



Full wwPDB EM Validation Report ⓘ

May 28, 2026 – 11:36 am BST

PDB ID : 9RU9 / pdb_00009ru9
EMDB ID : EMD-54267
Title : RPS26dC HEK mutant 80S ribosome bound to Kozak mRNA (RPS26dC-Kozak)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

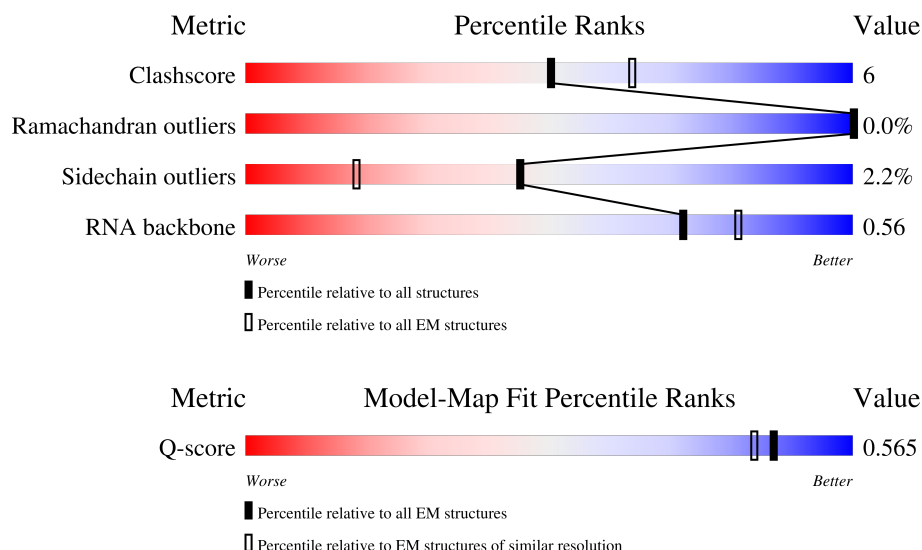
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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	LA	257	
2	SA	294	
3	LB	403	





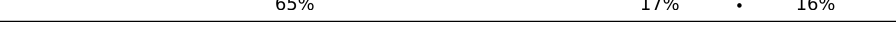
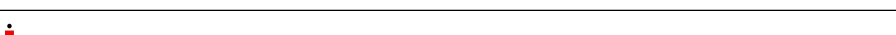



















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Mol	Chain	Length	Quality of chain
4	SB	264	
5	L8	156	
6	L7	120	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SF	204	
12	SH	194	
13	SW	130	
14	SI	208	
15	SQ	146	
16	SU	119	
17	SK	165	
18	SO	151	
19	SX	143	
20	SM	132	
21	SS	152	
22	Sd	56	
23	SN	151	
24	SL	158	
25	SR	135	
26	SP	145	
27	ST	145	
28	SV	82	

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Mol	Chain	Length	Quality of chain
29	SY	133	
30	SZ	125	
31	Sa	115	
32	Sb	84	
33	Sc	69	
34	Se	133	
35	Sf	156	
36	Sg	317	
37	LC	427	
38	LJ	178	
39	LH	192	
40	LE	288	
41	LG	266	
42	LO	203	
43	LL	211	
44	LV	140	
45	LM	215	
46	La	148	
47	LN	204	
48	LI	214	
49	LD	297	
50	LQ	188	
51	LR	196	
52	LS	176	
53	LT	160	





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Mol	Chain	Length	Quality of chain
54	LP	184	
55	LU	128	
56	LX	156	
57	LY	145	
58	LZ	136	
59	Lr	136	
60	Lh	123	
61	Lb	159	
62	LF	248	
63	Lc	115	
64	Ld	125	
65	Le	135	
66	Lf	110	
67	Lg	117	
68	Li	105	
69	Lj	97	
70	Lk	70	
71	Ll	51	
72	Lm	128	
73	Ln	25	
74	Lo	106	
75	Lp	92	
76	Pt	77	
77	mR	27	
78	S2	1869	

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Mol	Chain	Length	Quality of chain
79	L5	5069	 44% 22% . 30%
80	Et	75	 56% 36% 8%
81	LW	157	 35% . . 61%
82	SG	249	 71% 17% 12%

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 209052 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 Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LA	250	Total	C	N	O	S	1	0
			1921	1203	395	317	6		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SA	217	Total	C	N	O	S	0	0
			1692	1077	297	310	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	MET	-	initiating methionine	UNP P08865

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	394	Total	C	N	O	S	0	0
			3068	1956	583	515	14		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SB	221	Total	C	N	O	S	0	0
			1761	1118	319	310	14		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SD	224	Total	C	N	O	S	0	0
			1642	1049	293	293	7		

- Molecule 8 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SJ	179	Total	C	N	O	S	0	0
			1477	944	298	233	2		

- Molecule 9 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SE	258	Total	C	N	O	S	0	0
			2044	1308	378	350	8		

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SC	220	Total	C	N	O	S	1	0
			1685	1093	293	289	10		

- Molecule 11 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SF	182	Total	C	N	O	S	0	0
			1434	898	270	259	7		

- Molecule 12 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SH	183	Total	C	N	O	S	0	0
			1409	903	262	243	1		

- Molecule 13 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SW	129	Total	C	N	O	S	0	0
			1030	657	193	174	6		

- Molecule 14 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SI	206	Total	C	N	O	S	0	0
			1652	1036	328	283	5		

- Molecule 15 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SQ	140	Total	C	N	O	S	0	0
			1109	707	210	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SU	101	Total	C	N	O		0	0
			519	313	101	105			

- Molecule 17 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SK	96	Total	C	N	O	S	0	0
			678	437	122	114	5		

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SO	134	Total	C	N	O	S	0	0
			990	607	197	180	6		

- Molecule 19 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SX	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 20 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	SM	44	Total	C	N	O	0	0
			218	130	44	44		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	105	GLY	GLN	conflict	UNP P25398
SM	106	CYS	ILE	conflict	UNP P25398
SM	107	SER	ASN	conflict	UNP P25398
SM	108	CYS	LEU	conflict	UNP P25398
SM	109	VAL	ILE	conflict	UNP P25398
SM	110	VAL	LYS	conflict	UNP P25398

- Molecule 21 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SS	148	Total	C	N	O	S	0	0
			1184	746	244	193	1		

- 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
			458	286	94	73	5		

- Molecule 23 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 24 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SL	142	Total	C	N	O	S	0	0
			1148	731	215	196	6		

- Molecule 25 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SR	132	Total	C	N	O	S	0	0
			1038	653	195	186	4		

- Molecule 26 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SP	128	Total	C	N	O	S	0	0
			1049	665	198	179	7		

- Molecule 27 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	ST	141	Total	C	N	O	S	1	0
			1010	637	193	178	2		

- Molecule 28 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SV	82	Total	C	N	O	S	0	0
			628	388	116	120	4		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SY	122	Total	C	N	O	S	0	0
			972	617	193	157	5		

- Molecule 30 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SZ	77	Total	C	N	O	S	0	0
			592	382	109	100	1		

- Molecule 31 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Sa	98	Total	C	N	O	S	1	0
			782	488	164	125	5		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sb	83	Total	C	N	O	S	0	0
			642	403	118	114	7		

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sc	58	Total	C	N	O	S	0	0
			449	274	86	87	2		

- Molecule 34 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Se	48	Total	C	N	O	S	0	0
			373	227	84	61	1		

- Molecule 35 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	35	Total	C	N	O	S	0	0
			194	116	37	38	3		

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sg	311	Total	C	N	O	S	0	0
			2387	1508	417	451	11		

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 38 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LJ	170	Total	C	N	O	S	0	0
			1354	857	253	238	6		

- Molecule 39 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 40 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LE	223	Total	C	N	O	S	0	0
			1786	1150	339	293	4		

- Molecule 41 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LG	232	Total	C	N	O	S	0	0
			1856	1182	359	311	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LO	202	Total	C	N	O	S	0	0
			1642	1058	320	259	5		

- Molecule 43 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LL	206	Total	C	N	O	S	1	0
			1662	1041	348	269	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LL	112	ALA	THR	conflict	UNP A0A6V7HLS0

- Molecule 44 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LV	130	Total	C	N	O	S	0	0
			972	615	183	169	5		

- 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 uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	La	147	Total	C	N	O	S	0	0
			1152	729	235	185	3		

- Molecule 47 is a protein called 60S ribosomal protein L15.

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

- Molecule 48 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LI	203	Total	C	N	O	S	0	0
			1645	1045	317	270	13		

- Molecule 49 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 50 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 51 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LR	187	Total	C	N	O	S	0	0
			1476	914	317	236	9		

- Molecule 52 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 53 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LT	159	Total	C	N	O	S	2	0
			1311	833	256	216	6		

- Molecule 54 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LP	153	Total	C	N	O	S	1	0
			1249	781	243	216	9		

- Molecule 55 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LU	99	Total	C	N	O	S	0	0
			804	515	140	147	2		

- Molecule 56 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LX	118	Total	C	N	O	S	0	0
			966	618	181	166	1		

- Molecule 57 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LY	133	Total	C	N	O	S	0	0
			1102	691	223	185	3		

- Molecule 58 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 59 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lr	124	Total	C	N	O	S	1	0
			1002	624	207	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	2	MET	-	initiating methionine	UNP P46779

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 61 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lb	111	Total	C	N	O	S	0	0
			898	560	195	139	4		

- Molecule 62 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LF	225	Total	C	N	O	S	2	0
			1885	1212	364	300	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Lc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

- Molecule 64 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ld	107	Total	C	N	O	S	0	0
			589	361	112	116			

- Molecule 65 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Le	128	Total	C	N	O	S	1	0
			1061	672	219	165	5		

- Molecule 66 is a protein called 60S ribosomal protein L35a.

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

- Molecule 67 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lg	112	Total	C	N	O	S	0	0
			875	548	180	141	6		

- Molecule 68 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Li	102	Total	C	N	O	S	0	0
			821	513	174	129	5		

- Molecule 69 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 70 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lk	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 71 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ll	50	Total	C	N	O	S	0	0
			437	278	95	63	1		

- Molecule 72 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Lm	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

- Molecule 73 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 74 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Lp	91	Total	C	N	O	S	1	0
			715	450	139	119	7		

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

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

- Molecule 77 is a RNA chain called Kozak mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	mR	7	Total	C	N	O	P	0	0
			156	69	32	48	7		

- Molecule 78 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	S2	1635	Total	C	N	O	P	0	0
			34940	15627	6260	11419	1634		

- Molecule 79 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	L5	3523	Total	C	N	O	P	1	0
			75626	33716	13837	24550	3523		

- Molecule 80 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Et	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 81 is a protein called 60S ribosomal protein L24.

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

- Molecule 82 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	SG	220	Total	C	N	O	S	0	0
			1683	1053	337	286	7		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

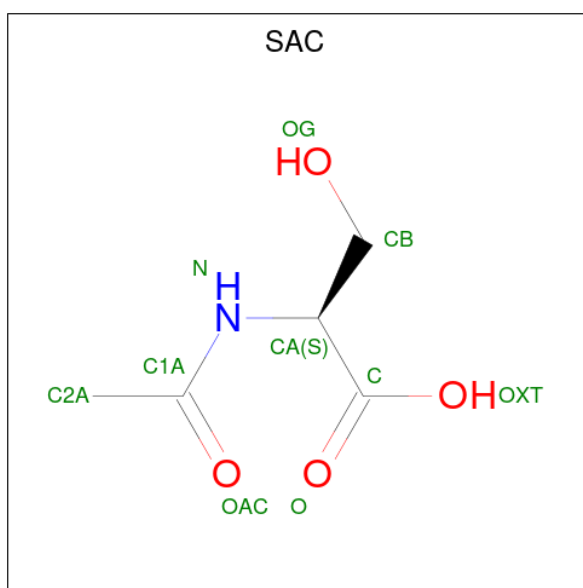
Mol	Chain	Residues	Atoms		AltConf
83	LA	3	Total	K	0
			3	3	
83	L8	3	Total	K	0
			3	3	
83	L7	4	Total	K	0
			4	4	
83	SO	1	Total	K	0
			1	1	
83	SL	1	Total	K	0
			1	1	
83	Sa	1	Total	K	0
			1	1	
83	LH	1	Total	K	0
			1	1	
83	LL	1	Total	K	0
			1	1	
83	LN	1	Total	K	0
			1	1	
83	LI	1	Total	K	0
			1	1	
83	LQ	1	Total	K	0
			1	1	
83	Lb	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
83	Le	1	Total	K	0
			1	1	
83	Lf	1	Total	K	0
			1	1	
83	Ll	1	Total	K	0
			1	1	
83	mR	1	Total	K	0
			1	1	
83	A	14	Total	K	0
			14	14	

- Molecule 84 is N-ACETYL-SERINE (CCD ID: SAC) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				AltConf
84	SA	1	Total	C	N	O	0
			9	5	1	3	
84	Lr	1	Total	C	N	O	0
			9	5	1	3	

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	LB	1	Total	Mg	0
			1	1	
85	L8	16	Total	Mg	0
			16	16	

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Mol	Chain	Residues	Atoms		AltConf
85	L7	15	Total 15	Mg 15	0
85	SX	1	Total 1	Mg 1	0
85	SS	2	Total 2	Mg 2	0
85	Sd	1	Total 1	Mg 1	0
85	SN	1	Total 1	Mg 1	0
85	ST	1	Total 1	Mg 1	0
85	LC	1	Total 1	Mg 1	0
85	LH	1	Total 1	Mg 1	0
85	LG	1	Total 1	Mg 1	0
85	LO	2	Total 2	Mg 2	0
85	LL	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	La	1	Total 1	Mg 1	0
85	LN	3	Total 3	Mg 3	0
85	LD	1	Total 1	Mg 1	0
85	LQ	2	Total 2	Mg 2	0
85	LR	1	Total 1	Mg 1	0
85	LS	1	Total 1	Mg 1	0
85	LP	2	Total 2	Mg 2	0
85	Lr	3	Total 3	Mg 3	0
85	LF	1	Total 1	Mg 1	0

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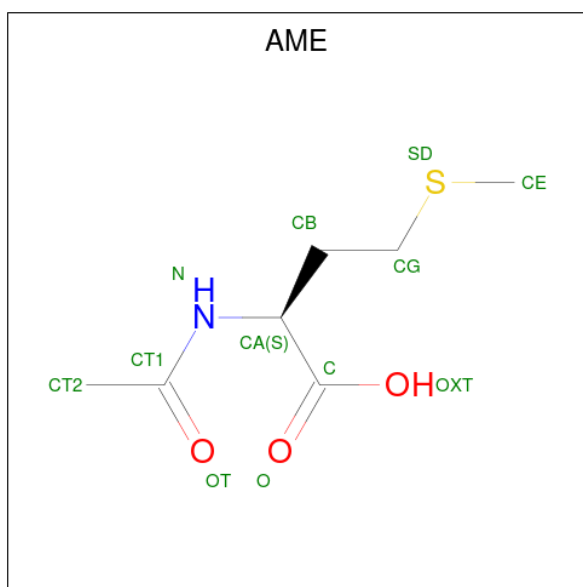
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Mol	Chain	Residues	Atoms		AltConf
85	Lc	1	Total 1	Mg 1	0
85	Lf	1	Total 1	Mg 1	0
85	Lg	1	Total 1	Mg 1	0
85	Lj	2	Total 2	Mg 2	0
85	Lo	1	Total 1	Mg 1	0
85	Lp	2	Total 2	Mg 2	0
85	Pt	1	Total 1	Mg 1	0
85	Et	1	Total 1	Mg 1	0
85	D	12	Total 12	Mg 12	0

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

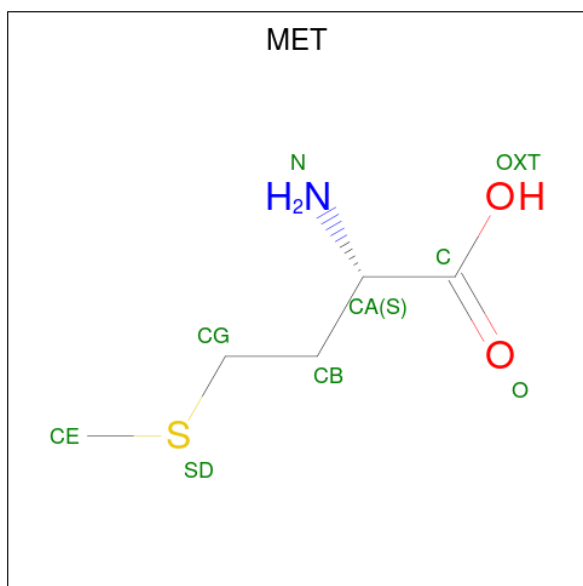
Mol	Chain	Residues	Atoms		AltConf
86	Sd	1	Total 1	Zn 1	0
86	Sa	1	Total 1	Zn 1	0
86	Sf	1	Total 1	Zn 1	0
86	Lg	1	Total 1	Zn 1	0
86	Lj	1	Total 1	Zn 1	0
86	Lm	1	Total 1	Zn 1	0
86	Lo	1	Total 1	Zn 1	0
86	Lp	1	Total 1	Zn 1	0

- Molecule 87 is N-ACETYLMETHIONINE (CCD ID: AME) (formula: C₇H₁₃NO₃S).



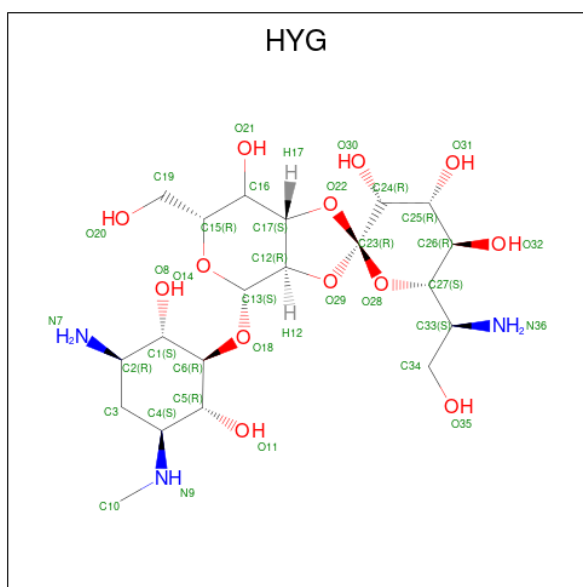
Mol	Chain	Residues	Atoms					AltConf
87	SV	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 88 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



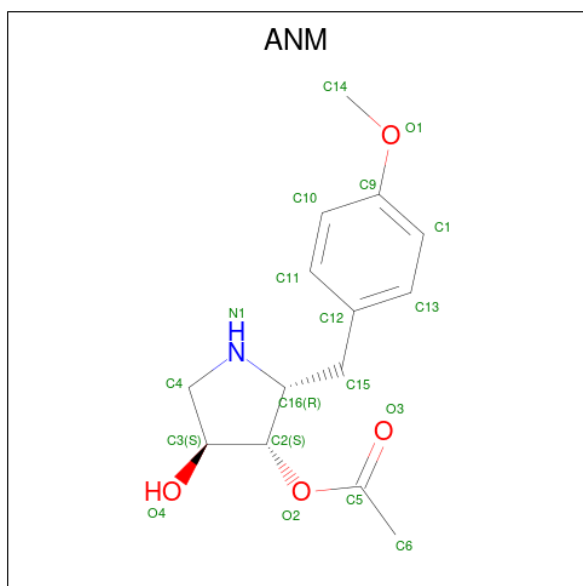
Mol	Chain	Residues	Atoms					AltConf
88	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



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

- Molecule 90 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



Mol	Chain	Residues	Atoms				AltConf
90	L5	1	Total	C	N	O	0
			19	14	1	4	

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

Mol	Chain	Residues	Atoms		AltConf
91	C	7	Total	Na	0
			7	7	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	LA	48	Total	O	0
			48	48	
92	LB	42	Total	O	0
			42	42	
92	L8	67	Total	O	0
			67	67	
92	L7	38	Total	O	0
			38	38	
92	SE	1	Total	O	0
			1	1	
92	SO	2	Total	O	0
			2	2	
92	SN	1	Total	O	0
			1	1	
92	SL	1	Total	O	0
			1	1	
92	Sa	2	Total	O	0
			2	2	
92	LC	59	Total	O	0
			59	59	
92	LJ	1	Total	O	0
			1	1	
92	LH	3	Total	O	0
			3	3	
92	LE	6	Total	O	0
			6	6	
92	LG	7	Total	O	0
			7	7	
92	LO	29	Total	O	0
			29	29	
92	LL	26	Total	O	0
			26	26	
92	LV	10	Total	O	0
			10	10	
92	LM	2	Total	O	0
			2	2	
92	La	26	Total	O	0
			26	26	

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Mol	Chain	Residues	Atoms		AltConf
92	LN	40	Total 40	O 40	0
92	LI	11	Total 11	O 11	0
92	LD	11	Total 11	O 11	0
92	LQ	36	Total 36	O 36	0
92	LR	17	Total 17	O 17	0
92	LS	14	Total 14	O 14	0
92	LT	18	Total 18	O 18	0
92	LP	17	Total 17	O 17	0
92	LU	1	Total 1	O 1	0
92	LX	7	Total 7	O 7	0
92	LY	10	Total 10	O 10	0
92	LZ	5	Total 5	O 5	0
92	Lr	12	Total 12	O 12	0
92	Lh	5	Total 5	O 5	0
92	Lb	10	Total 10	O 10	0
92	LF	30	Total 30	O 30	0
92	Lc	4	Total 4	O 4	0
92	Ld	9	Total 9	O 9	0
92	Le	28	Total 28	O 28	0
92	Lf	16	Total 16	O 16	0
92	Lg	22	Total 22	O 22	0

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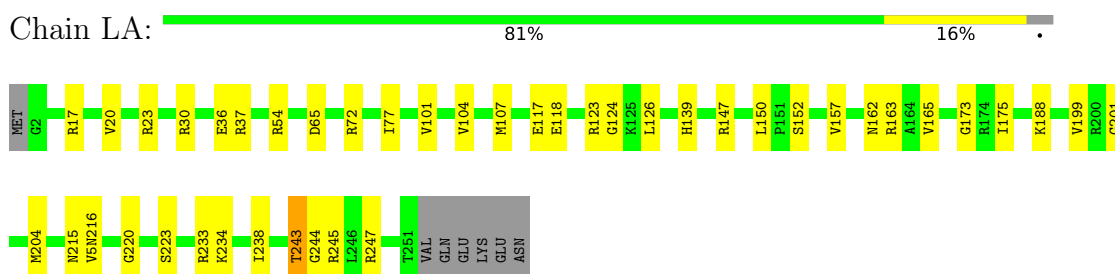
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Mol	Chain	Residues	Atoms		AltConf
92	Li	2	Total 2	O 2	0
92	Lj	19	Total 19	O 19	0
92	Lk	2	Total 2	O 2	0
92	Ll	8	Total 8	O 8	0
92	Lm	2	Total 2	O 2	0
92	Ln	1	Total 1	O 1	0
92	Lo	12	Total 12	O 12	0
92	Lp	14	Total 14	O 14	0
92	Pt	1	Total 1	O 1	0
92	B	18	Total 18	O 18	0

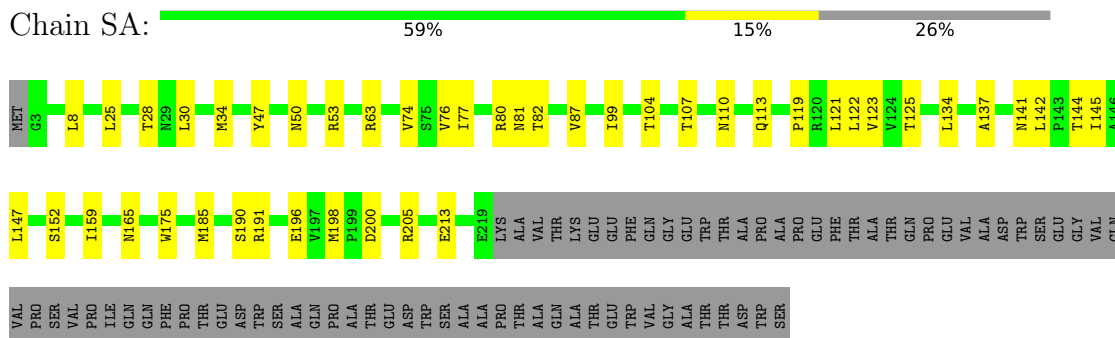
3 Residue-property plots

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.

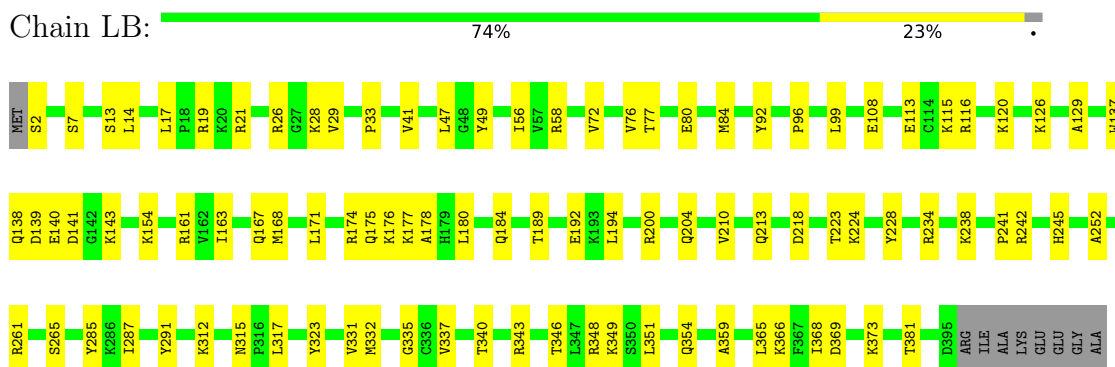
- Molecule 1: Large ribosomal subunit protein uL2



- Molecule 2: Small ribosomal subunit protein uS2

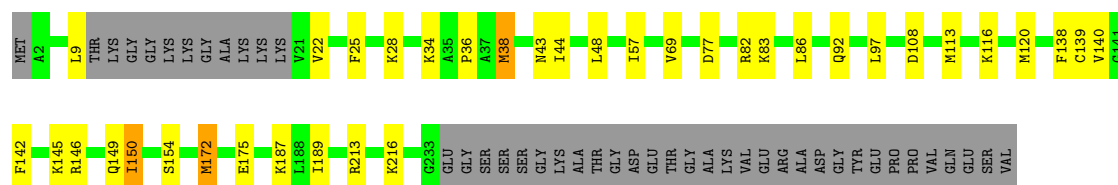


- Molecule 3: Large ribosomal subunit protein uL3



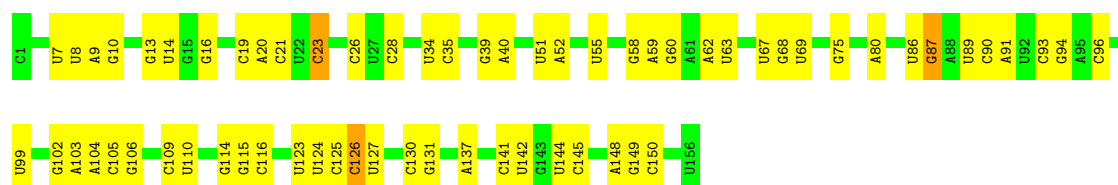
- Molecule 4: 40S ribosomal protein S3a

Chain SB:  70% 13% 16%



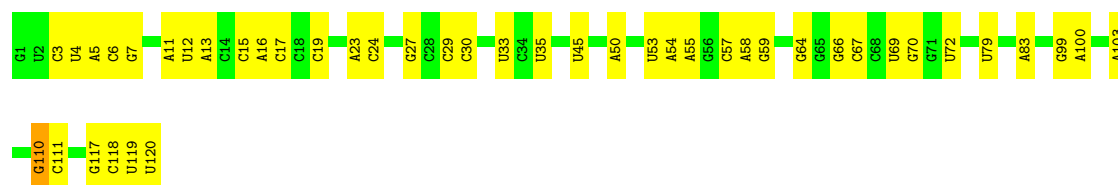
- Molecule 5: 5.8S rRNA

Chain L8:  59% 39%




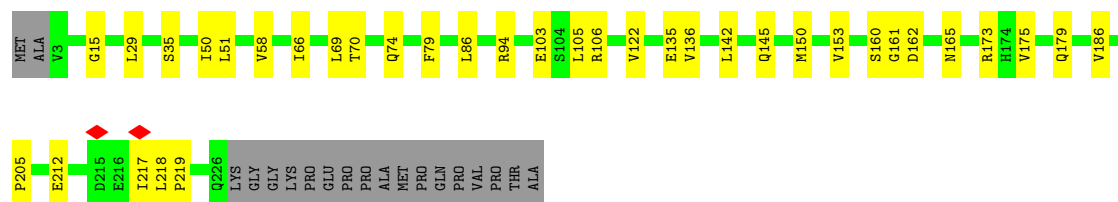
- Molecule 6: 5S rRNA

Chain L7:  63% 36%




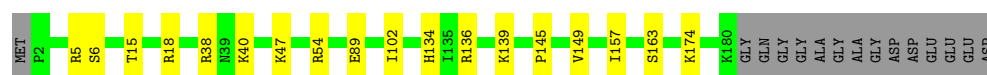
- Molecule 7: 40S ribosomal protein S3

Chain SD:  77% 15% 8%




- Molecule 8: 40S ribosomal protein S9

Chain SJ:  83% 9% 8%

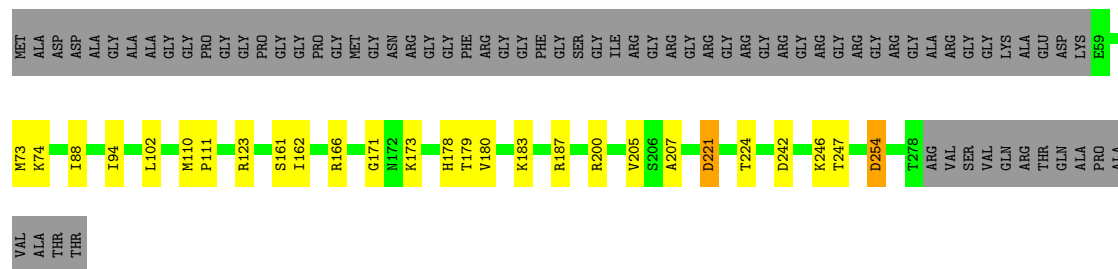


- Molecule 9: Small ribosomal subunit protein eS4, X isoform


Chain SE:  81% 17%

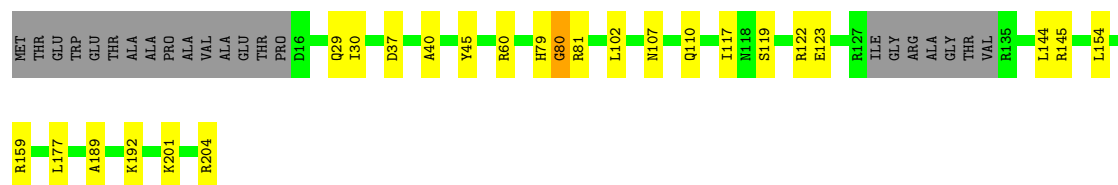
- Molecule 10: 40S ribosomal protein S2

Chain SC: 



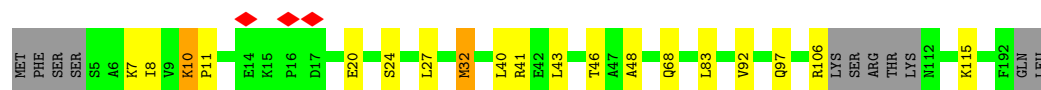
- Molecule 11: 40S ribosomal protein S5

Chain SF: 




- Molecule 12: 40S ribosomal protein S7

Chain SH: 85% 9% • 6%




- Molecule 13: 40S ribosomal protein S15a

Chain SW:  82% 17%



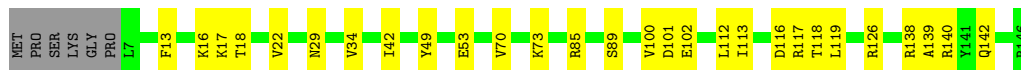
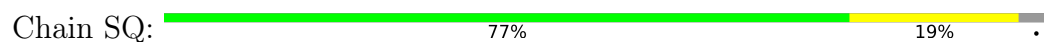
- Molecule 14: 40S ribosomal protein S8

Chain SI:  80% 19%

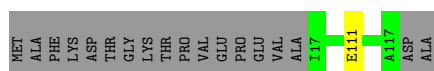




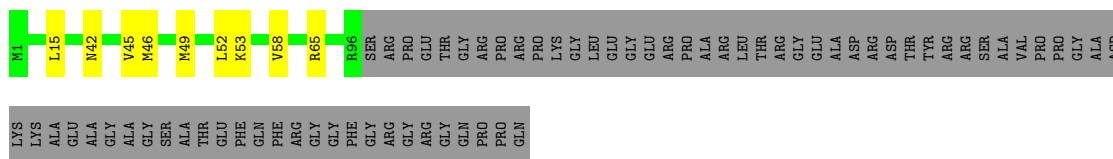
- Molecule 15: 40S ribosomal protein S16



- Molecule 16: 40S ribosomal protein S20



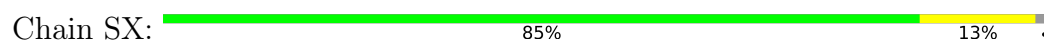
- Molecule 17: 40S ribosomal protein S10



- Molecule 18: 40S ribosomal protein S14

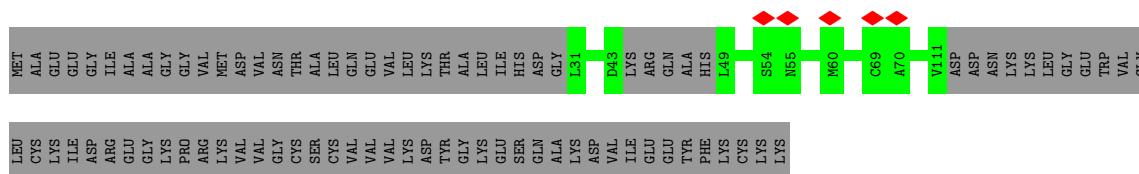


- Molecule 19: 40S ribosomal protein S23



- Molecule 20: Small ribosomal subunit protein eS12





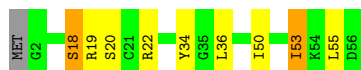
- Molecule 21: 40S ribosomal protein S18

Chain SS: 71% 26% .



- Molecule 22: 40S ribosomal protein S29

Chain Sd: 82% 12% . .



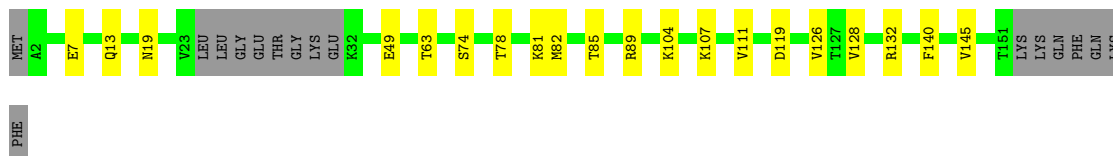
- Molecule 23: 40S ribosomal protein S13

Chain SN: 80% 19% .

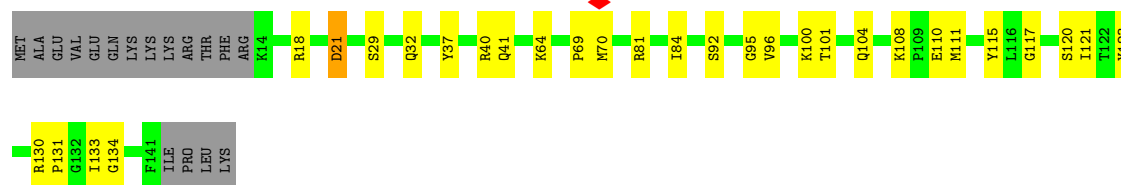


- Molecule 24: 40S ribosomal protein S11


Chain SL: 77% 13% 10%

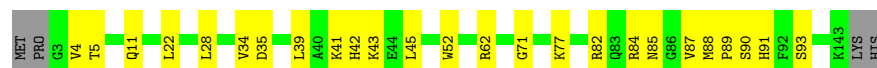


Chain SP:  68% 20% 12%




- Molecule 27: 40S ribosomal protein S19

Chain ST:  80% 17%




- Molecule 28: Small ribosomal subunit protein eS21

Chain SV:  89% 11%



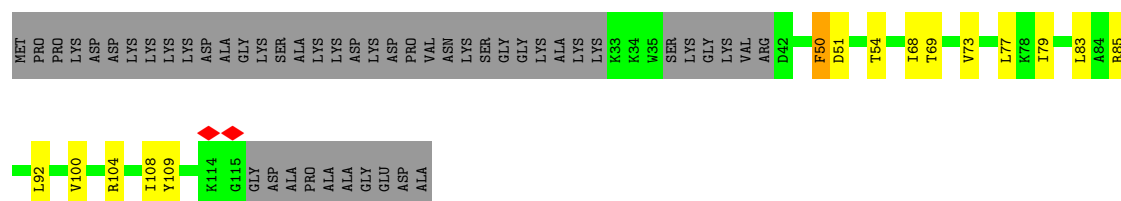
- Molecule 29: 40S ribosomal protein S24

Chain SY:  78% 14% 8%




- Molecule 30: 40S ribosomal protein S25

Chain SZ:  50% 11% 38%




- Molecule 31: 40S ribosomal protein S26

Chain Sa:  76% 10% 15%



- Molecule 32: 40S ribosomal protein S27

Chain Sb:  85% 14%



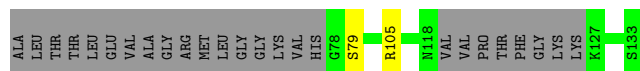
- Molecule 33: 40S ribosomal protein S28

Chain Sc:  65% 17% 16%



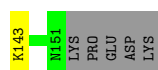
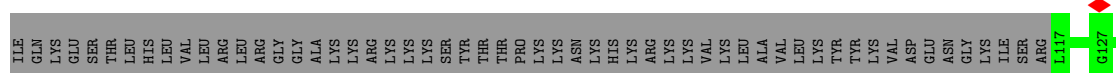
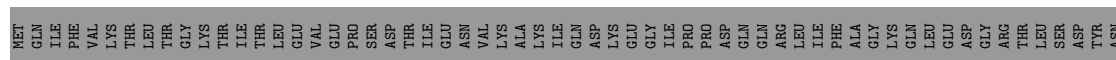
- Molecule 34: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:  35% 64%




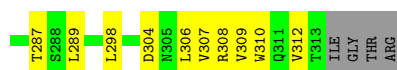
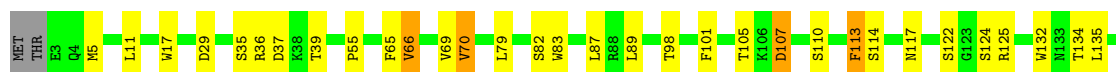
- Molecule 35: Ubiquitin

Chain Sf:  22% 78%

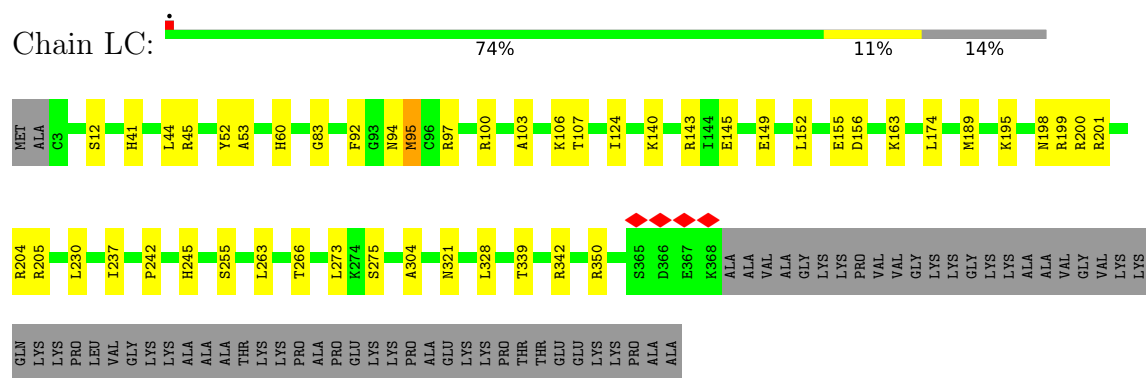


- Molecule 36: Receptor of activated protein C kinase 1

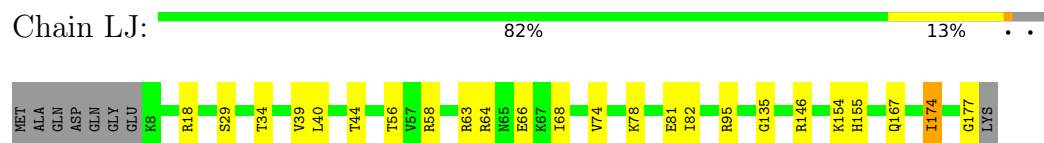
Chain Sg:  74% 23%



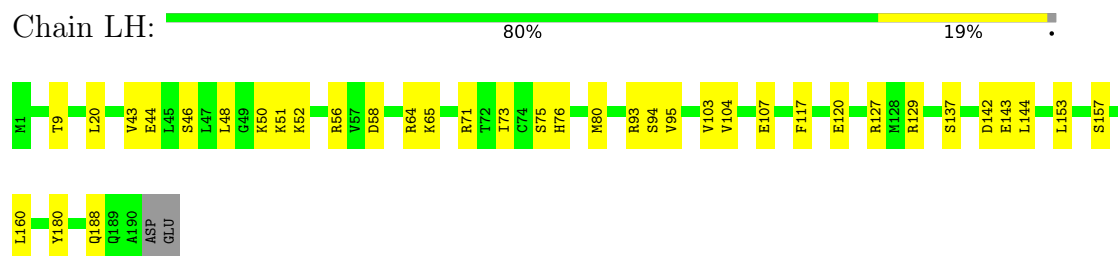
- Molecule 37: 60S ribosomal protein L4



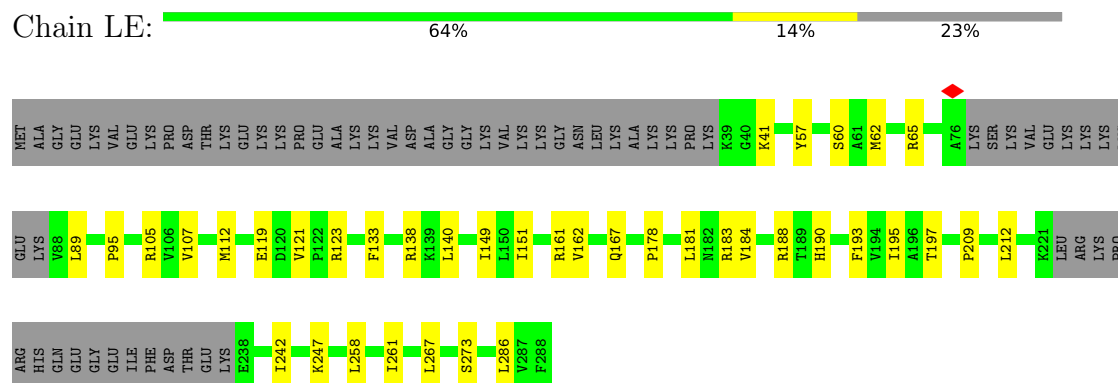
- Molecule 38: 60S ribosomal protein L11



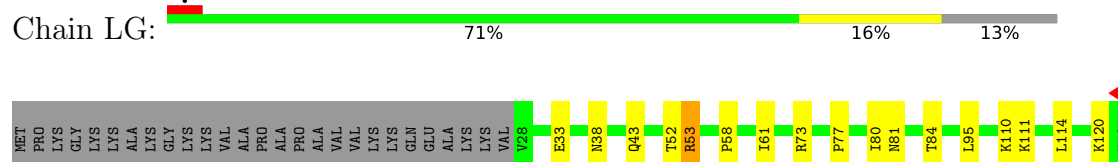
- Molecule 39: 60S ribosomal protein L9



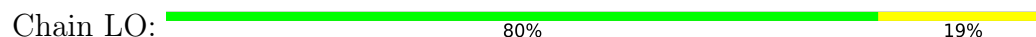
- Molecule 40: Large ribosomal subunit protein eL6



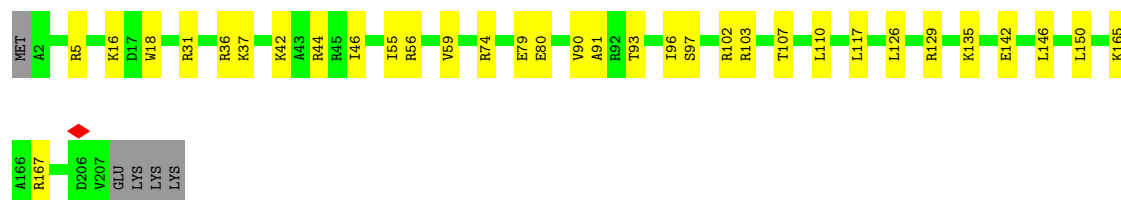
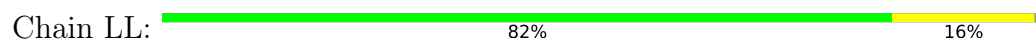
- Molecule 41: 60S ribosomal protein L7a



- Molecule 42: 60S ribosomal protein L13a



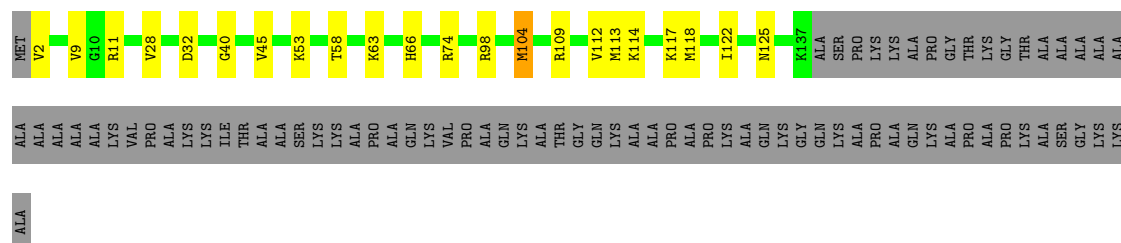
- Molecule 43: 60S ribosomal protein L13




- Molecule 44: 60S ribosomal protein L23

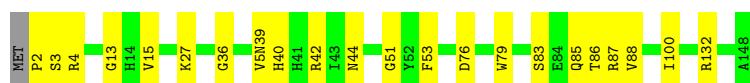


- Molecule 45: 60S ribosomal protein L14




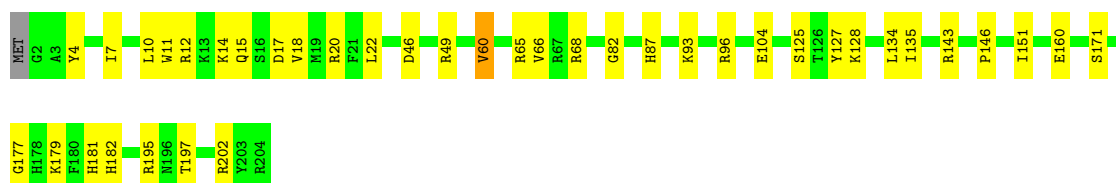
- Molecule 46: Large ribosomal subunit protein uL15

Chain La:  84% 15%




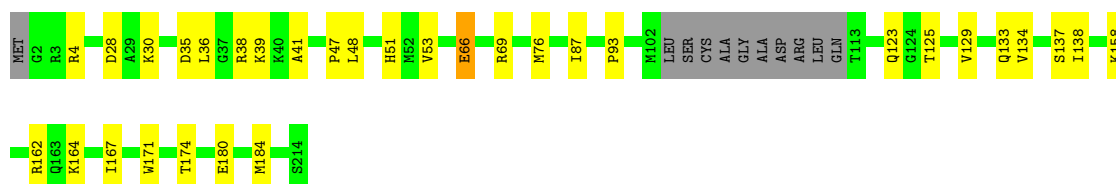
- Molecule 47: 60S ribosomal protein L15

Chain LN:  80% 19%




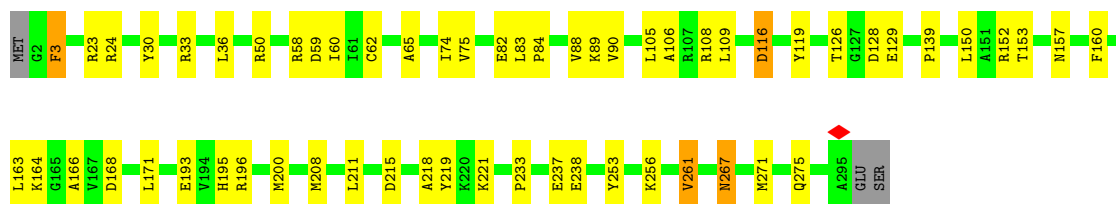
- Molecule 48: 60S ribosomal protein L10

Chain LI:  80% 14% 5%




- Molecule 49: 60S ribosomal protein L5

Chain LD:  79% 19% ..




- Molecule 50: 60S ribosomal protein L18

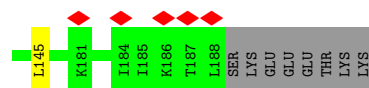
Chain LQ:  87% 13%



- Molecule 51: 60S ribosomal protein L19

Chain LR:  78% 17% 5%





- Molecule 52: 60S ribosomal protein L18a

Chain LS: 85% 15%



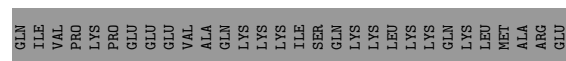
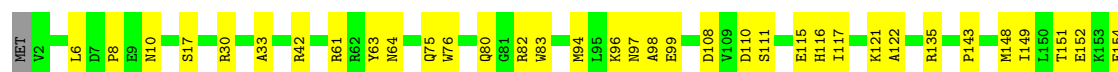
- Molecule 53: 60S ribosomal protein L21

Chain LT: 84% 14%



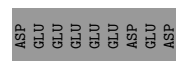
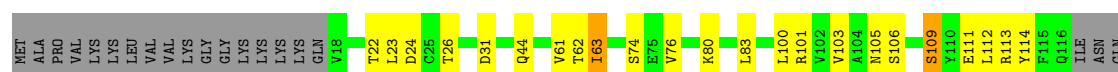
- Molecule 54: 60S ribosomal protein L17

Chain LP: 64% 19% 17%



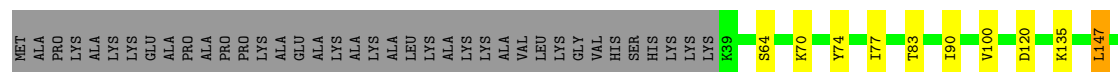
- Molecule 55: 60S ribosomal protein L22

Chain LU: 59% 16% 23%



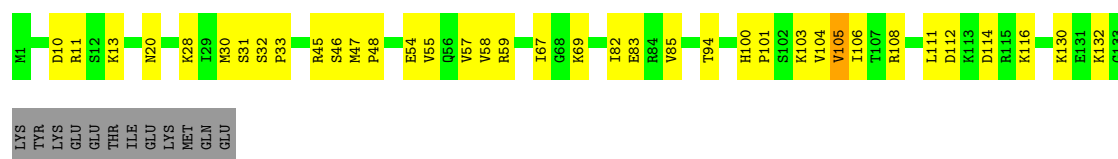
- Molecule 56: 60S ribosomal protein L23a

Chain LX: 69% 6% 24%



- Molecule 57: 60S ribosomal protein L26

Chain LY: 66% 25% 8%



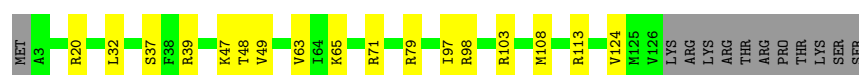
- Molecule 58: 60S ribosomal protein L27

Chain LZ: 82% 15% ..



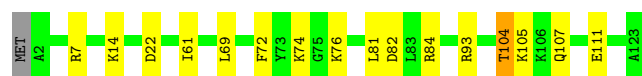
- Molecule 59: Large ribosomal subunit protein eL28

Chain Lr: 79% 12% 9%



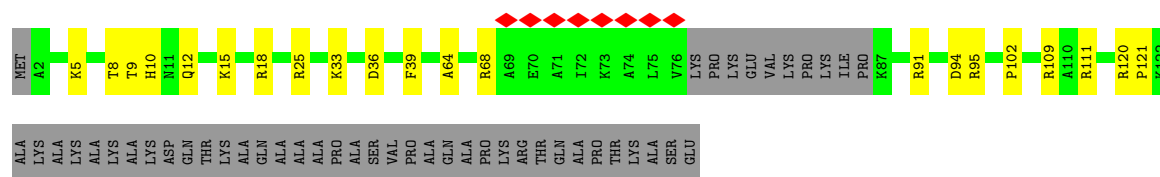
- Molecule 60: 60S ribosomal protein L35

Chain Lh: 86% 12% ..



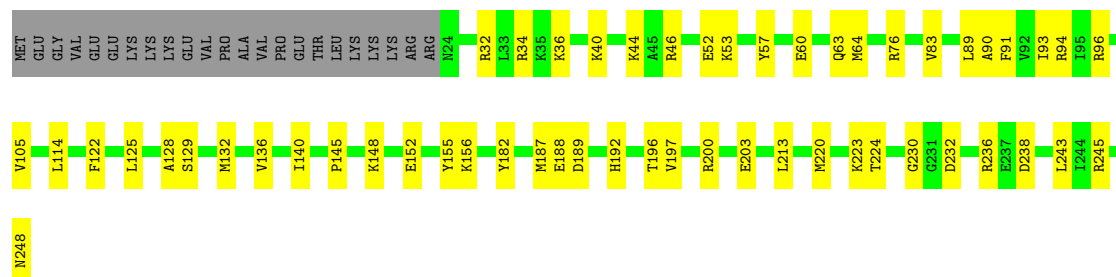
- Molecule 61: Large ribosomal subunit protein eL29

Chain Lb: 5% 57% 13% 30%



- Molecule 62: Large ribosomal subunit protein uL30

Chain LF: 69% 22% 9%



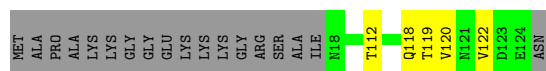
- Molecule 63: 60S ribosomal protein L30

Chain Lc:  73% 13% 14%




- Molecule 64: 60S ribosomal protein L31

Chain Ld:  82% 14%




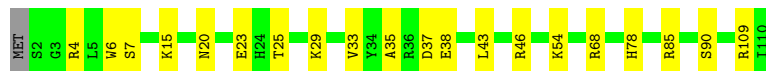
- Molecule 65: 60S ribosomal protein L32

Chain Le:  77% 18% 5%




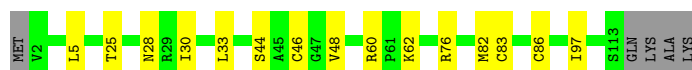
- Molecule 66: 60S ribosomal protein L35a

Chain Lf:  81% 18%



- Molecule 67: 60S ribosomal protein L34

Chain Lg:  83% 13%



- Molecule 68: 60S ribosomal protein L36

Chain Li:  86% 10%



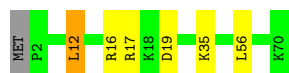
- Molecule 69: Large ribosomal subunit protein eL37

Chain Lj:  74% 14% 11%




- Molecule 70: 60S ribosomal protein L38

Chain Lk:  90% 7% ..




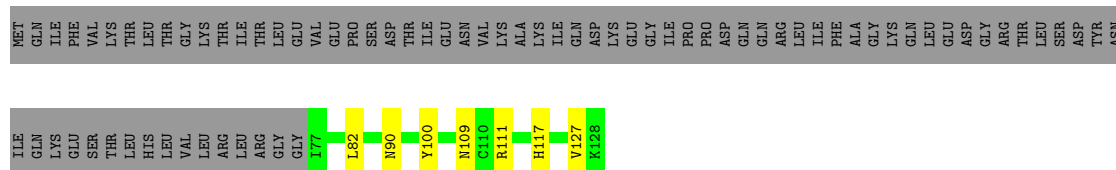
- Molecule 71: 60S ribosomal protein L39

Chain Ll:  76% 22% .




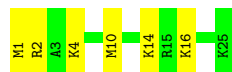
- Molecule 72: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  35% 5% 59%



- Molecule 73: 60S ribosomal protein L41

Chain Ln:  76% 24%



- Molecule 74: Large ribosomal subunit protein eL42

Chain Lo:  90% 9% .



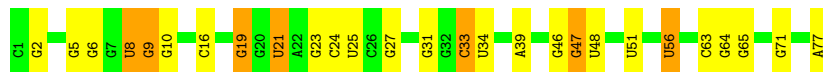
- Molecule 75: 60S ribosomal protein L37a

Chain Lp:  92% 7% .



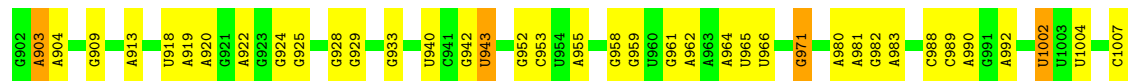
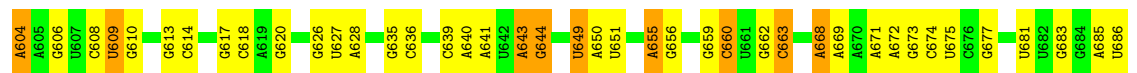
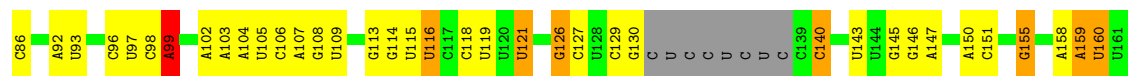
- Molecule 76: P site tRNA

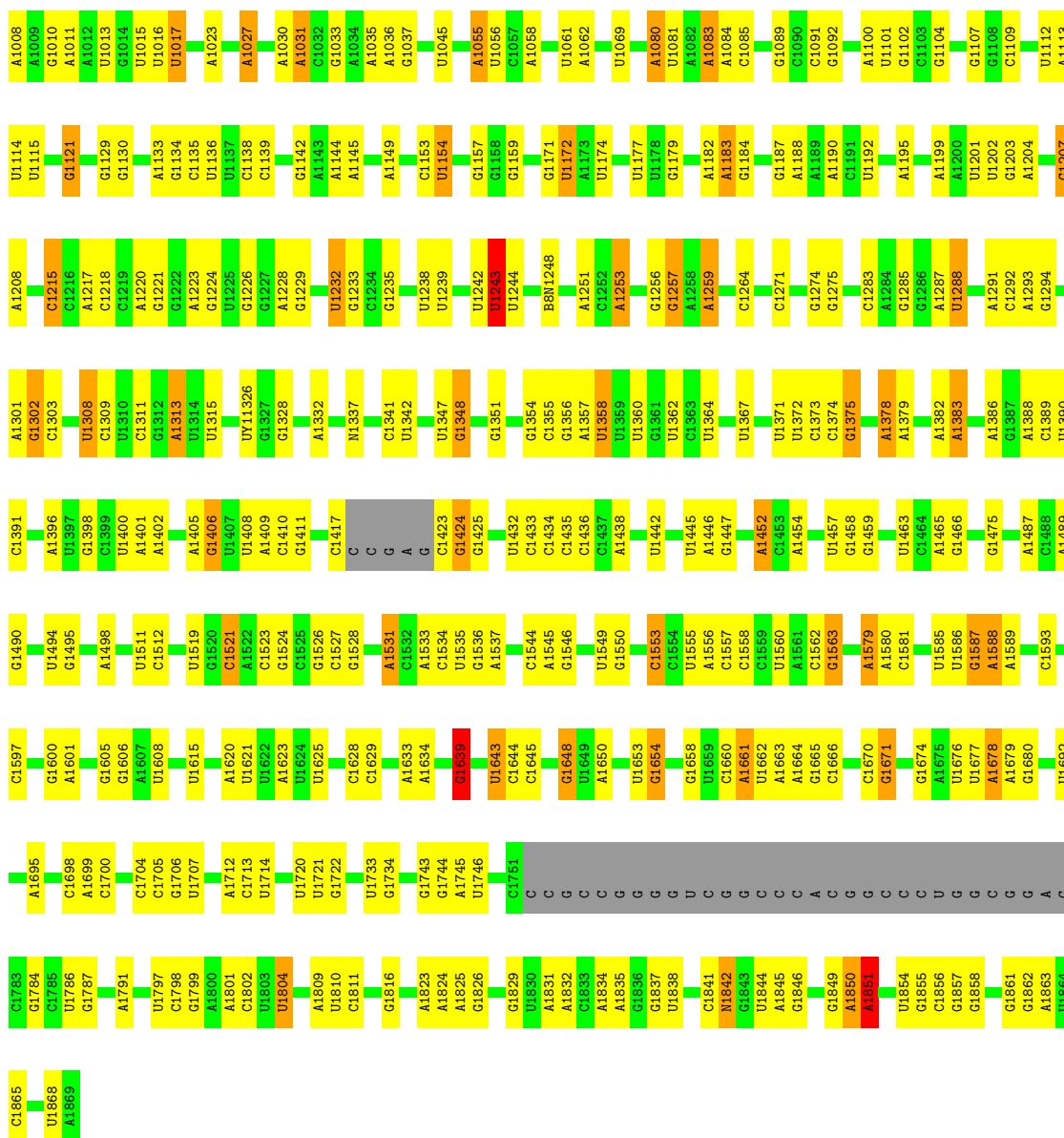
Chain Pt:  65% 26% 9%



A	G	A	U	C	C	G	C	U	A	C	C	G33	G34	G35	A36	A37	U38	G39	U	G	G	A	G	A	G	A
---	---	---	---	---	---	---	---	---	---	---	---	-----	-----	-----	-----	-----	-----	-----	---	---	---	---	---	---	---	---

Category	Count
U1	10
A2	10
C3	10
C4	10
U5	10
C6	10
U12	10
C13	10
C14	10
U15	10
C16	10
C17	10
A27	10
U28	10
C29	10
C30	10
C33	10
U34	10
C35	10
U36	10
C37	10
A38	10
C41	10
A42	10
U43	10
U44	10
A45	10
A46	10
U51	10
C52	10
C56	10
U57	10
C58	10
U59	10
C62	10
U63	10
A64	10
C65	10
C66	10
C67	10
A68	10
C73	10
G74	10
G75	10
U76	10
A77	10
C78	10
A79	10
C80	10
A84	10
A85	10

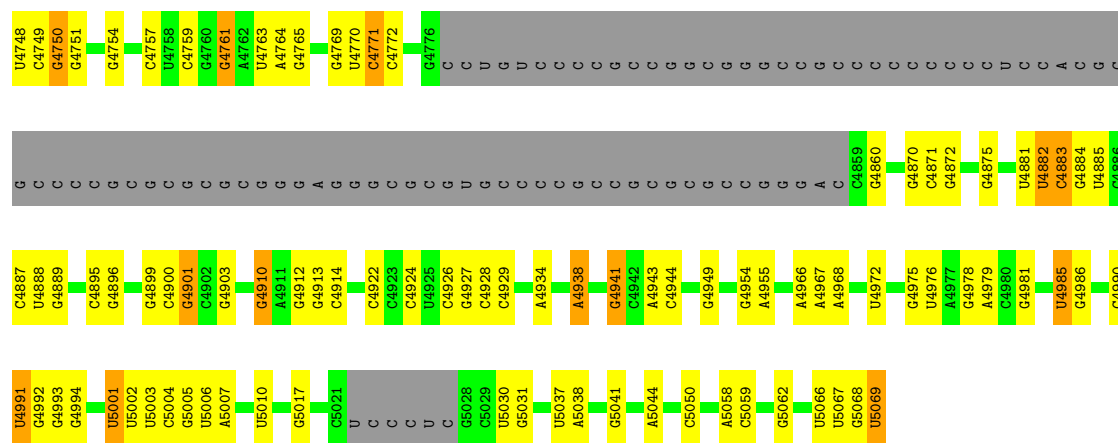




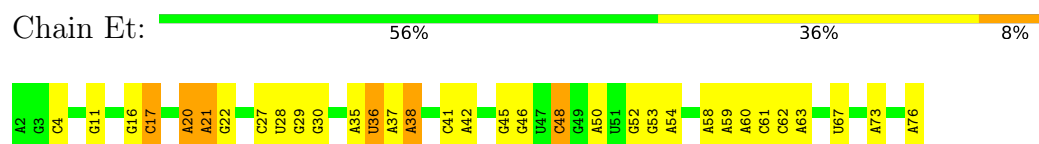




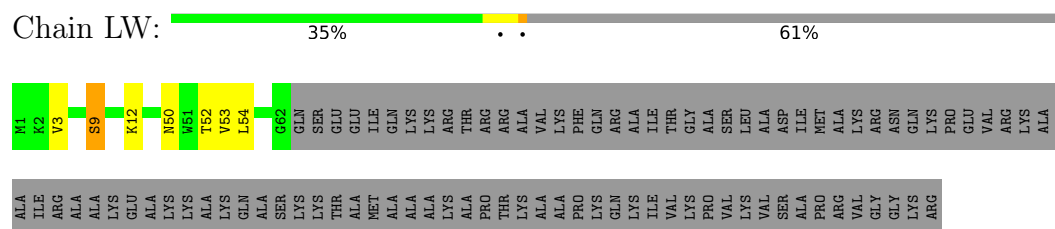




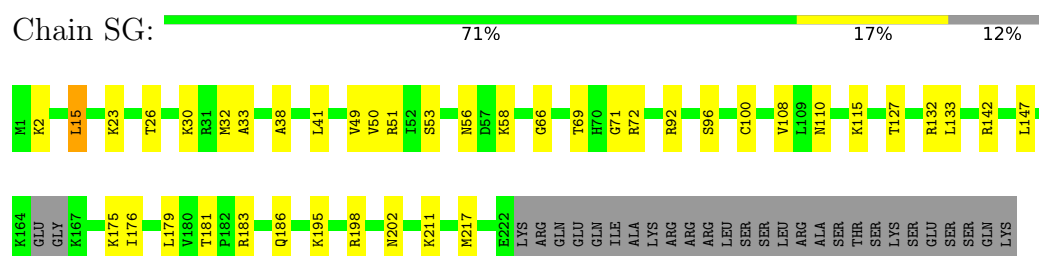
• Molecule 80: E site tRNA



• Molecule 81: 60S ribosomal protein L24



• Molecule 82: 40S ribosomal protein S6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59189	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	0.124	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANM, NA, UY1, AME, MG, H2U, 5MC, B8N, A2M, HIC, OMG, G7M, V5N, HY3, HYG, SAC, 4SU, UR3, OMC, 4AC, MA6, M3L, PSU, 6MZ, 1MA, OMU, MLZ, K, ZN

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	LA	0.16	0/1949	0.29	0/2610
2	SA	0.13	0/1728	0.27	0/2350
3	LB	0.16	0/3122	0.30	0/4191
4	SB	0.13	0/1787	0.31	1/2394 (0.0%)
5	L8	0.16	0/3631	0.28	0/5657
6	L7	0.16	0/2858	0.25	0/4455
7	SD	0.12	0/1667	0.31	0/2256
8	SJ	0.13	0/1502	0.29	0/2008
9	SE	0.13	0/2086	0.29	0/2809
10	SC	0.13	0/1721	0.29	0/2329
11	SF	0.12	0/1454	0.29	0/1956
12	SH	0.15	0/1429	0.37	0/1920
13	SW	0.15	0/1047	0.30	0/1401
14	SI	0.14	0/1680	0.30	0/2244
15	SQ	0.13	0/1126	0.30	0/1508
16	SU	0.09	0/519	0.28	0/722
17	SK	0.10	0/694	0.29	0/945
18	SO	0.13	0/1003	0.29	0/1347
19	SX	0.13	0/1096	0.28	0/1461
20	SM	0.06	0/215	0.19	0/295
21	SS	0.12	0/1202	0.30	0/1614
22	Sd	0.14	0/469	0.28	0/623
23	SN	0.13	0/1242	0.30	0/1671
24	SL	0.15	0/1168	0.27	0/1565
25	SR	0.13	0/1052	0.36	0/1413
26	SP	0.15	0/1070	0.40	0/1430
27	ST	0.15	0/1035	0.29	0/1402
28	SV	0.12	0/635	0.27	0/850
29	SY	0.13	0/988	0.28	0/1316
30	SZ	0.12	0/599	0.30	0/808
31	Sa	0.13	0/798	0.30	0/1070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.13	0/655	0.28	0/878
33	Sc	0.13	0/451	0.28	0/604
34	Se	0.11	0/375	0.26	0/491
35	Sf	0.11	0/194	0.36	0/265
36	Sg	0.15	0/2444	0.40	0/3332
37	LC	0.16	0/2968	0.30	0/3985
38	LJ	0.13	0/1377	0.28	0/1842
39	LH	0.15	0/1537	0.30	0/2066
40	LE	0.15	0/1820	0.31	0/2442
41	LG	0.15	0/1889	0.32	0/2545
42	LO	0.17	0/1674	0.32	0/2244
43	LL	0.16	0/1696	0.34	0/2271
44	LV	0.16	0/986	0.29	0/1324
45	LM	0.15	0/1138	0.31	0/1523
46	La	0.16	0/1168	0.30	0/1562
47	LN	0.17	0/1745	0.30	0/2338
48	LI	0.14	0/1683	0.27	0/2247
49	LD	0.15	0/2437	0.33	0/3263
50	LQ	0.16	0/1536	0.29	0/2052
51	LR	0.15	0/1492	0.27	0/1985
52	LS	0.16	0/1500	0.30	1/2013 (0.0%)
53	LT	0.17	0/1345	0.35	0/1795
54	LP	0.16	0/1279	0.29	0/1716
55	LU	0.15	0/818	0.36	0/1099
56	LX	0.14	0/983	0.27	0/1323
57	LY	0.14	0/1119	0.30	0/1489
58	LZ	0.15	0/1141	0.29	0/1521
59	Lr	0.14	0/1020	0.27	0/1367
60	Lh	0.13	0/1022	0.27	0/1351
61	Lb	0.13	0/900	0.30	0/1187
62	LF	0.16	0/1926	0.32	0/2567
63	Lc	0.14	0/780	0.27	0/1046
64	Ld	0.12	0/591	0.29	0/822
65	Le	0.16	0/1082	0.29	0/1443
66	Lf	0.16	0/894	0.27	0/1198
67	Lg	0.15	0/885	0.29	0/1182
68	Li	0.12	0/832	0.32	0/1101
69	Lj	0.16	0/731	0.31	0/967
70	Lk	0.15	0/574	0.29	0/761
71	Ll	0.13	0/447	0.24	0/592
72	Lm	0.15	0/433	0.31	0/575
73	Ln	0.18	0/240	0.36	0/305
74	Lo	0.14	0/877	0.25	0/1156

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lp	0.16	0/728	0.34	0/967
76	Pt	0.20	1/1721 (0.1%)	0.23	0/2679
77	mR	0.10	0/175	0.20	0/272
78	S2	0.18	0/37093	0.26	0/57803
79	L5	0.18	0/81582	0.27	0/127262
80	Et	0.11	0/1795	0.23	0/2798
81	LW	0.14	0/532	0.27	0/708
82	SG	0.12	0/1703	0.31	0/2285
All	All	0.17	1/218585 (0.0%)	0.28	2/321229 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	Pt	47	G7M	O3'-P	5.04	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	SB	150	ILE	N-CA-C	-5.14	107.40	113.42
52	LS	142	VAL	N-CA-C	-5.04	107.92	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	1921	0	2014	32	0
2	SA	1692	0	1689	27	0
3	LB	3068	0	3103	63	0
4	SB	1761	0	1816	25	0
5	L8	3315	0	1685	38	0
6	L7	2558	0	1294	31	0
7	SD	1642	0	1635	21	0
8	SJ	1477	0	1592	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	SE	2044	0	2145	27	0
10	SC	1685	0	1754	19	0
11	SF	1434	0	1471	17	0
12	SH	1409	0	1467	13	0
13	SW	1030	0	1076	17	0
14	SI	1652	0	1703	32	0
15	SQ	1109	0	1177	19	0
16	SU	519	0	254	0	0
17	SK	678	0	569	6	0
18	SO	990	0	1013	21	0
19	SX	1088	0	1149	9	0
20	SM	218	0	107	0	0
21	SS	1184	0	1240	27	0
22	Sd	458	0	448	8	0
23	SN	1214	0	1301	20	0
24	SL	1148	0	1194	13	0
25	SR	1038	0	1065	16	0
26	SP	1049	0	1092	22	0
27	ST	1010	0	935	17	0
28	SV	628	0	625	6	0
29	SY	972	0	1019	15	0
30	SZ	592	0	624	11	0
31	Sa	782	0	835	8	0
32	Sb	642	0	661	8	0
33	Sc	449	0	470	6	0
34	Se	373	0	401	1	0
35	Sf	194	0	121	1	0
36	Sg	2387	0	2316	45	0
37	LC	2914	0	3087	38	0
38	LJ	1354	0	1389	14	0
39	LH	1518	0	1600	24	0
40	LE	1786	0	1945	27	0
41	LG	1856	0	1985	31	0
42	LO	1642	0	1773	28	0
43	LL	1662	0	1773	26	0
44	LV	972	0	1034	18	0
45	LM	1116	0	1176	15	0
46	La	1152	0	1179	18	0
47	LN	1700	0	1749	30	0
48	LI	1645	0	1694	18	0
49	LD	2391	0	2425	40	0
50	LQ	1512	0	1628	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	LR	1476	0	1548	23	0
52	LS	1460	0	1502	18	0
53	LT	1311	0	1392	18	0
54	LP	1249	0	1276	22	0
55	LU	804	0	820	11	0
56	LX	966	0	1040	7	0
57	LY	1102	0	1181	23	0
58	LZ	1115	0	1195	16	0
59	Lr	1002	0	1076	13	0
60	Lh	1014	0	1148	13	0
61	Lb	898	0	983	15	0
62	LF	1885	0	2022	39	0
63	Lc	770	0	809	8	0
64	Ld	589	0	356	0	0
65	Le	1061	0	1160	18	0
66	Lf	875	0	911	11	0
67	Lg	875	0	951	10	0
68	Li	821	0	890	9	0
69	Lj	712	0	744	14	0
70	Lk	568	0	637	6	0
71	Ll	437	0	471	9	0
72	Lm	436	0	476	5	0
73	Ln	239	0	289	8	0
74	Lo	870	0	936	6	0
75	Lp	715	0	768	5	0
76	Pt	1645	0	844	16	0
77	mR	156	0	77	4	0
78	S2	34940	0	17689	363	0
79	L5	75626	0	38304	680	0
80	Et	1604	0	815	18	0
81	LW	519	0	533	4	0
82	SG	1683	0	1735	32	0
83	A	14	0	0	0	0
83	L7	4	0	0	0	0
83	L8	3	0	0	0	0
83	LA	3	0	0	0	0
83	LH	1	0	0	0	0
83	LI	1	0	0	0	0
83	LL	1	0	0	0	0
83	LN	1	0	0	0	0
83	LQ	1	0	0	0	0
83	Lb	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	Le	1	0	0	0	0
83	Lf	1	0	0	0	0
83	Ll	1	0	0	0	0
83	SL	1	0	0	0	0
83	SO	1	0	0	0	0
83	Sa	1	0	0	0	0
83	mR	1	0	0	0	0
84	Lr	9	0	8	0	0
84	SA	9	0	8	0	0
85	D	12	0	0	0	0
85	Et	1	0	0	0	0
85	L7	15	0	0	0	0
85	L8	16	0	0	0	0
85	LB	1	0	0	0	0
85	LC	1	0	0	0	0
85	LD	1	0	0	0	0
85	LF	1	0	0	0	0
85	LG	1	0	0	0	0
85	LH	1	0	0	0	0
85	LL	1	0	0	0	0
85	LN	3	0	0	0	0
85	LO	2	0	0	0	0
85	LP	2	0	0	0	0
85	LQ	2	0	0	0	0
85	LR	1	0	0	0	0
85	LS	1	0	0	0	0
85	LV	1	0	0	0	0
85	La	1	0	0	0	0
85	Lc	1	0	0	0	0
85	Lf	1	0	0	0	0
85	Lg	1	0	0	0	0
85	Lj	2	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	2	0	0	0	0
85	Lr	3	0	0	0	0
85	Pt	1	0	0	0	0
85	SN	1	0	0	0	0
85	SS	2	0	0	0	0
85	ST	1	0	0	0	0
85	SX	1	0	0	0	0
85	Sd	1	0	0	0	0
86	Lg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Lj	1	0	0	0	0
86	Lm	1	0	0	0	0
86	Lo	1	0	0	0	0
86	Lp	1	0	0	0	0
86	Sa	1	0	0	0	0
86	Sd	1	0	0	0	0
86	Sf	1	0	0	0	0
87	SV	11	0	12	0	0
88	Pt	8	0	8	0	0
89	S2	36	0	37	0	0
90	L5	19	0	18	1	0
91	C	7	0	0	0	0
92	B	18	0	0	0	0
92	L7	38	0	0	1	0
92	L8	67	0	0	1	0
92	LA	48	0	0	0	0
92	LB	42	0	0	2	0
92	LC	59	0	0	3	0
92	LD	11	0	0	0	0
92	LE	6	0	0	0	0
92	LF	30	0	0	1	0
92	LG	7	0	0	0	0
92	LH	3	0	0	0	0
92	LI	11	0	0	0	0
92	LJ	1	0	0	0	0
92	LL	26	0	0	2	0
92	LM	2	0	0	0	0
92	LN	40	0	0	2	0
92	LO	29	0	0	1	0
92	LP	17	0	0	1	0
92	LQ	36	0	0	1	0
92	LR	17	0	0	1	0
92	LS	14	0	0	0	0
92	LT	18	0	0	0	0
92	LU	1	0	0	0	0
92	LV	10	0	0	0	0
92	LX	7	0	0	1	0
92	LY	10	0	0	0	0
92	LZ	5	0	0	1	0
92	La	26	0	0	1	0
92	Lb	10	0	0	0	0
92	Lc	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	Ld	9	0	0	0	0
92	Le	28	0	0	1	0
92	Lf	16	0	0	1	0
92	Lg	22	0	0	0	0
92	Lh	5	0	0	0	0
92	Li	2	0	0	0	0
92	Lj	19	0	0	3	0
92	Lk	2	0	0	0	0
92	Ll	8	0	0	0	0
92	Lm	2	0	0	0	0
92	Ln	1	0	0	1	0
92	Lo	12	0	0	0	0
92	Lp	14	0	0	0	0
92	Lr	12	0	0	1	0
92	Pt	1	0	0	0	0
92	SE	1	0	0	0	0
92	SL	1	0	0	0	0
92	SN	1	0	0	0	0
92	SO	2	0	0	0	0
92	Sa	2	0	0	0	0
All	All	209052	0	152166	2016	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2016) 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)
26:SP:29:SER:HB3	26:SP:32:GLN:HE22	1.46	0.80
67:Lg:83:CYS:SG	67:Lg:86:CYS:HB2	2.22	0.80
38:LJ:95:ARG:HE	38:LJ:177:GLY:HA2	1.49	0.77
79:L5:2786:C:H5''	79:L5:2787:A:H5'	1.66	0.77
36:Sg:217:MET:HG2	36:Sg:229:THR:HG23	1.66	0.76
55:LU:23:LEU:HD21	55:LU:83:LEU:HB3	1.68	0.76
79:L5:2520:C:O2	79:L5:2640:G:N2	2.20	0.75
76:Pt:51:U:H3	76:Pt:65:G:H1	1.34	0.72
43:LL:167:ARG:HE	46:La:100:ILE:HD11	1.54	0.72
78:S2:191:A:H62	78:S2:208:G:H21	1.38	0.72
22:Sd:22:ARG:HH21	78:S2:1553:C:H41	1.37	0.72
36:Sg:153:CYS:HB2	36:Sg:168:CYS:H	1.55	0.72
36:Sg:87:LEU:HB2	36:Sg:101:PHE:HB2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:851:C:H5''	78:S2:852:G:H5'	1.70	0.71
21:SS:116:LYS:HA	79:L5:1766:A:H5''	1.73	0.70
39:LH:137:SER:HB3	39:LH:143:GLU:HB3	1.74	0.70
47:LN:60:VAL:HG22	47:LN:134:LEU:HB2	1.71	0.70
27:ST:85:ASN:HB2	27:ST:88:MET:HB2	1.73	0.70
63:Lc:34:THR:HG23	63:Lc:95:ALA:HB2	1.72	0.70
79:L5:3663:A:N6	79:L5:4168:G:O2'	2.24	0.70
79:L5:3717:A:H2'	79:L5:3718:A2M:H8	1.74	0.70
39:LH:56:ARG:NH1	39:LH:58:ASP:OD2	2.25	0.70
6:L7:72:U:O2	6:L7:103:A:N6	2.25	0.69
5:L8:99:U:O4	69:Lj:65:ARG:NH2	2.25	0.69
46:La:4:ARG:NH2	79:L5:2341:A:OP2	2.26	0.69
43:LL:36:ARG:NH2	79:L5:1364:U:OP2	2.26	0.69
59:Lr:98:ARG:NH1	79:L5:2262:G:N7	2.40	0.68
7:SD:105:LEU:HB2	7:SD:122:VAL:HG21	1.75	0.68
26:SP:40:ARG:NH2	78:S2:1615:U:O4	2.27	0.68
74:Lo:98:LYS:HE3	79:L5:4233:A:H4'	1.73	0.68
79:L5:4140:C:H2'	79:L5:4141:G:C4	2.29	0.68
66:Lf:33:VAL:HG13	66:Lf:38:GLU:HB2	1.76	0.68
44:LV:35:LYS:HD2	44:LV:67:LYS:HE2	1.76	0.68
41:LG:58:PRO:HD2	41:LG:61:ILE:HD12	1.76	0.67
52:LS:71:SER:O	52:LS:76:LYS:NZ	2.28	0.67
25:SR:70:SER:HB3	25:SR:73:LEU:HB2	1.76	0.67
39:LH:44:GLU:HG3	45:LM:2:VAL:HG12	1.77	0.67
39:LH:93:ARG:HD2	39:LH:143:GLU:HG3	1.77	0.66
79:L5:4573:G:N2	79:L5:4573:G:OP2	2.28	0.66
3:LB:126:LYS:NZ	79:L5:4966:A:OP2	2.28	0.66
43:LL:44:ARG:NH2	79:L5:186:G:OP2	2.28	0.66
79:L5:704:C:N4	79:L5:707:C:OP2	2.29	0.66
81:LW:52:THR:HG22	81:LW:54:LEU:H	1.61	0.66
13:SW:3:ARG:HH12	13:SW:28:ARG:HH21	1.44	0.66
49:LD:152:ARG:O	49:LD:157:ASN:ND2	2.29	0.66
79:L5:2562:G:N2	79:L5:2565:A:OP2	2.29	0.65
45:LM:74:ARG:NH2	79:L5:736:C:OP1	2.28	0.65
78:S2:326:C:H5''	78:S2:327:G:H5'	1.79	0.65
78:S2:99:A2M:N6	78:S2:433:A:N3	2.44	0.65
54:LP:42:ARG:NH1	54:LP:110:ASP:OD1	2.30	0.65
72:Lm:111:ARG:NH1	79:L5:4699:U:OP2	2.30	0.65
13:SW:107:SER:HB2	78:S2:860:G:H21	1.61	0.65
14:SI:98:LYS:HB3	78:S2:377:G:H5''	1.78	0.65
79:L5:3765:G:O2'	79:L5:3767:C:N4	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:SG:69:THR:HG22	82:SG:71:GLY:H	1.61	0.65
9:SE:44:LEU:HD13	9:SE:72:ILE:HD11	1.79	0.65
13:SW:12:LYS:O	13:SW:16:ASN:ND2	2.30	0.65
78:S2:126:G:H21	78:S2:180:G:H21	1.44	0.65
49:LD:126:THR:HG23	49:LD:128:ASP:H	1.62	0.65
7:SD:205:PRO:HA	25:SR:42:PRO:HG2	1.77	0.64
26:SP:37:TYR:HB3	26:SP:41:GLN:HB2	1.79	0.64
5:L8:40:A:N7	5:L8:104:A:N6	2.45	0.64
80:Et:11:G:O6	80:Et:45:G:N2	2.30	0.64
15:SQ:34:VAL:HG22	15:SQ:70:VAL:HB	1.80	0.64
79:L5:3722:G:H2'	79:L5:3723:A2M:H8	1.78	0.64
36:Sg:174:VAL:HB	36:Sg:188:HIS:HB2	1.79	0.64
72:Lm:100:TYR:O	79:L5:4472:G:O2'	2.15	0.64
7:SD:136:VAL:HG22	7:SD:186:VAL:HG22	1.78	0.64
82:SG:32:MET:HB2	82:SG:100:CYS:HB2	1.79	0.64
2:SA:80:ARG:NH2	2:SA:82:THR:OG1	2.30	0.64
42:LO:106:ASP:O	79:L5:4910:G:N2	2.31	0.64
78:S2:1139:C:H42	78:S2:1149:A:H62	1.43	0.64
54:LP:42:ARG:NH2	54:LP:99:GLU:OE2	2.31	0.63
62:LF:192:HIS:O	62:LF:196:THR:OG1	2.16	0.63
41:LG:209:SER:HA	41:LG:212:LYS:HG3	1.80	0.63
1:LA:215:ASN:ND2	79:L5:4546:A:N7	2.47	0.63
13:SW:2:VAL:N	78:S2:1091:C:HO2'	1.96	0.63
2:SA:77:ILE:HG12	2:SA:99:ILE:HB	1.81	0.63
79:L5:3641:U:OP2	79:L5:3646:A:N6	2.28	0.63
26:SP:100:LYS:HG2	26:SP:101:THR:HG23	1.81	0.63
55:LU:100:LEU:HD13	55:LU:112:LEU:HD23	1.80	0.63
1:LA:101:VAL:HG22	1:LA:165:VAL:HG22	1.81	0.63
80:Et:16:G:H22	80:Et:48:C:H42	1.45	0.63
47:LN:143:ARG:NH2	60:Lh:93:ARG:O	2.32	0.63
79:L5:2020:U:H2'	79:L5:2021:G:H8	1.64	0.63
11:SF:201:LYS:HG3	11:SF:204:ARG:HH21	1.63	0.63
50:LQ:11:ARG:HG3	79:L5:2081:C:H5''	1.81	0.63
18:SO:55:ARG:NH2	78:S2:953:C:O2	2.31	0.62
79:L5:4594:U:H2'	79:L5:4595:G:H8	1.64	0.62
3:LB:21:ARG:NH2	79:L5:4981:G:O6	2.32	0.62
14:SI:162:LEU:HD11	14:SI:191:GLU:HG2	1.80	0.62
22:Sd:18:SER:OG	78:S2:1556:A:N6	2.32	0.62
76:Pt:25:U:O2'	79:L5:3770:PSU:OP1	2.17	0.62
3:LB:261:ARG:NH2	92:LB:665:HOH:O	2.32	0.62
30:SZ:104:ARG:NH2	78:S2:1593:C:OP2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:LJ:18:ARG:HG3	38:LJ:135:GLY:HA3	1.81	0.62
61:Lb:120:ARG:NH2	79:L5:1241:C:N3	2.44	0.62
78:S2:43:U:OP2	78:S2:485:A:N6	2.33	0.62
79:L5:2485:U:H2'	79:L5:2486:G:C8	2.33	0.62
66:Lf:4:ARG:NH1	66:Lf:6:TRP:O	2.32	0.62
36:Sg:11:LEU:HB2	36:Sg:307:VAL:HB	1.82	0.62
79:L5:1332:C:H2'	79:L5:1333:A:H8	1.65	0.62
47:LN:160:GLU:OE2	47:LN:160:GLU:N	2.23	0.62
59:Lr:20:ARG:NH1	65:Le:78:LEU:O	2.33	0.62
78:S2:928:G:H2'	78:S2:929:G:C8	2.35	0.62
78:S2:1536:G:H2'	78:S2:1537:A:H8	1.64	0.62
79:L5:2360:A:N6	79:L5:3861:A:N7	2.45	0.62
51:LR:88:ARG:O	79:L5:2725:A:N6	2.32	0.62
81:LW:9:SER:HA	81:LW:52:THR:HG23	1.81	0.62
54:LP:17:SER:HB2	54:LP:98:ALA:HB2	1.81	0.61
9:SE:100:ARG:HH12	9:SE:122:LYS:HA	1.64	0.61
37:LC:189:MET:HE3	37:LC:200:ARG:HH21	1.64	0.61
38:LJ:68:ILE:HD11	79:L5:4258:C:H5'	1.83	0.61
41:LG:162:ASP:O	79:L5:150:U:N3	2.30	0.61
50:LQ:144:LYS:HG3	79:L5:1460:C:H5''	1.82	0.61
61:Lb:5:MLZ:HE3	61:Lb:8:THR:HB	1.83	0.61
78:S2:1854:U:H2'	78:S2:1855:G:H8	1.66	0.61
79:L5:1326:A2M:OP2	79:L5:4445:U:O2'	2.17	0.61
37:LC:204:ARG:NH1	92:LC:615:HOH:O	2.33	0.61
66:Lf:54:LYS:HE3	79:L5:4748:U:H5''	1.82	0.61
79:L5:308:G:OP2	79:L5:308:G:N2	2.29	0.61
44:LV:90:ARG:NH2	44:LV:140:ALA:O	2.33	0.61
47:LN:202:ARG:NH2	79:L5:1372:A:OP1	2.26	0.61
4:SB:216:LYS:NZ	78:S2:942:G:OP1	2.34	0.61
41:LG:38:ASN:OD1	41:LG:43:GLN:NE2	2.34	0.61
79:L5:62:A:N3	79:L5:77:U:O2'	2.29	0.61
54:LP:97:ASN:ND2	79:L5:393:U:O2	2.33	0.61
78:S2:958:G:N2	78:S2:965:U:O4	2.28	0.61
79:L5:181:C:H2'	79:L5:182:G:H8	1.65	0.61
79:L5:4620:OMU:OP2	79:L5:4670:C:N4	2.33	0.61
76:Pt:9:G:O2'	76:Pt:10:G:N7	2.31	0.61
3:LB:14:LEU:HD22	3:LB:17:LEU:HD11	1.82	0.61
3:LB:174:ARG:NH1	79:L5:4985:U:O2	2.34	0.61
11:SF:60:ARG:HD2	78:S2:1679:A:H2'	1.83	0.61
25:SR:43:SER:OG	78:S2:1389:C:OP1	2.17	0.60
39:LH:71:ARG:NH1	79:L5:4691:A:OP1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LZ:90:PRO:O	58:LZ:117:LYS:NZ	2.34	0.60
66:Lf:43:LEU:O	66:Lf:109:ARG:NH2	2.33	0.60
4:SB:138:PHE:O	4:SB:213:ARG:N	2.34	0.60
79:L5:1245:C:H2'	79:L5:1246:G:H8	1.65	0.60
79:L5:1562:G:N2	79:L5:1565:A:OP2	2.33	0.60
55:LU:44:GLN:HG2	55:LU:63:ILE:HD12	1.84	0.60
69:Lj:11:ARG:NH1	92:Lj:229:HOH:O	2.33	0.60
3:LB:213:GLN:NE2	3:LB:285:TYR:O	2.34	0.60
14:SI:57:ALA:HB2	14:SI:183:GLY:HA2	1.82	0.60
29:SY:29:HIS:HE2	29:SY:69:THR:HG1	1.47	0.60
43:LL:18:TRP:NE1	79:L5:1516:G:O2'	2.33	0.60
7:SD:106:ARG:HG3	7:SD:175:VAL:HG22	1.82	0.60
9:SE:19:MET:HG2	78:S2:846:G:H2'	1.83	0.60
14:SI:103:LEU:HD22	14:SI:170:LYS:HB3	1.83	0.60
52:LS:99:ASP:OD1	52:LS:108:GLN:NE2	2.34	0.60
69:Lj:30:GLN:NE2	79:L5:1621:A:OP2	2.35	0.60
71:Ll:2:SER:N	79:L5:2407:G:O6	2.34	0.60
80:Et:16:G:H1'	80:Et:20:A:H61	1.66	0.60
19:SX:127:ASN:O	19:SX:127:ASN:ND2	2.34	0.60
53:LT:39:ILE:HD12	53:LT:102:ARG:HG2	1.83	0.60
78:S2:1033:G:N1	78:S2:1080:A:O2'	2.26	0.60
78:S2:1283:C:O2'	78:S2:1313:A:N1	2.35	0.60
79:L5:453:G:N2	79:L5:1293:G:O6	2.33	0.60
37:LC:149:GLU:OE2	59:Lr:71:ARG:NH1	2.34	0.60
43:LL:31:ARG:NH2	92:LL:428:HOH:O	2.34	0.60
49:LD:23:ARG:NH1	49:LD:23:ARG:O	2.34	0.60
78:S2:1259:A:H1'	78:S2:1264:C:H42	1.65	0.60
57:LY:54:GLU:HB2	57:LY:108:ARG:HB3	1.84	0.60
21:SS:13:LEU:HB2	21:SS:20:ILE:HB	1.83	0.59
18:SO:61:LYS:NZ	18:SO:80:ASP:OD2	2.29	0.59
79:L5:1870:C:H2'	79:L5:1871:A2M:H8	1.84	0.59
42:LO:185:VAL:O	42:LO:187:LYS:N	2.36	0.59
61:Lb:36:ASP:OD1	79:L5:4314:C:O2'	2.20	0.59
78:S2:165:G:OP2	78:S2:165:G:N2	2.34	0.59
78:S2:1228:A:H2'	78:S2:1229:G:C8	2.37	0.59
13:SW:51:GLU:HG2	32:Sb:8:LEU:HD21	1.83	0.59
21:SS:22:GLY:HA2	21:SS:56:ALA:HB3	1.84	0.59
37:LC:189:MET:SD	37:LC:201:ARG:NH1	2.75	0.59
45:LM:53:LYS:NZ	79:L5:1924:C:OP1	2.29	0.59
40:LE:178:PRO:HD2	40:LE:181:LEU:HD12	1.83	0.59
42:LO:128:ARG:NH1	52:LS:162:GLN:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:1720:U:HO2'	79:L5:3796:U:HO2'	1.49	0.59
82:SG:23:LYS:HB3	82:SG:41:LEU:HA	1.83	0.59
8:SJ:38:ARG:NH1	78:S2:643:A:OP1	2.36	0.59
11:SF:80:GLY:H	78:S2:1223:A:H5''	1.67	0.59
57:LY:47:MET:HE3	57:LY:48:PRO:HD2	1.84	0.59
63:Lc:11:LEU:HD13	63:Lc:75:SER:HB2	1.83	0.59
1:LA:152:SER:OG	79:L5:3661:G:N7	2.35	0.59
7:SD:103:GLU:OE2	7:SD:173:ARG:NE	2.32	0.59
26:SP:40:ARG:NH1	78:S2:1620:A:O2'	2.36	0.59
33:Sc:44:ARG:NH1	33:Sc:63:ARG:O	2.36	0.59
40:LE:65:ARG:NH1	79:L5:1070:G:OP2	2.36	0.59
78:S2:928:G:H1	78:S2:1013:U:H3	1.50	0.59
78:S2:1400:U:O4	78:S2:1401:A:N6	2.35	0.59
4:SB:28:LYS:HD3	4:SB:48:LEU:HD12	1.83	0.59
41:LG:73:ARG:NE	79:L5:4076:G:OP1	2.32	0.59
50:LQ:14:ARG:NH2	79:L5:2083:C:OP2	2.32	0.59
73:Ln:4:LYS:NZ	92:Ln:102:HOH:O	2.35	0.59
13:SW:55:ASP:O	13:SW:57:ARG:NH1	2.35	0.59
18:SO:84:ARG:NH1	18:SO:87:GLU:OE2	2.36	0.59
79:L5:1320:U:O2'	79:L5:1891:A:N1	2.29	0.59
40:LE:161:ARG:NH1	40:LE:273:SER:OG	2.36	0.58
79:L5:4140:C:O2	79:L5:4144:C:N4	2.36	0.58
36:Sg:272:GLN:OE1	36:Sg:308:ARG:NH1	2.36	0.58
46:La:76:ASP:N	46:La:76:ASP:OD1	2.35	0.58
79:L5:4527:G:OP2	79:L5:4527:G:N2	2.34	0.58
26:SP:21:ASP:N	26:SP:21:ASP:OD1	2.30	0.58
45:LM:117:LYS:NZ	79:L5:4882:U:OP1	2.37	0.58
50:LQ:66:MET:HE3	50:LQ:98:LEU:HD13	1.83	0.58
56:LX:135:LYS:NZ	79:L5:2436:U:OP2	2.36	0.58
58:LZ:100:VAL:HG22	58:LZ:106:LEU:HB3	1.86	0.58
79:L5:2485:U:H2'	79:L5:2486:G:H8	1.68	0.58
36:Sg:284:PRO:HB3	36:Sg:304:ASP:HB2	1.85	0.58
42:LO:37:ARG:NH1	79:L5:4761:G:OP2	2.28	0.58
18:SO:147:ARG:HG2	18:SO:150:ARG:HD3	1.83	0.58
37:LC:321:ASN:ND2	79:L5:715:G:OP1	2.35	0.58
41:LG:165:GLU:HG3	47:LN:10:LEU:HD23	1.85	0.58
62:LF:155:TYR:OH	62:LF:188:GLU:OE2	2.19	0.58
53:LT:4:THR:OG1	79:L5:4208:U:OP2	2.20	0.58
79:L5:966:A:OP2	79:L5:2092:G:N2	2.36	0.58
79:L5:1700:G:N7	79:L5:1704:C:N4	2.51	0.58
79:L5:3718:A2M:H2	79:L5:3934:G:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SJ:54:ARG:NH1	10:SC:200:ARG:O	2.36	0.58
10:SC:178:HIS:ND1	10:SC:221:ASP:OD2	2.36	0.58
43:LL:16:LYS:NZ	79:L5:48:G:OP1	2.36	0.58
71:L1:44:TRP:O	71:L1:48:LYS:NZ	2.37	0.58
18:SO:34:PHE:HB3	18:SO:41:PHE:HB2	1.85	0.58
19:SX:119:ARG:NH2	78:S2:1192:U:OP2	2.36	0.58
46:La:44:ASN:ND2	79:L5:1683:PSU:OP1	2.37	0.58
49:LD:84:PRO:O	49:LD:89:LYS:NZ	2.35	0.58
4:SB:113:MET:HE3	4:SB:142:PHE:HE1	1.69	0.58
37:LC:304:ALA:HB1	79:L5:2096:G:H21	1.67	0.58
69:Lj:20:ARG:NH2	69:Lj:39:TYR:OH	2.34	0.58
78:S2:126:G:OP1	82:SG:198:ARG:NH1	2.33	0.58
79:L5:1697:G:N2	79:L5:2084:C:OP1	2.32	0.58
43:LL:5:ARG:NH2	79:L5:1850:A:OP2	2.36	0.58
59:Lr:37:SER:OG	79:L5:2267:U:OP1	2.19	0.58
78:S2:1662:U:O4	78:S2:1663:A:N6	2.37	0.58
79:L5:3723:A2M:H2'	79:L5:3724:A2M:H8	1.86	0.58
78:S2:155:G:H4'	82:SG:15:LEU:HD13	1.84	0.57
78:S2:1546:G:N2	78:S2:1670:C:O2	2.34	0.57
79:L5:1548:G:O2'	79:L5:2812:A:N3	2.35	0.57
79:L5:3823:G:OP2	79:L5:3823:G:N2	2.27	0.57
5:L8:67:U:H2'	5:L8:68:G:H8	1.69	0.57
69:Lj:55:ARG:NH2	79:L5:364:G:O6	2.37	0.57
3:LB:137:TRP:O	3:LB:143:LYS:NZ	2.37	0.57
12:SH:46:THR:HG21	12:SH:97:GLN:HG2	1.86	0.57
61:Lb:36:ASP:HB3	61:Lb:39:PHE:HB3	1.86	0.57
62:LF:105:VAL:HG13	62:LF:136:VAL:HG12	1.85	0.57
14:SI:64:ASN:ND2	78:S2:302:A:N3	2.53	0.57
18:SO:135:ILE:O	78:S2:943:U:O2'	2.22	0.57
73:Ln:10:MET:HE2	78:S2:1172:U:H5''	1.85	0.57
79:L5:307:A:N3	79:L5:310:G:O2'	2.35	0.57
7:SD:135:GLU:HG3	7:SD:153:VAL:HG22	1.85	0.57
22:Sd:18:SER:HG	78:S2:1556:A:N6	2.03	0.57
27:ST:82:ARG:HB2	78:S2:1589:A:H4'	1.86	0.57
66:Lf:29:LYS:NZ	92:Lf:308:HOH:O	2.36	0.57
78:S2:1745:A:H1'	82:SG:66:GLY:HA2	1.86	0.57
5:L8:126:C:H42	79:L5:2543:A:H4'	1.69	0.57
30:SZ:68:ILE:HB	30:SZ:109:TYR:HB2	1.86	0.57
40:LE:105:ARG:NH1	79:L5:469:C:O2	2.37	0.57
47:LN:49:ARG:NH1	92:LN:413:HOH:O	2.37	0.57
47:LN:182:HIS:NE2	79:L5:291:U:O2'	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:LR:116:ASP:OD1	51:LR:116:ASP:N	2.36	0.57
9:SE:43:PRO:HG2	9:SE:46:ILE:HG13	1.87	0.57
14:SI:6:ASP:OD1	14:SI:9:HIS:ND1	2.37	0.57
47:LN:17:ASP:OD2	47:LN:20:ARG:NH2	2.37	0.57
53:LT:87:LYS:NZ	79:L5:4305:G:N7	2.50	0.57
79:L5:1591:U:OP2	79:L5:2856:C:O2'	2.23	0.57
79:L5:4115:G:N2	79:L5:4115:G:OP2	2.36	0.57
80:Et:53:G:H2'	80:Et:54:A:H8	1.70	0.57
5:L8:93:C:OP1	69:Lj:76:HIS:NE2	2.31	0.57
78:S2:46:A:N6	78:S2:97:U:O2	2.37	0.57
78:S2:317:C:OP2	82:SG:183:ARG:NH2	2.32	0.57
79:L5:4474:A:OP2	79:L5:4476:C:N4	2.38	0.57
41:LG:154:LEU:HD13	41:LG:219:VAL:HG12	1.87	0.56
62:LF:52:GLU:OE2	79:L5:1238:A:O2'	2.22	0.56
78:S2:925:G:H1	78:S2:1017:U:H3	1.52	0.56
6:L7:6:C:N4	92:L7:424:HOH:O	2.39	0.56
18:SO:142:ARG:NH1	31:Sa:23:CYS:O	2.37	0.56
29:SY:29:HIS:NE2	29:SY:69:THR:OG1	2.33	0.56
78:S2:1536:G:H2'	78:S2:1537:A:C8	2.40	0.56
79:L5:1895:G:O2'	79:L5:1907:A:N3	2.33	0.56
79:L5:2335:C:H2'	79:L5:2336:G:H8	1.68	0.56
2:SA:104:THR:O	2:SA:107:THR:OG1	2.21	0.56
10:SC:254:ASP:N	10:SC:254:ASP:OD1	2.38	0.56
11:SF:102:LEU:HD21	30:SZ:100:VAL:HG21	1.86	0.56
15:SQ:142:GLN:NE2	78:S2:1527:C:OP1	2.36	0.56
48:LI:30:LYS:HG3	48:LI:66:GLU:HG3	1.86	0.56
69:Lj:49:TRP:O	79:L5:1646:A:O2'	2.21	0.56
78:S2:512:A2M:H4'	78:S2:576:A2M:H2	1.86	0.56
78:S2:1658:G:OP2	78:S2:1660:C:N4	2.38	0.56
79:L5:2848:G:O2'	79:L5:3838:U:O4	2.18	0.56
79:L5:4353:PSU:H5'	79:L5:4354:U:H5'	1.86	0.56
10:SC:179:THR:OG1	10:SC:180:VAL:N	2.39	0.56
36:Sg:149:GLU:HG2	36:Sg:171:ASP:HB3	1.87	0.56
77:mR:39:G:OP1	78:S2:1704:C:N4	2.37	0.56
78:S2:151:C:O2'	82:SG:132:ARG:NH2	2.38	0.56
79:L5:961:G:O2'	79:L5:963:G:N7	2.39	0.56
40:LE:119:GLU:HB3	65:Le:7:LEU:HD22	1.88	0.56
42:LO:176:ARG:HD2	79:L5:4769:G:H5''	1.88	0.56
52:LS:3:ALA:O	52:LS:111:ARG:NH2	2.39	0.56
78:S2:613:G:N2	78:S2:626:G:OP1	2.38	0.56
78:S2:1259:A:N6	78:S2:1519:U:OP1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:67:C:OP2	79:L5:312:G:N2	2.37	0.56
2:SA:205:ARG:NH2	2:SA:213:GLU:OE1	2.29	0.56
25:SR:79:GLU:O	25:SR:83:ASN:ND2	2.38	0.56
50:LQ:173:LYS:NZ	79:L5:88:A:N7	2.53	0.56
78:S2:84:A:N3	78:S2:150:A:O2'	2.38	0.56
79:L5:2809:G:O2'	79:L5:4644:G:OP1	2.23	0.56
4:SB:25:PHE:HA	4:SB:28:LYS:HD2	1.87	0.56
36:Sg:114:SER:O	36:Sg:117:ASN:ND2	2.39	0.56
42:LO:60:LYS:NZ	79:L5:2046:G:OP1	2.36	0.56
44:LV:107:ASN:HD21	44:LV:111:GLU:HB2	1.71	0.56
45:LM:118:MET:HE3	45:LM:122:ILE:HD11	1.88	0.56
52:LS:174:THR:HG1	79:L5:4763:U:HO2'	1.52	0.56
78:S2:106:C:OP1	78:S2:431:G:O2'	2.23	0.56
78:S2:1101:U:H2'	78:S2:1102:G:H8	1.71	0.56
79:L5:4589:A:N1	79:L5:4621:C:O2'	2.37	0.56
14:SI:3:ILE:O	14:SI:30:GLY:N	2.36	0.56
57:LY:28:LYS:NZ	79:L5:241:G:OP1	2.36	0.56
67:Lg:5:LEU:HD21	67:Lg:30:ILE:HG22	1.88	0.56
10:SC:187[B]:ARG:NH2	78:S2:1154:U:OP2	2.36	0.56
21:SS:145:THR:HA	78:S2:1523:C:H4'	1.87	0.56
23:SN:87:ASP:OD2	23:SN:87:ASP:N	2.37	0.56
43:LL:55:ILE:O	43:LL:97:SER:OG	2.21	0.56
50:LQ:65:ARG:NH1	79:L5:1459:A:OP1	2.38	0.56
78:S2:587:A:H5'	78:S2:592:C:H41	1.70	0.56
5:L8:102:G:OP2	5:L8:104:A:O2'	2.22	0.56
9:SE:88:ASP:OD2	9:SE:122:LYS:NZ	2.38	0.56
11:SF:145:ARG:HH12	78:S2:1220:A:H4'	1.71	0.56
82:SG:49:VAL:HG12	82:SG:115:LYS:HB3	1.88	0.56
3:LB:312:LYS:NZ	3:LB:368:ILE:O	2.38	0.55
6:L7:19:C:OP2	38:LJ:154:LYS:NZ	2.37	0.55
14:SI:101:ILE:HD12	14:SI:190:LEU:HD11	1.88	0.55
65:Le:9:LYS:HB3	79:L5:703:G:H5''	1.86	0.55
78:S2:562:U:H2'	78:S2:563:G:C8	2.41	0.55
78:S2:874:G:H2'	78:S2:875:A:H8	1.71	0.55
1:LA:223:SER:OG	79:L5:3748:A:O2'	2.20	0.55
3:LB:168:MET:HA	3:LB:171:LEU:HD12	1.88	0.55
24:SL:119:ASP:OD1	24:SL:119:ASP:N	2.37	0.55
78:S2:436:OMG:OP2	78:S2:471:G:O2'	2.24	0.55
78:S2:532:C:H2'	78:S2:533:A:C8	2.41	0.55
78:S2:1424:G:H2'	78:S2:1425:G:H8	1.71	0.55
79:L5:1332:C:H2'	79:L5:1333:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:4274:A:H2'	79:L5:4275:G:C8	2.41	0.55
79:L5:4993:G:H22	79:L5:5058:A:H2	1.55	0.55
36:Sg:213:ASP:OD1	36:Sg:213:ASP:N	2.37	0.55
56:LX:64:SER:HB2	60:Lh:69:LEU:HD22	1.89	0.55
79:L5:1705:G:H2'	79:L5:1706:A:C8	2.41	0.55
12:SH:20:GLU:HB2	12:SH:48:ALA:HB3	1.88	0.55
23:SN:5:HIS:HB3	23:SN:117:LEU:HD13	1.89	0.55
32:Sb:11:SER:OG	32:Sb:13:GLU:OE1	2.25	0.55
44:LV:84:GLN:HE21	44:LV:86:LYS:HB3	1.70	0.55
45:LM:9:VAL:HG11	45:LM:66:HIS:HA	1.89	0.55
79:L5:751:G:O6	79:L5:912:G:N2	2.33	0.55
79:L5:4537:C:H2'	79:L5:4538:G:H8	1.72	0.55
79:L5:4541:G:N2	79:L5:4544:A:OP2	2.32	0.55
3:LB:113:GLU:HA	3:LB:116:ARG:HD2	1.88	0.55
14:SI:142:SER:HB3	14:SI:145:ILE:HG22	1.87	0.55
41:LG:81:ASN:O	41:LG:84:THR:OG1	2.24	0.55
78:S2:165:G:H1'	82:SG:110:ASN:HD22	1.71	0.55
78:S2:420:G:O2'	78:S2:660:C:N3	2.40	0.55
78:S2:1550:G:O2'	78:S2:1558:C:O2	2.23	0.55
79:L5:5068:G:N2	79:L5:5069:U:O4	2.37	0.55
18:SO:101:GLY:HA3	18:SO:134:PRO:HD2	1.88	0.55
58:LZ:29:ILE:HG22	58:LZ:32:GLY:H	1.70	0.55
79:L5:1558:A:H2'	79:L5:1559:G:H8	1.71	0.55
79:L5:2407:G:OP2	79:L5:2407:G:N2	2.36	0.55
42:LO:125:LYS:HG3	42:LO:129:LEU:HD12	1.89	0.55
54:LP:116:HIS:HB3	54:LP:149:ILE:HB	1.87	0.55
60:Lh:81:LEU:HA	60:Lh:84:ARG:HD2	1.89	0.55
76:Pt:63:C:H2'	76:Pt:64:G:H8	1.71	0.55
79:L5:2045:G:O6	79:L5:3870:C:O2'	2.24	0.55
1:LA:234:LYS:HG2	1:LA:238:ILE:HG12	1.89	0.55
54:LP:82:ARG:NH1	92:LP:327:HOH:O	2.39	0.55
2:SA:191:ARG:NH2	28:SV:44:GLY:O	2.40	0.55
3:LB:26:ARG:NH1	92:LB:634:HOH:O	2.40	0.55
4:SB:44:ILE:HD11	4:SB:86:LEU:HD12	1.89	0.55
36:Sg:110:SER:HB3	36:Sg:154:VAL:HG22	1.89	0.55
49:LD:196:ARG:NH2	49:LD:237:GLU:OE2	2.32	0.55
51:LR:37:SER:OG	51:LR:40:GLN:NE2	2.38	0.55
65:Le:108:ARG:NH1	79:L5:2326:G:OP1	2.38	0.55
79:L5:4077:A:N1	79:L5:4171:C:N4	2.54	0.55
81:LW:3:VAL:HG11	81:LW:12:LYS:HE3	1.88	0.55
6:L7:99:G:N7	52:LS:55:LYS:NZ	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SO:56:VAL:HG13	18:SO:60:MET:HE2	1.89	0.55
23:SN:103:GLU:HG3	23:SN:104:ARG:HD2	1.89	0.55
63:Lc:38:ILE:HG21	63:Lc:63:TYR:HB3	1.88	0.55
78:S2:1396:A:O2'	78:S2:1398:G:N7	2.37	0.55
5:L8:150:C:N4	41:LG:52:THR:O	2.39	0.54
42:LO:49:ARG:NH1	79:L5:1930:U:OP2	2.36	0.54
79:L5:4309:G:H5'	79:L5:4338:G:H5''	1.88	0.54
6:L7:29:C:O2	6:L7:50:A:N6	2.38	0.54
21:SS:117:ILE:HD12	26:SP:111:MET:HG2	1.89	0.54
48:LI:76:MET:HE2	48:LI:138:ILE:HG21	1.89	0.54
79:L5:4519:C:H5''	79:L5:4520:G:H5''	1.89	0.54
79:L5:4734:A:H2'	79:L5:4735:G:C8	2.42	0.54
79:L5:4927:G:OP2	79:L5:4927:G:N2	2.39	0.54
14:SI:181:GLN:NE2	78:S2:380:G:OP2	2.40	0.54
39:LH:94:SER:HB2	39:LH:142:ASP:HB3	1.88	0.54
45:LM:11:ARG:NH1	45:LM:58:THR:O	2.41	0.54
47:LN:181:HIS:O	47:LN:195:ARG:NH2	2.29	0.54
48:LI:66:GLU:OE1	48:LI:69:ARG:NH2	2.35	0.54
54:LP:64:ASN:ND2	54:LP:80:GLN:OE1	2.33	0.54
57:LY:111:LEU:HB3	57:LY:116:LYS:HE3	1.89	0.54
78:S2:568:C:H2'	78:S2:569:A:C8	2.43	0.54
78:S2:1228:A:H2'	78:S2:1229:G:H8	1.73	0.54
1:LA:147:ARG:HG2	1:LA:157:VAL:HG22	1.89	0.54
2:SA:141:ASN:ND2	28:SV:31:SER:O	2.39	0.54
3:LB:242:ARG:NH2	79:L5:2856:C:O2	2.32	0.54
15:SQ:100:VAL:HG12	15:SQ:101:ASP:H	1.73	0.54
48:LI:4:ARG:NH1	79:L5:1866:U:OP1	2.29	0.54
78:S2:640:A:H2'	78:S2:641:A:C8	2.43	0.54
78:S2:1220:A:N3	78:S2:1677:U:O2'	2.35	0.54
79:L5:2579:G:N2	79:L5:2582:A:OP2	2.34	0.54
79:L5:2777:G:H5''	79:L5:2778:G:H5'	1.89	0.54
3:LB:77:THR:OG1	3:LB:335:GLY:O	2.23	0.54
40:LE:181:LEU:O	79:L5:4883:C:N4	2.35	0.54
51:LR:108:ARG:NH2	79:L5:2899:C:OP1	2.29	0.54
55:LU:80:LYS:N	79:L5:2620:G:OP1	2.27	0.54
3:LB:369:ASP:OD2	3:LB:373:LYS:NZ	2.40	0.54
4:SB:150:ILE:HD13	25:SR:129:LYS:HB2	1.89	0.54
5:L8:14:U:O2	79:L5:420:A:N6	2.41	0.54
8:SJ:18:ARG:NH1	78:S2:3:C:O2	2.40	0.54
21:SS:45:LEU:HD22	21:SS:50:ILE:HD11	1.89	0.54
62:LF:46:ARG:HH22	79:L5:1704:C:HO2'	1.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:44:U:O4	78:S2:485:A:N6	2.41	0.54
79:L5:1283:G:N1	79:L5:2076:G:OP1	2.36	0.54
79:L5:1739:G:N3	79:L5:1742:A:N6	2.55	0.54
79:L5:2758:G:O2'	79:L5:2765:A:N3	2.35	0.54
1:LA:247:ARG:HB3	78:S2:1069:U:H4'	1.89	0.54
3:LB:139:ASP:OD2	3:LB:141:ASP:N	2.40	0.54
5:L8:20:A:O2'	79:L5:2333:G:OP1	2.25	0.54
57:LY:45:ARG:NH2	79:L5:238:C:OP2	2.41	0.54
58:LZ:31:ASP:OD1	58:LZ:31:ASP:N	2.40	0.54
78:S2:491:C:O2	78:S2:493:A:N6	2.38	0.54
79:L5:3620:G:OP1	79:L5:3622:C:N4	2.41	0.54
80:Et:62:C:H2'	80:Et:63:A:C8	2.43	0.54
21:SS:88:LYS:O	26:SP:18:ARG:NH1	2.41	0.54
41:LG:234:ARG:HH11	41:LG:235:ARG:HH21	1.55	0.54
23:SN:83:ASP:N	23:SN:83:ASP:OD1	2.40	0.54
42:LO:87:MET:SD	79:L5:1912:G:N2	2.81	0.54
22:Sd:19:ARG:NH2	78:S2:1661:A:OP1	2.41	0.53
22:Sd:34:TYR:OH	78:S2:1549:U:OP1	2.24	0.53
25:SR:100:PRO:HG3	25:SR:122:PRO:HG3	1.89	0.53
78:S2:1030:A:H2'	78:S2:1031:A2M:H8	1.89	0.53
40:LE:190:HIS:HB3	40:LE:193:PHE:HD2	1.74	0.53
45:LM:40:GLY:HA3	45:LM:45:VAL:HB	1.91	0.53
65:Le:39:ARG:NH2	92:Le:311:HOH:O	2.36	0.53
73:Ln:4:LYS:NZ	78:S2:1844:U:O4	2.33	0.53
76:Pt:47:G7M:H2'	76:Pt:48:U:H5''	1.90	0.53
4:SB:175:GLU:OE2	4:SB:187:LYS:NZ	2.37	0.53
26:SP:69:PRO:O	26:SP:70:MET:HG2	2.08	0.53
37:LC:140:LYS:HE3	37:LC:245:HIS:HB2	1.90	0.53
59:Lr:32:LEU:O	59:Lr:113:ARG:NH1	2.41	0.53
67:Lg:76:ARG:NH2	79:L5:2583:C:OP2	2.40	0.53
79:L5:2416:G:N2	79:L5:2427:G:O6	2.40	0.53
82:SG:26:THR:O	82:SG:30:LYS:NZ	2.41	0.53
8:SJ:40:LYS:NZ	78:S2:641:A:OP1	2.40	0.53
36:Sg:5:MET:HA	36:Sg:312:VAL:HA	1.89	0.53
37:LC:103:ALA:HA	79:L5:1517:G:H22	1.72	0.53
41:LG:200:THR:OG1	79:L5:150:U:OP2	2.23	0.53
76:Pt:10:G:O6	76:Pt:46:G:N2	2.41	0.53
78:S2:106:C:H2'	78:S2:107:A:H8	1.72	0.53
78:S2:165:G:H4'	82:SG:53:SER:HB3	1.90	0.53
79:L5:1500:A:H5''	79:L5:1501:C:H5''	1.91	0.53
79:L5:2745:A:H2'	79:L5:2746:A:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:SI:99:ASN:HB2	78:S2:377:G:H5'	1.91	0.53
23:SN:2:GLY:N	78:S2:1092:G:OP1	2.42	0.53
7:SD:142:LEU:HD13	7:SD:150:MET:HE2	1.91	0.53
27:ST:85:ASN:ND2	27:ST:89:PRO:O	2.41	0.53
35:Sf:143:LYS:NZ	78:S2:1311:C:OP1	2.39	0.53
79:L5:3700:C:O2'	79:L5:3774:A:N3	2.37	0.53
80:Et:41:C:H2'	80:Et:42:A:H8	1.73	0.53
82:SG:142:ARG:HA	82:SG:147:LEU:HB3	1.90	0.53
1:LA:117:GLU:HG2	1:LA:124:GLY:H	1.73	0.53
7:SD:35:SER:HB2	7:SD:51:LEU:HD23	1.91	0.53
7:SD:212:GLU:H	7:SD:212:GLU:CD	2.17	0.53
48:LI:87:ILE:HG12	48:LI:138:ILE:HG23	1.89	0.53
62:LF:40:LYS:HE3	62:LF:44:LYS:HE2	1.89	0.53
79:L5:1503:A:H4'	79:L5:1504:G:H5'	1.91	0.53
14:SI:2:GLY:N	78:S2:441:C:OP2	2.41	0.53
37:LC:106:LYS:NZ	92:LC:619:HOH:O	2.33	0.53
61:Lb:33:LYS:NZ	79:L5:4299:PSU:OP1	2.42	0.53
2:SA:134:LEU:HD21	2:SA:144:THR:HG21	1.90	0.53
36:Sg:164:ILE:HG22	36:Sg:178:ASN:HA	1.91	0.53
49:LD:166:ALA:HB1	49:LD:171:LEU:HD12	1.91	0.53
58:LZ:21:ARG:NH1	92:LZ:201:HOH:O	2.39	0.53
78:S2:107:A:H2'	78:S2:108:G:C8	2.44	0.53
79:L5:489:C:O2	79:L5:667:A:N6	2.42	0.53
79:L5:2589:C:HO2'	79:L5:2767:U:HO2'	1.54	0.53
79:L5:4537:C:H2'	79:L5:4538:G:C8	2.44	0.53
30:SZ:79:ILE:HB	30:SZ:83:LEU:HD23	1.90	0.53
38:LJ:81:GLU:HG3	38:LJ:82:ILE:HD13	1.91	0.53
49:LD:108:ARG:HE	49:LD:253:TYR:HB2	1.73	0.53
55:LU:111:GLU:HG2	55:LU:113:ARG:HG3	1.91	0.53
74:Lo:34:TYR:O	74:Lo:39:ARG:NH1	2.41	0.53
79:L5:4750:G:H2'	79:L5:4751:G:H8	1.73	0.53
2:SA:50:ASN:HB3	2:SA:53:ARG:HG3	1.90	0.52
12:SH:83:LEU:HD13	12:SH:92:VAL:HG11	1.91	0.52
21:SS:88:LYS:HG2	26:SP:18:ARG:HD2	1.90	0.52
42:LO:130:LYS:HB2	42:LO:133:ARG:HG2	1.92	0.52
65:Le:89:LEU:HD13	65:Le:118:LEU:HD22	1.91	0.52
79:L5:4274:A:H2'	79:L5:4275:G:H8	1.73	0.52
3:LB:108:GLU:OE2	3:LB:138:GLN:NE2	2.32	0.52
45:LM:98:ARG:NH1	79:L5:4872:G:O6	2.43	0.52
52:LS:15:ARG:HB3	52:LS:27:LEU:HD23	1.90	0.52
79:L5:1414:C:H2'	79:L5:1415:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:Et:62:C:H2'	80:Et:63:A:H8	1.72	0.52
13:SW:55:ASP:OD1	13:SW:55:ASP:N	2.41	0.52
23:SN:64:ARG:NH1	78:S2:919:A:OP2	2.31	0.52
40:LE:123:ARG:NH2	79:L5:961:G:O6	2.37	0.52
43:LL:135:LYS:NZ	79:L5:170:C:O2'	2.42	0.52
49:LD:160:PHE:HA	49:LD:163:LEU:HB3	1.91	0.52
55:LU:101:ARG:HE	55:LU:103:VAL:HG22	1.75	0.52
62:LF:128:ALA:O	79:L5:1726:U:O2'	2.26	0.52
79:L5:1320:U:O2	79:L5:1891:A:N6	2.43	0.52
79:L5:2520:C:H2'	79:L5:2521:G:H8	1.74	0.52
79:L5:2640:G:H2'	79:L5:2641:A:C8	2.45	0.52
6:L7:11:A:N1	6:L7:66:G:O2'	2.40	0.52
15:SQ:89:SER:HB3	15:SQ:112:LEU:HD13	1.90	0.52
66:Lf:35:ALA:HB3	66:Lf:38:GLU:HG3	1.91	0.52
78:S2:1171:G:O2'	78:S2:1187:G:O6	2.22	0.52
79:L5:4598:C:O2	79:L5:4612:C:N4	2.36	0.52
82:SG:2:LYS:HB2	82:SG:108:VAL:HG23	1.91	0.52
1:LA:107:MET:O	1:LA:139:HIS:NE2	2.35	0.52
17:SK:15:LEU:HD22	17:SK:49:MET:HE1	1.92	0.52
23:SN:40:LEU:HB3	23:SN:45:LEU:HD12	1.92	0.52
63:Lc:28:VAL:HG21	63:Lc:37:MET:HG3	1.91	0.52
3:LB:154:LYS:HG3	3:LB:194:LEU:HD12	1.92	0.52
4:SB:77:ASP:OD1	4:SB:77:ASP:N	2.43	0.52
38:LJ:146:ARG:HG3	49:LD:150:LEU:HD12	1.91	0.52
79:L5:496:G:H2'	79:L5:497:G:C8	2.44	0.52
79:L5:2568:C:H2'	79:L5:2569:G:H8	1.73	0.52
50:LQ:42:THR:HB	79:L5:1428:U:H5''	1.90	0.52
56:LX:83:THR:HG22	79:L5:2434:G:H5''	1.91	0.52
78:S2:848:U:H2'	78:S2:849:A:H8	1.75	0.52
3:LB:167:GLN:NE2	3:LB:204:GLN:OE1	2.37	0.52
13:SW:11:LEU:HD22	13:SW:72:CYS:HB2	1.92	0.52
18:SO:98:ARG:HB3	18:SO:132:VAL:HG23	1.92	0.52
26:SP:81:ARG:NH2	26:SP:117:GLY:O	2.43	0.52
33:Sc:21:THR:OG1	33:Sc:22:GLY:N	2.43	0.52
42:LO:166:ILE:HG13	42:LO:169:ARG:HH21	1.74	0.52
70:Lk:19:ASP:OD2	70:Lk:19:ASP:N	2.36	0.52
79:L5:3861:A:H2'	79:L5:3862:A:H8	1.75	0.52
79:L5:4141:G:N2	79:L5:4143:G:O6	2.43	0.52
1:LA:36:GLU:OE2	1:LA:163:ARG:NH1	2.43	0.52
2:SA:147:LEU:O	2:SA:165:ASN:ND2	2.41	0.52
9:SE:27:PHE:O	78:S2:495:U:O2'	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:SY:108:LYS:NZ	78:S2:506:G:OP1	2.43	0.52
49:LD:267:ASN:N	49:LD:267:ASN:OD1	2.42	0.52
78:S2:140:C:H42	78:S2:313:A:H61	1.57	0.52
78:S2:981:A:H2'	78:S2:982:G:C8	2.44	0.52
79:L5:369:G:N2	79:L5:372:A:OP2	2.35	0.52
79:L5:1942:A:H2'	79:L5:1943:A:C8	2.45	0.52
1:LA:220:GLY:O	79:L5:3749:C:O2'	2.28	0.51
10:SC:161:SER:O	10:SC:161:SER:OG	2.26	0.51
53:LT:130:ARG:NE	79:L5:1837:A:OP2	2.40	0.51
55:LU:61:VAL:HG22	55:LU:74:SER:HB2	1.90	0.51
65:Le:16:ARG:NH1	79:L5:438:G:OP1	2.29	0.51
79:L5:2415:OMU:H2'	79:L5:2416:G:O4'	2.10	0.51
79:L5:3946:G:H1	79:L5:4067:U:H3	1.58	0.51
3:LB:140:GLU:N	3:LB:140:GLU:OE2	2.42	0.51
4:SB:139:CYS:SG	4:SB:172:MET:HE1	2.49	0.51
21:SS:134:GLN:NE2	78:S2:1608:U:OP1	2.44	0.51
27:ST:90:SER:O	27:ST:91:HIS:ND1	2.43	0.51
42:LO:9:LEU:HD23	42:LO:118:MET:HB2	1.91	0.51
92:Lj:205:HOH:O	79:L5:1600:A:OP1	2.19	0.51
79:L5:1480:C:O2'	79:L5:1482:G:OP2	2.24	0.51
79:L5:2745:A:H2'	79:L5:2746:A:C8	2.45	0.51
79:L5:3893:C:O2'	79:L5:4979:A:N1	2.41	0.51
3:LB:291:TYR:OH	3:LB:315:ASN:ND2	2.42	0.51
6:L7:35:U:O2	6:L7:45:U:O2'	2.27	0.51
10:SC:183:LYS:NZ	13:SW:91:ASN:O	2.42	0.51
21:SS:121:ARG:HG3	21:SS:131:VAL:HB	1.92	0.51
37:LC:205:ARG:HG2	79:L5:2297:G:H5'	1.91	0.51
51:LR:124:TYR:OH	79:L5:2666:U:OP2	2.20	0.51
62:LF:76:ARG:NE	79:L5:730:G:OP2	2.41	0.51
79:L5:158:A:H5''	79:L5:159:C:H2'	1.91	0.51
79:L5:3788:C:N4	79:L5:3812:C:OP2	2.41	0.51
79:L5:4670:C:O2'	79:L5:4672:A:OP2	2.25	0.51
79:L5:4967:A:H2'	79:L5:4968:A:H8	1.75	0.51
25:SR:129:LYS:NZ	78:S2:1100:A:OP1	2.35	0.51
29:SY:103:SER:HB3	29:SY:106:GLN:HG3	1.93	0.51
36:Sg:154:VAL:O	36:Sg:155:ARG:NE	2.43	0.51
36:Sg:249:CYS:HB3	36:Sg:289:LEU:HD13	1.93	0.51
53:LT:70:HIS:ND1	79:L5:4314:C:OP1	2.43	0.51
66:Lf:23:GLU:OE1	79:L5:438:G:N2	2.34	0.51
5:L8:26:C:O2'	37:LC:53:ALA:O	2.24	0.51
7:SD:29:LEU:HD21	7:SD:69:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SD:162:ASP:OD1	7:SD:165:ASN:ND2	2.42	0.51
11:SF:123:GLU:OE2	11:SF:204:ARG:NH1	2.43	0.51
11:SF:144:LEU:HD23	33:Sc:49:PRO:HG2	1.91	0.51
24:SL:81:LYS:HB3	78:S2:394:G:H5'	1.92	0.51
36:Sg:66:VAL:HA	36:Sg:82:SER:HA	1.93	0.51
43:LL:74:ARG:NH2	79:L5:109:G:OP2	2.44	0.51
78:S2:388:U:H2'	78:S2:389:A:H8	1.75	0.51
80:Et:41:C:H2'	80:Et:42:A:C8	2.45	0.51
3:LB:2:SER:N	79:L5:4517:A:OP2	2.44	0.51
9:SE:11:ARG:HA	9:SE:28:ALA:HB2	1.92	0.51
43:LL:80:GLU:HG3	43:LL:110:LEU:HD12	1.90	0.51
47:LN:96:ARG:NH2	47:LN:104:GLU:OE1	2.43	0.51
51:LR:105:LEU:HD13	51:LR:135:LYS:HE3	1.93	0.51
78:S2:1204:A:O2'	78:S2:1700:C:OP2	2.22	0.51
79:L5:300:A:H2'	79:L5:301:G:H8	1.75	0.51
78:S2:895:G:H2'	78:S2:896:U:H4'	1.93	0.51
78:S2:1084:A:OP1	78:S2:1858:G:O2'	2.27	0.51
79:L5:278:G:H5'	79:L5:329:A:N6	2.26	0.51
2:SA:8:LEU:HD11	28:SV:39:VAL:HG21	1.92	0.51
2:SA:76:VAL:HG12	2:SA:123:VAL:HB	1.93	0.51
3:LB:14:LEU:HD11	3:LB:265:SER:HB3	1.93	0.51
14:SI:5:ARG:NE	78:S2:379:C:O2	2.43	0.51
37:LC:95:MET:H	37:LC:95:MET:HE2	1.76	0.51
41:LG:165:GLU:HB3	47:LN:7:ILE:HG23	1.93	0.51
43:LL:80:GLU:OE1	43:LL:102:ARG:NH2	2.43	0.51
60:Lh:72:PHE:O	60:Lh:76:LYS:NZ	2.44	0.51
77:mR:35:G:H4'	77:mR:36:A:H5'	1.91	0.51
79:L5:926:G:H2'	79:L5:927:G:H8	1.76	0.51
79:L5:1582:PSU:O4	79:L5:2396:A:N6	2.44	0.51
79:L5:1764:G:O6	79:L5:1769:G:N1	2.44	0.51
79:L5:2574:G:N7	79:L5:2760:G:N2	2.58	0.51
2:SA:74:VAL:HG13	2:SA:121:LEU:HB3	1.93	0.51
12:SH:43:LEU:HD22	12:SH:68:GLN:HG3	1.92	0.51
78:S2:455:A:H2'	78:S2:456:C:H6	1.76	0.51
78:S2:1382:A:H2'	78:S2:1383:A2M:H8	1.93	0.51
79:L5:83:C:O2	79:L5:100:C:N4	2.34	0.51
79:L5:1097:C:H2'	79:L5:1098:G:H8	1.76	0.51
1:LA:118:GLU:OE1	79:L5:3662:A:O2'	2.26	0.51
14:SI:34:ALA:HB2	14:SI:56:ARG:HD2	1.92	0.51
29:SY:15:ASN:ND2	29:SY:22:GLN:OE1	2.43	0.51
60:Lh:76:LYS:O	79:L5:136:C:N4	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:65:C:N4	78:S2:169:U:O2'	2.44	0.51
78:S2:1354:G:N2	78:S2:1357:A:OP2	2.36	0.51
78:S2:1528:G:O2'	78:S2:1666:C:OP1	2.27	0.51
79:L5:93:G:H2'	79:L5:94:A:C8	2.46	0.51
79:L5:3900:G:O6	79:L5:4523:A2M:N6	2.41	0.51
1:LA:65:ASP:OD2	1:LA:72:ARG:NE	2.41	0.50
3:LB:161:ARG:HG2	3:LB:184:GLN:HA	1.93	0.50
9:SE:160:ILE:HD12	9:SE:169:ILE:HG12	1.92	0.50
21:SS:75:ARG:NH1	21:SS:81:ASP:OD1	2.44	0.50
72:Lm:109:ASN:ND2	72:Lm:117:HIS:O	2.43	0.50
78:S2:604:A:N3	78:S2:639:C:O2'	2.36	0.50
79:L5:1933:G:H2'	79:L5:1934:A:C8	2.45	0.50
11:SF:122:ARG:HD2	33:Sc:57:THR:HG21	1.92	0.50
21:SS:117:ILE:HD11	26:SP:110:GLU:HG2	1.94	0.50
41:LG:132:ARG:NH2	79:L5:119:G:OP1	2.39	0.50
46:La:36:GLY:HA3	46:La:40:HIS:CE1	2.46	0.50
49:LD:109:LEU:HD23	49:LD:171:LEU:HD21	1.92	0.50
53:LT:102:ARG:NH1	53:LT:105:PHE:HD2	2.09	0.50
78:S2:1259:A:H1'	78:S2:1264:C:N4	2.26	0.50
78:S2:1743:G:H21	78:S2:1791:A:H62	1.60	0.50
79:L5:717:U:H2'	79:L5:718:C:C6	2.45	0.50
79:L5:3910:C:H2'	79:L5:3911:C:H6	1.76	0.50
79:L5:5006:U:H4'	79:L5:5007:A:H5'	1.92	0.50
6:L7:7:G:OP1	49:LD:33:ARG:NH1	2.42	0.50
19:SX:24:ASP:HB3	19:SX:27:TYR:HB3	1.92	0.50
25:SR:47:ARG:NH1	25:SR:48:ASN:OD1	2.44	0.50
52:LS:17:LEU:HD11	53:LT:136:ARG:HH11	1.75	0.50
78:S2:1190:A:N3	78:S2:1714:U:O2'	2.42	0.50
79:L5:2494:U:H2'	79:L5:2495:U:O4'	2.11	0.50
5:L8:67:U:H2'	5:L8:68:G:C8	2.47	0.50
8:SJ:47:LYS:HG3	8:SJ:102:ILE:HD12	1.92	0.50
10:SC:123:ARG:NH2	78:S2:1358:U:OP2	2.45	0.50
51:LR:62:ARG:NH2	79:L5:4646:U:OP2	2.31	0.50
77:mR:33:G:H2'	78:S2:961:G:C2	2.46	0.50
78:S2:145:G:H2'	78:S2:146:G:C8	2.47	0.50
29:SY:37:LYS:NZ	78:S2:572:PSU:OP2	2.43	0.50
40:LE:209:PRO:HB2	40:LE:212:LEU:HD23	1.93	0.50
47:LN:68:ARG:HD2	47:LN:128:LYS:HG3	1.94	0.50
78:S2:1144:A:H5'	78:S2:1355:C:H41	1.75	0.50
3:LB:56:ILE:HD13	3:LB:365:LEU:HD22	1.92	0.50
3:LB:92:TYR:HB3	3:LB:99:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SE:112:HIS:NE2	9:SE:237:SER:O	2.45	0.50
50:LQ:50:ARG:NH1	92:LQ:314:HOH:O	2.45	0.50
15:SQ:13:PHE:HB3	15:SQ:22:VAL:HG22	1.94	0.50
23:SN:30:SER:HB2	23:SN:67:THR:HA	1.93	0.50
37:LC:60:HIS:HA	37:LC:92:PHE:HE1	1.75	0.50
47:LN:135:ILE:HG21	47:LN:151:ILE:HG21	1.92	0.50
62:LF:89:LEU:HD11	62:LF:122:PHE:HB3	1.93	0.50
70:Lk:35:LYS:NZ	79:L5:2693:G:OP1	2.33	0.50
78:S2:73:C:O2'	78:S2:74:G:N3	2.37	0.50
78:S2:1226:G:N1	78:S2:1639:G7M:OP2	2.37	0.50
1:LA:54:ARG:NH2	79:L5:3680:U:OP1	2.32	0.50
9:SE:107:GLY:HA2	9:SE:189:LEU:HG	1.93	0.50
9:SE:141:THR:OG1	9:SE:143:ASP:OD1	2.27	0.50
60:Lh:107:GLN:NE2	60:Lh:111:GLU:OE1	2.44	0.50
65:Le:21:ILE:HD13	65:Le:33[B]:ARG:HD3	1.93	0.50
79:L5:1669:A:H4'	79:L5:1685:G:N2	2.26	0.50
10:SC:242:ASP:O	10:SC:246:LYS:HG2	2.12	0.50
17:SK:65:ARG:HH12	22:Sd:20:SER:HB2	1.76	0.50
25:SR:66:VAL:HG23	25:SR:67:ARG:H	1.76	0.50
46:La:51:GLY:N	50:LQ:178:ARG:O	2.45	0.50
62:LF:96:ARG:NH1	79:L5:1895:G:OP1	2.44	0.50
69:Lj:13:ASN:ND2	79:L5:1618:G:OP1	2.36	0.50
78:S2:656:G:N2	78:S2:663:C:H5''	2.26	0.50
78:S2:1139:C:N4	78:S2:1149:A:H62	2.10	0.50
79:L5:4594:U:H2'	79:L5:4595:G:C8	2.44	0.50
79:L5:4967:A:H2'	79:L5:4968:A:C8	2.46	0.50
3:LB:175:GLN:NE2	3:LB:177:LYS:O	2.35	0.49
6:L7:24:C:O2	6:L7:117:G:N2	2.33	0.49
23:SN:13:GLN:HG3	32:Sb:21:LYS:HE3	1.93	0.49
25:SR:56:HIS:NE2	78:S2:1465:A:OP1	2.35	0.49
48:LI:47:PRO:HB3	48:LI:171:TRP:CZ2	2.47	0.49
66:Lf:78:HIS:HB2	66:Lf:85:ARG:HG2	1.94	0.49
78:S2:1101:U:H2'	78:S2:1102:G:C8	2.47	0.49
78:S2:1221:G:O2'	78:S2:1676:U:O2	2.25	0.49
79:L5:1328:G:O2'	79:L5:2349:A:OP1	2.29	0.49
79:L5:1577:G:O2'	79:L5:1612:G:H4'	2.11	0.49
79:L5:1700:G:N2	79:L5:2097:U:O4'	2.41	0.49
79:L5:4260:U:H2'	79:L5:4261:C:C6	2.47	0.49
1:LA:117:GLU:O	1:LA:162:ASN:ND2	2.45	0.49
11:SF:29:GLN:H	11:SF:110:GLN:NE2	2.09	0.49
11:SF:107:ASN:HB3	11:SF:110:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SH:32:MET:SD	12:SH:32:MET:N	2.85	0.49
29:SY:105:LYS:NZ	78:S2:52:G:O2'	2.37	0.49
49:LD:62:CYS:HB3	49:LD:105:LEU:HD22	1.94	0.49
78:S2:1351:G:O2'	78:S2:1378:A:N1	2.43	0.49
79:L5:445:U:O4	79:L5:1301:C:N4	2.42	0.49
3:LB:49:TYR:OH	3:LB:168:MET:SD	2.66	0.49
12:SH:106:ARG:NH1	78:S2:801:PSU:O2	2.39	0.49
13:SW:112:ASP:OD1	13:SW:112:ASP:N	2.38	0.49
28:SV:17:CYS:HB2	28:SV:56:CYS:HB3	1.93	0.49
43:LL:103:ARG:NH1	92:LL:426:HOH:O	2.44	0.49
62:LF:236:ARG:NH1	92:LF:441:HOH:O	2.46	0.49
5:L8:52:A:H5'	71:L1:21:ARG:HD3	1.93	0.49
53:LT:100:LYS:HB2	79:L5:1730:U:H4'	1.94	0.49
78:S2:116:OMU:O5'	78:S2:116:OMU:H6	2.13	0.49
79:L5:2090:U:H4'	79:L5:2091:C:H3'	1.94	0.49
31:Sa:32:LYS:NZ	78:S2:989:C:O2	2.45	0.49
47:LN:179:LYS:O	79:L5:297:U:O2'	2.31	0.49
49:LD:3:PHE:HB3	79:L5:1755:C:N3	2.28	0.49
65:Le:128:ARG:NH1	79:L5:2306:G:OP1	2.43	0.49
78:S2:940:U:H3	78:S2:1002:U:H3	1.61	0.49
79:L5:699:C:H2'	79:L5:700:G:H8	1.76	0.49
79:L5:4638:U:OP1	79:L5:5044:A:O2'	2.29	0.49
3:LB:28:LYS:NZ	79:L5:4582:C:OP2	2.35	0.49
12:SH:7:LYS:HZ1	12:SH:40:LEU:HD22	1.78	0.49
14:SI:22:HIS:HB3	78:S2:433:A:H5''	1.95	0.49
27:ST:77:LYS:HD3	78:S2:1587:G:H5''	1.95	0.49
51:LR:117:ARG:NH1	79:L5:2660:A:OP1	2.45	0.49
57:LY:82:ILE:HB	57:LY:85:VAL:HB	1.95	0.49
61:Lb:12:GLN:OE1	61:Lb:15:LYS:NZ	2.32	0.49
78:S2:528:A:H2'	78:S2:529:A:H8	1.78	0.49
79:L5:162:A:H2'	79:L5:163:A:C8	2.47	0.49
79:L5:1245:C:H2'	79:L5:1246:G:C8	2.45	0.49
79:L5:2459:G:N2	79:L5:2462:C:OP2	2.44	0.49
79:L5:3669:G:H21	79:L5:3672:G:H21	1.60	0.49
79:L5:3910:C:H2'	79:L5:3911:C:C6	2.47	0.49
3:LB:140:GLU:H	3:LB:140:GLU:CD	2.20	0.49
18:SO:116:LEU:HD13	31:Sa:45:VAL:HG12	1.93	0.49
26:SP:64:LYS:HE2	26:SP:92:SER:HB3	1.94	0.49
51:LR:20:LYS:NZ	79:L5:2822:G:N7	2.58	0.49
51:LR:38:ARG:NH2	79:L5:2527:A:OP1	2.39	0.49
51:LR:107:ARG:O	51:LR:111:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LZ:41:ALA:HB2	58:LZ:77:TYR:HE1	1.78	0.49
78:S2:28:U:H2'	78:S2:29:G:H8	1.77	0.49
79:L5:1442:C:H2'	79:L5:1443:A:C8	2.47	0.49
79:L5:1872:G:O2'	79:L5:4219:A:N3	2.44	0.49
79:L5:3717:A:H2'	79:L5:3718:A2M:C8	2.42	0.49
3:LB:176:LYS:HG3	79:L5:4986:G:H5''	1.94	0.49
3:LB:261:ARG:HB2	42:LO:64:THR:HG21	1.95	0.49
23:SN:3:ARG:HB2	23:SN:6:ALA:HB3	1.94	0.49
65:Le:3:ALA:HB1	65:Le:121:ARG:HH21	1.76	0.49
79:L5:1740:C:O2	79:L5:1786:A:N6	2.45	0.49
79:L5:2588:C:OP1	79:L5:2768:C:O2'	2.27	0.49
2:SA:77:ILE:HD11	2:SA:99:ILE:HD12	1.95	0.49
10:SC:166:ARG:HB3	10:SC:247:THR:HB	1.94	0.49
38:LJ:40:LEU:O	38:LJ:44:THR:OG1	2.27	0.49
39:LH:75:SER:OG	79:L5:4691:A:OP1	2.30	0.49
42:LO:53:LYS:NZ	92:LO:414:HOH:O	2.46	0.49
53:LT:4:THR:O	53:LT:9:ARG:NE	2.46	0.49
59:Lr:39:ARG:O	59:Lr:103:ARG:NH2	2.44	0.49
60:Lh:14:LYS:HZ1	60:Lh:61:ILE:HG23	1.78	0.49
62:LF:32:ARG:NH1	79:L5:962:C:O2	2.46	0.49
78:S2:15:U:H2'	78:S2:16:G:O4'	2.13	0.49
78:S2:453:C:O2'	82:SG:92:ARG:O	2.23	0.49
78:S2:528:A:H2'	78:S2:529:A:C8	2.48	0.49
78:S2:1348:G:N1	78:S2:1362:U:O4	2.40	0.49
79:L5:478:G:H2'	79:L5:479:G:H8	1.78	0.49
79:L5:1279:A:O2'	79:L5:1281:G:N7	2.41	0.49
79:L5:4228:OMG:N2	79:L5:4375:C:O2	2.36	0.49
3:LB:218:ASP:OD2	3:LB:348:ARG:NH2	2.33	0.49
4:SB:34:LYS:NZ	4:SB:43:ASN:OD1	2.46	0.49
18:SO:104:ARG:NH2	78:S2:959:G:OP1	2.46	0.49
36:Sg:37:ASP:OD1	36:Sg:39:THR:OG1	2.29	0.49
40:LE:261:ILE:HG23	40:LE:267:LEU:HD12	1.93	0.49
69:Lj:6:SER:OG	79:L5:2799:G:O2'	2.29	0.49
78:S2:982:G:H2'	78:S2:983:A:H8	1.77	0.49
5:L8:19:C:H2'	5:L8:20:A:C8	2.47	0.48
10:SC:88:ILE:HD13	10:SC:94:ILE:HD11	1.95	0.48
18:SO:147:ARG:HB3	18:SO:150:ARG:HH11	1.78	0.48
24:SL:111:VAL:HG12	24:SL:140:PHE:HB2	1.94	0.48
40:LE:247:LYS:HD3	79:L5:4938:A:H61	1.78	0.48
47:LN:146:PRO:HB2	60:Lh:104:THR:HG23	1.95	0.48
62:LF:156:LYS:NZ	62:LF:248:ASN:O	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:1333:A:H2'	79:L5:1334:A:C8	2.48	0.48
10:SC:205:VAL:O	10:SC:224:THR:OG1	2.31	0.48
42:LO:89:PRO:HD3	79:L5:1914:C:H4'	1.95	0.48
62:LF:129:SER:HA	62:LF:132:MET:HE3	1.94	0.48
78:S2:527:C:H2'	78:S2:528:A:H8	1.78	0.48
78:S2:838:G:H1'	78:S2:839:C:H5	1.78	0.48
78:S2:942:G:H2'	78:S2:943:U:C6	2.48	0.48
78:S2:1130:G:OP2	78:S2:1130:G:N2	2.43	0.48
78:S2:1232:PSU:H2'	78:S2:1233:G:C8	2.48	0.48
78:S2:1579:A:O2'	78:S2:1581:C:OP2	2.25	0.48
78:S2:1588:A:H2'	78:S2:1589:A:C8	2.48	0.48
79:L5:4208:U:OP1	79:L5:4334:U:O2'	2.30	0.48
2:SA:119:PRO:HG2	2:SA:142:LEU:HD21	1.94	0.48
30:SZ:92:LEU:HD12	30:SZ:109:TYR:HE1	1.78	0.48
41:LG:230:TYR:OH	68:Li:46:GLU:OE2	2.23	0.48
75:Lp:47:MET:HE2	75:Lp:57:CYS:HB2	1.94	0.48
78:S2:1534:C:N4	78:S2:1600:G:O6	2.45	0.48
78:S2:1834:A:N7	78:S2:1837:G:N2	2.61	0.48
79:L5:126:C:H2'	79:L5:127:G:H8	1.78	0.48
79:L5:1485:C:O4'	79:L5:4349:C:N4	2.47	0.48
11:SF:30:ILE:HG23	11:SF:117:ILE:HD11	1.95	0.48
23:SN:40:LEU:HD12	23:SN:50:ILE:HG23	1.94	0.48
24:SL:13:GLN:HE22	24:SL:63:THR:HB	1.78	0.48
37:LC:95:MET:HE1	79:L5:1521:C:H5'	1.96	0.48
41:LG:77:PRO:HG2	41:LG:80:ILE:HD12	1.95	0.48
41:LG:133:PRO:HD2	79:L5:119:G:H1	1.78	0.48
79:L5:1443:A:N6	79:L5:2103:G:O6	2.47	0.48
79:L5:2415:OMU:HM23	79:L5:2415:OMU:H1'	1.65	0.48
3:LB:77:THR:HG21	3:LB:337:VAL:HG22	1.95	0.48
3:LB:252:ALA:HB1	79:L5:4524:G:N3	2.28	0.48
7:SD:15:GLY:HA3	22:Sd:50:ILE:HG23	1.95	0.48
9:SE:126:VAL:HG22	9:SE:139:LEU:HD21	1.96	0.48
62:LF:182:TYR:HB3	62:LF:200:ARG:HG3	1.95	0.48
78:S2:158:A:H2'	78:S2:159:A2M:O4'	2.14	0.48
78:S2:890:U:H3	78:S2:897:U:H5	1.62	0.48
79:L5:4736:C:H2'	79:L5:4737:G:H8	1.77	0.48
92:L8:400:HOH:O	69:Lj:65:ARG:NH1	2.34	0.48
6:L7:117:G:H5'	49:LD:256:LYS:HD2	1.96	0.48
19:SX:93:PHE:HB3	19:SX:133:LEU:HD23	1.95	0.48
21:SS:110:ASP:OD1	21:SS:113:ARG:NH2	2.47	0.48
25:SR:37:GLU:OE1	36:Sg:150:TRP:NE1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SZ:73:VAL:HG12	30:SZ:79:ILE:HD11	1.95	0.48
37:LC:199:ARG:NH2	79:L5:350:C:OP2	2.45	0.48
50:LQ:35:LEU:O	50:LQ:39:THR:OG1	2.21	0.48
50:LQ:78:LYS:HD2	50:LQ:137:VAL:HG23	1.95	0.48
78:S2:476:A:N3	78:S2:488:U:O2'	2.34	0.48
78:S2:955:A:N7	78:S2:971:G:N2	2.61	0.48
78:S2:1243:PSU:O2	78:S2:1257:G:N2	2.42	0.48
79:L5:956:A:H1'	79:L5:2076:G:H5''	1.94	0.48
79:L5:1890:G:OP2	79:L5:1890:G:N2	2.38	0.48
79:L5:1916:G:N2	79:L5:2067:C:O2	2.47	0.48
79:L5:2411:C:H2'	79:L5:2412:A:H8	1.78	0.48
79:L5:3736:A:H2'	79:L5:3737:A:C8	2.48	0.48
82:SG:211:LYS:HD3	82:SG:211:LYS:HA	1.67	0.48
1:LA:173:GLY:O	75:Lp:69:TRP:NE1	2.43	0.48
3:LB:13:SER:HB2	79:L5:4622:A:H4'	1.94	0.48
15:SQ:102:GLU:HG2	36:Sg:55:PRO:HB2	1.95	0.48
23:SN:76:LYS:HE2	23:SN:76:LYS:HB2	1.62	0.48
26:SP:95:GLY:HA2	26:SP:104:GLN:HA	1.95	0.48
46:La:53:PHE:O	50:LQ:178:ARG:HB2	2.13	0.48
49:LD:83:LEU:HB3	49:LD:88:VAL:HB	1.94	0.48
62:LF:36:LYS:NZ	79:L5:1702:C:N3	2.62	0.48
67:Lg:62:LYS:HD3	79:L5:2517:A:H5'	1.96	0.48
78:S2:12:U:O2	78:S2:1356:G:N2	2.47	0.48
78:S2:1562:C:H2'	78:S2:1563:G:H8	1.79	0.48
79:L5:2845:A:H62	79:L5:3843:C:H42	1.61	0.48
79:L5:4258:C:H2'	79:L5:4259:C:H6	1.78	0.48
79:L5:4456:OMC:O2	79:L5:4524:G:N2	2.39	0.48
79:L5:4750:G:H2'	79:L5:4751:G:C8	2.48	0.48
2:SA:198:MET:HG2	2:SA:200:ASP:H	1.79	0.48
6:L7:79:U:O2'	79:L5:1795:A:N3	2.46	0.48
14:SI:56:ARG:HA	14:SI:180:GLY:HA2	1.95	0.48
19:SX:124:LYS:HA	19:SX:129:SER:HA	1.96	0.48
42:LO:54:TYR:OH	42:LO:73:PHE:O	2.31	0.48
46:La:85:GLN:HA	46:La:88:VAL:HG22	1.96	0.48
53:LT:36[A]:LYS:HE2	53:LT:67:VAL:HG23	1.96	0.48
61:Lb:91:ARG:HB2	61:Lb:94:ASP:HB2	1.95	0.48
78:S2:520:A:O2'	78:S2:825:A:N3	2.37	0.48
78:S2:1036:A:H4'	78:S2:1855:G:N2	2.28	0.48
79:L5:3715:PSU:OP1	80:Et:4:C:O2'	2.28	0.48
5:L8:13:G:O2'	54:LP:121:LYS:O	2.28	0.48
8:SJ:174:LYS:HB2	78:S2:560:A:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SE:124:CYS:HB3	9:SE:141:THR:HB	1.95	0.48
10:SC:207:ALA:HB2	78:S2:4:C:H4'	1.95	0.48
21:SS:98:VAL:HG11	21:SS:106:LYS:HG2	1.95	0.48
47:LN:65:ARG:HG3	47:LN:127:TYR:HB3	1.95	0.48
48:LI:35:ASP:HB3	48:LI:39:LYS:HG2	1.95	0.48
57:LY:31:SER:HA	57:LY:48:PRO:HA	1.95	0.48
67:Lg:62:LYS:NZ	79:L5:2516:G:O2'	2.46	0.48
79:L5:1558:A:H2'	79:L5:1559:G:C8	2.48	0.48
79:L5:1604:G:H2'	79:L5:1605:G:C8	2.48	0.48
79:L5:2411:C:H2'	79:L5:2412:A:C8	2.49	0.48
79:L5:4734:A:H2'	79:L5:4735:G:H8	1.78	0.48
14:SI:142:SER:OG	14:SI:143:LYS:N	2.45	0.48
36:Sg:207:CYS:HB2	36:Sg:221:LEU:HD21	1.96	0.48
48:LI:129:VAL:HG23	48:LI:133:GLN:HG2	1.96	0.48
70:Lk:35:LYS:NZ	79:L5:2695:A:OP1	2.38	0.48
78:S2:1203:G:H2'	78:S2:1204:A:C8	2.49	0.48
79:L5:3759:A:N6	79:L5:3764:PSU:O4	2.42	0.48
5:L8:148:A:H2'	5:L8:149:G:C8	2.49	0.47
46:La:2:PRO:HD2	79:L5:1509:C:H5''	1.96	0.47
59:Lr:108:MET:HG3	79:L5:2263:A:H5''	1.95	0.47
63:Lc:28:VAL:HB	63:Lc:33:GLN:HB3	1.95	0.47
66:Lf:20:ASN:ND2	79:L5:1885:G:OP1	2.40	0.47
78:S2:1850:MA6:H8	78:S2:1850:MA6:O5'	2.13	0.47
79:L5:1077:C:OP1	79:L5:1215:C:O2'	2.32	0.47
79:L5:1630:A:H5''	79:L5:1631:A:N7	2.30	0.47
79:L5:4733:C:H4'	79:L5:4734:A:H5'	1.96	0.47
79:L5:4743:G:H2'	79:L5:4744:A:C8	2.49	0.47
5:L8:87:G:N1	57:LY:114:ASP:OD2	2.36	0.47
6:L7:13:A:O2'	49:LD:24:ARG:NH2	2.46	0.47
32:Sb:20:LYS:NZ	78:S2:1015:U:OP2	2.47	0.47
36:Sg:248:LEU:HD23	36:Sg:259:TRP:HE3	1.80	0.47
37:LC:263:LEU:HG	37:LC:273:LEU:HD12	1.96	0.47
41:LG:165:GLU:HG2	47:LN:11:TRP:HE1	1.79	0.47
50:LQ:162:HIS:ND1	79:L5:1497:A:OP2	2.38	0.47
58:LZ:50:PRO:HD3	58:LZ:68:ILE:HG12	1.94	0.47
78:S2:191:A:H62	78:S2:208:G:N2	2.07	0.47
78:S2:1036:A:N3	78:S2:1844:U:O2'	2.45	0.47
78:S2:1845:A:H2'	78:S2:1846:G:C8	2.48	0.47
79:L5:433:A:C2	79:L5:3867:A2M:H4'	2.48	0.47
79:L5:3878:C:OP1	79:L5:4400:G:O2'	2.32	0.47
79:L5:4448:G:H5''	79:L5:4449:A:H5''	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:4459:U:H2'	79:L5:4460:U:C6	2.49	0.47
82:SG:176:ILE:HG22	82:SG:179:LEU:HB2	1.96	0.47
23:SN:4:MET:HE3	78:S2:924:G:H5'	1.95	0.47
30:SZ:85:ARG:NH2	78:S2:1597:C:OP2	2.46	0.47
43:LL:79:GLU:HG2	43:LL:110:LEU:HD11	1.96	0.47
51:LR:82:LYS:HE3	79:L5:2863:G:H1'	1.95	0.47
79:L5:162:A:H2'	79:L5:163:A:H8	1.79	0.47
79:L5:1893:C:H1'	79:L5:1937:C:O2	2.14	0.47
79:L5:2486:G:H2'	79:L5:2487:G:C8	2.50	0.47
79:L5:3656:A:H2'	79:L5:3657:U:H6	1.80	0.47
79:L5:3656:A:HO2'	79:L5:3747:A:HO2'	1.60	0.47
5:L8:144:U:H2'	5:L8:145:C:C6	2.50	0.47
36:Sg:107:ASP:HB2	36:Sg:125:ARG:HG3	1.97	0.47
37:LC:242:PRO:HB2	79:L5:2297:G:H4'	1.96	0.47
39:LH:117:PHE:O	39:LH:120:GLU:HG3	2.13	0.47
40:LE:60:SER:HB2	79:L5:1239:C:H5	1.79	0.47
47:LN:125:SER:HB2	79:L5:3937:C:H1'	1.95	0.47
53:LT:144:ASN:HB2	53:LT:146:LYS:HZ2	1.79	0.47
65:Le:124:ASN:OD1	65:Le:124:ASN:N	2.47	0.47
68:Li:28:ARG:NH2	79:L5:326:C:OP2	2.41	0.47
79:L5:478:G:H2'	79:L5:479:G:C8	2.50	0.47
79:L5:658:C:H2'	79:L5:659:G:C8	2.49	0.47
79:L5:4237:C:OP1	79:L5:4327:C:O2'	2.32	0.47
21:SS:89:ASP:OD2	21:SS:106:LYS:NZ	2.48	0.47
39:LH:153:LEU:O	39:LH:157:SER:OG	2.29	0.47
48:LI:158:LYS:NZ	79:L5:4413:C:O2	2.44	0.47
56:LX:77:ILE:HD13	56:LX:100:VAL:HG12	1.96	0.47
62:LF:93:ILE:HD12	62:LF:243:LEU:HD23	1.95	0.47
78:S2:952:G:H2'	78:S2:953:C:C6	2.49	0.47
79:L5:2486:G:H2'	79:L5:2487:G:H8	1.78	0.47
5:L8:58:G:N7	69:Lj:63:ARG:NH2	2.53	0.47
12:SH:83:LEU:HB3	12:SH:92:VAL:HG21	1.96	0.47
39:LH:43:VAL:HG21	39:LH:73:ILE:HD12	1.96	0.47
59:Lr:98:ARG:NH2	79:L5:2262:G:OP2	2.33	0.47
71:Li:37:TYR:O	79:L5:362:A:N6	2.47	0.47
78:S2:1423:C:H3'	78:S2:1424:G:H8	1.79	0.47
3:LB:76:VAL:HB	3:LB:332:MET:HG2	1.97	0.47
3:LB:80:GLU:OE1	3:LB:323:TYR:OH	2.33	0.47
5:L8:106:G:H4'	5:L8:137:A:H5'	1.97	0.47
24:SL:82:MET:HE1	78:S2:372:U:O2'	2.14	0.47
30:SZ:73:VAL:HG13	30:SZ:77:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Sa:98:PRO:O	78:S2:1868:U:N3	2.38	0.47
36:Sg:79:LEU:HD11	36:Sg:87:LEU:HD23	1.96	0.47
39:LH:64:ARG:NH1	79:L5:1949:U:OP1	2.48	0.47
40:LE:151:ILE:HB	40:LE:195:ILE:HB	1.95	0.47
43:LL:36:ARG:HH21	79:L5:1363:C:H3'	1.80	0.47
44:LV:24:ALA:HB3	44:LV:39:ILE:HD12	1.96	0.47
46:La:132:ARG:NH1	79:L5:1396:G:H5''	2.30	0.47
52:LS:96:GLU:HB3	52:LS:142:VAL:HG21	1.97	0.47
57:LY:10:ASP:HB3	57:LY:13:LYS:HB2	1.97	0.47
61:Lb:18:ARG:NH1	79:L5:1686:C:O2'	2.48	0.47
62:LF:91:PHE:HB2	62:LF:145:PRO:HG3	1.97	0.47
78:S2:1113:A:H2'	78:S2:1114:U:C6	2.50	0.47
78:S2:1531:A:H4'	78:S2:1605:G:H4'	1.95	0.47
79:L5:1538:U:H2'	79:L5:1539:G:H8	1.80	0.47
79:L5:3669:G:H21	79:L5:3672:G:N2	2.13	0.47
79:L5:4138:C:H2'	79:L5:4139:G:C8	2.50	0.47
1:LA:245[B]:ARG:HE	1:LA:245[B]:ARG:HB2	1.54	0.47
8:SJ:149:VAL:HG11	8:SJ:157:ILE:HD11	1.97	0.47
21:SS:105:ASN:OD1	21:SS:108:ARG:NH2	2.47	0.47
49:LD:65:ALA:HB2	49:LD:74:ILE:HD13	1.97	0.47
52:LS:62:VAL:HA	62:LF:83:VAL:HG22	1.97	0.47
57:LY:58:VAL:HG23	57:LY:59:ARG:HG2	1.97	0.47
68:Li:67:LYS:NZ	79:L5:3725:G:N7	2.41	0.47
78:S2:1288:OMU:HN3	78:S2:1311:C:H42	1.61	0.47
79:L5:256:G:H2'	79:L5:257:C:C6	2.50	0.47
79:L5:1188:C:H2'	79:L5:1189:G:H8	1.80	0.47
79:L5:2318:G:N2	79:L5:2321:G:OP2	2.41	0.47
79:L5:4924:C:H1'	79:L5:4926:C:N4	2.30	0.47
2:SA:110:ASN:HB3	2:SA:113:GLN:HB3	1.97	0.47
37:LC:321:ASN:OD1	79:L5:1280:C:O2'	2.22	0.47
42:LO:44:SER:OG	79:L5:2054:U:OP2	2.25	0.47
50:LQ:130:SER:O	50:LQ:130:SER:OG	2.25	0.47
65:Le:7:LEU:HB2	65:Le:93:LYS:HB3	1.96	0.47
78:S2:150:A:N6	78:S2:168:C:N3	2.62	0.47
78:S2:531:A:H2'	78:S2:532:C:C6	2.49	0.47
78:S2:891:G:O2'	78:S2:893:U:OP1	2.29	0.47
79:L5:2481:G:H2'	79:L5:2482:C:C6	2.49	0.47
80:Et:36:U:N3	80:Et:38:A:N7	2.62	0.47
2:SA:137:ALA:HB1	2:SA:142:LEU:HB3	1.97	0.47
54:LP:111:SER:HB2	54:LP:154:GLU:HB2	1.96	0.47
57:LY:32:SER:OG	57:LY:101:PRO:O	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LZ:48:ARG:H	58:LZ:69:LYS:HB3	1.80	0.47
62:LF:90:ALA:HB2	62:LF:125:LEU:HD11	1.97	0.47
62:LF:148:LYS:HD3	62:LF:245:ARG:HH21	1.79	0.47
79:L5:2845:A:N6	79:L5:3843:C:H42	2.13	0.47
79:L5:3732:A:H2'	79:L5:3733:A:H8	1.80	0.47
5:L8:8:U:H2'	5:L8:9:A:C8	2.50	0.46
8:SJ:89:GLU:H	8:SJ:89:GLU:CD	2.22	0.46
14:SI:170:LYS:HB2	14:SI:170:LYS:HE3	1.61	0.46
22:Sd:53:ILE:HD12	22:Sd:55:LEU:HD21	1.96	0.46
43:LL:90:VAL:O	43:LL:93:THR:OG1	2.31	0.46
49:LD:119:TYR:OH	49:LD:139:PRO:O	2.25	0.46
55:LU:105:ASN:OD1	55:LU:106:SER:N	2.48	0.46
78:S2:126:G:H5''	82:SG:195:LYS:HG2	1.97	0.46
78:S2:1010:G:H2'	78:S2:1011:A:H8	1.80	0.46
79:L5:3911:C:H2'	79:L5:3912:U:H6	1.80	0.46
18:SO:103:ASN:OD1	18:SO:103:ASN:N	2.44	0.46
29:SY:117:VAL:O	29:SY:122:LYS:NZ	2.48	0.46
31:Sa:33:ASP:OD1	31:Sa:34:LYS:N	2.49	0.46
37:LC:44:LEU:HD13	79:L5:1373:A:H5''	1.96	0.46
43:LL:165:LYS:HD3	43:LL:165:LYS:N	2.31	0.46
49:LD:208:MET:HE2	49:LD:233:PRO:HD3	1.98	0.46
58:LZ:36:ARG:HG2	58:LZ:38:TYR:CZ	2.51	0.46
78:S2:65:C:N3	82:SG:133:LEU:HB3	2.30	0.46
79:L5:3893:C:H2'	79:L5:3894:A:C8	2.50	0.46
3:LB:252:ALA:HB3	79:L5:4457:PSU:H1'	1.96	0.46
21:SS:35:GLY:O	21:SS:97:GLN:NE2	2.49	0.46
23:SN:55:ARG:HD3	78:S2:1017:U:H5'	1.97	0.46
36:Sg:139:LYS:HD3	36:Sg:139:LYS:HA	1.72	0.46
38:LJ:29:SER:OG	38:LJ:66:GLU:OE2	2.29	0.46
52:LS:2:LYS:HG3	79:L5:2062:C:OP1	2.15	0.46
62:LF:63:GLN:NE2	79:L5:1212:G:H5''	2.31	0.46
63:Lc:9:LYS:HD2	63:Lc:13:SER:HB3	1.96	0.46
67:Lg:25:THR:HG22	79:L5:2521:G:H5''	1.96	0.46
67:Lg:97:ILE:HD13	79:L5:4120:U:C4	2.50	0.46
78:S2:532:C:H2'	78:S2:533:A:H8	1.80	0.46
79:L5:2520:C:H2'	79:L5:2521:G:C8	2.50	0.46
79:L5:3785:A2M:HM'1	79:L5:4537:C:H1'	1.96	0.46
79:L5:4699:U:H1'	79:L5:4700:A:H5''	1.97	0.46
9:SE:128:LYS:HB3	9:SE:140:VAL:HB	1.97	0.46
39:LH:103:VAL:HG11	39:LH:144:LEU:HD11	1.97	0.46
78:S2:1037:G:H4'	78:S2:1845:A:H4'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:1662:C:H2'	79:L5:1663:C:C6	2.51	0.46
79:L5:1765:A:O2'	79:L5:1766:A:OP1	2.30	0.46
79:L5:4260:U:H2'	79:L5:4261:C:H6	1.79	0.46
82:SG:56:ASN:HB2	82:SG:108:VAL:HG12	1.96	0.46
3:LB:210:VAL:O	3:LB:349:LYS:NZ	2.48	0.46
15:SQ:140:ARG:HB2	78:S2:1644:C:H4'	1.97	0.46
27:ST:41:LYS:HE3	27:ST:93:SER:HB2	1.98	0.46
78:S2:121:OMU:N3	78:S2:343:A:N1	2.53	0.46
78:S2:484:A2M:H8	78:S2:484:A2M:O5'	2.15	0.46
78:S2:600:G:H2'	78:S2:601:OMG:H8	1.81	0.46
79:L5:257:C:H3'	79:L5:258:G:H8	1.79	0.46
79:L5:1173:G:H2'	79:L5:1174:G:C8	2.50	0.46
79:L5:1541:C:O2	79:L5:2448:G:N2	2.49	0.46
79:L5:3664:G:H2'	79:L5:3665:G:H8	1.80	0.46
79:L5:4188:U:H2'	79:L5:4189:U:C6	2.50	0.46
79:L5:4770:U:H2'	79:L5:4771:C:C6	2.50	0.46
3:LB:7:SER:OG	79:L5:4492:U:OP2	2.32	0.46
3:LB:139:ASP:OD2	3:LB:140:GLU:N	2.49	0.46
4:SB:83:LYS:HB2	4:SB:83:LYS:HE3	1.74	0.46
32:Sb:30:SER:OG	78:S2:1016:U:OP1	2.22	0.46
54:LP:10:ASN:N	54:LP:10:ASN:OD1	2.47	0.46
79:L5:9:C:O2	79:L5:2472:A:N6	2.48	0.46
79:L5:1617:G:H1'	79:L5:2513:A:N6	2.31	0.46
79:L5:4954:G:H2'	79:L5:4955:A:C8	2.51	0.46
80:Et:28:U:H2'	80:Et:29:G:C8	2.51	0.46
1:LA:188:LYS:NZ	79:L5:2739:C:O2	2.41	0.46
2:SA:196:GLU:OE2	2:SA:196:GLU:N	2.30	0.46
47:LN:49:ARG:NH2	79:L5:152:U:OP2	2.30	0.46
58:LZ:79:HIS:ND1	79:L5:2580:U:O2'	2.47	0.46
68:Li:79:THR:HG22	68:Li:82:ARG:H	1.81	0.46
79:L5:1333:A:H2'	79:L5:1334:A:H8	1.80	0.46
79:L5:1598:C:H2'	79:L5:1599:A:H8	1.80	0.46
79:L5:2103:G:H2'	79:L5:2104:G:H8	1.81	0.46
2:SA:134:LEU:HD23	2:SA:134:LEU:HA	1.76	0.46
5:L8:7:U:O2'	79:L5:1305:C:OP1	2.34	0.46
9:SE:148:ARG:NH2	82:SG:202:ASN:OD1	2.49	0.46
38:LJ:56:THR:OG1	38:LJ:64:ARG:N	2.45	0.46
44:LV:19:GLY:O	79:L5:2846:G:O2'	2.27	0.46
78:S2:367:U:H4'	78:S2:371:A:C8	2.51	0.46
78:S2:569:A:H2'	78:S2:570:C:O4'	2.15	0.46
78:S2:900:C:H2'	78:S2:901:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:1232:PSU:H2'	78:S2:1233:G:H8	1.81	0.46
79:L5:381:U:H4'	79:L5:415:G:H5'	1.98	0.46
79:L5:2079:G:H2'	79:L5:2080:U:C6	2.50	0.46
79:L5:4195:G:O2'	79:L5:4442:PSU:OP1	2.29	0.46
79:L5:4739:C:H2'	79:L5:4740:G:H5'	1.97	0.46
29:SY:29:HIS:ND1	29:SY:29:HIS:O	2.49	0.46
36:Sg:70:VAL:HG21	36:Sg:113:PHE:HB2	1.97	0.46
36:Sg:153:CYS:HB2	36:Sg:168:CYS:N	2.28	0.46
42:LO:197:LYS:HG2	42:LO:202:LEU:HB2	1.97	0.46
78:S2:1798:C:H2'	78:S2:1799:G:O4'	2.16	0.46
79:L5:3711:A:H4'	79:L5:3712:A:C8	2.51	0.46
80:Et:58:A:O2'	80:Et:60:A:OP2	2.22	0.46
1:LA:245[B]:ARG:HH12	79:L5:3698:G:P	2.39	0.46
5:L8:9:A:H2'	5:L8:10:G:H8	1.80	0.46
5:L8:141:C:H2'	5:L8:142:U:C6	2.50	0.46
12:SH:10:LYS:HG2	12:SH:11:PRO:HD2	1.98	0.46
24:SL:126:VAL:HG12	24:SL:145:VAL:HG22	1.97	0.46
27:ST:11:GLN:OE1	27:ST:62:ARG:NH1	2.39	0.46
39:LH:76:HIS:O	39:LH:80:MET:HG3	2.16	0.46
49:LD:164:LYS:NZ	49:LD:168:ASP:OD1	2.47	0.46
51:LR:136:ARG:O	51:LR:140:GLU:HG2	2.16	0.46
54:LP:135:ARG:NH2	79:L5:1596:U:O2'	2.39	0.46
66:Lf:68:ARG:NH1	79:L5:442:G:OP1	2.42	0.46
74:Lo:44:LYS:HE3	74:Lo:52:THR:HB	1.98	0.46
78:S2:116:OMU:N3	78:S2:347:G:O6	2.43	0.46
78:S2:649:PSU:H2'	78:S2:650:A:H8	1.81	0.46
79:L5:2434:G:O2'	79:L5:2527:A:N1	2.47	0.46
79:L5:4899:G:H2'	79:L5:4901:G:C8	2.51	0.46
14:SI:56:ARG:NH1	14:SI:180:GLY:O	2.46	0.45
19:SX:63:ASN:ND2	19:SX:114:ASP:OD2	2.39	0.45
23:SN:22:VAL:HG13	23:SN:66:VAL:HG22	1.99	0.45
38:LJ:78:LYS:HE3	38:LJ:82:ILE:HD11	1.98	0.45
39:LH:107:GLU:OE1	39:LH:127:ARG:NH1	2.36	0.45
42:LO:165:LYS:HD2	42:LO:165:LYS:HA	1.77	0.45
78:S2:530:U:H2'	78:S2:531:A:C8	2.51	0.45
79:L5:24:G:N2	79:L5:55:G:O6	2.50	0.45
79:L5:4088:C:H2'	79:L5:4089:G:C8	2.50	0.45
79:L5:4239:A:H2'	79:L5:4240:G:C8	2.51	0.45
79:L5:4620:OMU:HM23	79:L5:4620:OMU:H1'	1.68	0.45
79:L5:4637:OMG:HM23	79:L5:4637:OMG:H1'	1.69	0.45
6:L7:103:A:O2'	79:L5:1741:G:O6	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SW:31:SER:HB3	78:S2:685:A:H5''	1.97	0.45
30:SZ:69:THR:HG22	30:SZ:108:ILE:HA	1.98	0.45
42:LO:82:ARG:HH22	79:L5:3886:G:H5''	1.80	0.45
53:LT:115:LYS:HA	53:LT:115:LYS:HD2	1.64	0.45
54:LP:94:MET:HG2	54:LP:148:MET:HE3	1.97	0.45
79:L5:325:U:H2'	79:L5:326:C:C6	2.51	0.45
79:L5:703:G:H2'	79:L5:704:C:H5''	1.98	0.45
79:L5:1669:A:H4'	79:L5:1685:G:H22	1.81	0.45
79:L5:4991:U:H2'	79:L5:4992:G:H8	1.82	0.45
82:SG:38:ALA:HB2	82:SG:50:VAL:HG22	1.99	0.45
6:L7:30:C:O2'	49:LD:221:LYS:NZ	2.43	0.45
14:SI:139:LYS:HD2	14:SI:141:ARG:HE	1.81	0.45
21:SS:15:VAL:HG13	21:SS:68:ILE:HD11	1.98	0.45
27:ST:42:HIS:CD2	27:ST:43:LYS:HD3	2.51	0.45
31:Sa:66:LYS:HE2	31:Sa:66:LYS:HB3	1.85	0.45
41:LG:131:LYS:HA	41:LG:131:LYS:HD3	1.72	0.45
54:LP:33:ALA:HB1	54:LP:117:ILE:HG12	1.99	0.45
55:LU:22:THR:HB	55:LU:109:SER:HB2	1.98	0.45
57:LY:46:SER:OG	79:L5:239:C:OP1	2.34	0.45
75:Lp:48:LYS:HB2	75:Lp:48:LYS:HE2	1.75	0.45
78:S2:184:G:H2'	78:S2:185:G:C8	2.52	0.45
78:S2:1010:G:H2'	78:S2:1011:A:C8	2.51	0.45
78:S2:1013:U:OP1	78:S2:1129:G:O2'	2.31	0.45
79:L5:197:A:N3	79:L5:222:C:O2'	2.44	0.45
79:L5:1271:G:OP2	79:L5:1271:G:N2	2.36	0.45
79:L5:1437:C:N4	79:L5:2098:G:N3	2.65	0.45
79:L5:2444:U:O4	79:L5:2516:G:N2	2.49	0.45
79:L5:5004:C:H2'	79:L5:5005:G:O4'	2.17	0.45
82:SG:51:ARG:NH1	82:SG:53:SER:OG	2.49	0.45
4:SB:145:LYS:HG3	4:SB:149:GLN:NE2	2.32	0.45
11:SF:79:HIS:O	11:SF:81:ARG:N	2.50	0.45
14:SI:79:ILE:HG13	14:SI:170:LYS:HG2	1.98	0.45
29:SY:10:ARG:HG3	29:SY:11:LYS:HG3	1.97	0.45
29:SY:37:LYS:HD2	29:SY:57:VAL:HG23	1.97	0.45
49:LD:215:ASP:OD1	49:LD:218:ALA:N	2.38	0.45
57:LY:130:LYS:HE2	57:LY:130:LYS:HB2	1.62	0.45
59:Lr:20:ARG:NH2	65:Le:84:GLU:OE1	2.37	0.45
71:Ll:3:SER:O	79:L5:2781:G:O2'	2.34	0.45
74:Lo:23:VAL:HG22	74:Lo:70:LEU:HD23	1.98	0.45
78:S2:455:A:H2'	78:S2:456:C:C6	2.52	0.45
79:L5:462:G:H2'	79:L5:463:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:3720:G:H22	79:L5:3733:A:H2	1.65	0.45
79:L5:4088:C:H2'	79:L5:4089:G:H8	1.82	0.45
82:SG:154:ARG:HH11	82:SG:154:ARG:HB2	1.82	0.45
2:SA:125:THR:HG23	2:SA:175:TRP:HE1	1.81	0.45
9:SE:95:THR:HG22	29:SY:16:ARG:HB2	1.98	0.45
15:SQ:18:THR:HG21	78:S2:1546:G:H5'	1.99	0.45
18:SO:26:ASN:OD1	18:SO:26:ASN:N	2.48	0.45
46:La:27:LYS:HE3	79:L5:1518:A:H5'	1.98	0.45
46:La:42:ARG:NH2	79:L5:4377:G:N7	2.64	0.45
47:LN:14:LYS:HE2	79:L5:280:G:H5''	1.98	0.45
69:Lj:63:ARG:HE	69:Lj:65:ARG:HG3	1.82	0.45
78:S2:1035:A:O2'	78:S2:1856:C:O2	2.30	0.45
79:L5:1274:A:H2'	79:L5:1275:G:C8	2.52	0.45
79:L5:1683:PSU:H2'	79:L5:1684:A:C8	2.51	0.45
79:L5:1733:G:N3	79:L5:4214:A:H2'	2.31	0.45
79:L5:2521:G:H5'	79:L5:2640:G:H1'	1.98	0.45
79:L5:2539:C:H2'	79:L5:2540:C:C6	2.51	0.45
79:L5:4163:U:H5'	79:L5:4164:C:H5''	1.99	0.45
5:L8:21:C:OP1	37:LC:195:LYS:NZ	2.49	0.45
6:L7:55:A:H4'	38:LJ:155:HIS:HB2	1.98	0.45
10:SC:173:LYS:HB3	28:SV:3:ASN:HA	1.98	0.45
42:LO:81:TRP:HB2	42:LO:104:VAL:HG21	1.99	0.45
50:LQ:22:ASP:O	50:LQ:26:ARG:HG2	2.17	0.45
65:Le:11:LYS:HE2	65:Le:11:LYS:HB2	1.78	0.45
76:Pt:24:C:H2'	76:Pt:25:U:C6	2.52	0.45
79:L5:2517:A:N3	79:L5:2539:C:O2'	2.49	0.45
79:L5:3870:C:H2'	79:L5:3871:A:H8	1.82	0.45
79:L5:3938:G:N2	79:L5:4171:C:OP2	2.49	0.45
79:L5:4591:U:H2'	79:L5:4592:C:C6	2.52	0.45
24:SL:49:GLU:H	24:SL:49:GLU:CD	2.23	0.45
48:LI:36:LEU:HG	48:LI:87:ILE:HB	1.99	0.45
79:L5:156:G:N2	79:L5:157:U:O4	2.49	0.45
79:L5:1802:A:H5''	79:L5:1803:G:H5'	1.98	0.45
79:L5:2023:C:H2'	79:L5:2024:G:O4'	2.17	0.45
3:LB:168:MET:HG3	3:LB:178:ALA:HA	1.99	0.45
3:LB:228:TYR:O	79:L5:2835:A:O2'	2.25	0.45
9:SE:44:LEU:HD11	9:SE:70:ILE:HG21	1.98	0.45
14:SI:38:ILE:HD11	14:SI:81:VAL:HG23	1.98	0.45
39:LH:48:LEU:HD11	39:LH:56:ARG:HB2	1.98	0.45
45:LM:113:MET:HG3	79:L5:4881:U:N3	2.31	0.45
78:S2:1409:A:H2'	78:S2:1410:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:258:G:H2'	79:L5:259:C:C6	2.52	0.45
79:L5:732:A:H2'	79:L5:733:A:O4'	2.17	0.45
79:L5:1097:C:H2'	79:L5:1098:G:C8	2.52	0.45
79:L5:1249:C:H2'	79:L5:1250:C:C6	2.52	0.45
79:L5:1274:A:H2'	79:L5:1275:G:H8	1.80	0.45
79:L5:3707:U:H2'	79:L5:3708:C:C6	2.51	0.45
79:L5:3839:G:N2	79:L5:3843:C:O2'	2.50	0.45
79:L5:4619:U:H2'	79:L5:4620:OMU:H6	1.98	0.45
2:SA:30:LEU:HB2	2:SA:47:TYR:CE2	2.52	0.45
5:L8:60:G:OP1	56:LX:70:LYS:NZ	2.50	0.45
6:L7:69:U:H2'	6:L7:70:G:C8	2.52	0.45
14:SI:5:ARG:HB3	78:S2:386:C:H1'	1.99	0.45
24:SL:107:LYS:NZ	78:S2:354:OMU:OP2	2.50	0.45
36:Sg:65:PHE:O	36:Sg:83:TRP:N	2.44	0.45
36:Sg:298:LEU:HB3	36:Sg:310:TRP:HB2	1.99	0.45
38:LJ:167:GLN:HE21	38:LJ:174:ILE:HG12	1.80	0.45
54:LP:6:LEU:HD23	54:LP:6:LEU:HA	1.86	0.45
62:LF:36:LYS:HD2	62:LF:36:LYS:HA	1.70	0.45
78:S2:57:U:OP1	78:S2:504:G:O2'	2.35	0.45
78:S2:1801:A:H2'	78:S2:1802:C:C6	2.52	0.45
79:L5:153:G:H2'	79:L5:154:G:H8	1.82	0.45
79:L5:1346:C:H2'	79:L5:1347:G:H8	1.81	0.45
79:L5:1773:U:H2'	79:L5:1774:C:C6	2.52	0.45
4:SB:82:ARG:NH1	4:SB:189:ILE:O	2.50	0.45
78:S2:982:G:H2'	78:S2:983:A:C8	2.52	0.45
79:L5:394:G:N2	79:L5:397:G:OP2	2.37	0.45
79:L5:2505:C:H42	79:L5:4084:G:H4'	1.82	0.45
79:L5:3707:U:H2'	79:L5:3708:C:H6	1.81	0.45
79:L5:3848:U:H2'	79:L5:3849:A:H8	1.82	0.45
79:L5:4584:A:H2'	79:L5:4585:U:O4'	2.17	0.45
8:SJ:145:PRO:HD2	78:S2:522:A:H5''	1.99	0.44
10:SC:73:MET:HE3	10:SC:73:MET:HB3	1.80	0.44
23:SN:94:LYS:O	23:SN:98:VAL:HG23	2.17	0.44
24:SL:111:VAL:HG11	24:SL:128:VAL:HG11	1.99	0.44
40:LE:149:ILE:O	40:LE:197:THR:OG1	2.27	0.44
53:LT:80:VAL:HG21	79:L5:4305:G:C6	2.52	0.44
62:LF:32:ARG:HH12	79:L5:962:C:H1'	1.81	0.44
65:Le:16:ARG:NH2	65:Le:19:LYS:O	2.46	0.44
71:Ll:48:LYS:HE3	79:L5:2406:G:H4'	1.98	0.44
77:mR:35:G:H1'	78:S2:1207:G:C2	2.51	0.44
78:S2:5:U:H2'	78:S2:6:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:189:U:H2'	78:S2:190:G:O4'	2.17	0.44
78:S2:1410:C:H2'	78:S2:1411:G:H8	1.82	0.44
79:L5:223:G:H4'	79:L5:225:G:N7	2.32	0.44
80:Et:17:C:O2'	80:Et:61:C:OP1	2.34	0.44
4:SB:139:CYS:HA	4:SB:213:ARG:H	1.81	0.44
21:SS:148:VAL:HG22	26:SP:131:PRO:HB2	1.98	0.44
36:Sg:248:LEU:HD23	36:Sg:259:TRP:CE3	2.53	0.44
43:LL:56:ARG:NH1	43:LL:74:ARG:O	2.44	0.44
47:LN:4:TYR:OH	79:L5:151:G:OP2	2.21	0.44
49:LD:116:ASP:OD1	49:LD:116:ASP:N	2.43	0.44
51:LR:99:MET:HE1	51:LR:127:VAL:O	2.17	0.44
52:LS:17:LEU:HD23	52:LS:17:LEU:HA	1.87	0.44
54:LP:8:PRO:HD3	54:LP:149:ILE:HD13	1.98	0.44
59:Lr:63:VAL:HG22	59:Lr:79:ARG:HD2	1.99	0.44
68:Li:53:TYR:OH	68:Li:86:LYS:NZ	2.51	0.44
74:Lo:63:THR:OG1	79:L5:4229:U:OP1	2.28	0.44
78:S2:354:OMU:HM23	78:S2:354:OMU:H1'	1.63	0.44
78:S2:1215:C:O2'	78:S2:1645:C:OP2	2.33	0.44
79:L5:207:G:N3	79:L5:232:G:N2	2.58	0.44
79:L5:4389:C:H2'	79:L5:4390:A:C8	2.52	0.44
4:SB:116:LYS:HG3	78:S2:988:C:H5''	1.98	0.44
18:SO:151:LEU:HD23	18:SO:151:LEU:HA	1.81	0.44
36:Sg:134:THR:O	36:Sg:134:THR:OG1	2.34	0.44
37:LC:350:ARG:HD3	79:L5:724:C:OP1	2.18	0.44
39:LH:71:ARG:NH1	79:L5:4691:A:H5'	2.32	0.44
40:LE:133:PHE:O	40:LE:138:ARG:NH2	2.47	0.44
79:L5:257:C:H2'	79:L5:258:G:O4'	2.17	0.44
79:L5:1754:U:O2'	79:L5:1755:C:O5'	2.34	0.44
79:L5:1867:A:H2'	79:L5:1868:A:C8	2.52	0.44
79:L5:2900:U:H2'	79:L5:2901:G:C8	2.52	0.44
79:L5:4570:G:H2'	79:L5:4571:A2M:H8	1.99	0.44
79:L5:4694:G:OP1	79:L5:4694:G:N2	2.50	0.44
7:SD:219:PRO:HB2	36:Sg:190:GLY:HA2	2.00	0.44
11:SF:159:ARG:NH1	78:S2:1535:U:O4	2.50	0.44
12:SH:24:SER:HA	12:SH:27:LEU:HD12	1.98	0.44
27:ST:39:LEU:HA	27:ST:39:LEU:HD23	1.72	0.44
43:LL:126:LEU:HD12	43:LL:126:LEU:HA	1.85	0.44
46:La:132:ARG:HH12	79:L5:1396:G:H5''	1.82	0.44
57:LY:100:HIS:CD2	79:L5:231:U:H4'	2.52	0.44
68:Li:85:ARG:NH1	68:Li:85:ARG:HB2	2.33	0.44
79:L5:215:C:H5''	79:L5:216:C:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:456:C:H2'	79:L5:457:G:C8	2.53	0.44
79:L5:3861:A:H2'	79:L5:3862:A:C8	2.51	0.44
4:SB:36:PRO:HD2	4:SB:86:LEU:HD13	2.00	0.44
8:SJ:136:ARG:HH11	8:SJ:139:LYS:HA	1.82	0.44
12:SH:11:PRO:HD3	12:SH:46:THR:HG23	1.99	0.44
29:SY:8:ARG:HG2	29:SY:8:ARG:HH11	1.82	0.44
36:Sg:17:TRP:H	36:Sg:36:ARG:HB2	1.81	0.44
36:Sg:256:ILE:HB	36:Sg:270:LEU:HB2	1.99	0.44
48:LI:180:GLU:HG3	48:LI:184:MET:HE2	1.99	0.44
76:Pt:23:G:O6	76:Pt:47:G7M:N2	2.51	0.44
76:Pt:33:OMC:HM22	76:Pt:34:U:H5'	2.00	0.44
78:S2:1201:U:H2'	78:S2:1202:U:C6	2.52	0.44
79:L5:1194:G:OP2	79:L5:1194:G:N2	2.43	0.44
79:L5:1250:C:H2'	79:L5:1251:C:C6	2.52	0.44
79:L5:1846:G:H2'	79:L5:1847:C:C6	2.52	0.44
79:L5:3654:G:O2'	79:L5:3693:U:OP1	2.35	0.44
3:LB:224:LYS:HG2	3:LB:340:THR:HG23	1.99	0.44
6:L7:57:C:H2'	6:L7:58:A:H8	1.83	0.44
8:SJ:6:SER:OG	78:S2:828:G:OP1	2.35	0.44
27:ST:5:THR:HG21	78:S2:1425:G:H21	1.82	0.44
41:LG:242:LEU:HD23	41:LG:242:LEU:HA	1.89	0.44
67:Lg:60:ARG:HD2	67:Lg:60:ARG:HA	1.70	0.44
78:S2:609:PSU:H2'	78:S2:610:G:H8	1.83	0.44
78:S2:980:A:H2'	78:S2:981:A:C8	2.53	0.44
78:S2:1816:G:O2'	79:L5:3807:A:O2'	2.31	0.44
79:L5:177:G:H2'	79:L5:178:C:H5''	1.99	0.44
79:L5:1773:U:H2'	79:L5:1774:C:H6	1.82	0.44
79:L5:1967:A:H2'	79:L5:1968:G:C8	2.53	0.44
79:L5:2103:G:H2'	79:L5:2104:G:C8	2.53	0.44
79:L5:3721:U:H2'	79:L5:3722:G:H8	1.82	0.44
79:L5:4478:G:O2'	79:L5:4602:A:N1	2.45	0.44
13:SW:14:ILE:HG23	13:SW:65:LEU:HD21	1.99	0.44
24:SL:132:ARG:HD2	78:S2:383:G:H4'	2.00	0.44
25:SR:66:VAL:HG23	25:SR:67:ARG:N	2.33	0.44
43:LL:117:LEU:HD23	43:LL:117:LEU:HA	1.85	0.44
49:LD:238:GLU:OE1	49:LD:238:GLU:N	2.51	0.44
62:LF:182:TYR:CZ	62:LF:203:GLU:HG2	2.53	0.44
79:L5:653:U:H2'	79:L5:654:C:C6	2.52	0.44
79:L5:1696:C:H2'	79:L5:1697:G:O4'	2.18	0.44
1:LA:243:THR:N	79:L5:3745:U:O2'	2.47	0.44
3:LB:287:ILE:HD13	3:LB:331:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:146:ARG:HB2	4:SB:149:GLN:HB2	2.00	0.44
6:L7:4:U:H2'	6:L7:5:A:H8	1.83	0.44
6:L7:110:G:H2'	6:L7:111:C:C6	2.53	0.44
9:SE:18:TRP:O	9:SE:51:ARG:NH2	2.51	0.44
18:SO:95:ILE:HD12	18:SO:126:ILE:HG23	2.00	0.44
39:LH:65:LYS:HD3	39:LH:65:LYS:HA	1.75	0.44
42:LO:67:SER:HA	79:L5:4586:G:H4'	2.00	0.44
51:LR:14:VAL:HG11	51:LR:42:ARG:HG2	2.00	0.44
60:Lh:74:LYS:HE2	60:Lh:74:LYS:HB2	1.80	0.44
61:Lb:25:ARG:HA	61:Lb:25:ARG:HD2	1.69	0.44
62:LF:220:MET:HE1	62:LF:223:LYS:HB3	1.99	0.44
78:S2:1432:U:OP1	78:S2:1434:C:N4	2.50	0.44
79:L5:1316:OMG:HM23	79:L5:1316:OMG:H1'	1.79	0.44
79:L5:1327:C:H2'	79:L5:1328:G:C8	2.52	0.44
79:L5:2049:G:O2'	79:L5:3884:PSU:O2'	2.28	0.44
79:L5:2391:G:OP1	79:L5:4653:C:O2'	2.36	0.44
79:L5:2694:G:H5'	79:L5:2695:A:C2	2.52	0.44
1:LA:201:GLY:HA2	1:LA:204:MET:HG3	2.00	0.44
4:SB:120:MET:HB2	4:SB:142:PHE:CE2	2.53	0.44
5:L8:23:C:O2	57:LY:20:ASN:ND2	2.40	0.44
36:Sg:89:LEU:O	36:Sg:98:THR:N	2.51	0.44
37:LC:328:LEU:HD22	62:LF:187:MET:HG3	2.00	0.44
44:LV:45:ILE:HG21	44:LV:53:PRO:HB3	2.00	0.44
52:LS:2:LYS:HD3	62:LF:230:GLY:HA3	2.00	0.44
61:Lb:10:HIS:O	61:Lb:12:GLN:NE2	2.48	0.44
65:Le:106:LYS:HB3	65:Le:106:LYS:HE2	1.84	0.44
66:Lf:15:LYS:HB3	66:Lf:25:THR:HB	1.99	0.44
78:S2:1308:U:H2'	78:S2:1309:C:H6	1.83	0.44
79:L5:496:G:H2'	79:L5:497:G:H8	1.83	0.44
79:L5:1204:C:H2'	79:L5:1205:G:H8	1.82	0.44
79:L5:1734:G:N2	79:L5:1735:U:O4	2.40	0.44
79:L5:1787:A:N3	79:L5:4210:U:O2'	2.49	0.44
79:L5:3736:A:H2'	79:L5:3737:A:H8	1.83	0.44
79:L5:4991:U:H2'	79:L5:4992:G:C8	2.53	0.44
82:SG:58:LYS:H	82:SG:58:LYS:HG2	1.57	0.44
9:SE:174:LYS:HB3	9:SE:174:LYS:HE3	1.70	0.43
15:SQ:73:LYS:HE3	15:SQ:73:LYS:HB3	1.72	0.43
19:SX:98:ASP:OD2	19:SX:140:ARG:NH2	2.51	0.43
25:SR:132:ARG:NH2	78:S2:1100:A:OP1	2.51	0.43
31:Sa:12:LYS:HB2	31:Sa:33:ASP:OD2	2.18	0.43
41:LG:110:LYS:HG3	41:LG:114:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:LY:30:MET:HB3	57:LY:101:PRO:HG3	2.00	0.43
58:LZ:48:ARG:NH2	79:L5:2575:U:OP1	2.46	0.43
78:S2:1408:U:H2'	78:S2:1409:A:C8	2.53	0.43
79:L5:1253:G:N2	79:L5:1256:G:OP2	2.51	0.43
79:L5:1382:G:H2'	79:L5:1383:G:H8	1.83	0.43
79:L5:3848:U:H2'	79:L5:3849:A:C8	2.52	0.43
5:L8:87:G:P	60:Lh:7:ARG:HH22	2.41	0.43
6:L7:12:U:OP2	6:L7:67:C:O2'	2.36	0.43
9:SE:49:ARG:NH1	78:S2:496:C:OP2	2.50	0.43
36:Sg:152:SER:OG	36:Sg:168:CYS:SG	2.73	0.43
59:Lr:47:LYS:O	59:Lr:103:ARG:NH1	2.47	0.43
73:Ln:10:MET:HE1	73:Ln:14:LYS:HG3	2.00	0.43
78:S2:644:OMG:HM23	78:S2:644:OMG:H1'	1.81	0.43
79:L5:2052:G:O2'	79:L5:2057:A:N1	2.44	0.43
79:L5:5001:PSU:H2'	79:L5:5002:U:O4'	2.18	0.43
82:SG:154:ARG:HB2	82:SG:154:ARG:NH1	2.33	0.43
6:L7:3:C:H2'	6:L7:4:U:H6	1.83	0.43
10:SC:74:LYS:HD3	10:SC:74:LYS:HA	1.64	0.43
30:SZ:92:LEU:HD12	30:SZ:109:TYR:CE1	2.53	0.43
44:LV:16:ILE:HD11	44:LV:56:GLY:HA3	2.00	0.43
47:LN:15:GLN:O	47:LN:20:ARG:NH1	2.51	0.43
52:LS:9:GLU:HG3	52:LS:33:PHE:CE2	2.52	0.43
59:Lr:49:VAL:HG11	59:Lr:97:ILE:HD11	2.00	0.43
65:Le:90:MET:HE3	65:Le:90:MET:HB3	1.83	0.43
73:Ln:1:MET:HE3	78:S2:1851:MA6:H5'	1.99	0.43
78:S2:1589:A:N3	78:S2:1653:U:O2'	2.46	0.43
79:L5:1072:C:H2'	79:L5:1073:G:C8	2.53	0.43
79:L5:1278:C:H2'	79:L5:1279:A:O4'	2.18	0.43
79:L5:1741:G:N3	79:L5:1781:PSU:H5''	2.34	0.43
79:L5:5003:U:H2'	79:L5:5004:C:C6	2.53	0.43
80:Et:16:G:N2	80:Et:48:C:H42	2.15	0.43
5:L8:130:C:H2'	5:L8:131:G:H8	1.83	0.43
14:SI:190:LEU:HD22	14:SI:194:GLU:HG2	2.00	0.43
27:ST:71:GLY:HA3	78:S2:1562:C:H5''	2.00	0.43
39:LH:129:ARG:HH21	39:LH:160:LEU:HD21	1.82	0.43
40:LE:183:ARG:HA	40:LE:183:ARG:HD2	1.72	0.43
43:LL:42:LYS:HE3	43:LL:46:ILE:HD13	2.00	0.43
46:La:83:SER:OG	46:La:86:THR:OG1	2.33	0.43
62:LF:148:LYS:O	62:LF:152:GLU:HG2	2.19	0.43
75:Lp:4:ARG:NH1	79:L5:1555:G:O6	2.50	0.43
76:Pt:63:C:H2'	76:Pt:64:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:223:C:H2'	78:S2:224:A:C8	2.53	0.43
78:S2:1408:U:H2'	78:S2:1409:A:H8	1.82	0.43
78:S2:1447:OMG:HM23	78:S2:1447:OMG:H1'	1.81	0.43
79:L5:711:A:H2'	79:L5:712:C:C6	2.53	0.43
79:L5:1762:C:H42	79:L5:1770:A:H61	1.65	0.43
79:L5:2376:A:H2'	79:L5:2377:C:C6	2.54	0.43
79:L5:4578:G:H2'	79:L5:4579:PSU:C6	2.54	0.43
79:L5:5058:A:H2'	79:L5:5059:C:C6	2.52	0.43
7:SD:50:ILE:HD11	7:SD:86:LEU:HD23	2.01	0.43
15:SQ:53:GLU:HG3	15:SQ:85:ARG:HH21	1.83	0.43
40:LE:95:PRO:HG2	79:L5:687:U:C4	2.53	0.43
40:LE:140:LEU:HB2	40:LE:167:GLN:HE22	1.83	0.43
47:LN:171:SER:O	47:LN:171:SER:OG	2.36	0.43
49:LD:59:ASP:OD1	49:LD:60:ILE:N	2.51	0.43
51:LR:76:MET:HE2	51:LR:76:MET:HB3	1.86	0.43
54:LP:115:GLU:OE1	54:LP:151:THR:OG1	2.34	0.43
69:Lj:67:LEU:HD12	69:Lj:67:LEU:HA	1.88	0.43
71:Ll:24:PRO:HD2	71:Ll:27:ILE:HG13	2.01	0.43
78:S2:12:U:H2'	78:S2:13:C:C6	2.53	0.43
78:S2:844:U:H2'	78:S2:845:G:H8	1.82	0.43
78:S2:1139:C:H42	78:S2:1149:A:N6	2.13	0.43
78:S2:1390:U:H2'	78:S2:1391:OMC:C6	2.53	0.43
79:L5:492:U:H2'	79:L5:493:G:C8	2.54	0.43
79:L5:1177:U:H2'	79:L5:1178:G:C8	2.52	0.43
79:L5:1248:C:H2'	79:L5:1249:C:C6	2.53	0.43
79:L5:1662:C:H2'	79:L5:1663:C:H6	1.83	0.43
79:L5:2019:C:H2'	79:L5:2020:U:C6	2.54	0.43
79:L5:3656:A:H2'	79:L5:3657:U:C6	2.53	0.43
79:L5:4093:G:H2'	79:L5:4094:G:H8	1.83	0.43
79:L5:4460:U:H2'	79:L5:4461:C:H6	1.84	0.43
81:LW:50:ASN:OD1	81:LW:50:ASN:N	2.50	0.43
3:LB:241:PRO:HD3	79:L5:4456:OMC:HM21	2.00	0.43
17:SK:53:LYS:HB3	17:SK:53:LYS:HE2	1.59	0.43
18:SO:19:PRO:HG2	18:SO:27:VAL:HG21	2.00	0.43
32:Sb:68:GLY:O	78:S2:928:G:N2	2.47	0.43
39:LH:95:VAL:HG22	72:Lm:82:LEU:HD23	1.99	0.43
49:LD:271:MET:HG2	49:LD:275:GLN:HB2	1.99	0.43
62:LF:34:ARG:HD2	79:L5:1272:C:H5'	2.00	0.43
78:S2:495:U:H2'	78:S2:496:C:O4'	2.19	0.43
78:S2:1134:G:H2'	78:S2:1135:C:C6	2.54	0.43
79:L5:318:A:H2'	79:L5:319:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:1271:G:H21	79:L5:1271:G:P	2.39	0.43
79:L5:2323:C:H2'	79:L5:2324:C:H6	1.84	0.43
79:L5:2864:A:H2'	79:L5:2865:U:C6	2.54	0.43
79:L5:4992:G:H2'	79:L5:4993:G:C8	2.53	0.43
79:L5:5066:U:H2'	79:L5:5067:U:C6	2.54	0.43
80:Et:21:A:O4'	80:Et:48:C:N4	2.52	0.43
82:SG:72:ARG:HD3	82:SG:96:SER:HB3	2.01	0.43
1:LA:37:ARG:NH2	79:L5:4088:C:OP1	2.45	0.43
5:L8:90:C:H2'	5:L8:91:A:C8	2.54	0.43
14:SI:60:LEU:HD13	14:SI:185:ALA:HB2	2.00	0.43
21:SS:46:ARG:HG2	27:ST:35:ASP:HB2	2.00	0.43
25:SR:60:ARG:HB3	25:SR:66:VAL:HG11	2.01	0.43
42:LO:181:ALA:O	42:LO:185:VAL:HG22	2.18	0.43
47:LN:177:GLY:HA2	79:L5:67:C:O3'	2.18	0.43
48:LI:38:ARG:HG2	48:LI:41:ALA:HB2	2.00	0.43
48:LI:48:LEU:HD11	48:LI:167:ILE:HD12	2.00	0.43
53:LT:158:PHE:HD1	53:LT:159:MET:N	2.17	0.43
63:Lc:18:LEU:HD23	63:Lc:18:LEU:HA	1.86	0.43
78:S2:98:C:H2'	78:S2:426:A:H4'	2.00	0.43
78:S2:568:C:H42	78:S2:582:U:H3	1.67	0.43
78:S2:1007:C:H2'	78:S2:1008:A:C8	2.54	0.43
78:S2:1328:OMG:HM23	78:S2:1328:OMG:HI'	1.74	0.43
79:L5:1404:G:H2'	79:L5:1405:C:C6	2.53	0.43
79:L5:2568:C:H2'	79:L5:2569:G:C8	2.52	0.43
79:L5:2900:U:H2'	79:L5:2901:G:H8	1.83	0.43
1:LA:243:THR:HB	79:L5:3748:A:H5''	2.01	0.43
3:LB:47:LEU:HB2	3:LB:84:MET:SD	2.59	0.43
9:SE:127:ARG:HG3	9:SE:142:HIS:HA	2.01	0.43
21:SS:136:THR:OG1	78:S2:1521:C:OP2	2.32	0.43
23:SN:33:VAL:HG21	23:SN:66:VAL:HG11	2.00	0.43
33:Sc:36:ASP:OD2	33:Sc:37:ASP:N	2.52	0.43
37:LC:237:ILE:HD12	37:LC:237:ILE:HA	1.87	0.43
44:LV:123:LYS:HE3	44:LV:123:LYS:HB3	1.87	0.43
48:LI:162:ARG:HH21	48:LI:164:LYS:HE3	1.83	0.43
52:LS:37:HIS:NE2	62:LF:238:ASP:OD2	2.40	0.43
54:LP:83:TRP:O	79:L5:3856:A:H5''	2.18	0.43
61:Lb:95:ARG:HG3	79:L5:1266:G:C8	2.54	0.43
78:S2:51:U:H2'	78:S2:52:G:C8	2.54	0.43
78:S2:106:C:H2'	78:S2:107:A:C8	2.53	0.43
78:S2:1083:A:N7	78:S2:1841:C:O2'	2.44	0.43
79:L5:257:C:H3'	79:L5:258:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:268:G:H2'	79:L5:269:G:H8	1.83	0.43
79:L5:2894:A:H2'	79:L5:2895:A:C8	2.54	0.43
79:L5:4071:U:H2'	79:L5:4072:C:H6	1.84	0.43
79:L5:4538:G:H2'	79:L5:4539:U:C6	2.54	0.43
79:L5:4593:C:H2'	79:L5:4594:U:H6	1.84	0.43
1:LA:30:ARG:NH1	1:LA:36:GLU:OE1	2.52	0.43
3:LB:58:ARG:HA	3:LB:366:LYS:HG3	2.00	0.43
17:SK:45:VAL:O	17:SK:49:MET:HG2	2.18	0.43
25:SR:81:ARG:HD3	25:SR:81:ARG:HA	1.78	0.43
27:ST:39:LEU:HD21	27:ST:52:TRP:CZ3	2.54	0.43
28:SV:59:ILE:HD13	28:SV:62:MET:HE3	2.01	0.43
36:Sg:304:ASP:O	36:Sg:306:LEU:N	2.52	0.43
37:LC:60:HIS:NE2	37:LC:100:ARG:HD3	2.34	0.43
37:LC:230:LEU:HD23	37:LC:230:LEU:HA	1.88	0.43
40:LE:41:LYS:HB2	40:LE:41:LYS:HE2	1.82	0.43
49:LD:108:ARG:NE	49:LD:253:TYR:HB2	2.33	0.43
54:LP:108:ASP:N	54:LP:152:GLU:OE2	2.39	0.43
62:LF:53:LYS:NZ	62:LF:189:ASP:OD2	2.43	0.43
78:S2:118:C:H1'	78:S2:445:A:C5	2.54	0.43
78:S2:494:C:N4	78:S2:509:OMG:HN22	2.15	0.43
78:S2:1142:G:N2	78:S2:1145:A:OP2	2.42	0.43
78:S2:1410:C:H2'	78:S2:1411:G:C8	2.53	0.43
78:S2:1452:A:O2'	78:S2:1475:G:N2	2.52	0.43
78:S2:1545:A:N3	78:S2:1671:G:O2'	2.42	0.43
79:L5:223:G:H4'	79:L5:225:G:C8	2.54	0.43
79:L5:1676:C:H41	79:L5:4378:A:H5''	1.83	0.43
79:L5:2607:C:H2'	79:L5:2608:G:H8	1.84	0.43
79:L5:4578:G:H2'	79:L5:4579:PSU:H6	1.83	0.43
80:Et:53:G:H2'	80:Et:54:A:C8	2.51	0.43
3:LB:29:VAL:HG23	3:LB:346:THR:HG21	2.01	0.43
3:LB:72:VAL:HA	44:LV:92:ASP:HA	2.01	0.43
11:SF:154:LEU:HD22	11:SF:177:LEU:HD23	2.00	0.43
41:LG:165:GLU:OE2	47:LN:22:LEU:HD13	2.19	0.43
41:LG:213:GLY:O	41:LG:217:LYS:HG2	2.19	0.43
43:LL:142:GLU:HG3	43:LL:146:LEU:HD13	2.00	0.43
44:LV:33:GLY:HA3	44:LV:69:LYS:HD2	2.01	0.43
44:LV:51:ARG:NH1	79:L5:4620:OMU:OP1	2.48	0.43
48:LI:53:VAL:HG12	48:LI:134:VAL:HG22	2.00	0.43
51:LR:74:ARG:H	51:LR:74:ARG:HG2	1.66	0.43
57:LY:57:VAL:HA	57:LY:104:VAL:HG12	2.00	0.43
73:Ln:16:LYS:HD2	73:Ln:16:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:186:C:H2'	78:S2:187:G:H8	1.84	0.43
78:S2:1112:U:O2	78:S2:1121:G:O6	2.37	0.43
78:S2:1653:U:H2'	78:S2:1654:G:C8	2.54	0.43
79:L5:456:C:H2'	79:L5:457:G:H8	1.83	0.43
79:L5:3923:A:H2'	79:L5:3924:C:C6	2.54	0.43
79:L5:4069:U:H2'	79:L5:4070:U:H6	1.84	0.43
1:LA:244:GLY:HA3	79:L5:3746:A:H5''	2.00	0.42
2:SA:145:ILE:HG12	2:SA:159:ILE:HB	2.01	0.42
27:ST:22:LEU:HD13	27:ST:28:LEU:HD13	2.00	0.42
37:LC:52:TYR:O	92:LC:616:HOH:O	2.21	0.42
39:LH:43:VAL:O	79:L5:4764:A:O2'	2.34	0.42
40:LE:188:ARG:NH2	79:L5:4941:G:OP2	2.48	0.42
41:LG:176:LYS:HD3	68:Li:43:MET:HE1	2.00	0.42
48:LI:93:PRO:HB2	48:LI:125:THR:HB	2.01	0.42
51:LR:106:LEU:HB3	51:LR:120:TYR:CE1	2.55	0.42
57:LY:69:LYS:H	57:LY:83:GLU:HB2	1.84	0.42
61:Lb:102:PRO:HA	61:Lb:109:ARG:HH12	1.84	0.42
62:LF:232:ASP:OD2	62:LF:236:ARG:NH2	2.52	0.42
67:Lg:33:LEU:HD23	67:Lg:33:LEU:HA	1.94	0.42
92:Lj:205:HOH:O	79:L5:2794:C:OP1	2.21	0.42
78:S2:1643:PSU:H2'	78:S2:1644:C:C6	2.54	0.42
78:S2:1733:U:H2'	78:S2:1734:G:O4'	2.19	0.42
79:L5:132:G:O2'	79:L5:133:C:O4'	2.20	0.42
79:L5:3880:G:H2'	79:L5:3881:G:C8	2.54	0.42
79:L5:4504:C:H2'	79:L5:4505:C:C6	2.53	0.42
79:L5:4536:OMC:HM22	79:L5:4537:C:O4'	2.19	0.42
2:SA:63:ARG:HG3	2:SA:185:MET:HE1	2.01	0.42
6:L7:16:A:H2'	6:L7:17:C:C6	2.54	0.42
14:SI:3:ILE:H	14:SI:3:ILE:HG13	1.66	0.42
15:SQ:138:ARG:HD3	15:SQ:138:ARG:HA	1.76	0.42
27:ST:34:VAL:O	27:ST:52:TRP:NE1	2.40	0.42
37:LC:12:SER:HA	37:LC:155:GLU:HG2	2.02	0.42
40:LE:89:LEU:HD12	40:LE:89:LEU:HA	1.84	0.42
41:LG:120:LYS:HA	41:LG:120:LYS:HD3	1.74	0.42
42:LO:192:TYR:CZ	45:LM:118:MET:HG2	2.53	0.42
44:LV:21:PRO:HA	44:LV:54:ALA:HA	2.01	0.42
47:LN:82:GLY:O	47:LN:87:HIS:HE1	2.02	0.42
54:LP:122:ALA:HB3	54:LP:143:PRO:HG2	2.01	0.42
57:LY:11:ARG:HG3	79:L5:229:G:H5''	2.00	0.42
57:LY:103:LYS:NZ	79:L5:200:U:O4	2.31	0.42
78:S2:534:G:H2'	78:S2:535:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:655:A:H4'	78:S2:656:G:H3'	2.01	0.42
78:S2:659:G:O2'	78:S2:662:G:O2'	2.33	0.42
79:L5:459:C:H2'	79:L5:460:C:H6	1.83	0.42
79:L5:1086:C:H2'	79:L5:1087:A:H8	1.85	0.42
79:L5:2488:C:H2'	79:L5:2489:C:O4'	2.17	0.42
79:L5:2876:OMG:HM22	79:L5:2876:OMG:H1'	1.74	0.42
79:L5:4452:U:O4'	90:L5:5101:ANM:H10	2.19	0.42
18:SO:36:SER:OG	18:SO:37:PHE:N	2.51	0.42
31:Sa:2:THR:OG1	78:S2:1199:A:OP1	2.32	0.42
36:Sg:255:SER:HB3	36:Sg:271:LYS:HD2	2.00	0.42
37:LC:143:ARG:NH2	37:LC:145:GLU:OE2	2.52	0.42
37:LC:204:ARG:NH1	37:LC:205:ARG:O	2.52	0.42
45:LM:63:LYS:HB2	45:LM:63:LYS:HE2	1.72	0.42
47:LN:12:ARG:HD3	79:L5:279:A:C5	2.54	0.42
48:LI:51:HIS:ND1	48:LI:137:SER:HB3	2.34	0.42
49:LD:164:LYS:HD2	49:LD:164:LYS:HA	1.76	0.42
57:LY:33:PRO:HG2	57:LY:105:VAL:HG23	2.01	0.42
76:Pt:31:G:OP1	78:S2:1524:G:O2'	2.37	0.42
79:L5:25:A:N3	79:L5:339:C:O2'	2.44	0.42
79:L5:1260:G:H2'	79:L5:1261:G:C8	2.54	0.42
79:L5:3911:C:H4'	79:L5:4196:OMG:HM23	2.01	0.42
79:L5:4978:G:H2'	79:L5:4979:A:H5''	2.01	0.42
80:Et:27:C:H2'	80:Et:28:U:C6	2.54	0.42
6:L7:6:C:O2'	49:LD:50:ARG:NH2	2.52	0.42
10:SC:171:GLY:HA3	13:SW:97:ARG:HH21	1.82	0.42
15:SQ:16:LYS:HD2	15:SQ:17:LYS:H	1.83	0.42
15:SQ:34:VAL:HB	15:SQ:42:ILE:HD11	2.01	0.42
24:SL:78:THR:HG21	24:SL:89:ARG:HB2	2.01	0.42
27:ST:84:ARG:NH2	78:S2:1531:A:OP1	2.45	0.42
36:Sg:107:ASP:C	36:Sg:124:SER:HG	2.26	0.42
36:Sg:254:PRO:HB3	36:Sg:283:PRO:HB2	2.00	0.42
40:LE:112:MET:CE	79:L5:2261:G:H5''	2.50	0.42
43:LL:37:LYS:HD3	79:L5:1366:G:N7	2.34	0.42
45:LM:113:MET:HG3	79:L5:4881:U:C4	2.54	0.42
47:LN:93:LYS:HD3	79:L5:300:A:H2	1.85	0.42
74:Lo:30:LYS:HE2	74:Lo:30:LYS:HB2	1.92	0.42
78:S2:1511:U:H2'	78:S2:1512:C:C6	2.55	0.42
78:S2:1841:C:H2'	78:S2:1842:4AC:H6	2.00	0.42
79:L5:3627:OMG:HM23	79:L5:3627:OMG:H1'	1.88	0.42
79:L5:5002:U:H2'	79:L5:5003:U:C6	2.55	0.42
80:Et:54:A:N6	80:Et:58:A:N7	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:123:ARG:NH1	79:L5:4083:U:OP1	2.52	0.42
13:SW:32:LYS:HE2	13:SW:32:LYS:HB2	1.78	0.42
30:SZ:50:PHE:HB2	30:SZ:54:THR:HB	2.02	0.42
44:LV:82:ILE:HG22	44:LV:125:CYS:SG	2.60	0.42
49:LD:30:TYR:HA	49:LD:33:ARG:HB3	2.02	0.42
50:LQ:49:LYS:HE3	50:LQ:49:LYS:HB3	1.71	0.42
71:Ll:41:ARG:HD2	71:Ll:41:ARG:HA	1.75	0.42
78:S2:29:G:H2'	78:S2:30:C:C6	2.55	0.42
78:S2:96:C:H2'	78:S2:97:U:C6	2.54	0.42
78:S2:116:OMU:HM23	78:S2:116:OMU:H1'	1.76	0.42
78:S2:553:U:H2'	78:S2:555:A:C8	2.55	0.42
78:S2:1144:A:H2'	78:S2:1145:A:C8	2.55	0.42
78:S2:1458:G:H2'	78:S2:1459:G:C8	2.55	0.42
79:L5:90:G:OP2	79:L5:92:C:N4	2.46	0.42
79:L5:679:C:H2'	79:L5:680:G:H8	1.85	0.42
79:L5:1094:G:H2'	79:L5:1095:A:C8	2.55	0.42
79:L5:1341:U:H2'	79:L5:1342:A:C8	2.54	0.42
79:L5:1494:U:H2'	79:L5:1495:G:C8	2.54	0.42
3:LB:223:THR:O	3:LB:343:ARG:NH2	2.52	0.42
5:L8:60:G:O6	5:L8:96:C:O2'	2.32	0.42
6:L7:23:A:N3	6:L7:118:C:O2'	2.38	0.42
9:SE:213:ALA:HB3	9:SE:244:ILE:HD11	2.01	0.42
11:SF:192:LYS:HA	11:SF:192:LYS:HD2	1.82	0.42
33:Sc:34:PHE:CZ	33:Sc:61:SER:HB2	2.54	0.42
39:LH:50:LYS:O	39:LH:51:LYS:HG3	2.20	0.42
46:La:79:TRP:HB3	46:La:87:ARG:HH11	1.84	0.42
49:LD:82:GLU:OE1	49:LD:108:ARG:NH2	2.50	0.42
49:LD:164:LYS:HG2	49:LD:195:HIS:CE1	2.55	0.42
55:LU:24:ASP:OD2	55:LU:26:THR:OG1	2.37	0.42
69:Lj:43:ARG:HG2	79:L5:21:G:H5'	2.02	0.42
76:Pt:5:G:H2'	76:Pt:6:G:C8	2.55	0.42
78:S2:674:C:H2'	78:S2:675:U:C6	2.54	0.42
79:L5:1204:C:H2'	79:L5:1205:G:C8	2.55	0.42
79:L5:4884:G:H2'	79:L5:4885:U:C6	2.55	0.42
2:SA:81:ASN:OD1	2:SA:81:ASN:N	2.53	0.42
4:SB:92:GLN:HG3	4:SB:97:LEU:HD11	2.02	0.42
9:SE:197:ASN:HB2	9:SE:209:HIS:HB2	2.02	0.42
19:SX:87:ASN:N	78:S2:618:C:OP1	2.51	0.42
42:LO:76:PRO:HB3	42:LO:138:LEU:HG	2.02	0.42
46:La:4:ARG:H	46:La:4:ARG:HG2	1.61	0.42
73:Ln:2:ARG:NE	78:S2:1842:4AC:OP2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:S2:677:G:N1	78:S2:1027:A:OP2	2.32	0.42
78:S2:1293:A:N6	78:S2:1294:G:O6	2.52	0.42
78:S2:1678:A2M:H1'	78:S2:1678:A2M:HM'3	1.77	0.42
79:L5:106:A:H2'	79:L5:107:G:O4'	2.20	0.42
79:L5:381:U:O2	79:L5:385:A:N6	2.52	0.42
79:L5:490:C:H2'	79:L5:491:G:C8	2.55	0.42
79:L5:1475:G:H2'	79:L5:1476:C:C6	2.55	0.42
79:L5:1699:A:N1	79:L5:1705:G:H4'	2.35	0.42
79:L5:1763:C:H2'	79:L5:1764:G:C8	2.53	0.42
79:L5:2693:G:H2'	79:L5:2694:G:N2	2.34	0.42
79:L5:5030:U:H2'	79:L5:5031:G:H8	1.85	0.42
3:LB:19:ARG:HB2	3:LB:234:ARG:NH2	2.35	0.42
4:SB:146:ARG:HD3	4:SB:146:ARG:HA	1.87	0.42
17:SK:52:LEU:HB3	17:SK:58:VAL:HG22	2.02	0.42
18:SO:32:HIS:N	18:SO:43:HIS:O	2.50	0.42
23:SN:55:ARG:HH22	32:Sb:51:GLN:NE2	2.18	0.42
25:SR:82:ASP:OD2	25:SR:83:ASN:N	2.53	0.42
47:LN:46:ASP:OD2	92:LN:421:HOH:O	2.21	0.42
61:Lb:111:ARG:NH2	79:L5:1268:G:N7	2.67	0.42
78:S2:85:A:H2'	78:S2:86:C:H6	1.84	0.42
79:L5:173:C:H2'	79:L5:174:C:C6	2.55	0.42
79:L5:1878:G:H2'	79:L5:1879:C:C6	2.54	0.42
82:SG:147:LEU:HD23	82:SG:153:VAL:HG12	2.01	0.42
3:LB:120:LYS:HZ2	79:L5:4578:G:H5''	1.85	0.42
3:LB:200:ARG:HG2	3:LB:200:ARG:HH11	1.85	0.42
5:L8:28:C:O2'	79:L5:1371:A:N1	2.47	0.42
6:L7:27:G:N7	49:LD:58:ARG:NH1	2.61	0.42
9:SE:51:ARG:HD3	9:SE:51:ARG:HA	1.88	0.42
13:SW:50:PHE:HB3	13:SW:63:VAL:HG13	2.01	0.42
21:SS:14:ARG:HA	21:SS:14:ARG:HD2	1.87	0.42
37:LC:156:ASP:OD2	37:LC:255:SER:OG	2.31	0.42
46:La:13:GLY:HA2	79:L5:1660:U:H3'	2.01	0.42
92:La:345:HOH:O	79:L5:2282:A:OP2	2.22	0.42
54:LP:96:LYS:HE2	54:LP:96:LYS:HB3	1.72	0.42
61:Lb:64:ALA:HB1	61:Lb:68:ARG:CZ	2.50	0.42
62:LF:213:LEU:O	79:L5:2072:C:O2'	2.35	0.42
70:Lk:12:LEU:HB3	70:Lk:16:ARG:HH12	1.85	0.42
78:S2:77:A:H2	82:SG:175:LYS:HG3	1.85	0.42
78:S2:656:G:H5'	78:S2:662:G:N2	2.35	0.42
79:L5:2424:OMG:H1'	79:L5:2424:OMG:HM23	1.82	0.42
3:LB:96:PRO:HD3	42:LO:156:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L7:3:C:H2'	6:L7:4:U:C6	2.55	0.42
6:L7:69:U:H2'	6:L7:70:G:H8	1.85	0.42
15:SQ:126:ARG:HD3	15:SQ:126:ARG:HA	1.81	0.42
17:SK:42:ASN:O	17:SK:46:MET:HG3	2.20	0.42
52:LS:115:ALA:HB2	79:L5:2060:G:N2	2.35	0.42
54:LP:30:ARG:HD2	54:LP:63:TYR:HE1	1.85	0.42
55:LU:31:ASP:OD2	55:LU:114:TYR:OH	2.29	0.42
71:L1:48:LYS:HD2	71:L1:48:LYS:HA	1.74	0.42
78:S2:388:U:H2'	78:S2:389:A:C8	2.53	0.42
78:S2:440:G:OP1	78:S2:1798:C:O2'	2.34	0.42
78:S2:568:C:H2'	78:S2:569:A:H8	1.84	0.42
78:S2:903:A:H2'	78:S2:904:A:C8	2.54	0.42
78:S2:1217:A:H2'	78:S2:1218:C:C6	2.55	0.42
78:S2:1457:U:H2'	78:S2:1458:G:H8	1.84	0.42
78:S2:1458:G:H2'	78:S2:1459:G:H8	1.85	0.42
78:S2:1746:U:H5''	82:SG:33:ALA:HB3	2.02	0.42
79:L5:926:G:H2'	79:L5:927:G:C8	2.53	0.42
79:L5:2264:C:H2'	79:L5:2265:G:O4'	2.20	0.42
79:L5:4069:U:H2'	79:L5:4070:U:C6	2.55	0.42
79:L5:4460:U:H2'	79:L5:4461:C:C6	2.55	0.42
1:LA:20:VAL:HG12	1:LA:23:ARG:HD2	2.01	0.41
1:LA:126:LEU:HD13	1:LA:150:LEU:HD21	2.02	0.41
7:SD:70:THR:HA	7:SD:86:LEU:HD13	2.01	0.41
7:SD:74:GLN:NE2	7:SD:79:PHE:O	2.52	0.41
10:SC:94:ILE:HG21	10:SC:162:ILE:HD12	2.01	0.41
11:SF:40:ALA:HB1	11:SF:45:TYR:CG	2.55	0.41
12:SH:115:LYS:HE2	78:S2:868:G:C2	2.54	0.41
36:Sg:217:MET:HE2	36:Sg:219:TRP:CZ2	2.55	0.41
50:LQ:64:SER:OG	50:LQ:89:ASP:OD2	2.36	0.41
51:LR:128:LYS:NZ	92:LR:322:HOH:O	2.52	0.41
70:Lk:12:LEU:HB3	70:Lk:16:ARG:NH1	2.35	0.41
75:Lp:9:GLY:O	79:L5:1553:A:O2'	2.33	0.41
76:Pt:39:A:O2'	78:S2:1058:A:OP1	2.33	0.41
78:S2:300:U:H2'	78:S2:301:A:C8	2.55	0.41
78:S2:959:G:H1'	78:S2:964:A:N6	2.34	0.41
78:S2:1183:A:H2'	78:S2:1184:G:H8	1.85	0.41
78:S2:1856:C:H2'	78:S2:1857:G:C8	2.55	0.41
79:L5:186:G:H2'	79:L5:187:U:H4'	2.01	0.41
79:L5:446:C:H2'	79:L5:447:C:C6	2.54	0.41
79:L5:3910:C:O2'	79:L5:4196:OMG:N2	2.53	0.41
79:L5:3948:C:O2	79:L5:4065:G:N1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LB:238:LYS:HE2	3:LB:238:LYS:HB2	1.75	0.41
8:SJ:5:ARG:HG3	78:S2:38:A:OP1	2.20	0.41
14:SI:36:THR:HG21	14:SI:60:LEU:HD12	2.02	0.41
23:SN:125:LEU:HD12	23:SN:125:LEU:HA	1.88	0.41
26:SP:130:ARG:HG3	26:SP:130:ARG:HH11	1.85	0.41
37:LC:152:LEU:HD21	37:LC:174:LEU:HB3	2.02	0.41
39:LH:180:TYR:OH	72:Lm:90:ASN:ND2	2.50	0.41
40:LE:57:TYR:HB2	40:LE:62:MET:HG2	2.01	0.41
45:LM:114:LYS:HD3	79:L5:4929:C:H5''	2.02	0.41
68:Li:45:ARG:NH1	68:Li:49:GLY:O	2.41	0.41
78:S2:1786:U:H2'	78:S2:1787:G:H8	1.84	0.41
78:S2:1797:U:H2'	78:S2:1798:C:C6	2.55	0.41
78:S2:1810:U:H2'	78:S2:1811:C:C6	2.55	0.41
79:L5:1399:G:H2'	79:L5:1400:G:C8	2.55	0.41
79:L5:1751:A:H2'	79:L5:1752:G:H8	1.84	0.41
79:L5:1895:G:H2'	79:L5:1896:A:O4'	2.20	0.41
79:L5:2744:A:H2'	79:L5:2745:A:C8	2.55	0.41
79:L5:3925:OMU:H1'	79:L5:3925:OMU:HM23	1.62	0.41
7:SD:58:VAL:HG12	7:SD:66:ILE:HD13	2.03	0.41
38:LJ:174:ILE:HD13	38:LJ:174:ILE:HA	1.87	0.41
41:LG:53:ARG:HE	41:LG:53:ARG:HB3	1.43	0.41
59:Lr:65:LYS:NZ	92:Lr:322:HOH:O	2.51	0.41
76:Pt:10:G:N2	76:Pt:27:G:H1'	2.36	0.41
78:S2:1360:U:O2'	78:S2:1379:A:OP2	2.31	0.41
78:S2:1562:C:H2'	78:S2:1563:G:C8	2.54	0.41
78:S2:1804:OMU:HM23	78:S2:1804:OMU:H1'	1.73	0.41
79:L5:498:C:H2'	79:L5:499:G:C8	2.55	0.41
79:L5:2020:U:H2'	79:L5:2021:G:C8	2.50	0.41
79:L5:2413:U:H2'	79:L5:2414:G:H8	1.85	0.41
79:L5:3868:G:H22	79:L5:3900:G:H1'	1.84	0.41
79:L5:3911:C:H2'	79:L5:3912:U:C6	2.55	0.41
79:L5:4195:G:C8	79:L5:4442:PSU:H5'	2.55	0.41
8:SJ:38:ARG:HA	34:Se:105:ARG:HB2	2.03	0.41
21:SS:84:LEU:HD12	21:SS:95:TYR:HB3	2.02	0.41
36:Sg:207:CYS:O	36:Sg:219:TRP:HD1	2.03	0.41
37:LC:41:HIS:CE1	37:LC:45:ARG:HD3	2.55	0.41
52:LS:2:LYS:HE3	79:L5:2062:C:H5'	2.01	0.41
56:LX:74:TYR:OH	60:Lh:22:ASP:OD1	2.35	0.41
62:LF:60:GLU:O	62:LF:64:MET:HG3	2.21	0.41
78:S2:1706:G:H2'	78:S2:1707:U:H6	1.86	0.41
79:L5:699:C:H2'	79:L5:700:G:C8	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:2029:A:H2'	79:L5:2030:A:C8	2.56	0.41
79:L5:2362:U:H2'	79:L5:2363:A2M:H8	2.02	0.41
79:L5:4071:U:H2'	79:L5:4072:C:C6	2.55	0.41
79:L5:4313:A:H2'	79:L5:4314:C:O4'	2.20	0.41
1:LA:17:ARG:HE	1:LA:17:ARG:HB2	1.61	0.41
13:SW:12:LYS:HD3	13:SW:12:LYS:HA	1.78	0.41
29:SY:120:THR:OG1	78:S2:151:C:OP1	2.31	0.41
37:LC:163:LYS:HE3	37:LC:163:LYS:HB3	1.94	0.41
65:Le:104:SER:OG	65:Le:107:ASN:ND2	2.54	0.41
78:S2:1446:A:O2'	78:S2:1447:OMG:H5''	2.21	0.41
78:S2:1648:G:O2'	78:S2:1674:G:O6	2.35	0.41
78:S2:1809:A:H2'	78:S2:1810:U:C6	2.55	0.41
78:S2:1823:A:H2'	78:S2:1824:A:C8	2.55	0.41
79:L5:434:A:H2'	79:L5:435:A:O4'	2.20	0.41
79:L5:734:G:C2	79:L5:735:G:C8	3.08	0.41
79:L5:1086:C:H2'	79:L5:1087:A:C8	2.55	0.41
79:L5:2503:G:H21	79:L5:4084:G:H5'	1.85	0.41
79:L5:3893:C:H2'	79:L5:3894:A:H8	1.84	0.41
79:L5:4499:OMG:C2	79:L5:4529:G:H1'	2.56	0.41
82:SG:2:LYS:HD3	82:SG:15:LEU:HD21	2.02	0.41
2:SA:77:ILE:HD12	2:SA:122:LEU:HD11	2.03	0.41
3:LB:163:ILE:HG22	3:LB:180:LEU:HD22	2.02	0.41
6:L7:119:U:H2'	49:LD:261:VAL:HG21	2.01	0.41
9:SE:62:LYS:HB3	9:SE:62:LYS:HE2	1.84	0.41
15:SQ:113:ILE:HD13	15:SQ:113:ILE:HA	1.94	0.41
15:SQ:116:ASP:C	15:SQ:118:THR:H	2.29	0.41
41:LG:53:ARG:HD3	79:L5:4161:G:C6	2.56	0.41
42:LO:8:VAL:HG12	42:LO:117:ARG:HG3	2.02	0.41
48:LI:171:TRP:O	48:LI:174:THR:OG1	2.30	0.41
51:LR:7:GLN:HG2	51:LR:32:ILE:HG22	2.03	0.41
58:LZ:5:MET:O	58:LZ:28:ASN:ND2	2.53	0.41
58:LZ:47:ASP:N	58:LZ:69:LYS:O	2.50	0.41
60:Lh:82:ASP:OD1	60:Lh:82:ASP:N	2.40	0.41
78:S2:964:A:H2'	78:S2:965:U:H6	1.86	0.41
78:S2:1374:C:H2'	78:S2:1375:G:O4'	2.20	0.41
79:L5:272:U:H2'	79:L5:273:U:C6	2.56	0.41
79:L5:1661:C:H2'	79:L5:1662:C:H6	1.85	0.41
79:L5:1754:U:H1'	79:L5:1755:C:H5	1.85	0.41
79:L5:1762:C:H2'	79:L5:1763:C:C6	2.56	0.41
79:L5:1916:G:N3	79:L5:2067:C:O2'	2.51	0.41
1:LA:233:ARG:HB2	79:L5:4184:G:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LB:115:LYS:NZ	3:LB:129:ALA:O	2.46	0.41
4:SB:38:MET:H	4:SB:38:MET:HG3	1.65	0.41
5:L8:144:U:H2'	5:L8:145:C:H6	1.85	0.41
6:L7:58:A:H2'	6:L7:59:G:C8	2.56	0.41
6:L7:83:A:H4'	62:LF:224:THR:HB	2.02	0.41
7:SD:160:SER:OG	78:S2:1386:A:OP2	2.32	0.41
15:SQ:112:LEU:HD22	15:SQ:119:LEU:HD13	2.03	0.41
37:LC:83:GLY:O	79:L5:367:C:O2'	2.27	0.41
38:LJ:63:ARG:HE	38:LJ:63:ARG:HB2	1.73	0.41
41:LG:197:LYS:HG2	79:L5:6:C:H5''	2.02	0.41
49:LD:200:MET:HB3	49:LD:237:GLU:HG3	2.02	0.41
53:LT:71:ALA:HB3	79:L5:4313:A:H4'	2.02	0.41
58:LZ:35:ASP:OD2	58:LZ:35:ASP:N	2.54	0.41
58:LZ:60:LYS:HE2	58:LZ:60:LYS:HB3	1.82	0.41
61:Lb:120:ARG:HA	61:Lb:121:PRO:HD3	1.92	0.41
67:Lg:44:SER:OG	67:Lg:46:CYS:SG	2.75	0.41
78:S2:76:U:H5'	78:S2:77:A:OP2	2.21	0.41
78:S2:160:U:O2'	78:S2:162:C:O5'	2.38	0.41
78:S2:443:U:H2'	78:S2:444:G:O4'	2.20	0.41
79:L5:86:U:H2'	79:L5:87:A:C8	2.54	0.41
79:L5:323:C:H2'	79:L5:324:A:H8	1.86	0.41
79:L5:2079:G:H2'	79:L5:2080:U:H6	1.85	0.41
79:L5:2448:G:H2'	79:L5:2449:A:C8	2.55	0.41
8:SJ:18:ARG:NH2	78:S2:4:C:O2'	2.50	0.41
9:SE:22:LYS:HG3	9:SE:23:LEU:HD23	2.03	0.41
26:SP:96:VAL:HG13	26:SP:120:SER:HB2	2.02	0.41
44:LV:106:VAL:HG12	44:LV:112:MET:HG2	2.02	0.41
49:LD:153:THR:HG21	79:L5:4323:A:C6	2.56	0.41
49:LD:193:GLU:OE2	49:LD:196:ARG:NH1	2.53	0.41
53:LT:102:ARG:HD2	53:LT:102:ARG:HA	1.77	0.41
53:LT:124:THR:OG1	53:LT:125:TRP:N	2.54	0.41
68:Li:35:LYS:HB3	68:Li:35:LYS:HE3	1.68	0.41
76:Pt:5:G:H2'	76:Pt:6:G:H8	1.84	0.41
78:S2:656:G:H21	78:S2:663:C:H5''	1.86	0.41
78:S2:1179:G:N2	78:S2:1182:A:OP2	2.37	0.41
79:L5:288:G:H2'	79:L5:289:C:C6	2.55	0.41
79:L5:1967:A:H2'	79:L5:1968:G:H8	1.86	0.41
79:L5:2844:A:O2'	79:L5:4631:G:H4'	2.20	0.41
79:L5:2884:G:H2'	79:L5:2885:A:C8	2.55	0.41
79:L5:3732:A:H2'	79:L5:3733:A:C8	2.56	0.41
79:L5:4239:A:H2'	79:L5:4240:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:4458:C:H2'	79:L5:4459:U:C6	2.55	0.41
1:LA:175:ILE:H	1:LA:175:ILE:HG13	1.66	0.41
3:LB:33:PRO:HA	3:LB:351:LEU:HD23	2.02	0.41
5:L8:89:U:H2'	5:L8:90:C:C6	2.55	0.41
7:SD:161:GLY:HA3	78:S2:1388:A:H61	1.85	0.41
7:SD:218:LEU:HA	7:SD:219:PRO:HD3	1.96	0.41
14:SI:80:ASP:OD2	14:SI:81:VAL:N	2.50	0.41
14:SI:103:LEU:HD23	14:SI:103:LEU:HA	1.94	0.41
19:SX:40:PRO:HA	19:SX:79:LYS:HD2	2.02	0.41
21:SS:120:HIS:NE2	26:SP:123:TYR:OH	2.42	0.41
26:SP:84:ILE:HG12	26:SP:115:TYR:HE1	1.85	0.41
26:SP:134:GLY:O	78:S2:1235:G:O2'	2.37	0.41
37:LC:339:THR:OG1	37:LC:342:ARG:NH2	2.54	0.41
40:LE:121:VAL:HG21	79:L5:702:U:H5'	2.02	0.41
41:LG:147:VAL:HG13	41:LG:179:VAL:HG21	2.03	0.41
44:LV:43:LYS:HG3	44:LV:60:MET:HG2	2.02	0.41
46:La:3:SER:OG	79:L5:2344:U:O4	2.37	0.41
51:LR:145:LEU:HD23	51:LR:145:LEU:HA	1.91	0.41
53:LT:14:MET:HE3	53:LT:14:MET:HB2	1.88	0.41
57:LY:55:VAL:HG12	57:LY:106:ILE:HA	2.03	0.41
57:LY:132:LYS:HE3	79:L5:247:G:H5'	2.01	0.41
78:S2:28:U:H2'	78:S2:29:G:C8	2.56	0.41
78:S2:454:U:H2'	78:S2:455:A:C8	2.55	0.41
78:S2:553:U:H3'	78:S2:555:A:H5''	2.03	0.41
78:S2:563:G:O2'	78:S2:564:A:H8	2.04	0.41
78:S2:863:PSU:H2'	78:S2:864:A:H8	1.85	0.41
78:S2:1292:C:N4	78:S2:1302:G:O6	2.51	0.41
78:S2:1628:C:H2'	78:S2:1629:C:C6	2.56	0.41
78:S2:1633:A:H2'	78:S2:1634:A:C8	2.56	0.41
78:S2:1705:C:H2'	78:S2:1706:G:C8	2.56	0.41
79:L5:459:C:H2'	79:L5:460:C:C6	2.56	0.41
79:L5:1317:U:H2'	79:L5:1318:C:C6	2.55	0.41
79:L5:1661:C:H2'	79:L5:1662:C:C6	2.56	0.41
79:L5:4378:A:O2'	79:L5:4379:A:H2'	2.20	0.41
79:L5:4887:C:H2'	79:L5:4888:U:O4'	2.21	0.41
2:SA:25:LEU:HD23	2:SA:25:LEU:HA	1.86	0.41
5:L8:130:C:H2'	5:L8:131:G:C8	2.55	0.41
6:L7:15:C:H2'	6:L7:16:A:H8	1.86	0.41
14:SI:153:LYS:HB2	14:SI:153:LYS:HE2	1.81	0.41
26:SP:108:LYS:HB2	26:SP:111:MET:HG3	2.02	0.41
36:Sg:122:SER:HB3	36:Sg:132:TRP:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LE:258:LEU:HD23	40:LE:258:LEU:HA	1.89	0.41
51:LR:44:LEU:HD22	51:LR:49:LEU:HD22	2.02	0.41
62:LF:94:ARG:NH1	62:LF:114:LEU:O	2.54	0.41
62:LF:136:VAL:O	62:LF:140:ILE:HG12	2.21	0.41
78:S2:1253:A:OP2	78:S2:1526:G:N2	2.40	0.41
79:L5:1693:U:H2'	79:L5:1694:C:O4'	2.20	0.41
79:L5:2884:G:H2'	79:L5:2885:A:H8	1.85	0.41
79:L5:3934:G:H2'	79:L5:3935:C:C6	2.56	0.41
79:L5:5037:U:H2'	79:L5:5038:A:C8	2.55	0.41
3:LB:194:LEU:HA	3:LB:194:LEU:HD23	1.78	0.40
4:SB:44:ILE:HG23	4:SB:69:VAL:HG11	2.02	0.40
5:L8:39:G:O2'	5:L8:104:A:N1	2.54	0.40
7:SD:145:GLN:O	78:S2:1332:A:O2'	2.36	0.40
10:SC:110:MET:HA	10:SC:111:PRO:HD3	1.89	0.40
32:Sb:15:GLU:HG3	32:Sb:23:ARG:HG2	2.02	0.40
36:Sg:35:SER:OG	36:Sg:36:ARG:N	2.54	0.40
41:LG:136:LEU:HD12	41:LG:136:LEU:HA	1.92	0.40
43:LL:91:ALA:HB1	43:LL:96:ILE:HB	2.03	0.40
43:LL:129:ARG:HD3	79:L5:173:C:OP1	2.21	0.40
43:LL:150:LEU:HD12	43:LL:150:LEU:HA	1.92	0.40
44:LV:90:ARG:NH2	44:LV:96:LEU:HD22	2.36	0.40
49:LD:106:ALA:HB2	49:LD:166:ALA:HA	2.02	0.40
49:LD:211:LEU:HB3	49:LD:219:TYR:HB2	2.04	0.40
56:LX:90:ILE:HG22	56:LX:147:LEU:HD22	2.03	0.40
58:LZ:36:ARG:NH1	79:L5:2580:U:OP1	2.40	0.40
60:Lh:105:LYS:HE3	60:Lh:105:LYS:HB2	1.87	0.40
73:Ln:4:LYS:HB2	78:S2:1842:4AC:OP2	2.20	0.40
78:S2:96:C:O2	78:S2:473:A:O2'	2.35	0.40
78:S2:102:A:H4'	78:S2:104:A:C8	2.56	0.40
78:S2:836:G:H21	78:S2:837:A:H3'	1.85	0.40
78:S2:1712:A:H2'	78:S2:1713:C:C6	2.56	0.40
79:L5:23:C:H2'	79:L5:24:G:O4'	2.21	0.40
79:L5:426:A:H2'	79:L5:427:A:C8	2.56	0.40
79:L5:1346:C:H2'	79:L5:1347:G:C8	2.56	0.40
79:L5:3619:G:H22	79:L5:3624:A:H1'	1.85	0.40
79:L5:4178:A:H2'	79:L5:4179:G:C8	2.56	0.40
3:LB:189:THR:OG1	3:LB:192:GLU:HG3	2.21	0.40
9:SE:89:VAL:HG13	9:SE:114:ILE:HD11	2.03	0.40
12:SH:41:ARG:HE	12:SH:41:ARG:HB3	1.62	0.40
14:SI:160:SER:HA	14:SI:163:GLU:HB2	2.03	0.40
15:SQ:139:ALA:HB2	78:S2:1650:A:H5''	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:SS:38:ARG:HB3	27:ST:45:LEU:HD21	2.03	0.40
36:Sg:29:ASP:N	36:Sg:29:ASP:OD2	2.54	0.40
39:LH:52:LYS:HD3	39:LH:52:LYS:HA	1.86	0.40
40:LE:242:ILE:H	40:LE:242:ILE:HG12	1.72	0.40
44:LV:13:LYS:NZ	44:LV:59:ASP:OD2	2.54	0.40
45:LM:104:MET:HE3	45:LM:109:ARG:HG2	2.02	0.40
51:LR:98:ARG:NH1	51:LR:132:PHE:O	2.54	0.40
52:LS:94:TYR:OH	52:LS:96:GLU:OE2	2.34	0.40
54:LP:61:ARG:NH2	54:LP:76:TRP:HB3	2.36	0.40
92:LX:205:HOH:O	79:L5:2782:U:O4	2.21	0.40
62:LF:57:TYR:HD2	62:LF:188:GLU:HB3	1.86	0.40
78:S2:454:U:H2'	78:S2:455:A:H8	1.86	0.40
78:S2:929:G:N2	78:S2:1104:G:H4'	2.36	0.40
78:S2:962:A:N1	78:S2:1055:A:O2'	2.53	0.40
78:S2:1856:C:H2'	78:S2:1857:G:H8	1.86	0.40
79:L5:365:U:H2'	79:L5:366:A:H8	1.85	0.40
79:L5:1416:G:H2'	79:L5:1417:C:C6	2.57	0.40
79:L5:2484:A:H2'	79:L5:2485:U:C6	2.56	0.40
79:L5:3663:A:N6	79:L5:4168:G:HO2'	2.18	0.40
79:L5:4238:G:H2'	79:L5:4239:A:C8	2.57	0.40
79:L5:4454:G:O2'	79:L5:4500:PSU:O2'	2.29	0.40
3:LB:354:GLN:HB3	3:LB:359:ALA:HB1	2.02	0.40
4:SB:9:LEU:H	4:SB:9:LEU:HD12	1.87	0.40
4:SB:140:VAL:HG12	4:SB:213:ARG:HB2	2.03	0.40
14:SI:104:ILE:HD13	14:SI:173:ALA:HB2	2.04	0.40
21:SS:101:ASN:O	21:SS:105:ASN:ND2	2.54	0.40
26:SP:133:ILE:HD13	26:SP:133:ILE:HA	1.87	0.40
29:SY:8:ARG:HG2	29:SY:8:ARG:NH1	2.36	0.40
37:LC:97:ARG:HG3	79:L5:354:U:H1'	2.03	0.40
37:LC:201:ARG:HE	37:LC:201:ARG:HB3	1.69	0.40
37:LC:275:SER:N	79:L5:1376:C:OP1	2.42	0.40
63:Lc:90:ARG:NH1	92:Lc:302:HOH:O	2.52	0.40
78:S2:635:G:H2'	78:S2:636:C:C6	2.57	0.40
78:S2:1405:A:H2'	78:S2:1406:G:O4'	2.21	0.40
78:S2:1845:A:H2'	78:S2:1846:G:H8	1.85	0.40
79:L5:318:A:H2'	79:L5:319:A:C8	2.56	0.40
79:L5:1405:C:H2'	79:L5:1406:G:C8	2.56	0.40
79:L5:1701:A:H5'	79:L5:2096:G:N2	2.36	0.40
79:L5:2508:PSU:H2'	79:L5:2509:C:C6	2.56	0.40
79:L5:3907:G:H1'	79:L5:3908[A]:A:N7	2.37	0.40
79:L5:4068:U:H2'	79:L5:4069:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:L5:4749:C:H2'	79:L5:4750:G:O4'	2.22	0.40
1:LA:199:VAL:HG21	79:L5:1631:A:N7	2.36	0.40
2:SA:34:MET:HE3	2:SA:34:MET:HB3	1.84	0.40
3:LB:245:HIC:HB2	79:L5:4525:C:H5''	2.04	0.40
18:SO:59:GLY:HA2	18:SO:68:GLU:HG2	2.03	0.40
21:SS:127:TRP:HE3	21:SS:129:LEU:HD12	1.86	0.40
23:SN:124:ARG:HD2	78:S2:677:G:OP1	2.21	0.40
24:SL:82:MET:HG3	24:SL:85:THR:O	2.22	0.40
24:SL:104:LYS:HB3	24:SL:104:LYS:HE3	1.93	0.40
36:Sg:227:LEU:HB3	36:Sg:228:TYR:CD1	2.56	0.40
39:LH:20:LEU:HD23	39:LH:20:LEU:HA	1.94	0.40
40:LE:162:VAL:HG11	40:LE:184:VAL:HG11	2.04	0.40
42:LO:78:ARG:HA	42:LO:78:ARG:HD2	1.95	0.40
70:Lk:17:ARG:HB3	70:Lk:19:ASP:OD2	2.22	0.40
76:Pt:19:G:N1	76:Pt:56:PSU:O4	2.46	0.40
78:S2:300:U:H2'	78:S2:301:A:H8	1.87	0.40
78:S2:312:G:OP2	82:SG:195:LYS:NZ	2.54	0.40
78:S2:509:OMG:HM23	78:S2:509:OMG:H1'	1.85	0.40
78:S2:639:C:H2'	78:S2:640:A:C8	2.57	0.40
78:S2:1291:A:OP2	78:S2:1302:G:O2'	2.37	0.40
79:L5:3870:C:H2'	79:L5:3871:A:C8	2.57	0.40
5:L8:75:OMG:HM23	5:L8:75:OMG:H1'	1.84	0.40
5:L8:115:G:H2'	5:L8:116:C:H6	1.85	0.40
5:L8:115:G:H2'	5:L8:116:C:C6	2.57	0.40
8:SJ:134:HIS:ND1	8:SJ:163:SER:HB2	2.36	0.40
11:SF:119:SER:OG	11:SF:189:ALA:HB1	2.21	0.40
13:SW:76:SER:OG	78:S2:1159:G:OP1	2.37	0.40
15:SQ:117:ARG:HD3	15:SQ:117:ARG:O	2.21	0.40
41:LG:165:GLU:HG2	47:LN:11:TRP:NE1	2.35	0.40
41:LG:193:LEU:HD12	41:LG:193:LEU:HA	1.89	0.40
78:S2:531:A:H2'	78:S2:532:C:H6	1.86	0.40
78:S2:1220:A:H2'	78:S2:1221:G:O4'	2.21	0.40
79:L5:1431:C:H2'	79:L5:1432:G:O4'	2.21	0.40
79:L5:2508:PSU:H2'	79:L5:2509:C:H6	1.86	0.40
79:L5:3711:A:N6	79:L5:3736:A:OP1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	LA	248/257 (96%)	238 (96%)	10 (4%)	0	100	100
2	SA	215/294 (73%)	211 (98%)	4 (2%)	0	100	100
3	LB	391/403 (97%)	383 (98%)	8 (2%)	0	100	100
4	SB	217/264 (82%)	212 (98%)	5 (2%)	0	100	100
7	SD	222/243 (91%)	211 (95%)	11 (5%)	0	100	100
8	SJ	177/194 (91%)	170 (96%)	7 (4%)	0	100	100
9	SE	256/263 (97%)	253 (99%)	3 (1%)	0	100	100
10	SC	219/293 (75%)	211 (96%)	8 (4%)	0	100	100
11	SF	178/204 (87%)	174 (98%)	3 (2%)	1 (1%)	21	53
12	SH	179/194 (92%)	171 (96%)	8 (4%)	0	100	100
13	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	SI	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
15	SQ	138/146 (94%)	134 (97%)	4 (3%)	0	100	100
16	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
17	SK	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
18	SO	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
19	SX	137/143 (96%)	131 (96%)	6 (4%)	0	100	100
20	SM	38/132 (29%)	37 (97%)	1 (3%)	0	100	100
21	SS	146/152 (96%)	141 (97%)	5 (3%)	0	100	100
22	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
23	SN	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
24	SL	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
25	SR	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
26	SP	126/145 (87%)	120 (95%)	6 (5%)	0	100	100
27	ST	141/145 (97%)	135 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	SV	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
29	SY	120/133 (90%)	119 (99%)	1 (1%)	0	100	100
30	SZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
31	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
32	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
33	Sc	56/69 (81%)	54 (96%)	2 (4%)	0	100	100
34	Se	44/133 (33%)	42 (96%)	2 (4%)	0	100	100
35	Sf	33/156 (21%)	30 (91%)	3 (9%)	0	100	100
36	Sg	309/317 (98%)	282 (91%)	27 (9%)	0	100	100
37	LC	364/427 (85%)	357 (98%)	7 (2%)	0	100	100
38	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
39	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
40	LE	217/288 (75%)	207 (95%)	10 (5%)	0	100	100
41	LG	230/266 (86%)	223 (97%)	7 (3%)	0	100	100
42	LO	200/203 (98%)	199 (100%)	0	1 (0%)	24	58
43	LL	205/211 (97%)	201 (98%)	4 (2%)	0	100	100
44	LV	128/140 (91%)	126 (98%)	2 (2%)	0	100	100
45	LM	134/215 (62%)	128 (96%)	6 (4%)	0	100	100
46	La	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
47	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
48	LI	199/214 (93%)	196 (98%)	3 (2%)	0	100	100
49	LD	292/297 (98%)	285 (98%)	7 (2%)	0	100	100
50	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
51	LR	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
52	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
53	LT	159/160 (99%)	155 (98%)	4 (2%)	0	100	100
54	LP	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
55	LU	97/128 (76%)	93 (96%)	4 (4%)	0	100	100
56	LX	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
57	LY	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
58	LZ	134/136 (98%)	129 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	Lr	123/136 (90%)	121 (98%)	2 (2%)	0	100	100
60	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
61	Lb	106/159 (67%)	104 (98%)	2 (2%)	0	100	100
62	LF	225/248 (91%)	218 (97%)	6 (3%)	1 (0%)	30	62
63	Lc	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
64	Ld	105/125 (84%)	105 (100%)	0	0	100	100
65	Le	127/135 (94%)	125 (98%)	2 (2%)	0	100	100
66	Lf	107/110 (97%)	107 (100%)	0	0	100	100
67	Lg	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
68	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
69	Lj	85/97 (88%)	85 (100%)	0	0	100	100
70	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
71	Ll	48/51 (94%)	48 (100%)	0	0	100	100
72	Lm	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
73	Ln	23/25 (92%)	23 (100%)	0	0	100	100
74	Lo	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
75	Lp	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
81	LW	60/157 (38%)	60 (100%)	0	0	100	100
82	SG	216/249 (87%)	211 (98%)	5 (2%)	0	100	100
All	All	11012/12759 (86%)	10698 (97%)	311 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	LO	186	GLU
11	SF	80	GLY
62	LF	197	VAL

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	LA	191/198 (96%)	188 (98%)	3 (2%)	55	78
2	SA	175/242 (72%)	171 (98%)	4 (2%)	44	72
3	LB	309/348 (89%)	306 (99%)	3 (1%)	68	83
4	SB	192/231 (83%)	186 (97%)	6 (3%)	35	66
7	SD	160/202 (79%)	157 (98%)	3 (2%)	50	75
8	SJ	155/168 (92%)	154 (99%)	1 (1%)	78	88
9	SE	220/225 (98%)	218 (99%)	2 (1%)	70	85
10	SC	177/225 (79%)	174 (98%)	3 (2%)	53	77
11	SF	152/170 (89%)	151 (99%)	1 (1%)	76	87
12	SH	147/174 (84%)	144 (98%)	3 (2%)	48	75
13	SW	111/113 (98%)	110 (99%)	1 (1%)	70	85
14	SI	168/180 (93%)	168 (100%)	0	100	100
15	SQ	114/121 (94%)	112 (98%)	2 (2%)	51	76
16	SU	7/107 (6%)	6 (86%)	1 (14%)	3	14
17	SK	51/136 (38%)	51 (100%)	0	100	100
18	SO	101/119 (85%)	100 (99%)	1 (1%)	68	83
19	SX	111/114 (97%)	109 (98%)	2 (2%)	51	76
21	SS	120/132 (91%)	117 (98%)	3 (2%)	42	71
22	Sd	48/49 (98%)	45 (94%)	3 (6%)	16	46
23	SN	131/131 (100%)	127 (97%)	4 (3%)	35	66
24	SL	124/142 (87%)	121 (98%)	3 (2%)	43	72
25	SR	109/122 (89%)	105 (96%)	4 (4%)	30	62
26	SP	114/130 (88%)	112 (98%)	2 (2%)	51	76
27	ST	84/115 (73%)	82 (98%)	2 (2%)	43	72
28	SV	66/66 (100%)	65 (98%)	1 (2%)	57	79
29	SY	98/115 (85%)	97 (99%)	1 (1%)	68	83
30	SZ	61/103 (59%)	59 (97%)	2 (3%)	33	65
31	Sa	84/98 (86%)	82 (98%)	2 (2%)	43	72
32	Sb	73/76 (96%)	71 (97%)	2 (3%)	39	70
33	Sc	51/62 (82%)	47 (92%)	4 (8%)	11	37
34	Se	36/104 (35%)	35 (97%)	1 (3%)	38	69
35	Sf	8/140 (6%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Sg	260/275 (94%)	247 (95%)	13 (5%)	22	54
37	LC	305/348 (88%)	299 (98%)	6 (2%)	48	75
38	LJ	141/149 (95%)	136 (96%)	5 (4%)	32	63
39	LH	169/171 (99%)	165 (98%)	4 (2%)	43	72
40	LE	196/252 (78%)	194 (99%)	2 (1%)	68	83
41	LG	195/223 (87%)	186 (95%)	9 (5%)	24	57
42	LO	170/174 (98%)	168 (99%)	2 (1%)	63	82
43	LL	170/177 (96%)	168 (99%)	2 (1%)	63	82
44	LV	100/107 (94%)	98 (98%)	2 (2%)	48	75
45	LM	115/161 (71%)	110 (96%)	5 (4%)	26	58
46	La	116/120 (97%)	115 (99%)	1 (1%)	70	85
47	LN	171/172 (99%)	167 (98%)	4 (2%)	44	72
48	LI	173/181 (96%)	170 (98%)	3 (2%)	53	77
49	LD	247/250 (99%)	239 (97%)	8 (3%)	34	65
50	LQ	164/165 (99%)	161 (98%)	3 (2%)	51	76
51	LR	144/175 (82%)	142 (99%)	2 (1%)	59	80
52	LS	157/157 (100%)	151 (96%)	6 (4%)	29	61
53	LT	141/140 (101%)	136 (96%)	5 (4%)	32	63
54	LP	135/163 (83%)	134 (99%)	1 (1%)	76	87
55	LU	88/115 (76%)	84 (96%)	4 (4%)	24	57
56	LX	106/133 (80%)	104 (98%)	2 (2%)	50	75
57	LY	122/135 (90%)	118 (97%)	4 (3%)	33	65
58	LZ	118/118 (100%)	115 (98%)	3 (2%)	42	71
59	Lr	109/120 (91%)	107 (98%)	2 (2%)	51	76
60	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	85
61	Lb	90/125 (72%)	89 (99%)	1 (1%)	65	82
62	LF	196/215 (91%)	196 (100%)	0	100	100
63	Lc	84/97 (87%)	82 (98%)	2 (2%)	43	72
64	Ld	20/110 (18%)	15 (75%)	5 (25%)	0	3
65	Le	115/121 (95%)	113 (98%)	2 (2%)	53	77
66	Lf	88/89 (99%)	84 (96%)	4 (4%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	Lg	92/100 (92%)	89 (97%)	3 (3%)	33	65
68	Li	83/89 (93%)	82 (99%)	1 (1%)	63	82
69	Lj	74/80 (92%)	72 (97%)	2 (3%)	39	70
70	Lk	64/65 (98%)	62 (97%)	2 (3%)	35	66
71	Ll	46/48 (96%)	44 (96%)	2 (4%)	26	58
72	Lm	48/115 (42%)	47 (98%)	1 (2%)	47	74
73	Ln	24/24 (100%)	24 (100%)	0	100	100
74	Lo	93/93 (100%)	92 (99%)	1 (1%)	65	82
75	Lp	75/75 (100%)	75 (100%)	0	100	100
81	LW	54/126 (43%)	52 (96%)	2 (4%)	30	62
82	SG	167/218 (77%)	161 (96%)	6 (4%)	31	63
All	All	9082/10739 (85%)	8879 (98%)	203 (2%)	45	73

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LA	77	ILE
1	LA	104	VAL
1	LA	243	THR
2	SA	28	THR
2	SA	87	VAL
2	SA	152	SER
2	SA	190	SER
3	LB	41	VAL
3	LB	317	LEU
3	LB	381	THR
4	SB	22	VAL
4	SB	38	MET
4	SB	57	ILE
4	SB	108	ASP
4	SB	154	SER
4	SB	172	MET
7	SD	94	ARG
7	SD	179	GLN
7	SD	217	ILE
8	SJ	15	THR
9	SE	117	GLU
9	SE	220	THR

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Mol	Chain	Res	Type
10	SC	102	LEU
10	SC	221	ASP
10	SC	254	ASP
11	SF	37	ASP
12	SH	8	ILE
12	SH	10	LYS
12	SH	32	MET
13	SW	105	THR
15	SQ	29	ASN
15	SQ	49	TYR
16	SU	111	GLU
18	SO	36	SER
19	SX	105	PHE
19	SX	115	ILE
21	SS	83	PHE
21	SS	99	LEU
21	SS	118	ARG
22	Sd	18	SER
22	Sd	36	LEU
22	Sd	53	ILE
23	SN	123[A]	HIS
23	SN	123[B]	HIS
23	SN	144	SER
23	SN	145	THR
24	SL	7	GLU
24	SL	19	ASN
24	SL	74	SER
25	SR	22	THR
25	SR	80	ARG
25	SR	85	VAL
25	SR	105	MET
26	SP	21	ASP
26	SP	121	ILE
27	ST	4	VAL
27	ST	87	VAL
28	SV	10	ASP
29	SY	24	VAL
30	SZ	50	PHE
30	SZ	51	ASP
31	Sa	76	SER
31	Sa	88	SER
32	Sb	26	GLN

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Mol	Chain	Res	Type
32	Sb	34	ASP
33	Sc	18	LEU
33	Sc	21	THR
33	Sc	40	ARG
33	Sc	50	VAL
34	Se	79	SER
36	Sg	66	VAL
36	Sg	69	VAL
36	Sg	70	VAL
36	Sg	105	THR
36	Sg	107	ASP
36	Sg	113	PHE
36	Sg	135	LEU
36	Sg	142	VAL
36	Sg	173	LEU
36	Sg	199	THR
36	Sg	213	ASP
36	Sg	287	THR
36	Sg	309	VAL
37	LC	94	ASN
37	LC	95	MET
37	LC	107	THR
37	LC	124	ILE
37	LC	198	ASN
37	LC	266	THR
38	LJ	34	THR
38	LJ	39	VAL
38	LJ	58	ARG
38	LJ	74	VAL
38	LJ	174	ILE
39	LH	9	THR
39	LH	46	SER
39	LH	104	VAL
39	LH	188	GLN
40	LE	107	VAL
40	LE	286	LEU
41	LG	33	GLU
41	LG	53	ARG
41	LG	95	LEU
41	LG	111	LYS
41	LG	198	THR
41	LG	201	THR

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Mol	Chain	Res	Type
41	LG	231	ASP
41	LG	253	LEU
41	LG	257	LYS
42	LO	125	LYS
42	LO	179	LYS
43	LL	59	VAL
43	LL	107	THR
44	LV	101	ASN
44	LV	123	LYS
45	LM	28	VAL
45	LM	32	ASP
45	LM	104	MET
45	LM	112	VAL
45	LM	125	ASN
46	La	15	VAL
47	LN	18	VAL
47	LN	60	VAL
47	LN	66	VAL
47	LN	197	THR
48	LI	28	ASP
48	LI	66	GLU
48	LI	123	GLN
49	LD	3	PHE
49	LD	36	LEU
49	LD	75	VAL
49	LD	90	VAL
49	LD	116	ASP
49	LD	129	GLU
49	LD	261	VAL
49	LD	267	ASN
50	LQ	45	GLN
50	LQ	76	GLU
50	LQ	183	SER
51	LR	37	SER
51	LR	122	SER
52	LS	16	CYS
52	LS	48	VAL
52	LS	75	VAL
52	LS	85	ASP
52	LS	129	VAL
52	LS	158	VAL
53	LT	36[A]	LYS

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Mol	Chain	Res	Type
53	LT	36[B]	LYS
53	LT	127	GLN
53	LT	142[A]	ARG
53	LT	142[B]	ARG
54	LP	75	GLN
55	LU	62	THR
55	LU	63	ILE
55	LU	76	VAL
55	LU	109	SER
56	LX	120	ASP
56	LX	147	LEU
57	LY	67	ILE
57	LY	94	THR
57	LY	105	VAL
57	LY	112	ASP
58	LZ	35	ASP
58	LZ	100	VAL
58	LZ	109	LYS
59	Lr	48	THR
59	Lr	124	VAL
60	Lh	104	THR
61	Lb	9	THR
63	Lc	94	LEU
63	Lc	103	ASP
64	Ld	112	THR
64	Ld	118	GLN
64	Ld	119	THR
64	Ld	120	VAL
64	Ld	122	VAL
65	Le	53	ILE
65	Le	81	ASN
66	Lf	7	SER
66	Lf	37	ASP
66	Lf	46	ARG
66	Lf	90	SER
67	Lg	28	ASN
67	Lg	48	VAL
67	Lg	82	MET
68	Li	35	LYS
69	Lj	66[A]	HIS
69	Lj	66[B]	HIS
70	Lk	12	LEU

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Mol	Chain	Res	Type
70	Lk	56	LEU
71	Ll	11	ARG
71	Ll	23	ILE
72	Lm	127	VAL
74	Lo	25	GLN
81	LW	9	SER
81	LW	53	VAL
82	SG	15	LEU
82	SG	127	THR
82	SG	163	ASN
82	SG	181	THR
82	SG	186	GLN
82	SG	217	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	LA	22	HIS
2	SA	9	GLN
2	SA	50	ASN
2	SA	164	ASN
3	LB	121	ASN
3	LB	145	GLN
4	SB	149	GLN
7	SD	57	ASN
7	SD	101	GLN
7	SD	159	HIS
8	SJ	177	ASN
9	SE	50	ASN
9	SE	67	GLN
9	SE	157	ASN
9	SE	224	ASN
10	SC	136	HIS
10	SC	172	ASN
11	SF	79	HIS
11	SF	186	ASN
12	SH	33	ASN
12	SH	44	ASN
12	SH	112	ASN
15	SQ	11	GLN
15	SQ	86	GLN
17	SK	42	ASN

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Mol	Chain	Res	Type
21	SS	19	ASN
21	SS	72	GLN
22	Sd	26	ASN
24	SL	141	ASN
25	SR	74	GLN
28	SV	33	GLN
28	SV	35	ASN
29	SY	89	HIS
32	Sb	26	GLN
33	Sc	29	GLN
34	Se	89	GLN
36	Sg	237	ASN
37	LC	38	ASN
37	LC	299	GLN
37	LC	317	ASN
38	LJ	42	GLN
38	LJ	167	GLN
39	LH	7	ASN
39	LH	102	ASN
39	LH	169	ASN
40	LE	167	GLN
40	LE	284	HIS
41	LG	141	ASN
42	LO	26	GLN
42	LO	46	ASN
42	LO	180	GLN
43	LL	19	GLN
43	LL	149	GLN
45	LM	20	HIS
45	LM	33	GLN
45	LM	34	ASN
45	LM	48	GLN
47	LN	15	GLN
47	LN	87	HIS
47	LN	99	GLN
47	LN	196	ASN
50	LQ	45	GLN
51	LR	40	GLN
52	LS	125	GLN
54	LP	97	ASN
56	LX	107	HIS
57	LY	96	HIS

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Mol	Chain	Res	Type
59	Lr	4	HIS
59	Lr	30	ASN
61	Lb	6	ASN
63	Lc	19	GLN
64	Ld	118	GLN
65	Le	34	ASN
65	Le	107	ASN
65	Le	126	ASN
66	Lf	99	HIS
68	Li	15	HIS
82	SG	177	GLN
82	SG	186	GLN
82	SG	197	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L8	155/156 (99%)	22 (14%)	0
6	L7	119/120 (99%)	7 (5%)	0
76	Pt	76/77 (98%)	8 (10%)	0
77	mR	6/27 (22%)	3 (50%)	0
78	S2	1627/1869 (87%)	264 (16%)	0
79	L5	3504/5069 (69%)	531 (15%)	5 (0%)
80	Et	74/75 (98%)	17 (22%)	0
All	All	5561/7393 (75%)	852 (15%)	5 (0%)

All (852) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L8	16	G
5	L8	23	C
5	L8	34	U
5	L8	35	C
5	L8	51	U
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	80	A
5	L8	86	U
5	L8	87	G
5	L8	94	G

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Mol	Chain	Res	Type
5	L8	103	A
5	L8	105	C
5	L8	109	C
5	L8	110	U
5	L8	114	G
5	L8	123	U
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U
6	L7	33	U
6	L7	53	U
6	L7	54	A
6	L7	64	G
6	L7	100	A
6	L7	110	G
6	L7	120	U
76	Pt	2	G
76	Pt	8	4SU
76	Pt	9	G
76	Pt	16	C
76	Pt	19	G
76	Pt	21	H2U
76	Pt	71	G
76	Pt	77	A
77	mR	35	G
77	mR	36	A
77	mR	37	A
78	S2	3	C
78	S2	17	C
78	S2	33	G
78	S2	41	G
78	S2	42	A
78	S2	46	A
78	S2	56	G
78	S2	59	U
78	S2	62	G
78	S2	64	A
78	S2	65	C
78	S2	67	C
78	S2	68	A
78	S2	74	G

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Mol	Chain	Res	Type
78	S2	75	G
78	S2	76	U
78	S2	79	A
78	S2	80	G
78	S2	92	A
78	S2	99	A2M
78	S2	103	A
78	S2	113	G
78	S2	114	G
78	S2	115	U
78	S2	126	G
78	S2	127	C
78	S2	129	C
78	S2	130	G
78	S2	140	C
78	S2	143	U
78	S2	147	A
78	S2	155	G
78	S2	160	U
78	S2	162	C
78	S2	168	C
78	S2	182	C
78	S2	183	G
78	S2	184	G
78	S2	215	G
78	S2	225	G
78	S2	302	A
78	S2	306	C
78	S2	309	G
78	S2	312	G
78	S2	319	C
78	S2	320	G
78	S2	323	C
78	S2	324	C
78	S2	327	G
78	S2	328	U
78	S2	335	G
78	S2	347	G
78	S2	361	U
78	S2	362	C
78	S2	364	A
78	S2	370	G

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Mol	Chain	Res	Type
78	S2	385	G
78	S2	386	C
78	S2	407	G
78	S2	409	C
78	S2	436	OMG
78	S2	441	C
78	S2	448	A
78	S2	449	A
78	S2	450	C
78	S2	465	A
78	S2	466	G
78	S2	467	G
78	S2	471	G
78	S2	472	C
78	S2	474	G
78	S2	482	G
78	S2	487	U
78	S2	492	C
78	S2	493	A
78	S2	496	C
78	S2	508	A
78	S2	509	OMG
78	S2	512	A2M
78	S2	516	A
78	S2	525	A
78	S2	533	A
78	S2	534	G
78	S2	554	A
78	S2	555	A
78	S2	563	G
78	S2	564	A
78	S2	576	A2M
78	S2	587	A
78	S2	590	A2M
78	S2	591	U
78	S2	594	A
78	S2	604	A
78	S2	606	G
78	S2	608	C
78	S2	614	C
78	S2	617	G
78	S2	620	G

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Mol	Chain	Res	Type
78	S2	628	A
78	S2	643	A
78	S2	644	OMG
78	S2	655	A
78	S2	660	C
78	S2	663	C
78	S2	668	A2M
78	S2	669	A
78	S2	671	A
78	S2	672	A
78	S2	673	G
78	S2	683	OMG
78	S2	688	U
78	S2	809	A
78	S2	821	G
78	S2	822	PSU
78	S2	827	A
78	S2	830	A
78	S2	831	G
78	S2	835	C
78	S2	836	G
78	S2	838	G
78	S2	847	A
78	S2	870	A
78	S2	871	U
78	S2	872	A
78	S2	878	G
78	S2	888	U
78	S2	889	U
78	S2	891	G
78	S2	892	U
78	S2	895	G
78	S2	896	U
78	S2	897	U
78	S2	903	A
78	S2	909	G
78	S2	913	A
78	S2	920	A
78	S2	922	A
78	S2	933	G
78	S2	943	U
78	S2	971	G

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Mol	Chain	Res	Type
78	S2	990	A
78	S2	992	A
78	S2	1002	U
78	S2	1017	U
78	S2	1023	A
78	S2	1027	A
78	S2	1045	U
78	S2	1055	A
78	S2	1061	U
78	S2	1062	A
78	S2	1080	A
78	S2	1083	A
78	S2	1085	C
78	S2	1089	G
78	S2	1107	G
78	S2	1109	C
78	S2	1115	U
78	S2	1121	G
78	S2	1133	A
78	S2	1138	C
78	S2	1153	C
78	S2	1154	U
78	S2	1157	G
78	S2	1172	U
78	S2	1183	A
78	S2	1188	A
78	S2	1195	A
78	S2	1207	G
78	S2	1208	A
78	S2	1215	C
78	S2	1224	G
78	S2	1242	U
78	S2	1243	PSU
78	S2	1251	A
78	S2	1253	A
78	S2	1256	G
78	S2	1257	G
78	S2	1259	A
78	S2	1271	C
78	S2	1274	G
78	S2	1275	G
78	S2	1285	G

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Mol	Chain	Res	Type
78	S2	1287	A
78	S2	1301	A
78	S2	1302	G
78	S2	1303	C
78	S2	1308	U
78	S2	1313	A
78	S2	1315	U
78	S2	1341	C
78	S2	1342	U
78	S2	1348	G
78	S2	1358	U
78	S2	1364	U
78	S2	1371	U
78	S2	1372	U
78	S2	1373	C
78	S2	1375	G
78	S2	1378	A
78	S2	1402	A
78	S2	1406	G
78	S2	1417	C
78	S2	1424	G
78	S2	1433	C
78	S2	1435	C
78	S2	1436	C
78	S2	1438	A
78	S2	1442	U
78	S2	1452	A
78	S2	1454	A
78	S2	1463	U
78	S2	1466	G
78	S2	1487	A
78	S2	1489	A
78	S2	1490	OMG
78	S2	1494	U
78	S2	1495	G
78	S2	1498	A
78	S2	1521	C
78	S2	1531	A
78	S2	1533	A
78	S2	1544	C
78	S2	1553	C
78	S2	1555	U

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Mol	Chain	Res	Type
78	S2	1557	C
78	S2	1560	U
78	S2	1563	G
78	S2	1579	A
78	S2	1580	A
78	S2	1585	U
78	S2	1586	U
78	S2	1587	G
78	S2	1588	A
78	S2	1601	A
78	S2	1606	G
78	S2	1621	U
78	S2	1623	A
78	S2	1639	G7M
78	S2	1648	G
78	S2	1654	G
78	S2	1661	A
78	S2	1664	A
78	S2	1665	G
78	S2	1671	G
78	S2	1680	G
78	S2	1695	A
78	S2	1698	C
78	S2	1699	A
78	S2	1721	U
78	S2	1722	G
78	S2	1744	G
78	S2	1784	G
78	S2	1825	A
78	S2	1826	G
78	S2	1829	G
78	S2	1831	A
78	S2	1835	A
78	S2	1838	U
78	S2	1849	G
78	S2	1851	MA6
78	S2	1861	G
78	S2	1862	G
78	S2	1863	A
78	S2	1865	C
79	L5	2	G
79	L5	21	G

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Mol	Chain	Res	Type
79	L5	25	A
79	L5	39	A
79	L5	42	A
79	L5	48	G
79	L5	59	A
79	L5	64	A
79	L5	65	A
79	L5	66	A
79	L5	73	A
79	L5	74	G
79	L5	75	G
79	L5	85	G
79	L5	91	G
79	L5	108	A
79	L5	109	G
79	L5	110	C
79	L5	119	G
79	L5	120	A
79	L5	132	G
79	L5	133	C
79	L5	134	G
79	L5	136	C
79	L5	140	G
79	L5	141	C
79	L5	143	C
79	L5	159	C
79	L5	178	C
79	L5	181	C
79	L5	184	U
79	L5	186	G
79	L5	187	U
79	L5	189	G
79	L5	200	U
79	L5	209	U
79	L5	210	C
79	L5	234	G
79	L5	253	G
79	L5	257	C
79	L5	259	C
79	L5	262	G
79	L5	266	C
79	L5	278	G

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Mol	Chain	Res	Type
79	L5	280	G
79	L5	297	U
79	L5	306	A
79	L5	315	G
79	L5	316	U
79	L5	328	A
79	L5	340	C
79	L5	387	G
79	L5	398	A2M
79	L5	409	G
79	L5	410	A
79	L5	412	G
79	L5	413	G
79	L5	440	U
79	L5	449	C
79	L5	450	G
79	L5	451	C
79	L5	453	G
79	L5	454	U
79	L5	461	G
79	L5	467	U
79	L5	496	G
79	L5	498	C
79	L5	504	G
79	L5	509	A
79	L5	510	U
79	L5	644	G
79	L5	669	C
79	L5	686	A
79	L5	687	U
79	L5	692	A
79	L5	696	C
79	L5	705	G
79	L5	708	G
79	L5	731	G
79	L5	738	C
79	L5	739	G
79	L5	740	G
79	L5	747	A
79	L5	757	G
79	L5	759	G
79	L5	904	C

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Mol	Chain	Res	Type
79	L5	915	A
79	L5	916	C
79	L5	917	A
79	L5	925	C
79	L5	926	G
79	L5	932	A
79	L5	933	G
79	L5	936	C
79	L5	937	U
79	L5	944	A
79	L5	945	U
79	L5	956	A
79	L5	958	G
79	L5	959	G
79	L5	960	A
79	L5	961	G
79	L5	962	C
79	L5	964	A
79	L5	965	G
79	L5	967	C
79	L5	968	C
79	L5	969	C
79	L5	970	G
79	L5	1070	G
79	L5	1072	C
79	L5	1092	G
79	L5	1094	G
79	L5	1101	C
79	L5	1168	G
79	L5	1171	G
79	L5	1182	C
79	L5	1183	C
79	L5	1187	G
79	L5	1199	G
79	L5	1200	G
79	L5	1211	G
79	L5	1215	C
79	L5	1216	C
79	L5	1241	C
79	L5	1253	G
79	L5	1254	A
79	L5	1257	A

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Mol	Chain	Res	Type
79	L5	1262	G
79	L5	1266	G
79	L5	1270	A
79	L5	1272	C
79	L5	1273	G
79	L5	1284	G
79	L5	1287	G
79	L5	1293	G
79	L5	1302	U
79	L5	1303	A
79	L5	1326	A2M
79	L5	1354	A
79	L5	1359	G
79	L5	1366	G
79	L5	1379	C
79	L5	1381	U
79	L5	1387	A
79	L5	1397	A
79	L5	1398	A
79	L5	1403	G
79	L5	1408	G
79	L5	1410	U
79	L5	1411	C
79	L5	1417	C
79	L5	1420	A
79	L5	1435	G
79	L5	1439	C
79	L5	1442	C
79	L5	1443	A
79	L5	1444	G
79	L5	1446	C
79	L5	1457	G
79	L5	1484	G
79	L5	1498	G
79	L5	1502	G
79	L5	1516	G
79	L5	1518	A
79	L5	1525	A
79	L5	1534	A2M
79	L5	1547	A
79	L5	1566	C
79	L5	1578	U

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Mol	Chain	Res	Type
79	L5	1591	U
79	L5	1596	U
79	L5	1612	G
79	L5	1614	C
79	L5	1624	G
79	L5	1625	OMG
79	L5	1631	A
79	L5	1633	G
79	L5	1634	A
79	L5	1638	A
79	L5	1640	C
79	L5	1641	G
79	L5	1642	A
79	L5	1654	G
79	L5	1661	C
79	L5	1676	C
79	L5	1677	PSU
79	L5	1680	G
79	L5	1691	G
79	L5	1699	A
79	L5	1701	A
79	L5	1703	C
79	L5	1721	G
79	L5	1741	G
79	L5	1755	C
79	L5	1761	G
79	L5	1766	A
79	L5	1767	A
79	L5	1768	C
79	L5	1785	C
79	L5	1787	A
79	L5	1789	C
79	L5	1792	PSU
79	L5	1804	A
79	L5	1806	G
79	L5	1815	G
79	L5	1821	G
79	L5	1833	G
79	L5	1834	U
79	L5	1836	G
79	L5	1837	A
79	L5	1842	G

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Mol	Chain	Res	Type
79	L5	1855	G
79	L5	1869	G
79	L5	1882	U
79	L5	1892	A
79	L5	1897	A
79	L5	1918	U
79	L5	1919	G
79	L5	1920	C
79	L5	1921	C
79	L5	1922	G
79	L5	1925	G
79	L5	1931	C
79	L5	1932	A
79	L5	1940	G
79	L5	1941	A
79	L5	1945	G
79	L5	1948	G
79	L5	1955	G
79	L5	1960	A
79	L5	1961	G
79	L5	1966	C
79	L5	1967	A
79	L5	1969	G
79	L5	2018	C
79	L5	2019	C
79	L5	2025	A
79	L5	2026	A
79	L5	2044	U
79	L5	2046	G
79	L5	2048	U
79	L5	2055	G
79	L5	2056	G
79	L5	2069	A
79	L5	2071	A
79	L5	2084	C
79	L5	2090	U
79	L5	2092	G
79	L5	2093	A
79	L5	2095	A
79	L5	2096	G
79	L5	2097	U
79	L5	2098	G

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Mol	Chain	Res	Type
79	L5	2099	G
79	L5	2100	A
79	L5	2102	G
79	L5	2105	A
79	L5	2106	G
79	L5	2107	C
79	L5	2289	C
79	L5	2300	A
79	L5	2301	G
79	L5	2306	G
79	L5	2313	A
79	L5	2316	G
79	L5	2331	G
79	L5	2333	G
79	L5	2345	G
79	L5	2348	G
79	L5	2351	OMC
79	L5	2360	A
79	L5	2395	A
79	L5	2397	G
79	L5	2402	G
79	L5	2408	U
79	L5	2417	A
79	L5	2421	G
79	L5	2450	G
79	L5	2469	C
79	L5	2470	C
79	L5	2471	G
79	L5	2474	G
79	L5	2478	C
79	L5	2483	G
79	L5	2488	C
79	L5	2492	C
79	L5	2496	G
79	L5	2503	G
79	L5	2504	C
79	L5	2505	C
79	L5	2506	G
79	L5	2513	A
79	L5	2519	U
79	L5	2520	C
79	L5	2554	U

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Mol	Chain	Res	Type
79	L5	2566	G
79	L5	2567	G
79	L5	2573	A
79	L5	2583	C
79	L5	2586	G
79	L5	2587	A
79	L5	2589	C
79	L5	2601	A
79	L5	2612	G
79	L5	2627	C
79	L5	2653	C
79	L5	2660	A
79	L5	2662	G
79	L5	2669	C
79	L5	2687	U
79	L5	2694	G
79	L5	2695	A
79	L5	2696	A
79	L5	2705	G
79	L5	2708	U
79	L5	2711	G
79	L5	2724	G
79	L5	2735	G
79	L5	2739	C
79	L5	2743	A
79	L5	2754	G
79	L5	2759	G
79	L5	2761	U
79	L5	2764	A
79	L5	2770	C
79	L5	2787	A
79	L5	2788	U
79	L5	2790	U
79	L5	2814	C
79	L5	2815	A2M
79	L5	2826	U
79	L5	2827	G
79	L5	2842	G
79	L5	2855	G
79	L5	2856	C
79	L5	2877	G
79	L5	3597	G

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Mol	Chain	Res	Type
79	L5	3605	C
79	L5	3615	G
79	L5	3616	U
79	L5	3619	G
79	L5	3626	G
79	L5	3635	A
79	L5	3644	U
79	L5	3648	A
79	L5	3662	A
79	L5	3664	G
79	L5	3672	G
79	L5	3673	C
79	L5	3710	G
79	L5	3711	A
79	L5	3712	A
79	L5	3729	PSU
79	L5	3748	A
79	L5	3753	G
79	L5	3754	G
79	L5	3760	A
79	L5	3776	G
79	L5	3777	G
79	L5	3784	A
79	L5	3785	A2M
79	L5	3788	C
79	L5	3811	G
79	L5	3812	C
79	L5	3814	U
79	L5	3817	A
79	L5	3819	G
79	L5	3838	U
79	L5	3839	G
79	L5	3840	U
79	L5	3877	A
79	L5	3878	C
79	L5	3879	G
79	L5	3892	U
79	L5	3897	G
79	L5	3901	A
79	L5	3906	A
79	L5	3907	G
79	L5	3915	U

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Mol	Chain	Res	Type
79	L5	3938	G
79	L5	3946	G
79	L5	4066	U
79	L5	4076	G
79	L5	4096	C
79	L5	4097	G
79	L5	4111	U
79	L5	4119	C
79	L5	4121	G
79	L5	4122	G
79	L5	4127	A
79	L5	4139	G
79	L5	4140	C
79	L5	4141	G
79	L5	4142	C
79	L5	4145	C
79	L5	4158	C
79	L5	4162	C
79	L5	4163	U
79	L5	4164	C
79	L5	4170	A
79	L5	4183	G
79	L5	4184	G
79	L5	4191	G
79	L5	4203	A
79	L5	4212	A
79	L5	4222	G
79	L5	4225	G
79	L5	4228	OMG
79	L5	4229	U
79	L5	4233	A
79	L5	4235	G
79	L5	4251	A
79	L5	4254	G
79	L5	4266	G
79	L5	4268	A
79	L5	4273	A
79	L5	4281	A
79	L5	4282	A
79	L5	4291	G
79	L5	4304	A
79	L5	4305	G

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Mol	Chain	Res	Type
79	L5	4314	C
79	L5	4329	G
79	L5	4330	G
79	L5	4332	C
79	L5	4338	G
79	L5	4354	U
79	L5	4373	G
79	L5	4376	A
79	L5	4377	G
79	L5	4378	A
79	L5	4380	A
79	L5	4387	C
79	L5	4391	G
79	L5	4394	A
79	L5	4415	A
79	L5	4416	G
79	L5	4420	PSU
79	L5	4421	C
79	L5	4422	A
79	L5	4437	U
79	L5	4440	G
79	L5	4448	G
79	L5	4453	C
79	L5	4464	A
79	L5	4465	U
79	L5	4466	C
79	L5	4475	G
79	L5	4500	PSU
79	L5	4510	A
79	L5	4512	U
79	L5	4513	A
79	L5	4515	G
79	L5	4519	C
79	L5	4524	G
79	L5	4529	G
79	L5	4532	PSU
79	L5	4548	A
79	L5	4560	C
79	L5	4567	G
79	L5	4573	G
79	L5	4574	U
79	L5	4575	G

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Mol	Chain	Res	Type
79	L5	4590	A2M
79	L5	4600	G
79	L5	4627	U
79	L5	4636	PSU
79	L5	4637	OMG
79	L5	4652	G
79	L5	4656	A
79	L5	4657	U
79	L5	4670	C
79	L5	4672	A
79	L5	4677	U
79	L5	4700	A
79	L5	4708	A
79	L5	4709	U
79	L5	4720	C
79	L5	4730	C
79	L5	4731	G
79	L5	4732	G
79	L5	4733	C
79	L5	4740	G
79	L5	4741	C
79	L5	4742	G
79	L5	4743	G
79	L5	4745	G
79	L5	4750	G
79	L5	4754	G
79	L5	4757	C
79	L5	4759	C
79	L5	4761	G
79	L5	4765	G
79	L5	4771	C
79	L5	4772	C
79	L5	4860	G
79	L5	4870	G
79	L5	4871	C
79	L5	4875	G
79	L5	4882	U
79	L5	4883	C
79	L5	4889	G
79	L5	4895	C
79	L5	4896	G
79	L5	4900	C

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Mol	Chain	Res	Type
79	L5	4901	G
79	L5	4903	G
79	L5	4910	G
79	L5	4912	G
79	L5	4913	G
79	L5	4914	C
79	L5	4922	C
79	L5	4928	C
79	L5	4934	A
79	L5	4938	A
79	L5	4941	G
79	L5	4943	A
79	L5	4944	C
79	L5	4949	G
79	L5	4975	G
79	L5	4976	U
79	L5	4985	U
79	L5	4990	C
79	L5	4991	U
79	L5	4994	G
79	L5	5017	G
79	L5	5041	G
79	L5	5050	C
79	L5	5062	G
79	L5	5069	U
80	Et	17	C
80	Et	20	A
80	Et	21	A
80	Et	22	G
80	Et	30	G
80	Et	35	A
80	Et	36	U
80	Et	37	A
80	Et	38	A
80	Et	46	G
80	Et	48	C
80	Et	50	A
80	Et	52	G
80	Et	59	A
80	Et	67	U
80	Et	73	A
80	Et	76	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
79	L5	132	G
79	L5	1633	G
79	L5	1754	U
79	L5	1765	A
79	L5	4699	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

225 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
78	A2M	S2	1678	-	22,25,26	3.94	10 (45%)	31,36,39	3.82	14 (45%)
79	PSU	L5	4579	-	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
78	OMG	S2	644	-	23,26,27	0.49	0	33,38,41	0.52	0
78	OMU	S2	428	-	19,22,23	3.05	8 (42%)	26,31,34	1.71	4 (15%)
78	PSU	S2	1232	-	18,21,22	1.11	1 (5%)	22,30,33	1.77	4 (18%)
79	PSU	L5	1782	-	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
79	PSU	L5	4576	-	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
78	PSU	S2	1367	-	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
78	PSU	S2	1239	-	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
78	PSU	S2	36	-	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
78	PSU	S2	573	-	18,21,22	1.11	1 (5%)	22,30,33	1.75	4 (18%)
78	OMU	S2	1288	-	19,22,23	3.02	8 (42%)	26,31,34	1.65	4 (15%)
79	OMG	L5	1625	-	23,26,27	0.54	0	33,38,41	0.54	0
79	A2M	L5	3718	-	22,25,26	3.90	11 (50%)	31,36,39	3.66	14 (45%)
76	4SU	Pt	8	-	18,21,22	3.74	8 (44%)	26,30,33	2.22	4 (15%)
79	OMU	L5	2415	-	19,22,23	3.00	8 (42%)	26,31,34	1.70	4 (15%)
79	A2M	L5	4523	-	22,25,26	3.91	11 (50%)	31,36,39	3.70	15 (48%)
79	A2M	L5	1524	-	22,25,26	3.97	9 (40%)	31,36,39	3.94	14 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
78	OMC	S2	517	-	19,22,23	0.54	0	26,31,34	0.64	0
79	OMU	L5	4620	-	19,22,23	2.94	8 (42%)	26,31,34	1.69	5 (19%)
78	PSU	S2	109	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
78	PSU	S2	649	-	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
79	PSU	L5	3639	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
79	OMU	L5	4498	-	19,22,23	2.99	8 (42%)	26,31,34	1.71	5 (19%)
79	5MC	L5	4447	-	18,22,23	0.73	0	26,32,35	0.67	0
79	OMG	L5	4618	-	23,26,27	0.50	0	33,38,41	0.54	0
79	A2M	L5	1326	-	22,25,26	3.92	10 (45%)	31,36,39	3.69	14 (45%)
79	PSU	L5	3729	-	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
79	PSU	L5	4636	-	18,21,22	1.04	1 (5%)	22,30,33	1.71	5 (22%)
78	PSU	S2	1244	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	A2M	S2	27	-	22,25,26	3.91	10 (45%)	31,36,39	3.68	13 (41%)
79	PSU	L5	3762	-	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
78	OMC	S2	462	-	19,22,23	0.53	0	26,31,34	0.68	0
78	MA6	S2	1851	-	23,26,27	1.46	4 (17%)	34,38,41	3.48	12 (35%)
79	PSU	L5	4972	-	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
78	PSU	S2	1136	-	18,21,22	1.05	1 (5%)	22,30,33	1.83	5 (22%)
79	OMC	L5	3701	-	19,22,23	0.53	0	26,31,34	0.57	0
79	OMU	L5	2837	-	19,22,23	3.01	8 (42%)	26,31,34	1.77	5 (19%)
78	PSU	S2	681	-	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
79	OMG	L5	3944	-	23,26,27	0.49	0	33,38,41	0.55	0
78	OMU	S2	172	-	19,22,23	3.02	8 (42%)	26,31,34	1.76	5 (19%)
79	A2M	L5	2815	-	22,25,26	3.93	10 (45%)	31,36,39	3.78	14 (45%)
79	PSU	L5	4689	-	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
79	A2M	L5	1534	-	22,25,26	3.93	11 (50%)	31,36,39	3.81	15 (48%)
79	PSU	L5	2839	-	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
79	PSU	L5	5001	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
78	PSU	S2	1643	-	18,21,22	1.07	1 (5%)	22,30,33	1.78	6 (27%)
79	PSU	L5	3637	-	18,21,22	1.04	1 (5%)	22,30,33	1.83	4 (18%)
79	A2M	L5	2401	-	22,25,26	3.94	10 (45%)	31,36,39	3.74	16 (51%)
78	PSU	S2	1174	-	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
79	OMG	L5	1316	-	23,26,27	0.54	0	33,38,41	0.58	0
79	A2M	L5	2363	-	22,25,26	3.93	10 (45%)	31,36,39	3.73	14 (45%)
79	PSU	L5	3695	-	18,21,22	1.09	1 (5%)	22,30,33	1.80	4 (18%)
79	PSU	L5	4493	-	18,21,22	1.05	1 (5%)	22,30,33	1.71	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
78	PSU	S2	1445	-	18,21,22	1.06	1 (5%)	22,30,33	1.78	5 (22%)
78	PSU	S2	1243	-	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
79	OMG	L5	3627	-	23,26,27	0.52	0	33,38,41	0.64	0
78	PSU	S2	814	-	18,21,22	1.03	1 (5%)	22,30,33	1.69	4 (18%)
79	PSU	L5	4673	-	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
79	A2M	L5	4571	-	22,25,26	3.93	10 (45%)	31,36,39	3.74	14 (45%)
78	PSU	S2	918	-	18,21,22	1.09	2 (11%)	22,30,33	1.79	5 (22%)
79	PSU	L5	3758	-	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
78	A2M	S2	99	-	22,25,26	3.93	11 (50%)	31,36,39	3.70	15 (48%)
79	PSU	L5	1536	-	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
79	PSU	L5	4420	-	18,21,22	1.06	1 (5%)	22,30,33	1.60	5 (22%)
78	PSU	S2	572	-	18,21,22	1.03	1 (5%)	22,30,33	1.71	4 (18%)
79	OMC	L5	2804	-	19,22,23	0.55	0	26,31,34	0.71	0
78	PSU	S2	966	-	18,21,22	1.01	1 (5%)	22,30,33	1.67	4 (18%)
79	PSU	L5	3853	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
79	A2M	L5	1871	-	22,25,26	3.93	10 (45%)	31,36,39	3.67	15 (48%)
78	A2M	S2	590	-	22,25,26	3.97	9 (40%)	31,36,39	3.93	13 (41%)
79	OMC	L5	2824	-	19,22,23	0.56	0	26,31,34	0.75	1 (3%)
79	PSU	L5	4552	-	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	3715	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	5 (22%)
79	PSU	L5	4293	-	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	3844	-	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
79	PSU	L5	4569	-	18,21,22	1.06	1 (5%)	22,30,33	1.66	4 (18%)
79	OMG	L5	3899	-	23,26,27	0.56	0	33,38,41	0.60	0
76	G7M	Pt	47	-	23,26,27	2.79	8 (34%)	35,39,42	2.29	10 (28%)
78	OMG	S2	1328	-	23,26,27	0.49	0	33,38,41	0.48	0
79	OMC	L5	1881	-	19,22,23	0.57	0	26,31,34	0.67	0
79	PSU	L5	3920	-	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
46	V5N	La	39	-	9,11,12	2.66	2 (22%)	9,14,16	1.23	1 (11%)
78	PSU	S2	651	-	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
79	OMC	L5	1340	-	19,22,23	0.56	0	26,31,34	0.66	0
79	PSU	L5	1779	-	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
78	A2M	S2	1383	-	22,25,26	3.95	10 (45%)	31,36,39	3.69	15 (48%)
79	PSU	L5	1860	-	18,21,22	1.03	1 (5%)	22,30,33	1.74	4 (18%)
78	PSU	S2	863	-	18,21,22	1.10	1 (5%)	22,30,33	1.72	4 (18%)
78	A2M	S2	166	-	22,25,26	3.93	9 (40%)	31,36,39	3.74	16 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	OMG	L5	2876	-	23,26,27	0.57	0	33,38,41	0.74	1 (3%)
79	OMG	L5	3744	-	23,26,27	0.50	0	33,38,41	0.48	0
1	V5N	LA	216	-	9,11,12	2.71	2 (22%)	9,14,16	1.25	1 (11%)
74	MLZ	Lo	53	-	8,9,10	0.75	0	4,9,11	0.61	0
79	OMG	L5	4370	-	23,26,27	0.51	0	33,38,41	0.51	0
78	OMG	S2	1447	-	23,26,27	0.48	0	33,38,41	0.50	0
79	OMU	L5	3925	-	19,22,23	2.99	8 (42%)	26,31,34	1.74	5 (19%)
78	PSU	S2	406	-	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
78	PSU	S2	815	-	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
78	PSU	S2	1347	-	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
78	A2M	S2	468	-	22,25,26	3.92	11 (50%)	31,36,39	3.65	15 (48%)
78	OMC	S2	174	-	19,22,23	0.52	0	26,31,34	0.65	0
78	PSU	S2	1004	-	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
79	PSU	L5	1792	-	18,21,22	1.01	1 (5%)	22,30,33	1.70	4 (18%)
79	OMC	L5	2365	-	19,22,23	0.56	0	26,31,34	0.65	0
79	A2M	L5	3825	-	22,25,26	3.92	10 (45%)	31,36,39	3.65	14 (45%)
78	A2M	S2	576	-	22,25,26	3.93	11 (50%)	31,36,39	3.71	15 (48%)
78	PSU	S2	119	-	18,21,22	1.05	1 (5%)	22,30,33	1.61	4 (18%)
78	4AC	S2	1842	-	21,24,25	3.45	10 (47%)	29,34,37	1.11	4 (13%)
78	6MZ	S2	1832	-	22,25,26	2.54	3 (13%)	30,36,39	3.51	12 (40%)
78	MA6	S2	1850	-	23,26,27	1.48	4 (17%)	34,38,41	3.28	11 (32%)
79	PSU	L5	4442	-	18,21,22	1.07	1 (5%)	22,30,33	1.77	5 (22%)
79	PSU	L5	1744	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	OMG	S2	436	-	23,26,27	0.53	0	33,38,41	0.54	0
78	PSU	S2	822	-	18,21,22	1.04	1 (5%)	22,30,33	1.76	5 (22%)
79	OMC	L5	4456	-	19,22,23	0.60	0	26,31,34	0.79	1 (3%)
78	PSU	S2	1081	-	18,21,22	1.02	1 (5%)	22,30,33	1.70	5 (22%)
76	OMC	Pt	33	-	19,22,23	0.57	0	26,31,34	1.01	2 (7%)
76	PSU	Pt	56	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	PSU	S2	105	-	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
78	PSU	S2	1177	-	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
78	OMU	S2	116	-	19,22,23	2.97	8 (42%)	26,31,34	1.64	5 (19%)
78	PSU	S2	1238	-	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
79	PSU	L5	4353	-	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
76	H2U	Pt	21	-	18,21,22	0.45	0	21,30,33	1.02	1 (4%)
79	OMU	L5	4227	-	19,22,23	2.99	8 (42%)	26,31,34	1.73	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	A2M	L5	3724	-	22,25,26	3.94	11 (50%)	31,36,39	3.72	14 (45%)
79	A2M	L5	3830	-	22,25,26	3.92	10 (45%)	31,36,39	3.63	14 (45%)
79	5MC	L5	3782	-	18,22,23	0.57	0	26,32,35	0.72	0
79	OMG	L5	4637	-	23,26,27	0.53	0	33,38,41	0.50	0
78	PSU	S2	866	-	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
79	OMC	L5	4536	-	19,22,23	0.57	0	26,31,34	0.76	0
79	PSU	L5	3851	-	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	4628	-	18,21,22	1.05	1 (5%)	22,30,33	1.88	5 (22%)
79	UR3	L5	4530	-	19,22,23	2.76	8 (42%)	26,32,35	1.29	2 (7%)
78	PSU	S2	686	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
79	A2M	L5	4590	-	22,25,26	3.94	9 (40%)	31,36,39	3.76	16 (51%)
79	OMG	L5	2424	-	23,26,27	0.52	0	33,38,41	0.44	0
78	A2M	S2	1031	-	22,25,26	3.92	10 (45%)	31,36,39	3.71	15 (48%)
78	OMG	S2	509	-	23,26,27	0.51	0	33,38,41	0.53	0
79	OMG	L5	3792	-	23,26,27	0.51	0	33,38,41	0.47	0
78	PSU	S2	1625	-	18,21,22	1.10	1 (5%)	22,30,33	1.71	4 (18%)
79	PSU	L5	2508	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
79	1MA	L5	1322	-	21,25,26	0.51	0	31,37,40	0.76	1 (3%)
79	PSU	L5	1677	-	18,21,22	1.13	1 (5%)	22,30,33	1.79	5 (22%)
79	PSU	L5	4361	-	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
3	HIC	LB	245	-	10,11,12	0.53	0	8,14,16	0.45	0
79	OMC	L5	2351	-	19,22,23	0.59	0	26,31,34	1.23	2 (7%)
78	A2M	S2	512	-	22,25,26	3.92	10 (45%)	31,36,39	3.70	15 (48%)
79	PSU	L5	4312	-	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
79	OMC	L5	3887	-	19,22,23	0.56	0	26,31,34	0.66	0
78	UY1	S2	1326	-	19,22,23	4.20	8 (42%)	22,31,34	1.81	5 (22%)
78	OMU	S2	1804	-	19,22,23	2.99	8 (42%)	26,31,34	1.77	5 (19%)
79	OMC	L5	3869	-	19,22,23	0.58	0	26,31,34	0.74	0
61	MLZ	Lb	5	-	8,9,10	0.78	0	4,9,11	0.68	0
72	M3L	Lm	98	-	10,11,12	0.40	0	9,14,16	0.28	0
78	OMG	S2	1490	-	23,26,27	0.54	0	33,38,41	0.51	0
79	PSU	L5	2632	-	18,21,22	1.05	1 (5%)	22,30,33	1.66	4 (18%)
79	OMG	L5	4499	-	23,26,27	0.52	0	33,38,41	0.47	0
79	OMG	L5	1522	-	23,26,27	0.51	0	33,38,41	0.61	0
78	A2M	S2	159	-	22,25,26	3.89	10 (45%)	31,36,39	3.69	13 (41%)
79	PSU	L5	4299	-	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
79	OMG	L5	4623	-	23,26,27	0.53	0	33,38,41	0.59	0
78	PSU	S2	609	-	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
78	OMC	S2	1391	-	19,22,23	0.53	0	26,31,34	0.65	0
79	PSU	L5	4521	-	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
79	PSU	L5	3734	-	18,21,22	1.01	1 (5%)	22,30,33	1.63	4 (18%)
79	PSU	L5	5010	-	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
78	G7M	S2	1639	-	23,26,27	2.76	8 (34%)	35,39,42	2.32	10 (28%)
79	PSU	L5	4403	-	18,21,22	1.00	1 (5%)	22,30,33	1.82	5 (22%)
79	OMC	L5	2861	-	19,22,23	0.58	0	26,31,34	0.83	1 (3%)
79	A2M	L5	3867	-	22,25,26	3.94	10 (45%)	31,36,39	3.75	14 (45%)
79	PSU	L5	3768	-	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
79	PSU	L5	4531	-	18,21,22	1.08	1 (5%)	22,30,33	1.81	5 (22%)
78	OMG	S2	601	-	23,26,27	0.49	0	33,38,41	0.46	0
79	PSU	L5	3770	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
78	OMU	S2	627	-	19,22,23	3.04	8 (42%)	26,31,34	1.67	4 (15%)
79	OMC	L5	3841	-	19,22,23	0.57	0	26,31,34	0.65	0
79	OMG	L5	4392	-	23,26,27	0.50	0	33,38,41	0.45	0
79	6MZ	L5	4220	-	22,25,26	2.61	3 (13%)	30,36,39	3.46	9 (30%)
79	OMG	L5	4494	-	23,26,27	0.53	0	33,38,41	0.49	0
79	PSU	L5	2843	-	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
79	PSU	L5	4471	-	18,21,22	1.06	1 (5%)	22,30,33	1.67	4 (18%)
78	OMC	S2	1703	-	19,22,23	0.55	0	26,31,34	0.62	0
79	PSU	L5	4296	-	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
78	PSU	S2	1692	-	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
79	PSU	L5	4532	-	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
79	OMC	L5	2422	-	19,22,23	0.58	0	26,31,34	0.77	1 (3%)
79	OMC	L5	3808	-	19,22,23	0.64	0	26,31,34	0.90	2 (7%)
79	PSU	L5	1862	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
79	A2M	L5	3785	-	22,25,26	3.94	11 (50%)	31,36,39	3.76	14 (45%)
78	PSU	S2	34	-	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
78	A2M	S2	668	-	22,25,26	3.91	11 (50%)	31,36,39	3.63	14 (45%)
79	OMG	L5	2364	-	23,26,27	0.51	0	33,38,41	0.47	0
78	B8N	S2	1248	-	24,29,30	3.02	6 (25%)	29,42,45	1.75	5 (17%)
79	UY1	L5	3818	-	19,22,23	4.18	8 (42%)	22,31,34	1.80	5 (22%)
79	PSU	L5	4423	-	18,21,22	1.07	1 (5%)	22,30,33	1.74	4 (18%)
19	HY3	SX	62	-	6,8,9	7.80	3 (50%)	5,10,12	0.98	0
78	OMU	S2	121	-	19,22,23	2.99	8 (42%)	26,31,34	1.66	5 (19%)
78	OMU	S2	354	-	19,22,23	2.96	8 (42%)	26,31,34	1.71	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	PSU	L5	4457	-	18,21,22	1.04	1 (5%)	22,30,33	1.80	5 (22%)
5	PSU	L8	55	-	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
79	A2M	L5	3723	-	22,25,26	3.93	10 (45%)	31,36,39	3.74	14 (45%)
78	4AC	S2	1337	-	21,24,25	3.46	10 (47%)	29,34,37	1.09	3 (10%)
78	OMG	S2	683	-	23,26,27	0.51	0	33,38,41	0.57	0
79	A2M	L5	398	-	22,25,26	3.88	10 (45%)	31,36,39	3.69	13 (41%)
79	PSU	L5	1781	-	18,21,22	1.08	1 (5%)	22,30,33	1.65	4 (18%)
79	PSU	L5	4500	-	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
79	PSU	L5	3764	-	18,21,22	1.06	1 (5%)	22,30,33	1.74	5 (22%)
78	PSU	S2	218	-	18,21,22	1.06	1 (5%)	22,30,33	1.69	5 (22%)
78	PSU	S2	296	-	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
78	PSU	S2	1056	-	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
5	PSU	L8	69	-	18,21,22	1.07	1 (5%)	22,30,33	1.75	5 (22%)
79	A2M	L5	400	-	22,25,26	3.93	10 (45%)	31,36,39	3.71	14 (45%)
79	OMU	L5	4306	-	19,22,23	2.99	8 (42%)	26,31,34	1.70	5 (19%)
78	A2M	S2	484	-	22,25,26	3.85	11 (50%)	31,36,39	3.68	13 (41%)
79	OMG	L5	4228	-	23,26,27	0.50	0	33,38,41	0.55	0
78	PSU	S2	93	-	18,21,22	1.05	1 (5%)	22,30,33	1.65	4 (18%)
79	PSU	L5	4431	-	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
79	PSU	L5	1582	-	18,21,22	1.07	1 (5%)	22,30,33	1.70	4 (18%)
78	PSU	S2	801	-	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
79	PSU	L5	1683	-	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
5	OMG	L8	75	-	23,26,27	0.49	0	33,38,41	0.49	0
79	PSU	L5	3884	-	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
79	OMG	L5	4196	-	23,26,27	0.52	0	33,38,41	0.54	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
78	A2M	S2	1678	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	4579	-	-	0/7/25/26	0/2/2/2
78	OMG	S2	644	-	-	3/9/27/28	0/3/3/3
78	OMU	S2	428	-	-	6/9/27/28	0/2/2/2
78	PSU	S2	1232	-	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	PSU	L5	1782	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4576	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1367	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1239	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	36	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	573	-	-	0/7/25/26	0/2/2/2
78	OMU	S2	1288	-	-	0/9/27/28	0/2/2/2
79	OMG	L5	1625	-	-	1/9/27/28	0/3/3/3
79	A2M	L5	3718	-	-	0/9/27/28	0/3/3/3
76	4SU	Pt	8	-	-	0/7/25/26	0/2/2/2
79	OMU	L5	2415	-	-	1/9/27/28	0/2/2/2
79	A2M	L5	4523	-	-	2/9/27/28	0/3/3/3
79	A2M	L5	1524	-	-	2/9/27/28	0/3/3/3
78	OMC	S2	517	-	-	0/9/27/28	0/2/2/2
79	OMU	L5	4620	-	-	1/9/27/28	0/2/2/2
78	PSU	S2	109	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	649	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3639	-	-	0/7/25/26	0/2/2/2
79	OMU	L5	4498	-	-	0/9/27/28	0/2/2/2
79	5MC	L5	4447	-	-	4/7/25/26	0/2/2/2
79	OMG	L5	4618	-	-	0/9/27/28	0/3/3/3
79	A2M	L5	1326	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	3729	-	-	2/7/25/26	0/2/2/2
79	PSU	L5	4636	-	-	2/7/25/26	0/2/2/2
78	PSU	S2	1244	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	27	-	-	2/9/27/28	0/3/3/3
79	PSU	L5	3762	-	-	0/7/25/26	0/2/2/2
78	OMC	S2	462	-	-	0/9/27/28	0/2/2/2
78	MA6	S2	1851	-	-	3/11/29/30	0/3/3/3
79	PSU	L5	4972	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1136	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	3701	-	-	4/9/27/28	0/2/2/2
79	OMU	L5	2837	-	-	0/9/27/28	0/2/2/2
78	PSU	S2	681	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	3944	-	-	0/9/27/28	0/3/3/3
78	OMU	S2	172	-	-	0/9/27/28	0/2/2/2
79	A2M	L5	2815	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	4689	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	1534	-	-	2/9/27/28	0/3/3/3
79	PSU	L5	2839	-	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	PSU	L5	5001	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1643	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3637	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	2401	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	1174	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	1316	-	-	1/9/27/28	0/3/3/3
79	A2M	L5	2363	-	-	0/9/27/28	0/3/3/3
79	PSU	L5	3695	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4493	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1445	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1243	-	-	2/7/25/26	0/2/2/2
79	OMG	L5	3627	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	814	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4673	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	4571	-	-	1/9/27/28	0/3/3/3
78	PSU	S2	918	-	-	2/7/25/26	0/2/2/2
79	PSU	L5	3758	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	99	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	1536	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4420	-	-	4/7/25/26	0/2/2/2
78	PSU	S2	572	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	2804	-	-	0/9/27/28	0/2/2/2
78	PSU	S2	966	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3853	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	1871	-	-	0/9/27/28	0/3/3/3
78	A2M	S2	590	-	-	6/9/27/28	0/3/3/3
79	OMC	L5	2824	-	-	1/9/27/28	0/2/2/2
79	PSU	L5	4552	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3715	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4293	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	3844	-	-	1/7/25/26	0/2/2/2
79	PSU	L5	4569	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	3899	-	-	0/9/27/28	0/3/3/3
76	G7M	Pt	47	-	-	2/7/25/26	0/3/3/3
78	OMG	S2	1328	-	-	1/9/27/28	0/3/3/3
79	OMC	L5	1881	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	3920	-	-	0/7/25/26	0/2/2/2
46	V5N	La	39	-	-	1/9/10/12	0/1/1/1
78	PSU	S2	651	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	1340	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	1779	-	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
78	A2M	S2	1383	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	1860	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	863	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	166	-	-	1/9/27/28	0/3/3/3
79	OMG	L5	2876	-	-	3/9/27/28	0/3/3/3
79	OMG	L5	3744	-	-	0/9/27/28	0/3/3/3
1	V5N	LA	216	-	-	1/9/10/12	0/1/1/1
74	MLZ	Lo	53	-	-	2/7/8/10	-
79	OMG	L5	4370	-	-	2/9/27/28	0/3/3/3
78	OMG	S2	1447	-	-	2/9/27/28	0/3/3/3
79	OMU	L5	3925	-	-	1/9/27/28	0/2/2/2
78	PSU	S2	406	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	815	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1347	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	468	-	-	2/9/27/28	0/3/3/3
78	OMC	S2	174	-	-	0/9/27/28	0/2/2/2
78	PSU	S2	1004	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1792	-	-	2/7/25/26	0/2/2/2
79	OMC	L5	2365	-	-	0/9/27/28	0/2/2/2
79	A2M	L5	3825	-	-	1/9/27/28	0/3/3/3
78	A2M	S2	576	-	-	3/9/27/28	0/3/3/3
78	PSU	S2	119	-	-	1/7/25/26	0/2/2/2
78	4AC	S2	1842	-	-	0/11/29/30	0/2/2/2
78	6MZ	S2	1832	-	-	0/9/27/28	0/3/3/3
78	MA6	S2	1850	-	-	0/11/29/30	0/3/3/3
79	PSU	L5	4442	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1744	-	-	0/7/25/26	0/2/2/2
78	OMG	S2	436	-	-	2/9/27/28	0/3/3/3
78	PSU	S2	822	-	-	2/7/25/26	0/2/2/2
79	OMC	L5	4456	-	-	0/9/27/28	0/2/2/2
78	PSU	S2	1081	-	-	0/7/25/26	0/2/2/2
76	OMC	Pt	33	-	-	1/9/27/28	0/2/2/2
76	PSU	Pt	56	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	105	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1177	-	-	0/7/25/26	0/2/2/2
78	OMU	S2	116	-	-	1/9/27/28	0/2/2/2
78	PSU	S2	1238	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4353	-	-	0/7/25/26	0/2/2/2
76	H2U	Pt	21	-	-	6/7/38/39	0/2/2/2
79	OMU	L5	4227	-	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	A2M	L5	3724	-	-	1/9/27/28	0/3/3/3
79	A2M	L5	3830	-	-	0/9/27/28	0/3/3/3
79	5MC	L5	3782	-	-	1/7/25/26	0/2/2/2
79	OMG	L5	4637	-	-	3/9/27/28	0/3/3/3
78	PSU	S2	866	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	4536	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	3851	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4628	-	-	0/7/25/26	0/2/2/2
79	UR3	L5	4530	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	686	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	4590	-	-	1/9/27/28	0/3/3/3
79	OMG	L5	2424	-	-	0/9/27/28	0/3/3/3
78	A2M	S2	1031	-	-	0/9/27/28	0/3/3/3
78	OMG	S2	509	-	-	2/9/27/28	0/3/3/3
79	OMG	L5	3792	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	1625	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	2508	-	-	0/7/25/26	0/2/2/2
79	1MA	L5	1322	-	-	2/7/25/26	0/3/3/3
79	PSU	L5	1677	-	-	1/7/25/26	0/2/2/2
79	PSU	L5	4361	-	-	1/7/25/26	0/2/2/2
3	HIC	LB	245	-	-	0/5/6/8	0/1/1/1
79	OMC	L5	2351	-	-	4/9/27/28	0/2/2/2
78	A2M	S2	512	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	4312	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	3887	-	-	1/9/27/28	0/2/2/2
78	UY1	S2	1326	-	-	2/9/27/28	0/2/2/2
78	OMU	S2	1804	-	-	1/9/27/28	0/2/2/2
79	OMC	L5	3869	-	-	0/9/27/28	0/2/2/2
61	MLZ	Lb	5	-	-	4/7/8/10	-
72	M3L	Lm	98	-	-	0/9/10/12	-
78	OMG	S2	1490	-	-	2/9/27/28	0/3/3/3
79	PSU	L5	2632	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	4499	-	-	0/9/27/28	0/3/3/3
79	OMG	L5	1522	-	-	0/9/27/28	0/3/3/3
78	A2M	S2	159	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	4299	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	4623	-	-	0/9/27/28	0/3/3/3
78	PSU	S2	609	-	-	0/7/25/26	0/2/2/2
78	OMC	S2	1391	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	4521	-	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	PSU	L5	3734	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	5010	-	-	0/7/25/26	0/2/2/2
78	G7M	S2	1639	-	-	2/7/25/26	0/3/3/3
79	PSU	L5	4403	-	-	0/7/25/26	0/2/2/2
79	OMC	L5	2861	-	-	0/9/27/28	0/2/2/2
79	A2M	L5	3867	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	3768	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4531	-	-	0/7/25/26	0/2/2/2
78	OMG	S2	601	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	3770	-	-	0/7/25/26	0/2/2/2
78	OMU	S2	627	-	-	0/9/27/28	0/2/2/2
79	OMC	L5	3841	-	-	0/9/27/28	0/2/2/2
79	OMG	L5	4392	-	-	0/9/27/28	0/3/3/3
79	6MZ	L5	4220	-	-	2/9/27/28	0/3/3/3
79	OMG	L5	4494	-	-	1/9/27/28	0/3/3/3
79	PSU	L5	2843	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4471	-	-	0/7/25/26	0/2/2/2
78	OMC	S2	1703	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	4296	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1692	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4532	-	-	2/7/25/26	0/2/2/2
79	OMC	L5	2422	-	-	2/9/27/28	0/2/2/2
79	OMC	L5	3808	-	-	0/9/27/28	0/2/2/2
79	PSU	L5	1862	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	3785	-	-	4/9/27/28	0/3/3/3
78	PSU	S2	34	-	-	0/7/25/26	0/2/2/2
78	A2M	S2	668	-	-	2/9/27/28	0/3/3/3
79	OMG	L5	2364	-	-	2/9/27/28	0/3/3/3
78	B8N	S2	1248	-	-	6/16/34/35	0/2/2/2
79	UY1	L5	3818	-	-	3/9/27/28	0/2/2/2
79	PSU	L5	4423	-	-	0/7/25/26	0/2/2/2
19	HY3	SX	62	-	-	0/1/12/14	0/1/1/1
78	OMU	S2	121	-	-	0/9/27/28	0/2/2/2
78	OMU	S2	354	-	-	1/9/27/28	0/2/2/2
79	PSU	L5	4457	-	-	0/7/25/26	0/2/2/2
5	PSU	L8	55	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	3723	-	-	1/9/27/28	0/3/3/3
78	4AC	S2	1337	-	-	0/11/29/30	0/2/2/2
78	OMG	S2	683	-	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	A2M	L5	398	-	-	3/9/27/28	0/3/3/3
79	PSU	L5	1781	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4500	-	-	1/7/25/26	0/2/2/2
79	PSU	L5	3764	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	218	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	296	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	1056	-	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	-	-	0/7/25/26	0/2/2/2
79	A2M	L5	400	-	-	0/9/27/28	0/3/3/3
79	OMU	L5	4306	-	-	0/9/27/28	0/2/2/2
78	A2M	S2	484	-	-	1/9/27/28	0/3/3/3
79	OMG	L5	4228	-	-	2/9/27/28	0/3/3/3
78	PSU	S2	93	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	4431	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1582	-	-	0/7/25/26	0/2/2/2
78	PSU	S2	801	-	-	0/7/25/26	0/2/2/2
79	PSU	L5	1683	-	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	-	-	0/9/27/28	0/3/3/3
79	PSU	L5	3884	-	-	0/7/25/26	0/2/2/2
79	OMG	L5	4196	-	-	1/9/27/28	0/3/3/3

All (646) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	SX	62	HY3	C3-CA	-17.99	1.37	1.55
78	S2	590	A2M	C3'-C2'	-12.71	1.24	1.52
78	S2	1383	A2M	C3'-C2'	-12.67	1.24	1.52
79	L5	4590	A2M	C3'-C2'	-12.67	1.24	1.52
79	L5	3785	A2M	C3'-C2'	-12.67	1.24	1.52
79	L5	3867	A2M	C3'-C2'	-12.66	1.24	1.52
79	L5	1534	A2M	C3'-C2'	-12.64	1.24	1.52
79	L5	2363	A2M	C3'-C2'	-12.62	1.24	1.52
79	L5	1871	A2M	C3'-C2'	-12.62	1.24	1.52
78	S2	99	A2M	C3'-C2'	-12.58	1.24	1.52
78	S2	27	A2M	C3'-C2'	-12.56	1.24	1.52
78	S2	468	A2M	C3'-C2'	-12.56	1.24	1.52
79	L5	3825	A2M	C3'-C2'	-12.56	1.24	1.52
79	L5	3830	A2M	C3'-C2'	-12.56	1.24	1.52
79	L5	1524	A2M	C3'-C2'	-12.55	1.25	1.52
79	L5	3724	A2M	C3'-C2'	-12.55	1.25	1.52
79	L5	4571	A2M	C3'-C2'	-12.55	1.25	1.52
79	L5	2815	A2M	C3'-C2'	-12.55	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	400	A2M	C3'-C2'	-12.54	1.25	1.52
79	L5	2401	A2M	C3'-C2'	-12.54	1.25	1.52
78	S2	166	A2M	C3'-C2'	-12.54	1.25	1.52
79	L5	1326	A2M	C3'-C2'	-12.53	1.25	1.52
78	S2	1031	A2M	C3'-C2'	-12.53	1.25	1.52
78	S2	512	A2M	C3'-C2'	-12.52	1.25	1.52
79	L5	3723	A2M	C3'-C2'	-12.50	1.25	1.52
78	S2	1678	A2M	C3'-C2'	-12.50	1.25	1.52
78	S2	576	A2M	C3'-C2'	-12.47	1.25	1.52
79	L5	3718	A2M	C3'-C2'	-12.45	1.25	1.52
79	L5	398	A2M	C3'-C2'	-12.43	1.25	1.52
79	L5	4523	A2M	C3'-C2'	-12.39	1.25	1.52
78	S2	159	A2M	C3'-C2'	-12.34	1.25	1.52
78	S2	668	A2M	C3'-C2'	-12.11	1.25	1.52
78	S2	484	A2M	C3'-C2'	-12.11	1.26	1.52
78	S2	1326	UY1	C6-C5	11.06	1.48	1.35
79	L5	3818	UY1	C6-C5	10.99	1.48	1.35
79	L5	4220	6MZ	C6-N6	10.85	1.45	1.34
78	S2	1832	6MZ	C6-N6	10.47	1.45	1.34
78	S2	1326	UY1	C2-N1	9.59	1.49	1.36
79	L5	3818	UY1	C2-N1	9.51	1.49	1.36
76	Pt	8	4SU	C4-N3	7.96	1.46	1.37
78	S2	1248	B8N	C4-N3	-7.84	1.25	1.40
78	S2	1248	B8N	C6-N1	7.57	1.55	1.36
78	S2	1326	UY1	C2-N3	7.36	1.50	1.37
79	L5	3818	UY1	C2-N3	7.29	1.50	1.37
79	L5	4530	UR3	C2-N1	7.21	1.48	1.38
78	S2	428	OMU	C2-N1	7.19	1.50	1.38
79	L5	2415	OMU	C2-N1	7.12	1.49	1.38
78	S2	627	OMU	C2-N1	7.07	1.49	1.38
78	S2	1842	4AC	C4-N3	7.06	1.45	1.32
79	L5	4227	OMU	C2-N1	7.03	1.49	1.38
78	S2	1337	4AC	C4-N3	7.02	1.45	1.32
78	S2	172	OMU	C2-N1	7.02	1.49	1.38
78	S2	1288	OMU	C2-N1	7.01	1.49	1.38
79	L5	2837	OMU	C2-N1	7.01	1.49	1.38
76	Pt	8	4SU	C2-N3	6.97	1.50	1.38
78	S2	668	A2M	O4'-C4'	-6.96	1.29	1.45
79	L5	4498	OMU	C2-N1	6.93	1.49	1.38
78	S2	1804	OMU	C2-N1	6.90	1.49	1.38
78	S2	121	OMU	C2-N1	6.89	1.49	1.38
79	L5	4306	OMU	C2-N1	6.88	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	3925	OMU	C2-N1	6.88	1.49	1.38
78	S2	627	OMU	C2-N3	6.86	1.50	1.38
78	S2	172	OMU	C2-N3	6.83	1.50	1.38
78	S2	428	OMU	C2-N3	6.82	1.50	1.38
78	S2	116	OMU	C2-N3	6.79	1.50	1.38
78	S2	121	OMU	C2-N3	6.79	1.50	1.38
76	Pt	8	4SU	C2-N1	6.77	1.49	1.38
78	S2	354	OMU	C2-N1	6.77	1.49	1.38
79	L5	1524	A2M	O4'-C4'	-6.76	1.29	1.45
78	S2	116	OMU	C2-N1	6.76	1.49	1.38
79	L5	4620	OMU	C2-N1	6.76	1.49	1.38
79	L5	2837	OMU	C2-N3	6.75	1.50	1.38
78	S2	1288	OMU	C2-N3	6.75	1.50	1.38
78	S2	1337	4AC	C2-N3	6.74	1.50	1.36
78	S2	1842	4AC	C2-N3	6.73	1.50	1.36
79	L5	3867	A2M	O4'-C4'	-6.73	1.30	1.45
79	L5	2415	OMU	C2-N3	6.72	1.49	1.38
79	L5	4306	OMU	C2-N3	6.72	1.49	1.38
78	S2	354	OMU	C2-N3	6.71	1.49	1.38
78	S2	1804	OMU	C2-N3	6.71	1.49	1.38
76	Pt	47	G7M	C4-N3	6.70	1.50	1.34
78	S2	1678	A2M	O4'-C4'	-6.70	1.30	1.45
79	L5	3925	OMU	C2-N3	6.68	1.49	1.38
79	L5	4227	OMU	C2-N3	6.66	1.49	1.38
79	L5	4498	OMU	C2-N3	6.63	1.49	1.38
79	L5	4620	OMU	C2-N3	6.63	1.49	1.38
79	L5	400	A2M	O4'-C4'	-6.62	1.30	1.45
78	S2	1639	G7M	C4-N3	6.61	1.50	1.34
79	L5	4571	A2M	O4'-C4'	-6.60	1.30	1.45
79	L5	2815	A2M	O4'-C4'	-6.60	1.30	1.45
79	L5	1326	A2M	O4'-C4'	-6.59	1.30	1.45
79	L5	4523	A2M	O4'-C4'	-6.58	1.30	1.45
78	S2	512	A2M	O4'-C4'	-6.56	1.30	1.45
79	L5	2363	A2M	O4'-C4'	-6.56	1.30	1.45
1	LA	216	V5N	CG-ND1	-6.55	1.31	1.37
79	L5	3724	A2M	O4'-C4'	-6.54	1.30	1.45
78	S2	159	A2M	O4'-C4'	-6.53	1.30	1.45
78	S2	27	A2M	O4'-C4'	-6.52	1.30	1.45
79	L5	4590	A2M	O4'-C4'	-6.52	1.30	1.45
79	L5	3723	A2M	O4'-C4'	-6.51	1.30	1.45
78	S2	590	A2M	O4'-C4'	-6.50	1.30	1.45
79	L5	3825	A2M	O4'-C4'	-6.50	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	S2	576	A2M	O4'-C4'	-6.50	1.30	1.45
78	S2	484	A2M	O4'-C4'	-6.47	1.30	1.45
79	L5	1871	A2M	O4'-C4'	-6.46	1.30	1.45
78	S2	166	A2M	O4'-C4'	-6.46	1.30	1.45
46	La	39	V5N	CG-ND1	-6.45	1.31	1.37
78	S2	99	A2M	O4'-C4'	-6.44	1.30	1.45
78	S2	1031	A2M	O4'-C4'	-6.43	1.30	1.45
79	L5	2401	A2M	O4'-C4'	-6.42	1.30	1.45
79	L5	398	A2M	O4'-C4'	-6.40	1.30	1.45
78	S2	1383	A2M	O4'-C4'	-6.39	1.30	1.45
78	S2	468	A2M	O4'-C4'	-6.39	1.30	1.45
79	L5	3718	A2M	O4'-C4'	-6.35	1.30	1.45
78	S2	1337	4AC	C6-C5	6.34	1.49	1.35
79	L5	3785	A2M	O4'-C4'	-6.34	1.30	1.45
79	L5	3830	A2M	O4'-C4'	-6.34	1.30	1.45
79	L5	1534	A2M	O4'-C4'	-6.30	1.30	1.45
78	S2	1842	4AC	C6-C5	6.26	1.49	1.35
79	L5	4530	UR3	C6-C5	6.08	1.49	1.35
78	S2	1248	B8N	C6-C5	5.90	1.43	1.34
78	S2	1248	B8N	C2-N1	5.89	1.56	1.39
76	Pt	47	G7M	C2-N2	5.86	1.48	1.34
78	S2	1639	G7M	C2-N2	5.82	1.48	1.34
76	Pt	8	4SU	C6-C5	5.81	1.48	1.35
78	S2	627	OMU	C6-C5	5.72	1.48	1.35
78	S2	1288	OMU	C6-C5	5.70	1.48	1.35
78	S2	172	OMU	C6-C5	5.68	1.48	1.35
79	L5	4498	OMU	C6-C5	5.68	1.48	1.35
78	S2	428	OMU	C6-C5	5.68	1.48	1.35
79	L5	2837	OMU	C6-C5	5.67	1.48	1.35
79	L5	4227	OMU	C6-C5	5.66	1.48	1.35
79	L5	3925	OMU	C6-C5	5.63	1.48	1.35
79	L5	4306	OMU	C6-C5	5.62	1.48	1.35
78	S2	121	OMU	C6-C5	5.61	1.48	1.35
78	S2	354	OMU	C6-C5	5.60	1.48	1.35
78	S2	1804	OMU	C6-C5	5.60	1.48	1.35
79	L5	3785	A2M	C3'-C4'	5.59	1.67	1.53
79	L5	2415	OMU	C6-C5	5.58	1.48	1.35
79	L5	4620	OMU	C6-C5	5.58	1.48	1.35
78	S2	116	OMU	C6-C5	5.58	1.48	1.35
76	Pt	47	G7M	C2-N3	5.52	1.46	1.33
79	L5	4571	A2M	C6-N6	5.48	1.47	1.34
78	S2	1337	4AC	C4-N4	5.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	S2	1842	4AC	C4-N4	5.44	1.47	1.39
78	S2	576	A2M	C6-N6	5.43	1.47	1.34
78	S2	468	A2M	C6-N6	5.43	1.47	1.34
78	S2	590	A2M	C6-N6	5.43	1.47	1.34
78	S2	1383	A2M	C6-N6	5.42	1.47	1.34
79	L5	3724	A2M	C6-N6	5.42	1.47	1.34
78	S2	166	A2M	C6-N6	5.42	1.47	1.34
79	L5	3723	A2M	C6-N6	5.42	1.47	1.34
78	S2	484	A2M	C6-N6	5.41	1.47	1.34
78	S2	159	A2M	C6-N6	5.41	1.47	1.34
78	S2	1031	A2M	C6-N6	5.41	1.47	1.34
78	S2	512	A2M	C6-N6	5.41	1.47	1.34
78	S2	27	A2M	C6-N6	5.41	1.47	1.34
78	S2	668	A2M	C6-N6	5.41	1.47	1.34
78	S2	1639	G7M	C2-N3	5.41	1.46	1.33
79	L5	1871	A2M	C6-N6	5.40	1.47	1.34
79	L5	3867	A2M	C6-N6	5.40	1.47	1.34
79	L5	400	A2M	C6-N6	5.39	1.47	1.34
78	S2	1678	A2M	C6-N6	5.39	1.47	1.34
79	L5	1524	A2M	C6-N6	5.39	1.47	1.34
79	L5	3718	A2M	C6-N6	5.39	1.47	1.34
79	L5	4590	A2M	C6-N6	5.38	1.47	1.34
79	L5	4523	A2M	C6-N6	5.38	1.47	1.34
79	L5	2401	A2M	C6-N6	5.38	1.47	1.34
79	L5	398	A2M	C6-N6	5.37	1.47	1.34
79	L5	2815	A2M	C6-N6	5.36	1.47	1.34
79	L5	3825	A2M	C6-N6	5.35	1.47	1.34
79	L5	3830	A2M	C6-N6	5.35	1.47	1.34
79	L5	1326	A2M	C6-N6	5.34	1.47	1.34
79	L5	2363	A2M	C6-N6	5.33	1.47	1.34
78	S2	99	A2M	C6-N6	5.33	1.47	1.34
79	L5	3785	A2M	C6-N6	5.33	1.47	1.34
79	L5	1534	A2M	C3'-C4'	5.32	1.66	1.53
78	S2	668	A2M	C3'-C4'	5.28	1.66	1.53
79	L5	1534	A2M	C6-N6	5.27	1.47	1.34
78	S2	159	A2M	C3'-C4'	5.27	1.66	1.53
78	S2	468	A2M	C3'-C4'	5.27	1.66	1.53
79	L5	3830	A2M	C3'-C4'	5.25	1.66	1.53
78	S2	1326	UY1	C6-N1	5.24	1.44	1.36
78	S2	1678	A2M	C3'-C4'	5.24	1.66	1.53
78	S2	484	A2M	C3'-C4'	5.22	1.66	1.53
79	L5	3724	A2M	C3'-C4'	5.22	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	S2	99	A2M	C3'-C4'	5.20	1.66	1.53
79	L5	1326	A2M	C3'-C4'	5.20	1.66	1.53
79	L5	3723	A2M	C3'-C4'	5.20	1.66	1.53
79	L5	3818	UY1	C6-N1	5.19	1.44	1.36
79	L5	4523	A2M	C3'-C4'	5.17	1.66	1.53
78	S2	1031	A2M	C3'-C4'	5.17	1.66	1.53
79	L5	2363	A2M	C3'-C4'	5.17	1.66	1.53
78	S2	590	A2M	C3'-C4'	5.16	1.66	1.53
79	L5	4571	A2M	C3'-C4'	5.16	1.66	1.53
79	L5	3718	A2M	C3'-C4'	5.15	1.66	1.53
79	L5	3825	A2M	C3'-C4'	5.15	1.66	1.53
79	L5	398	A2M	C3'-C4'	5.13	1.66	1.53
79	L5	400	A2M	C3'-C4'	5.13	1.66	1.53
79	L5	1871	A2M	C3'-C4'	5.11	1.66	1.53
78	S2	576	A2M	C3'-C4'	5.09	1.66	1.53
79	L5	2401	A2M	C3'-C4'	5.09	1.66	1.53
78	S2	27	A2M	C3'-C4'	5.08	1.66	1.53
78	S2	1383	A2M	C3'-C4'	5.07	1.66	1.53
79	L5	2815	A2M	C3'-C4'	5.07	1.65	1.53
79	L5	4590	A2M	C3'-C4'	5.06	1.65	1.53
78	S2	166	A2M	C3'-C4'	5.04	1.65	1.53
78	S2	512	A2M	C3'-C4'	5.04	1.65	1.53
79	L5	1524	A2M	C1'-N9	-5.03	1.32	1.46
79	L5	1524	A2M	C3'-C4'	5.02	1.65	1.53
79	L5	3867	A2M	C3'-C4'	5.02	1.65	1.53
79	L5	4530	UR3	C2-N3	5.01	1.48	1.39
76	Pt	8	4SU	C5-C4	4.96	1.49	1.42
78	S2	590	A2M	C1'-N9	-4.91	1.32	1.46
78	S2	1850	MA6	C6-N6	4.69	1.50	1.36
78	S2	1851	MA6	C6-N6	4.66	1.50	1.36
78	S2	576	A2M	C1'-N9	-4.61	1.33	1.46
76	Pt	8	4SU	C4-S4	-4.60	1.59	1.68
79	L5	4590	A2M	C1'-N9	-4.56	1.33	1.46
78	S2	1383	A2M	O4'-C1'	4.53	1.52	1.42
78	S2	1337	4AC	C5-C4	4.53	1.50	1.40
79	L5	2401	A2M	C1'-N9	-4.50	1.33	1.46
79	L5	3718	A2M	O4'-C1'	4.49	1.52	1.42
79	L5	1534	A2M	C1'-N9	-4.48	1.33	1.46
78	S2	166	A2M	O4'-C1'	4.47	1.52	1.42
79	L5	1871	A2M	C1'-N9	-4.46	1.33	1.46
79	L5	3724	A2M	O4'-C1'	4.46	1.52	1.42
79	L5	3830	A2M	O4'-C1'	4.46	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	398	A2M	O4'-C1'	4.46	1.52	1.42
78	S2	99	A2M	O4'-C1'	4.46	1.52	1.42
79	L5	2401	A2M	O4'-C1'	4.44	1.52	1.42
78	S2	1031	A2M	O4'-C1'	4.44	1.52	1.42
79	L5	3785	A2M	C1'-N9	-4.44	1.33	1.46
78	S2	166	A2M	C1'-N9	-4.44	1.33	1.46
79	L5	4590	A2M	O4'-C1'	4.44	1.52	1.42
78	S2	1842	4AC	C5-C4	4.44	1.50	1.40
79	L5	3723	A2M	O4'-C1'	4.43	1.52	1.42
79	L5	2815	A2M	C1'-N9	-4.42	1.33	1.46
79	L5	2815	A2M	O4'-C1'	4.42	1.52	1.42
78	S2	1678	A2M	O4'-C1'	4.42	1.52	1.42
78	S2	576	A2M	O4'-C1'	4.42	1.52	1.42
78	S2	1842	4AC	C2-N1	4.41	1.49	1.40
78	S2	1678	A2M	C1'-N9	-4.41	1.33	1.46
79	L5	1871	A2M	O4'-C1'	4.40	1.52	1.42
78	S2	1031	A2M	C1'-N9	-4.39	1.33	1.46
78	S2	512	A2M	C1'-N9	-4.39	1.33	1.46
78	S2	468	A2M	O4'-C1'	4.39	1.52	1.42
79	L5	3724	A2M	C1'-N9	-4.38	1.33	1.46
79	L5	1326	A2M	C1'-N9	-4.38	1.33	1.46
79	L5	2363	A2M	C1'-N9	-4.38	1.33	1.46
78	S2	1337	4AC	C2-N1	4.38	1.49	1.40
78	S2	99	A2M	C1'-N9	-4.38	1.33	1.46
79	L5	4571	A2M	O4'-C1'	4.38	1.52	1.42
78	S2	1383	A2M	C1'-N9	-4.37	1.33	1.46
79	L5	3825	A2M	O4'-C1'	4.37	1.52	1.42
79	L5	2363	A2M	O4'-C1'	4.36	1.52	1.42
78	S2	27	A2M	C1'-N9	-4.35	1.34	1.46
78	S2	668	A2M	C1'-N9	-4.35	1.34	1.46
79	L5	3830	A2M	C1'-N9	-4.35	1.34	1.46
79	L5	1534	A2M	O4'-C1'	4.35	1.52	1.42
79	L5	3723	A2M	C1'-N9	-4.34	1.34	1.46
79	L5	3867	A2M	O4'-C1'	4.34	1.52	1.42
79	L5	400	A2M	C1'-N9	-4.34	1.34	1.46
78	S2	468	A2M	C1'-N9	-4.34	1.34	1.46
79	L5	400	A2M	O4'-C1'	4.34	1.52	1.42
78	S2	512	A2M	O4'-C1'	4.33	1.52	1.42
79	L5	4523	A2M	O4'-C1'	4.32	1.52	1.42
79	L5	3825	A2M	C1'-N9	-4.31	1.34	1.46
79	L5	3867	A2M	C1'-N9	-4.31	1.34	1.46
79	L5	1326	A2M	O4'-C1'	4.31	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	4523	A2M	C1'-N9	-4.31	1.34	1.46
78	S2	159	A2M	C1'-N9	-4.30	1.34	1.46
79	L5	4571	A2M	C1'-N9	-4.29	1.34	1.46
78	S2	27	A2M	O4'-C1'	4.29	1.52	1.42
78	S2	590	A2M	O4'-C1'	4.26	1.52	1.42
78	S2	1337	4AC	C7-N4	4.22	1.45	1.37
79	L5	398	A2M	C1'-N9	-4.21	1.34	1.46
1	LA	216	V5N	CD2-NE2	-4.20	1.31	1.37
78	S2	159	A2M	O4'-C1'	4.19	1.51	1.42
78	S2	484	A2M	O4'-C1'	4.19	1.51	1.42
78	S2	1842	4AC	C7-N4	4.19	1.44	1.37
78	S2	484	A2M	C1'-N9	-4.18	1.34	1.46
78	S2	627	OMU	C4-N3	4.18	1.46	1.38
78	S2	428	OMU	C4-N3	4.14	1.46	1.38
79	L5	3718	A2M	C1'-N9	-4.14	1.34	1.46
78	S2	1639	G7M	C5-N7	-4.13	1.34	1.39
19	SX	62	HY3	C4-C5	4.13	1.59	1.53
78	S2	1288	OMU	C4-N3	4.12	1.45	1.38
19	SX	62	HY3	C5-N	-4.11	1.34	1.49
78	S2	1804	OMU	C4-N3	4.11	1.45	1.38
76	Pt	47	G7M	C5-C6	4.10	1.54	1.43
79	L5	1524	A2M	O4'-C1'	4.09	1.51	1.42
78	S2	172	OMU	C4-N3	4.09	1.45	1.38
78	S2	121	OMU	C4-N3	4.07	1.45	1.38
78	S2	116	OMU	C4-N3	4.07	1.45	1.38
46	La	39	V5N	CD2-NE2	-4.06	1.31	1.37
79	L5	4306	OMU	C4-N3	4.05	1.45	1.38
78	S2	1639	G7M	C5-C6	4.04	1.54	1.43
78	S2	354	OMU	C4-N3	4.03	1.45	1.38
79	L5	2837	OMU	C4-N3	4.02	1.45	1.38
79	L5	3925	OMU	C4-N3	4.02	1.45	1.38
79	L5	2415	OMU	C4-N3	3.97	1.45	1.38
79	L5	3785	A2M	O4'-C1'	3.94	1.51	1.42
79	L5	4620	OMU	C4-N3	3.93	1.45	1.38
76	Pt	47	G7M	C5-N7	-3.91	1.34	1.39
78	S2	668	A2M	O4'-C1'	3.91	1.51	1.42
79	L5	4498	OMU	C4-N3	3.91	1.45	1.38
79	L5	4227	OMU	C4-N3	3.91	1.45	1.38
78	S2	1326	UY1	C4-N3	3.84	1.46	1.38
79	L5	3818	UY1	C4-N3	3.75	1.45	1.38
78	S2	1232	PSU	C6-C5	3.62	1.39	1.35
78	S2	573	PSU	C6-C5	3.59	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	1677	PSU	C6-C5	3.59	1.39	1.35
78	S2	1842	4AC	C6-N1	3.59	1.46	1.38
78	S2	1625	PSU	C6-C5	3.58	1.39	1.35
78	S2	1337	4AC	C6-N1	3.58	1.46	1.38
78	S2	609	PSU	C6-C5	3.57	1.39	1.35
79	L5	4420	PSU	C6-C5	3.57	1.39	1.35
76	Pt	47	G7M	C2-N1	3.56	1.46	1.37
79	L5	1781	PSU	C6-C5	3.56	1.39	1.35
78	S2	801	PSU	C6-C5	3.56	1.39	1.35
78	S2	863	PSU	C6-C5	3.53	1.39	1.35
78	S2	119	PSU	C6-C5	3.52	1.39	1.35
76	Pt	56	PSU	C6-C5	3.49	1.39	1.35
78	S2	1177	PSU	C6-C5	3.48	1.39	1.35
79	L5	4471	PSU	C6-C5	3.48	1.39	1.35
78	S2	1004	PSU	C6-C5	3.48	1.39	1.35
78	S2	1239	PSU	C6-C5	3.48	1.39	1.35
79	L5	1779	PSU	C6-C5	3.47	1.39	1.35
79	L5	3758	PSU	C6-C5	3.47	1.39	1.35
79	L5	3762	PSU	C6-C5	3.46	1.39	1.35
79	L5	1744	PSU	C6-C5	3.46	1.39	1.35
78	S2	1639	G7M	C2-N1	3.45	1.46	1.37
79	L5	5010	PSU	C6-C5	3.45	1.39	1.35
78	S2	649	PSU	C6-C5	3.45	1.39	1.35
79	L5	2632	PSU	C6-C5	3.44	1.39	1.35
79	L5	2839	PSU	C6-C5	3.43	1.39	1.35
78	S2	93	PSU	C6-C5	3.43	1.39	1.35
78	S2	1174	PSU	C6-C5	3.43	1.39	1.35
79	L5	4293	PSU	C6-C5	3.43	1.39	1.35
78	S2	36	PSU	C6-C5	3.43	1.39	1.35
79	L5	3844	PSU	C6-C5	3.42	1.39	1.35
79	L5	4531	PSU	C6-C5	3.42	1.39	1.35
78	S2	1244	PSU	C6-C5	3.41	1.39	1.35
78	S2	1238	PSU	C6-C5	3.41	1.39	1.35
79	L5	2843	PSU	C6-C5	3.41	1.39	1.35
78	S2	1692	PSU	C6-C5	3.40	1.39	1.35
79	L5	1582	PSU	C6-C5	3.40	1.39	1.35
79	L5	3764	PSU	C6-C5	3.40	1.39	1.35
78	S2	406	PSU	C6-C5	3.40	1.39	1.35
79	L5	1862	PSU	C6-C5	3.40	1.39	1.35
79	L5	4296	PSU	C6-C5	3.39	1.39	1.35
79	L5	3768	PSU	C6-C5	3.39	1.39	1.35
78	S2	34	PSU	C6-C5	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	4532	PSU	C6-C5	3.38	1.39	1.35
79	L5	4312	PSU	C6-C5	3.38	1.39	1.35
78	S2	686	PSU	C6-C5	3.38	1.39	1.35
78	S2	1367	PSU	C6-C5	3.38	1.39	1.35
5	L8	69	PSU	C6-C5	3.38	1.39	1.35
79	L5	3884	PSU	C6-C5	3.38	1.39	1.35
78	S2	109	PSU	C6-C5	3.38	1.39	1.35
79	L5	4493	PSU	C6-C5	3.37	1.39	1.35
79	L5	4423	PSU	C6-C5	3.37	1.39	1.35
79	L5	2508	PSU	C6-C5	3.37	1.39	1.35
78	S2	822	PSU	C6-C5	3.37	1.39	1.35
79	L5	1683	PSU	C6-C5	3.37	1.39	1.35
79	L5	4431	PSU	C6-C5	3.37	1.39	1.35
79	L5	4636	PSU	C6-C5	3.37	1.39	1.35
79	L5	4673	PSU	C6-C5	3.37	1.39	1.35
79	L5	5001	PSU	C6-C5	3.37	1.39	1.35
78	S2	866	PSU	C6-C5	3.36	1.39	1.35
78	S2	218	PSU	C6-C5	3.36	1.39	1.35
79	L5	1536	PSU	C6-C5	3.35	1.39	1.35
79	L5	4361	PSU	C6-C5	3.35	1.39	1.35
78	S2	1347	PSU	C6-C5	3.35	1.39	1.35
78	S2	814	PSU	C6-C5	3.34	1.39	1.35
79	L5	1792	PSU	C6-C5	3.34	1.39	1.35
79	L5	3639	PSU	C6-C5	3.34	1.39	1.35
78	S2	1643	PSU	C6-C5	3.34	1.39	1.35
78	S2	815	PSU	C6-C5	3.34	1.39	1.35
78	S2	105	PSU	C6-C5	3.33	1.39	1.35
79	L5	3715	PSU	C6-C5	3.33	1.39	1.35
78	S2	1243	PSU	C6-C5	3.33	1.39	1.35
79	L5	4299	PSU	C6-C5	3.33	1.39	1.35
79	L5	3695	PSU	C6-C5	3.32	1.39	1.35
79	L5	4569	PSU	C6-C5	3.32	1.39	1.35
78	S2	651	PSU	C6-C5	3.32	1.39	1.35
78	S2	966	PSU	C6-C5	3.31	1.39	1.35
78	S2	918	PSU	C6-C5	3.30	1.39	1.35
79	L5	3729	PSU	C6-C5	3.30	1.39	1.35
79	L5	4521	PSU	C6-C5	3.30	1.39	1.35
5	L8	55	PSU	C6-C5	3.30	1.39	1.35
79	L5	3853	PSU	C6-C5	3.30	1.39	1.35
79	L5	4353	PSU	C6-C5	3.30	1.39	1.35
78	S2	572	PSU	C6-C5	3.28	1.39	1.35
79	L5	3851	PSU	C6-C5	3.28	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	1782	PSU	C6-C5	3.28	1.39	1.35
79	L5	4442	PSU	C6-C5	3.27	1.39	1.35
78	S2	296	PSU	C6-C5	3.27	1.39	1.35
79	L5	3734	PSU	C6-C5	3.27	1.39	1.35
79	L5	4576	PSU	C6-C5	3.27	1.39	1.35
79	L5	4628	PSU	C6-C5	3.27	1.39	1.35
78	S2	1445	PSU	C6-C5	3.27	1.39	1.35
79	L5	3637	PSU	C6-C5	3.26	1.39	1.35
79	L5	1860	PSU	C6-C5	3.26	1.39	1.35
78	S2	1056	PSU	C6-C5	3.25	1.39	1.35
78	S2	681	PSU	C6-C5	3.25	1.39	1.35
79	L5	3920	PSU	C6-C5	3.23	1.39	1.35
79	L5	4972	PSU	C6-C5	3.22	1.39	1.35
78	S2	1081	PSU	C6-C5	3.21	1.39	1.35
79	L5	4689	PSU	C6-C5	3.21	1.39	1.35
78	S2	1136	PSU	C6-C5	3.21	1.39	1.35
79	L5	3770	PSU	C6-C5	3.20	1.39	1.35
79	L5	4579	PSU	C6-C5	3.17	1.39	1.35
79	L5	4457	PSU	C6-C5	3.16	1.39	1.35
79	L5	4552	PSU	C6-C5	3.11	1.38	1.35
79	L5	4530	UR3	C6-N1	3.10	1.45	1.38
78	S2	668	A2M	C2'-C1'	3.10	1.61	1.53
76	Pt	8	4SU	C6-N1	3.09	1.45	1.38
79	L5	3723	A2M	O2'-C2'	3.04	1.50	1.42
78	S2	1639	G7M	O6-C6	-3.04	1.17	1.23
79	L5	4500	PSU	C6-C5	3.02	1.38	1.35
79	L5	3724	A2M	O2'-C2'	3.01	1.50	1.42
79	L5	4620	OMU	O4-C4	-3.01	1.18	1.24
79	L5	1524	A2M	O2'-C2'	3.00	1.50	1.42
79	L5	2401	A2M	O2'-C2'	3.00	1.50	1.42
78	S2	1678	A2M	O2'-C2'	3.00	1.50	1.42
76	Pt	47	G7M	O6-C6	-2.99	1.17	1.23
79	L5	4227	OMU	O4-C4	-2.99	1.18	1.24
79	L5	2415	OMU	O4-C4	-2.98	1.18	1.24
79	L5	3718	A2M	O2'-C2'	2.98	1.50	1.42
78	S2	590	A2M	O2'-C2'	2.98	1.50	1.42
79	L5	400	A2M	O2'-C2'	2.98	1.50	1.42
78	S2	1383	A2M	O2'-C2'	2.98	1.50	1.42
78	S2	484	A2M	O2'-C2'	2.97	1.50	1.42
78	S2	159	A2M	O2'-C2'	2.97	1.50	1.42
78	S2	1804	OMU	O4-C4	-2.97	1.18	1.24
78	S2	116	OMU	O4-C4	-2.97	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	4571	A2M	O2'-C2'	2.97	1.50	1.42
79	L5	1326	A2M	O2'-C2'	2.96	1.50	1.42
78	S2	354	OMU	O4-C4	-2.95	1.18	1.24
79	L5	4523	A2M	O2'-C2'	2.95	1.50	1.42
78	S2	668	A2M	O2'-C2'	2.95	1.50	1.42
78	S2	166	A2M	O2'-C2'	2.95	1.50	1.42
78	S2	468	A2M	O2'-C2'	2.95	1.50	1.42
79	L5	3825	A2M	O2'-C2'	2.95	1.50	1.42
79	L5	4498	OMU	O4-C4	-2.95	1.18	1.24
78	S2	484	A2M	C2'-C1'	2.95	1.60	1.53
78	S2	1031	A2M	O2'-C2'	2.94	1.50	1.42
78	S2	428	OMU	O4-C4	-2.94	1.18	1.24
79	L5	4306	OMU	O4-C4	-2.94	1.18	1.24
78	S2	576	A2M	O2'-C2'	2.94	1.50	1.42
79	L5	3925	OMU	O4-C4	-2.94	1.18	1.24
79	L5	2837	OMU	O4-C4	-2.93	1.18	1.24
79	L5	2363	A2M	O2'-C2'	2.92	1.50	1.42
78	S2	1832	6MZ	C5-C4	-2.92	1.33	1.39
79	L5	4590	A2M	O2'-C2'	2.92	1.50	1.42
78	S2	172	OMU	O4-C4	-2.92	1.18	1.24
79	L5	3830	A2M	O2'-C2'	2.92	1.50	1.42
78	S2	1383	A2M	C2'-C1'	2.92	1.60	1.53
79	L5	3785	A2M	O2'-C2'	2.92	1.50	1.42
78	S2	27	A2M	O2'-C2'	2.91	1.50	1.42
78	S2	121	OMU	O4-C4	-2.91	1.18	1.24
78	S2	512	A2M	O2'-C2'	2.91	1.50	1.42
79	L5	2815	A2M	O2'-C2'	2.90	1.50	1.42
79	L5	2401	A2M	C2'-C1'	2.90	1.60	1.53
79	L5	1871	A2M	O2'-C2'	2.90	1.50	1.42
78	S2	99	A2M	O2'-C2'	2.89	1.50	1.42
78	S2	1288	OMU	O4-C4	-2.88	1.18	1.24
78	S2	627	OMU	O4-C4	-2.88	1.18	1.24
79	L5	1534	A2M	O2'-C2'	2.88	1.50	1.42
79	L5	4220	6MZ	C5-C4	-2.86	1.33	1.39
79	L5	3867	A2M	O2'-C2'	2.85	1.49	1.42
78	S2	166	A2M	C2'-C1'	2.85	1.60	1.53
79	L5	4403	PSU	C6-C5	2.84	1.38	1.35
79	L5	398	A2M	O2'-C2'	2.84	1.49	1.42
78	S2	1288	OMU	C6-N1	2.84	1.44	1.38
78	S2	627	OMU	C6-N1	2.84	1.44	1.38
78	S2	428	OMU	C6-N1	2.83	1.44	1.38
79	L5	4306	OMU	C6-N1	2.82	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	S2	159	A2M	C2'-C1'	2.81	1.60	1.53
79	L5	3723	A2M	C2'-C1'	2.81	1.60	1.53
79	L5	4220	6MZ	C5-N7	-2.81	1.33	1.39
78	S2	1804	OMU	C6-N1	2.80	1.44	1.38
79	L5	3718	A2M	C2'-C1'	2.80	1.60	1.53
78	S2	576	A2M	C2'-C1'	2.80	1.60	1.53
79	L5	3785	A2M	C2'-C1'	2.80	1.60	1.53
78	S2	121	OMU	C6-N1	2.79	1.44	1.38
78	S2	468	A2M	C2'-C1'	2.79	1.60	1.53
79	L5	3785	A2M	C5-C4	-2.78	1.33	1.39
79	L5	3925	OMU	C6-N1	2.78	1.44	1.38
79	L5	1524	A2M	C2'-C1'	2.78	1.60	1.53
79	L5	398	A2M	C2'-C1'	2.77	1.60	1.53
79	L5	3830	A2M	C2'-C1'	2.77	1.60	1.53
79	L5	4523	A2M	C2'-C1'	2.77	1.60	1.53
79	L5	2837	OMU	C6-N1	2.76	1.44	1.38
78	S2	1326	UY1	C1'-C5	2.76	1.56	1.50
78	S2	512	A2M	C2'-C1'	2.76	1.60	1.53
78	S2	1851	MA6	C5-C4	-2.76	1.33	1.39
79	L5	4498	OMU	C6-N1	2.76	1.44	1.38
79	L5	2815	A2M	C2'-C1'	2.75	1.60	1.53
78	S2	172	OMU	C6-N1	2.74	1.44	1.38
79	L5	3818	UY1	C1'-C5	2.74	1.56	1.50
79	L5	4227	OMU	C6-N1	2.74	1.44	1.38
79	L5	1871	A2M	C5-C4	-2.74	1.33	1.39
78	S2	1031	A2M	C2'-C1'	2.74	1.60	1.53
79	L5	3724	A2M	C2'-C1'	2.73	1.60	1.53
79	L5	400	A2M	C2'-C1'	2.73	1.60	1.53
79	L5	2415	OMU	C6-N1	2.73	1.44	1.38
79	L5	4523	A2M	C5-C4	-2.72	1.33	1.39
78	S2	1031	A2M	C5-C4	-2.72	1.33	1.39
78	S2	99	A2M	C2'-C1'	2.72	1.60	1.53
78	S2	116	OMU	C6-N1	2.71	1.44	1.38
78	S2	354	OMU	C6-N1	2.71	1.44	1.38
78	S2	1832	6MZ	C5-N7	-2.71	1.33	1.39
78	S2	27	A2M	C2'-C1'	2.70	1.60	1.53
79	L5	1326	A2M	C2'-C1'	2.69	1.60	1.53
79	L5	1534	A2M	C5-C4	-2.69	1.34	1.39
76	Pt	47	G7M	C6-N1	2.69	1.43	1.38
78	S2	1678	A2M	C5-C4	-2.68	1.34	1.39
79	L5	2401	A2M	C5-C4	-2.68	1.34	1.39
79	L5	3867	A2M	C2'-C1'	2.68	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	L5	4590	A2M	C5-C4	-2.67	1.34	1.39
79	L5	1326	A2M	C5-C4	-2.67	1.34	1.39
79	L5	3825	A2M	C2'-C1'	2.67	1.59	1.53
78	S2	668	A2M	C5-C4	-2.67	1.34	1.39
79	L5	1524	A2M	C5-C4	-2.67	1.34	1.39
78	S2	1850	MA6	C5-C4	-2.67	1.34	1.39
78	S2	99	A2M	C5-C4	-2.66	1.34	1.39
79	L5	4571	A2M	C2'-C1'	2.66	1.59	1.53
78	S2	590	A2M	C2'-C1'	2.66	1.59	1.53
79	L5	4590	A2M	C2'-C1'	2.66	1.59	1.53
78	S2	512	A2M	C5-C4	-2.66	1.34	1.39
79	L5	4620	OMU	C6-N1	2.64	1.44	1.38
79	L5	2815	A2M	C5-C4	-2.64	1.34	1.39
79	L5	2363	A2M	C5-C4	-2.64	1.34	1.39
79	L5	3830	A2M	C5-C4	-2.64	1.34	1.39
79	L5	3724	A2M	C5-C4	-2.63	1.34	1.39
78	S2	1383	A2M	C5-C4	-2.63	1.34	1.39
78	S2	166	A2M	C5-C4	-2.63	1.34	1.39
78	S2	576	A2M	C5-C4	-2.62	1.34	1.39
78	S2	27	A2M	C5-C4	-2.62	1.34	1.39
79	L5	2363	A2M	C2'-C1'	2.62	1.59	1.53
79	L5	1871	A2M	C2'-C1'	2.61	1.59	1.53
78	S2	590	A2M	C5-C4	-2.61	1.34	1.39
79	L5	400	A2M	C5-C4	-2.61	1.34	1.39
79	L5	3825	A2M	C5-C4	-2.60	1.34	1.39
79	L5	398	A2M	C5-C4	-2.59	1.34	1.39
79	L5	3867	A2M	C5-C4	-2.59	1.34	1.39
79	L5	3723	A2M	C5-C4	-2.58	1.34	1.39
79	L5	4571	A2M	C5-C4	-2.58	1.34	1.39
78	S2	1639	G7M	C6-N1	2.58	1.43	1.38
78	S2	1326	UY1	O4-C4	-2.56	1.18	1.23
78	S2	468	A2M	C5-C4	-2.55	1.34	1.39
79	L5	3718	A2M	C5-C4	-2.54	1.34	1.39
78	S2	159	A2M	C5-C4	-2.53	1.34	1.39
78	S2	484	A2M	C5-C4	-2.53	1.34	1.39
79	L5	3818	UY1	O4-C4	-2.53	1.18	1.23
78	S2	1678	A2M	C2'-C1'	2.52	1.59	1.53
79	L5	1534	A2M	C2'-C1'	2.49	1.59	1.53
78	S2	1842	4AC	O2-C2	-2.48	1.19	1.23
78	S2	627	OMU	C5-C4	2.46	1.49	1.43
78	S2	1337	4AC	O2-C2	-2.46	1.19	1.23
79	L5	2837	OMU	C5-C4	2.44	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	S2	1288	OMU	C5-C4	2.44	1.49	1.43
78	S2	428	OMU	C5-C4	2.40	1.48	1.43
79	L5	4498	OMU	O2-C2	-2.40	1.18	1.23
78	S2	172	OMU	C5-C4	2.39	1.48	1.43
79	L5	4498	OMU	C5-C4	2.38	1.48	1.43
79	L5	4227	OMU	C5-C4	2.37	1.48	1.43
78	S2	1850	MA6	C5-N7	-2.36	1.34	1.39
79	L5	3925	OMU	C5-C4	2.36	1.48	1.43
79	L5	3925	OMU	O2-C2	-2.34	1.18	1.23
78	S2	1804	OMU	C5-C4	2.33	1.48	1.43
78	S2	1804	OMU	O2-C2	-2.32	1.18	1.23
79	L5	4306	OMU	C5-C4	2.31	1.48	1.43
78	S2	121	OMU	C5-C4	2.29	1.48	1.43
78	S2	354	OMU	C5-C4	2.28	1.48	1.43
79	L5	3718	A2M	C5-N7	-2.28	1.34	1.39
79	L5	4306	OMU	O2-C2	-2.27	1.18	1.23
79	L5	4620	OMU	O2-C2	-2.27	1.18	1.23
79	L5	4227	OMU	O2-C2	-2.27	1.18	1.23
78	S2	116	OMU	C5-C4	2.27	1.48	1.43
79	L5	2415	OMU	C5-C4	2.27	1.48	1.43
79	L5	2837	OMU	O2-C2	-2.25	1.18	1.23
78	S2	116	OMU	O2-C2	-2.24	1.18	1.23
78	S2	1842	4AC	O7-C7	-2.24	1.18	1.23
78	S2	428	OMU	O2-C2	-2.24	1.19	1.23
78	S2	354	OMU	O2-C2	-2.23	1.19	1.23
79	L5	4530	UR3	O4-C4	-2.21	1.18	1.23
79	L5	4620	OMU	C5-C4	2.21	1.48	1.43
79	L5	2415	OMU	O2-C2	-2.21	1.19	1.23
78	S2	121	OMU	O2-C2	-2.21	1.19	1.23
78	S2	172	OMU	O2-C2	-2.21	1.19	1.23
79	L5	4530	UR3	C5-C4	2.19	1.49	1.43
78	S2	1326	UY1	O2-C2	-2.18	1.18	1.23
79	L5	4530	UR3	O2-C2	-2.18	1.18	1.22
78	S2	1850	MA6	C8-N9	-2.17	1.33	1.37
78	S2	627	OMU	O2-C2	-2.16	1.19	1.23
78	S2	1337	4AC	O7-C7	-2.16	1.18	1.23
78	S2	1851	MA6	C5-N7	-2.16	1.34	1.39
78	S2	1288	OMU	O2-C2	-2.16	1.19	1.23
79	L5	3830	A2M	C5-N7	-2.15	1.35	1.39
79	L5	4530	UR3	C4-N3	2.15	1.45	1.40
79	L5	3818	UY1	O2-C2	-2.15	1.18	1.23
79	L5	3867	A2M	C5-N7	-2.15	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	S2	1248	B8N	O2-C2	-2.15	1.18	1.22
78	S2	484	A2M	C5-N7	-2.14	1.35	1.39
78	S2	668	A2M	C5-N7	-2.13	1.35	1.39
79	L5	2401	A2M	C5-N7	-2.13	1.35	1.39
79	L5	398	A2M	C5-N7	-2.13	1.35	1.39
78	S2	512	A2M	C5-N7	-2.12	1.35	1.39
78	S2	918	PSU	O4'-C1'	-2.12	1.40	1.43
79	L5	1871	A2M	C5-N7	-2.11	1.35	1.39
79	L5	400	A2M	C5-N7	-2.10	1.35	1.39
78	S2	668	A2M	O3'-C3'	2.09	1.47	1.43
79	L5	4571	A2M	C5-N7	-2.09	1.35	1.39
79	L5	4523	A2M	C5-N7	-2.09	1.35	1.39
79	L5	3724	A2M	C5-N7	-2.08	1.35	1.39
78	S2	1678	A2M	C5-N7	-2.08	1.35	1.39
78	S2	484	A2M	O3'-C3'	2.08	1.47	1.43
78	S2	1383	A2M	C5-N7	-2.08	1.35	1.39
79	L5	3785	A2M	C5-N7	-2.07	1.35	1.39
78	S2	27	A2M	C5-N7	-2.07	1.35	1.39
78	S2	1851	MA6	C8-N9	-2.06	1.33	1.37
78	S2	159	A2M	C5-N7	-2.06	1.35	1.39
78	S2	576	A2M	C5-N7	-2.06	1.35	1.39
79	L5	1326	A2M	C5-N7	-2.06	1.35	1.39
79	L5	1534	A2M	O3'-C3'	2.06	1.47	1.43
78	S2	468	A2M	C5-N7	-2.06	1.35	1.39
78	S2	99	A2M	C5-N7	-2.05	1.35	1.39
79	L5	3785	A2M	O3'-C3'	2.05	1.47	1.43
79	L5	3825	A2M	C5-N7	-2.05	1.35	1.39
76	Pt	8	4SU	O2-C2	-2.05	1.19	1.23
79	L5	1534	A2M	C5-N7	-2.04	1.35	1.39
79	L5	2363	A2M	C5-N7	-2.03	1.35	1.39
79	L5	4523	A2M	O3'-C3'	2.03	1.47	1.43
79	L5	2815	A2M	C5-N7	-2.03	1.35	1.39
78	S2	1031	A2M	C5-N7	-2.02	1.35	1.39
78	S2	99	A2M	O3'-C3'	2.02	1.47	1.43
79	L5	3723	A2M	C5-N7	-2.02	1.35	1.39
78	S2	576	A2M	O3'-C3'	2.01	1.47	1.43
78	S2	1248	B8N	C32-C31	2.01	1.56	1.52
79	L5	3724	A2M	O3'-C3'	2.00	1.47	1.43
79	L5	3718	A2M	O3'-C3'	2.00	1.47	1.43
78	S2	468	A2M	O3'-C3'	2.00	1.47	1.43

All (1072) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1851	MA6	N1-C6-N6	-14.02	101.76	117.08
78	S2	1850	MA6	N1-C6-N6	-12.80	103.09	117.08
79	L5	1524	A2M	C1'-N9-C8	-12.49	98.93	127.14
78	S2	590	A2M	C1'-N9-C8	-12.39	99.15	127.14
78	S2	1678	A2M	C1'-N9-C8	-11.53	101.09	127.14
79	L5	1534	A2M	C1'-N9-C8	-11.46	101.26	127.14
79	L5	3867	A2M	C1'-N9-C8	-11.41	101.36	127.14
79	L5	2815	A2M	C1'-N9-C8	-11.31	101.59	127.14
79	L5	3785	A2M	C1'-N9-C8	-11.20	101.85	127.14
79	L5	4571	A2M	C1'-N9-C8	-11.19	101.87	127.14
79	L5	3723	A2M	C1'-N9-C8	-11.11	102.04	127.14
79	L5	4220	6MZ	C1'-N9-C8	-11.11	102.06	127.14
79	L5	3724	A2M	C1'-N9-C8	-11.05	102.19	127.14
79	L5	400	A2M	C1'-N9-C8	-11.03	102.22	127.14
79	L5	2401	A2M	C1'-N9-C8	-11.02	102.25	127.14
79	L5	2363	A2M	C1'-N9-C8	-11.01	102.27	127.14
79	L5	1326	A2M	C1'-N9-C8	-11.01	102.27	127.14
79	L5	4590	A2M	C1'-N9-C8	-10.98	102.35	127.14
78	S2	1832	6MZ	C1'-N9-C8	-10.96	102.38	127.14
78	S2	159	A2M	C1'-N9-C8	-10.90	102.53	127.14
78	S2	1031	A2M	C1'-N9-C8	-10.88	102.56	127.14
78	S2	484	A2M	C1'-N9-C8	-10.87	102.58	127.14
79	L5	398	A2M	C1'-N9-C8	-10.87	102.60	127.14
78	S2	576	A2M	C1'-N9-C8	-10.83	102.68	127.14
78	S2	166	A2M	C1'-N9-C8	-10.81	102.72	127.14
78	S2	99	A2M	C1'-N9-C8	-10.77	102.81	127.14
79	L5	4523	A2M	C1'-N9-C8	-10.76	102.85	127.14
78	S2	27	A2M	C1'-N9-C8	-10.75	102.86	127.14
78	S2	512	A2M	C1'-N9-C8	-10.75	102.87	127.14
79	L5	3718	A2M	C1'-N9-C8	-10.71	102.95	127.14
78	S2	1383	A2M	C1'-N9-C8	-10.66	103.07	127.14
79	L5	1524	A2M	C4-N9-C1'	10.64	151.94	126.59
78	S2	468	A2M	C1'-N9-C8	-10.62	103.16	127.14
78	S2	590	A2M	C4-N9-C1'	10.62	151.89	126.59
79	L5	3825	A2M	C1'-N9-C8	-10.55	103.32	127.14
79	L5	1871	A2M	C1'-N9-C8	-10.52	103.39	127.14
78	S2	668	A2M	C1'-N9-C8	-10.51	103.40	127.14
79	L5	3830	A2M	C1'-N9-C8	-10.48	103.46	127.14
79	L5	3867	A2M	C4-N9-C1'	10.23	150.96	126.59
79	L5	4220	6MZ	C4-N9-C1'	10.16	150.81	126.59
78	S2	1678	A2M	C4-N9-C1'	10.11	150.67	126.59
79	L5	1534	A2M	C4-N9-C1'	10.06	150.57	126.59
79	L5	2815	A2M	C4-N9-C1'	10.05	150.53	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	4571	A2M	C4-N9-C1'	9.98	150.38	126.59
78	S2	1832	6MZ	C4-N9-C1'	9.94	150.26	126.59
78	S2	484	A2M	C4-N9-C1'	9.90	150.18	126.59
79	L5	3718	A2M	C4-N9-C1'	9.88	150.14	126.59
79	L5	3723	A2M	C4-N9-C1'	9.86	150.08	126.59
79	L5	3785	A2M	C4-N9-C1'	9.84	150.04	126.59
79	L5	400	A2M	C4-N9-C1'	9.83	150.02	126.59
79	L5	1326	A2M	C4-N9-C1'	9.81	149.97	126.59
79	L5	3724	A2M	C4-N9-C1'	9.80	149.95	126.59
78	S2	159	A2M	C4-N9-C1'	9.79	149.91	126.59
79	L5	2363	A2M	C4-N9-C1'	9.78	149.91	126.59
79	L5	398	A2M	C4-N9-C1'	9.76	149.85	126.59
79	L5	2401	A2M	C4-N9-C1'	9.75	149.83	126.59
78	S2	1031	A2M	C4-N9-C1'	9.64	149.56	126.59
78	S2	512	A2M	C4-N9-C1'	9.61	149.49	126.59
79	L5	4590	A2M	C4-N9-C1'	9.59	149.45	126.59
78	S2	27	A2M	C4-N9-C1'	9.59	149.44	126.59
78	S2	576	A2M	C4-N9-C1'	9.57	149.39	126.59
78	S2	99	A2M	C4-N9-C1'	9.55	149.34	126.59
78	S2	1383	A2M	C4-N9-C1'	9.54	149.31	126.59
78	S2	166	A2M	C4-N9-C1'	9.53	149.31	126.59
79	L5	4523	A2M	C4-N9-C1'	9.53	149.30	126.59
78	S2	468	A2M	C4-N9-C1'	9.48	149.19	126.59
79	L5	3825	A2M	C4-N9-C1'	9.45	149.11	126.59
79	L5	3830	A2M	C4-N9-C1'	9.38	148.93	126.59
78	S2	668	A2M	C4-N9-C1'	9.32	148.81	126.59
79	L5	1871	A2M	C4-N9-C1'	9.32	148.79	126.59
76	Pt	8	4SU	C4-N3-C2	-7.80	119.77	127.34
78	S2	1851	MA6	C5-C6-N6	7.62	138.58	125.30
78	S2	1850	MA6	C5-C6-N6	6.94	137.38	125.30
79	L5	1534	A2M	N6-C6-N1	-6.17	104.84	118.35
79	L5	4590	A2M	N6-C6-N1	-6.08	105.03	118.35
79	L5	3825	A2M	N6-C6-N1	-6.08	105.04	118.35
79	L5	2363	A2M	N6-C6-N1	-6.08	105.04	118.35
78	S2	590	A2M	N6-C6-N1	-6.06	105.07	118.35
78	S2	668	A2M	N6-C6-N1	-6.04	105.12	118.35
76	Pt	47	G7M	CN7-N7-C5	6.03	134.26	126.77
79	L5	2815	A2M	N6-C6-N1	-5.99	105.23	118.35
78	S2	166	A2M	N6-C6-N1	-5.99	105.24	118.35
78	S2	1639	G7M	CN7-N7-C5	5.99	134.21	126.77
78	S2	27	A2M	N6-C6-N1	-5.96	105.30	118.35
78	S2	159	A2M	N6-C6-N1	-5.96	105.31	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	400	A2M	N6-C6-N1	-5.95	105.31	118.35
79	L5	1524	A2M	N6-C6-N1	-5.95	105.33	118.35
79	L5	3718	A2M	N6-C6-N1	-5.94	105.34	118.35
79	L5	1871	A2M	N6-C6-N1	-5.93	105.35	118.35
78	S2	512	A2M	N6-C6-N1	-5.90	105.42	118.35
79	L5	3830	A2M	N6-C6-N1	-5.89	105.45	118.35
78	S2	99	A2M	N6-C6-N1	-5.88	105.46	118.35
78	S2	1031	A2M	N6-C6-N1	-5.88	105.47	118.35
79	L5	1326	A2M	N6-C6-N1	-5.88	105.48	118.35
79	L5	4523	A2M	N6-C6-N1	-5.87	105.49	118.35
79	L5	2401	A2M	N6-C6-N1	-5.87	105.50	118.35
79	L5	3723	A2M	N6-C6-N1	-5.86	105.51	118.35
78	S2	1678	A2M	N6-C6-N1	-5.86	105.52	118.35
79	L5	4571	A2M	N6-C6-N1	-5.84	105.55	118.35
79	L5	398	A2M	N6-C6-N1	-5.84	105.56	118.35
78	S2	484	A2M	N6-C6-N1	-5.82	105.60	118.35
78	S2	1383	A2M	N6-C6-N1	-5.81	105.62	118.35
79	L5	3867	A2M	N6-C6-N1	-5.81	105.63	118.35
79	L5	3724	A2M	N6-C6-N1	-5.80	105.64	118.35
78	S2	468	A2M	N6-C6-N1	-5.79	105.66	118.35
78	S2	576	A2M	N6-C6-N1	-5.77	105.71	118.35
79	L5	1871	A2M	N3-C2-N1	-5.74	119.62	128.60
79	L5	3785	A2M	N6-C6-N1	-5.74	105.79	118.35
78	S2	1851	MA6	N1-C2-N3	-5.72	119.65	128.60
79	L5	3724	A2M	N3-C2-N1	-5.64	119.79	128.60
78	S2	512	A2M	N3-C2-N1	-5.61	119.83	128.60
78	S2	166	A2M	N3-C2-N1	-5.61	119.83	128.60
79	L5	4590	A2M	N3-C2-N1	-5.60	119.83	128.60
78	S2	27	A2M	N3-C2-N1	-5.60	119.84	128.60
79	L5	4220	6MZ	N1-C2-N3	-5.60	119.85	128.60
79	L5	400	A2M	N3-C2-N1	-5.59	119.85	128.60
78	S2	1383	A2M	N3-C2-N1	-5.59	119.85	128.60
79	L5	3830	A2M	N3-C2-N1	-5.59	119.86	128.60
76	Pt	8	4SU	C5-C4-N3	5.57	119.86	114.69
78	S2	590	A2M	N3-C2-N1	-5.57	119.88	128.60
79	L5	3785	A2M	N3-C2-N1	-5.57	119.89	128.60
78	S2	1031	A2M	N3-C2-N1	-5.56	119.90	128.60
79	L5	1326	A2M	N3-C2-N1	-5.55	119.92	128.60
79	L5	1534	A2M	N3-C2-N1	-5.54	119.94	128.60
78	S2	99	A2M	N3-C2-N1	-5.54	119.94	128.60
79	L5	398	A2M	N3-C2-N1	-5.54	119.94	128.60
79	L5	4523	A2M	N3-C2-N1	-5.53	119.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	2363	A2M	N3-C2-N1	-5.52	119.97	128.60
78	S2	1832	6MZ	N1-C2-N3	-5.51	119.98	128.60
79	L5	2401	A2M	N3-C2-N1	-5.51	119.99	128.60
79	L5	2815	A2M	N3-C2-N1	-5.49	120.02	128.60
79	L5	3723	A2M	N3-C2-N1	-5.47	120.04	128.60
78	S2	159	A2M	N3-C2-N1	-5.46	120.06	128.60
78	S2	668	A2M	N3-C2-N1	-5.45	120.07	128.60
79	L5	1524	A2M	N3-C2-N1	-5.44	120.09	128.60
78	S2	468	A2M	N3-C2-N1	-5.43	120.11	128.60
79	L5	3718	A2M	C5-C4-N3	-5.42	119.67	126.75
79	L5	2837	OMU	C4-N3-C2	-5.42	119.43	126.58
78	S2	1678	A2M	N3-C2-N1	-5.41	120.14	128.60
78	S2	484	A2M	N3-C2-N1	-5.41	120.14	128.60
78	S2	1850	MA6	N1-C2-N3	-5.40	120.15	128.60
79	L5	4571	A2M	N3-C2-N1	-5.40	120.16	128.60
78	S2	1804	OMU	C4-N3-C2	-5.39	119.47	126.58
78	S2	668	A2M	C5-C6-N6	5.39	135.15	123.43
79	L5	4227	OMU	C4-N3-C2	-5.38	119.49	126.58
78	S2	172	OMU	C4-N3-C2	-5.36	119.51	126.58
79	L5	3867	A2M	C5-C4-N3	-5.34	119.78	126.75
79	L5	4590	A2M	C5-C6-N6	5.34	135.04	123.43
79	L5	2363	A2M	C5-C6-N6	5.33	135.03	123.43
78	S2	484	A2M	C5-C4-N3	-5.32	119.81	126.75
78	S2	576	A2M	N3-C2-N1	-5.32	120.28	128.60
79	L5	4498	OMU	C4-N3-C2	-5.32	119.57	126.58
78	S2	1850	MA6	C5-C4-N3	-5.30	119.83	126.75
78	S2	590	A2M	C5-C6-N6	5.30	134.95	123.43
79	L5	3825	A2M	C5-C6-N6	5.29	134.95	123.43
79	L5	3825	A2M	N3-C2-N1	-5.28	120.35	128.60
79	L5	2415	OMU	C4-N3-C2	-5.27	119.63	126.58
79	L5	1871	A2M	C5-C6-N6	5.26	134.89	123.43
79	L5	400	A2M	C5-C6-N6	5.26	134.88	123.43
79	L5	1534	A2M	C5-C6-N6	5.26	134.88	123.43
78	S2	159	A2M	C5-C6-N6	5.26	134.87	123.43
79	L5	3925	OMU	C4-N3-C2	-5.25	119.65	126.58
78	S2	27	A2M	C5-C6-N6	5.25	134.85	123.43
78	S2	428	OMU	C4-N3-C2	-5.25	119.66	126.58
79	L5	1524	A2M	C5-C6-N6	5.25	134.85	123.43
78	S2	166	A2M	C5-C6-N6	5.22	134.80	123.43
78	S2	1678	A2M	C5-C4-N3	-5.22	119.94	126.75
78	S2	354	OMU	C4-N3-C2	-5.21	119.70	126.58
79	L5	3718	A2M	C5-C6-N6	5.21	134.78	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	3830	A2M	C5-C6-N6	5.20	134.75	123.43
78	S2	1248	B8N	C5-C4-N3	5.20	125.80	116.17
78	S2	512	A2M	C5-C6-N6	5.20	134.75	123.43
79	L5	398	A2M	C5-C4-N3	-5.20	119.97	126.75
79	L5	2815	A2M	C5-C4-N3	-5.19	119.98	126.75
79	L5	4571	A2M	C5-C4-N3	-5.19	119.98	126.75
79	L5	4306	OMU	C4-N3-C2	-5.18	119.74	126.58
79	L5	2815	A2M	C5-C6-N6	5.18	134.71	123.43
79	L5	3867	A2M	N3-C2-N1	-5.18	120.50	128.60
78	S2	627	OMU	C4-N3-C2	-5.16	119.77	126.58
78	S2	576	A2M	C5-C6-N6	5.16	134.66	123.43
79	L5	3723	A2M	C5-C4-N3	-5.16	120.02	126.75
79	L5	2401	A2M	C5-C6-N6	5.16	134.65	123.43
79	L5	4571	A2M	C5-C6-N6	5.15	134.64	123.43
79	L5	3785	A2M	C5-C4-N3	-5.14	120.05	126.75
79	L5	1326	A2M	C5-C6-N6	5.13	134.59	123.43
79	L5	398	A2M	C5-C6-N6	5.12	134.57	123.43
79	L5	4523	A2M	C5-C6-N6	5.12	134.57	123.43
78	S2	1383	A2M	C5-C6-N6	5.12	134.56	123.43
78	S2	1832	6MZ	C5-C4-N3	-5.11	120.08	126.75
78	S2	1031	A2M	C5-C6-N6	5.10	134.54	123.43
79	L5	3723	A2M	C5-C6-N6	5.10	134.53	123.43
79	L5	3724	A2M	C5-C6-N6	5.10	134.53	123.43
79	L5	1534	A2M	C5-C4-N3	-5.09	120.11	126.75
78	S2	99	A2M	C5-C4-N3	-5.09	120.11	126.75
78	S2	468	A2M	C5-C6-N6	5.08	134.50	123.43
78	S2	159	A2M	C5-C4-N3	-5.08	120.12	126.75
79	L5	3724	A2M	C5-C4-N3	-5.08	120.13	126.75
78	S2	1678	A2M	C5-C6-N6	5.07	134.47	123.43
78	S2	512	A2M	C5-C4-N3	-5.07	120.14	126.75
78	S2	1031	A2M	C5-C4-N3	-5.06	120.14	126.75
79	L5	2401	A2M	C5-C4-N3	-5.06	120.14	126.75
79	L5	1326	A2M	C5-C4-N3	-5.06	120.15	126.75
78	S2	484	A2M	C5-C6-N6	5.06	134.44	123.43
78	S2	99	A2M	C5-C6-N6	5.06	134.44	123.43
78	S2	1288	OMU	C4-N3-C2	-5.05	119.92	126.58
79	L5	3867	A2M	C5-C6-N6	5.04	134.40	123.43
79	L5	3825	A2M	C5-C4-N3	-5.04	120.17	126.75
79	L5	400	A2M	C5-C4-N3	-5.04	120.18	126.75
79	L5	4523	A2M	C5-C4-N3	-5.03	120.19	126.75
79	L5	4220	6MZ	C5-C4-N3	-5.03	120.19	126.75
78	S2	1383	A2M	C5-C4-N3	-5.02	120.20	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	2363	A2M	C5-C4-N3	-5.01	120.21	126.75
78	S2	468	A2M	C5-C4-N3	-4.99	120.23	126.75
78	S2	166	A2M	C5-C4-N3	-4.99	120.24	126.75
78	S2	121	OMU	C4-N3-C2	-4.99	120.00	126.58
79	L5	4620	OMU	C4-N3-C2	-4.98	120.01	126.58
78	S2	27	A2M	C5-C4-N3	-4.98	120.25	126.75
78	S2	116	OMU	C4-N3-C2	-4.97	120.02	126.58
79	L5	3637	PSU	N1-C2-N3	4.97	120.76	115.13
79	L5	3718	A2M	N3-C2-N1	-4.93	120.90	128.60
79	L5	3830	A2M	C5-C4-N3	-4.88	120.38	126.75
79	L5	4628	PSU	N1-C2-N3	4.87	120.65	115.13
79	L5	3785	A2M	C5-C6-N6	4.86	134.02	123.43
78	S2	1851	MA6	C5-C4-N3	-4.85	120.42	126.75
79	L5	1524	A2M	N9-C8-N7	-4.84	107.30	113.91
79	L5	4457	PSU	C4-N3-C2	-4.83	119.37	126.34
78	S2	590	A2M	C5-C4-N3	-4.83	120.45	126.75
78	S2	668	A2M	C5-C4-N3	-4.83	120.45	126.75
79	L5	4590	A2M	C5-C4-N3	-4.82	120.47	126.75
78	S2	590	A2M	N9-C8-N7	-4.80	107.35	113.91
78	S2	576	A2M	C5-C4-N3	-4.80	120.49	126.75
79	L5	1871	A2M	C5-C4-N3	-4.79	120.50	126.75
79	L5	4403	PSU	C4-N3-C2	-4.78	119.45	126.34
78	S2	1326	UY1	C4-N3-C2	-4.70	119.57	126.34
79	L5	4500	PSU	N1-C2-N3	4.69	120.45	115.13
79	L5	4293	PSU	N1-C2-N3	4.69	120.44	115.13
79	L5	4521	PSU	C4-N3-C2	-4.68	119.59	126.34
76	Pt	47	G7M	CN7-N7-C8	-4.68	117.62	124.84
79	L5	1524	A2M	C5-C4-N3	-4.67	120.65	126.75
78	S2	1136	PSU	C4-N3-C2	-4.67	119.61	126.34
79	L5	3695	PSU	C4-N3-C2	-4.65	119.63	126.34
79	L5	4500	PSU	C4-N3-C2	-4.64	119.65	126.34
79	L5	4296	PSU	C4-N3-C2	-4.63	119.67	126.34
78	S2	1851	MA6	N9-C8-N7	-4.62	107.60	113.91
79	L5	4531	PSU	N1-C2-N3	4.61	120.36	115.13
78	S2	651	PSU	C4-N3-C2	-4.61	119.69	126.34
79	L5	4531	PSU	C4-N3-C2	-4.61	119.70	126.34
78	S2	1243	PSU	C4-N3-C2	-4.61	119.70	126.34
79	L5	3762	PSU	C4-N3-C2	-4.61	119.70	126.34
79	L5	4576	PSU	N1-C2-N3	4.60	120.34	115.13
78	S2	1239	PSU	C4-N3-C2	-4.60	119.71	126.34
79	L5	3851	PSU	N1-C2-N3	4.59	120.33	115.13
78	S2	1238	PSU	C4-N3-C2	-4.59	119.72	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	3637	PSU	C4-N3-C2	-4.59	119.73	126.34
79	L5	4628	PSU	C4-N3-C2	-4.59	119.73	126.34
79	L5	1862	PSU	C4-N3-C2	-4.59	119.73	126.34
79	L5	4293	PSU	C4-N3-C2	-4.59	119.73	126.34
79	L5	4552	PSU	C4-N3-C2	-4.59	119.73	126.34
79	L5	5001	PSU	N1-C2-N3	4.58	120.32	115.13
78	S2	1445	PSU	C4-N3-C2	-4.58	119.74	126.34
78	S2	815	PSU	C4-N3-C2	-4.58	119.75	126.34
78	S2	1639	G7M	CN7-N7-C8	-4.57	117.78	124.84
79	L5	4576	PSU	C4-N3-C2	-4.57	119.75	126.34
79	L5	3695	PSU	N1-C2-N3	4.57	120.31	115.13
79	L5	4353	PSU	C4-N3-C2	-4.57	119.75	126.34
78	S2	1347	PSU	C4-N3-C2	-4.57	119.75	126.34
78	S2	573	PSU	C4-N3-C2	-4.57	119.75	126.34
78	S2	406	PSU	C4-N3-C2	-4.56	119.76	126.34
78	S2	686	PSU	C4-N3-C2	-4.56	119.76	126.34
79	L5	4530	UR3	C4-N3-C2	-4.56	120.27	124.56
79	L5	5001	PSU	C4-N3-C2	-4.56	119.77	126.34
79	L5	2508	PSU	C4-N3-C2	-4.56	119.77	126.34
79	L5	3758	PSU	C4-N3-C2	-4.56	119.77	126.34
76	Pt	56	PSU	C4-N3-C2	-4.55	119.78	126.34
79	L5	3851	PSU	C4-N3-C2	-4.55	119.78	126.34
79	L5	1536	PSU	N1-C2-N3	4.55	120.29	115.13
79	L5	4457	PSU	N1-C2-N3	4.55	120.29	115.13
79	L5	3770	PSU	C4-N3-C2	-4.55	119.78	126.34
78	S2	1367	PSU	C4-N3-C2	-4.55	119.78	126.34
78	S2	1136	PSU	N1-C2-N3	4.54	120.28	115.13
79	L5	3639	PSU	N1-C2-N3	4.54	120.28	115.13
78	S2	1177	PSU	C4-N3-C2	-4.54	119.80	126.34
79	L5	3884	PSU	N1-C2-N3	4.53	120.27	115.13
79	L5	4296	PSU	N1-C2-N3	4.53	120.26	115.13
79	L5	4521	PSU	N1-C2-N3	4.53	120.26	115.13
78	S2	1056	PSU	C4-N3-C2	-4.53	119.81	126.34
78	S2	406	PSU	N1-C2-N3	4.53	120.26	115.13
79	L5	4552	PSU	N1-C2-N3	4.53	120.26	115.13
79	L5	2843	PSU	C4-N3-C2	-4.53	119.82	126.34
79	L5	3818	UY1	C4-N3-C2	-4.52	119.82	126.34
79	L5	3920	PSU	N1-C2-N3	4.52	120.25	115.13
78	S2	866	PSU	C4-N3-C2	-4.52	119.82	126.34
78	S2	1639	G7M	C2-N3-C4	4.52	120.36	112.30
79	L5	4353	PSU	N1-C2-N3	4.52	120.25	115.13
78	S2	649	PSU	C4-N3-C2	-4.52	119.83	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	1677	PSU	C4-N3-C2	-4.52	119.83	126.34
78	S2	1232	PSU	C4-N3-C2	-4.52	119.83	126.34
78	S2	1232	PSU	N1-C2-N3	4.52	120.25	115.13
78	S2	1243	PSU	N1-C2-N3	4.51	120.24	115.13
79	L5	1779	PSU	C4-N3-C2	-4.51	119.84	126.34
78	S2	1367	PSU	N1-C2-N3	4.51	120.24	115.13
78	S2	801	PSU	C4-N3-C2	-4.51	119.84	126.34
78	S2	109	PSU	C4-N3-C2	-4.51	119.84	126.34
79	L5	1536	PSU	C4-N3-C2	-4.51	119.84	126.34
79	L5	4972	PSU	C4-N3-C2	-4.51	119.84	126.34
79	L5	3762	PSU	N1-C2-N3	4.51	120.24	115.13
79	L5	4423	PSU	C4-N3-C2	-4.51	119.85	126.34
79	L5	4442	PSU	C4-N3-C2	-4.51	119.85	126.34
78	S2	1347	PSU	N1-C2-N3	4.50	120.23	115.13
79	L5	3853	PSU	C4-N3-C2	-4.50	119.86	126.34
78	S2	1244	PSU	C4-N3-C2	-4.50	119.86	126.34
78	S2	1004	PSU	N1-C2-N3	4.49	120.22	115.13
79	L5	3920	PSU	C4-N3-C2	-4.49	119.87	126.34
78	S2	34	PSU	C4-N3-C2	-4.49	119.87	126.34
78	S2	822	PSU	N1-C2-N3	4.49	120.22	115.13
79	L5	4673	PSU	C4-N3-C2	-4.49	119.87	126.34
78	S2	1643	PSU	N1-C2-N3	4.49	120.22	115.13
78	S2	651	PSU	N1-C2-N3	4.49	120.22	115.13
78	S2	815	PSU	N1-C2-N3	4.49	120.22	115.13
78	S2	1004	PSU	C4-N3-C2	-4.49	119.87	126.34
78	S2	1643	PSU	C4-N3-C2	-4.49	119.88	126.34
79	L5	1677	PSU	N1-C2-N3	4.49	120.21	115.13
79	L5	3884	PSU	C4-N3-C2	-4.48	119.88	126.34
79	L5	4423	PSU	N1-C2-N3	4.48	120.21	115.13
78	S2	1174	PSU	C4-N3-C2	-4.48	119.88	126.34
78	S2	218	PSU	C4-N3-C2	-4.48	119.89	126.34
79	L5	1744	PSU	C4-N3-C2	-4.48	119.89	126.34
78	S2	105	PSU	C4-N3-C2	-4.48	119.89	126.34
79	L5	4442	PSU	N1-C2-N3	4.48	120.20	115.13
78	S2	649	PSU	N1-C2-N3	4.47	120.20	115.13
79	L5	1779	PSU	N1-C2-N3	4.47	120.20	115.13
79	L5	4532	PSU	C4-N3-C2	-4.47	119.89	126.34
79	L5	4493	PSU	C4-N3-C2	-4.47	119.89	126.34
78	S2	1445	PSU	N1-C2-N3	4.47	120.20	115.13
78	S2	1081	PSU	C4-N3-C2	-4.47	119.90	126.34
79	L5	1782	PSU	C4-N3-C2	-4.47	119.90	126.34
79	L5	4361	PSU	C4-N3-C2	-4.47	119.90	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	1744	PSU	N1-C2-N3	4.47	120.19	115.13
78	S2	1692	PSU	C4-N3-C2	-4.47	119.90	126.34
79	L5	4431	PSU	C4-N3-C2	-4.47	119.90	126.34
79	L5	3715	PSU	C4-N3-C2	-4.46	119.91	126.34
78	S2	1238	PSU	N1-C2-N3	4.46	120.19	115.13
79	L5	1782	PSU	N1-C2-N3	4.46	120.19	115.13
5	L8	69	PSU	C4-N3-C2	-4.46	119.92	126.34
79	L5	1582	PSU	C4-N3-C2	-4.46	119.92	126.34
79	L5	3639	PSU	C4-N3-C2	-4.46	119.92	126.34
5	L8	69	PSU	N1-C2-N3	4.45	120.17	115.13
78	S2	34	PSU	N1-C2-N3	4.45	120.17	115.13
78	S2	1244	PSU	N1-C2-N3	4.45	120.17	115.13
79	L5	1860	PSU	N1-C2-N3	4.45	120.17	115.13
79	L5	3844	PSU	N1-C2-N3	4.45	120.17	115.13
5	L8	55	PSU	C4-N3-C2	-4.45	119.93	126.34
79	L5	1862	PSU	N1-C2-N3	4.44	120.17	115.13
79	L5	4312	PSU	N1-C2-N3	4.44	120.17	115.13
79	L5	4673	PSU	N1-C2-N3	4.44	120.16	115.13
5	L8	55	PSU	N1-C2-N3	4.44	120.16	115.13
79	L5	3715	PSU	N1-C2-N3	4.44	120.16	115.13
79	L5	2508	PSU	N1-C2-N3	4.44	120.16	115.13
79	L5	3853	PSU	N1-C2-N3	4.44	120.16	115.13
78	S2	36	PSU	N1-C2-N3	4.44	120.16	115.13
78	S2	1177	PSU	N1-C2-N3	4.44	120.16	115.13
79	L5	3764	PSU	N1-C2-N3	4.44	120.16	115.13
79	L5	4532	PSU	N1-C2-N3	4.44	120.16	115.13
78	S2	686	PSU	N1-C2-N3	4.44	120.16	115.13
78	S2	573	PSU	N1-C2-N3	4.43	120.15	115.13
78	S2	822	PSU	C4-N3-C2	-4.43	119.95	126.34
79	L5	3758	PSU	N1-C2-N3	4.43	120.15	115.13
79	L5	2843	PSU	N1-C2-N3	4.43	120.15	115.13
79	L5	4312	PSU	C4-N3-C2	-4.43	119.96	126.34
79	L5	4220	6MZ	C4-C5-C6	4.43	120.24	116.81
79	L5	1792	PSU	C4-N3-C2	-4.42	119.97	126.34
78	S2	918	PSU	N1-C2-N3	4.42	120.14	115.13
79	L5	3770	PSU	N1-C2-N3	4.41	120.13	115.13
76	Pt	47	G7M	C2-N3-C4	4.41	120.16	112.30
79	L5	2839	PSU	C4-N3-C2	-4.41	119.98	126.34
79	L5	4361	PSU	N1-C2-N3	4.41	120.13	115.13
79	L5	4636	PSU	N1-C2-N3	4.41	120.13	115.13
79	L5	2839	PSU	N1-C2-N3	4.41	120.13	115.13
79	L5	1860	PSU	C4-N3-C2	-4.41	119.99	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1625	PSU	C4-N3-C2	-4.41	119.99	126.34
78	S2	681	PSU	N1-C2-N3	4.41	120.12	115.13
78	S2	681	PSU	C4-N3-C2	-4.41	119.99	126.34
78	S2	109	PSU	N1-C2-N3	4.40	120.12	115.13
79	L5	4471	PSU	N1-C2-N3	4.40	120.12	115.13
78	S2	1056	PSU	N1-C2-N3	4.40	120.11	115.13
79	L5	4689	PSU	C4-N3-C2	-4.40	120.00	126.34
79	L5	1792	PSU	N1-C2-N3	4.39	120.11	115.13
78	S2	801	PSU	N1-C2-N3	4.39	120.11	115.13
76	Pt	56	PSU	N1-C2-N3	4.39	120.10	115.13
79	L5	4431	PSU	N1-C2-N3	4.39	120.10	115.13
79	L5	3764	PSU	C4-N3-C2	-4.39	120.01	126.34
79	L5	5010	PSU	C4-N3-C2	-4.39	120.01	126.34
79	L5	4590	A2M	N9-C8-N7	-4.39	107.91	113.91
79	L5	1582	PSU	N1-C2-N3	4.39	120.10	115.13
79	L5	4579	PSU	C4-N3-C2	-4.39	120.02	126.34
78	S2	572	PSU	C4-N3-C2	-4.38	120.02	126.34
78	S2	1174	PSU	N1-C2-N3	4.38	120.09	115.13
79	L5	4299	PSU	C4-N3-C2	-4.38	120.03	126.34
78	S2	36	PSU	C4-N3-C2	-4.38	120.03	126.34
78	S2	1239	PSU	N1-C2-N3	4.38	120.09	115.13
79	L5	4972	PSU	N1-C2-N3	4.38	120.09	115.13
79	L5	4299	PSU	N1-C2-N3	4.37	120.09	115.13
78	S2	1625	PSU	N1-C2-N3	4.37	120.08	115.13
78	S2	609	PSU	C4-N3-C2	-4.37	120.04	126.34
78	S2	572	PSU	N1-C2-N3	4.37	120.08	115.13
78	S2	609	PSU	N1-C2-N3	4.37	120.08	115.13
78	S2	863	PSU	N1-C2-N3	4.37	120.08	115.13
78	S2	1692	PSU	N1-C2-N3	4.37	120.08	115.13
78	S2	1678	A2M	N9-C8-N7	-4.36	107.95	113.91
79	L5	3768	PSU	C4-N3-C2	-4.36	120.05	126.34
79	L5	1683	PSU	C4-N3-C2	-4.36	120.06	126.34
78	S2	1248	B8N	C4-N3-C2	-4.36	119.95	125.46
79	L5	4493	PSU	N1-C2-N3	4.35	120.06	115.13
79	L5	3785	A2M	N9-C8-N7	-4.35	107.96	113.91
78	S2	863	PSU	C4-N3-C2	-4.35	120.07	126.34
78	S2	105	PSU	N1-C2-N3	4.35	120.06	115.13
78	S2	814	PSU	N1-C2-N3	4.35	120.06	115.13
79	L5	5010	PSU	N1-C2-N3	4.35	120.06	115.13
78	S2	918	PSU	C4-N3-C2	-4.35	120.08	126.34
78	S2	296	PSU	C4-N3-C2	-4.34	120.08	126.34
78	S2	814	PSU	C4-N3-C2	-4.34	120.08	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	166	A2M	N9-C8-N7	-4.34	107.98	113.91
78	S2	1081	PSU	N1-C2-N3	4.34	120.05	115.13
79	L5	1871	A2M	O4'-C1'-N9	4.34	116.61	108.06
79	L5	4403	PSU	N1-C2-N3	4.33	120.04	115.13
78	S2	866	PSU	N1-C2-N3	4.33	120.04	115.13
79	L5	3844	PSU	C4-N3-C2	-4.33	120.10	126.34
79	L5	3768	PSU	N1-C2-N3	4.32	120.03	115.13
78	S2	576	A2M	C2'-C1'-N9	-4.32	106.25	113.53
79	L5	4689	PSU	N1-C2-N3	4.32	120.02	115.13
79	L5	1683	PSU	N1-C2-N3	4.32	120.02	115.13
79	L5	1781	PSU	N1-C2-N3	4.31	120.02	115.13
79	L5	4579	PSU	N1-C2-N3	4.31	120.02	115.13
79	L5	1534	A2M	N9-C8-N7	-4.31	108.02	113.91
79	L5	4569	PSU	C4-N3-C2	-4.31	120.13	126.34
78	S2	93	PSU	N1-C2-N3	4.31	120.01	115.13
78	S2	966	PSU	N1-C2-N3	4.30	120.01	115.13
79	L5	2632	PSU	N1-C2-N3	4.30	120.00	115.13
79	L5	3729	PSU	C4-N3-C2	-4.30	120.14	126.34
78	S2	966	PSU	C4-N3-C2	-4.30	120.14	126.34
79	L5	4569	PSU	N1-C2-N3	4.29	119.99	115.13
78	S2	218	PSU	N1-C2-N3	4.29	119.98	115.13
79	L5	3830	A2M	O4'-C1'-N9	4.28	116.50	108.06
78	S2	93	PSU	C4-N3-C2	-4.28	120.17	126.34
78	S2	296	PSU	N1-C2-N3	4.27	119.97	115.13
79	L5	3729	PSU	N1-C2-N3	4.27	119.97	115.13
79	L5	4636	PSU	C4-N3-C2	-4.26	120.19	126.34
79	L5	1781	PSU	C4-N3-C2	-4.24	120.23	126.34
79	L5	2401	A2M	N9-C8-N7	-4.23	108.13	113.91
79	L5	2632	PSU	C4-N3-C2	-4.22	120.25	126.34
79	L5	4523	A2M	N9-C8-N7	-4.22	108.14	113.91
78	S2	99	A2M	N9-C8-N7	-4.22	108.15	113.91
79	L5	4471	PSU	C4-N3-C2	-4.21	120.27	126.34
79	L5	3723	A2M	N9-C8-N7	-4.21	108.16	113.91
78	S2	1850	MA6	N9-C8-N7	-4.21	108.16	113.91
78	S2	1031	A2M	N9-C8-N7	-4.20	108.17	113.91
78	S2	99	A2M	O4'-C1'-N9	4.20	116.34	108.06
79	L5	2363	A2M	N9-C8-N7	-4.20	108.17	113.91
78	S2	1639	G7M	C1'-N9-C4	4.19	138.96	126.50
79	L5	2815	A2M	N9-C8-N7	-4.18	108.19	113.91
78	S2	119	PSU	N1-C2-N3	4.18	119.87	115.13
78	S2	1639	G7M	C1'-N9-C8	-4.18	112.62	126.74
78	S2	576	A2M	N9-C8-N7	-4.18	108.19	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	3734	PSU	N1-C2-N3	4.18	119.86	115.13
78	S2	468	A2M	O4'-C1'-N9	4.18	116.29	108.06
78	S2	1639	G7M	C5-C4-N3	-4.17	120.14	128.15
79	L5	3718	A2M	O4'-C1'-N9	4.16	116.26	108.06
79	L5	1871	A2M	N9-C8-N7	-4.14	108.25	113.91
79	L5	3734	PSU	C4-N3-C2	-4.14	120.38	126.34
79	L5	3724	A2M	N9-C8-N7	-4.13	108.27	113.91
78	S2	1326	UY1	N1-C2-N3	4.12	119.80	115.13
78	S2	668	A2M	N9-C8-N7	-4.12	108.28	113.91
79	L5	3825	A2M	O4'-C1'-N9	4.11	116.17	108.06
78	S2	27	A2M	N9-C8-N7	-4.11	108.29	113.91
79	L5	400	A2M	N9-C8-N7	-4.10	108.31	113.91
79	L5	4571	A2M	N9-C8-N7	-4.09	108.31	113.91
79	L5	1326	A2M	N9-C8-N7	-4.08	108.33	113.91
79	L5	4498	OMU	N3-C2-N1	4.08	120.31	114.89
79	L5	4523	A2M	O4'-C1'-N9	4.08	116.10	108.06
78	S2	512	A2M	N9-C8-N7	-4.07	108.35	113.91
79	L5	3825	A2M	N9-C8-N7	-4.07	108.35	113.91
78	S2	119	PSU	C4-N3-C2	-4.07	120.48	126.34
76	Pt	47	G7M	C5-C4-N3	-4.05	120.39	128.15
78	S2	1383	A2M	N9-C8-N7	-4.05	108.38	113.91
78	S2	468	A2M	N9-C8-N7	-4.05	108.38	113.91
79	L5	4420	PSU	N1-C2-N3	4.05	119.71	115.13
78	S2	1031	A2M	O4'-C1'-N9	4.04	116.03	108.06
78	S2	166	A2M	O4'-C1'-N9	4.03	116.00	108.06
78	S2	1850	MA6	C4-C5-C6	4.03	120.39	115.88
79	L5	3818	UY1	N1-C2-N3	4.01	119.68	115.13
79	L5	4590	A2M	O4'-C1'-N9	4.00	115.95	108.06
78	S2	27	A2M	O4'-C1'-N9	4.00	115.95	108.06
79	L5	3830	A2M	N9-C8-N7	-3.99	108.45	113.91
79	L5	2837	OMU	N3-C2-N1	3.97	120.16	114.89
79	L5	398	A2M	N9-C8-N7	-3.97	108.49	113.91
79	L5	398	A2M	O4'-C1'-N9	3.96	115.87	108.06
78	S2	159	A2M	N9-C8-N7	-3.96	108.50	113.91
76	Pt	47	G7M	C1'-N9-C8	-3.96	113.38	126.74
79	L5	4420	PSU	C4-N3-C2	-3.95	120.64	126.34
78	S2	1383	A2M	O4'-C1'-N9	3.94	115.82	108.06
78	S2	1832	6MZ	N9-C8-N7	-3.94	108.53	113.91
78	S2	1639	G7M	C5-C6-N1	3.94	120.01	111.79
79	L5	3867	A2M	N9-C8-N7	-3.93	108.53	113.91
78	S2	172	OMU	N3-C2-N1	3.90	120.07	114.89
78	S2	512	A2M	O4'-C1'-N9	3.90	115.75	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	Pt	47	G7M	C5-C6-N1	3.89	119.92	111.79
79	L5	4227	OMU	N3-C2-N1	3.89	120.05	114.89
76	Pt	47	G7M	C1'-N9-C4	3.89	138.04	126.50
78	S2	1832	6MZ	C4-C5-C6	3.88	119.82	116.81
79	L5	3925	OMU	N3-C2-N1	3.88	120.04	114.89
79	L5	3723	A2M	O4'-C1'-N9	3.88	115.70	108.06
79	L5	3724	A2M	O4'-C1'-N9	3.87	115.69	108.06
79	L5	2363	A2M	O4'-C1'-N9	3.86	115.67	108.06
79	L5	2401	A2M	O4'-C1'-N9	3.81	115.57	108.06
78	S2	428	OMU	N3-C2-N1	3.76	119.89	114.89
78	S2	1804	OMU	N3-C2-N1	3.74	119.85	114.89
78	S2	484	A2M	N9-C8-N7	-3.73	108.81	113.91
76	Pt	8	4SU	N3-C2-N1	3.73	119.84	114.89
78	S2	1851	MA6	C2-N1-C6	3.73	120.56	111.75
78	S2	354	OMU	N3-C2-N1	3.72	119.82	114.89
79	L5	4571	A2M	O4'-C1'-N9	3.71	115.37	108.06
79	L5	4306	OMU	N3-C2-N1	3.68	119.78	114.89
79	L5	2415	OMU	N3-C2-N1	3.68	119.77	114.89
78	S2	1678	A2M	O4'-C1'-N9	3.66	115.28	108.06
78	S2	1832	6MZ	C9-N6-C6	-3.66	119.72	122.87
78	S2	627	OMU	N3-C2-N1	3.65	119.73	114.89
79	L5	1534	A2M	C2-N3-C4	3.64	120.35	111.75
79	L5	3785	A2M	C2-N3-C4	3.64	120.34	111.75
79	L5	2815	A2M	C2-N3-C4	3.63	120.32	111.75
79	L5	4620	OMU	N3-C2-N1	3.62	119.69	114.89
78	S2	484	A2M	C2-N3-C4	3.61	120.29	111.75
78	S2	166	A2M	C2-N3-C4	3.61	120.29	111.75
78	S2	1031	A2M	C2-N3-C4	3.61	120.28	111.75
79	L5	398	A2M	C2-N3-C4	3.61	120.27	111.75
78	S2	99	A2M	C2-N3-C4	3.60	120.27	111.75
78	S2	121	OMU	N3-C2-N1	3.60	119.67	114.89
78	S2	116	OMU	N3-C2-N1	3.59	119.66	114.89
78	S2	512	A2M	C2-N3-C4	3.59	120.23	111.75
79	L5	3724	A2M	C2-N3-C4	3.59	120.23	111.75
78	S2	159	A2M	O4'-C1'-N9	3.59	115.12	108.06
78	S2	1851	MA6	C2-N3-C4	3.58	120.21	111.75
79	L5	2351	OMC	C1'-N1-C2	3.58	126.41	118.42
79	L5	3723	A2M	C2-N3-C4	3.58	120.21	111.75
79	L5	1326	A2M	C2-N3-C4	3.57	120.19	111.75
78	S2	1678	A2M	C2-N3-C4	3.57	120.19	111.75
79	L5	400	A2M	C2-N3-C4	3.57	120.19	111.75
78	S2	27	A2M	C2-N3-C4	3.57	120.18	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1288	OMU	N3-C2-N1	3.57	119.62	114.89
78	S2	1850	MA6	C2-N1-C6	3.57	120.17	111.75
79	L5	4523	A2M	C2-N3-C4	3.57	120.17	111.75
79	L5	4571	A2M	C2-N3-C4	3.56	120.16	111.75
78	S2	1639	G7M	O6-C6-C5	-3.56	120.03	128.06
79	L5	2363	A2M	C2-N3-C4	3.56	120.15	111.75
78	S2	1383	A2M	C2-N3-C4	3.55	120.14	111.75
79	L5	4590	A2M	C2-N3-C4	3.55	120.14	111.75
78	S2	590	A2M	C2-N3-C4	3.55	120.13	111.75
76	Pt	47	G7M	O6-C6-C5	-3.54	120.07	128.06
79	L5	1871	A2M	C2-N3-C4	3.54	120.12	111.75
79	L5	3867	A2M	C2-N3-C4	3.54	120.12	111.75
79	L5	4220	6MZ	N9-C8-N7	-3.54	109.08	113.91
79	L5	2401	A2M	C2-N3-C4	3.54	120.10	111.75
78	S2	159	A2M	C2-N3-C4	3.52	120.08	111.75
78	S2	1832	6MZ	C2-N3-C4	3.51	120.05	111.75
78	S2	468	A2M	C2-N3-C4	3.51	120.05	111.75
79	L5	3718	A2M	N9-C8-N7	-3.50	109.13	113.91
79	L5	2815	A2M	O4'-C1'-N9	3.50	114.95	108.06
79	L5	3825	A2M	C2-N3-C4	3.49	120.01	111.75
78	S2	1804	OMU	C5-C4-N3	3.49	120.07	114.84
79	L5	3830	A2M	C2-N3-C4	3.48	119.98	111.75
79	L5	1326	A2M	O4'-C1'-N9	3.48	114.92	108.06
78	S2	576	A2M	O4'-C1'-N9	3.47	114.90	108.06
78	S2	1850	MA6	C2-N3-C4	3.46	119.92	111.75
79	L5	400	A2M	O4'-C1'-N9	3.46	114.87	108.06
79	L5	3718	A2M	C2-N3-C4	3.45	119.90	111.75
79	L5	2415	OMU	C5-C4-N3	3.44	119.98	114.84
78	S2	484	A2M	O4'-C1'-N9	3.43	114.82	108.06
79	L5	1524	A2M	C2-N3-C4	3.43	119.86	111.75
78	S2	668	A2M	C2-N3-C4	3.42	119.84	111.75
76	Pt	8	4SU	C5-C4-S4	-3.41	120.07	124.47
78	S2	576	A2M	C2-N3-C4	3.40	119.78	111.75
79	L5	4220	6MZ	C2-N3-C4	3.39	119.77	111.75
78	S2	428	OMU	C5-C4-N3	3.36	119.87	114.84
79	L5	4227	OMU	C5-C4-N3	3.36	119.87	114.84
79	L5	3925	OMU	C5-C4-N3	3.35	119.86	114.84
78	S2	354	OMU	C5-C4-N3	3.34	119.84	114.84
79	L5	4306	OMU	C5-C4-N3	3.34	119.84	114.84
78	S2	668	A2M	C2'-C1'-N9	3.33	119.14	113.53
79	L5	2837	OMU	C5-C4-N3	3.33	119.83	114.84
78	S2	1850	MA6	N3-C4-N9	3.31	132.53	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	627	OMU	C5-C4-N3	3.31	119.79	114.84
79	L5	3867	A2M	O4'-C1'-N9	3.29	114.54	108.06
79	L5	4620	OMU	C5-C4-N3	3.29	119.76	114.84
78	S2	1288	OMU	C5-C4-N3	3.29	119.76	114.84
79	L5	4498	OMU	C5-C4-N3	3.27	119.73	114.84
78	S2	590	A2M	C5-N7-C8	3.26	108.14	103.51
78	S2	116	OMU	C5-C4-N3	3.26	119.72	114.84
78	S2	121	OMU	C5-C4-N3	3.25	119.70	114.84
78	S2	1851	MA6	C5-N7-C8	3.25	108.13	103.51
78	S2	1851	MA6	C4-C5-C6	3.24	119.50	115.88
78	S2	172	OMU	C5-C4-N3	3.23	119.68	114.84
78	S2	1678	A2M	C5-N7-C8	3.18	108.03	103.51
78	S2	668	A2M	C4'-O4'-C1'	-3.18	102.46	109.47
79	L5	4590	A2M	C4'-O4'-C1'	-3.17	102.49	109.47
79	L5	1524	A2M	C5-N7-C8	3.16	108.00	103.51
76	Pt	21	H2U	C5-C4-N3	-3.16	113.10	116.65
79	L5	3818	UY1	C6-C5-C4	3.15	120.40	118.20
79	L5	1524	A2M	C4-N9-C8	3.14	109.13	105.73
78	S2	166	A2M	C5-N7-C8	3.09	107.90	103.51
79	L5	2363	A2M	C5-N7-C8	3.09	107.90	103.51
79	L5	3785	A2M	O4'-C1'-C2'	-3.07	101.18	106.57
79	L5	3867	A2M	N3-C4-N9	3.07	132.15	127.08
78	S2	1639	G7M	C2-N1-C6	-3.07	119.50	125.10
76	Pt	33	OMC	C1'-N1-C2	3.06	125.25	118.42
78	S2	1850	MA6	C5-N7-C8	3.06	107.85	103.51
79	L5	3723	A2M	C5-N7-C8	3.06	107.85	103.51
79	L5	4523	A2M	C4'-O4'-C1'	-3.05	102.73	109.47
79	L5	4523	A2M	C5-N7-C8	3.05	107.85	103.51
79	L5	2401	A2M	C5-N7-C8	3.04	107.83	103.51
79	L5	1534	A2M	C5-N7-C8	3.03	107.82	103.51
79	L5	4571	A2M	C5-N7-C8	3.03	107.82	103.51
78	S2	99	A2M	C5-N7-C8	3.02	107.80	103.51
79	L5	4590	A2M	C5-N7-C8	3.01	107.79	103.51
78	S2	1678	A2M	N3-C4-N9	3.01	132.05	127.08
76	Pt	47	G7M	C2-N1-C6	-3.01	119.61	125.10
79	L5	2815	A2M	C5-N7-C8	3.01	107.79	103.51
79	L5	3785	A2M	C5-N7-C8	3.01	107.78	103.51
78	S2	1031	A2M	C5-N7-C8	2.99	107.76	103.51
79	L5	3825	A2M	C5-N7-C8	2.99	107.76	103.51
78	S2	1639	G7M	N9-C4-N3	2.99	131.95	125.94
79	L5	3785	A2M	N3-C4-N9	2.99	132.00	127.08
79	L5	400	A2M	C5-N7-C8	2.98	107.75	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1326	UY1	C6-C5-C4	2.98	120.28	118.20
78	S2	590	A2M	C4-N9-C8	2.98	108.96	105.73
79	L5	2415	OMU	O4-C4-C5	-2.98	119.93	125.16
78	S2	1804	OMU	O4-C4-C5	-2.97	119.93	125.16
78	S2	166	A2M	C2'-C1'-N9	-2.97	108.53	113.53
78	S2	27	A2M	C5-N7-C8	2.96	107.72	103.51
78	S2	428	OMU	O4-C4-C5	-2.96	119.95	125.16
79	L5	1524	A2M	C2'-C1'-N9	-2.95	108.57	113.53
78	S2	576	A2M	C5-N7-C8	2.94	107.68	103.51
79	L5	4552	PSU	O2-C2-N1	-2.94	119.56	122.79
78	S2	1832	6MZ	C5-N7-C8	2.94	107.68	103.51
78	S2	512	A2M	C5-N7-C8	2.93	107.67	103.51
78	S2	668	A2M	C5-N7-C8	2.93	107.67	103.51
79	L5	1536	PSU	O2-C2-N1	-2.92	119.58	122.79
79	L5	1326	A2M	C5-N7-C8	2.92	107.66	103.51
79	L5	398	A2M	C5-N7-C8	2.91	107.65	103.51
79	L5	3724	A2M	C5-N7-C8	2.91	107.64	103.51
78	S2	468	A2M	C5-N7-C8	2.90	107.63	103.51
78	S2	512	A2M	C2'-C1'-N9	-2.90	108.65	113.53
78	S2	159	A2M	C5-N7-C8	2.89	107.61	103.51
79	L5	4620	OMU	O4-C4-C5	-2.88	120.09	125.16
79	L5	1871	A2M	C5-N7-C8	2.88	107.60	103.51
79	L5	4628	PSU	O2-C2-N1	-2.88	119.62	122.79
79	L5	4306	OMU	O4-C4-C5	-2.88	120.10	125.16
78	S2	1383	A2M	C5-N7-C8	2.88	107.60	103.51
78	S2	1248	B8N	N3-C2-N1	2.88	120.82	116.76
78	S2	354	OMU	O4-C4-C5	-2.88	120.10	125.16
79	L5	3867	A2M	C5-N7-C8	2.87	107.59	103.51
79	L5	3808	OMC	C1'-N1-C2	2.87	124.83	118.42
78	S2	590	A2M	N3-C4-N9	2.87	131.81	127.08
78	S2	172	OMU	O4-C4-C5	-2.87	120.12	125.16
76	Pt	47	G7M	N9-C4-N3	2.87	131.69	125.94
78	S2	590	A2M	C2'-C1'-N9	-2.86	108.71	113.53
79	L5	3925	OMU	O4-C4-C5	-2.86	120.13	125.16
78	S2	484	A2M	N3-C4-N9	2.86	131.79	127.08
79	L5	3830	A2M	C5-N7-C8	2.86	107.57	103.51
78	S2	627	OMU	O4-C4-C5	-2.85	120.15	125.16
79	L5	1524	A2M	N3-C4-N9	2.84	131.77	127.08
78	S2	121	OMU	O4-C4-C5	-2.84	120.16	125.16
79	L5	398	A2M	N3-C4-N9	2.84	131.77	127.08
79	L5	3723	A2M	N3-C4-N9	2.84	131.77	127.08
79	L5	2815	A2M	N3-C4-N9	2.84	131.76	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1842	4AC	C6-C5-C4	2.83	120.43	116.96
78	S2	116	OMU	O4-C4-C5	-2.83	120.18	125.16
79	L5	4220	6MZ	N3-C4-N9	2.83	131.74	127.08
79	L5	4571	A2M	N3-C4-N9	2.83	131.74	127.08
79	L5	1534	A2M	N3-C4-N9	2.82	131.74	127.08
79	L5	4576	PSU	O2-C2-N1	-2.82	119.69	122.79
78	S2	1337	4AC	C6-C5-C4	2.81	120.41	116.96
79	L5	3718	A2M	N3-C4-N9	2.81	131.72	127.08
79	L5	3724	A2M	N3-C4-N9	2.81	131.72	127.08
79	L5	4531	PSU	O2-C2-N1	-2.81	119.70	122.79
79	L5	3762	PSU	O2-C2-N1	-2.81	119.70	122.79
79	L5	3851	PSU	O2-C2-N1	-2.81	119.70	122.79
79	L5	2837	OMU	O4-C4-C5	-2.80	120.23	125.16
78	S2	1288	OMU	O4-C4-C5	-2.80	120.23	125.16
5	L8	55	PSU	O2-C2-N1	-2.78	119.72	122.79
78	S2	484	A2M	C5-N7-C8	2.78	107.46	103.51
78	S2	99	A2M	N3-C4-N9	2.78	131.67	127.08
79	L5	2401	A2M	N3-C4-N9	2.78	131.66	127.08
78	S2	1004	PSU	O2-C2-N1	-2.77	119.74	122.79
79	L5	2839	PSU	O2-C2-N1	-2.77	119.74	122.79
78	S2	36	PSU	O2-C2-N1	-2.77	119.74	122.79
78	S2	1031	A2M	N3-C4-N9	2.77	131.64	127.08
78	S2	1678	A2M	C4'-O4'-C1'	-2.77	103.37	109.47
79	L5	4227	OMU	O4-C4-C5	-2.77	120.30	125.16
79	L5	3844	PSU	O2-C2-N1	-2.76	119.75	122.79
78	S2	1383	A2M	C2'-C1'-N9	-2.76	108.88	113.53
79	L5	1326	A2M	N3-C4-N9	2.75	131.62	127.08
79	L5	3785	A2M	O4'-C1'-N9	2.75	113.48	108.06
79	L5	1779	PSU	O2-C2-N1	-2.75	119.76	122.79
79	L5	4523	A2M	N3-C4-N9	2.75	131.61	127.08
79	L5	3818	UY1	C6-N1-C2	-2.74	119.88	122.68
79	L5	3785	A2M	C4'-O4'-C1'	-2.74	103.43	109.47
78	S2	1832	6MZ	N3-C4-N9	2.73	131.57	127.08
78	S2	822	PSU	O2-C2-N1	-2.72	119.79	122.79
79	L5	3853	PSU	O2-C2-N1	-2.72	119.79	122.79
79	L5	400	A2M	N3-C4-N9	2.72	131.56	127.08
79	L5	4403	PSU	O2-C2-N1	-2.72	119.80	122.79
79	L5	3867	A2M	C4'-O4'-C1'	-2.71	103.48	109.47
78	S2	1232	PSU	O2-C2-N1	-2.71	119.80	122.79
78	S2	863	PSU	O2-C2-N1	-2.71	119.81	122.79
79	L5	1677	PSU	O2-C2-N1	-2.71	119.81	122.79
79	L5	3718	A2M	C5-N7-C8	2.71	107.36	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1326	UY1	C6-N1-C2	-2.71	119.91	122.68
78	S2	159	A2M	N3-C4-N9	2.71	131.55	127.08
78	S2	406	PSU	O2-C2-N1	-2.70	119.81	122.79
78	S2	1643	PSU	O2-C2-N1	-2.70	119.82	122.79
79	L5	4689	PSU	O2-C2-N1	-2.70	119.82	122.79
78	S2	1851	MA6	N3-C4-N9	2.69	131.52	127.08
78	S2	1136	PSU	O2-C2-N1	-2.69	119.83	122.79
78	S2	1243	PSU	O2-C2-N1	-2.69	119.83	122.79
78	S2	512	A2M	N3-C4-N9	2.69	131.52	127.08
78	S2	649	PSU	O2-C2-N1	-2.69	119.83	122.79
79	L5	3729	PSU	O2-C2-N1	-2.69	119.83	122.79
79	L5	1860	PSU	O2-C2-N1	-2.68	119.84	122.79
78	S2	1383	A2M	N3-C4-N9	2.68	131.50	127.08
78	S2	609	PSU	O2-C2-N1	-2.67	119.85	122.79
79	L5	4353	PSU	O2-C2-N1	-2.67	119.86	122.79
78	S2	1174	PSU	O2-C2-N1	-2.66	119.86	122.79
78	S2	1238	PSU	O2-C2-N1	-2.66	119.87	122.79
78	S2	1367	PSU	O2-C2-N1	-2.65	119.87	122.79
79	L5	3724	A2M	C4'-O4'-C1'	-2.65	103.62	109.47
79	L5	3764	PSU	O2-C2-N1	-2.65	119.87	122.79
79	L5	4628	PSU	C6-N1-C2	-2.65	119.97	122.68
78	S2	1692	PSU	O2-C2-N1	-2.65	119.87	122.79
79	L5	3770	PSU	O2-C2-N1	-2.65	119.88	122.79
79	L5	4498	OMU	O4-C4-C5	-2.65	120.50	125.16
5	L8	69	PSU	O2-C2-N1	-2.65	119.88	122.79
79	L5	4500	PSU	O2-C2-N1	-2.64	119.88	122.79
78	S2	468	A2M	N3-C4-N9	2.64	131.44	127.08
79	L5	2363	A2M	N3-C4-N9	2.64	131.44	127.08
78	S2	166	A2M	N3-C4-N9	2.64	131.43	127.08
79	L5	3884	PSU	O2-C2-N1	-2.64	119.88	122.79
78	S2	27	A2M	N3-C4-N9	2.64	131.43	127.08
78	S2	918	PSU	O2-C2-N1	-2.64	119.89	122.79
78	S2	801	PSU	O2-C2-N1	-2.63	119.89	122.79
79	L5	3639	PSU	O2-C2-N1	-2.63	119.89	122.79
79	L5	2351	OMC	C1'-N1-C6	-2.62	115.13	120.84
79	L5	1683	PSU	O2-C2-N1	-2.61	119.91	122.79
79	L5	4500	PSU	C6-C5-C4	2.61	120.03	118.20
79	L5	1782	PSU	O2-C2-N1	-2.61	119.91	122.79
78	S2	686	PSU	O2-C2-N1	-2.60	119.92	122.79
78	S2	1248	B8N	O4-C4-N3	-2.60	115.56	119.98
78	S2	651	PSU	O2-C2-N1	-2.60	119.93	122.79
79	L5	4220	6MZ	C5-N7-C8	2.59	107.19	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	1534	A2M	O4'-C1'-C2'	-2.59	102.03	106.57
79	L5	4312	PSU	O2-C2-N1	-2.58	119.95	122.79
79	L5	4636	PSU	O2-C2-N1	-2.58	119.95	122.79
79	L5	4673	PSU	O2-C2-N1	-2.58	119.95	122.79
78	S2	1244	PSU	O2-C2-N1	-2.58	119.95	122.79
78	S2	1177	PSU	O2-C2-N1	-2.58	119.95	122.79
79	L5	1871	A2M	C2'-C1'-N9	-2.57	109.20	113.53
79	L5	4590	A2M	N3-C4-N9	2.57	131.32	127.08
79	L5	1534	A2M	C2'-C1'-N9	2.57	117.86	113.53
78	S2	814	PSU	O2-C2-N1	-2.57	119.96	122.79
79	L5	3830	A2M	N3-C4-N9	2.57	131.31	127.08
78	S2	1347	PSU	O2-C2-N1	-2.57	119.97	122.79
78	S2	34	PSU	O2-C2-N1	-2.56	119.97	122.79
79	L5	2861	OMC	C1'-N1-C2	2.56	124.14	118.42
79	L5	1744	PSU	O2-C2-N1	-2.56	119.97	122.79
79	L5	4296	PSU	O2-C2-N1	-2.56	119.97	122.79
79	L5	4972	PSU	O2-C2-N1	-2.56	119.97	122.79
78	S2	1056	PSU	O2-C2-N1	-2.55	119.98	122.79
79	L5	3825	A2M	N3-C4-N9	2.55	131.29	127.08
78	S2	109	PSU	O2-C2-N1	-2.55	119.98	122.79
78	S2	1445	PSU	O2-C2-N1	-2.54	119.99	122.79
78	S2	296	PSU	O2-C2-N1	-2.54	119.99	122.79
79	L5	4521	PSU	O2-C2-N1	-2.54	119.99	122.79
79	L5	2401	A2M	C4'-O4'-C1'	-2.54	103.86	109.47
79	L5	4442	PSU	O2-C2-N1	-2.54	119.99	122.79
79	L5	4531	PSU	C6-C5-C4	2.53	119.97	118.20
79	L5	3758	PSU	O2-C2-N1	-2.53	120.00	122.79
79	L5	1871	A2M	N3-C4-N9	2.53	131.25	127.08
79	L5	1536	PSU	C6-N1-C2	-2.52	120.11	122.68
78	S2	572	PSU	O2-C2-N1	-2.52	120.02	122.79
79	L5	1792	PSU	O2-C2-N1	-2.52	120.02	122.79
79	L5	2401	A2M	C2'-C1'-N9	-2.52	109.29	113.53
78	S2	576	A2M	N3-C4-N9	2.52	131.23	127.08
78	S2	966	PSU	O2-C2-N1	-2.51	120.02	122.79
79	L5	4471	PSU	O2-C2-N1	-2.51	120.03	122.79
79	L5	4431	PSU	O2-C2-N1	-2.51	120.03	122.79
78	S2	573	PSU	O2-C2-N1	-2.51	120.03	122.79
78	S2	918	PSU	O4'-C1'-C2'	2.51	108.68	105.14
79	L5	2508	PSU	O2-C2-N1	-2.50	120.03	122.79
79	L5	3637	PSU	C6-N1-C2	-2.50	120.13	122.68
79	L5	4361	PSU	O2-C2-N1	-2.50	120.04	122.79
79	L5	4493	PSU	O2-C2-N1	-2.50	120.04	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	2632	PSU	O2-C2-N1	-2.50	120.04	122.79
78	S2	1851	MA6	C4-N9-C8	2.50	108.43	105.73
79	L5	4530	UR3	C6-N1-C2	-2.49	119.56	121.79
78	S2	1625	PSU	O2-C2-N1	-2.49	120.05	122.79
78	S2	863	PSU	C6-N1-C2	-2.49	120.14	122.68
76	Pt	56	PSU	O2-C2-N1	-2.48	120.06	122.79
78	S2	668	A2M	N3-C4-N9	2.48	131.18	127.08
79	L5	3734	PSU	O2-C2-N1	-2.48	120.06	122.79
79	L5	3768	PSU	O2-C2-N1	-2.48	120.06	122.79
79	L5	4532	PSU	O2-C2-N1	-2.48	120.06	122.79
79	L5	3715	PSU	O2-C2-N1	-2.47	120.07	122.79
78	S2	93	PSU	O2-C2-N1	-2.47	120.07	122.79
78	S2	36	PSU	C6-N1-C2	-2.46	120.17	122.68
79	L5	3844	PSU	C6-N1-C2	-2.46	120.17	122.68
79	L5	1524	A2M	C4'-O4'-C1'	-2.45	104.06	109.47
78	S2	119	PSU	C6-N1-C2	-2.45	120.18	122.68
78	S2	918	PSU	C6-N1-C2	-2.45	120.18	122.68
79	L5	3695	PSU	O2-C2-N1	-2.45	120.09	122.79
78	S2	1004	PSU	C6-N1-C2	-2.44	120.19	122.68
79	L5	3884	PSU	C6-N1-C2	-2.44	120.19	122.68
78	S2	166	A2M	C4'-O4'-C1'	-2.44	104.10	109.47
79	L5	4636	PSU	C6-N1-C2	-2.43	120.19	122.68
79	L5	4299	PSU	O2-C2-N1	-2.43	120.11	122.79
79	L5	5001	PSU	O2-C2-N1	-2.43	120.12	122.79
78	S2	609	PSU	C6-N1-C2	-2.43	120.20	122.68
79	L5	2876	OMG	CM2-O2'-C2'	2.43	120.89	114.52
79	L5	3718	A2M	C5-C4-N9	2.43	108.61	105.78
78	S2	815	PSU	O2-C2-N1	-2.43	120.12	122.79
79	L5	4420	PSU	O2-C2-N1	-2.43	120.12	122.79
79	L5	4579	PSU	O2-C2-N1	-2.43	120.12	122.79
79	L5	4590	A2M	C2'-C1'-N9	-2.42	109.45	113.53
78	S2	681	PSU	O2-C2-N1	-2.42	120.13	122.79
79	L5	2839	PSU	C6-N1-C2	-2.41	120.22	122.68
78	S2	1337	4AC	C5-C4-N3	-2.41	118.72	122.59
79	L5	4423	PSU	O2-C2-N1	-2.41	120.14	122.79
78	S2	1842	4AC	C5-C4-N3	-2.41	118.72	122.59
78	S2	1326	UY1	O2-C2-N1	-2.41	120.14	122.79
78	S2	866	PSU	O2-C2-N1	-2.40	120.15	122.79
79	L5	1781	PSU	O2-C2-N1	-2.40	120.15	122.79
79	L5	4293	PSU	C6-N1-C2	-2.40	120.23	122.68
79	L5	5001	PSU	C6-N1-C2	-2.40	120.23	122.68
79	L5	3920	PSU	O2-C2-N1	-2.40	120.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1232	PSU	C6-N1-C2	-2.40	120.23	122.68
79	L5	4500	PSU	C6-N1-C2	-2.39	120.24	122.68
78	S2	1383	A2M	C4'-O4'-C1'	-2.39	104.20	109.47
79	L5	3639	PSU	C6-N1-C2	-2.39	120.24	122.68
79	L5	3729	PSU	C6-N1-C2	-2.39	120.24	122.68
79	L5	1326	A2M	C4'-O4'-C1'	-2.39	104.21	109.47
78	S2	119	PSU	O2-C2-N1	-2.38	120.17	122.79
79	L5	1683	PSU	C6-N1-C2	-2.38	120.25	122.68
79	L5	4457	PSU	O2-C2-N1	-2.38	120.17	122.79
79	L5	4471	PSU	C6-N1-C2	-2.38	120.25	122.68
79	L5	5010	PSU	O2-C2-N1	-2.38	120.17	122.79
79	L5	2632	PSU	C6-N1-C2	-2.37	120.26	122.68
78	S2	296	PSU	C6-N1-C2	-2.37	120.26	122.68
79	L5	4569	PSU	O2-C2-N1	-2.37	120.18	122.79
79	L5	3825	A2M	C5-C4-N9	2.37	108.54	105.78
79	L5	3734	PSU	C6-N1-C2	-2.37	120.26	122.68
78	S2	1174	PSU	C6-N1-C2	-2.36	120.27	122.68
79	L5	1582	PSU	O2-C2-N1	-2.36	120.19	122.79
79	L5	2363	A2M	C4-C5-N7	-2.35	107.76	110.62
78	S2	105	PSU	O2-C2-N1	-2.34	120.21	122.79
79	L5	1862	PSU	O2-C2-N1	-2.34	120.21	122.79
5	L8	69	PSU	C6-N1-C2	-2.34	120.29	122.68
79	L5	4579	PSU	C6-N1-C2	-2.34	120.29	122.68
79	L5	4689	PSU	C6-N1-C2	-2.34	120.29	122.68
78	S2	406	PSU	C6-N1-C2	-2.33	120.30	122.68
79	L5	4293	PSU	O2-C2-N1	-2.33	120.22	122.79
79	L5	4673	PSU	C6-N1-C2	-2.33	120.30	122.68
76	Pt	33	OMC	C1'-N1-C6	-2.33	115.77	120.84
78	S2	1851	MA6	C4-C5-N7	-2.33	107.78	110.62
79	L5	3764	PSU	C6-N1-C2	-2.33	120.31	122.68
79	L5	3825	A2M	C4-C5-N7	-2.33	107.79	110.62
79	L5	3770	PSU	C6-N1-C2	-2.32	120.31	122.68
79	L5	3830	A2M	C2'-C1'-N9	-2.32	109.62	113.53
78	S2	649	PSU	C6-N1-C2	-2.32	120.31	122.68
79	L5	4312	PSU	C6-N1-C2	-2.32	120.31	122.68
78	S2	99	A2M	C4'-O4'-C1'	-2.31	104.36	109.47
78	S2	1239	PSU	O2-C2-N1	-2.31	120.24	122.79
78	S2	1248	B8N	O4'-C1'-C2'	2.31	108.40	105.14
5	L8	55	PSU	C6-N1-C2	-2.31	120.32	122.68
79	L5	4403	PSU	O4'-C1'-C2'	2.31	108.40	105.14
78	S2	590	A2M	C4-C5-N7	-2.30	107.81	110.62
79	L5	3768	PSU	C6-N1-C2	-2.30	120.33	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	166	A2M	C4-C5-N7	-2.30	107.82	110.62
79	L5	3920	PSU	C6-N1-C2	-2.30	120.33	122.68
79	L5	4552	PSU	C6-N1-C2	-2.29	120.34	122.68
78	S2	1244	PSU	C6-N1-C2	-2.29	120.34	122.68
78	S2	1643	PSU	C6-N1-C2	-2.29	120.34	122.68
79	L5	1779	PSU	C6-N1-C2	-2.29	120.34	122.68
79	L5	4423	PSU	C6-N1-C2	-2.29	120.34	122.68
79	L5	4442	PSU	C6-N1-C2	-2.29	120.34	122.68
78	S2	572	PSU	C6-N1-C2	-2.29	120.35	122.68
78	S2	681	PSU	C6-N1-C2	-2.29	120.35	122.68
78	S2	814	PSU	C6-N1-C2	-2.28	120.35	122.68
78	S2	1625	PSU	C6-N1-C2	-2.28	120.35	122.68
79	L5	2843	PSU	O2-C2-N1	-2.28	120.28	122.79
79	L5	4590	A2M	C4-N9-C8	2.28	108.20	105.73
78	S2	1367	PSU	C6-N1-C2	-2.28	120.35	122.68
79	L5	1860	PSU	C6-N1-C2	-2.28	120.35	122.68
78	S2	218	PSU	O2-C2-N1	-2.28	120.28	122.79
79	L5	4456	OMC	C1'-N1-C2	2.28	123.50	118.42
79	L5	3695	PSU	C6-N1-C2	-2.27	120.36	122.68
79	L5	4299	PSU	C6-N1-C2	-2.27	120.36	122.68
79	L5	1781	PSU	C6-N1-C2	-2.27	120.36	122.68
78	S2	1081	PSU	O2-C2-N1	-2.27	120.29	122.79
79	L5	3762	PSU	C6-N1-C2	-2.27	120.36	122.68
79	L5	1744	PSU	C6-N1-C2	-2.27	120.36	122.68
78	S2	1692	PSU	C6-N1-C2	-2.26	120.37	122.68
79	L5	4571	A2M	C4-C5-N7	-2.26	107.87	110.62
79	L5	4403	PSU	C6-C5-C4	2.26	119.78	118.20
79	L5	1677	PSU	C6-N1-C2	-2.26	120.38	122.68
79	L5	4353	PSU	C6-N1-C2	-2.26	120.38	122.68
78	S2	1678	A2M	C4-C5-N7	-2.25	107.87	110.62
79	L5	4531	PSU	C6-N1-C2	-2.25	120.38	122.68
79	L5	3718	A2M	C6-C5-C4	2.25	120.21	117.18
78	S2	573	PSU	C6-N1-C2	-2.25	120.38	122.68
79	L5	4361	PSU	C6-N1-C2	-2.25	120.38	122.68
78	S2	484	A2M	C5-C4-N9	2.25	108.40	105.78
78	S2	109	PSU	C6-N1-C2	-2.25	120.39	122.68
79	L5	4576	PSU	C6-N1-C2	-2.25	120.39	122.68
79	L5	4590	A2M	C4-C5-N7	-2.25	107.88	110.62
79	L5	4420	PSU	C6-N1-C2	-2.24	120.39	122.68
79	L5	2422	OMC	C1'-N1-C2	2.24	123.42	118.42
79	L5	4569	PSU	C6-N1-C2	-2.24	120.39	122.68
78	S2	172	OMU	O2-C2-N1	-2.24	119.81	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	822	PSU	C6-N1-C2	-2.24	120.39	122.68
78	S2	1804	OMU	O2-C2-N1	-2.23	119.82	122.79
79	L5	2815	A2M	C4-C5-N7	-2.23	107.90	110.62
79	L5	4532	PSU	C6-N1-C2	-2.23	120.40	122.68
78	S2	93	PSU	C6-N1-C2	-2.23	120.40	122.68
79	L5	3723	A2M	C4-C5-N7	-2.23	107.90	110.62
78	S2	34	PSU	C6-N1-C2	-2.23	120.41	122.68
78	S2	1136	PSU	C6-N1-C2	-2.23	120.41	122.68
79	L5	1782	PSU	C6-N1-C2	-2.23	120.41	122.68
78	S2	1678	A2M	C4-N9-C8	2.23	108.14	105.73
78	S2	1850	MA6	C4-N9-C8	2.23	108.14	105.73
78	S2	1177	PSU	C6-N1-C2	-2.23	120.41	122.68
78	S2	668	A2M	C5-C4-N9	2.22	108.37	105.78
78	S2	1238	PSU	C6-N1-C2	-2.22	120.41	122.68
79	L5	3715	PSU	C6-N1-C2	-2.22	120.42	122.68
78	S2	1031	A2M	C2'-C1'-N9	-2.22	109.80	113.53
78	S2	576	A2M	C4-C5-N7	-2.21	107.92	110.62
79	L5	1534	A2M	C4-C5-N7	-2.21	107.93	110.62
78	S2	686	PSU	C6-N1-C2	-2.21	120.42	122.68
79	L5	2363	A2M	C5-C4-N9	2.21	108.35	105.78
78	S2	512	A2M	C5-C4-N9	2.21	108.35	105.78
79	L5	2401	A2M	C4-C5-N7	-2.20	107.93	110.62
78	S2	1056	PSU	C6-N1-C2	-2.20	120.43	122.68
78	S2	1832	6MZ	C5-C4-N9	2.20	108.34	105.78
78	S2	668	A2M	C4-C5-N7	-2.20	107.94	110.62
79	L5	400	A2M	C4-C5-N7	-2.20	107.94	110.62
79	L5	5010	PSU	C6-N1-C2	-2.20	120.44	122.68
78	S2	966	PSU	C6-N1-C2	-2.20	120.44	122.68
79	L5	3785	A2M	C4-N9-C8	2.20	108.11	105.73
78	S2	801	PSU	C6-N1-C2	-2.19	120.44	122.68
79	L5	4431	PSU	C6-N1-C2	-2.19	120.44	122.68
78	S2	159	A2M	C5-C4-N9	2.19	108.33	105.78
79	L5	400	A2M	C4'-O4'-C1'	-2.19	104.64	109.47
79	L5	2815	A2M	C4'-O4'-C1'	-2.19	104.64	109.47
78	S2	166	A2M	C5-C4-N9	2.19	108.33	105.78
78	S2	468	A2M	C5-C4-N9	2.19	108.33	105.78
79	L5	4523	A2M	C4-C5-N7	-2.19	107.96	110.62
78	S2	1347	PSU	C6-N1-C2	-2.19	120.45	122.68
79	L5	3853	PSU	C6-N1-C2	-2.18	120.45	122.68
78	S2	27	A2M	C5-C4-N9	2.18	108.32	105.78
79	L5	2837	OMU	O2-C2-N1	-2.18	119.88	122.79
79	L5	4523	A2M	O4'-C4'-C3'	-2.18	100.80	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	4628	PSU	C6-C5-C4	2.18	119.72	118.20
78	S2	27	A2M	C4-C5-N7	-2.18	107.96	110.62
78	S2	1842	4AC	N4-C4-N3	2.18	117.51	113.85
78	S2	512	A2M	O4'-C1'-C2'	-2.18	102.75	106.57
78	S2	815	PSU	C6-N1-C2	-2.18	120.46	122.68
78	S2	354	OMU	O2-C2-N1	-2.17	119.89	122.79
79	L5	3818	UY1	O2-C2-N1	-2.17	120.40	122.79
79	L5	4521	PSU	C6-N1-C2	-2.17	120.46	122.68
79	L5	4420	PSU	O4'-C1'-C2'	2.17	108.21	105.14
78	S2	116	OMU	O2-C2-N1	-2.17	119.90	122.79
79	L5	3830	A2M	C5-C4-N9	2.17	108.31	105.78
78	S2	1136	PSU	C6-C5-C4	2.17	119.72	118.20
78	S2	1031	A2M	C4-C5-N7	-2.17	107.98	110.62
79	L5	3925	OMU	O2-C2-N1	-2.17	119.90	122.79
79	L5	1534	A2M	C4-N9-C8	2.17	108.08	105.73
78	S2	99	A2M	C4-C5-N7	-2.17	107.98	110.62
78	S2	1243	PSU	C6-N1-C2	-2.16	120.47	122.68
78	S2	1445	PSU	C6-N1-C2	-2.16	120.47	122.68
78	S2	651	PSU	C6-N1-C2	-2.16	120.47	122.68
79	L5	2843	PSU	C6-N1-C2	-2.16	120.47	122.68
78	S2	105	PSU	C6-N1-C2	-2.16	120.47	122.68
78	S2	468	A2M	C4'-O4'-C1'	-2.16	104.71	109.47
79	L5	3718	A2M	C4-C5-N7	-2.16	107.99	110.62
78	S2	1383	A2M	C5-C4-N9	2.16	108.29	105.78
79	L5	4442	PSU	O4'-C1'-C2'	2.16	108.19	105.14
78	S2	468	A2M	C2'-C1'-N9	-2.16	109.90	113.53
79	L5	3723	A2M	C4'-O4'-C1'	-2.16	104.72	109.47
79	L5	1524	A2M	C4-C5-N7	-2.15	107.99	110.62
79	L5	3758	PSU	C6-N1-C2	-2.15	120.48	122.68
78	S2	159	A2M	C4-C5-N7	-2.15	108.00	110.62
78	S2	512	A2M	C4-C5-N7	-2.15	108.00	110.62
79	L5	1322	1MA	N1-C6-N6	2.15	125.23	119.77
79	L5	3851	PSU	C6-N1-C2	-2.15	120.49	122.68
78	S2	468	A2M	C4-C5-N7	-2.14	108.01	110.62
78	S2	576	A2M	C5-C4-N9	2.14	108.28	105.78
79	L5	3808	OMC	C1'-N1-C6	-2.14	116.17	120.84
79	L5	4571	A2M	C5-C4-N9	2.14	108.27	105.78
79	L5	4296	PSU	C6-N1-C2	-2.14	120.50	122.68
79	L5	3764	PSU	O4'-C1'-C2'	2.13	108.15	105.14
79	L5	2508	PSU	C6-N1-C2	-2.13	120.50	122.68
79	L5	4306	OMU	O2-C2-N1	-2.13	119.95	122.79
79	L5	398	A2M	C5-C4-N9	2.13	108.26	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	L5	400	A2M	C5-C4-N9	2.13	108.26	105.78
79	L5	1792	PSU	C6-N1-C2	-2.13	120.51	122.68
79	L5	2815	A2M	C5-C4-N9	2.13	108.26	105.78
79	L5	1871	A2M	C5-C4-N9	2.13	108.25	105.78
79	L5	2824	OMC	C1'-N1-C2	2.13	123.16	118.42
79	L5	1326	A2M	C4-C5-N7	-2.13	108.03	110.62
79	L5	3637	PSU	O2-C2-N1	-2.12	120.45	122.79
79	L5	1871	A2M	C4'-O4'-C1'	-2.12	104.80	109.47
78	S2	1239	PSU	C6-N1-C2	-2.11	120.52	122.68
79	L5	3825	A2M	C4'-O4'-C1'	-2.11	104.81	109.47
79	L5	4620	OMU	O2-C2-N1	-2.11	119.98	122.79
79	L5	398	A2M	C4-C5-N7	-2.11	108.05	110.62
5	L8	69	PSU	O4'-C1'-C2'	2.11	108.12	105.14
79	L5	2363	A2M	C4'-O4'-C1'	-2.11	104.82	109.47
79	L5	1326	A2M	C5-C4-N9	2.11	108.23	105.78
78	S2	822	PSU	O4'-C1'-C2'	2.11	108.11	105.14
79	L5	4636	PSU	O4'-C1'-C2'	2.10	108.11	105.14
79	L5	4493	PSU	C6-N1-C2	-2.10	120.54	122.68
78	S2	218	PSU	C6-N1-C2	-2.10	120.54	122.68
79	L5	3830	A2M	C4-C5-N7	-2.10	108.06	110.62
78	S2	99	A2M	C2'-C1'-N9	-2.09	110.00	113.53
78	S2	99	A2M	C5-C4-N9	2.09	108.22	105.78
78	S2	1031	A2M	C5-C4-N9	2.09	108.22	105.78
79	L5	1871	A2M	C4-C5-N7	-2.09	108.07	110.62
79	L5	3867	A2M	C6-C5-C4	2.09	119.99	117.18
79	L5	4590	A2M	C5-C4-N9	2.09	108.21	105.78
79	L5	3723	A2M	C5-C4-N9	2.09	108.21	105.78
79	L5	4523	A2M	C5-C4-N9	2.08	108.20	105.78
79	L5	2401	A2M	C5-C4-N9	2.07	108.19	105.78
79	L5	3724	A2M	C4-C5-N7	-2.07	108.09	110.62
78	S2	166	A2M	C4-N9-C8	2.07	107.97	105.73
78	S2	484	A2M	C4-C5-N7	-2.07	108.09	110.62
78	S2	1832	6MZ	C4-C5-N7	-2.07	108.10	110.62
78	S2	1081	PSU	C6-N1-C2	-2.07	120.57	122.68
78	S2	121	OMU	O2-C2-N1	-2.07	120.04	122.79
79	L5	4457	PSU	C6-N1-C2	-2.06	120.58	122.68
79	L5	4972	PSU	C6-N1-C2	-2.06	120.58	122.68
79	L5	1862	PSU	C6-N1-C2	-2.06	120.58	122.68
78	S2	1445	PSU	C6-C5-C4	2.06	119.64	118.20
79	L5	1582	PSU	C6-N1-C2	-2.06	120.58	122.68
78	S2	1031	A2M	C4'-O4'-C1'	-2.06	104.93	109.47
79	L5	4457	PSU	O4'-C1'-C2'	2.06	108.04	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1383	A2M	C4-C5-N7	-2.05	108.12	110.62
79	L5	4227	OMU	O2-C2-N1	-2.05	120.06	122.79
78	S2	218	PSU	O4'-C1'-C2'	2.04	108.02	105.14
79	L5	1534	A2M	C5-C4-N9	2.04	108.15	105.78
79	L5	3724	A2M	C5-C4-N9	2.04	108.15	105.78
79	L5	3715	PSU	O4'-C1'-C2'	2.03	108.01	105.14
78	S2	576	A2M	C4-N9-C8	2.03	107.92	105.73
79	L5	4571	A2M	C6-C5-C4	2.03	119.91	117.18
78	S2	866	PSU	C6-N1-C2	-2.03	120.61	122.68
79	L5	1677	PSU	C6-C5-C4	2.02	119.61	118.20
79	L5	2401	A2M	C4-N9-C8	2.02	107.92	105.73
46	La	39	V5N	O-C-CA	-2.02	119.48	124.78
78	S2	1337	4AC	N4-C4-N3	2.02	117.24	113.85
79	L5	3867	A2M	C4-C5-N7	-2.02	108.16	110.62
76	Pt	56	PSU	C6-N1-C2	-2.01	120.62	122.68
1	LA	216	V5N	O-C-CA	-2.01	119.50	124.78
78	S2	1081	PSU	O4'-C1'-C2'	2.01	107.98	105.14
78	S2	1643	PSU	C6-C5-C4	2.01	119.60	118.20
79	L5	4498	OMU	O2-C2-N1	-2.00	120.12	122.79
78	S2	1643	PSU	O4'-C1'-C2'	2.00	107.97	105.14
78	S2	1842	4AC	CM7-C7-N4	2.00	118.75	115.29

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	LA	216	V5N	O-C-CA-CB
46	La	39	V5N	O2-CB-CG-CD2
61	Lb	5	MLZ	N-CA-CB-CG
61	Lb	5	MLZ	C-CA-CB-CG
74	Lo	53	MLZ	O-C-CA-CB
76	Pt	21	H2U	O4'-C1'-N1-C6
78	S2	27	A2M	C1'-C2'-O2'-CM'
78	S2	99	A2M	O4'-C4'-C5'-O5'
78	S2	99	A2M	C1'-C2'-O2'-CM'
78	S2	354	OMU	C1'-C2'-O2'-CM2
78	S2	468	A2M	C1'-C2'-O2'-CM'
78	S2	484	A2M	C1'-C2'-O2'-CM'
78	S2	512	A2M	O4'-C4'-C5'-O5'
78	S2	512	A2M	C1'-C2'-O2'-CM'
78	S2	576	A2M	C3'-C4'-C5'-O5'
78	S2	601	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
78	S2	644	OMG	O4'-C4'-C5'-O5'
78	S2	668	A2M	C3'-C4'-C5'-O5'
78	S2	683	OMG	O4'-C4'-C5'-O5'
78	S2	683	OMG	C3'-C4'-C5'-O5'
78	S2	822	PSU	C3'-C4'-C5'-O5'
78	S2	822	PSU	O4'-C4'-C5'-O5'
78	S2	1248	B8N	N34-C33-C34-O35
78	S2	1248	B8N	C31-C32-C33-N34
78	S2	1326	UY1	C2'-C1'-C5-C6
78	S2	1326	UY1	O4'-C1'-C5-C6
78	S2	1328	OMG	C1'-C2'-O2'-CM2
78	S2	1383	A2M	C1'-C2'-O2'-CM'
78	S2	1678	A2M	C1'-C2'-O2'-CM'
78	S2	1804	OMU	C1'-C2'-O2'-CM2
78	S2	1851	MA6	O4'-C4'-C5'-O5'
79	L5	398	A2M	O4'-C4'-C5'-O5'
79	L5	398	A2M	C1'-C2'-O2'-CM'
79	L5	2351	OMC	C1'-C2'-O2'-CM2
79	L5	2415	OMU	C1'-C2'-O2'-CM2
79	L5	2815	A2M	C3'-C4'-C5'-O5'
79	L5	2824	OMC	C1'-C2'-O2'-CM2
79	L5	2876	OMG	C1'-C2'-O2'-CM2
79	L5	3701	OMC	C2'-C1'-N1-C6
79	L5	3723	A2M	C1'-C2'-O2'-CM'
79	L5	3724	A2M	C1'-C2'-O2'-CM'
79	L5	3825	A2M	C1'-C2'-O2'-CM'
79	L5	3867	A2M	C1'-C2'-O2'-CM'
79	L5	3925	OMU	C1'-C2'-O2'-CM2
79	L5	4220	6MZ	C5-C6-N6-C9
79	L5	4220	6MZ	N1-C6-N6-C9
79	L5	4420	PSU	C2'-C1'-C5-C4
79	L5	4420	PSU	C2'-C1'-C5-C6
79	L5	4523	A2M	C1'-C2'-O2'-CM'
79	L5	4571	A2M	C1'-C2'-O2'-CM'
79	L5	4620	OMU	C1'-C2'-O2'-CM2
79	L5	4636	PSU	C3'-C4'-C5'-O5'
79	L5	4637	OMG	O4'-C4'-C5'-O5'
79	L5	4637	OMG	C1'-C2'-O2'-CM2
79	L5	3701	OMC	C2'-C1'-N1-C2
79	L5	4590	A2M	C4'-C5'-O5'-P
78	S2	99	A2M	C3'-C4'-C5'-O5'
78	S2	590	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
78	S2	590	A2M	C3'-C4'-C5'-O5'
78	S2	644	OMG	C3'-C4'-C5'-O5'
78	S2	668	A2M	O4'-C4'-C5'-O5'
78	S2	918	PSU	O4'-C4'-C5'-O5'
78	S2	1243	PSU	O4'-C4'-C5'-O5'
78	S2	1851	MA6	C3'-C4'-C5'-O5'
79	L5	2876	OMG	C3'-C4'-C5'-O5'
79	L5	3785	A2M	O4'-C4'-C5'-O5'
79	L5	3785	A2M	C3'-C4'-C5'-O5'
79	L5	4636	PSU	O4'-C4'-C5'-O5'
79	L5	4637	OMG	C3'-C4'-C5'-O5'
61	Lb	5	MLZ	CG-CD-CE-NZ
78	S2	159	A2M	O4'-C4'-C5'-O5'
78	S2	468	A2M	O4'-C4'-C5'-O5'
78	S2	512	A2M	C3'-C4'-C5'-O5'
78	S2	576	A2M	O4'-C4'-C5'-O5'
78	S2	918	PSU	C3'-C4'-C5'-O5'
78	S2	1243	PSU	C3'-C4'-C5'-O5'
79	L5	398	A2M	C3'-C4'-C5'-O5'
79	L5	2815	A2M	O4'-C4'-C5'-O5'
79	L5	2876	OMG	O4'-C4'-C5'-O5'
79	L5	3729	PSU	O4'-C4'-C5'-O5'
79	L5	4228	OMG	O4'-C4'-C5'-O5'
79	L5	4228	OMG	C3'-C4'-C5'-O5'
79	L5	4420	PSU	O4'-C4'-C5'-O5'
79	L5	4532	PSU	C3'-C4'-C5'-O5'
76	Pt	21	H2U	C2'-C1'-N1-C6
78	S2	428	OMU	C2'-C1'-N1-C6
78	S2	1639	G7M	C3'-C4'-C5'-O5'
78	S2	1248	B8N	N34-C33-C34-O36
76	Pt	21	H2U	C2'-C1'-N1-C2
78	S2	1447	OMG	C3'-C4'-C5'-O5'
79	L5	4532	PSU	O4'-C4'-C5'-O5'
61	Lb	5	MLZ	CE-CD-CG-CB
78	S2	428	OMU	O4'-C4'-C5'-O5'
78	S2	1639	G7M	O4'-C4'-C5'-O5'
79	L5	2364	OMG	O4'-C4'-C5'-O5'
79	L5	4447	5MC	C2'-C1'-N1-C6
79	L5	3729	PSU	C3'-C4'-C5'-O5'
79	L5	4420	PSU	C3'-C4'-C5'-O5'
79	L5	1792	PSU	O4'-C4'-C5'-O5'
79	L5	3867	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
78	S2	428	OMU	C2'-C1'-N1-C2
76	Pt	47	G7M	O4'-C4'-C5'-O5'
78	S2	27	A2M	O4'-C4'-C5'-O5'
78	S2	428	OMU	O4'-C1'-N1-C6
78	S2	428	OMU	C3'-C4'-C5'-O5'
78	S2	166	A2M	C1'-C2'-O2'-CM'
79	L5	1316	OMG	C1'-C2'-O2'-CM2
79	L5	3785	A2M	C1'-C2'-O2'-CM'
74	Lo	53	MLZ	CG-CD-CE-NZ
79	L5	4447	5MC	O4'-C1'-N1-C6
76	Pt	21	H2U	O4'-C1'-N1-C2
79	L5	1326	A2M	C4'-C5'-O5'-P
79	L5	3844	PSU	C4'-C5'-O5'-P
78	S2	436	OMG	O4'-C4'-C5'-O5'
78	S2	1447	OMG	O4'-C4'-C5'-O5'
78	S2	1490	OMG	O4'-C4'-C5'-O5'
79	L5	1625	OMG	C3'-C4'-C5'-O5'
79	L5	3867	A2M	O4'-C4'-C5'-O5'
78	S2	1248	B8N	C31-C32-C33-C34
79	L5	1524	A2M	C3'-C2'-O2'-CM'
79	L5	3785	A2M	C3'-C2'-O2'-CM'
79	L5	4494	OMG	C3'-C2'-O2'-CM2
79	L5	2815	A2M	C4'-C5'-O5'-P
79	L5	3818	UY1	C4'-C5'-O5'-P
79	L5	4500	PSU	C4'-C5'-O5'-P
79	L5	3701	OMC	O4'-C1'-N1-C6
79	L5	1534	A2M	C4'-C5'-O5'-P
79	L5	4447	5MC	O4'-C1'-N1-C2
78	S2	509	OMG	O4'-C4'-C5'-O5'
78	S2	1248	B8N	C32-C33-C34-O35
78	S2	428	OMU	O4'-C1'-N1-C2
79	L5	3701	OMC	O4'-C1'-N1-C2
76	Pt	21	H2U	C4'-C5'-O5'-P
78	S2	1490	OMG	C4'-C5'-O5'-P
79	L5	3887	OMC	C4'-C5'-O5'-P
78	S2	1248	B8N	C32-C33-C34-O36
78	S2	644	OMG	C4'-C5'-O5'-P
76	Pt	21	H2U	O4'-C4'-C5'-O5'
79	L5	4447	5MC	C2'-C1'-N1-C2
78	S2	576	A2M	C4'-C5'-O5'-P
78	S2	590	A2M	C3'-C2'-O2'-CM'
79	L5	3818	UY1	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
79	L5	2351	OMC	C2'-C1'-N1-C6
79	L5	1322	1MA	C2'-C1'-N9-C8
79	L5	1322	1MA	C2'-C1'-N9-C4
78	S2	119	PSU	O4'-C4'-C5'-O5'
79	L5	3782	5MC	O4'-C4'-C5'-O5'
79	L5	2351	OMC	C2'-C1'-N1-C2
78	S2	590	A2M	C2'-C1'-N9-C8
78	S2	159	A2M	C3'-C4'-C5'-O5'
79	L5	1792	PSU	C3'-C4'-C5'-O5'
79	L5	2364	OMG	C3'-C4'-C5'-O5'
78	S2	116	OMU	C1'-C2'-O2'-CM2
78	S2	159	A2M	C1'-C2'-O2'-CM'
79	L5	4370	OMG	C1'-C2'-O2'-CM2
79	L5	3818	UY1	C1'-C2'-O2'-CM2
79	L5	4370	OMG	C3'-C2'-O2'-CM2
76	Pt	33	OMC	C2'-C1'-N1-C2
78	S2	590	A2M	O4'-C1'-N9-C8
79	L5	1524	A2M	O4'-C1'-N9-C8
79	L5	2422	OMC	C3'-C4'-C5'-O5'
79	L5	1677	PSU	O4'-C1'-C5-C6
76	Pt	47	G7M	C3'-C4'-C5'-O5'
79	L5	1534	A2M	O4'-C4'-C5'-O5'
79	L5	4523	A2M	O4'-C4'-C5'-O5'
78	S2	590	A2M	C2'-C1'-N9-C4
78	S2	1851	MA6	C4'-C5'-O5'-P
78	S2	436	OMG	C3'-C4'-C5'-O5'
78	S2	509	OMG	C3'-C4'-C5'-O5'
79	L5	2351	OMC	O4'-C4'-C5'-O5'
79	L5	2422	OMC	O4'-C4'-C5'-O5'
79	L5	4361	PSU	O4'-C4'-C5'-O5'
79	L5	4196	OMG	C4'-C5'-O5'-P

There are no ring outliers.

76 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
78	S2	1678	A2M	1	0
79	L5	4579	PSU	2	0
78	S2	644	OMG	1	0
78	S2	1232	PSU	2	0
78	S2	1288	OMU	1	0
79	L5	3718	A2M	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
79	L5	2415	OMU	2	0
79	L5	4523	A2M	1	0
79	L5	4620	OMU	4	0
78	S2	649	PSU	1	0
79	L5	1326	A2M	1	0
78	S2	1851	MA6	1	0
79	L5	5001	PSU	1	0
78	S2	1643	PSU	1	0
79	L5	1316	OMG	1	0
79	L5	2363	A2M	1	0
78	S2	1243	PSU	1	0
79	L5	3627	OMG	1	0
79	L5	4571	A2M	1	0
78	S2	99	A2M	1	0
78	S2	572	PSU	1	0
79	L5	1871	A2M	1	0
79	L5	3715	PSU	1	0
76	Pt	47	G7M	2	0
78	S2	1328	OMG	1	0
78	S2	1383	A2M	1	0
78	S2	863	PSU	1	0
79	L5	2876	OMG	1	0
78	S2	1447	OMG	2	0
79	L5	3925	OMU	1	0
78	S2	576	A2M	1	0
78	S2	1842	4AC	3	0
78	S2	1850	MA6	1	0
79	L5	4442	PSU	2	0
78	S2	436	OMG	1	0
79	L5	4456	OMC	2	0
76	Pt	33	OMC	1	0
76	Pt	56	PSU	1	0
78	S2	116	OMU	3	0
79	L5	4353	PSU	1	0
79	L5	3724	A2M	1	0
79	L5	4637	OMG	1	0
79	L5	4536	OMC	1	0
79	L5	2424	OMG	1	0
78	S2	1031	A2M	1	0
78	S2	509	OMG	2	0
79	L5	2508	PSU	2	0
3	LB	245	HIC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
78	S2	512	A2M	1	0
78	S2	1804	OMU	1	0
61	Lb	5	MLZ	1	0
79	L5	4499	OMG	1	0
78	S2	159	A2M	1	0
79	L5	4299	PSU	1	0
78	S2	609	PSU	1	0
78	S2	1391	OMC	1	0
78	S2	1639	G7M	1	0
79	L5	3867	A2M	1	0
78	S2	601	OMG	1	0
79	L5	3770	PSU	1	0
79	L5	3785	A2M	1	0
78	S2	121	OMU	1	0
78	S2	354	OMU	2	0
79	L5	4457	PSU	1	0
79	L5	3723	A2M	2	0
79	L5	1781	PSU	1	0
79	L5	4500	PSU	1	0
79	L5	3764	PSU	1	0
78	S2	484	A2M	1	0
79	L5	4228	OMG	1	0
79	L5	1582	PSU	1	0
78	S2	801	PSU	1	0
79	L5	1683	PSU	2	0
5	L8	75	OMG	1	0
79	L5	3884	PSU	1	0
79	L5	4196	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 140 ligands modelled in this entry, 134 are monoatomic - leaving 6 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$
89	HYG	S2	1901	-	35,39,39	3.09	11 (31%)	43,60,60	1.51	7 (16%)
88	MET	Pt	78	-	6,7,8	0.46	0	2,7,9	0.21	0
84	SAC	SA	2	-	7,8,9	0.41	0	8,9,11	1.66	1 (12%)
84	SAC	Lr	2	-	7,8,9	0.36	0	8,9,11	1.14	1 (12%)
90	ANM	L5	5101	-	20,20,20	4.06	10 (50%)	22,27,27	1.53	4 (18%)
87	AME	SV	1	-	9,10,11	1.44	1 (11%)	9,11,13	1.53	2 (22%)

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
89	HYG	S2	1901	-	-	4/12/87/87	0/4/4/4
88	MET	Pt	78	-	-	1/5/6/8	-
84	SAC	SA	2	-	-	3/7/8/10	-
84	SAC	Lr	2	-	-	2/7/8/10	-
90	ANM	L5	5101	-	-	4/10/23/23	0/2/2/2
87	AME	SV	1	-	-	3/9/10/12	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5101	ANM	C2-C16	-11.68	1.30	1.53
89	S2	1901	HYG	O29-C12	10.88	1.61	1.43
90	L5	5101	ANM	C16-N1	8.95	1.67	1.48
89	S2	1901	HYG	O22-C17	6.61	1.53	1.43
89	S2	1901	HYG	O14-C13	6.55	1.58	1.41
89	S2	1901	HYG	O28-C23	6.01	1.47	1.40
90	L5	5101	ANM	O4-C3	-5.11	1.32	1.43
89	S2	1901	HYG	C16-C15	4.33	1.62	1.53
90	L5	5101	ANM	O2-C5	4.25	1.44	1.35
89	S2	1901	HYG	C17-C12	-4.16	1.44	1.53
90	L5	5101	ANM	C4-N1	-3.85	1.33	1.47
90	L5	5101	ANM	O2-C2	3.71	1.50	1.44
87	SV	1	AME	CT1-N	3.21	1.45	1.34
89	S2	1901	HYG	O28-C27	3.15	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5101	ANM	C15-C12	2.93	1.58	1.51
90	L5	5101	ANM	C3-C2	2.91	1.59	1.53
89	S2	1901	HYG	C25-C24	-2.63	1.48	1.53
89	S2	1901	HYG	O18-C13	-2.62	1.34	1.41
89	S2	1901	HYG	O30-C24	2.43	1.47	1.42
90	L5	5101	ANM	C4-C3	2.29	1.56	1.53
90	L5	5101	ANM	C15-C16	2.23	1.58	1.53
89	S2	1901	HYG	O31-C25	2.19	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	L5	5101	ANM	O2-C5-C6	5.02	120.32	111.09
89	S2	1901	HYG	O29-C12-C13	4.74	123.29	110.86
89	S2	1901	HYG	O22-C17-C16	4.15	121.33	111.22
84	SA	2	SAC	CA-N-C1A	4.08	130.68	123.15
89	S2	1901	HYG	O28-C27-C26	3.12	112.95	108.52
89	S2	1901	HYG	C13-O18-C6	-2.67	111.35	117.96
89	S2	1901	HYG	O14-C15-C16	2.56	114.33	109.69
87	SV	1	AME	CE-SD-CG	2.54	109.13	100.40
89	S2	1901	HYG	O22-C17-C12	2.44	107.49	103.58
84	Lr	2	SAC	CA-N-C1A	2.37	127.52	123.15
87	SV	1	AME	CT2-CT1-N	2.25	119.91	116.10
90	L5	5101	ANM	C2-O2-C5	-2.18	114.35	117.72
90	L5	5101	ANM	C12-C15-C16	-2.11	109.67	113.33
89	S2	1901	HYG	C19-C15-C16	-2.09	108.12	113.00
90	L5	5101	ANM	C3-C2-C16	-2.08	101.29	104.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	SA	2	SAC	CB-CA-N-C1A
84	SA	2	SAC	C-CA-CB-OG
87	SV	1	AME	O-C-CA-CB
88	Pt	78	MET	N-CA-CB-CG
89	S2	1901	HYG	C27-C33-C34-O35
89	S2	1901	HYG	O14-C13-O18-C6
90	L5	5101	ANM	C1-C9-O1-C14
90	L5	5101	ANM	C10-C9-O1-C14
84	Lr	2	SAC	C2A-C1A-N-CA
84	Lr	2	SAC	OAC-C1A-N-CA

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Mol	Chain	Res	Type	Atoms
87	SV	1	AME	CB-CG-SD-CE
87	SV	1	AME	N-CA-CB-CG
89	S2	1901	HYG	O28-C27-C33-C34
84	SA	2	SAC	N-CA-CB-OG
89	S2	1901	HYG	N36-C33-C34-O35
90	L5	5101	ANM	C13-C12-C15-C16
90	L5	5101	ANM	C11-C12-C15-C16

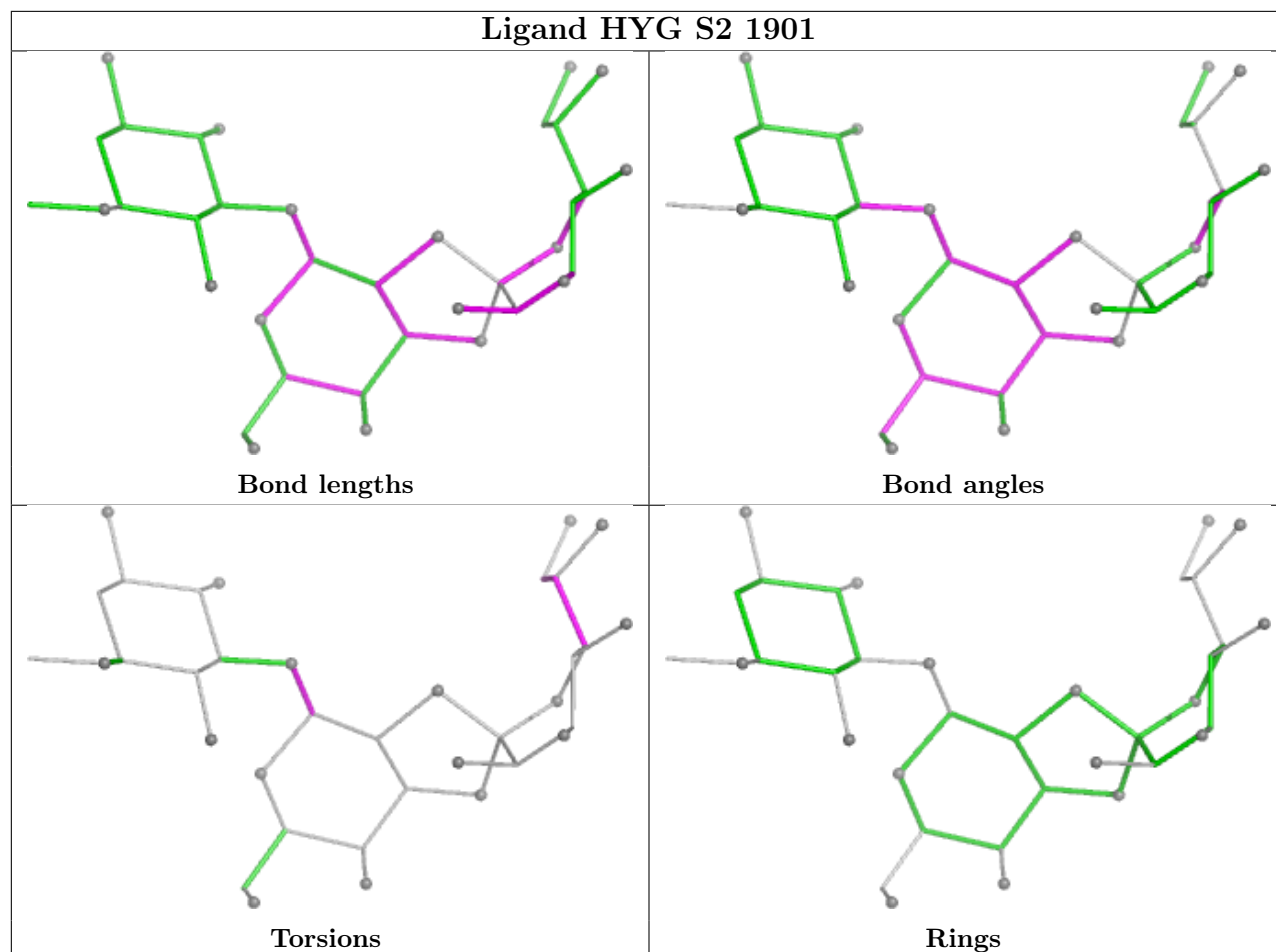
There are no ring outliers.

1 monomer is involved in 1 short contact:

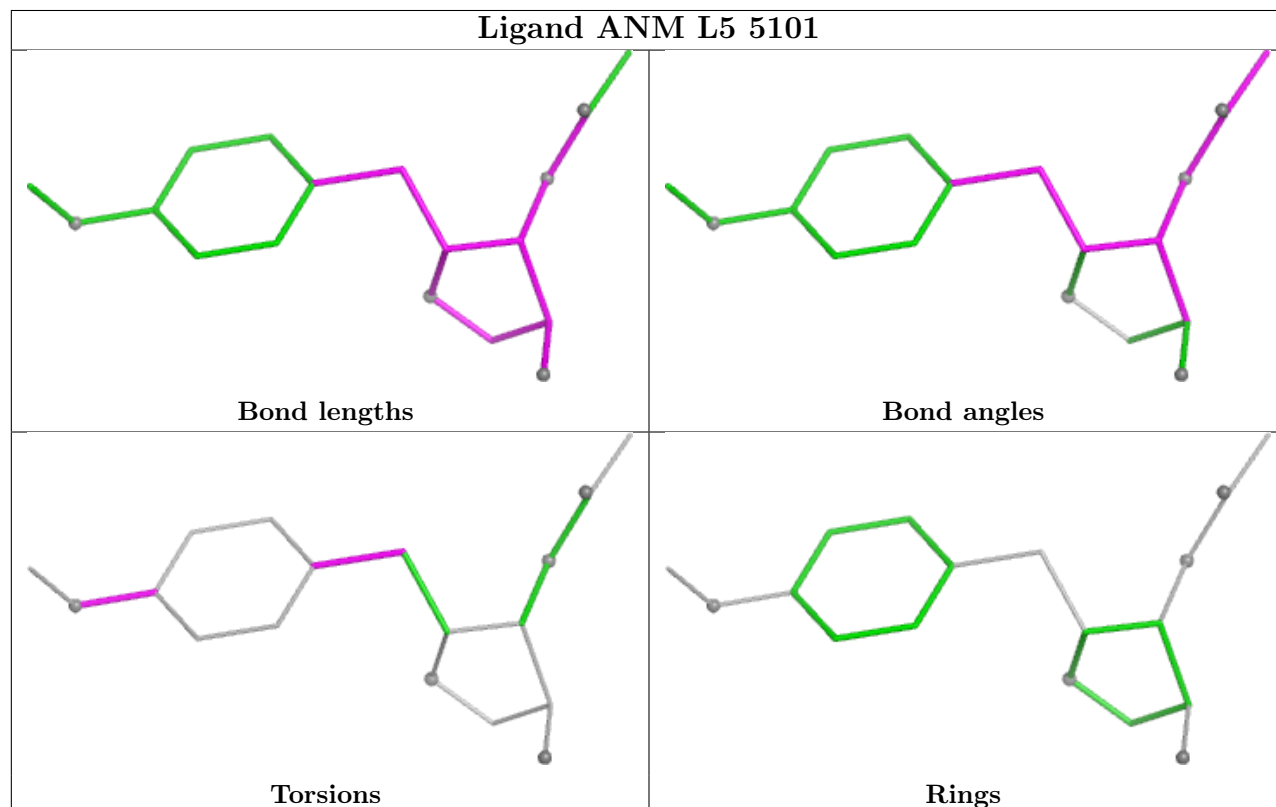
Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	L5	5101	ANM	1	0

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

Ligand HYG S2 1901



Ligand ANM L5 5101



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
20	SM	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SM	72:HIS	C	105:GLY	N	25.35

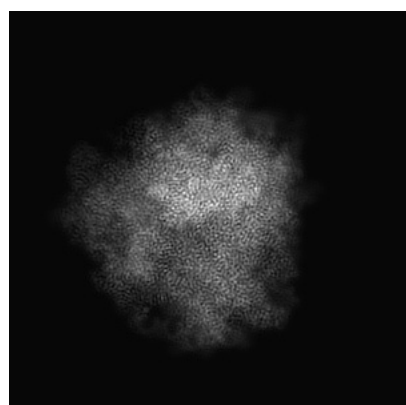
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54267. These allow visual inspection of the internal detail of the map and identification of artifacts.

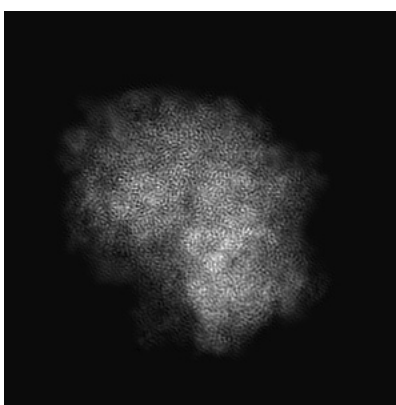
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

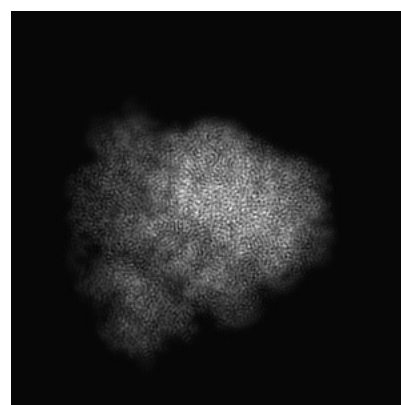
6.1.1 Primary map



X



Y

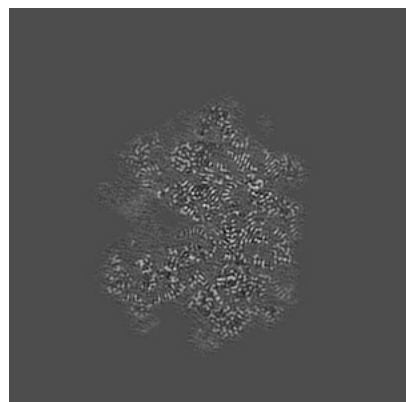


Z

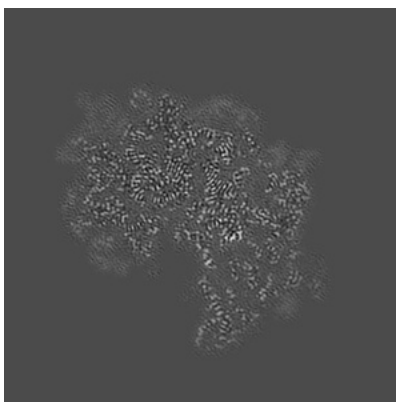
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

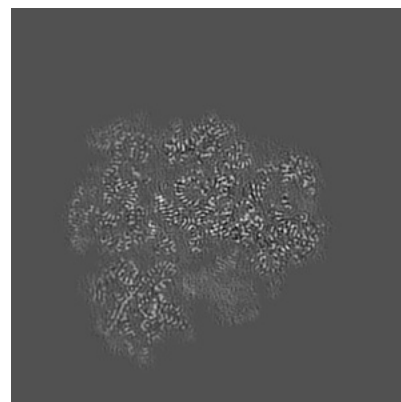
6.2.1 Primary map



X Index: 240



Y Index: 240

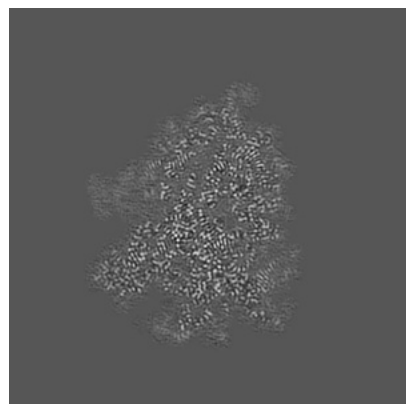


Z Index: 240

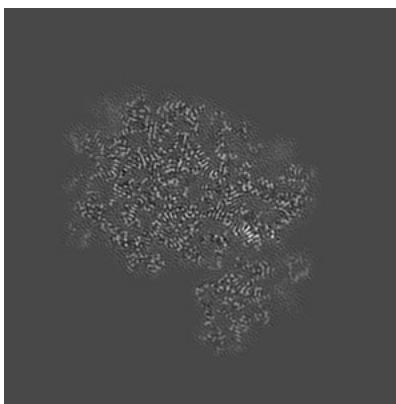
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

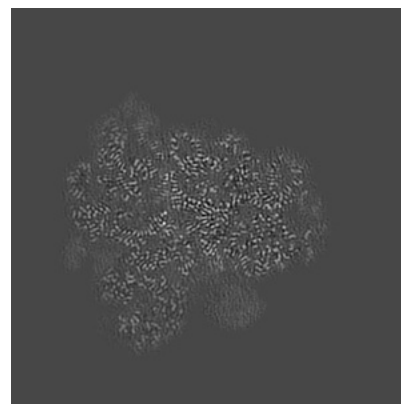
6.3.1 Primary map



X Index: 272



Y Index: 258

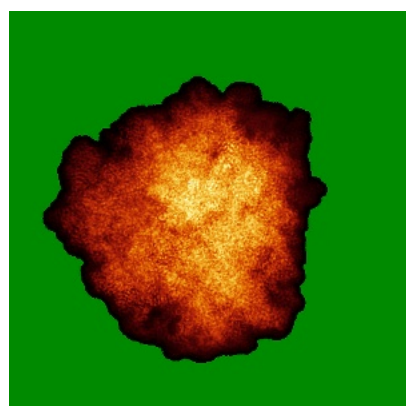


Z Index: 261

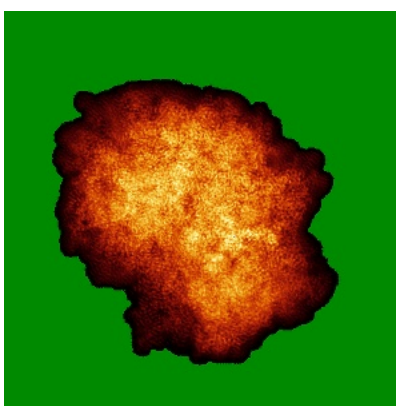
The images above show the largest variance slices of the map in three orthogonal directions.

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

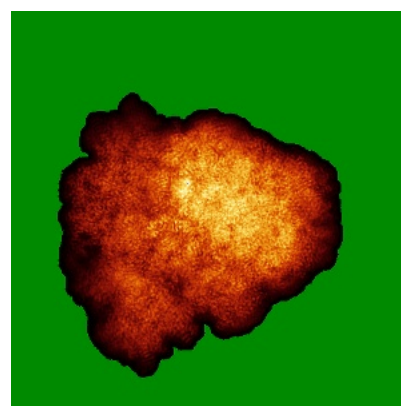
6.4.1 Primary map



X



Y

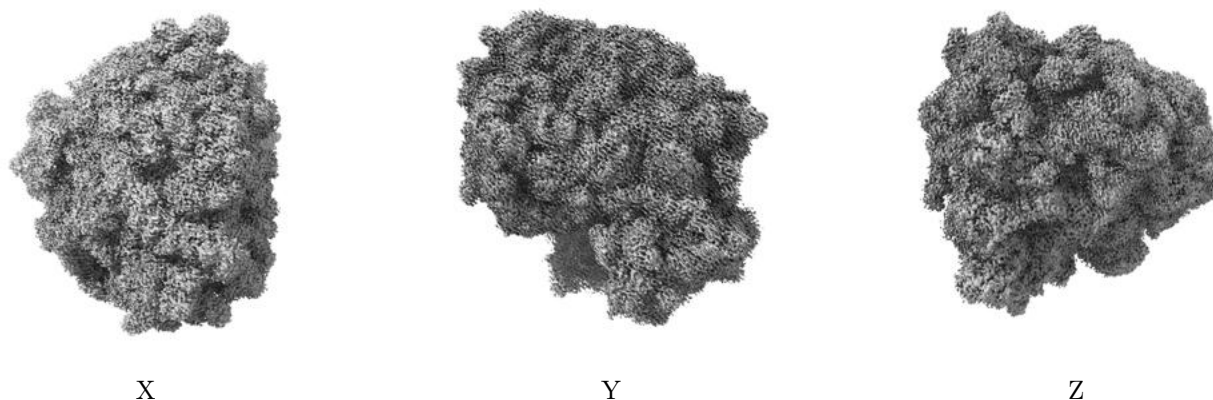


Z

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.

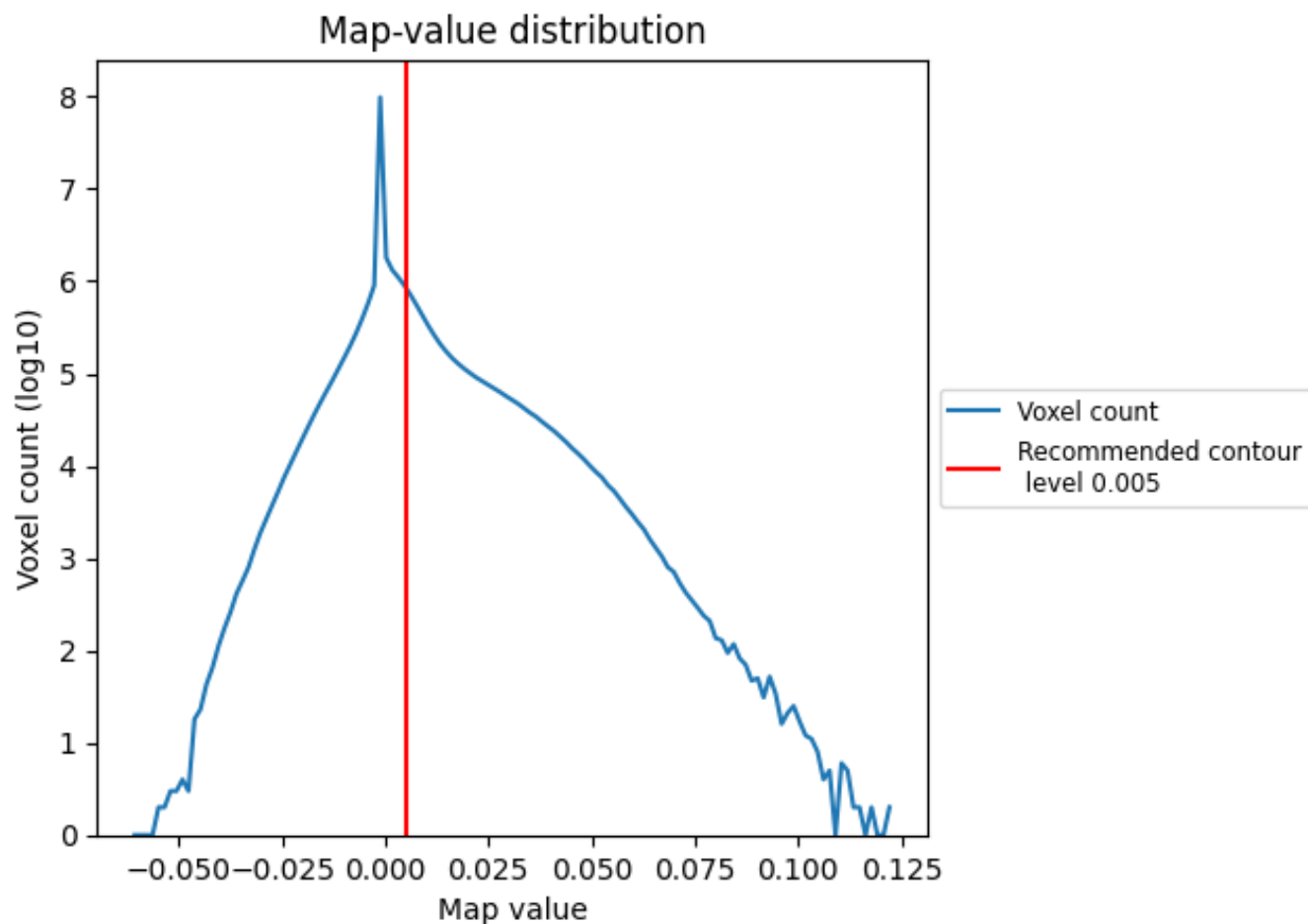
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

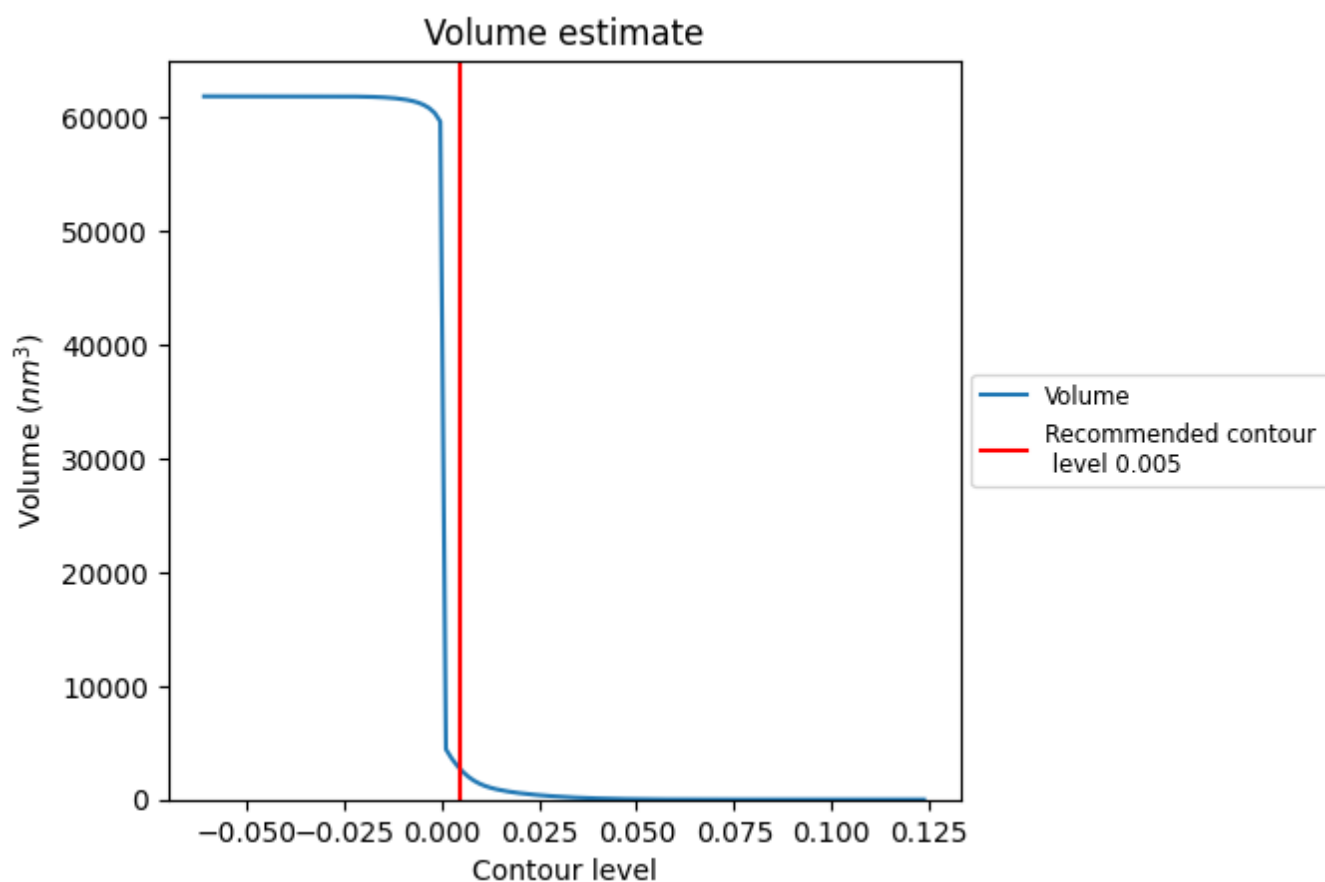
This section contains the results of statistical analysis of the map.

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.

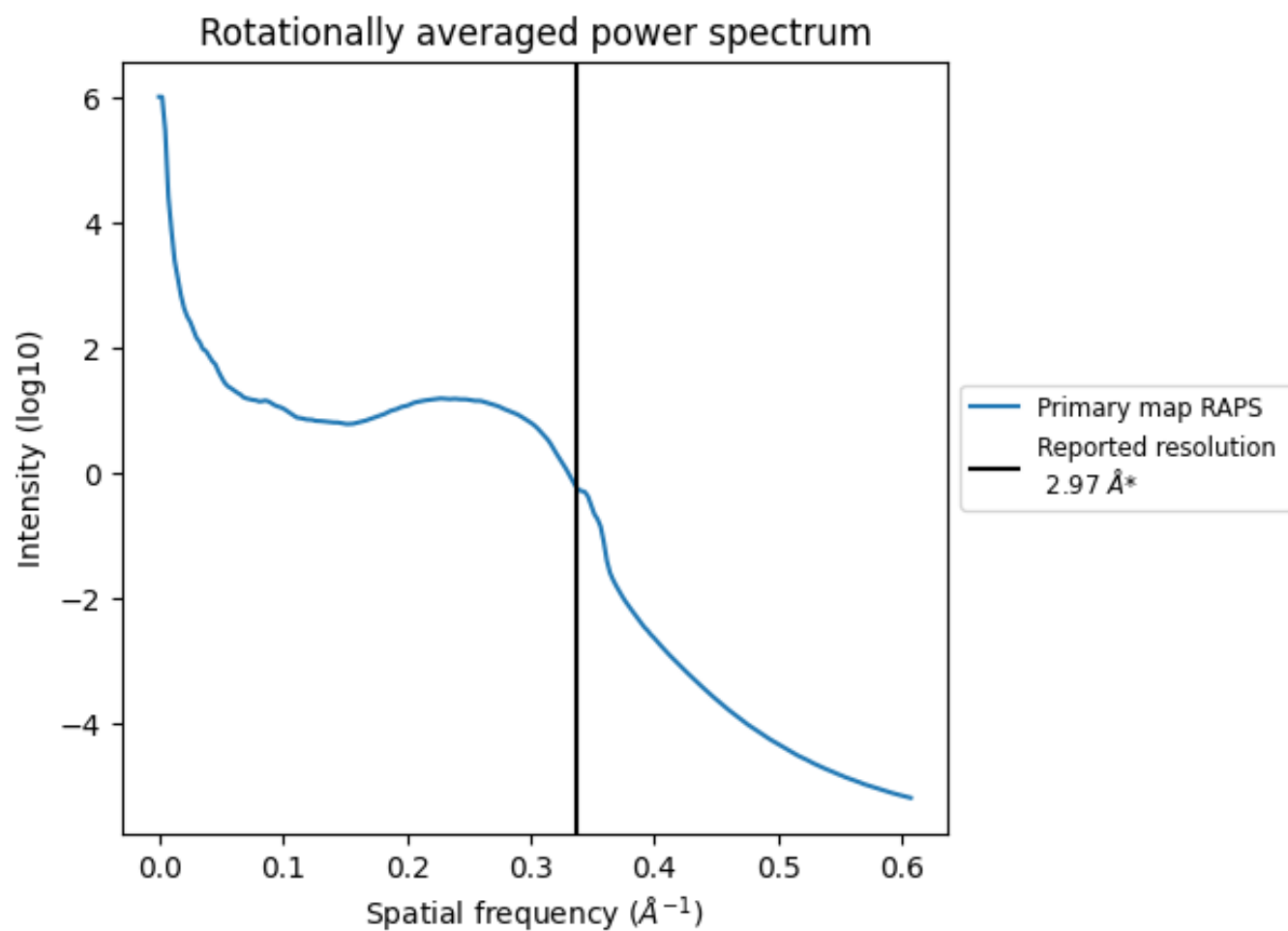
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2631 nm^3 ; this corresponds to an approximate mass of 2376 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 0.337 Å⁻¹

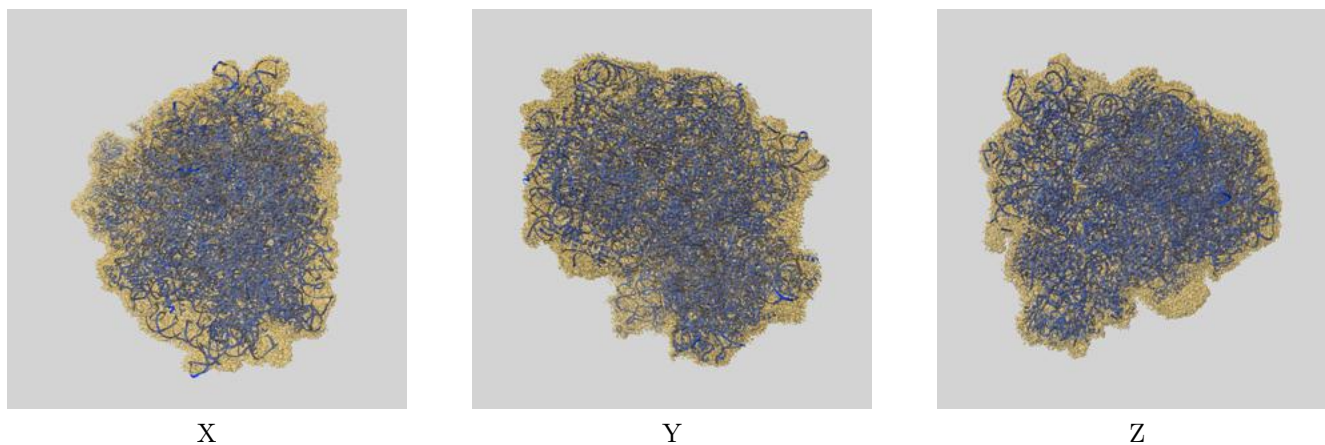
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

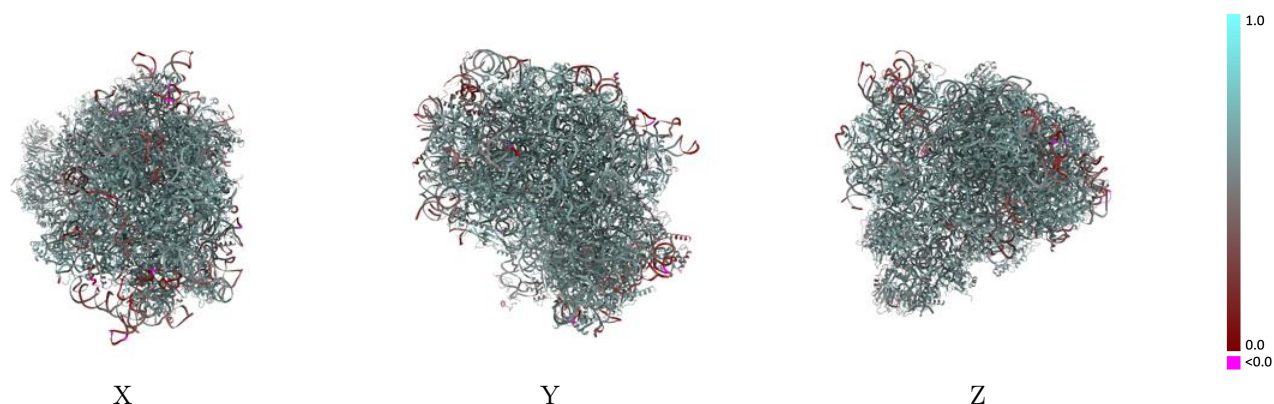
This section contains information regarding the fit between EMDB map EMD-54267 and PDB model 9RU9. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



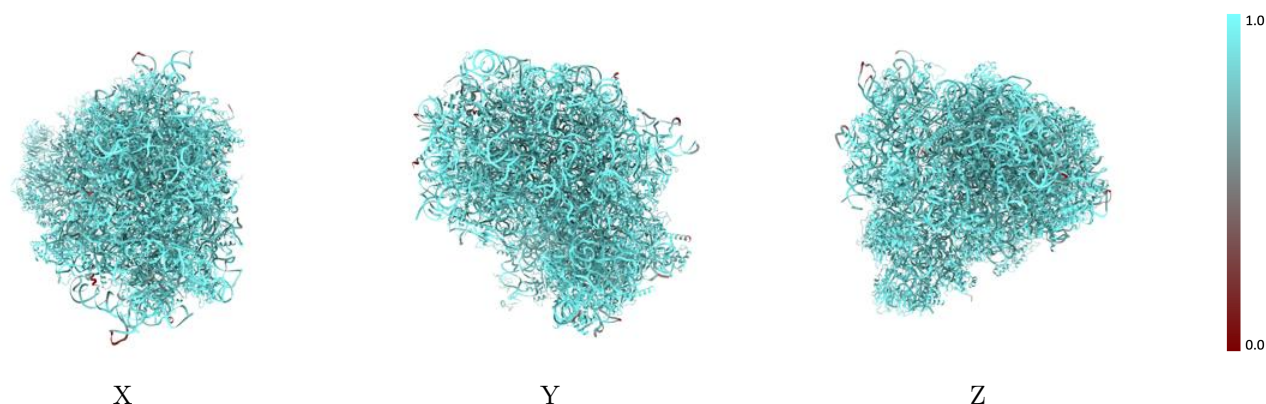
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



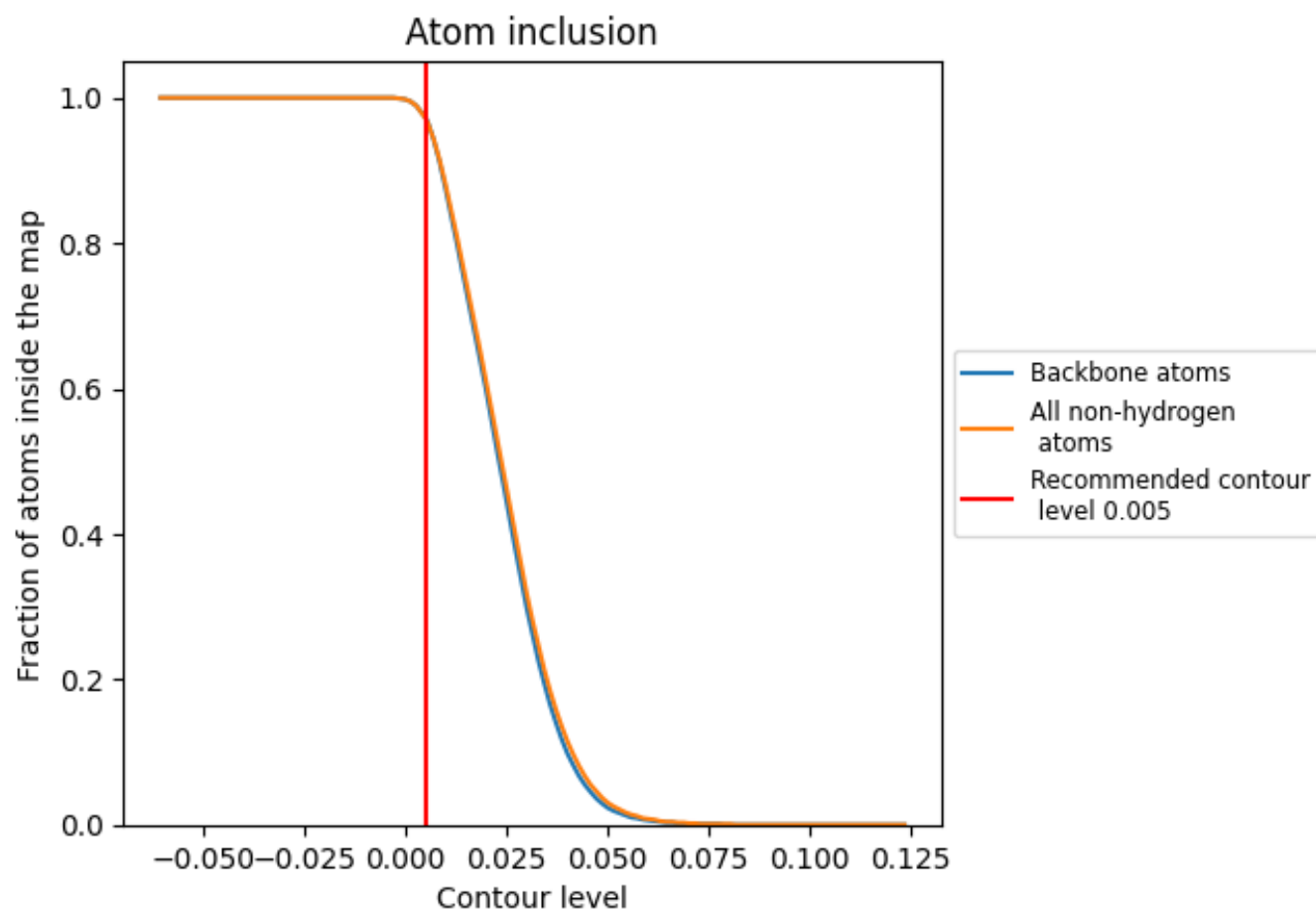
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9710	 0.5650
A	 1.0000	 0.7620
C	 1.0000	 0.7760
D	 1.0000	 0.7260
Et	 0.8770	 0.2960
L5	 0.9710	 0.5520
L7	 0.9930	 0.5930
L8	 0.9860	 0.5690
LA	 0.9960	 0.6190
LB	 0.9900	 0.6130
LC	 0.9720	 0.6010
LD	 0.9710	 0.5870
LE	 0.9720	 0.5740
LF	 0.9890	 0.6070
LG	 0.9380	 0.5550
LH	 0.9830	 0.6030
LI	 0.9830	 0.6100
LJ	 0.9750	 0.5830
LL	 0.9750	 0.5850
LM	 0.9800	 0.5940
LN	 0.9960	 0.6230
LO	 0.9880	 0.6100
LP	 0.9880	 0.6080
LQ	 0.9910	 0.6150
LR	 0.9650	 0.5760
LS	 0.9940	 0.6160
LT	 0.9870	 0.5970
LU	 0.9710	 0.5460
LV	 0.9960	 0.6130
LW	 0.9960	 0.6150
LX	 0.9900	 0.5990
LY	 0.9890	 0.6130
LZ	 0.9830	 0.5910
La	 0.9940	 0.6180
Lb	 0.9070	 0.5270





















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Chain	Atom inclusion	Q-score
Lc	 0.9920	 0.5940
Ld	 0.9920	 0.5840
Le	 0.9940	 0.6150
Lf	 0.9940	 0.6240
Lg	 0.9920	 0.6000
Lh	 0.9790	 0.6020
Li	 0.9710	 0.5820
Lj	 0.9970	 0.6150
Lk	 0.9780	 0.5700
Ll	 0.9950	 0.6080
Lm	 0.9860	 0.5940
Ln	 0.9950	 0.5800
Lo	 0.9860	 0.6070
Lp	 0.9930	 0.6040
Lr	 0.9850	 0.6100
Pt	 0.9200	 0.4720
S2	 0.9700	 0.5510
SA	 0.9720	 0.5860
SB	 0.9830	 0.5870
SC	 0.9770	 0.5950
SD	 0.9400	 0.5480
SE	 0.9780	 0.5930
SF	 0.9740	 0.5790
SG	 0.9640	 0.5490
SH	 0.9310	 0.5370
SI	 0.9660	 0.5680
SJ	 0.9660	 0.5880
SK	 0.9430	 0.5400
SL	 0.9830	 0.5990
SM	 0.7800	 0.3940
SN	 0.9860	 0.5910
SO	 0.9810	 0.5920
SP	 0.9500	 0.5460
SQ	 0.9710	 0.5830
SR	 0.9200	 0.5470
SS	 0.9680	 0.5670
ST	 0.9780	 0.5800
SU	 0.9440	 0.5380
SV	 0.9660	 0.5820
SW	 0.9800	 0.6030
SX	 0.9900	 0.5990
SY	 0.9750	 0.5790

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Chain	Atom inclusion	Q-score
SZ	 0.9520	 0.5560
Sa	 0.9770	 0.5840
Sb	 0.9590	 0.5620
Sc	 0.9660	 0.5780
Sd	 0.9860	 0.5980
Se	 0.9750	 0.5780
Sf	 0.8510	 0.4260
Sg	 0.9150	 0.5300
mR	 0.8790	 0.4760