76	S2	1056	PSU	N1-C2-N3	4.51	120.24	115.13
76	S2	36	PSU	N1-C2-N3	4.51	120.24	115.13
72	L5	1782	PSU	C4-N3-C2	-4.51	119.84	126.34
72	L5	4493	PSU	C4-N3-C2	-4.51	119.85	126.34
72	L5	4299	PSU	N1-C2-N3	4.51	120.23	115.13
72	L5	4579	PSU	C4-N3-C2	-4.50	119.85	126.34
76	S2	1136	PSU	N1-C2-N3	4.50	120.23	115.13
76	S2	1367	PSU	C4-N3-C2	-4.50	119.85	126.34
76	S2	1643	PSU	C4-N3-C2	-4.50	119.86	126.34
76	S2	105	PSU	C4-N3-C2	-4.50	119.86	126.34
72	L5	2839	PSU	N1-C2-N3	4.50	120.23	115.13
71	L8	55	PSU	C4-N3-C2	-4.49	119.86	126.34
76	S2	686	PSU	N1-C2-N3	4.49	120.22	115.13
76	S2	1347	PSU	C4-N3-C2	-4.49	119.87	126.34
76	S2	1244	PSU	C4-N3-C2	-4.49	119.87	126.34
72	L5	4493	PSU	N1-C2-N3	4.49	120.22	115.13
72	L5	4673	PSU	C4-N3-C2	-4.49	119.87	126.34
72	L5	4431	PSU	N1-C2-N3	4.49	120.22	115.13
76	S2	1081	PSU	C4-N3-C2	-4.49	119.87	126.34
76	S2	815	PSU	N1-C2-N3	4.48	120.21	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	4361	PSU	C4-N3-C2	-4.48	119.88	126.34
76	S2	649	PSU	C4-N3-C2	-4.48	119.89	126.34
72	L5	4532	PSU	C4-N3-C2	-4.48	119.89	126.34
76	S2	866	PSU	N1-C2-N3	4.48	120.20	115.13
76	S2	1692	PSU	N1-C2-N3	4.47	120.20	115.13
72	L5	4532	PSU	N1-C2-N3	4.47	120.19	115.13
76	S2	34	PSU	N1-C2-N3	4.47	120.19	115.13
72	L5	4423	PSU	C4-N3-C2	-4.47	119.90	126.34
72	L5	1744	PSU	C4-N3-C2	-4.47	119.90	126.34
76	S2	863	PSU	N1-C2-N3	4.47	120.19	115.13
72	L5	4552	PSU	C4-N3-C2	-4.47	119.90	126.34
72	L5	1534	A2M	N9-C8-N7	-4.47	107.81	113.91
72	L5	5010	PSU	N1-C2-N3	4.46	120.19	115.13
69	Pt	47	G7M	CN7-N7-C8	-4.46	117.95	124.84
72	L5	4361	PSU	N1-C2-N3	4.46	120.19	115.13
72	L5	4972	PSU	C4-N3-C2	-4.46	119.91	126.34
72	L5	3770	PSU	N1-C2-N3	4.46	120.18	115.13
72	L5	3715	PSU	N1-C2-N3	4.46	120.18	115.13
72	L5	3844	PSU	N1-C2-N3	4.46	120.18	115.13
76	S2	609	PSU	C4-N3-C2	-4.46	119.92	126.34
76	S2	1832	6MZ	N9-C8-N7	-4.45	107.82	113.91
72	L5	3770	PSU	C4-N3-C2	-4.45	119.92	126.34
76	S2	681	PSU	C4-N3-C2	-4.45	119.92	126.34
72	L5	4972	PSU	N1-C2-N3	4.45	120.17	115.13
76	S2	105	PSU	N1-C2-N3	4.45	120.17	115.13
72	L5	1860	PSU	C4-N3-C2	-4.45	119.92	126.34
72	L5	4403	PSU	N1-C2-N3	4.45	120.17	115.13
76	S2	109	PSU	N1-C2-N3	4.45	120.17	115.13
76	S2	609	PSU	N1-C2-N3	4.45	120.17	115.13
76	S2	651	PSU	N1-C2-N3	4.45	120.17	115.13
72	L5	4471	PSU	C4-N3-C2	-4.45	119.93	126.34
76	S2	918	PSU	C4-N3-C2	-4.45	119.93	126.34
72	L5	4353	PSU	N1-C2-N3	4.44	120.17	115.13
72	L5	4590	A2M	N9-C8-N7	-4.44	107.84	113.91
72	L5	1779	PSU	N1-C2-N3	4.44	120.16	115.13
76	S2	966	PSU	N1-C2-N3	4.44	120.16	115.13
72	L5	3762	PSU	C4-N3-C2	-4.44	119.94	126.34
72	L5	1683	PSU	C4-N3-C2	-4.44	119.95	126.34
72	L5	4423	PSU	N1-C2-N3	4.44	120.16	115.13
76	S2	649	PSU	N1-C2-N3	4.43	120.15	115.13
76	S2	681	PSU	N1-C2-N3	4.43	120.15	115.13
72	L5	4457	PSU	N1-C2-N3	4.43	120.15	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1174	PSU	N1-C2-N3	4.43	120.15	115.13
72	L5	1683	PSU	N1-C2-N3	4.43	120.15	115.13
76	S2	1347	PSU	N1-C2-N3	4.43	120.15	115.13
72	L5	1744	PSU	N1-C2-N3	4.43	120.15	115.13
76	S2	1177	PSU	N1-C2-N3	4.43	120.15	115.13
76	S2	93	PSU	C4-N3-C2	-4.43	119.96	126.34
76	S2	814	PSU	C4-N3-C2	-4.43	119.96	126.34
76	S2	1643	PSU	N1-C2-N3	4.42	120.14	115.13
76	S2	296	PSU	N1-C2-N3	4.42	120.14	115.13
72	L5	4312	PSU	N1-C2-N3	4.42	120.14	115.13
72	L5	3768	PSU	C4-N3-C2	-4.42	119.97	126.34
72	L5	4576	PSU	N1-C2-N3	4.42	120.14	115.13
76	S2	93	PSU	N1-C2-N3	4.42	120.13	115.13
71	L8	55	PSU	N1-C2-N3	4.41	120.12	115.13
76	S2	1625	PSU	C4-N3-C2	-4.41	119.99	126.34
76	S2	801	PSU	N1-C2-N3	4.41	120.12	115.13
76	S2	918	PSU	N1-C2-N3	4.41	120.12	115.13
72	L5	1781	PSU	N1-C2-N3	4.40	120.12	115.13
76	S2	1004	PSU	C4-N3-C2	-4.40	120.00	126.34
76	S2	573	PSU	N1-C2-N3	4.40	120.12	115.13
72	L5	5001	PSU	C4-N3-C2	-4.40	120.00	126.34
76	S2	1232	PSU	N1-C2-N3	4.40	120.11	115.13
76	S2	1367	PSU	N1-C2-N3	4.40	120.11	115.13
76	S2	1243	PSU	N1-C2-N3	4.39	120.11	115.13
76	S2	1639	G7M	C2-N3-C4	4.39	120.12	112.30
72	L5	5001	PSU	N1-C2-N3	4.39	120.10	115.13
72	L5	4569	PSU	N1-C2-N3	4.38	120.09	115.13
69	Pt	56	PSU	N1-C2-N3	4.38	120.09	115.13
76	S2	1851	MA6	N9-C8-N7	-4.38	107.93	113.91
72	L5	4579	PSU	N1-C2-N3	4.37	120.09	115.13
72	L5	3785	A2M	N9-C8-N7	-4.37	107.93	113.91
76	S2	572	PSU	N1-C2-N3	4.37	120.08	115.13
76	S2	814	PSU	N1-C2-N3	4.36	120.07	115.13
72	L5	1871	A2M	O4'-C1'-N9	4.36	116.64	108.06
76	S2	1004	PSU	N1-C2-N3	4.35	120.06	115.13
72	L5	3762	PSU	N1-C2-N3	4.35	120.06	115.13
72	L5	2815	A2M	N9-C8-N7	-4.35	107.96	113.91
76	S2	1244	PSU	N1-C2-N3	4.35	120.06	115.13
72	L5	1781	PSU	C4-N3-C2	-4.35	120.08	126.34
76	S2	1243	PSU	C4-N3-C2	-4.35	120.08	126.34
76	S2	1238	PSU	N1-C2-N3	4.34	120.05	115.13
76	S2	218	PSU	C4-N3-C2	-4.33	120.09	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	L8	69	PSU	N1-C2-N3	4.33	120.03	115.13
72	L5	4569	PSU	C4-N3-C2	-4.32	120.11	126.34
72	L5	3768	PSU	N1-C2-N3	4.32	120.03	115.13
76	S2	1081	PSU	N1-C2-N3	4.32	120.03	115.13
76	S2	572	PSU	C4-N3-C2	-4.31	120.12	126.34
72	L5	3734	PSU	C4-N3-C2	-4.31	120.13	126.34
72	L5	2632	PSU	N1-C2-N3	4.30	120.00	115.13
71	L8	69	PSU	C4-N3-C2	-4.30	120.15	126.34
72	L5	3729	PSU	N1-C2-N3	4.29	119.99	115.13
76	S2	1239	PSU	N1-C2-N3	4.29	119.99	115.13
72	L5	1792	PSU	N1-C2-N3	4.27	119.97	115.13
76	S2	576	A2M	N9-C8-N7	-4.26	108.08	113.91
72	L5	3764	PSU	N1-C2-N3	4.26	119.96	115.13
72	L5	2508	PSU	N1-C2-N3	4.24	119.94	115.13
72	L5	2632	PSU	C4-N3-C2	-4.24	120.23	126.34
72	L5	4523	A2M	O4'-C1'-N9	4.24	116.41	108.06
72	L5	3734	PSU	N1-C2-N3	4.23	119.93	115.13
76	S2	99	A2M	O4'-C1'-N9	4.22	116.38	108.06
72	L5	3764	PSU	C4-N3-C2	-4.22	120.26	126.34
72	L5	4220	6MZ	C4-C5-C6	4.22	120.08	116.81
72	L5	1582	PSU	N1-C2-N3	4.22	119.91	115.13
72	L5	3830	A2M	O4'-C1'-N9	4.21	116.36	108.06
69	Pt	47	G7M	C2-N3-C4	4.21	119.80	112.30
76	S2	1639	G7M	C1'-N9-C8	-4.21	112.53	126.74
72	L5	2508	PSU	C4-N3-C2	-4.20	120.28	126.34
72	L5	1792	PSU	C4-N3-C2	-4.20	120.29	126.34
72	L5	3830	A2M	N9-C8-N7	-4.20	108.17	113.91
76	S2	1383	A2M	O4'-C1'-N9	4.20	116.33	108.06
76	S2	1639	G7M	C1'-N9-C4	4.19	138.94	126.50
72	L5	3718	A2M	O4'-C1'-N9	4.19	116.31	108.06
76	S2	218	PSU	N1-C2-N3	4.16	119.84	115.13
72	L5	3729	PSU	C4-N3-C2	-4.16	120.35	126.34
76	S2	468	A2M	O4'-C1'-N9	4.14	116.22	108.06
72	L5	3853	PSU	N1-C2-N3	4.14	119.82	115.13
76	S2	1678	A2M	N9-C8-N7	-4.13	108.27	113.91
72	L5	3853	PSU	C4-N3-C2	-4.12	120.40	126.34
72	L5	4420	PSU	C4-N3-C2	-4.11	120.42	126.34
76	S2	1383	A2M	N9-C8-N7	-4.11	108.30	113.91
76	S2	27	A2M	O4'-C1'-N9	4.11	116.15	108.06
72	L5	2401	A2M	N9-C8-N7	-4.10	108.31	113.91
72	L5	4420	PSU	N1-C2-N3	4.10	119.77	115.13
72	L5	1582	PSU	C4-N3-C2	-4.09	120.44	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1639	G7M	C5-C4-N3	-4.08	120.32	128.15
76	S2	119	PSU	N1-C2-N3	4.08	119.75	115.13
76	S2	27	A2M	N9-C8-N7	-4.07	108.35	113.91
72	L5	400	A2M	N9-C8-N7	-4.07	108.35	113.91
76	S2	468	A2M	N9-C8-N7	-4.07	108.35	113.91
72	L5	4590	A2M	O4'-C1'-N9	4.06	116.07	108.06
76	S2	668	A2M	N9-C8-N7	-4.06	108.36	113.91
76	S2	512	A2M	N9-C8-N7	-4.04	108.38	113.91
76	S2	1832	6MZ	C2-N3-C4	4.03	121.28	111.75
72	L5	3825	A2M	N9-C8-N7	-4.03	108.40	113.91
72	L5	4227	OMU	N3-C2-N1	4.01	120.21	114.89
76	S2	1031	A2M	O4'-C1'-N9	4.01	115.96	108.06
72	L5	2363	A2M	N9-C8-N7	-4.01	108.43	113.91
72	L5	1871	A2M	N9-C8-N7	-4.00	108.44	113.91
76	S2	119	PSU	C4-N3-C2	-3.99	120.59	126.34
72	L5	398	A2M	O4'-C1'-N9	3.98	115.90	108.06
76	S2	99	A2M	N9-C8-N7	-3.98	108.47	113.91
72	L5	398	A2M	N9-C8-N7	-3.97	108.48	113.91
76	S2	1031	A2M	N9-C8-N7	-3.97	108.48	113.91
72	L5	3925	OMU	N3-C2-N1	3.97	120.16	114.89
72	L5	3825	A2M	O4'-C1'-N9	3.97	115.87	108.06
76	S2	428	OMU	N3-C2-N1	3.94	120.11	114.89
72	L5	3724	A2M	N9-C8-N7	-3.93	108.53	113.91
72	L5	3724	A2M	O4'-C1'-N9	3.93	115.80	108.06
69	Pt	47	G7M	C5-C6-N1	3.92	119.98	111.79
72	L5	1326	A2M	N9-C8-N7	-3.92	108.56	113.91
72	L5	4571	A2M	N9-C8-N7	-3.92	108.56	113.91
72	L5	2401	A2M	O4'-C1'-N9	3.92	115.78	108.06
72	L5	3867	A2M	N9-C8-N7	-3.92	108.56	113.91
72	L5	2363	A2M	O4'-C1'-N9	3.91	115.77	108.06
76	S2	576	A2M	C2'-C1'-N9	-3.91	106.95	113.53
76	S2	1639	G7M	C5-C6-N1	3.89	119.91	111.79
72	L5	4498	OMU	N3-C2-N1	3.85	120.00	114.89
72	L5	3830	A2M	C2'-C1'-N9	-3.84	107.06	113.53
72	L5	4523	A2M	N9-C8-N7	-3.84	108.66	113.91
72	L5	2837	OMU	N3-C2-N1	3.79	119.93	114.89
72	L5	400	A2M	O4'-C1'-N9	3.78	115.52	108.06
69	Pt	8	4SU	N3-C2-N1	3.78	119.91	114.89
76	S2	1804	OMU	N3-C2-N1	3.75	119.87	114.89
72	L5	3785	A2M	O4'-C1'-N9	3.75	115.45	108.06
76	S2	512	A2M	O4'-C1'-N9	3.71	115.38	108.06
76	S2	1850	MA6	C4-C5-C6	3.70	120.03	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	1534	A2M	C2-N3-C4	3.66	120.40	111.75
76	S2	1678	A2M	O4'-C1'-N9	3.65	115.25	108.06
72	L5	3785	A2M	O4'-C1'-C2'	-3.64	100.17	106.57
72	L5	2815	A2M	C2-N3-C4	3.64	120.35	111.75
76	S2	484	A2M	N9-C8-N7	-3.64	108.94	113.91
76	S2	1851	MA6	C2-N1-C6	3.63	120.33	111.75
76	S2	627	OMU	N3-C2-N1	3.61	119.68	114.89
76	S2	1678	A2M	C2-N3-C4	3.61	120.27	111.75
76	S2	484	A2M	C2-N3-C4	3.61	120.27	111.75
76	S2	1850	MA6	C2-N1-C6	3.60	120.26	111.75
76	S2	99	A2M	C2-N3-C4	3.60	120.25	111.75
76	S2	116	OMU	N3-C2-N1	3.59	119.66	114.89
72	L5	3785	A2M	C2-N3-C4	3.59	120.24	111.75
72	L5	2363	A2M	C2-N3-C4	3.59	120.24	111.75
72	L5	4523	A2M	C2-N3-C4	3.59	120.22	111.75
72	L5	3760	A2M	C2-N3-C4	3.58	120.20	111.75
76	S2	1383	A2M	C2-N3-C4	3.58	120.20	111.75
72	L5	4571	A2M	C2-N3-C4	3.56	120.17	111.75
76	S2	590	A2M	C2-N3-C4	3.56	120.17	111.75
76	S2	1031	A2M	C2-N3-C4	3.56	120.15	111.75
72	L5	398	A2M	C2-N3-C4	3.55	120.15	111.75
72	L5	3724	A2M	C2-N3-C4	3.55	120.15	111.75
72	L5	3825	A2M	C2-N3-C4	3.55	120.14	111.75
76	S2	27	A2M	C2-N3-C4	3.55	120.14	111.75
72	L5	400	A2M	C2-N3-C4	3.55	120.14	111.75
72	L5	1326	A2M	C2-N3-C4	3.54	120.11	111.75
72	L5	3830	A2M	C2-N3-C4	3.53	120.09	111.75
69	Pt	47	G7M	C5-C4-N3	-3.53	121.38	128.15
72	L5	1326	A2M	O4'-C1'-N9	3.53	115.02	108.06
72	L5	3867	A2M	C2-N3-C4	3.53	120.08	111.75
76	S2	1851	MA6	C2-N3-C4	3.52	120.07	111.75
72	L5	2401	A2M	C2-N3-C4	3.52	120.07	111.75
76	S2	468	A2M	C2-N3-C4	3.52	120.06	111.75
76	S2	512	A2M	C2-N3-C4	3.51	120.05	111.75
72	L5	2815	A2M	O4'-C1'-N9	3.51	114.97	108.06
72	L5	1871	A2M	C2-N3-C4	3.50	120.02	111.75
72	L5	4620	OMU	N3-C2-N1	3.50	119.54	114.89
72	L5	3718	A2M	N9-C8-N7	-3.50	109.13	113.91
76	S2	1851	MA6	C4-C5-C6	3.50	119.80	115.88
72	L5	3867	A2M	O4'-C1'-N9	3.49	114.94	108.06
76	S2	1639	G7M	O6-C6-C5	-3.48	120.21	128.06
72	L5	4571	A2M	O4'-C1'-N9	3.47	114.90	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	4220	6MZ	C2-N3-C4	3.47	119.95	111.75
76	S2	1832	6MZ	C5-N7-C8	3.47	108.44	103.51
76	S2	484	A2M	O4'-C1'-N9	3.47	114.89	108.06
76	S2	668	A2M	C2-N3-C4	3.46	119.92	111.75
69	Pt	47	G7M	O6-C6-C5	-3.46	120.26	128.06
72	L5	3718	A2M	C2-N3-C4	3.45	119.89	111.75
76	S2	576	A2M	O4'-C1'-N9	3.43	114.82	108.06
69	Pt	8	4SU	C5-C4-S4	-3.43	120.05	124.47
76	S2	576	A2M	C2-N3-C4	3.43	119.85	111.75
72	L5	4590	A2M	C2-N3-C4	3.43	119.85	111.75
72	L5	2837	OMU	C5-C4-N3	3.42	119.95	114.84
72	L5	4227	OMU	C5-C4-N3	3.41	119.94	114.84
72	L5	4498	OMU	C5-C4-N3	3.39	119.91	114.84
76	S2	1850	MA6	C2-N3-C4	3.38	119.74	111.75
72	L5	1524	A2M	C2-N3-C4	3.37	119.72	111.75
72	L5	3925	OMU	C5-C4-N3	3.35	119.85	114.84
76	S2	627	OMU	C5-C4-N3	3.34	119.84	114.84
76	S2	428	OMU	C5-C4-N3	3.34	119.84	114.84
69	Pt	21	H2U	C5-C4-N3	-3.32	112.92	116.65
76	S2	668	A2M	C2'-C1'-N9	3.32	119.11	113.53
76	S2	1804	OMU	C5-C4-N3	3.31	119.80	114.84
76	S2	1832	6MZ	C4-C5-N7	-3.31	106.58	110.62
72	L5	4220	6MZ	N9-C8-N7	-3.25	109.47	113.91
76	S2	116	OMU	C5-C4-N3	3.24	119.69	114.84
72	L5	3760	A2M	C5-N7-C8	3.23	108.09	103.51
76	S2	512	A2M	C2'-C1'-N9	-3.21	108.12	113.53
72	L5	2815	A2M	C5-N7-C8	3.20	108.06	103.51
72	L5	1524	A2M	C5-N7-C8	3.19	108.04	103.51
76	S2	590	A2M	C5-N7-C8	3.19	108.04	103.51
72	L5	4590	A2M	C2'-C1'-N9	-3.15	108.22	113.53
72	L5	1534	A2M	C5-N7-C8	3.15	107.99	103.51
72	L5	3760	A2M	N3-C4-N9	3.15	132.27	127.08
72	L5	4220	6MZ	C9-N6-C6	-3.14	120.17	122.87
76	S2	1850	MA6	C5-N7-C8	3.13	107.95	103.51
72	L5	4620	OMU	C5-C4-N3	3.11	119.49	114.84
76	S2	1678	A2M	N3-C4-N9	3.10	132.20	127.08
72	L5	3825	A2M	C5-N7-C8	3.09	107.91	103.51
76	S2	590	A2M	N3-C4-N9	3.09	132.17	127.08
69	Pt	47	G7M	C2-N1-C6	-3.08	119.48	125.10
76	S2	1678	A2M	C5-N7-C8	3.08	107.89	103.51
72	L5	4590	A2M	C5-N7-C8	3.07	107.87	103.51
76	S2	1851	MA6	C5-N7-C8	3.07	107.87	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1850	MA6	N3-C4-N9	3.06	132.13	127.08
72	L5	3760	A2M	C4-N9-C8	3.06	109.05	105.73
72	L5	3867	A2M	N3-C4-N9	3.06	132.12	127.08
72	L5	1524	A2M	N3-C4-N9	3.06	132.12	127.08
76	S2	1832	6MZ	C5-C4-N9	3.05	109.33	105.78
76	S2	1851	MA6	N3-C4-N9	3.04	132.09	127.08
76	S2	1639	G7M	C2-N1-C6	-3.04	119.56	125.10
76	S2	116	OMU	O4-C4-C5	-3.03	119.83	125.16
72	L5	3758	PSU	O2-C2-N1	-3.01	119.47	122.79
72	L5	3925	OMU	O4-C4-C5	-2.98	119.92	125.16
76	S2	1383	A2M	C5-N7-C8	2.97	107.73	103.51
76	S2	576	A2M	C5-N7-C8	2.97	107.73	103.51
76	S2	1625	PSU	O2-C2-N1	-2.97	119.52	122.79
72	L5	2401	A2M	C5-N7-C8	2.96	107.71	103.51
72	L5	1524	A2M	C4-N9-C8	2.96	108.93	105.73
72	L5	2363	A2M	C5-N7-C8	2.95	107.70	103.51
72	L5	3830	A2M	C5-N7-C8	2.95	107.70	103.51
76	S2	1639	G7M	N9-C4-N3	2.93	131.83	125.94
76	S2	590	A2M	C4-N9-C8	2.93	108.91	105.73
76	S2	27	A2M	C5-N7-C8	2.93	107.67	103.51
72	L5	3867	A2M	C5-N7-C8	2.93	107.67	103.51
72	L5	400	A2M	C5-N7-C8	2.93	107.67	103.51
72	L5	3785	A2M	C5-N7-C8	2.93	107.67	103.51
72	L5	1871	A2M	C2'-C1'-N9	-2.92	108.61	113.53
72	L5	398	A2M	C5-N7-C8	2.92	107.66	103.51
76	S2	468	A2M	C5-N7-C8	2.92	107.66	103.51
76	S2	428	OMU	O4-C4-C5	-2.92	120.03	125.16
76	S2	1804	OMU	O4-C4-C5	-2.91	120.03	125.16
76	S2	627	OMU	O4-C4-C5	-2.91	120.04	125.16
72	L5	4590	A2M	C4'-O4'-C1'	-2.91	103.06	109.47
72	L5	4571	A2M	N3-C4-N9	2.91	131.87	127.08
76	S2	668	A2M	C5-N7-C8	2.91	107.64	103.51
76	S2	99	A2M	C5-N7-C8	2.89	107.62	103.51
72	L5	3724	A2M	C5-N7-C8	2.88	107.60	103.51
72	L5	3770	PSU	O2-C2-N1	-2.88	119.62	122.79
76	S2	1248	B8N	N3-C2-N1	2.87	120.82	116.76
72	L5	1871	A2M	C5-N7-C8	2.87	107.59	103.51
76	S2	1031	A2M	C5-N7-C8	2.87	107.59	103.51
72	L5	4498	OMU	O4-C4-C5	-2.87	120.12	125.16
72	L5	3808	OMC	C1'-N1-C2	2.87	124.82	118.42
72	L5	4571	A2M	C5-N7-C8	2.85	107.56	103.51
72	L5	3785	A2M	N3-C4-N9	2.85	131.78	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1842	4AC	C6-C5-C4	2.85	120.45	116.96
72	L5	2837	OMU	O4-C4-C5	-2.85	120.16	125.16
72	L5	3724	A2M	N3-C4-N9	2.84	131.76	127.08
76	S2	1337	4AC	C6-C5-C4	2.84	120.43	116.96
76	S2	512	A2M	C5-N7-C8	2.83	107.53	103.51
72	L5	4523	A2M	C5-N7-C8	2.83	107.53	103.51
76	S2	822	PSU	O2-C2-N1	-2.83	119.68	122.79
76	S2	484	A2M	N3-C4-N9	2.82	131.73	127.08
72	L5	2351	OMC	C1'-N1-C2	2.82	124.72	118.42
76	S2	484	A2M	C5-N7-C8	2.81	107.50	103.51
72	L5	398	A2M	N3-C4-N9	2.81	131.71	127.08
76	S2	1174	PSU	O2-C2-N1	-2.80	119.70	122.79
72	L5	2363	A2M	N3-C4-N9	2.80	131.70	127.08
72	L5	1326	A2M	C5-N7-C8	2.80	107.48	103.51
76	S2	99	A2M	N3-C4-N9	2.80	131.69	127.08
72	L5	3825	A2M	N3-C4-N9	2.80	131.69	127.08
72	L5	2815	A2M	N3-C4-N9	2.79	131.67	127.08
76	S2	1383	A2M	N3-C4-N9	2.79	131.67	127.08
72	L5	4689	PSU	O2-C2-N1	-2.78	119.73	122.79
72	L5	400	A2M	N3-C4-N9	2.78	131.66	127.08
72	L5	4220	6MZ	N3-C4-N9	2.78	131.66	127.08
72	L5	1326	A2M	N3-C4-N9	2.78	131.66	127.08
72	L5	3718	A2M	C5-N7-C8	2.76	107.44	103.51
72	L5	3718	A2M	N3-C4-N9	2.76	131.64	127.08
72	L5	1534	A2M	N3-C4-N9	2.76	131.63	127.08
72	L5	4523	A2M	N3-C4-N9	2.75	131.62	127.08
76	S2	1004	PSU	O2-C2-N1	-2.75	119.77	122.79
76	S2	27	A2M	N3-C4-N9	2.75	131.61	127.08
76	S2	1248	B8N	O4-C4-N3	-2.74	115.32	119.98
76	S2	109	PSU	O2-C2-N1	-2.74	119.77	122.79
72	L5	1536	PSU	O2-C2-N1	-2.73	119.78	122.79
72	L5	2401	A2M	N3-C4-N9	2.73	131.58	127.08
72	L5	2815	A2M	C2'-C1'-N9	-2.72	108.95	113.53
76	S2	609	PSU	O2-C2-N1	-2.72	119.80	122.79
72	L5	4227	OMU	O4-C4-C5	-2.72	120.38	125.16
72	L5	3830	A2M	N3-C4-N9	2.71	131.54	127.08
76	S2	512	A2M	N3-C4-N9	2.71	131.54	127.08
72	L5	4620	OMU	O4-C4-C5	-2.71	120.40	125.16
76	S2	668	A2M	C4'-O4'-C1'	-2.70	103.51	109.47
72	L5	3884	PSU	O2-C2-N1	-2.70	119.82	122.79
69	Pt	47	G7M	C1'-N9-C8	-2.70	117.63	126.74
76	S2	468	A2M	N3-C4-N9	2.70	131.53	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	4500	PSU	O2-C2-N1	-2.69	119.83	122.79
76	S2	1031	A2M	N3-C4-N9	2.69	131.51	127.08
69	Pt	33	OMC	C1'-N1-C2	2.69	124.42	118.42
76	S2	1850	MA6	C4-N9-C8	2.68	108.64	105.73
72	L5	4628	PSU	O2-C2-N1	-2.68	119.84	122.79
76	S2	1238	PSU	O2-C2-N1	-2.67	119.85	122.79
76	S2	1243	PSU	O2-C2-N1	-2.67	119.85	122.79
72	L5	5010	PSU	O2-C2-N1	-2.67	119.85	122.79
72	L5	1677	PSU	O2-C2-N1	-2.67	119.86	122.79
72	L5	4531	PSU	O2-C2-N1	-2.66	119.86	122.79
76	S2	649	PSU	O2-C2-N1	-2.65	119.87	122.79
72	L5	3715	PSU	O2-C2-N1	-2.65	119.87	122.79
76	S2	36	PSU	O2-C2-N1	-2.65	119.87	122.79
76	S2	1445	PSU	O2-C2-N1	-2.65	119.87	122.79
72	L5	4471	PSU	O2-C2-N1	-2.64	119.88	122.79
72	L5	1860	PSU	O2-C2-N1	-2.64	119.89	122.79
72	L5	4523	A2M	C4'-O4'-C1'	-2.63	103.66	109.47
76	S2	1832	6MZ	C4-N9-C1'	-2.63	120.32	126.59
71	L8	69	PSU	O2-C2-N1	-2.63	119.90	122.79
72	L5	3762	PSU	O2-C2-N1	-2.62	119.90	122.79
72	L5	4431	PSU	O2-C2-N1	-2.62	119.91	122.79
76	S2	1136	PSU	O2-C2-N1	-2.62	119.91	122.79
72	L5	4532	PSU	O2-C2-N1	-2.61	119.91	122.79
76	S2	1643	PSU	O2-C2-N1	-2.61	119.91	122.79
76	S2	573	PSU	O2-C2-N1	-2.61	119.92	122.79
76	S2	918	PSU	O2-C2-N1	-2.61	119.92	122.79
76	S2	296	PSU	O2-C2-N1	-2.61	119.92	122.79
76	S2	1244	PSU	O2-C2-N1	-2.60	119.93	122.79
76	S2	815	PSU	O2-C2-N1	-2.60	119.93	122.79
72	L5	1683	PSU	O2-C2-N1	-2.59	119.94	122.79
72	L5	2839	PSU	O2-C2-N1	-2.59	119.94	122.79
72	L5	3729	PSU	O2-C2-N1	-2.59	119.94	122.79
76	S2	1692	PSU	O2-C2-N1	-2.59	119.94	122.79
72	L5	4220	6MZ	C5-N7-C8	2.58	107.18	103.51
72	L5	3729	PSU	C6-N1-C2	-2.58	120.04	122.68
76	S2	651	PSU	O2-C2-N1	-2.58	119.95	122.79
72	L5	4972	PSU	O2-C2-N1	-2.58	119.95	122.79
72	L5	4531	PSU	C6-C5-C4	2.57	120.00	118.20
76	S2	668	A2M	N3-C4-N9	2.57	131.32	127.08
72	L5	4442	PSU	O2-C2-N1	-2.57	119.96	122.79
72	L5	4493	PSU	O2-C2-N1	-2.57	119.96	122.79
76	S2	681	PSU	O2-C2-N1	-2.57	119.96	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	866	PSU	O2-C2-N1	-2.57	119.96	122.79
72	L5	4293	PSU	O2-C2-N1	-2.57	119.97	122.79
76	S2	34	PSU	O2-C2-N1	-2.56	119.97	122.79
72	L5	4403	PSU	O2-C2-N1	-2.55	119.98	122.79
72	L5	4576	PSU	O2-C2-N1	-2.55	119.98	122.79
72	L5	1782	PSU	O2-C2-N1	-2.55	119.98	122.79
72	L5	4689	PSU	C6-N1-C2	-2.55	120.08	122.68
76	S2	1248	B8N	C31-N3-C2	2.55	121.49	117.67
72	L5	3734	PSU	O2-C2-N1	-2.55	119.99	122.79
72	L5	2401	A2M	C2'-C1'-N9	-2.55	109.24	113.53
72	L5	4636	PSU	C6-C5-C4	2.54	119.98	118.20
76	S2	1232	PSU	O2-C2-N1	-2.54	119.99	122.79
72	L5	4296	PSU	O2-C2-N1	-2.54	119.99	122.79
72	L5	4579	PSU	O2-C2-N1	-2.54	119.99	122.79
71	L8	55	PSU	O2-C2-N1	-2.54	120.00	122.79
76	S2	1239	PSU	O2-C2-N1	-2.54	120.00	122.79
72	L5	4673	PSU	O2-C2-N1	-2.53	120.01	122.79
72	L5	1792	PSU	O2-C2-N1	-2.52	120.01	122.79
72	L5	1871	A2M	N3-C4-N9	2.52	131.23	127.08
76	S2	1625	PSU	C6-N1-C2	-2.52	120.11	122.68
72	L5	3851	PSU	O2-C2-N1	-2.51	120.02	122.79
72	L5	4361	PSU	O2-C2-N1	-2.51	120.02	122.79
76	S2	1056	PSU	O2-C2-N1	-2.51	120.03	122.79
76	S2	576	A2M	N3-C4-N9	2.51	131.22	127.08
72	L5	1781	PSU	O2-C2-N1	-2.51	120.03	122.79
76	S2	1347	PSU	O2-C2-N1	-2.51	120.03	122.79
72	L5	4312	PSU	O2-C2-N1	-2.51	120.03	122.79
76	S2	406	PSU	O2-C2-N1	-2.51	120.03	122.79
76	S2	1367	PSU	O2-C2-N1	-2.50	120.03	122.79
72	L5	3639	PSU	O2-C2-N1	-2.50	120.03	122.79
76	S2	966	PSU	O2-C2-N1	-2.50	120.03	122.79
72	L5	4353	PSU	O2-C2-N1	-2.50	120.04	122.79
72	L5	4299	PSU	O2-C2-N1	-2.50	120.04	122.79
76	S2	863	PSU	O2-C2-N1	-2.50	120.04	122.79
72	L5	2632	PSU	O2-C2-N1	-2.49	120.04	122.79
76	S2	814	PSU	O2-C2-N1	-2.49	120.05	122.79
76	S2	468	A2M	C4'-O4'-C1'	-2.49	103.97	109.47
76	S2	105	PSU	O2-C2-N1	-2.49	120.05	122.79
72	L5	1862	PSU	O2-C2-N1	-2.49	120.05	122.79
72	L5	1744	PSU	O2-C2-N1	-2.49	120.05	122.79
72	L5	4423	PSU	O2-C2-N1	-2.49	120.05	122.79
72	L5	4457	PSU	O2-C2-N1	-2.49	120.05	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1832	6MZ	C6-C5-N7	2.48	135.08	132.39
76	S2	1678	A2M	C4'-O4'-C1'	-2.48	103.99	109.47
72	L5	3695	PSU	O2-C2-N1	-2.48	120.06	122.79
72	L5	1779	PSU	O2-C2-N1	-2.47	120.07	122.79
72	L5	3718	A2M	C5-C4-N9	2.47	108.66	105.78
72	L5	4552	PSU	O2-C2-N1	-2.47	120.07	122.79
72	L5	1534	A2M	O4'-C1'-C2'	-2.47	102.24	106.57
76	S2	572	PSU	O2-C2-N1	-2.46	120.08	122.79
76	S2	590	A2M	C4'-O4'-C1'	-2.45	104.06	109.47
76	S2	119	PSU	C6-N1-C2	-2.45	120.17	122.68
72	L5	3768	PSU	O2-C2-N1	-2.45	120.10	122.79
76	S2	218	PSU	O2-C2-N1	-2.44	120.10	122.79
72	L5	2843	PSU	O2-C2-N1	-2.44	120.10	122.79
76	S2	119	PSU	O2-C2-N1	-2.44	120.11	122.79
76	S2	686	PSU	O2-C2-N1	-2.44	120.11	122.79
72	L5	3920	PSU	O2-C2-N1	-2.44	120.11	122.79
72	L5	4521	PSU	O2-C2-N1	-2.44	120.11	122.79
72	L5	4590	A2M	N3-C4-N9	2.44	131.10	127.08
69	Pt	47	G7M	C1'-N9-C4	2.43	133.73	126.50
76	S2	918	PSU	O4'-C1'-C2'	2.43	108.58	105.14
76	S2	93	PSU	O2-C2-N1	-2.43	120.12	122.79
72	L5	4420	PSU	O2-C2-N1	-2.43	120.12	122.79
76	S2	428	OMU	O2-C2-N1	-2.43	119.56	122.79
69	Pt	56	PSU	O2-C2-N1	-2.42	120.12	122.79
76	S2	572	PSU	C6-N1-C2	-2.42	120.21	122.68
76	S2	1177	PSU	O2-C2-N1	-2.41	120.14	122.79
72	L5	3844	PSU	O2-C2-N1	-2.41	120.14	122.79
76	S2	801	PSU	O2-C2-N1	-2.41	120.14	122.79
72	L5	3760	A2M	C2'-C1'-N9	-2.40	109.48	113.53
72	L5	3825	A2M	C4-C5-N7	-2.40	107.69	110.62
72	L5	1860	PSU	C6-N1-C2	-2.40	120.23	122.68
72	L5	4471	PSU	C6-N1-C2	-2.40	120.23	122.68
72	L5	3853	PSU	O2-C2-N1	-2.39	120.16	122.79
72	L5	4552	PSU	C6-N1-C2	-2.39	120.24	122.68
72	L5	3758	PSU	C6-N1-C2	-2.39	120.24	122.68
76	S2	1004	PSU	C6-N1-C2	-2.38	120.25	122.68
72	L5	3764	PSU	C6-N1-C2	-2.38	120.25	122.68
76	S2	822	PSU	C6-N1-C2	-2.38	120.25	122.68
72	L5	3637	PSU	C6-N1-C2	-2.38	120.25	122.68
76	S2	484	A2M	C5-C4-N9	2.38	108.55	105.78
72	L5	3764	PSU	O2-C2-N1	-2.38	120.18	122.79
72	L5	5001	PSU	O2-C2-N1	-2.37	120.18	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	590	A2M	C2'-C1'-N9	-2.37	109.54	113.53
72	L5	2815	A2M	C4-C5-N7	-2.35	107.75	110.62
72	L5	4456	OMC	C1'-N1-C2	2.35	123.67	118.42
76	S2	609	PSU	C6-N1-C2	-2.35	120.28	122.68
72	L5	3867	A2M	C4'-O4'-C1'	-2.35	104.28	109.47
72	L5	1534	A2M	C4-N9-C8	2.35	108.28	105.73
72	L5	3639	PSU	C6-N1-C2	-2.34	120.29	122.68
76	S2	1383	A2M	C4'-O4'-C1'	-2.34	104.30	109.47
72	L5	3825	A2M	C5-C4-N9	2.34	108.50	105.78
72	L5	3762	PSU	C6-N1-C2	-2.34	120.29	122.68
76	S2	1851	MA6	C4-N9-C8	2.33	108.26	105.73
72	L5	4423	PSU	C6-N1-C2	-2.33	120.30	122.68
72	L5	1677	PSU	C6-C5-C4	2.33	119.83	118.20
72	L5	1534	A2M	C4-C5-N7	-2.32	107.79	110.62
72	L5	2401	A2M	C4'-O4'-C1'	-2.32	104.36	109.47
72	L5	1792	PSU	C6-N1-C2	-2.31	120.32	122.68
71	L8	69	PSU	C6-N1-C2	-2.31	120.32	122.68
72	L5	3770	PSU	C6-N1-C2	-2.31	120.33	122.68
72	L5	4628	PSU	C6-N1-C2	-2.30	120.33	122.68
72	L5	4293	PSU	C6-N1-C2	-2.30	120.33	122.68
76	S2	918	PSU	C6-N1-C2	-2.30	120.34	122.68
72	L5	4673	PSU	C6-N1-C2	-2.29	120.34	122.68
72	L5	1536	PSU	C6-N1-C2	-2.29	120.34	122.68
72	L5	2861	OMC	C1'-N1-C2	2.29	123.54	118.42
76	S2	1842	4AC	C5-C4-N3	-2.29	118.91	122.59
76	S2	99	A2M	C2'-C1'-N9	-2.29	109.67	113.53
72	L5	4590	A2M	C4-C5-N7	-2.29	107.83	110.62
72	L5	3884	PSU	C6-N1-C2	-2.29	120.34	122.68
76	S2	1337	4AC	C5-C4-N3	-2.28	118.92	122.59
76	S2	863	PSU	C6-N1-C2	-2.28	120.35	122.68
76	S2	649	PSU	C6-N1-C2	-2.28	120.35	122.68
72	L5	3718	A2M	C2'-C1'-N9	-2.28	109.70	113.53
72	L5	3718	A2M	C4-C5-N7	-2.28	107.85	110.62
72	L5	4636	PSU	O2-C2-N1	-2.28	120.28	122.79
72	L5	1744	PSU	C6-N1-C2	-2.28	120.36	122.68
72	L5	4500	PSU	C6-N1-C2	-2.28	120.36	122.68
72	L5	3853	PSU	C6-N1-C2	-2.27	120.36	122.68
72	L5	4590	A2M	C4-N9-C8	2.27	108.19	105.73
72	L5	1683	PSU	C6-N1-C2	-2.27	120.36	122.68
76	S2	406	PSU	C6-N1-C2	-2.27	120.37	122.68
72	L5	2632	PSU	C6-N1-C2	-2.27	120.37	122.68
76	S2	681	PSU	C6-N1-C2	-2.26	120.37	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	1582	PSU	C6-N1-C2	-2.26	120.37	122.68
72	L5	3768	PSU	C6-N1-C2	-2.26	120.37	122.68
72	L5	4403	PSU	O4'-C1'-C2'	2.26	108.33	105.14
72	L5	4569	PSU	C6-N1-C2	-2.26	120.37	122.68
76	S2	1243	PSU	C6-N1-C2	-2.26	120.37	122.68
76	S2	105	PSU	C6-N1-C2	-2.26	120.37	122.68
72	L5	3718	A2M	C6-C5-C4	2.26	120.22	117.18
76	S2	36	PSU	C6-N1-C2	-2.25	120.38	122.68
76	S2	573	PSU	C6-N1-C2	-2.25	120.38	122.68
72	L5	4493	PSU	C6-N1-C2	-2.25	120.38	122.68
72	L5	3695	PSU	C6-N1-C2	-2.25	120.38	122.68
72	L5	4532	PSU	C6-N1-C2	-2.25	120.38	122.68
76	S2	576	A2M	C4-C5-N7	-2.25	107.88	110.62
72	L5	1782	PSU	C6-N1-C2	-2.25	120.39	122.68
72	L5	1582	PSU	O2-C2-N1	-2.25	120.32	122.79
76	S2	1056	PSU	C6-N1-C2	-2.24	120.39	122.68
76	S2	1832	6MZ	C9-N6-C6	2.24	124.81	122.87
72	L5	3785	A2M	C4-N9-C8	2.24	108.16	105.73
72	L5	1871	A2M	C5-C4-N9	2.24	108.39	105.78
76	S2	1692	PSU	C6-N1-C2	-2.24	120.39	122.68
72	L5	4227	OMU	O2-C2-N1	-2.24	119.81	122.79
72	L5	2508	PSU	O2-C2-N1	-2.24	120.32	122.79
72	L5	4420	PSU	O4'-C1'-C2'	2.24	108.31	105.14
72	L5	4431	PSU	C6-N1-C2	-2.24	120.39	122.68
72	L5	1781	PSU	C6-N1-C2	-2.24	120.39	122.68
72	L5	2508	PSU	C6-N1-C2	-2.24	120.39	122.68
72	L5	3734	PSU	C6-N1-C2	-2.24	120.39	122.68
72	L5	3715	PSU	C6-N1-C2	-2.24	120.40	122.68
72	L5	2839	PSU	C6-N1-C2	-2.23	120.40	122.68
76	S2	1232	PSU	C6-N1-C2	-2.23	120.40	122.68
72	L5	3808	OMC	C1'-N1-C6	-2.23	115.97	120.84
76	S2	1842	4AC	N4-C4-N3	2.23	117.60	113.85
72	L5	1322	1MA	N1-C6-N6	2.23	125.44	119.77
76	S2	1031	A2M	C5-C4-N9	2.23	108.38	105.78
72	L5	4361	PSU	C6-N1-C2	-2.23	120.40	122.68
76	S2	1445	PSU	C6-C5-C4	2.23	119.76	118.20
72	L5	4530	UR3	C6-N1-C2	-2.23	119.79	121.79
76	S2	1174	PSU	C6-N1-C2	-2.23	120.40	122.68
76	S2	93	PSU	C6-N1-C2	-2.23	120.41	122.68
72	L5	3851	PSU	C6-N1-C2	-2.22	120.41	122.68
76	S2	109	PSU	C6-N1-C2	-2.22	120.41	122.68
76	S2	1347	PSU	C6-N1-C2	-2.22	120.41	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	668	A2M	C5-C4-N9	2.22	108.36	105.78
72	L5	4972	PSU	C6-N1-C2	-2.22	120.42	122.68
72	L5	5001	PSU	C6-N1-C2	-2.22	120.42	122.68
72	L5	3920	PSU	C6-N1-C2	-2.21	120.42	122.68
72	L5	4500	PSU	C6-C5-C4	2.21	119.74	118.20
72	L5	5010	PSU	C6-N1-C2	-2.21	120.43	122.68
76	S2	815	PSU	C6-N1-C2	-2.21	120.43	122.68
72	L5	4569	PSU	O2-C2-N1	-2.21	120.36	122.79
72	L5	4442	PSU	O4'-C1'-C2'	2.20	108.25	105.14
76	S2	1643	PSU	C6-N1-C2	-2.20	120.43	122.68
72	L5	1524	A2M	C2'-C1'-N9	-2.20	109.83	113.53
72	L5	4531	PSU	C6-N1-C2	-2.19	120.44	122.68
76	S2	814	PSU	C6-N1-C2	-2.19	120.44	122.68
76	S2	99	A2M	C5-C4-N9	2.19	108.33	105.78
76	S2	576	A2M	C5-C4-N9	2.19	108.33	105.78
72	L5	4299	PSU	C6-N1-C2	-2.18	120.45	122.68
76	S2	1337	4AC	N4-C4-N3	2.18	117.52	113.85
72	L5	2824	OMC	C1'-N1-C2	2.18	123.29	118.42
72	L5	4220	6MZ	C5-C4-N9	2.18	108.31	105.78
72	L5	4442	PSU	C6-N1-C2	-2.18	120.46	122.68
76	S2	1445	PSU	C6-N1-C2	-2.18	120.46	122.68
76	S2	1678	A2M	C4-C5-N7	-2.18	107.97	110.62
72	L5	4523	A2M	C5-C4-N9	2.17	108.31	105.78
72	L5	4579	PSU	C6-N1-C2	-2.17	120.46	122.68
72	L5	2363	A2M	C4-C5-N7	-2.17	107.97	110.62
76	S2	296	PSU	C6-N1-C2	-2.17	120.46	122.68
76	S2	1367	PSU	C6-N1-C2	-2.17	120.47	122.68
76	S2	1383	A2M	C5-C4-N9	2.17	108.31	105.78
72	L5	1779	PSU	C6-N1-C2	-2.17	120.47	122.68
72	L5	4312	PSU	C6-N1-C2	-2.17	120.47	122.68
72	L5	2815	A2M	C5-C4-N9	2.16	108.30	105.78
76	S2	484	A2M	C4-C5-N7	-2.16	107.99	110.62
72	L5	3760	A2M	C4-C5-N7	-2.16	107.99	110.62
76	S2	34	PSU	C6-N1-C2	-2.16	120.48	122.68
72	L5	398	A2M	C5-C4-N9	2.16	108.29	105.78
76	S2	1383	A2M	C4-C5-N7	-2.16	107.99	110.62
76	S2	1248	B8N	O4'-C1'-C2'	2.16	108.18	105.14
76	S2	822	PSU	O4'-C1'-C2'	2.15	108.18	105.14
72	L5	2363	A2M	C5-C4-N9	2.15	108.29	105.78
76	S2	651	PSU	C6-N1-C2	-2.15	120.48	122.68
76	S2	468	A2M	C5-C4-N9	2.15	108.28	105.78
71	L8	55	PSU	C6-N1-C2	-2.15	120.48	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1081	PSU	O2-C2-N1	-2.15	120.42	122.79
76	S2	1136	PSU	C6-N1-C2	-2.15	120.48	122.68
72	L5	2401	A2M	C4-C5-N7	-2.15	108.00	110.62
76	S2	668	A2M	C4-C5-N7	-2.15	108.00	110.62
72	L5	1524	A2M	C4-C5-N7	-2.14	108.01	110.62
72	L5	4590	A2M	C5-C4-N9	2.14	108.27	105.78
76	S2	590	A2M	C4-C5-N7	-2.14	108.02	110.62
72	L5	3925	OMU	O2-C2-N1	-2.14	119.95	122.79
76	S2	966	PSU	C6-N1-C2	-2.14	120.50	122.68
72	L5	4576	PSU	C6-N1-C2	-2.13	120.50	122.68
72	L5	400	A2M	C4-C5-N7	-2.13	108.02	110.62
72	L5	3867	A2M	C6-C5-C4	2.13	120.05	117.18
76	S2	1031	A2M	C4-C5-N7	-2.13	108.02	110.62
72	L5	1871	A2M	C4-C5-N7	-2.13	108.02	110.62
76	S2	1832	6MZ	C2-N1-C6	2.13	122.41	115.25
72	L5	4521	PSU	C6-N1-C2	-2.13	120.51	122.68
76	S2	1238	PSU	C6-N1-C2	-2.13	120.51	122.68
71	L8	69	PSU	O4'-C1'-C2'	2.13	108.14	105.14
72	L5	2401	A2M	C5-C4-N9	2.12	108.25	105.78
72	L5	3724	A2M	C4-C5-N7	-2.12	108.03	110.62
76	S2	686	PSU	C6-N1-C2	-2.12	120.51	122.68
76	S2	576	A2M	C4'-O4'-C1'	-2.12	104.80	109.47
76	S2	1244	PSU	C6-N1-C2	-2.11	120.52	122.68
72	L5	1862	PSU	C6-N1-C2	-2.11	120.52	122.68
76	S2	468	A2M	C4-C5-N7	-2.11	108.05	110.62
72	L5	3844	PSU	C6-N1-C2	-2.11	120.53	122.68
76	S2	866	PSU	C6-N1-C2	-2.11	120.53	122.68
72	L5	1326	A2M	C4'-O4'-C1'	-2.11	104.83	109.47
72	L5	400	A2M	C5-C4-N9	2.10	108.23	105.78
76	S2	99	A2M	C4-C5-N7	-2.10	108.06	110.62
72	L5	398	A2M	C4-C5-N7	-2.10	108.06	110.62
72	L5	4457	PSU	C6-N1-C2	-2.10	120.53	122.68
76	S2	1177	PSU	C6-N1-C2	-2.10	120.53	122.68
76	S2	27	A2M	C4-C5-N7	-2.10	108.06	110.62
76	S2	1081	PSU	O4'-C1'-C2'	2.10	108.10	105.14
72	L5	3724	A2M	C5-C4-N9	2.10	108.22	105.78
72	L5	3867	A2M	C4-C5-N7	-2.09	108.07	110.62
72	L5	4571	A2M	C4-C5-N7	-2.09	108.07	110.62
76	S2	1804	OMU	O2-C2-N1	-2.09	120.00	122.79
76	S2	27	A2M	C5-C4-N9	2.09	108.22	105.78
72	L5	2422	OMC	C1'-N1-C2	2.09	123.09	118.42
69	Pt	56	PSU	C6-N1-C2	-2.09	120.55	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	S2	1678	A2M	C6-C5-C4	2.09	119.99	117.18
76	S2	1832	6MZ	C1'-N9-C8	2.09	131.85	127.14
69	Pt	33	OMC	C1'-N1-C6	-2.09	116.29	120.84
72	L5	3830	A2M	C5-C4-N9	2.08	108.21	105.78
72	L5	4636	PSU	C6-N1-C2	-2.08	120.55	122.68
72	L5	3830	A2M	C4-C5-N7	-2.08	108.08	110.62
76	S2	1239	PSU	C6-N1-C2	-2.08	120.55	122.68
72	L5	4636	PSU	O4'-C1'-C2'	2.08	108.08	105.14
76	S2	627	OMU	O2-C2-N1	-2.08	120.02	122.79
76	S2	576	A2M	C4-N9-C8	2.08	107.98	105.73
76	S2	484	A2M	C6-C5-C4	2.08	119.97	117.18
72	L5	4296	PSU	C6-N1-C2	-2.07	120.57	122.68
69	Pt	8	4SU	O2-C2-N1	-2.06	120.04	122.79
76	S2	1031	A2M	C2'-C1'-N9	-2.06	110.06	113.53
69	Pt	47	G7M	N9-C8-N7	-2.06	107.12	112.21
76	S2	218	PSU	C6-N1-C2	-2.06	120.58	122.68
72	L5	2837	OMU	O2-C2-N1	-2.05	120.06	122.79
72	L5	1326	A2M	C5-C4-N9	2.05	108.17	105.78
72	L5	3715	PSU	O4'-C1'-C2'	2.05	108.04	105.14
72	L5	4420	PSU	C6-N1-C2	-2.05	120.59	122.68
72	L5	400	A2M	C4'-O4'-C1'	-2.05	104.95	109.47
72	L5	2843	PSU	C6-N1-C2	-2.05	120.59	122.68
72	L5	2815	A2M	C4'-O4'-C1'	-2.05	104.95	109.47
76	S2	668	A2M	C3'-C2'-C1'	2.04	106.72	102.89
72	L5	4220	6MZ	C4-C5-N7	-2.04	108.14	110.62
72	L5	2815	A2M	C4-N9-C8	2.03	107.93	105.73
72	L5	1677	PSU	C6-N1-C2	-2.03	120.61	122.68
76	S2	801	PSU	C6-N1-C2	-2.03	120.61	122.68
72	L5	3764	PSU	O4'-C1'-C2'	2.03	108.01	105.14
72	L5	4457	PSU	O4'-C1'-C2'	2.03	108.00	105.14
72	L5	3825	A2M	C6-C5-C4	2.03	119.91	117.18
76	S2	572	PSU	O4'-C1'-C2'	2.03	108.00	105.14
72	L5	1534	A2M	C5-C4-N9	2.02	108.14	105.78
72	L5	4523	A2M	C4-C5-N7	-2.02	108.15	110.62
69	Pt	47	G7M	N2-C2-N1	2.02	121.02	116.71
72	L5	4571	A2M	C5-C4-N9	2.02	108.14	105.78
72	L5	1340	OMC	C1'-N1-C2	2.02	122.93	118.42
72	L5	4498	OMU	O2-C2-N1	-2.02	120.10	122.79
76	S2	1850	MA6	C4-C5-N7	-2.02	108.16	110.62
72	L5	3867	A2M	C5-C4-N9	2.02	108.13	105.78
76	S2	218	PSU	O4'-C1'-C2'	2.01	107.98	105.14
76	S2	1136	PSU	C6-C5-C4	2.01	119.60	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	L5	1534	A2M	O4'-C1'-N9	2.01	112.02	108.06
67	La	39	V5N	O-C-CA	-2.00	119.53	124.78
76	S2	1643	PSU	O4'-C1'-C2'	2.00	107.97	105.14
72	L5	4571	A2M	C2'-C1'-N9	-2.00	110.16	113.53
72	L5	3724	A2M	C6-C5-C4	2.00	119.87	117.18
72	L5	4571	A2M	C6-C5-C4	2.00	119.87	117.18

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Lo	53	MLZ	N-CA-CB-CG
3	Lo	53	MLZ	C-CA-CB-CG
65	Lb	5	MLZ	N-CA-CB-CG
65	Lb	5	MLZ	C-CA-CB-CG
72	L5	398	A2M	O4'-C4'-C5'-O5'
72	L5	398	A2M	C1'-C2'-O2'-CM'
72	L5	400	A2M	C1'-C2'-O2'-CM'
72	L5	1625	OMG	O4'-C4'-C5'-O5'
72	L5	2824	OMC	C1'-C2'-O2'-CM2
72	L5	3701	OMC	C2'-C1'-N1-C6
72	L5	3718	A2M	C1'-C2'-O2'-CM'
72	L5	3724	A2M	C1'-C2'-O2'-CM'
72	L5	3760	A2M	C2'-C1'-N9-C4
72	L5	3808	OMC	C1'-C2'-O2'-CM2
72	L5	3867	A2M	C1'-C2'-O2'-CM'
72	L5	3925	OMU	C1'-C2'-O2'-CM2
72	L5	4196	OMG	C1'-C2'-O2'-CM2
72	L5	4420	PSU	C2'-C1'-C5-C4
72	L5	4523	A2M	C1'-C2'-O2'-CM'
72	L5	4590	A2M	C4'-C5'-O5'-P
72	L5	4636	PSU	C2'-C1'-C5-C6
72	L5	4637	OMG	C1'-C2'-O2'-CM2
71	L8	69	PSU	C3'-C4'-C5'-O5'
71	L8	75	OMG	C1'-C2'-O2'-CM2
76	S2	27	A2M	C1'-C2'-O2'-CM'
76	S2	116	OMU	C1'-C2'-O2'-CM2
76	S2	468	A2M	C1'-C2'-O2'-CM'
76	S2	484	A2M	C1'-C2'-O2'-CM'
76	S2	512	A2M	O4'-C4'-C5'-O5'
76	S2	576	A2M	C3'-C4'-C5'-O5'
76	S2	644	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
76	S2	668	A2M	C1'-C2'-O2'-CM'
76	S2	683	OMG	C3'-C4'-C5'-O5'
76	S2	867	OMG	C1'-C2'-O2'-CM2
76	S2	1248	B8N	N34-C33-C34-O35
76	S2	1383	A2M	C1'-C2'-O2'-CM'
76	S2	1447	OMG	O4'-C4'-C5'-O5'
76	S2	1447	OMG	C3'-C4'-C5'-O5'
76	S2	1678	A2M	C1'-C2'-O2'-CM'
76	S2	1832	6MZ	O4'-C4'-C5'-O5'
76	S2	1832	6MZ	C3'-C4'-C5'-O5'
69	Pt	21	H2U	O4'-C4'-C5'-O5'
72	L5	1625	OMG	C3'-C4'-C5'-O5'
72	L5	3729	PSU	O4'-C4'-C5'-O5'
72	L5	3760	A2M	O4'-C4'-C5'-O5'
72	L5	3844	PSU	C3'-C4'-C5'-O5'
72	L5	3844	PSU	O4'-C4'-C5'-O5'
72	L5	4420	PSU	C3'-C4'-C5'-O5'
72	L5	4420	PSU	O4'-C4'-C5'-O5'
71	L8	69	PSU	O4'-C4'-C5'-O5'
76	S2	99	A2M	O4'-C4'-C5'-O5'
76	S2	512	A2M	C3'-C4'-C5'-O5'
76	S2	590	A2M	O4'-C4'-C5'-O5'
76	S2	590	A2M	C3'-C4'-C5'-O5'
76	S2	644	OMG	C3'-C4'-C5'-O5'
76	S2	668	A2M	O4'-C4'-C5'-O5'
76	S2	668	A2M	C3'-C4'-C5'-O5'
72	L5	3760	A2M	C2'-C1'-N9-C8
72	L5	3701	OMC	C2'-C1'-N1-C2
76	S2	1248	B8N	N34-C33-C34-O36
72	L5	398	A2M	C3'-C4'-C5'-O5'
72	L5	1677	PSU	C3'-C4'-C5'-O5'
72	L5	1677	PSU	O4'-C4'-C5'-O5'
72	L5	2364	OMG	O4'-C4'-C5'-O5'
72	L5	3729	PSU	C3'-C4'-C5'-O5'
76	S2	576	A2M	O4'-C4'-C5'-O5'
76	S2	683	OMG	O4'-C4'-C5'-O5'
76	S2	428	OMU	C2'-C1'-N1-C6
69	Pt	21	H2U	C3'-C4'-C5'-O5'
72	L5	3760	A2M	C3'-C4'-C5'-O5'
76	S2	468	A2M	O4'-C4'-C5'-O5'
76	S2	428	OMU	C2'-C1'-N1-C2
72	L5	2364	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
72	L5	3867	A2M	C3'-C4'-C5'-O5'
76	S2	99	A2M	C3'-C4'-C5'-O5'
76	S2	1639	G7M	C3'-C4'-C5'-O5'
3	Lo	53	MLZ	CD-CE-NZ-CM
72	L5	2422	OMC	O4'-C4'-C5'-O5'
72	L5	3758	PSU	C3'-C4'-C5'-O5'
72	L5	3785	A2M	O4'-C4'-C5'-O5'
72	L5	3867	A2M	O4'-C4'-C5'-O5'
76	S2	1639	G7M	O4'-C4'-C5'-O5'
76	S2	627	OMU	O4'-C4'-C5'-O5'
76	S2	1243	PSU	C3'-C4'-C5'-O5'
72	L5	3785	A2M	C3'-C4'-C5'-O5'
72	L5	2422	OMC	C3'-C4'-C5'-O5'
72	L5	4637	OMG	O4'-C4'-C5'-O5'
76	S2	644	OMG	C1'-C2'-O2'-CM2
69	Pt	21	H2U	C4'-C5'-O5'-P
72	L5	1534	A2M	C4'-C5'-O5'-P
72	L5	4500	PSU	C4'-C5'-O5'-P
76	S2	1851	MA6	C4'-C5'-O5'-P
72	L5	2508	PSU	C3'-C4'-C5'-O5'
72	L5	3758	PSU	O4'-C4'-C5'-O5'
76	S2	119	PSU	O4'-C4'-C5'-O5'
72	L5	2876	OMG	C3'-C2'-O2'-CM2
72	L5	4370	OMG	C3'-C2'-O2'-CM2
76	S2	428	OMU	O4'-C1'-N1-C6
72	L5	4447	5MC	C2'-C1'-N1-C6
72	L5	1326	A2M	C4'-C5'-O5'-P
76	S2	918	PSU	O4'-C4'-C5'-O5'
65	Lb	5	MLZ	CE-CD-CG-CB
76	S2	428	OMU	O4'-C1'-N1-C2
76	S2	1248	B8N	N3-C31-C32-C33
72	L5	4447	5MC	O4'-C1'-N1-C6
72	L5	3701	OMC	O4'-C1'-N1-C2
72	L5	3844	PSU	C4'-C5'-O5'-P
76	S2	1447	OMG	C4'-C5'-O5'-P
76	S2	1243	PSU	O4'-C4'-C5'-O5'
72	L5	3701	OMC	O4'-C1'-N1-C6
76	S2	1248	B8N	C32-C31-N3-C4
76	S2	644	OMG	C4'-C5'-O5'-P
76	S2	1490	OMG	C4'-C5'-O5'-P
72	L5	3785	A2M	C3'-C2'-O2'-CM'
69	Pt	47	G7M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
76	S2	576	A2M	C4'-C5'-O5'-P
76	S2	822	PSU	O4'-C4'-C5'-O5'
76	S2	1232	PSU	O4'-C1'-C5-C4
76	S2	1238	PSU	O4'-C1'-C5-C4
72	L5	1322	1MA	C2'-C1'-N9-C8
72	L5	4447	5MC	O4'-C1'-N1-C2
76	S2	627	OMU	O4'-C1'-N1-C6
72	L5	1322	1MA	C2'-C1'-N9-C4
76	S2	627	OMU	C2'-C1'-N1-C6
72	L5	2508	PSU	O4'-C4'-C5'-O5'
76	S2	509	OMG	O4'-C4'-C5'-O5'
72	L5	3887	OMC	C4'-C5'-O5'-P
76	S2	1239	PSU	O4'-C4'-C5'-O5'
72	L5	2876	OMG	C1'-C2'-O2'-CM2
76	S2	1850	MA6	C5-C6-N6-C10
76	S2	590	A2M	C3'-C2'-O2'-CM'
76	S2	590	A2M	O4'-C1'-N9-C8
69	Pt	21	H2U	C2'-C1'-N1-C2
72	L5	1677	PSU	O4'-C1'-C5-C6
72	L5	4636	PSU	O4'-C1'-C5-C6
76	S2	1232	PSU	O4'-C1'-C5-C6
72	L5	2815	A2M	C4'-C5'-O5'-P
72	L5	4636	PSU	C4'-C5'-O5'-P
72	L5	1534	A2M	O4'-C4'-C5'-O5'
72	L5	2351	OMC	O4'-C4'-C5'-O5'
72	L5	4361	PSU	O4'-C4'-C5'-O5'
72	L5	4636	PSU	O4'-C4'-C5'-O5'
72	L5	4637	OMG	C3'-C4'-C5'-O5'
76	S2	119	PSU	C3'-C4'-C5'-O5'
76	S2	590	A2M	C2'-C1'-N9-C8
76	S2	428	OMU	O4'-C4'-C5'-O5'
76	S2	918	PSU	C3'-C4'-C5'-O5'
66	LA	216	V5N	O-C-CA-CB
69	Pt	33	OMC	C2'-C1'-N1-C2
72	L5	2351	OMC	C2'-C1'-N1-C2
72	L5	4447	5MC	C2'-C1'-N1-C2
76	S2	590	A2M	C2'-C1'-N9-C4
76	S2	627	OMU	C2'-C1'-N1-C2

There are no ring outliers.

60 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	S2	116	OMU	2	0
72	L5	1340	OMC	2	0
76	S2	576	A2M	1	0
76	S2	801	PSU	1	0
72	L5	1316	OMG	1	0
76	S2	1383	A2M	1	0
76	S2	509	OMG	1	0
76	S2	1445	PSU	1	0
76	S2	484	A2M	1	0
72	L5	3770	PSU	1	0
76	S2	1447	OMG	1	0
72	L5	3867	A2M	2	0
72	L5	1871	A2M	1	0
72	L5	4353	PSU	1	0
72	L5	4536	OMC	1	0
76	S2	436	OMG	1	0
76	S2	649	PSU	1	0
72	L5	2351	OMC	2	0
69	Pt	21	H2U	2	0
76	S2	468	A2M	1	0
72	L5	1326	A2M	1	0
76	S2	1678	A2M	1	0
72	L5	3785	A2M	2	0
76	S2	218	PSU	1	0
72	L5	4447	5MC	1	0
72	L5	4392	OMG	1	0
76	S2	512	A2M	1	0
76	S2	1248	B8N	1	0
72	L5	1683	PSU	1	0
72	L5	2824	OMC	1	0
72	L5	3925	OMU	1	0
72	L5	4299	PSU	1	0
72	L5	4523	A2M	1	0
72	L5	2363	A2M	1	0
69	Pt	33	OMC	1	0
72	L5	4579	PSU	2	0
76	S2	1639	G7M	1	0
76	S2	1391	OMC	1	0
76	S2	681	PSU	1	0
71	L8	75	OMG	2	0
72	L5	3724	A2M	1	0
72	L5	4620	OMU	3	0
76	S2	1692	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	L5	3825	A2M	1	0
72	L5	2424	OMG	1	0
72	L5	3718	A2M	3	0
76	S2	867	OMG	1	0
76	S2	1031	A2M	1	0
69	Pt	47	G7M	1	0
76	S2	668	A2M	1	0
72	L5	4571	A2M	1	0
72	L5	1677	PSU	1	0
76	S2	1004	PSU	2	0
76	S2	644	OMG	1	0
72	L5	1781	PSU	1	0
76	S2	1337	4AC	1	0
72	L5	4457	PSU	1	0
72	L5	3808	OMC	1	0
76	S2	1244	PSU	1	0
76	S2	27	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 261 ligands modelled in this entry, 260 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
85	SPD	L5	5103	-	9,9,9	0.44	0	8,8,8	0.15	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	SPD	L5	5103	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	L5	5103	SPD	N1-C2-C3-C4
85	L5	5103	SPD	C8-C7-N6-C5
85	L5	5103	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
76	S2	2
38	Lr	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lr	2(A):SER	C	3:ALA	N	4.82
1	S2	1832:6MZ	O3'	1833:C	P	4.80
1	S2	1831:A	O3'	1832:6MZ	P	4.40

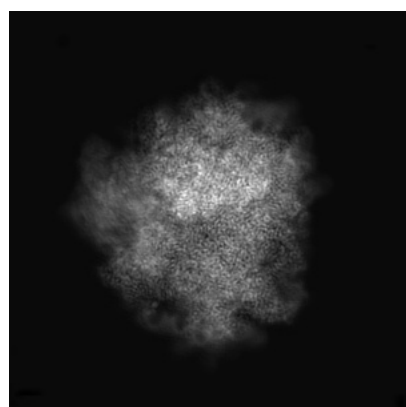
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54268. These allow visual inspection of the internal detail of the map and identification of artifacts.

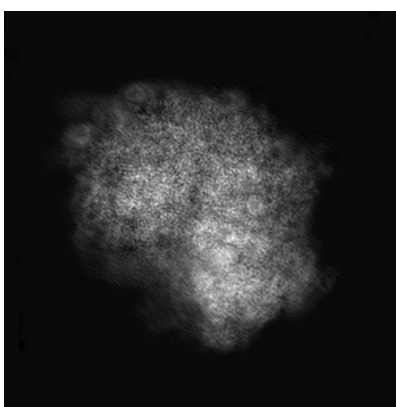
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

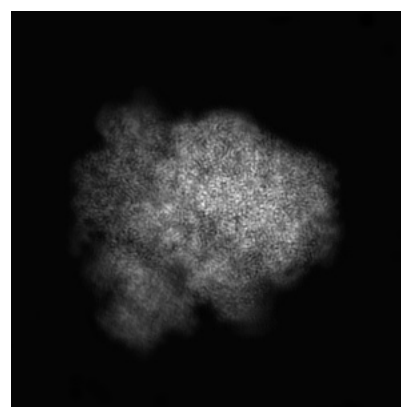
6.1.1 Primary map



X



Y

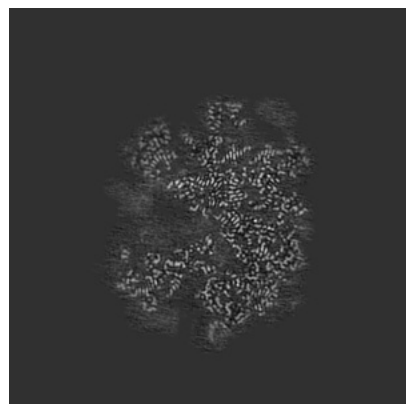


Z

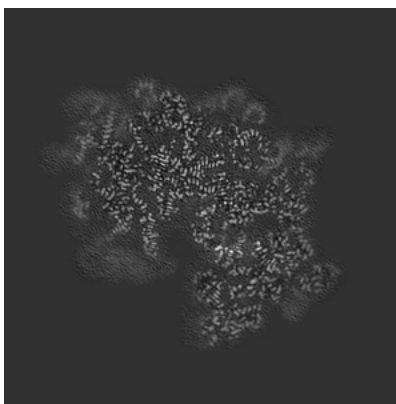
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

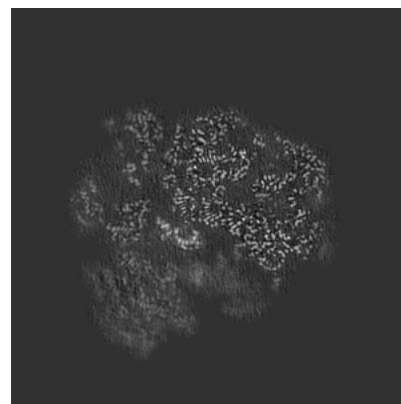
6.2.1 Primary map



X Index: 240



Y Index: 240

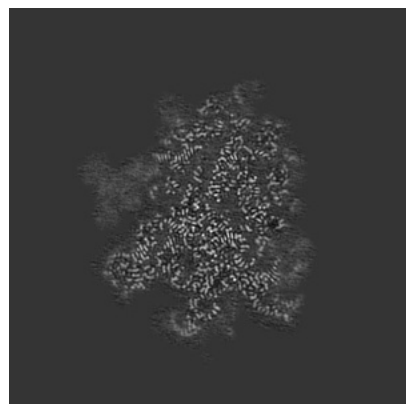


Z Index: 240

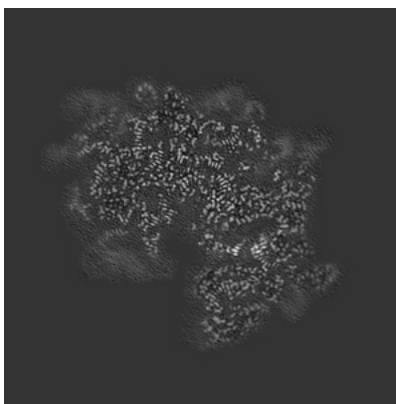
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

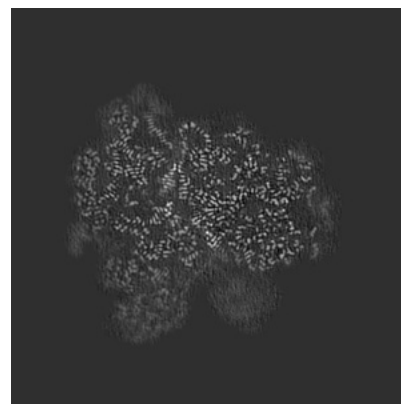
6.3.1 Primary map



X Index: 279



Y Index: 244

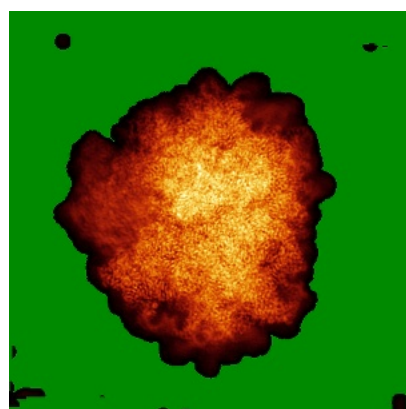


Z Index: 268

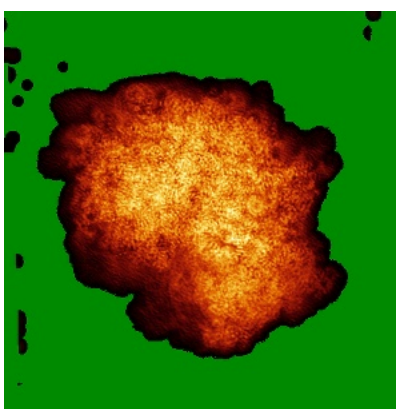
The images above show the largest variance slices of the map in three orthogonal directions.

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

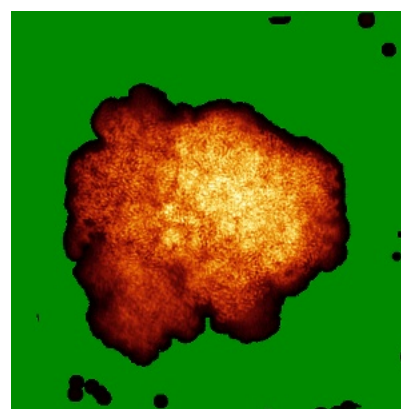
6.4.1 Primary map



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.

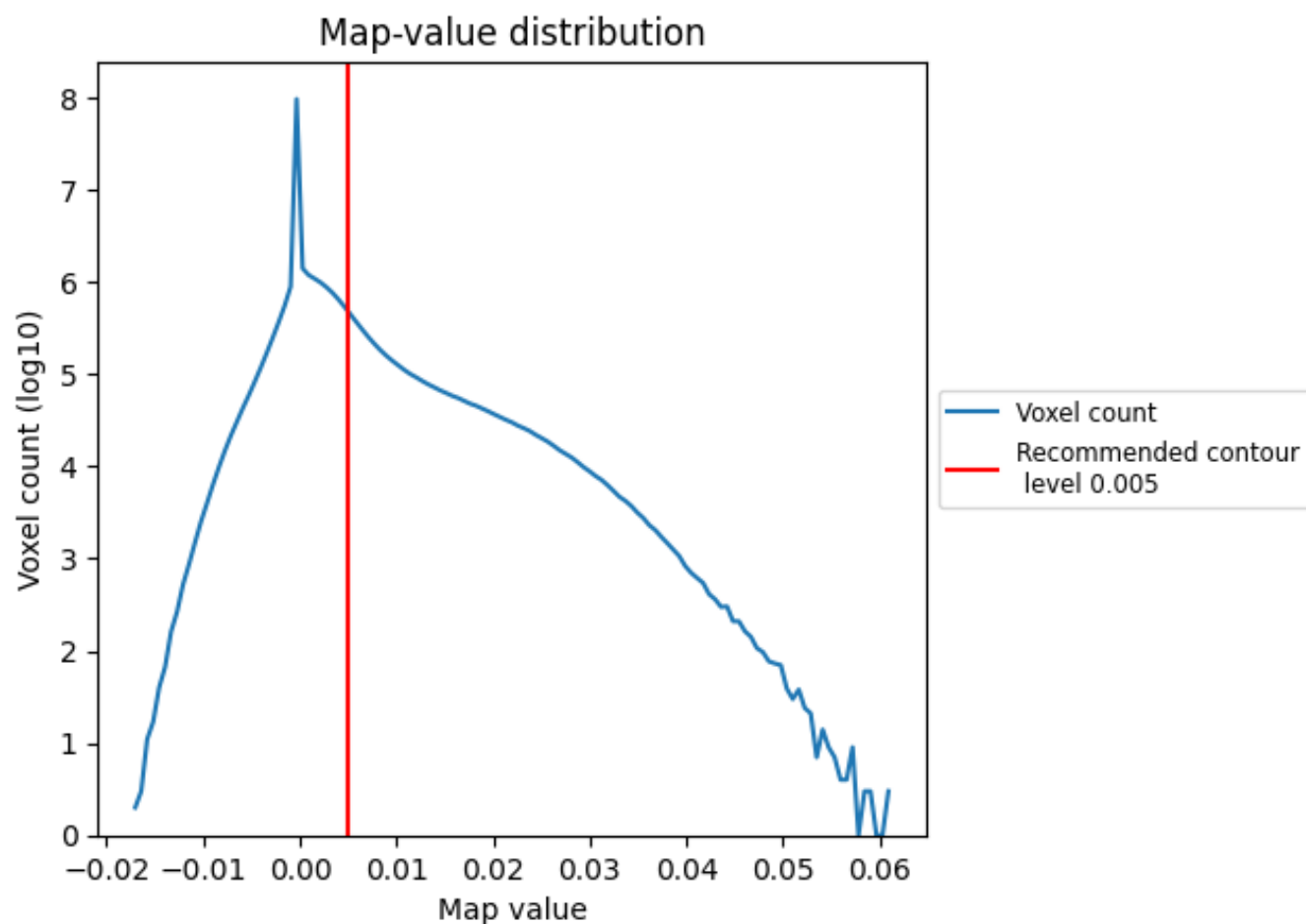
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

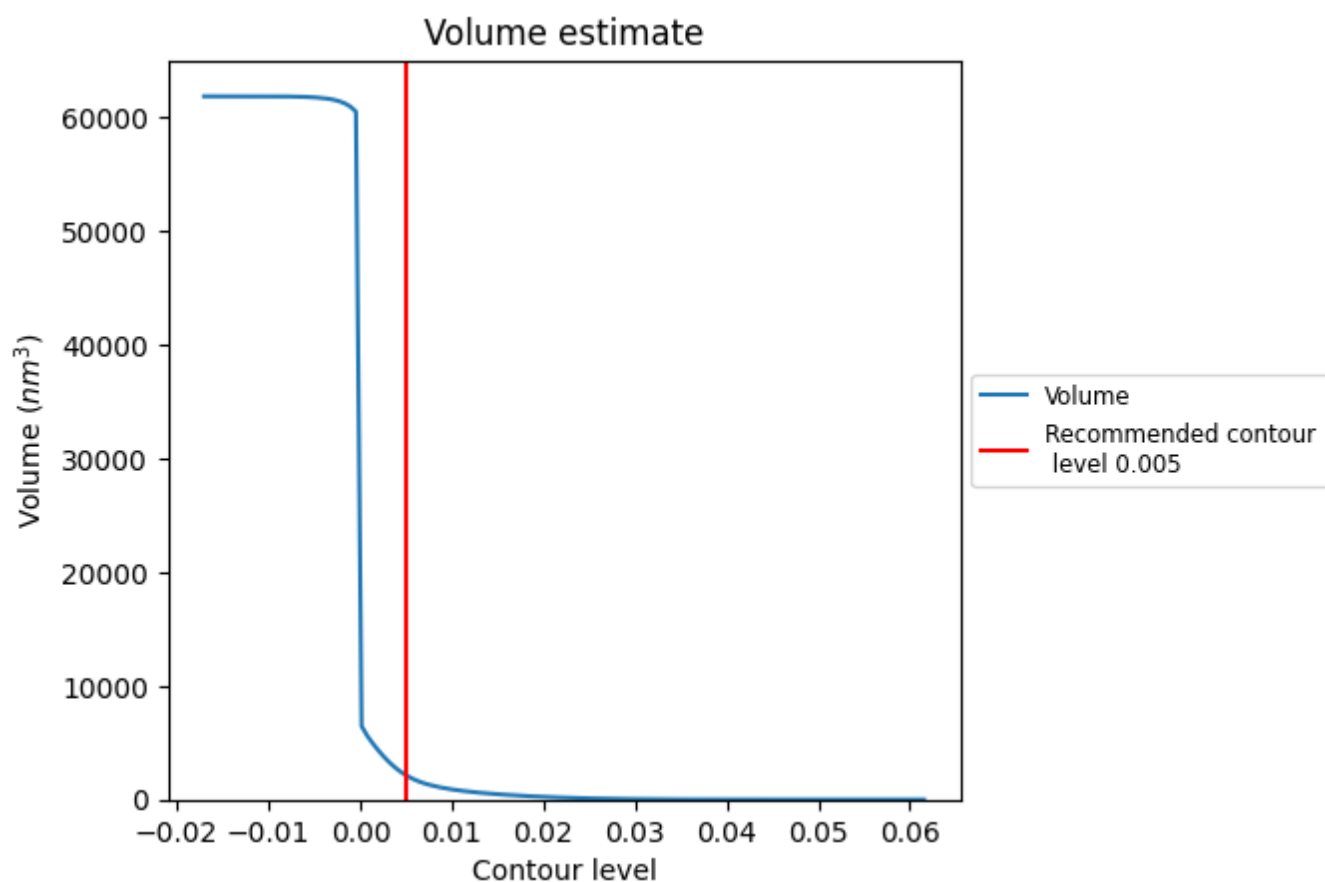
This section contains the results of statistical analysis of the map.

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.

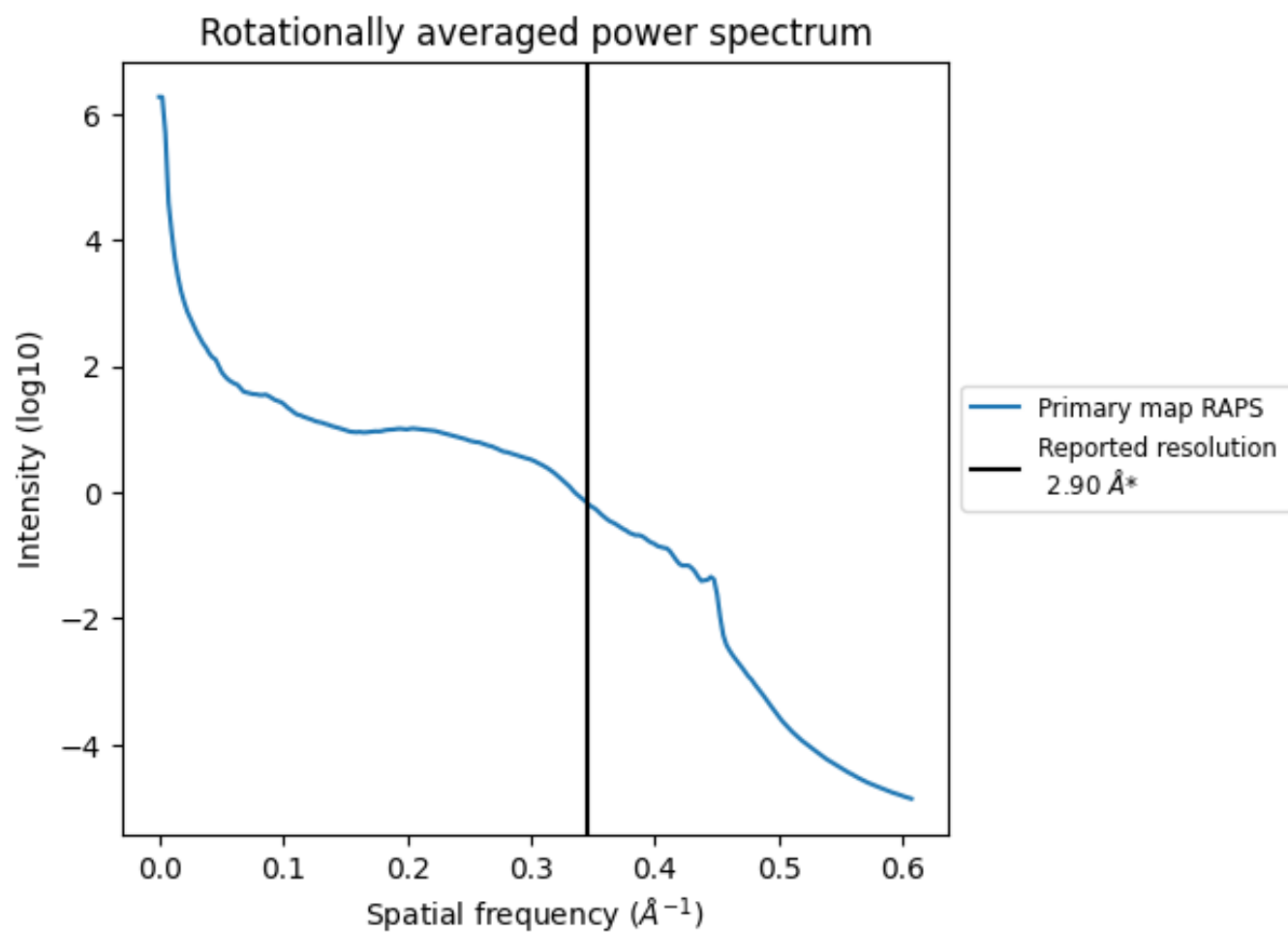
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2149 nm³; this corresponds to an approximate mass of 1941 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 0.345 Å⁻¹

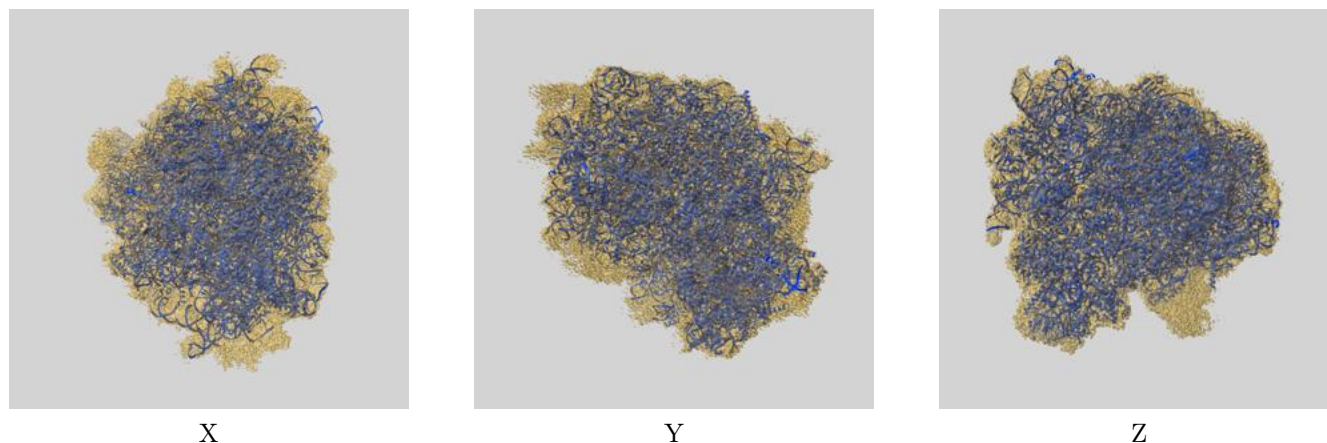
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

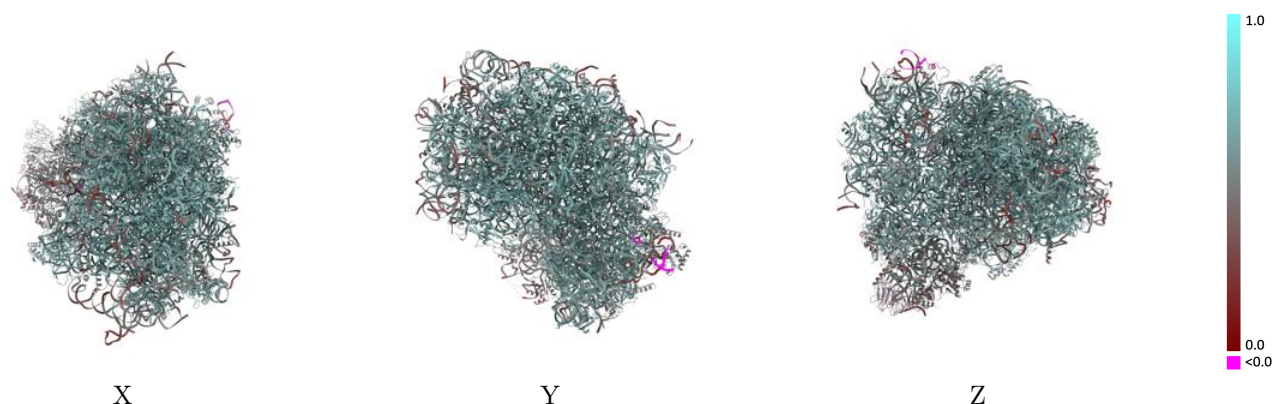
This section contains information regarding the fit between EMDB map EMD-54268 and PDB model 9RUA. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



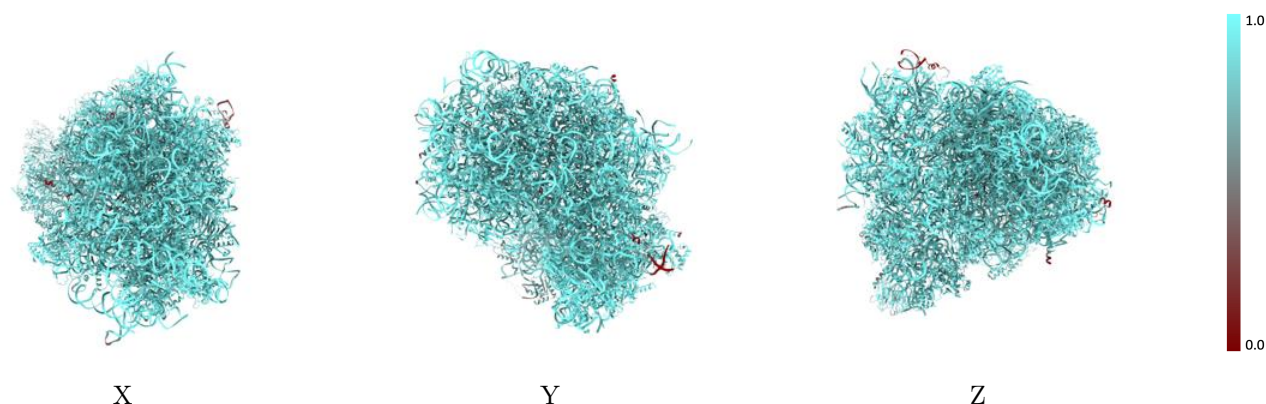
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



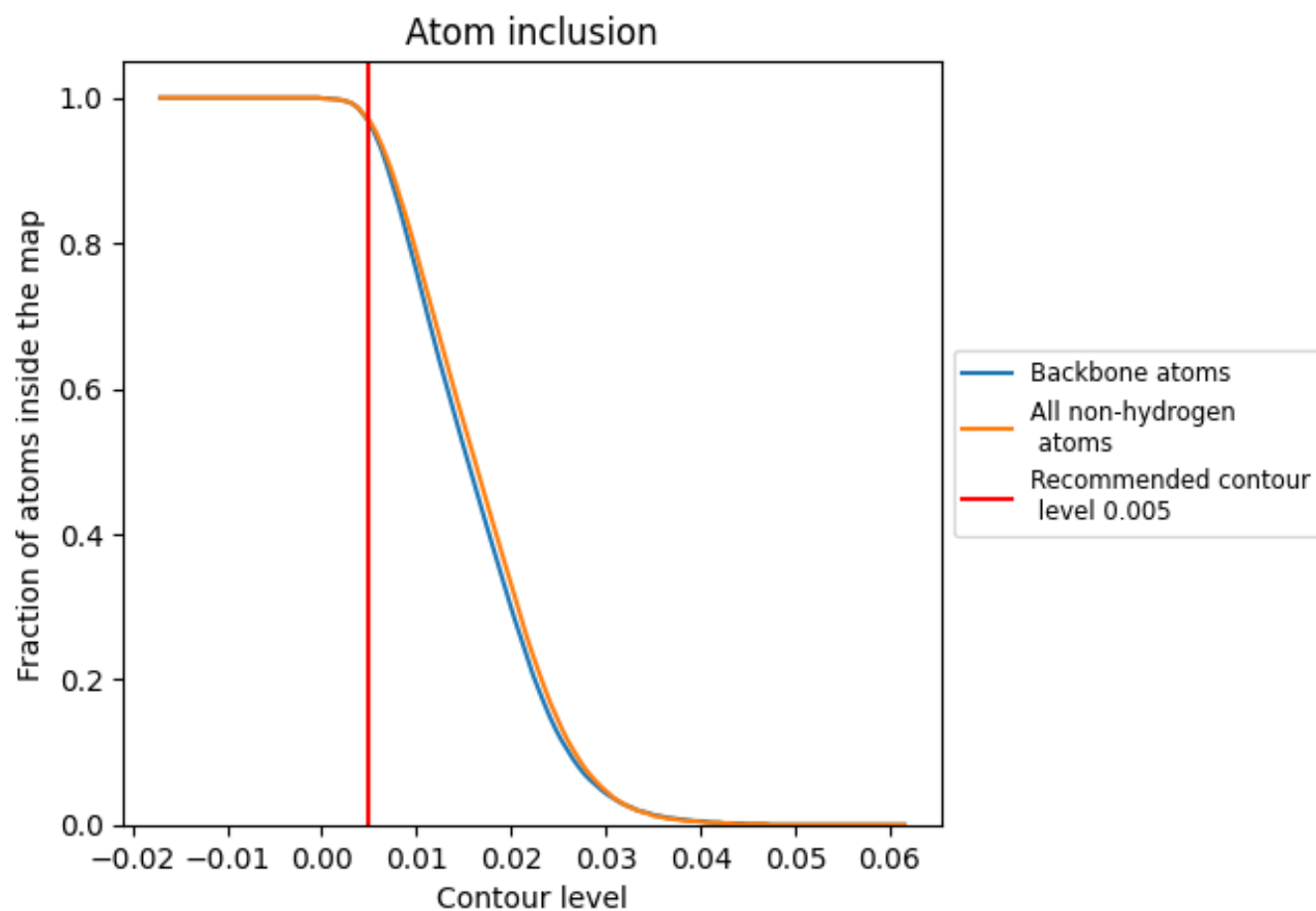
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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	 0.9690	 0.5880
L5	 0.9860	 0.5980
L7	 1.0000	 0.6230
L8	 0.9860	 0.6080
LA	 0.9940	 0.6530
LB	 0.9800	 0.6420
LC	 0.9830	 0.6470
LD	 0.9760	 0.6070
LE	 0.9830	 0.6140
LF	 0.9880	 0.6460
LG	 0.9150	 0.5870
LH	 0.9760	 0.6280
LI	 0.9780	 0.6330
LJ	 0.9490	 0.5590
LL	 0.9390	 0.6150
LM	 0.9770	 0.6240
LN	 0.9990	 0.6660
LO	 0.9890	 0.6510
LP	 0.9850	 0.6510
LQ	 0.9950	 0.6560
LR	 0.9730	 0.6070
LS	 0.9890	 0.6480
LT	 0.9760	 0.6330
LU	 0.9590	 0.5590
LV	 0.9890	 0.6450
LW	 0.9940	 0.6380
LX	 0.9760	 0.6310
LY	 0.9860	 0.6390
LZ	 0.9840	 0.6210
La	 0.9900	 0.6580
Lb	 0.9730	 0.5990
Lc	 0.9760	 0.5980
Ld	 0.9890	 0.6370
Le	 0.9890	 0.6590
Lf	 0.9880	 0.6560











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Chain	Atom inclusion	Q-score
Lg	 0.9920	 0.6410
Lh	 0.9530	 0.6170
Li	 0.9740	 0.6150
Lj	 0.9970	 0.6610
Lk	 0.9410	 0.5990
Ll	 0.9860	 0.6340
Lm	 0.9920	 0.6410
Ln	 0.9860	 0.6020
Lo	 0.9890	 0.6420
Lp	 0.9880	 0.6350
Lr	 0.9940	 0.6420
Pt	 0.5970	 0.3410
S2	 0.9680	 0.5530
S6	 0.8700	 0.3220
SA	 0.9450	 0.5880
SB	 0.9490	 0.5950
SC	 0.9660	 0.6040
SD	 0.8770	 0.4980
SE	 0.9720	 0.6030
SF	 0.9240	 0.4950
SG	 0.9500	 0.5620
SH	 0.9180	 0.5460
SI	 0.9170	 0.5690
SJ	 0.9690	 0.5950
SK	 0.8330	 0.4010
SL	 0.9680	 0.6160
SN	 0.9810	 0.6090
SO	 0.9830	 0.5950
SP	 0.8380	 0.4200
SQ	 0.9430	 0.4690
SR	 0.8880	 0.5180
SS	 0.9380	 0.4480
ST	 0.9520	 0.4590
SU	 0.8720	 0.5090
SV	 0.9390	 0.5970
SW	 0.9840	 0.6240
SX	 0.9850	 0.6150
SY	 0.9910	 0.6000
SZ	 0.9290	 0.4260
Sa	 0.9720	 0.6050
Sb	 0.9620	 0.5810
Sc	 0.9210	 0.5260

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Chain	Atom inclusion	Q-score
Sd	 0.9280	 0.4880
Se	 0.9580	 0.5770
Sg	 0.8170	 0.4430
mR	 0.7510	 0.4250