



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:24 am BST

PDB ID : 9SPF / pdb_00009spf
EMDB ID : EMD-55083
Title : CRYO-EM STRUCTURE OF HUMAN 80S RIBOSOME WITH A/P/E-SITE
TRNA AND MRNA CONTAINING N1-METHYLPSEUDOURIDINE
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-09-17
Resolution : 2.40 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

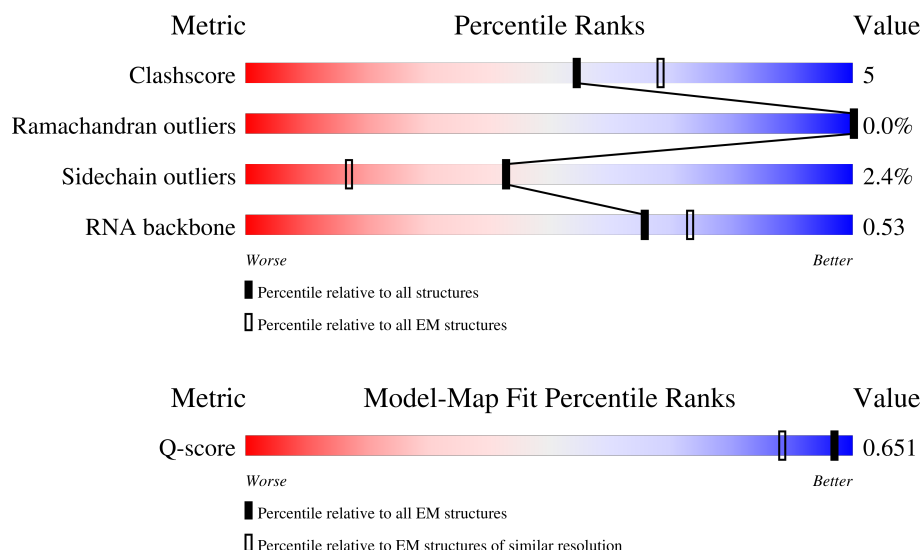
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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.



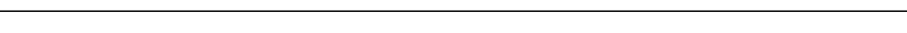
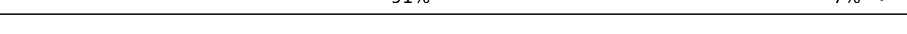
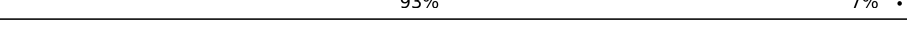
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	At	77	
2	Et	75	
3	L5	5069	

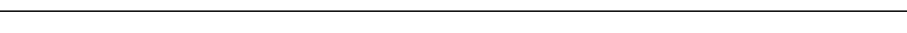
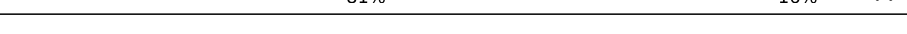
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LB	403	
7	LC	427	
8	LD	297	
9	LE	288	
10	LF	248	
11	LG	266	
12	LH	192	
13	LI	214	
14	LJ	178	
15	LL	211	
16	LM	215	
17	LN	204	
18	LO	203	
19	LP	184	
20	LQ	188	
21	LR	196	
22	LS	176	
23	LT	160	
24	LU	128	
25	LV	140	
26	LW	157	
27	LX	156	
28	LY	145	

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Mol	Chain	Length	Quality of chain
29	LZ	136	
30	La	148	
31	Lb	159	
32	Lc	115	
33	Ld	125	
34	Le	135	
35	Lf	110	
36	Lg	117	
37	Lh	123	
38	Li	105	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	Mr	7	
47	Pt	76	
48	S2	1869	
49	SB	264	
50	SC	293	
51	SD	243	
52	SE	263	
53	SF	204	

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Mol	Chain	Length	Quality of chain
54	SG	249	
55	SH	194	
56	SI	208	
57	SJ	194	
58	SK	165	
59	SL	158	
60	SM	132	
61	SN	151	
62	SO	151	
63	SP	145	
64	SQ	146	
65	SR	135	
66	SS	152	
67	ST	145	
68	SU	119	
69	SV	83	
70	SW	130	
71	SY	133	
72	SZ	125	
73	Sa	115	
74	Sb	84	
75	Sc	69	
76	Sd	56	
77	Se	133	
78	Sf	156	

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Mol	Chain	Length	Quality of chain
79	Sg	317	
80	LA	257	
81	SA	295	
82	SX	143	
83	Lj	97	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	ZN	Sd	102	-	-	X	-
90	HYG	S2	2021	X	-	-	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 211463 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called A-site-tRNA-Ile-AAT-9-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	At	73	Total	C	N	O	P	0	0
			1559	697	280	510	72		

- Molecule 2 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Et	54	Total	C	N	O	P	0	0
			1155	516	214	372	53		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3466	Total	C	N	O	P	1	0
			74397	33170	13604	24157	3466		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- 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
			3316	1482	585	1094	155		

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LB	399	Total	C	N	O	S	0	0
			3221	2051	605	551	14		

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD	294	Total	C	N	O	S	0	0
			2385	1507	436	428	14		

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	223	Total	C	N	O	S	0	0
			1782	1147	338	293	4		

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LF	225	Total	C	N	O	S	0	0
			1856	1193	357	297	9		

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	232	Total	C	N	O	S	0	0
			1846	1175	356	311	4		

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	207	Total	C	N	O	S	0	0
			1672	1062	322	275	13		

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LL	206	Total	C	N	O	S	1	0
			1672	1046	348	274	4		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 17 is a protein called 60S ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	200	Total	C	N	O	S	0	0
			1640	1058	320	257	5		

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

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

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	180	Total	C	N	O	S	0	0
			1449	898	311	231	9		

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	159	Total	C	N	O	S	1	0
			1303	828	253	216	6		

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 25 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LV	133	Total	C	N	O	S	0	0
			988	623	186	174	5		

- Molecule 26 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LW	105	Total	C	N	O	S	0	0
			847	532	171	140	4		

- Molecule 27 is a protein called 60S ribosomal protein L23a.

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

- Molecule 28 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LY	132	Total	C	N	O	S	0	0
			1098	689	222	184	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lb	105	Total	C	N	O	S	0	0
			846	526	185	131	4		

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lc	99	Total	C	N	O	S	0	0
			766	485	135	140	6		

- Molecule 33 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lf	110	Total	C	N	O	S	0	0
			880	558	175	144	3		

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lg	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lk	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 41 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	1	0
			432	269	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	2	0
			875	548	181	140	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lp	90	Total	C	N	O	S	0	0
			698	440	134	117	7		

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 46 is a RNA chain called synthetic mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Mr	7	Total	C	N	O	P	0	0
			147	67	23	50	7		

- Molecule 47 is a RNA chain called P-site tRNA-Arg-ACG.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Pt	74	Total	C	N	O	P	0	0
			1587	710	285	518	74		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1619	Total	C	N	O	P	0	0
			34624	15485	6221	11300	1618		

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	221	Total	C	N	O	S	0	0
			1793	1138	323	318	14		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SC	219	Total	C	N	O	S	0	0
			1700	1100	292	298	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	225	Total	C	N	O	S	0	0
			1742	1112	312	311	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	259	Total	C	N	O	S	0	0
			2059	1316	383	352	8		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	183	Total	C	N	O	S	0	0
			1443	905	269	262	7		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SG	216	Total	C	N	O	S	0	0
			1721	1078	341	295	7		

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SH	186	Total	C	N	O	S	0	0
			1486	947	271	267	1		

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SJ	175	Total	C	N	O	S	0	0
			1424	905	284	233	2		

- Molecule 58 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SK	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 59 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SL	143	Total	C	N	O	S	0	0
			1171	746	221	198	6		

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SM	109	Total	C	N	O	S	0	0
			754	469	135	144	6		

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SN	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SO	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SP	130	Total	C	N	O	S	0	0
			1071	680	203	181	7		

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SQ	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 65 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SR	133	Total	C	N	O	S	0	0
			1075	675	200	196	4		

- Molecule 66 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 67 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	142	Total	C	N	O	S	1	0
			1121	707	212	199	3		

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 70 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SY	121	Total	C	N	O	S	0	0
			995	631	195	164	5		

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SZ	87	Total	C	N	O	S	0	0
			693	445	130	117	1		

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 75 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sc	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 76 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 77 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	49	Total	C	N	O	S	0	0
			390	239	87	63	1		

- Molecule 78 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	61	Total	C	N	O	S	0	0
			480	300	91	83	6		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sg	312	Total	C	N	O	S	0	0
			2427	1531	423	463	10		

- Molecule 80 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	LA	250	Total	C	N	O	S	1	0
			1923	1204	395	318	6		

- Molecule 81 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SA	220	Total	C	N	O	S	0	0
			1730	1099	303	321	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	ACE	-	acetylation	UNP P08865

- Molecule 82 is a protein called 40S ribosomal protein S23.

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

- Molecule 83 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
84	L5	86	Total	K	0
			86	86	
84	L7	2	Total	K	0
			2	2	
84	L8	1	Total	K	0
			1	1	
84	LH	1	Total	K	0
			1	1	
84	LI	1	Total	K	0
			1	1	
84	Lb	1	Total	K	0
			1	1	
84	Le	1	Total	K	0
			1	1	
84	Lf	1	Total	K	0
			1	1	
84	Lg	1	Total	K	0
			1	1	
84	Pt	1	Total	K	0
			1	1	
84	S2	48	Total	K	0
			48	48	
84	SF	1	Total	K	0
			1	1	
84	SL	1	Total	K	0
			1	1	
84	SO	1	Total	K	0
			1	1	
84	SS	1	Total	K	0
			1	1	
84	Sd	1	Total	K	0
			1	1	
84	LA	2	Total	K	0
			2	2	

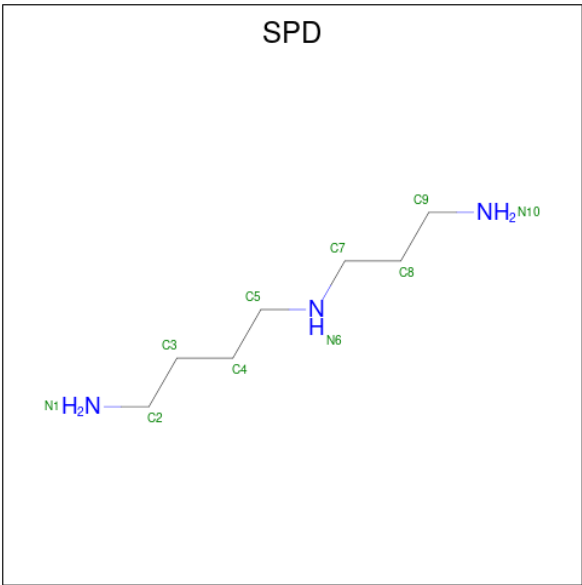
- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	L5	160	Total 160	Mg 160	0
85	L7	3	Total 3	Mg 3	0
85	L8	2	Total 2	Mg 2	0
85	LI	1	Total 1	Mg 1	0
85	LP	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	Ln	2	Total 2	Mg 2	0
85	Pt	1	Total 1	Mg 1	0
85	S2	54	Total 54	Mg 54	0

- Molecule 86 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	L5	22	Total 22	Na 22	0
86	L8	1	Total 1	Na 1	0
86	La	1	Total 1	Na 1	0
86	S2	11	Total 11	Na 11	0

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



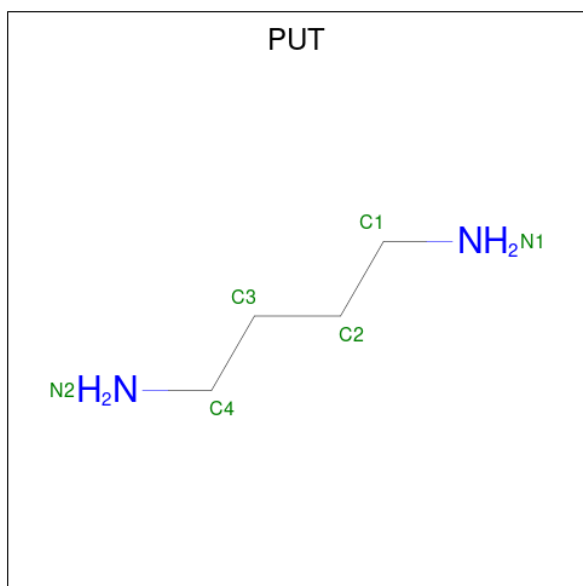
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L8	1	Total	C	N	0
			10	7	3	
87	LN	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	
87	S2	1	Total	C	N	0
			10	7	3	

- Molecule 88 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	
88	L5	1	Total	C	N	0
			6	4	2	

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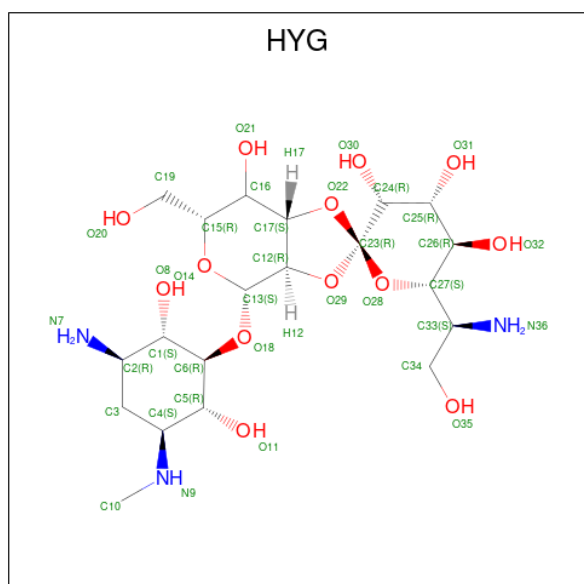
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Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			6	4	2	
88	S2	1	Total	C	N	0
			6	4	2	
88	S2	1	Total	C	N	0
			6	4	2	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 90 is HYGROMYCIN B (CCD ID: HYG) (formula: C₂₀H₃₇N₃O₁₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 91 is water.

Mol	Chain	Residues	Atoms		AltConf
91	At	1	Total	O	0
			1	1	
91	Et	1	Total	O	0
			1	1	
91	L5	281	Total	O	0
			281	281	
91	L7	1	Total	O	0
			1	1	
91	L8	6	Total	O	0
			6	6	
91	LC	1	Total	O	0
			1	1	
91	LI	1	Total	O	0
			1	1	
91	LN	1	Total	O	0
			1	1	
91	LP	1	Total	O	0
			1	1	
91	LQ	1	Total	O	0
			1	1	
91	LY	1	Total	O	0
			1	1	
91	La	3	Total	O	0
			3	3	
91	Ld	1	Total	O	0
			1	1	
91	Le	3	Total	O	0
			3	3	
91	Ln	7	Total	O	0
			7	7	
91	Lo	4	Total	O	0
			4	4	
91	Lp	1	Total	O	0
			1	1	
91	Mr	11	Total	O	0
			11	11	
91	Pt	11	Total	O	0
			11	11	

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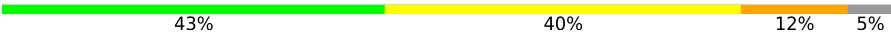
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Mol	Chain	Residues	Atoms		AltConf
91	S2	171	Total 171	O 171	0
91	SN	1	Total 1	O 1	0
91	SO	1	Total 1	O 1	0
91	SQ	1	Total 1	O 1	0
91	SW	1	Total 1	O 1	0
91	LA	4	Total 4	O 4	0
91	SX	1	Total 1	O 1	0

3 Residue-property plots

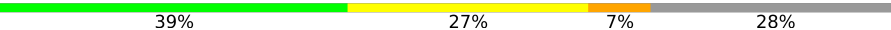
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

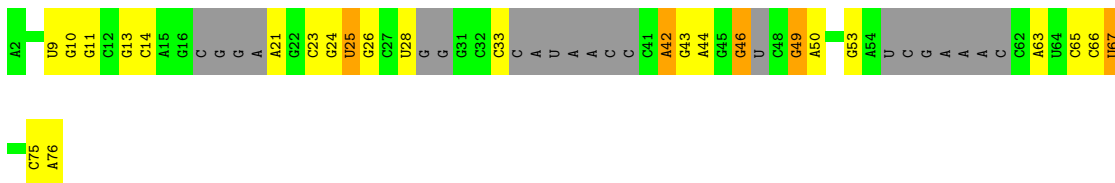
• Molecule 1: A-site-tRNA-Ile-AAT-9-1

Chain At: 



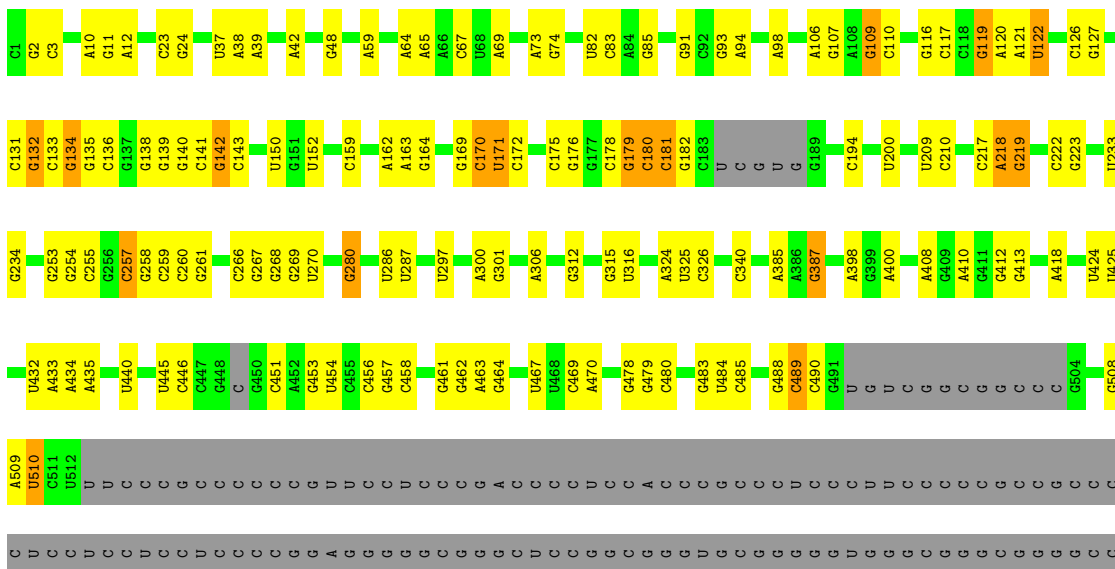
• Molecule 2: E site tRNA

Chain Et: 



• Molecule 3: 28S rRNA

Chain L5: 







C4883	C4741	G4590	C4314	G4196	C4112	C	C	C3906	C3808	U3694	C
C4887	G4742	U4521	G4415	A4203	U4113	C	C	G3907	G3811	U3695	G
U4888	G4743	G4522	C4327	A4203	C4114	G	G	C3908	G3811	C3696	G
	G4744	A4523	G4328	U4208	G4115	C	G	C3909	U3814	U3697	C
A4893	A4611	G4524	G4329	U4208	C4119	C	G	C3910	U3814	C3701	C
A4894	A4422	G4525	G4330	A4214	U4120	G	G	C3911	A3817	C3701	C
C4895	U4423		G4331	A4214	U4120	G	G	U3912	U113818	U3707	C
	U4431	G4528	C4332	A4219	G4121	U	U	U3915	G3819	C3708	C
G4900	U4620	G4529	C4333	A4219	G4122	G	G	G3916	U113818	C3708	C
G4901	U4530	U4531	U4334	A4220	G4123	A	A	C3917	G3823	A3712	C
C4902	C4621	U4531	C4335	C4221	C4124	A	A	G3918	G3823	A3712	C
G4903	A4622	U4532	A4336	G4222	G4124	A	A	C3919	A3824	A3717	C
	G4623	U4532	C4337	G4222	A4127	U	U	U3920	A3825	A3717	C
	A4624	C4536	G4338	U4227	A4128	A	A		A3830	A3718	C
G4910	C4625	C4537	A4339	U4228	G4135	C	C	A3923	A3830	A3719	C
A4911	U4626	U4445	U4340	U4228	G4136	C	C	A3924	G3720	A3719	C
G4912	U4627	U4446	C4342	U4229	C4137	A	A	U3925	U3838	G3721	C
G4913	U4628	C4447	U4343	U4232	G4138	C	C	G3926	G3839	G3722	C
	U4629	C4448	U4344	A4233	C4138	U	U	A3927	U3840	A3723	C
	U4630		C4345	A4234	G4139	A	A	A3928	C3841	A3724	C
C4918	G4631	U4546	U4346	U4235	C	C	C	G3929	U3844	G3725	C
G4919	G4631	C4547	G4347	G4236	C	C	C	U3930	U3844	A3726	C
C4920	A4635	G4549	A4348	G4236	G	U	U	C3931	U3844	A3727	C
C4921	G4636	G4550	A4348	G4236	C	C	C		U3844	A3727	C
C4922	U4636	U4551	A4348	G4236	C	C	C		U3844	A3727	C
C4923	G4637	U4552	U4352	G4239	C	U	G		U3844	A3728	C
	U4638		U4353	G4240	G	U	G	G3934	U3849	A3728	C
	A4656	C4560	U4353	G4240	C4145	A	A	C3935	A3850	A3732	C
G4927	C		U4353	A4251	G4146	U	U	A3936	U3851	U3733	C
C4928	C		U4353	C4252	G4147	U	U	C3937	U3851	U3734	C
A4934	C4670	U4563	A4361	A4253	G4147	U	U		U3853	G3735	C
C4935	G4671	U4564	A4363	G4254	G4150	G	G	G3946	U4066	A3736	C
	U4672		A4363	G4254	G4150	G	G	A3947	U4067	A3737	C
C4938	U4673	G4567	G4370	C4258	C4155	C	C	C3948	U4068	U3640	C
	C4674	A4568	G4370	U4259	G4156	C	C	A	U4069	G3744	C
	U4675	U4569	G4373	C4261	A4157	C	C	U	A3861	U3745	C
		G4570	G4373	C4261	G4158	C	C	U	A3862	U3745	C
A4943	U4689	A4571	G4377	G4266	C4162	C	C	G	A3862	A3748	C
G4954	G4694	U4572	A4378	G4267	U4163	G	G	A	A3867	G3753	C
A4955	C	U4573	A4379	A4268	U4163	G	G	A	G3868	G3753	C
C4957	G4694	G4574	A4383	U4268	C4164	C	C	G	C3869	U3758	C
C4958	U4699	U4575	U4384	A4273	G4168	G	G	U	G3873	A3759	C
	A4700	U4576	U4384	A4274	G4169	G	G	U	G3874	A3760	C
	A4708	U4577	C4387	G4275	A4170	U	U	A	G3874	G3654	C
A4966	U4708	U4578	C4387	G4275	A4170	U	U	A	G3874	G3654	C
A4967	U4709	U4579	G4391	A4281	U4174	C	C	G	A3877	U3768	C
C4968	C	U4580	G4392	U4296	G4175	C	C	G	C3877	G3769	C
C4969	G4719	A4584	G4393	U4296	G4175	C	C	A	C3878	U3770	C
C4970	C4720	U4585	A4394	G4291	A4178	C	C	A	G3879	C3771	C
A4971	C	U4585	U4395	U4293	G4179	C	C	U	G3880	U3772	C
U4972	C4730	A4589	U4401	U4296	U4183	C	C	A	G3881	G3776	C
	G	U4590	C4402	U4296	G4183	C	C	A	U3884	G3777	C
U4976	C	U4591	C4403	U4299	G4184	C	C	U	C3887	G3777	C
U4988	A4734	C4592	U4404	U4299	U4188	C	C	U	C3887	C3782	C
U	C4735	C4593	U4405	A4304	U4189	A	A	G	G3887	A3783	C
C	G4737	G4594	U4406	A4304	U4190	G	G	C	G3888	A3784	C
U4991	C4738	G4595	G4407	U4306	G4191	C	C	A	G3889	A3785	C
G4992	C4739	G4600	A4513	U4312	A4192	C	C	G	G3899	U3786	C
G4993	G4740	A4602	C4413	U4312	A4193	C	C	C	A3901	G3792	C
			A4414	A4313	C4193	G	G	C			C
						U4111	G	C			C



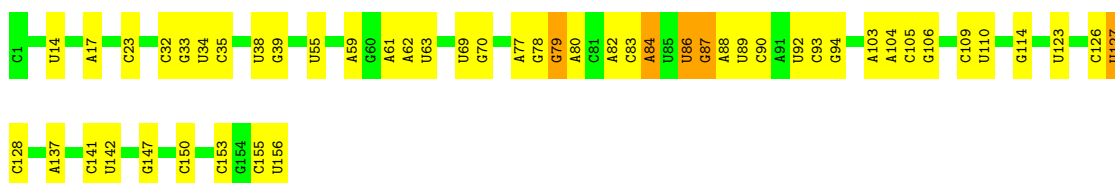
• Molecule 4: 5S rRNA

Chain L7: 78% 21% ..



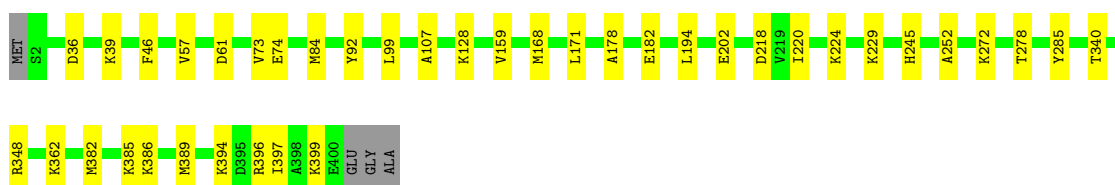
• Molecule 5: 5.8S rRNA

Chain L8: 68% 29% .



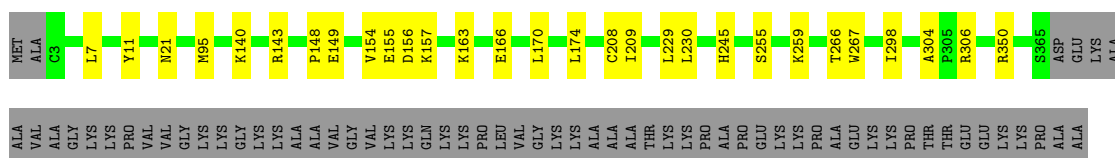
• Molecule 6: Large ribosomal subunit protein uL3

Chain LB: 89% 10% .



• Molecule 7: 60S ribosomal protein L4

Chain LC: 78% 7% 15%

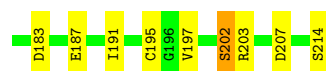


• Molecule 8: 60S ribosomal protein L5

Chain LD: 86% 12% ..

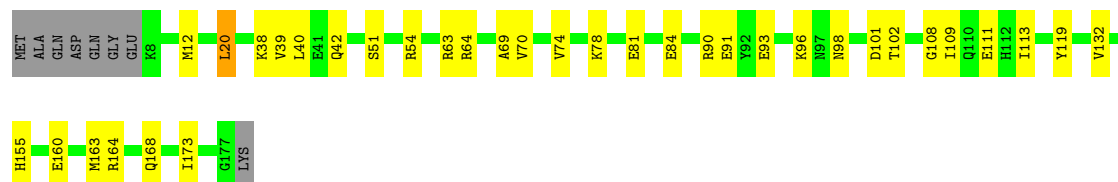


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|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|
| MET | G2 | R7 | R32 | I33 | L36 | K39 | L48 | S54 | S61 | S62 | A64 | L65 | R69 | K74 | V77 | G81 | K82 | I87 | P93 | L103 | SER | CYS | ALA | GLY | ALA | ASP | R110 | T113 | T125 | I135 | R139 | K145 | E146 | I149 | L152 | I161 |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|



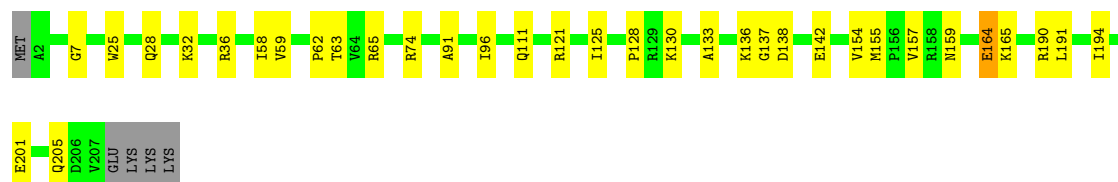
- Molecule 14: 60S ribosomal protein L11

Chain LJ: 76% 19% . .



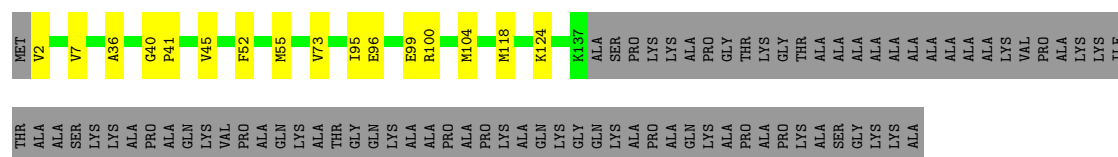
- Molecule 15: Large ribosomal subunit protein eL13

Chain LL: 82% 16% .



- Molecule 16: 60S ribosomal protein L14

Chain LM: 56% 7% 37%



- Molecule 17: 60S ribosomal protein L15

Chain LN: 88% 12%



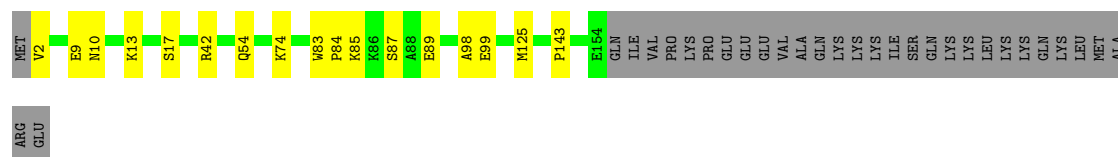
- Molecule 18: 60S ribosomal protein L13a

Chain LO: 91% 7% .



- Molecule 19: 60S ribosomal protein L17

Chain LP: 74% 9% 17%



- Molecule 20: 60S ribosomal protein L18

Chain LQ: 93% 7%



- Molecule 21: 60S ribosomal protein L19

Chain LR: 85% 7% 8%



- Molecule 22: 60S ribosomal protein L18a

Chain LS: 90% 10%



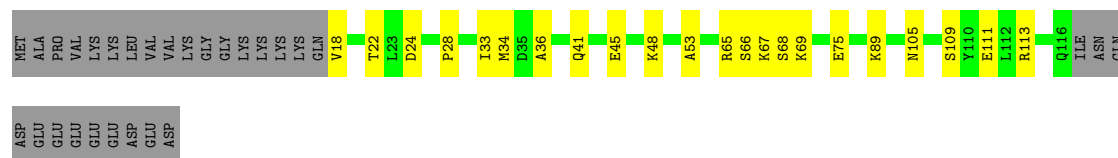
- Molecule 23: 60S ribosomal protein L21

Chain LT: 87% 12%



- Molecule 24: 60S ribosomal protein L22

Chain LU: 60% 17% 23%



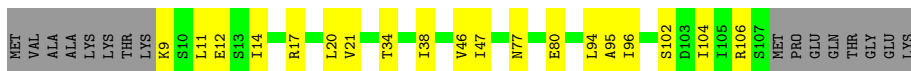
- Molecule 25: 60S ribosomal protein L23

Chain LV: 87% 8% 5%



- Molecule 32: 60S ribosomal protein L30

Chain Lc:  70% 17% 14%



- Molecule 33: 60S ribosomal protein L31

Chain Ld:  73% 12% 14%

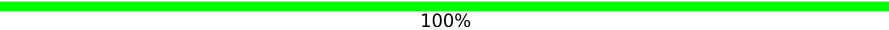


- Molecule 34: 60S ribosomal protein L32

Chain Le:  84% 10% 5%



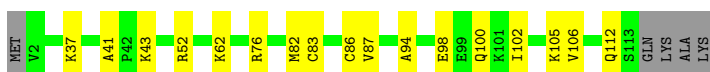
- Molecule 35: 60S ribosomal protein L35a

Chain Lf:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 60S ribosomal protein L34

Chain Lg:  81% 15%



- Molecule 37: 60S ribosomal protein L35

Chain Lh:  81% 18%



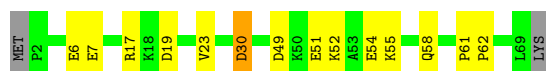
- Molecule 38: 60S ribosomal protein L36

Chain Li:  82% 15%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  77% 19%



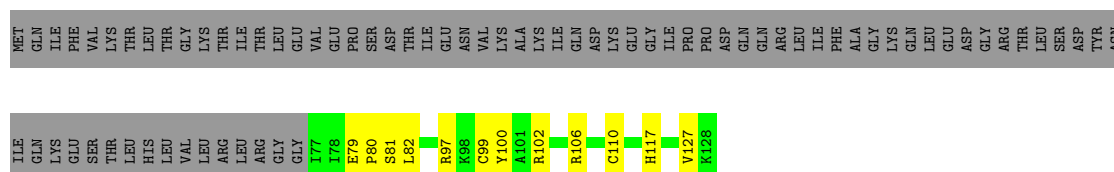
- Molecule 40: 60S ribosomal protein L39

Chain Ll: 80% 18% .



- Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm: 31% 9% 59%



- Molecule 42: 60S ribosomal protein L41

Chain Ln: 88% 12%



- Molecule 43: Large ribosomal subunit protein eL42

Chain Lo: 81% 16% ..



- Molecule 44: 60S ribosomal protein L37a

Chain Lp: 91% 5% ..



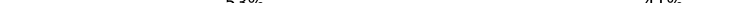
- Molecule 45: 60S ribosomal protein L28

Chain Lr: 81% 10% 9%



- Molecule 46: synthetic mRNA

C2	A5	U6	C7	C8
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- Chain Pt:  53% 41% . .

G1	G2	G3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15	G16	G17	G18	A	U	A21	A22	C23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35	G36	G37	G38	G39	G40	G41	G42	A43	A44	G45	G46	U47	U48	G49	G50	G51	G52	G53	G54	G55	G56	G57	G58	A59	C60	G61	G62	G63	G64	G65	G66	G67	G68	G69	G70	U71	G72	G73	G74	G75	A76	G77	G78	G79	G80	G81	G82	G83	G84	G85	G86	G87	G88	G89	G90	G91	G92	G93	G94	G95	G96	G97	G98	G99	G100
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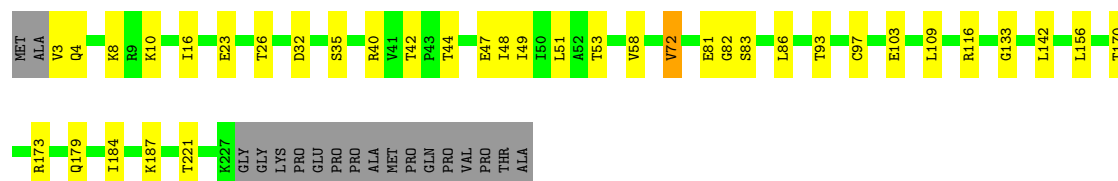
- Chain S2:

U800	C	G673	A587	A512	C417	G309	G	U172	A103	U1
A810	C	U681	G588	A516	C417	G312	G	A173	A104	A2
A811	U	G682	G589	C517	U428	A313	U	C174	U105	C3
A812	G	G683	U591	G518	C429	A313	A	A175	G106	C4
A813	C	C592	C592	A523	G316	G316	G	U176	A107	U15
U814	U	C593	C593	U524	A433	C317	C	G177	G108	G16
U815	C	C687	A594	U525	G434	A318	C	C179	U109	C17
G821	C	U688	C598	A526	G437	C319	C	G184	G113	U21
U822	C	G690	C527	C527	G438	C323	U	G185	G114	A22
U823	G	G691	A528	A528	C441	C324	U	C186	U115	G23
C824	G	G692	A529	A529	C442	C325	U	G187	U116	G27
A827	C	G	U530	U530	C442	C326	C	C	C117	A27
C	C	G	A531	A531	A445	U328	C	G190	C118	G33
A830	C	C	A532	A532	A445	U328	G	A191	U119	U34
A831	C	G	A533	A533	A448	G335	C	C195	U120	C35
C	C	G	G534	G534	A449	G335	C	C196	U121	G36
C	C	G	G535	G535	C450	U344	C	U	G122	U36
C834	C	C	A536	A536	C450	U344	C	U	G126	G41
C	U	G	C	C	A455	U345	G	C	C127	C
A	C	G	U	U	C456	C346	G	C	U128	U44
G	A	U	U	U	C456	G347	C	C	C129	A45
C	U	G	U	U	C463	G351	C	G	G130	A46
C	C	U	U	U	A464	C362	G	G203	C	C
G841	C	U	C	C	A465	C362	G	G204	U	U51
C842	C	U	G	G	C466	A363	G	G205	C	G52
C843	C	C	A	A	G467	A364	G	G206	C	C
U844	U	G	G	G	C470	U367	G	G207	U	G56
G845	A	C	A629	C	G470	C368	C	G208	C	U59
G846	U	C	C	C	C471	C369	C	A209	U	A60
A847	C	C	C632	C549	A472	G370	G	C	C	A61
C	C	C	C	C550	A473	G370	G	C212	C	C
U857	G	C	C	U551	G474	A371	C	G213	C140	A64
A858	U	A	C639	G552	C475	G377	G	U214	A141	A64
A861	A	G	A640	U553	A476	G377	C	G215	C142	C65
A862	G	G	U642	A554	G480	C378	C	C216	U143	G66
U863	U	C	A543	A555	C481	U379	C	A217	U144	C67
C	G	G	G644	A555	G482	C380	G	U218	G145	A68
U	U	A	C	G559	C483	C382	C	U219	C59	C69
C	C	G	U649	C	C483	C382	C	U220	A147	G70
G867	C	C	U650	U562	U487	G383	G	C	U148	G71
G868	C	C	G651	C563	U488	C384	C	C223	C72	C
A869	G	A	A655	A564	A489	C385	U	A224	A150	C
A870	C	C	G656	C568	C492	C387	U	G225	C151	G
U871	G	C	C	A569	A493	U388	U	A	G155	U76
A872	C	G	C660	C	A494	C389	C	C	A77	A77
G873	G	C	C	U572	C494	C390	U	U290	U160	C78
C874	C	C	U661	U573	U495	C391	A	A	U161	A79
A875	G	C	G662	U573	C496	C391	A	A	C162	G80
C876	C	U	C663	A576	A500	G394	A	A	U163	U81
C877	C	C	A664	C	C501	C400	C	C	A164	G82
C878	G	C	C	C	A508	C	C	A	G165	C
C										



- Molecule 51: 40S ribosomal protein S3

Chain SD: 



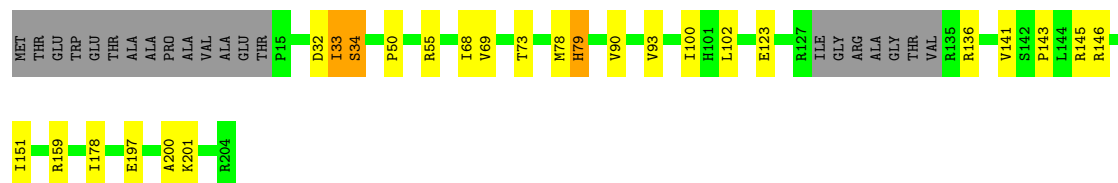
- Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE:  83% 15%



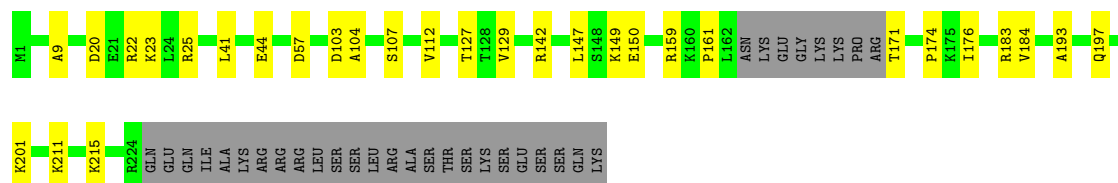
- Molecule 53: 40S ribosomal protein S5

Chain SF: 77% 11% • 10%



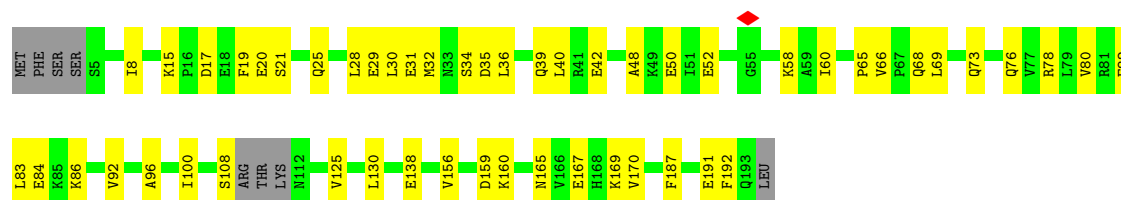
- Molecule 54: 40S ribosomal protein S6

Chain SG: 75% 12% 13%



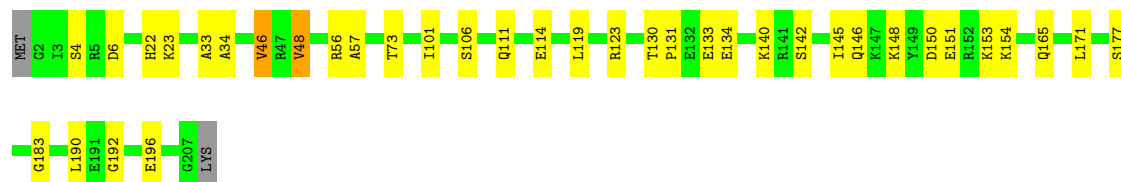
- Molecule 55: 40S ribosomal protein S7

Chain SH:  69% 27% .



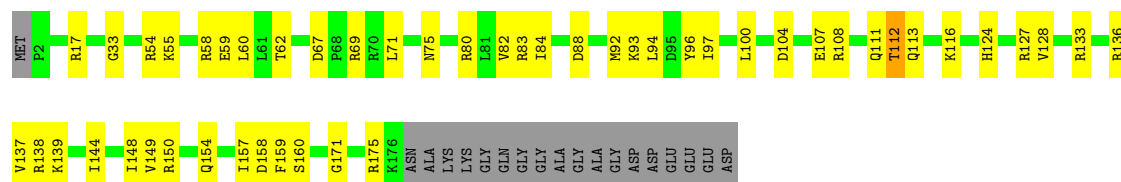
• Molecule 56: 40S ribosomal protein S8

Chain SI: 81% 17% ..



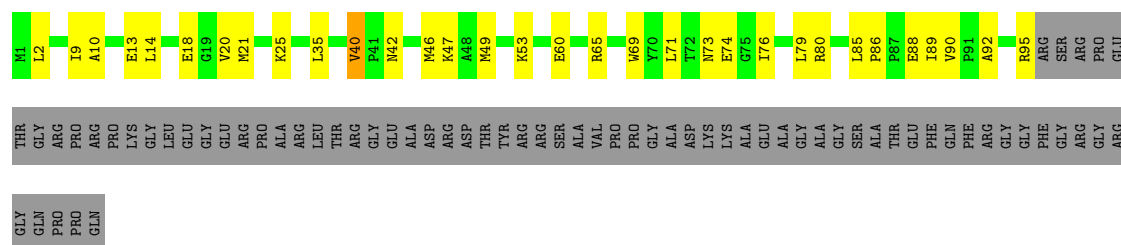
• Molecule 57: 40S ribosomal protein S9

Chain SJ: 65% 25% 10%



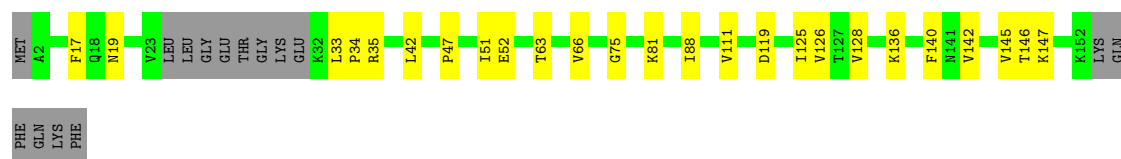
• Molecule 58: 40S ribosomal protein S10

Chain SK: 38% 19% 42%



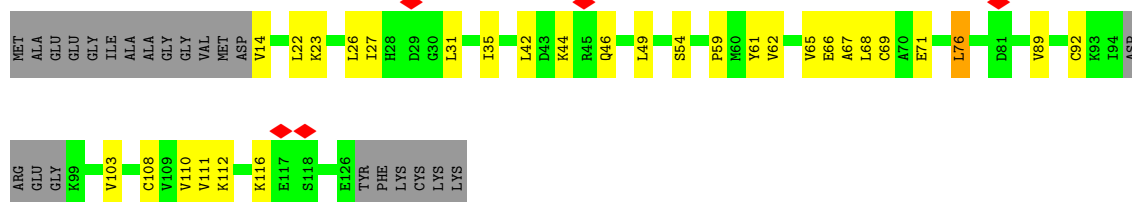
• Molecule 59: 40S ribosomal protein S11

Chain SL: 75% 16% 9%



• Molecule 60: 40S ribosomal protein S12

Chain SM:  60% 22% 17%



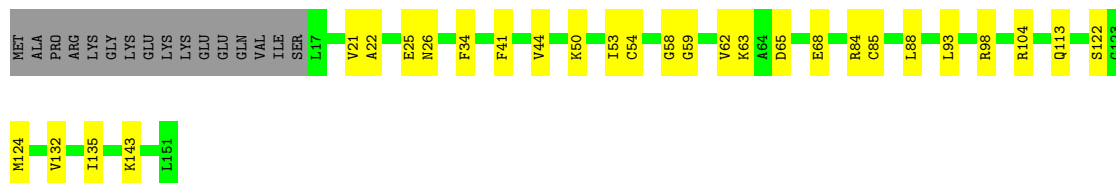
- Molecule 61: 40S ribosomal protein S13

Chain SN:  83% 16%



- Molecule 62: 40S ribosomal protein S14

Chain SO:  71% 19% 11%



- Molecule 63: 40S ribosomal protein S15

Chain SP:  81% 6% 10%



- Molecule 64: 40S ribosomal protein S16

Chain SQ:  82% 12% 6%



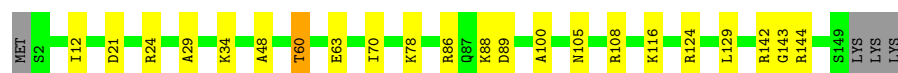
- Molecule 65: 40S ribosomal protein S17

Chain SR:  76% 21% 3%



- Molecule 66: 40S ribosomal protein S18

Chain SS:  83% 14% ..



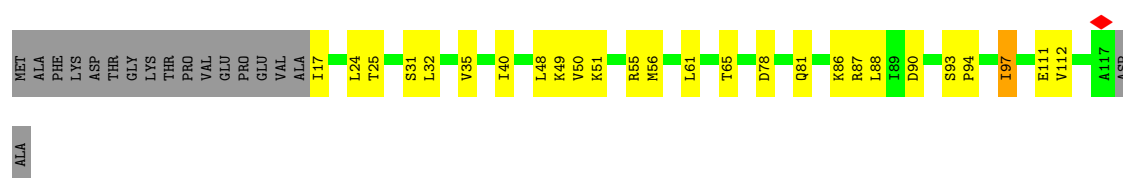
- Molecule 67: 40S ribosomal protein S19

Chain ST:  87% 10% ..



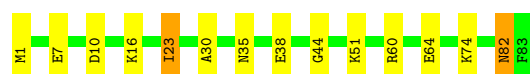
- Molecule 68: 40S ribosomal protein S20

Chain SU:  63% 21% • 15%



- Molecule 69: 40S ribosomal protein S21

Chain SV:  83% 14% •



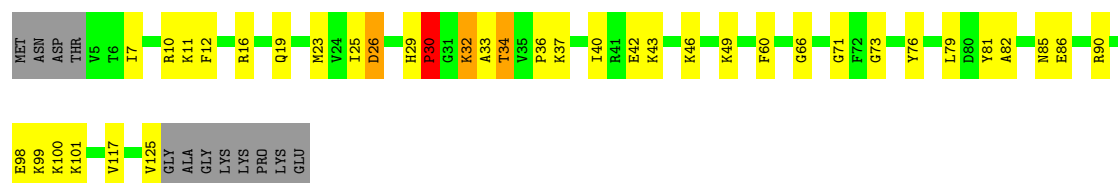
- Molecule 70: 40S ribosomal protein S15a

Chain SW:  86% 12% ..



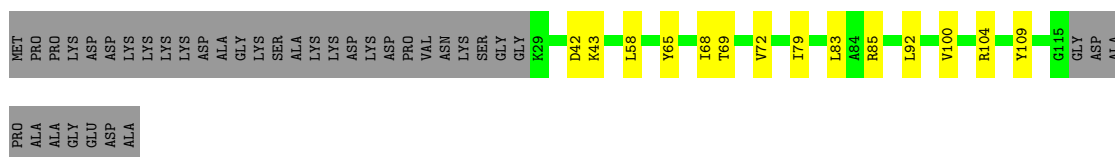
- Molecule 71: 40S ribosomal protein S24

Chain SY:  62% 26% •• 9%



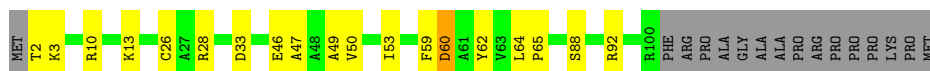
- Molecule 72: 40S ribosomal protein S25

Chain SZ:  58% 11% 30%



- Molecule 73: 40S ribosomal protein S26

Chain Sa: 70% 16% 14%



- Molecule 74: 40S ribosomal protein S27

Chain Sb: 80% 18% ..



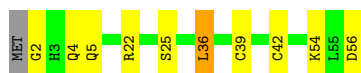
- Molecule 75: 40S ribosomal protein S28

Chain Sc: 65% 26% 9%



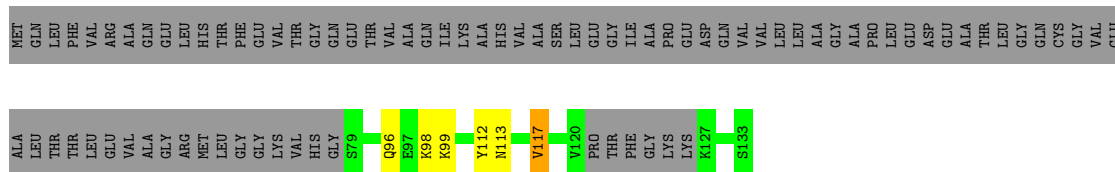
- Molecule 76: 40S ribosomal protein S29

Chain Sd: 80% 16% ..



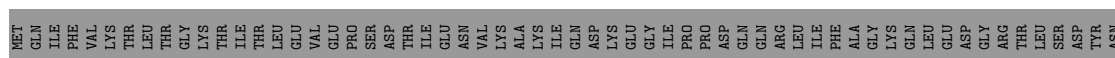
- Molecule 77: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se: 32% 63%



- Molecule 78: Ubiquitin

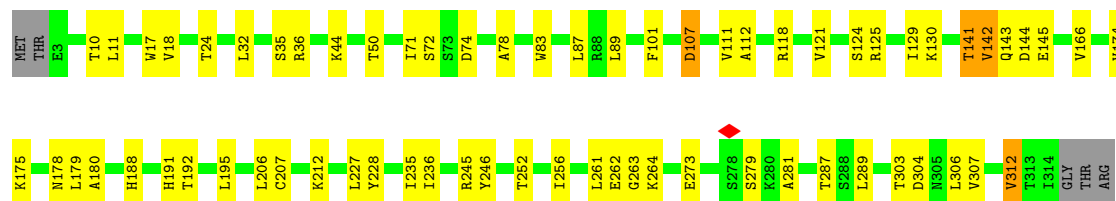
Chain Sf: 29% 10% 61%





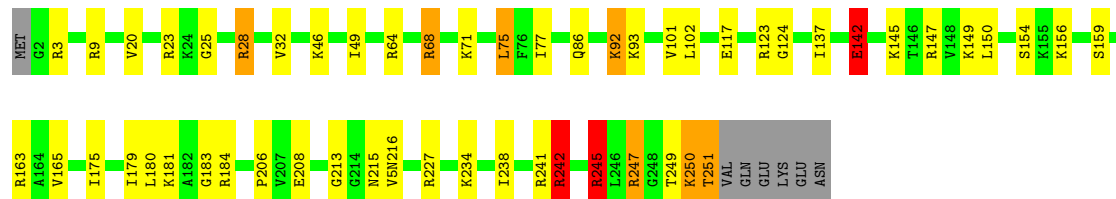
- Molecule 79: Receptor of activated protein C kinase 1

Chain Sg: 77% 20% ..



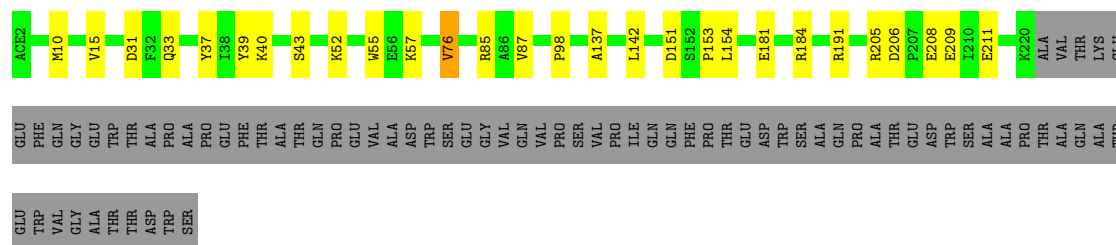
- Molecule 80: Large ribosomal subunit protein uL2

Chain LA: 76% 17% . . .



- Molecule 81: Small ribosomal subunit protein uS2

Chain SA: 65% 9% 25%



- Molecule 82: 40S ribosomal protein S23

Chain SX: 84% 12% ..



- Molecule 83: Large ribosomal subunit protein eL37

Chain Lj: 81% 7% 11%

MET	T2	S7	R20	K36	Y39 P40	W49	K87	ARG	ALA	ALA	VAL	ALA	ALA	SER	SER	SER
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121901	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 ($e^-/\text{\AA}^2$)	1.077	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, PUT, UR3, A2M, UY1, M3L, ACE, SPD, 6MZ, HIC, MA7, B8H, MG, OMC, M2G, 1MA, K, OMU, NA, OMG, 5MC, V5N, MA6, HY3, 1MG, PSU, B8N, 4AC, HYG, ZN, G7M

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	At	0.70	0/1714	0.99	1/2662 (0.0%)
2	Et	0.20	0/1287	0.28	0/1994
3	L5	0.29	0/80395	0.32	2/125381 (0.0%)
4	L7	0.66	0/2836	0.84	0/4421
5	L8	0.66	0/3609	0.84	0/5623
6	LB	0.22	0/3276	0.31	0/4382
7	LC	0.22	0/2942	0.31	0/3951
8	LD	0.20	0/2430	0.30	0/3254
9	LE	0.19	0/1816	0.28	0/2438
10	LF	0.23	0/1890	0.32	0/2521
11	LG	0.21	0/1877	0.31	0/2532
12	LH	0.21	0/1537	0.33	0/2066
13	LI	0.33	0/1710	0.52	1/2284 (0.0%)
14	LJ	0.19	0/1385	0.39	0/1852
15	LL	0.20	0/1706	0.30	0/2284
16	LM	0.21	0/1142	0.32	0/1527
17	LN	0.25	0/1745	0.33	0/2338
18	LO	0.22	0/1672	0.31	0/2238
19	LP	0.22	0/1279	0.34	0/1716
20	LQ	0.23	0/1536	0.31	0/2052
21	LR	0.20	0/1465	0.31	0/1945
22	LS	0.24	0/1500	0.32	0/2013
23	LT	0.22	0/1334	0.34	0/1781
24	LU	0.18	0/822	0.36	0/1103
25	LV	0.21	0/1002	0.32	0/1345
26	LW	0.21	0/861	0.39	0/1146
27	LX	0.21	0/983	0.33	0/1323
28	LY	0.21	0/1115	0.33	0/1484
29	LZ	0.21	0/1130	0.27	0/1507
30	La	0.24	0/1178	0.32	0/1573
31	Lb	0.20	0/848	0.35	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.20	0/776	0.29	0/1042
33	Ld	0.21	0/903	0.30	0/1216
34	Le	0.22	0/1082	0.29	0/1443
35	Lf	0.23	0/899	0.29	0/1205
36	Lg	0.21	0/898	0.32	0/1197
37	Lh	0.20	0/1022	0.29	0/1351
38	Li	0.19	0/843	0.30	0/1115
39	Lk	0.21	0/565	0.36	0/750
40	Ll	0.23	0/453	0.29	0/599
41	Lm	0.56	0/429	0.73	0/571
42	Ln	0.39	0/240	0.31	0/305
43	Lo	0.29	0/881	0.38	0/1161
44	Lp	0.22	0/708	0.33	0/941
45	Lr	0.22	0/1017	0.31	0/1364
46	Mr	0.60	0/114	0.96	0/170
47	Pt	0.71	0/1663	0.90	1/2585 (0.0%)
48	S2	0.67	0/36806	0.86	5/57350 (0.0%)
49	SB	0.20	0/1819	0.31	0/2432
50	SC	0.22	0/1737	0.33	0/2347
51	SD	0.20	0/1770	0.30	0/2385
52	SE	0.20	0/2101	0.32	0/2828
53	SF	0.23	0/1464	0.35	0/1969
54	SG	0.18	0/1742	0.33	0/2326
55	SH	0.17	0/1508	0.34	0/2022
56	SI	0.22	0/1715	0.37	0/2287
57	SJ	0.23	0/1446	0.40	0/1937
58	SK	0.23	0/823	0.41	0/1111
59	SL	0.23	0/1191	0.35	0/1593
60	SM	0.15	0/758	0.40	0/1028
61	SN	0.20	0/1231	0.29	0/1656
62	SO	0.28	0/1022	0.42	0/1372
63	SP	0.32	0/1093	0.48	1/1460 (0.1%)
64	SQ	0.24	0/1133	0.38	0/1517
65	SR	0.22	0/1090	0.41	1/1464 (0.1%)
66	SS	0.21	0/1232	0.33	0/1651
67	ST	0.21	0/1148	0.32	0/1540
68	SU	0.20	0/813	0.30	0/1092
69	SV	0.19	0/643	0.31	0/860
70	SW	0.23	0/1051	0.36	0/1406
71	SY	0.32	0/1012	0.48	0/1344
72	SZ	0.20	0/701	0.35	0/936
73	Sa	0.38	0/805	0.52	0/1079
74	Sb	0.46	0/665	0.61	1/891 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sc	0.22	0/497	0.34	0/666
76	Sd	0.50	0/469	0.63	0/623
77	Se	0.16	0/392	0.31	0/514
78	Sf	0.13	0/489	0.37	0/650
79	Sg	0.20	0/2484	0.39	0/3382
80	LA	1.03	2/1951 (0.1%)	1.23	8/2613 (0.3%)
81	SA	0.31	0/1765	0.47	0/2398
82	SX	0.35	0/1096	0.45	0/1461
83	Lj	0.41	0/720	0.61	0/952
All	All	0.40	2/220897 (0.0%)	0.52	21/324011 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	LI	0	2
41	Lm	0	2
57	SJ	0	1
63	SP	0	1
74	Sb	0	1
80	LA	0	15
82	SX	0	1
83	Lj	0	1
All	All	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	LA	245[A]	ARG	C-O	10.29	1.36	1.23
80	LA	245[B]	ARG	C-O	10.29	1.36	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1581	G	OP1-P-O3'	-24.59	34.24	108.00
80	LA	245[A]	ARG	CA-C-O	11.07	132.03	120.95
80	LA	245[B]	ARG	CA-C-O	11.07	132.03	120.95
80	LA	245[A]	ARG	O-C-N	-7.47	114.74	123.11
80	LA	245[B]	ARG	O-C-N	-7.47	114.74	123.11
48	S2	1825	A	O3'-P-O5'	-6.85	93.72	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	LA	245[A]	ARG	N-CA-C	6.71	120.21	110.42
80	LA	245[B]	ARG	N-CA-C	6.71	120.21	110.42
48	S2	1705	C	O3'-P-O5'	6.21	113.32	104.00
3	L5	4531	U	C4'-C3'-O3'	5.57	117.75	109.40
80	LA	25	GLY	CA-C-O	-5.46	118.39	122.37
13	LI	81	GLY	CA-C-O	-5.46	117.87	122.29
47	Pt	32	C	P-O3'-C3'	5.19	127.98	120.20
48	S2	589	G	OP2-P-O3'	5.17	123.52	108.00
74	Sb	29	ASN	N-CA-C	-5.12	106.71	113.17
65	SR	109	LEU	O-C-N	5.09	129.49	122.46
48	S2	1824	A	C4'-C3'-O3'	-5.07	105.39	113.00
48	S2	1252	C	O3'-P-O5'	-5.07	96.40	104.00
80	LA	142	GLU	CA-C-O	-5.05	116.05	121.56
63	SP	133	ILE	CA-C-O	-5.05	115.70	120.95
1	At	17	G	C4'-C3'-O3'	5.05	116.97	109.40

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
80	LA	123	ARG	Sidechain
80	LA	147	ARG	Sidechain
80	LA	163	ARG	Sidechain
80	LA	184	ARG	Sidechain
80	LA	227	ARG	Sidechain
80	LA	241	ARG	Sidechain
80	LA	242	ARG	Sidechain
80	LA	245[A]	ARG	Sidechain
80	LA	245[B]	ARG	Sidechain
80	LA	247	ARG	Sidechain
80	LA	28	ARG	Sidechain
80	LA	3	ARG	Sidechain
80	LA	64	ARG	Sidechain
80	LA	68	ARG	Sidechain
80	LA	9	ARG	Sidechain
13	LI	32	ARG	Sidechain
13	LI	69	ARG	Sidechain
83	Lj	20	ARG	Sidechain
41	Lm	102	ARG	Sidechain
41	Lm	97	ARG	Sidechain
57	SJ	133	ARG	Sidechain
63	SP	130	ARG	Sidechain

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Mol	Chain	Res	Type	Group
82	SX	61	GLN	Peptide
74	Sb	81	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	At	1559	0	793	13	0
2	Et	1155	0	593	15	0
3	L5	74397	0	37669	646	0
4	L7	2538	0	1284	9	0
5	L8	3316	0	1687	15	0
6	LB	3221	0	3363	24	0
7	LC	2888	0	3064	21	0
8	LD	2385	0	2419	23	0
9	LE	1782	0	1934	17	0
10	LF	1856	0	1981	17	0
11	LG	1846	0	1954	22	0
12	LH	1518	0	1600	15	0
13	LI	1672	0	1717	20	0
14	LJ	1362	0	1399	23	0
15	LL	1672	0	1786	30	0
16	LM	1120	0	1187	13	0
17	LN	1700	0	1749	16	0
18	LO	1640	0	1788	10	0
19	LP	1249	0	1276	10	0
20	LQ	1512	0	1628	13	0
21	LR	1449	0	1549	7	0
22	LS	1460	0	1502	14	0
23	LT	1303	0	1379	17	0
24	LU	808	0	831	12	0
25	LV	988	0	1047	8	0
26	LW	847	0	873	22	0
27	LX	966	0	1040	5	0
28	LY	1098	0	1178	11	0
29	LZ	1107	0	1182	14	0
30	La	1162	0	1206	13	0
31	Lb	846	0	914	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Lc	766	0	798	9	0
33	Ld	888	0	930	9	0
34	Le	1061	0	1160	8	0
35	Lf	880	0	916	0	0
36	Lg	888	0	977	12	0
37	Lh	1014	0	1148	16	0
38	Li	832	0	917	8	0
39	Lk	559	0	624	9	0
40	Ll	443	0	483	6	0
41	Lm	432	0	465	7	0
42	Ln	239	0	289	4	0
43	Lo	875	0	941	14	0
44	Lp	698	0	748	3	0
45	Lr	1002	0	1068	11	0
46	Mr	147	0	56	0	0
47	Pt	1587	0	810	10	0
48	S2	34624	0	17520	262	0
49	SB	1793	0	1879	21	0
50	SC	1700	0	1784	20	0
51	SD	1742	0	1833	18	0
52	SE	2059	0	2164	28	0
53	SF	1443	0	1483	18	0
54	SG	1721	0	1840	19	0
55	SH	1486	0	1560	35	0
56	SI	1686	0	1772	23	0
57	SJ	1424	0	1499	31	0
58	SK	799	0	823	22	0
59	SL	1171	0	1241	13	0
60	SM	754	0	705	20	0
61	SN	1207	0	1293	15	0
62	SO	1009	0	1034	19	0
63	SP	1071	0	1114	8	0
64	SQ	1116	0	1185	14	0
65	SR	1075	0	1128	21	0
66	SS	1214	0	1275	14	0
67	ST	1121	0	1151	15	0
68	SU	803	0	873	15	0
69	SV	636	0	637	13	0
70	SW	1034	0	1080	9	0
71	SY	995	0	1068	31	0
72	SZ	693	0	768	11	0
73	Sa	792	0	841	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	Sb	651	0	672	16	0
75	Sc	495	0	523	9	0
76	Sd	458	0	449	9	0
77	Se	390	0	431	6	0
78	Sf	480	0	469	10	0
79	Sg	2427	0	2380	37	0
80	LA	1923	0	2019	17	0
81	SA	1730	0	1731	20	0
82	SX	1088	0	1149	8	0
83	Lj	705	0	737	3	0
84	L5	86	0	0	0	0
84	L7	2	0	0	0	0
84	L8	1	0	0	0	0
84	LA	2	0	0	0	0
84	LH	1	0	0	0	0
84	LI	1	0	0	0	0
84	Lb	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lf	1	0	0	0	0
84	Lg	1	0	0	0	0
84	Pt	1	0	0	0	0
84	S2	48	0	0	0	0
84	SF	1	0	0	0	0
84	SL	1	0	0	0	0
84	SO	1	0	0	0	0
84	SS	1	0	0	0	0
84	Sd	1	0	0	0	0
85	L5	160	0	0	0	0
85	L7	3	0	0	0	0
85	L8	2	0	0	0	0
85	LI	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Ln	2	0	0	0	0
85	Pt	1	0	0	0	0
85	S2	54	0	0	0	0
86	L5	22	0	0	0	0
86	L8	1	0	0	0	0
86	La	1	0	0	0	0
86	S2	11	0	0	0	0
87	L5	120	0	228	7	0
87	L8	10	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LN	10	0	19	0	0
87	S2	50	0	95	3	0
88	L5	42	0	84	3	0
88	S2	12	0	24	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	1	0	0	2	0
90	S2	36	0	37	1	0
91	At	1	0	0	0	0
91	Et	1	0	0	0	0
91	L5	281	0	0	2	0
91	L7	1	0	0	0	0
91	L8	6	0	0	0	0
91	LA	4	0	0	0	0
91	LC	1	0	0	0	0
91	LI	1	0	0	0	0
91	LN	1	0	0	0	0
91	LP	1	0	0	0	0
91	LQ	1	0	0	0	0
91	LY	1	0	0	0	0
91	La	3	0	0	0	0
91	Ld	1	0	0	0	0
91	Le	3	0	0	0	0
91	Ln	7	0	0	0	0
91	Lo	4	0	0	0	0
91	Lp	1	0	0	0	0
91	Mr	11	0	0	0	0
91	Pt	11	0	0	0	0
91	S2	171	0	0	0	0
91	SN	1	0	0	0	0
91	SO	1	0	0	0	0
91	SQ	1	0	0	0	0
91	SW	1	0	0	0	0
91	SX	1	0	0	0	0
All	All	211463	0	156518	1844	0

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

All (1844) 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)
48:S2:551:U:H2'	48:S2:552:G:C8	1.98	0.98
48:S2:857:U:H2'	48:S2:858:A:C8	2.04	0.91
3:L5:4095:G:H1	3:L5:4113:U:H3	0.89	0.89
50:SC:249:SER:HA	69:SV:23:ILE:HD11	1.56	0.88
48:S2:394:G:H5'	59:SL:81:LYS:HB3	1.57	0.86
58:SK:65:ARG:HG3	76:Sd:22:ARG:O	1.74	0.86
48:S2:307:G:H4'	48:S2:308:G:OP2	1.75	0.86
3:L5:1759:G:H1	3:L5:1773:U:H3	1.24	0.84
3:L5:2557:G:H1	3:L5:2570:U:H3	1.24	0.84
15:LL:63:THR:HG21	30:La:66:ASN:HB3	1.59	0.83
48:S2:190:G:HO2'	48:S2:191:A:H8	0.84	0.82
48:S2:1308:U:H1'	78:Sf:135:HIS:CE1	2.15	0.82
3:L5:3946:G:H1	3:L5:4067:U:H3	1.26	0.80
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.46	0.80
48:S2:190:G:O2'	48:S2:191:A:H8	1.63	0.79
3:L5:1762:C:H42	3:L5:1770:A:H61	1.29	0.78
76:Sd:39:CYS:SG	76:Sd:42:CYS:SG	2.82	0.77
82:SX:51:VAL:HG22	82:SX:98:ASP:H	1.50	0.77
69:SV:7:GLU:N	69:SV:7:GLU:OE2	2.18	0.77
48:S2:70:G:H21	48:S2:79:A:H2	1.31	0.75
15:LL:63:THR:HG22	15:LL:65:ARG:H	1.52	0.75
3:L5:4115:G:OP2	3:L5:4115:G:N2	2.17	0.75
48:S2:797:C:H2'	48:S2:798:G:C8	2.20	0.75
58:SK:74:GLU:OE2	58:SK:74:GLU:N	2.20	0.74
79:Sg:118:ARG:HA	79:Sg:118:ARG:HH11	1.51	0.74
48:S2:940:U:H3	48:S2:1002:U:H3	1.36	0.74
14:LJ:63:ARG:HH22	43:Lo:105:GLN:HA	1.52	0.74
3:L5:181:C:H2'	3:L5:182:G:H8	1.51	0.74
59:SL:119:ASP:O	59:SL:147:LYS:NZ	2.21	0.74
3:L5:3823:G:N2	3:L5:3823:G:OP2	2.21	0.74
53:SF:55:ARG:HH11	53:SF:55:ARG:HG3	1.53	0.74
60:SM:31:LEU:HD12	60:SM:89:VAL:HG13	1.71	0.73
19:LP:42:ARG:NH2	19:LP:99:GLU:OE2	2.22	0.73
48:S2:190:G:O2'	48:S2:191:A:C8	2.41	0.72
48:S2:925:G:H1	48:S2:1017:U:H3	1.39	0.71
79:Sg:273:GLU:OE2	79:Sg:273:GLU:N	2.20	0.71
76:Sd:42:CYS:SG	89:Sd:102:ZN:ZN	1.79	0.71
53:SF:33:ILE:HD11	75:Sc:35:MET:HE1	1.73	0.71
57:SJ:83:ARG:HG2	57:SJ:150:ARG:HD3	1.73	0.70
52:SE:165:GLU:OE1	52:SE:165:GLU:N	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2800:G:N7	88:L5:5387:PUT:N2	2.40	0.70
61:SN:101:HIS:HA	61:SN:104:ARG:HH21	1.56	0.70
4:L7:28:C:H2'	4:L7:29:C:H5'	1.72	0.69
3:L5:5040:U:OP2	6:LB:396:ARG:NH2	2.25	0.69
55:SH:52:GLU:HG2	55:SH:58:LYS:HZ3	1.58	0.69
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.57	0.69
24:LU:28:PRO:HB2	24:LU:34:MET:HG2	1.75	0.69
39:Lk:52:LYS:HA	39:Lk:55:LYS:HE3	1.75	0.69
70:SW:28:ARG:HB3	70:SW:29:PRO:HD3	1.74	0.69
3:L5:4918:C:H2'	3:L5:4919:G:H8	1.58	0.69
19:LP:10:ASN:OD1	19:LP:13:LYS:NZ	2.26	0.69
49:SB:83:LYS:HD3	49:SB:106:THR:HG22	1.74	0.69
69:SV:44:GLY:O	81:SA:191:ARG:NH2	2.26	0.69
52:SE:133:THR:HG22	52:SE:134:LYS:HG2	1.74	0.69
48:S2:928:G:H1	48:S2:1013:U:H3	1.40	0.69
32:Lc:21:VAL:HG11	32:Lc:96:ILE:HD12	1.75	0.68
66:SS:105:ASN:OD1	66:SS:108:ARG:NH2	2.26	0.68
63:SP:31:GLU:OE1	63:SP:31:GLU:N	2.26	0.68
48:S2:326:C:H5''	48:S2:327:G:H5'	1.75	0.68
37:Lh:15:GLU:OE2	37:Lh:15:GLU:N	2.18	0.68
26:LW:106:GLU:HA	26:LW:109:ILE:HG22	1.76	0.67
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.77	0.67
20:LQ:14:ARG:HG2	20:LQ:14:ARG:HH11	1.58	0.67
22:LS:99:ASP:OD2	22:LS:108:GLN:NE2	2.28	0.67
58:SK:42:ASN:O	58:SK:46:MET:HG3	1.94	0.67
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.30	0.67
3:L5:2861:OMC:OP2	87:L5:5373:SPD:N10	2.28	0.67
3:L5:2017:A:H2'	3:L5:2018:C:C6	2.30	0.66
6:LB:168:MET:HG3	6:LB:178:ALA:HA	1.76	0.66
47:Pt:26:M2G:HM12	47:Pt:44:A:H2	1.60	0.66
48:S2:115:U:H2'	48:S2:116:OMU:C6	2.26	0.66
3:L5:1480:C:O2'	3:L5:1482:G:OP2	2.14	0.66
49:SB:165:ARG:HG2	49:SB:169:MET:HE2	1.77	0.66
79:Sg:145:GLU:OE2	79:Sg:145:GLU:N	2.28	0.66
62:SO:59:GLY:HA2	62:SO:68:GLU:HG2	1.78	0.66
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.24	0.66
3:L5:989:U:H3	3:L5:1064:G:H1	1.43	0.66
48:S2:640:A:H2'	48:S2:641:A:C8	2.31	0.66
32:Lc:9:LYS:N	32:Lc:12:GLU:OE1	2.29	0.65
2:Et:33:C:H4'	53:SF:136:ARG:HD2	1.78	0.65
3:L5:4251:A:H5''	14:LJ:108:GLY:HA3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Sg:129:ILE:HB	79:Sg:142:VAL:HG22	1.77	0.65
65:SR:75:GLU:OE1	65:SR:78:ARG:NH1	2.29	0.65
29:LZ:90:PRO:O	29:LZ:117:LYS:NZ	2.29	0.65
3:L5:4124:G:N2	11:LG:43:GLN:O	2.30	0.65
57:SJ:58:ARG:O	57:SJ:62:THR:HG23	1.97	0.65
3:L5:705:G:OP2	34:Le:5:ARG:NH2	2.30	0.64
49:SB:224:GLU:HB2	49:SB:227:LYS:HB2	1.78	0.64
70:SW:80:ASP:OD1	70:SW:124:LYS:NZ	2.26	0.64
3:L5:4918:C:H2'	3:L5:4919:G:C8	2.32	0.64
54:SG:142:ARG:HA	54:SG:147:LEU:HD23	1.80	0.64
3:L5:2899:C:OP1	21:LR:108:ARG:NH2	2.29	0.64
19:LP:85:LYS:O	19:LP:89:GLU:HG2	1.96	0.64
32:Lc:20:LEU:HB3	32:Lc:102:SER:HB2	1.80	0.64
58:SK:53:LYS:HE2	58:SK:60:GLU:HB3	1.79	0.64
21:LR:7:GLN:NE2	21:LR:35:ALA:O	2.31	0.64
55:SH:39:GLN:OE1	55:SH:39:GLN:N	2.31	0.64
71:SY:7:ILE:HD13	71:SY:43:LYS:HD2	1.79	0.64
7:LC:140:LYS:HE3	7:LC:245:HIS:HB2	1.79	0.64
62:SO:25:GLU:OE1	62:SO:25:GLU:N	2.30	0.64
3:L5:2095:A:O2'	10:LF:32:ARG:NH1	2.31	0.64
3:L5:4734:A:H2'	3:L5:4735:G:C8	2.33	0.64
23:LT:102:ARG:O	23:LT:106:LEU:HG	1.98	0.64
3:L5:74:G:H5'	15:LL:59:VAL:HB	1.80	0.63
10:LF:182:TYR:HB3	10:LF:200:ARG:HG3	1.80	0.63
39:Lk:30:ASP:OD1	39:Lk:30:ASP:N	2.31	0.63
3:L5:1727:U:OP1	10:LF:131:ASN:ND2	2.31	0.63
55:SH:60:ILE:HB	55:SH:92:VAL:HG12	1.80	0.63
13:LI:146:GLU:N	13:LI:146:GLU:OE2	2.30	0.63
3:L5:1759:G:N2	3:L5:1773:U:O2	2.29	0.63
74:Sb:83:GLN:OE1	74:Sb:83:GLN:N	2.31	0.63
3:L5:1757:U:H2'	3:L5:1758:G:H8	1.63	0.63
14:LJ:160:GLU:OE2	14:LJ:164:ARG:NH1	2.32	0.63
71:SY:19:GLN:HG3	71:SY:81:TYR:CD2	2.33	0.63
61:SN:29:THR:OG1	61:SN:32:ASP:OD2	2.14	0.63
68:SU:51:LYS:HB3	68:SU:90:ASP:HB2	1.80	0.63
79:Sg:32:LEU:HD12	79:Sg:71:ILE:HG12	1.80	0.63
3:L5:1761:G:H1	3:L5:1771:U:H3	1.47	0.63
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.78	0.63
3:L5:4095:G:N2	3:L5:4113:U:O2	2.25	0.63
44:Lp:84:ARG:O	44:Lp:88:GLU:HG2	1.98	0.63
53:SF:73:THR:HG22	53:SF:93:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82: SX:70: VAL: HG11	82: SX:94: ILE: HG21	1.81	0.62
13: LI:183: ASP: O	13: LI:187: GLU: HG2	1.99	0.62
54: SG:103: ASP: OD1	54: SG:104: ALA: N	2.30	0.62
65: SR:111: PHE: HD2	81: SA:15: VAL: HG21	1.62	0.62
3: L5:4076: G: OP1	11: LG:73: ARG: NE	2.20	0.62
33: Ld:19: GLU: OE1	33: Ld:92: ARG: NH1	2.32	0.62
48: S2:1228: A: H2'	48: S2:1229: G: C8	2.34	0.62
3: L5:1697: G: N2	3: L5:2084: C: OP1	2.32	0.62
3: L5:4260: U: H2'	3: L5:4261: C: C6	2.34	0.62
48: S2:1545: A: H2'	48: S2:1546: G: C8	2.34	0.62
3: L5:169: G: O2'	15: LL:136: LYS: NZ	2.33	0.62
3: L5:4967: A: H2'	3: L5:4968: A: H8	1.65	0.62
3: L5:257: C: H2'	3: L5:258: G: H8	1.63	0.62
8: LD:204: VAL: O	8: LD:208: MET: HG3	2.00	0.62
39: Lk:51: GLU: N	39: Lk:51: GLU: OE2	2.33	0.62
52: SE:100: ARG: HH12	52: SE:118: GLU: HG3	1.64	0.62
57: SJ:149: VAL: HG11	57: SJ:157: ILE: HD11	1.81	0.62
3: L5:1188: C: H2'	3: L5:1189: G: C8	2.35	0.62
61: SN:19: ARG: HG2	74: Sb:84: HIS: CE1	2.34	0.62
3: L5:257: C: H2'	3: L5:258: G: C8	2.34	0.61
3: L5:920: C: H2'	3: L5:921: C: H6	1.65	0.61
3: L5:4274: A: H2'	3: L5:4275: G: C8	2.36	0.61
65: SR:31: ASN: HD22	65: SR:55: THR: HG22	1.65	0.61
2: Et:26: G: H22	2: Et:44: A: H2	1.48	0.61
3: L5:3936: A: H2	17: LN:125: SER: HG	1.48	0.61
3: L5:4352: U: OP1	15: LL:190[B]: ARG: NH2	2.29	0.61
3: L5:4299: PSU: OP1	20: LQ:160: HIS: HE1	1.84	0.61
9: LE:180: VAL: HG11	9: LE:258: LEU: HD11	1.82	0.61
24: LU:105: ASN: OD1	24: LU:109: SER: OG	2.18	0.61
58: SK:73: ASN: O	58: SK:76: ILE: HG22	2.01	0.61
48: S2:145: G: H2'	48: S2:146: G: C8	2.35	0.61
74: Sb:75: GLU: N	74: Sb:75: GLU: OE2	2.31	0.61
43: Lo:11: PHE: O	43: Lo:81: ARG: NH2	2.33	0.61
3: L5:1460: C: H5''	20: LQ:144: LYS: HG2	1.83	0.61
48: S2:1239: PSU: H5'	63: SP:124: LYS: HD2	1.82	0.61
24: LU:48: LYS: HG2	24: LU:53: ALA: HB2	1.81	0.61
26: LW:91: MET: HE2	26: LW:91: MET: HA	1.82	0.61
3: L5:699: C: H2'	3: L5:700: G: H8	1.66	0.61
66: SS:24: ARG: HB2	66: SS:29: ALA: HB2	1.83	0.61
24: LU:24: ASP: OD2	24: LU:69: LYS: NZ	2.32	0.60
49: SB:47: THR: OG1	49: SB:65: ARG: NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LB:74:GLU:OE1	6:LB:285:TYR:OH	2.16	0.60
19:LP:125:MET:HE3	19:LP:143:PRO:HG3	1.83	0.60
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.34	0.60
21:LR:135:LYS:O	21:LR:139:MET:HG3	2.01	0.60
47:Pt:21:A:H61	47:Pt:46:A:H2'	1.67	0.60
50:SC:169:TYR:OH	50:SC:175:GLY:O	2.17	0.60
41:Lm:79:GLU:OE2	41:Lm:81:SER:N	2.33	0.60
52:SE:176:ASP:OD1	52:SE:179:ASN:ND2	2.34	0.60
58:SK:86:PRO:HG2	58:SK:89:ILE:HD11	1.83	0.60
3:L5:217:C:H3'	3:L5:218:A:H2'	1.83	0.60
3:L5:2091:C:O2	3:L5:2094:G:O2'	2.11	0.60
3:L5:1699:A:H2'	3:L5:1700:G:O4'	2.02	0.60
3:L5:480:C:OP1	45:Lr:67:ARG:NH1	2.34	0.60
3:L5:658:C:H2'	3:L5:659:G:H8	1.67	0.60
2:Et:42:A:H2'	2:Et:43:G:C8	2.37	0.60
14:LJ:12:MET:HA	14:LJ:12:MET:HE3	1.84	0.60
54:SG:20:ASP:OD1	54:SG:23:LYS:N	2.28	0.60
68:SU:40:ILE:HG12	68:SU:50:VAL:HG11	1.83	0.60
44:Lp:38:THR:HA	44:Lp:45:THR:HA	1.84	0.59
48:S2:1308:U:H1'	78:Sf:135:HIS:HE1	1.64	0.59
50:SC:187:ARG:HD3	50:SC:192:LEU:HD12	1.84	0.59
3:L5:3786:U:OP1	3:L5:4550:G:O2'	2.20	0.59
7:LC:154:VAL:HG11	7:LC:174:LEU:HD11	1.85	0.59
15:LL:25:TRP:HE1	17:LN:199:GLN:HG3	1.67	0.59
3:L5:1188:C:H2'	3:L5:1189:G:H8	1.67	0.59
3:L5:1769:G:H2'	3:L5:1770:A:C8	2.37	0.59
3:L5:4095:G:O6	3:L5:4113:U:O4	2.20	0.59
15:LL:128:PRO:HA	15:LL:138:ASP:OD2	2.01	0.59
24:LU:18:VAL:HG12	24:LU:75:GLU:HA	1.83	0.59
3:L5:690:C:OP1	45:Lr:87:ARG:NH1	2.36	0.59
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.68	0.59
16:LM:118:MET:HE2	16:LM:118:MET:HA	1.84	0.59
3:L5:462:G:H2'	3:L5:463:A:C8	2.37	0.59
30:La:76:ASP:HB3	30:La:115:GLY:HA3	1.83	0.59
12:LH:44:GLU:OE1	16:LM:2:VAL:N	2.35	0.59
12:LH:59:LYS:HE2	12:LH:66:GLU:HB3	1.85	0.59
23:LT:103:ASP:OD1	23:LT:104:SER:N	2.36	0.59
3:L5:1418:C:H2'	3:L5:1419:G:O4'	2.03	0.59
78:Sf:137:ASP:HA	78:Sf:150:PHE:HD2	1.66	0.59
3:L5:1769:G:H2'	3:L5:1770:A:H8	1.68	0.59
12:LH:94:SER:HB2	12:LH:142:ASP:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1588:A:H2'	48:S2:1589:A:C8	2.37	0.58
71:SY:117:VAL:HG21	71:SY:125:VAL:HG21	1.85	0.58
64:SQ:61:GLU:H	64:SQ:61:GLU:CD	2.10	0.58
3:L5:1293:G:OP2	3:L5:1293:G:N2	2.29	0.58
48:S2:1091:C:HO2'	70:SW:2:VAL:N	2.00	0.58
3:L5:4694:G:OP1	3:L5:4694:G:N2	2.35	0.58
48:S2:65:C:H5'	54:SG:174:PRO:HA	1.85	0.58
48:S2:1144:A:H2'	48:S2:1145:A:C8	2.38	0.58
53:SF:102:LEU:HD11	72:SZ:100:VAL:HG21	1.85	0.58
55:SH:42:GLU:OE2	55:SH:42:GLU:N	2.24	0.58
8:LD:208:MET:HB2	8:LD:233:PRO:HG3	1.84	0.58
11:LG:58:PRO:HD2	11:LG:61:ILE:HD12	1.84	0.58
3:L5:1405:C:N4	3:L5:1406:G:O6	2.37	0.58
41:Lm:79:GLU:OE2	41:Lm:81:SER:OG	2.22	0.58
57:SJ:82:VAL:HG21	57:SJ:92:MET:HE1	1.84	0.58
3:L5:1100:U:H3	3:L5:1195:G:H1	1.50	0.58
48:S2:582:U:H2'	48:S2:583:A:C8	2.38	0.58
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.38	0.58
3:L5:4392:OMG:H2'	3:L5:4447:5MC:HM51	1.86	0.58
13:LI:36:LEU:HD12	13:LI:87:ILE:HB	1.84	0.58
3:L5:1708:G:OP1	31:Lb:101:HIS:NE2	2.33	0.58
3:L5:1768:C:H2'	3:L5:1769:G:C8	2.38	0.58
9:LE:114:ARG:HH21	45:Lr:87:ARG:HH22	1.49	0.58
48:S2:958:G:O6	49:SB:5:LYS:NZ	2.37	0.58
80:LA:117:GLU:HG2	80:LA:124:GLY:H	1.69	0.58
16:LM:55:MET:O	22:LS:157:ARG:NH2	2.36	0.58
3:L5:669:C:H5'	45:Lr:68:SER:HB2	1.85	0.57
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.38	0.57
9:LE:161:ARG:NH1	9:LE:273:SER:OG	2.37	0.57
32:Lc:34:THR:HG23	32:Lc:95:ALA:HB2	1.86	0.57
48:S2:1140:G:O2'	48:S2:1141:G:H5'	2.04	0.57
56:SI:34:ALA:HB2	56:SI:56:ARG:HD2	1.86	0.57
57:SJ:108:ARG:NH1	57:SJ:113:GLN:OE1	2.36	0.57
48:S2:1314:U:H2'	58:SK:2:LEU:HD23	1.86	0.57
13:LI:202:SER:O	13:LI:202:SER:OG	2.22	0.57
48:S2:120:U:H2'	48:S2:121:OMU:C6	2.33	0.57
48:S2:582:U:H1'	71:SY:33:ALA:HB2	1.86	0.57
52:SE:141:THR:OG1	52:SE:143:ASP:OD1	2.21	0.57
79:Sg:18:VAL:O	79:Sg:287:THR:OG1	2.22	0.57
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.38	0.57
3:L5:2583:C:OP2	36:Lg:76:ARG:NH1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.39	0.57
44:Lp:74:THR:O	44:Lp:78:THR:HG22	2.05	0.57
48:S2:811:A:H2'	48:S2:812:A:C8	2.39	0.57
78:Sf:121:CYS:HG	78:Sf:126:CYS:HG	1.51	0.57
48:S2:885:U:H2'	48:S2:886:A:C8	2.39	0.57
58:SK:9:ILE:HD12	58:SK:10:ALA:N	2.18	0.57
3:L5:170:C:O2'	3:L5:171:U:OP1	2.23	0.57
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.39	0.57
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.39	0.57
3:L5:4927:G:H5''	3:L5:4928:C:H5	1.69	0.57
31:Lb:117:ARG:HA	31:Lb:117:ARG:HE	1.69	0.57
64:SQ:53:GLU:OE2	64:SQ:85:ARG:NH2	2.31	0.57
3:L5:1241:C:H1'	31:Lb:119:CYS:HA	1.87	0.57
9:LE:258:LEU:HD22	9:LE:262:LYS:HE3	1.87	0.57
47:Pt:63:U:H2'	47:Pt:64:G:C8	2.40	0.57
48:S2:433:A:H5''	56:SI:22:HIS:HB3	1.86	0.57
55:SH:167:GLU:OE1	55:SH:167:GLU:N	2.35	0.57
3:L5:1591:U:OP2	3:L5:2856:C:O2'	2.19	0.57
3:L5:2756:G:N7	29:LZ:51:ARG:NH2	2.48	0.57
6:LB:36:ASP:HB3	6:LB:39:LYS:HG3	1.87	0.57
48:S2:582:U:H2'	48:S2:583:A:H8	1.69	0.57
10:LF:41:MET:HE2	31:Lb:113:ALA:HB2	1.86	0.56
3:L5:961:G:O2'	3:L5:963:G:N7	2.36	0.56
3:L5:2018:C:H2'	3:L5:2019:C:C6	2.41	0.56
15:LL:154:VAL:HG12	15:LL:155:MET:HG3	1.86	0.56
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.41	0.56
3:L5:1700:G:H5'	7:LC:306:ARG:HD2	1.86	0.56
3:L5:1927:U:OP1	3:L5:1949:U:O2'	2.22	0.56
3:L5:2023:C:H2'	3:L5:2024:G:C4	2.40	0.56
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.40	0.56
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.70	0.56
3:L5:4739:C:H2'	3:L5:4740:G:H5'	1.87	0.56
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.40	0.56
18:LO:4:VAL:HG12	18:LO:31:ARG:HH21	1.68	0.56
48:S2:59:U:H5'	48:S2:501:C:H4'	1.86	0.56
71:SY:101:LYS:HD2	71:SY:101:LYS:N	2.21	0.56
3:L5:2414:G:H2'	3:L5:2415:OMU:H6	1.88	0.56
25:LV:43:LYS:HG3	25:LV:60:MET:HG2	1.87	0.56
41:Lm:79:GLU:HG2	41:Lm:80:PRO:HD2	1.86	0.56
51:SD:103:GLU:OE2	51:SD:173:ARG:NE	2.39	0.56
57:SJ:59:GLU:OE1	57:SJ:69:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SK:80:ARG:HG2	58:SK:85:LEU:HB2	1.86	0.56
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.41	0.56
3:L5:4927:G:H5''	3:L5:4928:C:C5	2.40	0.56
48:S2:1536:G:H2'	48:S2:1537:A:C8	2.40	0.56
79:Sg:11:LEU:HB2	79:Sg:307:VAL:HB	1.86	0.56
81:SA:10:MET:CE	81:SA:55:TRP:HB2	2.35	0.56
3:L5:711:A:H2'	3:L5:712:C:C6	2.40	0.56
3:L5:2814:C:H5'	3:L5:2815:A2M:OP2	2.05	0.56
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.70	0.56
53:SF:55:ARG:HG3	53:SF:55:ARG:NH1	2.20	0.56
56:SI:57:ALA:HB2	56:SI:183:GLY:HA2	1.87	0.56
65:SR:109:LEU:HD23	81:SA:52:LYS:HB2	1.88	0.56
3:L5:143:C:O4'	11:LG:108:GLN:NE2	2.38	0.56
25:LV:39:ILE:HD12	25:LV:61:VAL:HG21	1.88	0.56
3:L5:1435:G:O2'	3:L5:1707:C:N3	2.33	0.56
3:L5:3663:A:N6	3:L5:4168:G:O2'	2.39	0.56
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.41	0.56
12:LH:14:GLU:H	12:LH:14:GLU:CD	2.14	0.56
48:S2:981:A:H2'	48:S2:982:G:C8	2.40	0.56
82:SX:95:GLU:O	82:SX:98:ASP:HB2	2.06	0.56
3:L5:3937:C:H1'	17:LN:125:SER:HB2	1.87	0.56
3:L5:4860:G:H2'	3:L5:4861:G:H8	1.71	0.56
4:L7:28:C:C2'	4:L7:29:C:H5'	2.36	0.56
71:SY:26:ASP:N	71:SY:26:ASP:OD1	2.36	0.56
79:Sg:304:ASP:O	79:Sg:306:LEU:N	2.39	0.56
3:L5:2758:G:O2'	3:L5:2765:A:N3	2.33	0.56
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.41	0.56
48:S2:120:U:H2'	48:S2:121:OMU:H6	1.86	0.56
48:S2:811:A:H2'	48:S2:812:A:H8	1.71	0.56
54:SG:161:PRO:HA	54:SG:171:THR:HG22	1.87	0.56
3:L5:93:G:H2'	3:L5:94:A:C8	2.40	0.55
3:L5:1459:A:OP1	20:LQ:65:ARG:NH1	2.39	0.55
5:L8:127:U:H3'	5:L8:128:C:H6	1.71	0.55
38:Li:84:LYS:O	38:Li:88:GLU:HG2	2.06	0.55
48:S2:107:A:H2'	48:S2:108:G:C8	2.41	0.55
48:S2:115:U:H2'	48:S2:116:OMU:H6	1.87	0.55
3:L5:963:G:H2'	3:L5:964:A:C4	2.41	0.55
3:L5:4910:G:N2	18:LO:106:ASP:O	2.39	0.55
6:LB:396:ARG:HG2	6:LB:399:LYS:HE3	1.86	0.55
71:SY:86:GLU:OE2	71:SY:90:ARG:NE	2.39	0.55
3:L5:1100:U:O2	3:L5:1195:G:N2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LS:133:ALA:HB3	22:LS:136:LYS:HD3	1.87	0.55
48:S2:1462:U:H2'	48:S2:1464:C:C4	2.42	0.55
3:L5:1921:C:O2'	22:LS:160:ARG:NH2	2.33	0.55
47:Pt:9:1MG:H2'	47:Pt:11:C:H41	1.70	0.55
48:S2:1417:C:H2'	48:S2:1421:A:C2	2.40	0.55
3:L5:2306:G:OP1	34:Le:128:ARG:NH1	2.40	0.55
8:LD:235:MET:N	8:LD:235:MET:HE3	2.21	0.55
26:LW:80:ARG:NH1	54:SG:129:VAL:O	2.40	0.55
27:LX:129:ARG:NH2	27:LX:131:ASP:OD2	2.35	0.55
47:Pt:61:C:H2'	47:Pt:62:C:C6	2.42	0.55
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.88	0.55
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.42	0.55
13:LI:62:SER:HA	13:LI:65:LEU:HD12	1.88	0.55
59:SL:125:ILE:HG13	59:SL:146:THR:HB	1.88	0.55
76:Sd:2:GLY:N	76:Sd:5:GLN:OE1	2.39	0.55
3:L5:162:A:H2'	3:L5:163:A:C8	2.41	0.55
3:L5:4635:A:OP1	3:L5:4636:U:O2'	2.25	0.55
6:LB:218:ASP:OD2	6:LB:348:ARG:NH2	2.29	0.55
48:S2:553:U:H2'	48:S2:555:A:C8	2.42	0.55
52:SE:182:MET:HE3	52:SE:190:GLY:HA2	1.89	0.55
74:Sb:16:LYS:HD2	74:Sb:16:LYS:C	2.32	0.55
3:L5:194:C:O2	28:LY:121:ARG:NH2	2.39	0.55
3:L5:1326:A2M:OP2	3:L5:4445:U:O2'	2.25	0.55
7:LC:209:ILE:HB	7:LC:229:LEU:HD13	1.89	0.55
48:S2:1421:A:H4'	48:S2:1422:G:OP1	2.06	0.55
50:SC:272:HIS:O	50:SC:276:THR:OG1	2.24	0.55
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.41	0.55
55:SH:19:PHE:O	55:SH:19:PHE:HD1	1.91	0.55
57:SJ:113:GLN:OE1	57:SJ:154:GLN:NE2	2.39	0.55
71:SY:76:TYR:OH	71:SY:86:GLU:OE1	2.20	0.55
80:LA:20:VAL:HA	80:LA:23:ARG:HG3	1.89	0.55
3:L5:1857:C:H2'	3:L5:1858:A:H8	1.72	0.54
22:LS:15:ARG:HB3	22:LS:27:LEU:HD23	1.89	0.54
48:S2:1217:A:H2'	48:S2:1218:C:C6	2.41	0.54
75:Sc:36:ASP:OD1	75:Sc:37:ASP:N	2.40	0.54
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.42	0.54
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.70	0.54
3:L5:734:G:C2	3:L5:735:G:C8	2.95	0.54
3:L5:2887:U:O4	87:L5:5373:SPD:N1	2.40	0.54
48:S2:1511:U:H2'	48:S2:1512:C:C6	2.42	0.54
68:SU:31:SER:O	68:SU:35:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.42	0.54
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.42	0.54
48:S2:1550:G:H3'	48:S2:1579:A:H61	1.71	0.54
59:SL:33:LEU:HD12	59:SL:34:PRO:HD2	1.88	0.54
62:SO:34:PHE:HB3	62:SO:41:PHE:HB2	1.90	0.54
69:SV:16:LYS:HG2	69:SV:23:ILE:HG22	1.90	0.54
3:L5:1563:A:N6	48:S2:1028:A:N1	2.56	0.54
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.43	0.54
80:LA:250:LYS:O	80:LA:251:THR:C	2.50	0.54
3:L5:660:A:H2'	3:L5:661:C:C2	2.43	0.54
5:L8:127:U:H3'	5:L8:128:C:C6	2.43	0.54
14:LJ:81:GLU:O	14:LJ:84:GLU:HG3	2.07	0.54
25:LV:42:VAL:HB	25:LV:45:ILE:HG13	1.90	0.54
68:SU:56:MET:HB2	68:SU:86:LYS:HB3	1.89	0.54
79:Sg:212:LYS:HA	79:Sg:235:ILE:HG23	1.89	0.54
3:L5:2884:G:O2'	48:S2:1731:A:O2'	2.16	0.54
3:L5:5002:U:OP2	6:LB:385:LYS:NZ	2.40	0.54
48:S2:562:U:H2'	48:S2:563:G:C8	2.42	0.54
48:S2:959:G:OP1	62:SO:104:ARG:NH2	2.41	0.54
48:S2:1545:A:H5''	64:SQ:74:GLY:HA2	1.89	0.54
3:L5:691:C:H2'	3:L5:692:A:C8	2.43	0.54
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.43	0.54
15:LL:58:ILE:HG12	15:LL:157:VAL:HG22	1.90	0.54
26:LW:77:LYS:NZ	26:LW:78:PHE:O	2.41	0.54
59:SL:51:ILE:HB	59:SL:52:GLU:OE2	2.08	0.54
3:L5:218:A:H1'	3:L5:219:G:H5'	1.90	0.54
3:L5:325:U:H2'	3:L5:326:C:C6	2.43	0.54
3:L5:4415:A:H2'	3:L5:4416:G:O4'	2.08	0.54
9:LE:117:PRO:O	45:Lr:112:ARG:NH1	2.39	0.54
14:LJ:40:LEU:HD12	14:LJ:70:VAL:HG22	1.90	0.54
48:S2:215:G:H2'	48:S2:216:C:C6	2.43	0.54
57:SJ:107:GLU:O	57:SJ:112:THR:OG1	2.26	0.54
83:Lj:2:THR:O	83:Lj:7:SER:OG	2.24	0.54
15:LL:91:ALA:HB1	15:LL:96:ILE:HB	1.90	0.54
57:SJ:33:GLY:HA3	77:Se:112:TYR:CG	2.43	0.54
60:SM:44:LYS:HD3	78:Sf:128:ALA:HB3	1.89	0.54
3:L5:418:A:C2	5:L8:17:A:H1'	2.43	0.53
3:L5:4145:C:H2'	3:L5:4146:G:H8	1.73	0.53
10:LF:70:ARG:O	10:LF:74:MET:HG3	2.07	0.53
39:Lk:54:GLU:O	39:Lk:58:GLN:HG2	2.07	0.53
43:Lo:22:LYS:NZ	43:Lo:22:LYS:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SH:30:LEU:HD11	55:SH:82:GLU:HG3	1.90	0.53
55:SH:73:GLN:HA	55:SH:76:GLN:HB2	1.90	0.53
69:SV:1:MET:HA	69:SV:10:ASP:OD1	2.09	0.53
71:SY:99:LYS:HG2	71:SY:100:LYS:H	1.73	0.53
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.73	0.53
3:L5:4096:C:O2	36:Lg:112:GLN:NE2	2.40	0.53
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.43	0.53
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.08	0.53
3:L5:4145:C:H2'	3:L5:4146:G:C8	2.42	0.53
48:S2:190:G:H1'	48:S2:209:A:H61	1.73	0.53
62:SO:21:VAL:HG22	62:SO:22:ALA:H	1.72	0.53
3:L5:109:G:OP2	15:LL:74:ARG:NH2	2.38	0.53
3:L5:254:G:H2'	3:L5:255:C:C6	2.43	0.53
3:L5:3656:A:H2'	3:L5:3657:U:H6	1.73	0.53
40:Ll:23:ILE:HD12	40:Ll:27:ILE:HD11	1.91	0.53
48:S2:164:A:H3'	48:S2:165:G:H21	1.74	0.53
51:SD:10:LYS:HE3	68:SU:111:GLU:CD	2.34	0.53
55:SH:25:GLN:O	55:SH:29:GLU:HG3	2.08	0.53
57:SJ:93:LYS:HB2	57:SJ:96:TYR:HD2	1.73	0.53
29:LZ:88:ASP:OD1	29:LZ:88:ASP:N	2.34	0.53
58:SK:71:LEU:HD11	58:SK:79:LEU:HD12	1.90	0.53
58:SK:89:ILE:HD12	58:SK:89:ILE:H	1.72	0.53
3:L5:1294:A:H1'	3:L5:1295:C:H5	1.73	0.53
3:L5:4260:U:H2'	3:L5:4261:C:H6	1.71	0.53
31:Lb:117:ARG:HA	31:Lb:117:ARG:NE	2.22	0.53
50:SC:146:GLU:OE1	51:SD:116:ARG:NH2	2.42	0.53
18:LO:168:TYR:CE2	18:LO:172:LYS:HD2	2.43	0.53
28:LY:31:SER:HA	28:LY:48:PRO:HA	1.90	0.53
3:L5:4299:PSU:OP1	20:LQ:160:HIS:CE1	2.62	0.53
3:L5:4499:OMG:HM23	3:L5:4528:G:N2	2.24	0.53
6:LB:220:ILE:HG12	6:LB:278:THR:HG23	1.91	0.53
28:LY:37:GLU:H	28:LY:37:GLU:CD	2.17	0.53
56:SI:106:SER:HB3	56:SI:171:LEU:HG	1.91	0.53
60:SM:22:LEU:HD13	60:SM:89:VAL:HG22	1.91	0.53
3:L5:724:C:OP1	7:LC:350:ARG:HD2	2.09	0.53
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.91	0.53
48:S2:552:G:H2'	48:S2:553:U:C6	2.44	0.53
3:L5:653:U:H2'	3:L5:654:C:C6	2.44	0.52
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.44	0.52
3:L5:3619:G:N7	87:L5:5373:SPD:H42	2.24	0.52
3:L5:4966:A:H5''	6:LB:128:LYS:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LP:54:GLN:HA	19:LP:83:TRP:CD1	2.44	0.52
29:LZ:68:ILE:O	29:LZ:115:LYS:NZ	2.40	0.52
48:S2:1594:A:N7	72:SZ:104:ARG:HD3	2.24	0.52
55:SH:17:ASP:HB3	55:SH:21:SER:HB3	1.90	0.52
57:SJ:136:ARG:HD3	57:SJ:139:LYS:H	1.73	0.52
2:Et:42:A:H2'	2:Et:43:G:H8	1.73	0.52
3:L5:1405:C:H2'	3:L5:1406:G:C8	2.44	0.52
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.44	0.52
37:Lh:6:ALA:O	37:Lh:10:ARG:HG2	2.09	0.52
51:SD:4:GLN:OE1	51:SD:4:GLN:N	2.38	0.52
67:ST:116:ASP:OD1	67:ST:117:GLN:N	2.42	0.52
72:SZ:42:ASP:N	72:SZ:42:ASP:OD1	2.42	0.52
3:L5:162:A:H2'	3:L5:163:A:H8	1.73	0.52
3:L5:4392:OMG:N2	3:L5:4395:U:O2	2.40	0.52
52:SE:233:LYS:HB2	52:SE:233:LYS:NZ	2.24	0.52
55:SH:165:ASN:O	55:SH:169:LYS:NZ	2.35	0.52
82:SX:98:ASP:OD2	82:SX:140:ARG:NH2	2.33	0.52
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.25	0.52
3:L5:1818:G:O2'	3:L5:1820:C:OP2	2.25	0.52
3:L5:4928:C:O2	16:LM:118:MET:HE1	2.09	0.52
9:LE:94:LYS:HE2	9:LE:107:VAL:HG21	1.90	0.52
73:Sa:10:ARG:HB2	73:Sa:33:ASP:OD2	2.09	0.52
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.45	0.52
3:L5:4299:PSU:OP1	31:Lb:33:LYS:NZ	2.30	0.52
8:LD:223:PHE:HB3	8:LD:226:TYR:HB2	1.90	0.52
10:LF:105:VAL:HG13	10:LF:136:VAL:HG12	1.90	0.52
43:Lo:74:GLU:HB3	43:Lo:77:CYS:HB3	1.91	0.52
81:SA:184:ARG:HD3	81:SA:191:ARG:HD3	1.91	0.52
3:L5:1695:U:H2'	3:L5:1696:C:C6	2.44	0.52
8:LD:116:ASP:OD1	8:LD:116:ASP:N	2.39	0.52
12:LH:7:ASN:HB3	12:LH:58:ASP:OD1	2.09	0.52
48:S2:207:G:H3'	48:S2:208:G:H8	1.74	0.52
48:S2:1543:U:OP1	64:SQ:37:ARG:NH2	2.34	0.52
64:SQ:21:ALA:HB2	64:SQ:72:VAL:HG13	1.92	0.52
1:At:1:G:H3'	1:At:2:G:H5''	1.90	0.52
3:L5:659:G:H2'	3:L5:660:A:C8	2.45	0.52
32:Lc:77:ASN:OD1	32:Lc:80:GLU:HG3	2.10	0.52
48:S2:996:A:H2'	48:S2:997:A:C8	2.44	0.52
48:S2:1665:G:C8	67:ST:88:MET:HE3	2.45	0.52
48:S2:1861:G:H5''	73:Sa:3:LYS:HA	1.90	0.52
49:SB:26:SER:O	49:SB:51:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SJ:60:LEU:HB3	57:SJ:94:LEU:HD11	1.92	0.52
61:SN:87:ASP:OD1	61:SN:87:ASP:N	2.41	0.52
3:L5:1743:A:O4'	8:LD:15:ARG:HD2	2.10	0.52
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.74	0.52
29:LZ:41:ALA:HB2	29:LZ:77:TYR:HE1	1.74	0.52
48:S2:1667:U:H2'	48:S2:1668:U:C6	2.45	0.52
2:Et:43:G:H2'	2:Et:44:A:C8	2.45	0.52
3:L5:1498:G:OP1	20:LQ:150:ARG:NH1	2.40	0.52
3:L5:3720:G:H22	3:L5:3733:A:H2	1.58	0.52
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.45	0.52
60:SM:46:GLN:HB3	60:SM:112:LYS:HG3	1.91	0.52
19:LP:9:GLU:OE1	19:LP:9:GLU:N	2.35	0.52
34:Le:82:VAL:HG13	34:Le:114:ARG:HG2	1.92	0.52
48:S2:530:U:H2'	48:S2:531:A:C8	2.44	0.52
52:SE:19:MET:SD	52:SE:108:ARG:HD2	2.50	0.52
55:SH:78:ARG:O	55:SH:82:GLU:HG2	2.09	0.52
81:SA:37:TYR:OH	81:SA:57:LYS:NZ	2.41	0.52
3:L5:181:C:H2'	3:L5:182:G:C8	2.40	0.51
3:L5:1202:C:H2'	3:L5:1203:G:C8	2.45	0.51
48:S2:207:G:H3'	48:S2:208:G:C8	2.45	0.51
66:SS:86:ARG:NH2	66:SS:89:ASP:OD2	2.29	0.51
8:LD:235:MET:HE3	8:LD:235:MET:H	1.74	0.51
16:LM:40:GLY:HA3	16:LM:45:VAL:HB	1.91	0.51
33:Ld:36:VAL:HG21	33:Ld:44:ARG:HG2	1.92	0.51
48:S2:1322:G:C2'	48:S2:1323:U:H5'	2.41	0.51
64:SQ:40:GLU:N	64:SQ:40:GLU:OE2	2.44	0.51
3:L5:1420:A:OP1	20:LQ:71:LYS:NZ	2.43	0.51
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.93	0.51
20:LQ:14:ARG:HG2	20:LQ:14:ARG:NH1	2.25	0.51
51:SD:8:LYS:HG2	68:SU:61:LEU:HD11	1.91	0.51
65:SR:51:ALA:O	65:SR:55:THR:HG23	2.10	0.51
48:S2:1421:A:H1'	48:S2:1422:G:C2	2.46	0.51
72:SZ:65:TYR:HB2	72:SZ:68:ILE:HG12	1.92	0.51
3:L5:445:U:H2'	3:L5:446:C:O4'	2.10	0.51
3:L5:1411:C:H2'	3:L5:1412:G:C8	2.46	0.51
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.45	0.51
31:Lb:92:LYS:HG2	31:Lb:95:ARG:HH12	1.76	0.51
57:SJ:111:GLN:NE2	57:SJ:127:ARG:HB2	2.25	0.51
57:SJ:136:ARG:HG2	57:SJ:160:SER:HA	1.93	0.51
69:SV:82:ASN:HB2	81:SA:52:LYS:HE3	1.92	0.51
3:L5:4146:G:H2'	3:L5:4147:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LC:350:ARG:NH1	7:LC:350:ARG:HB2	2.25	0.51
24:LU:68:SER:O	24:LU:68:SER:OG	2.22	0.51
38:Li:54:GLU:HG2	38:Li:90:LEU:HD21	1.92	0.51
48:S2:190:G:H1'	48:S2:209:A:N6	2.26	0.51
48:S2:441:C:H2'	48:S2:442:C:C6	2.45	0.51
48:S2:672:A:N1	48:S2:1027:A:OP1	2.44	0.51
48:S2:1446:A:H1'	68:SU:55:ARG:HD2	1.92	0.51
53:SF:68:ILE:HD11	53:SF:151:ILE:HD11	1.92	0.51
62:SO:44:VAL:HG12	62:SO:53:ILE:HB	1.91	0.51
69:SV:64:GLU:OE2	81:SA:33:GLN:NE2	2.32	0.51
3:L5:106:A:H2'	3:L5:107:G:O4'	2.11	0.51
3:L5:1198:G:H2'	3:L5:1200:G:H8	1.76	0.51
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.46	0.51
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.46	0.51
13:LI:203:ARG:NH1	13:LI:203:ARG:HB2	2.25	0.51
26:LW:102:LYS:HG2	26:LW:105:ARG:HH21	1.76	0.51
47:Pt:2:G:H1	47:Pt:71:U:H3	1.58	0.51
48:S2:379:C:H5'	56:SI:33:ALA:HA	1.92	0.51
63:SP:12:PHE:C	63:SP:13:ARG:HE	2.18	0.51
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.46	0.51
32:Lc:38:ILE:HD11	32:Lc:46:VAL:HG21	1.93	0.51
55:SH:52:GLU:HG2	55:SH:58:LYS:NZ	2.25	0.51
13:LI:203:ARG:HB2	13:LI:203:ARG:HH11	1.76	0.51
48:S2:551:U:C2'	48:S2:552:G:C8	2.83	0.51
7:LC:155:GLU:HG3	7:LC:157:LYS:HG2	1.93	0.50
14:LJ:111:GLU:HB3	14:LJ:113:ILE:HG22	1.93	0.50
50:SC:167:ARG:HB3	50:SC:177:PRO:HB2	1.92	0.50
51:SD:40:ARG:NH2	51:SD:47:GLU:OE1	2.44	0.50
81:SA:10:MET:HE3	81:SA:55:TRP:HB2	1.92	0.50
12:LH:37:ASP:OD1	12:LH:39:ASN:ND2	2.24	0.50
33:Ld:64:ILE:HG23	33:Ld:68:LEU:HD23	1.92	0.50
48:S2:1308:U:O2'	78:Sf:133:ALA:HB1	2.11	0.50
51:SD:170:THR:HG23	51:SD:187:LYS:HG2	1.94	0.50
65:SR:21:TYR:CE1	65:SR:58:MET:HE1	2.46	0.50
71:SY:10:ARG:HG2	71:SY:11:LYS:HG3	1.93	0.50
76:Sd:4:GLN:H	76:Sd:4:GLN:CD	2.18	0.50
3:L5:1703:C:N3	10:LF:39:GLN:NE2	2.59	0.50
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.45	0.50
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.10	0.50
3:L5:4957:C:H2'	3:L5:4958:C:H6	1.76	0.50
4:L7:55:A:H4'	14:LJ:155:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LM:118:MET:HG2	18:LO:192:TYR:CZ	2.47	0.50
48:S2:581:U:H4'	71:SY:66:GLY:HA2	1.91	0.50
48:S2:1417:C:H2'	48:S2:1421:A:H2	1.75	0.50
79:Sg:87:LEU:HB2	79:Sg:101:PHE:HB2	1.92	0.50
3:L5:1202:C:H2'	3:L5:1203:G:H8	1.76	0.50
3:L5:2848:G:O2'	3:L5:3838:U:O4	2.25	0.50
3:L5:4524:G:C2	6:LB:252:ALA:HB1	2.46	0.50
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.46	0.50
42:Ln:6:ARG:NH2	48:S2:1169:G:OP1	2.45	0.50
53:SF:69:VAL:O	53:SF:73:THR:HG23	2.11	0.50
59:SL:35:ARG:HH21	59:SL:63:THR:HG21	1.75	0.50
82:SX:48:LYS:HD3	82:SX:99:GLU:OE2	2.11	0.50
3:L5:138:G:H2'	3:L5:139:G:C8	2.47	0.50
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	1.91	0.50
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.92	0.50
48:S2:1323:U:H2'	48:S2:1324:G:C8	2.47	0.50
65:SR:97:GLU:HG2	65:SR:120:THR:HG22	1.93	0.50
65:SR:127:ASN:O	65:SR:127:ASN:ND2	2.43	0.50
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.11	0.50
5:L8:82:A:H5''	37:Lh:3:LYS:HG2	1.94	0.50
48:S2:898:U:H2'	48:S2:899:U:O4'	2.11	0.50
70:SW:28:ARG:HH11	70:SW:28:ARG:HG3	1.76	0.50
77:Se:96:GLN:O	77:Se:98:LYS:NZ	2.43	0.50
1:At:17:G:C8	1:At:58:MA7:HN2	2.47	0.50
2:Et:75:C:O2'	43:Lo:54:PRO:O	2.23	0.50
3:L5:126:C:H2'	3:L5:127:G:C8	2.46	0.50
3:L5:258:G:H2'	3:L5:259:C:H6	1.76	0.50
3:L5:267:G:H2'	3:L5:268:G:H8	1.75	0.50
26:LW:105:ARG:NH1	54:SG:150:GLU:O	2.41	0.50
43:Lo:59:LYS:NZ	43:Lo:61:LYS:O	2.43	0.50
47:Pt:63:U:H2'	47:Pt:64:G:H8	1.77	0.50
49:SB:134:LEU:HG	49:SB:218:LEU:HD12	1.93	0.50
51:SD:35:SER:HB2	51:SD:51:LEU:HD12	1.92	0.50
80:LA:137:ILE:HD11	80:LA:149:LYS:HB2	1.94	0.50
3:L5:1407:C:H2'	3:L5:1408:G:C8	2.47	0.50
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.47	0.50
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.12	0.50
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.47	0.50
11:LG:80:ILE:HD11	17:LN:18:VAL:HG13	1.94	0.50
65:SR:31:ASN:ND2	65:SR:55:THR:HG22	2.26	0.50
67:ST:117:GLN:CD	67:ST:117:GLN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:258:G:H2'	3:L5:259:C:C6	2.47	0.50
16:LM:95:ILE:O	16:LM:99:GLU:HG2	2.12	0.50
72:SZ:79:ILE:HB	72:SZ:83:LEU:HD23	1.93	0.50
3:L5:1509:C:H5''	30:La:2:PRO:HD2	1.93	0.49
17:LN:96:ARG:NH1	17:LN:100:SER:OG	2.45	0.49
26:LW:71:ARG:N	26:LW:73:ARG:HH22	2.10	0.49
48:S2:463:C:H2'	48:S2:465:A:N7	2.27	0.49
48:S2:824:C:H1'	57:SJ:144:ILE:HG21	1.93	0.49
55:SH:31:GLU:HB2	55:SH:40:LEU:HD22	1.93	0.49
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.48	0.49
6:LB:394:LYS:O	6:LB:397:ILE:HG13	2.12	0.49
41:Lm:99:CYS:O	41:Lm:100:TYR:HB2	2.12	0.49
56:SI:131:PRO:HA	56:SI:134:GLU:HB3	1.95	0.49
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.47	0.49
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.48	0.49
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.47	0.49
26:LW:80:ARG:HD3	54:SG:9:ALA:O	2.12	0.49
49:SB:124:HIS:HA	49:SB:137:LEU:O	2.12	0.49
55:SH:69:LEU:HD22	55:SH:96:ALA:HB2	1.93	0.49
65:SR:72:LYS:HE2	65:SR:76:GLU:CD	2.38	0.49
3:L5:1773:U:H2'	3:L5:1774:C:H6	1.77	0.49
3:L5:3654:G:O2'	3:L5:3693:U:OP1	2.26	0.49
8:LD:264:LYS:HD2	8:LD:266:TRP:CZ2	2.47	0.49
48:S2:35:C:H5''	48:S2:579:C:H5''	1.94	0.49
59:SL:75:GLY:HA3	59:SL:88:ILE:HD12	1.94	0.49
79:Sg:174:VAL:HB	79:Sg:188:HIS:HB2	1.94	0.49
3:L5:1409:C:H2'	3:L5:1410:U:O4'	2.13	0.49
3:L5:4457:PSU:H1'	6:LB:252:ALA:HB3	1.94	0.49
14:LJ:164:ARG:O	14:LJ:168:GLN:HG3	2.12	0.49
23:LT:122:LYS:O	23:LT:122:LYS:NZ	2.34	0.49
40:Ll:20:ASN:ND2	40:Ll:42:ARG:O	2.44	0.49
48:S2:1798:C:H2'	48:S2:1799:G:O4'	2.13	0.49
55:SH:192:PHE:CD2	74:Sb:12:PRO:HB3	2.47	0.49
79:Sg:236:ILE:HG12	79:Sg:252:THR:HG22	1.94	0.49
3:L5:180:C:H2'	3:L5:181:C:C1'	2.42	0.49
3:L5:508:G:O2'	3:L5:510:U:OP2	2.14	0.49
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.47	0.49
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.78	0.49
3:L5:4893:A:OP1	18:LO:188:LYS:NZ	2.37	0.49
13:LI:54:SER:HB2	13:LI:135:ILE:HD11	1.93	0.49
17:LN:159:ARG:HB3	17:LN:164:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Lg:83:CYS:SG	36:Lg:86:CYS:HB2	2.52	0.49
48:S2:553:U:H3'	48:S2:555:A:H5''	1.93	0.49
48:S2:928:G:H2'	48:S2:929:G:C8	2.47	0.49
52:SE:151:ASP:HB3	52:SE:154:ILE:HG13	1.94	0.49
52:SE:175:PHE:HE1	52:SE:225:ILE:HG21	1.76	0.49
53:SF:78:MET:HB2	53:SF:159:ARG:CZ	2.43	0.49
79:Sg:124:SER:OG	79:Sg:125:ARG:N	2.45	0.49
3:L5:1410:U:H4'	3:L5:1411:C:O5'	2.13	0.49
3:L5:1584:G:N7	87:L5:5371:SPD:N10	2.60	0.49
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.48	0.49
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.48	0.49
14:LJ:119:TYR:CD1	66:SS:12:ILE:HG13	2.47	0.49
45:Lr:63:VAL:HG22	45:Lr:79:ARG:HG2	1.95	0.49
52:SE:11:ARG:HA	52:SE:28:ALA:HB2	1.95	0.49
57:SJ:58:ARG:HG3	57:SJ:58:ARG:HH11	1.78	0.49
3:L5:661:C:H2'	3:L5:662:C:C6	2.48	0.49
3:L5:2539:C:H2'	3:L5:2540:C:H6	1.78	0.49
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.27	0.49
3:L5:4208:U:OP1	3:L5:4334:U:O2'	2.29	0.49
3:L5:4635:A:O2'	3:L5:4637:OMG:OP1	2.28	0.49
75:Sc:28:THR:HG21	75:Sc:50:VAL:HG12	1.94	0.49
3:L5:38:A:H5''	30:La:35:ALA:HB2	1.95	0.49
3:L5:142:G:OP1	11:LG:111:LYS:NZ	2.45	0.49
3:L5:1757:U:H2'	3:L5:1758:G:C8	2.46	0.49
3:L5:1855:G:OP1	31:Lb:4:SER:HB2	2.13	0.49
48:S2:1395:C:H1'	48:S2:1474:A:C4	2.48	0.49
58:SK:92:ALA:HA	58:SK:95:ARG:HD3	1.95	0.49
65:SR:82:ASP:O	81:SA:85:ARG:NH2	2.46	0.49
65:SR:111:PHE:CD2	81:SA:15:VAL:HG21	2.47	0.49
71:SY:33:ALA:O	71:SY:34:THR:C	2.56	0.49
74:Sb:34:ASP:O	74:Sb:79:PHE:HA	2.13	0.49
82:SX:101:LEU:HB3	82:SX:123:VAL:O	2.12	0.49
2:Et:23:C:H2'	2:Et:24:G:C8	2.48	0.49
2:Et:49:G:H2'	2:Et:50:A:H8	1.77	0.49
3:L5:2097:U:C4	10:LF:35:LYS:HD3	2.48	0.49
3:L5:2415:OMU:H2'	3:L5:2416:G:O4'	2.13	0.49
39:Lk:54:GLU:HA	39:Lk:54:GLU:OE2	2.12	0.49
48:S2:943:U:O2'	62:SO:135:ILE:O	2.28	0.49
71:SY:25:ILE:HG21	71:SY:40:ILE:HD11	1.95	0.49
2:Et:43:G:H2'	2:Et:44:A:H8	1.78	0.48
3:L5:1399:G:N2	3:L5:1419:G:H1'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2515:G:OP1	36:Lg:37:LYS:NZ	2.36	0.48
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.48	0.48
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.48	0.48
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.77	0.48
3:L5:4499:OMG:HM23	3:L5:4528:G:C2	2.48	0.48
15:LL:164:GLU:HB2	30:La:100:ILE:HD12	1.95	0.48
23:LT:51:GLY:HA3	23:LT:92:ARG:HG3	1.95	0.48
48:S2:1017:U:H5'	61:SN:55:ARG:HD3	1.95	0.48
70:SW:104:LEU:HD23	70:SW:125:ILE:HA	1.95	0.48
79:Sg:256:ILE:HG12	79:Sg:289:LEU:HD21	1.95	0.48
3:L5:1625:OMG:H3'	17:LN:81:TYR:OH	2.13	0.48
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.48	0.48
8:LD:53:VAL:HG11	8:LD:159:VAL:HA	1.94	0.48
17:LN:166:SER:O	17:LN:170:LYS:HG2	2.13	0.48
30:La:84:GLU:HA	30:La:84:GLU:OE2	2.13	0.48
48:S2:1404:U:C5	68:SU:88:LEU:HD21	2.48	0.48
3:L5:142:G:P	11:LG:111:LYS:HZ1	2.36	0.48
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.13	0.48
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.13	0.48
3:L5:4336:A:H5''	3:L5:4337:C:H5'	1.95	0.48
12:LH:91:LYS:HB3	12:LH:143:GLU:OE2	2.14	0.48
36:Lg:105:LYS:HD2	36:Lg:105:LYS:C	2.38	0.48
39:Lk:49:ASP:HB2	39:Lk:52:LYS:HG3	1.94	0.48
48:S2:388:U:H2'	48:S2:389:A:C8	2.48	0.48
65:SR:104:GLU:HG3	81:SA:39:TYR:OH	2.13	0.48
3:L5:2300:A:N7	7:LC:143:ARG:NH1	2.61	0.48
3:L5:2434:G:O2'	3:L5:2527:A:N1	2.46	0.48
54:SG:22:ARG:HA	54:SG:25:ARG:HD2	1.96	0.48
3:L5:10:A:H2'	3:L5:11:G:C8	2.48	0.48
3:L5:2500:U:H2'	3:L5:2501:C:C6	2.49	0.48
32:Lc:47:ILE:HB	32:Lc:94:LEU:HG	1.95	0.48
48:S2:798:G:H2'	55:SH:108:SER:C	2.38	0.48
3:L5:67:C:OP2	3:L5:312:G:N2	2.46	0.48
3:L5:126:C:H2'	3:L5:127:G:H8	1.78	0.48
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.49	0.48
9:LE:190:HIS:HB3	9:LE:193:PHE:HD1	1.78	0.48
55:SH:20:GLU:HG3	55:SH:48:ALA:HB3	1.96	0.48
79:Sg:35:SER:OG	79:Sg:36:ARG:N	2.47	0.48
79:Sg:143:GLN:NE2	79:Sg:144:ASP:OD1	2.45	0.48
3:L5:1660:U:OP1	91:L5:5401:HOH:O	2.19	0.48
3:L5:1846:G:H2'	3:L5:1847:C:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.49	0.48
3:L5:3598:C:H2'	3:L5:3599:A:H8	1.78	0.48
3:L5:4344:U:H2'	3:L5:4345:C:H6	1.79	0.48
26:LW:101:ARG:O	26:LW:105:ARG:HG3	2.13	0.48
48:S2:21:U:O2	57:SJ:17:ARG:NH2	2.46	0.48
48:S2:1405:A:H2'	48:S2:1406:G:O4'	2.14	0.48
56:SI:114:GLU:OE2	56:SI:123:ARG:NE	2.46	0.48
68:SU:24:LEU:HD23	68:SU:112:VAL:HG22	1.96	0.48
3:L5:1359:G:H4'	17:LN:203:TYR:HB2	1.96	0.48
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.14	0.48
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.95	0.48
3:L5:2394:G:O2'	3:L5:2819:U:O4	2.28	0.48
3:L5:2412:A:H2'	3:L5:2413:U:C6	2.48	0.48
3:L5:2415:OMU:H2'	3:L5:2416:G:C8	2.48	0.48
3:L5:3656:A:H2'	3:L5:3657:U:C6	2.48	0.48
8:LD:156:GLY:HA2	8:LD:181:PRO:HG3	1.95	0.48
48:S2:44:U:O2	48:S2:482:G:H1'	2.14	0.48
48:S2:568:C:H2'	48:S2:569:A:C8	2.48	0.48
48:S2:867:OMG:HM23	48:S2:867:OMG:H1'	1.58	0.48
49:SB:28:LYS:HD3	49:SB:48:LEU:HD12	1.95	0.48
50:SC:196:ILE:HB	50:SC:223:TYR:HB2	1.95	0.48
3:L5:131:C:N4	3:L5:132:G:N7	2.61	0.48
3:L5:280:G:H5''	17:LN:14:LYS:HE2	1.96	0.48
3:L5:1199:G:N1	23:LT:142:ARG:HG3	2.29	0.48
3:L5:1249:C:H2'	3:L5:1250:C:C6	2.49	0.48
3:L5:1296:G:H2'	3:L5:1297:U:C6	2.49	0.48
11:LG:130:THR:OG1	11:LG:131:LYS:N	2.42	0.48
13:LI:207:ASP:N	13:LI:207:ASP:OD1	2.47	0.48
26:LW:107:GLN:CD	26:LW:110:ARG:HH21	2.21	0.48
79:Sg:145:GLU:H	79:Sg:145:GLU:CD	2.18	0.48
3:L5:133:C:H5''	3:L5:134:G:C6	2.49	0.48
3:L5:1249:C:H2'	3:L5:1250:C:H6	1.78	0.48
3:L5:2516:G:O2'	36:Lg:62:LYS:NZ	2.47	0.48
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.49	0.48
19:LP:17:SER:HB2	19:LP:98:ALA:HB2	1.96	0.48
54:SG:211:LYS:O	54:SG:215:LYS:HG2	2.14	0.48
58:SK:35:LEU:HB3	58:SK:40:VAL:HG13	1.95	0.48
3:L5:169:G:O3'	15:LL:136:LYS:NZ	2.36	0.47
3:L5:1087:A:H2'	3:L5:1088:C:C6	2.49	0.47
3:L5:3689:G:O2'	3:L5:3818:UY1:OP2	2.30	0.47
3:L5:4093:G:H2'	3:L5:4094:G:C8	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.48	0.47
3:L5:4266:G:N3	3:L5:4266:G:H2'	2.29	0.47
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.79	0.47
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.13	0.47
3:L5:4970:C:OP1	19:LP:74:LYS:NZ	2.42	0.47
11:LG:163:PRO:HB2	11:LG:165:GLU:OE2	2.13	0.47
37:Lh:103:LYS:O	37:Lh:108:GLN:NE2	2.47	0.47
48:S2:215:G:H2'	48:S2:216:C:H6	1.79	0.47
48:S2:573:PSU:H6	48:S2:576:A2M:H8	1.78	0.47
48:S2:639:C:H2'	48:S2:640:A:C8	2.48	0.47
51:SD:16:ILE:HD11	76:Sd:36:LEU:HD23	1.96	0.47
65:SR:101:ASP:OD2	81:SA:40:LYS:HD2	2.14	0.47
81:SA:208:GLU:O	81:SA:211:GLU:HG3	2.14	0.47
3:L5:37:U:H2'	3:L5:38:A:O4'	2.15	0.47
3:L5:1787:A:H4'	88:L5:5381:PUT:H11	1.96	0.47
3:L5:4342:C:O3'	43:Lo:37:GLY:HA3	2.14	0.47
3:L5:4637:OMG:H2'	3:L5:4638:U:C6	2.49	0.47
3:L5:4860:G:H2'	3:L5:4861:G:C8	2.50	0.47
8:LD:211:LEU:HB3	8:LD:219:TYR:HB2	1.96	0.47
14:LJ:20:LEU:HD23	14:LJ:132:VAL:HG22	1.96	0.47
48:S2:1566:G:O6	67:ST:97:LYS:HB2	2.14	0.47
65:SR:28:PHE:HA	65:SR:55:THR:HG21	1.96	0.47
3:L5:133:C:H2'	3:L5:134:G:C2	2.49	0.47
3:L5:653:U:H2'	3:L5:654:C:H6	1.79	0.47
3:L5:690:C:H2'	3:L5:691:C:H6	1.80	0.47
3:L5:968:C:O5'	9:LE:110:ARG:NH2	2.45	0.47
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.14	0.47
3:L5:1564:A:N1	48:S2:1029:G:O2'	2.46	0.47
3:L5:1672:U:H2'	3:L5:1673:U:C6	2.49	0.47
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.49	0.47
3:L5:2382:A:N1	3:L5:2829:U:O2'	2.45	0.47
3:L5:2566:G:H2'	3:L5:2567:G:H8	1.79	0.47
4:L7:35:U:O2	4:L7:45:U:O2'	2.30	0.47
13:LI:33:ILE:HB	13:LI:69:ARG:HH21	1.79	0.47
48:S2:1464:C:H2'	48:S2:1465:A:C8	2.49	0.47
3:L5:286:U:H2'	3:L5:287:U:C6	2.50	0.47
15:LL:201:GLU:O	15:LL:205:GLN:HG2	2.14	0.47
48:S2:51:U:H2'	48:S2:52:G:C8	2.50	0.47
57:SJ:124:HIS:O	57:SJ:128:VAL:HG23	2.15	0.47
67:ST:108:GLU:OE2	67:ST:121:ARG:NH1	2.47	0.47
69:SV:38:GLU:OE2	69:SV:51:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:Sb:16:LYS:HD2	74:Sb:16:LYS:O	2.14	0.47
81:SA:76:VAL:HG23	81:SA:98:PRO:HA	1.95	0.47
3:L5:2084:C:H1'	20:LQ:14:ARG:HH21	1.79	0.47
3:L5:4258:C:OP2	14:LJ:54:ARG:NH1	2.47	0.47
3:L5:4861:G:H2'	3:L5:4862:G:C8	2.50	0.47
48:S2:27:A2M:HM'3	48:S2:27:A2M:H1'	1.59	0.47
48:S2:367:U:H4'	48:S2:371:A:C8	2.49	0.47
48:S2:551:U:H4'	77:Se:117:VAL:HG21	1.97	0.47
48:S2:877:C:H2'	48:S2:878:G:C8	2.50	0.47
3:L5:2284:G:OP1	30:La:7:LYS:NZ	2.44	0.47
3:L5:2303:C:OP1	34:Le:107:ASN:ND2	2.42	0.47
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.13	0.47
3:L5:4734:A:H2'	3:L5:4735:G:H8	1.77	0.47
3:L5:4743:G:H2'	3:L5:4744:A:H8	1.79	0.47
34:Le:35:TRP:CZ2	34:Le:56:PRO:HD2	2.49	0.47
48:S2:195:C:H2'	48:S2:196:C:C6	2.49	0.47
52:SE:124:CYS:HB3	52:SE:141:THR:HB	1.96	0.47
54:SG:23:LYS:HZ2	54:SG:41:LEU:HA	1.80	0.47
77:Se:99:LYS:HB2	77:Se:99:LYS:HE3	1.73	0.47
79:Sg:166:VAL:HG11	79:Sg:207:CYS:SG	2.55	0.47
3:L5:268:G:H2'	3:L5:269:G:H8	1.79	0.47
3:L5:1689:G:OP2	88:L5:5380:PUT:N1	2.45	0.47
3:L5:1699:A:O2'	7:LC:306:ARG:NH1	2.48	0.47
3:L5:2262:G:OP2	45:Lr:98:ARG:NH2	2.37	0.47
3:L5:4589:A:N1	3:L5:4621:C:O2'	2.46	0.47
3:L5:4927:G:OP2	3:L5:4927:G:N2	2.33	0.47
12:LH:137:SER:HB3	12:LH:143:GLU:HG2	1.97	0.47
48:S2:988:C:H5''	49:SB:116:LYS:HG2	1.96	0.47
51:SD:42:THR:HG22	51:SD:44:THR:H	1.79	0.47
56:SI:165:GLN:HB3	56:SI:171:LEU:HD23	1.97	0.47
62:SO:63:LYS:H	62:SO:63:LYS:HE2	1.80	0.47
67:ST:102:ARG:HD3	67:ST:102:ARG:HA	1.72	0.47
71:SY:98:GLU:OE1	71:SY:101:LYS:HD3	2.15	0.47
81:SA:137:ALA:HB1	81:SA:142:LEU:HB3	1.96	0.47
82:SX:124:LYS:HG2	82:SX:129:SER:HA	1.96	0.47
2:Et:11:G:C2	2:Et:26:G:H1'	2.50	0.47
3:L5:1646:A:O2'	83:Lj:49:TRP:O	2.31	0.47
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.50	0.47
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.49	0.47
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.79	0.47
5:L8:70:G:H5''	28:LY:27:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LL:63:THR:CG2	30:La:66:ASN:HB3	2.37	0.47
56:SI:154:LYS:C	56:SI:154:LYS:HD2	2.40	0.47
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.50	0.47
3:L5:1548:G:O2'	3:L5:2812:A:N3	2.43	0.47
3:L5:4621:C:OP1	25:LV:48:ARG:HD2	2.15	0.47
3:L5:4739:C:C2'	3:L5:4740:G:H5'	2.45	0.47
37:Lh:103:LYS:NZ	37:Lh:111:GLU:OE2	2.47	0.47
48:S2:796:G:H2'	48:S2:797:C:H1'	1.96	0.47
56:SI:148:LYS:O	56:SI:151:GLU:HG3	2.15	0.47
77:Se:113:ASN:O	77:Se:117:VAL:HG22	2.14	0.47
1:At:43:A:H3'	1:At:44:A:H5''	1.96	0.47
3:L5:152:U:OP2	17:LN:49:ARG:NH2	2.35	0.47
3:L5:732:A:H2'	3:L5:733:A:O4'	2.15	0.47
3:L5:1719:A:H2'	3:L5:1720:C:C6	2.49	0.47
3:L5:1761:G:O6	3:L5:1771:U:O4	2.33	0.47
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.15	0.47
48:S2:535:G:H2'	48:S2:536:A:O4'	2.15	0.47
48:S2:1037:G:H4'	48:S2:1845:A:H4'	1.95	0.47
52:SE:100:ARG:HG2	52:SE:102:ILE:HG12	1.97	0.47
3:L5:23:C:H2'	3:L5:24:G:O4'	2.15	0.46
3:L5:4069:U:H2'	3:L5:4070:U:H6	1.80	0.46
11:LG:143:VAL:O	11:LG:147:VAL:HG13	2.15	0.46
15:LL:165:LYS:HE3	15:LL:165:LYS:HB2	1.72	0.46
48:S2:186:C:H2'	48:S2:187:G:C8	2.50	0.46
48:S2:527:C:H2'	48:S2:528:A:C8	2.50	0.46
73:Sa:13:LYS:HD3	73:Sa:13:LYS:HA	1.67	0.46
3:L5:1756:U:H2'	3:L5:1757:U:C6	2.51	0.46
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.15	0.46
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.50	0.46
10:LF:241:ASN:O	10:LF:245:ARG:HG2	2.15	0.46
12:LH:63:ASN:O	12:LH:67:LEU:HG	2.15	0.46
23:LT:159:MET:HE2	23:LT:159:MET:HB3	1.85	0.46
48:S2:870:A:H5'	48:S2:915:G:N2	2.29	0.46
48:S2:1639:G7M:H2'	48:S2:1640:A:C8	2.49	0.46
82:SX:68:LYS:HB3	82:SX:91:LEU:HD22	1.96	0.46
3:L5:4745:G:H22	3:L5:4955:A:H2	1.63	0.46
33:Ld:32:ARG:HB3	33:Ld:48:GLU:HG3	1.98	0.46
48:S2:799:U:H2'	48:S2:800:U:C6	2.50	0.46
48:S2:1285:G:O5'	60:SM:35:ILE:HD13	2.15	0.46
50:SC:193:VAL:HG11	50:SC:240:THR:HG22	1.98	0.46
52:SE:44:LEU:HD21	52:SE:72:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:At:49:G:H1	1:At:65:U:H3	1.64	0.46
3:L5:2095:A:O2'	10:LF:28:LEU:HD11	2.14	0.46
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.79	0.46
3:L5:4093:G:H2'	3:L5:4094:G:H8	1.80	0.46
4:L7:111:C:H2'	4:L7:112:U:O4'	2.15	0.46
15:LL:62:PRO:O	15:LL:63:THR:HB	2.14	0.46
18:LO:61:ARG:HA	18:LO:70:PRO:HD2	1.97	0.46
24:LU:67:LYS:HE2	24:LU:67:LYS:HB2	1.70	0.46
29:LZ:29:ILE:HG22	29:LZ:32:GLY:H	1.80	0.46
48:S2:118:C:H1'	48:S2:445:A:C5	2.51	0.46
57:SJ:67:ASP:O	57:SJ:71:LEU:HG	2.15	0.46
64:SQ:89:SER:HB3	64:SQ:112:LEU:HD13	1.98	0.46
72:SZ:68:ILE:HB	72:SZ:109:TYR:HB2	1.96	0.46
3:L5:699:C:H2'	3:L5:700:G:C8	2.49	0.46
3:L5:1406:G:N1	3:L5:1412:G:C6	2.83	0.46
3:L5:4065:G:H2'	3:L5:4066:U:C6	2.51	0.46
3:L5:4522:G:O2'	3:L5:4525:C:OP2	2.27	0.46
38:Li:45:ARG:NH1	38:Li:49:GLY:O	2.45	0.46
42:Ln:1:MET:HE3	48:S2:1851:MA6:H5'	1.98	0.46
48:S2:15:U:H2'	48:S2:16:G:O4'	2.15	0.46
48:S2:509:OMG:H1'	48:S2:509:OMG:HM23	1.68	0.46
48:S2:1328:OMG:HM23	48:S2:1328:OMG:H1'	1.64	0.46
48:S2:1705:C:H2'	48:S2:1706:G:C8	2.51	0.46
53:SF:141:VAL:HG13	53:SF:145:ARG:HG2	1.95	0.46
54:SG:57:ASP:O	54:SG:107:SER:OG	2.21	0.46
55:SH:192:PHE:HD2	74:Sb:12:PRO:HB3	1.80	0.46
59:SL:47:PRO:O	59:SL:51:ILE:HG12	2.15	0.46
59:SL:128:VAL:HG12	59:SL:142:VAL:HA	1.96	0.46
3:L5:1246:G:H2'	3:L5:1247:U:C6	2.51	0.46
3:L5:4401:G:H2'	3:L5:4402:C:H6	1.80	0.46
3:L5:4460:U:H2'	3:L5:4461:C:H6	1.81	0.46
3:L5:4770:U:H2'	3:L5:4771:C:C5	2.49	0.46
3:L5:4771:C:O2'	3:L5:4772:C:H6	1.99	0.46
34:Le:89:LEU:HD13	34:Le:118:LEU:HD22	1.98	0.46
34:Le:98:GLU:OE1	34:Le:123:THR:OG1	2.25	0.46
48:S2:1802:C:H2'	48:S2:1803:U:C6	2.51	0.46
51:SD:133:GLY:HA3	51:SD:156:LEU:O	2.16	0.46
53:SF:32:ASP:OD1	53:SF:34:SER:OG	2.33	0.46
56:SI:140:LYS:N	56:SI:140:LYS:HD2	2.30	0.46
57:SJ:171:GLY:O	57:SJ:175:ARG:HG3	2.16	0.46
59:SL:111:VAL:HG12	59:SL:140:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SN:19:ARG:HG2	74:Sb:84:HIS:HE1	1.81	0.46
3:L5:163:A:H2'	3:L5:164:G:C8	2.51	0.46
3:L5:2020:U:H2'	3:L5:2021:G:C8	2.44	0.46
3:L5:4861:G:H2'	3:L5:4862:G:H8	1.81	0.46
17:LN:61:ILE:CG2	17:LN:131:GLU:HG2	2.45	0.46
50:SC:176:LYS:HB2	50:SC:176:LYS:NZ	2.31	0.46
50:SC:200:ARG:HA	50:SC:221:ASP:OD2	2.14	0.46
3:L5:980:U:H2'	3:L5:981:C:C6	2.49	0.46
3:L5:1411:C:H2'	3:L5:1412:G:H8	1.80	0.46
3:L5:2363:A2M:HM'2	3:L5:2364:OMG:H5'	1.97	0.46
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.51	0.46
11:LG:182:CYS:HB3	11:LG:222:ILE:HG12	1.97	0.46
48:S2:598:G:N3	48:S2:605:A:H2	2.14	0.46
48:S2:615:C:H2'	48:S2:616:A:C8	2.51	0.46
48:S2:907:G:H2'	48:S2:908:A:C8	2.50	0.46
58:SK:10:ALA:HA	58:SK:13:GLU:HG3	1.98	0.46
3:L5:488:G:H2'	3:L5:489:C:O4'	2.16	0.46
3:L5:683:C:H2'	3:L5:684:G:O4'	2.16	0.46
3:L5:4460:U:H2'	3:L5:4461:C:C6	2.51	0.46
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.15	0.46
20:LQ:178:ARG:HA	20:LQ:184:ARG:O	2.16	0.46
27:LX:143:ASP:N	27:LX:143:ASP:OD1	2.34	0.46
43:Lo:14:LYS:HE3	43:Lo:77:CYS:SG	2.56	0.46
48:S2:1223:A:OP1	53:SF:79:HIS:HA	2.16	0.46
48:S2:1356:G:H2'	48:S2:1357:A:C8	2.50	0.46
48:S2:1520:G:N3	48:S2:1520:G:H2'	2.31	0.46
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.51	0.46
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.81	0.46
11:LG:251:ALA:HA	11:LG:254:GLU:HG3	1.98	0.46
12:LH:173:ARG:HB3	41:Lm:127:VAL:HG22	1.98	0.46
14:LJ:96:LYS:HE2	14:LJ:96:LYS:HB3	1.81	0.46
15:LL:130:LYS:HB3	15:LL:133:ALA:HB3	1.98	0.46
36:Lg:100:GLN:OE1	36:Lg:100:GLN:HA	2.16	0.46
48:S2:306:C:H5'	48:S2:308:G:H5'	1.98	0.46
48:S2:847:A:C2	52:SE:248:ILE:HD11	2.51	0.46
48:S2:951:C:O2'	62:SO:50:LYS:NZ	2.49	0.46
48:S2:1606:G:N2	48:S2:1632:G:H1'	2.31	0.46
49:SB:131:ASP:CG	49:SB:180:ASP:HB2	2.41	0.46
62:SO:21:VAL:HG22	62:SO:22:ALA:N	2.29	0.46
62:SO:93:LEU:HG	62:SO:124:MET:HE3	1.98	0.46
68:SU:94:PRO:HD2	68:SU:97:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Sa:88:SER:O	73:Sa:92:ARG:HG3	2.16	0.46
3:L5:1246:G:H2'	3:L5:1247:U:H6	1.81	0.45
3:L5:2691:U:C2	3:L5:2692:U:C5	3.04	0.45
6:LB:386:LYS:HE2	6:LB:386:LYS:HB2	1.81	0.45
11:LG:97:LYS:HE3	11:LG:97:LYS:HB3	1.69	0.45
13:LI:93:PRO:HB2	13:LI:125:THR:HB	1.96	0.45
13:LI:152:LEU:HB3	13:LI:165:ILE:HD12	1.98	0.45
48:S2:1139:C:H2'	48:S2:1140:G:O4'	2.16	0.45
48:S2:1305:C:H2'	48:S2:1306:U:C6	2.51	0.45
51:SD:72:VAL:HG23	58:SK:20:VAL:HB	1.98	0.45
60:SM:23:LYS:O	60:SM:27:ILE:HG12	2.16	0.45
65:SR:27:ASP:OD2	65:SR:30:THR:OG1	2.26	0.45
69:SV:1:MET:HB3	69:SV:1:MET:HE2	1.74	0.45
69:SV:30:ALA:O	69:SV:60:ARG:HD3	2.16	0.45
79:Sg:144:ASP:HB2	79:Sg:145:GLU:OE2	2.16	0.45
1:At:10:G:H3'	1:At:11:U:H5''	1.98	0.45
3:L5:1472:C:H2'	3:L5:1473:U:C6	2.50	0.45
3:L5:2520:C:O2	3:L5:2640:G:N2	2.49	0.45
3:L5:4070:U:H2'	3:L5:4071:U:H6	1.81	0.45
13:LI:61:SER:OG	13:LI:63:GLU:OE1	2.34	0.45
29:LZ:35:ASP:OD1	29:LZ:35:ASP:N	2.47	0.45
48:S2:1595:U:H5	72:SZ:104:ARG:HG3	1.81	0.45
48:S2:1797:U:H2'	48:S2:1798:C:C6	2.51	0.45
74:Sb:33:MET:HB2	74:Sb:79:PHE:HD2	1.81	0.45
1:At:11:U:H3	1:At:24:G:H22	1.65	0.45
3:L5:163:A:H2'	3:L5:164:G:H8	1.80	0.45
3:L5:1247:U:H2'	3:L5:1248:C:C6	2.52	0.45
3:L5:1625:OMG:H4'	3:L5:1626:G:O5'	2.17	0.45
3:L5:4546:A:N7	80:LA:215:ASN:ND2	2.64	0.45
15:LL:121:ARG:HH11	15:LL:121:ARG:HG3	1.82	0.45
18:LO:181:ALA:O	18:LO:185:VAL:HG22	2.16	0.45
29:LZ:50:PRO:HD3	29:LZ:68:ILE:HG12	1.97	0.45
37:Lh:110:LYS:HB2	37:Lh:110:LYS:HE3	1.70	0.45
48:S2:1271:C:OP1	78:Sf:92:LYS:HD3	2.16	0.45
48:S2:1600:G:H4'	72:SZ:43:LYS:HD2	1.99	0.45
58:SK:47:LYS:HD3	58:SK:47:LYS:HA	1.64	0.45
64:SQ:82:TYR:O	64:SQ:85:ARG:HG2	2.16	0.45
71:SY:43:LYS:HE2	71:SY:43:LYS:HB2	1.58	0.45
73:Sa:47:ALA:O	73:Sa:50:VAL:HG12	2.16	0.45
3:L5:4563:U:H2'	3:L5:4564:A:C8	2.51	0.45
3:L5:4771:C:O2'	3:L5:4772:C:O5'	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LC:266:THR:O	7:LC:267:TRP:HB2	2.16	0.45
26:LW:72:THR:O	26:LW:73:ARG:HG3	2.16	0.45
37:Lh:77:LYS:HD3	37:Lh:78:TYR:CZ	2.52	0.45
48:S2:456:C:O2'	48:S2:1801:A:H4'	2.17	0.45
57:SJ:137:VAL:HG12	57:SJ:138:ARG:HG3	1.98	0.45
62:SO:98:ARG:HB3	62:SO:132:VAL:HG23	1.99	0.45
63:SP:37:TYR:HB3	63:SP:41:GLN:HB2	1.99	0.45
78:Sf:107:LYS:HE2	78:Sf:115:SER:OG	2.17	0.45
79:Sg:44:LYS:HB2	79:Sg:44:LYS:HE3	1.86	0.45
2:Et:65:C:N4	2:Et:66:C:H41	2.14	0.45
3:L5:300:A:H2'	3:L5:301:G:H8	1.81	0.45
3:L5:4770:U:H2'	3:L5:4771:C:C6	2.52	0.45
11:LG:105:GLU:OE2	11:LG:113:ARG:NH1	2.50	0.45
16:LM:41:PRO:HG3	16:LM:73:VAL:HG12	1.98	0.45
17:LN:9:GLU:HB2	38:Li:44:ILE:HG13	1.98	0.45
48:S2:1438:A:H2'	48:S2:1439:A:C8	2.52	0.45
55:SH:34:SER:OG	55:SH:35:ASP:N	2.48	0.45
66:SS:21:ASP:HB3	66:SS:24:ARG:HG3	1.99	0.45
71:SY:23:MET:HE3	71:SY:23:MET:HB3	1.86	0.45
71:SY:29:HIS:O	71:SY:30:PRO:C	2.57	0.45
74:Sb:81:ARG:HE	74:Sb:81:ARG:HB3	1.43	0.45
79:Sg:112:ALA:HB3	79:Sg:121:VAL:HG12	1.98	0.45
3:L5:3652:A:H2'	3:L5:3653:A:C5	2.52	0.45
3:L5:3856:A:H5''	19:LP:83:TRP:O	2.16	0.45
3:L5:4481:U:H2'	3:L5:4482:U:H6	1.81	0.45
9:LE:210:LYS:HE3	9:LE:210:LYS:HB2	1.83	0.45
36:Lg:41:ALA:O	36:Lg:52:ARG:HD3	2.17	0.45
48:S2:525:A:H2'	48:S2:526:A:H8	1.80	0.45
48:S2:549:C:H2'	48:S2:550:C:C6	2.51	0.45
48:S2:1199:A:OP1	73:Sa:2:THR:N	2.50	0.45
48:S2:1597:C:OP2	72:SZ:85:ARG:NH2	2.49	0.45
87:S2:2016:SPD:H42	87:S2:2016:SPD:H72	1.53	0.45
3:L5:424:U:H2'	3:L5:425:U:C6	2.51	0.45
3:L5:982:U:H2'	3:L5:983:C:C6	2.51	0.45
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.52	0.45
3:L5:1433:A:N6	3:L5:1451:G:O2'	2.48	0.45
3:L5:1952:G:OP1	22:LS:139:ARG:NE	2.50	0.45
3:L5:4174:U:H2'	3:L5:4175:G:H8	1.82	0.45
3:L5:4405:G:OP2	13:LI:7:ARG:NH2	2.43	0.45
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.51	0.45
48:S2:61:A:H1'	48:S2:316:G:H1'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:326:C:H4'	48:S2:327:G:C4	2.51	0.45
48:S2:1140:G:C2'	48:S2:1141:G:H5'	2.46	0.45
48:S2:1349:G:H2'	48:S2:1350:U:C6	2.52	0.45
50:SC:77:SER:HB2	50:SC:79:GLU:HG2	1.98	0.45
52:SE:95:THR:O	52:SE:97:GLU:HG3	2.16	0.45
66:SS:143:GLY:O	66:SS:144:ARG:HB2	2.15	0.45
3:L5:964:A:H2'	3:L5:965:G:H4'	1.98	0.45
3:L5:2500:U:H2'	3:L5:2501:C:H6	1.82	0.45
16:LM:96:GLU:OE2	16:LM:100:ARG:NE	2.46	0.45
37:Lh:94:ARG:HE	37:Lh:94:ARG:HB2	1.61	0.45
47:Pt:23:C:H2'	47:Pt:24:G:C8	2.52	0.45
48:S2:302:A:H1'	56:SI:73:THR:HG23	1.99	0.45
48:S2:644:OMG:HM23	48:S2:644:OMG:H1'	1.64	0.45
48:S2:884:C:H2'	48:S2:885:U:C6	2.51	0.45
63:SP:127:LYS:HA	63:SP:127:LYS:HD3	1.66	0.45
64:SQ:48:GLN:O	64:SQ:52:LEU:HG	2.17	0.45
1:At:21:A:C5	1:At:48:C:C4	3.05	0.45
3:L5:10:A:H2'	3:L5:11:G:H8	1.82	0.45
3:L5:119:G:O4'	11:LG:132:ARG:NH1	2.49	0.45
3:L5:654:C:H2'	3:L5:655:C:C6	2.51	0.45
3:L5:1320:U:O2'	3:L5:1891:A:N1	2.44	0.45
3:L5:1472:C:H2'	3:L5:1473:U:H6	1.82	0.45
3:L5:3934:G:H2'	3:L5:3935:C:C6	2.51	0.45
6:LB:46:PHE:CZ	6:LB:84:MET:HG3	2.51	0.45
6:LB:224:LYS:HG2	6:LB:340:THR:HG22	1.98	0.45
22:LS:71:SER:O	22:LS:76:LYS:NZ	2.49	0.45
38:Li:63:VAL:HG12	38:Li:65:LYS:HG3	1.98	0.45
72:SZ:69:THR:H	72:SZ:72:VAL:HG22	1.81	0.45
79:Sg:78:ALA:O	79:Sg:89:LEU:HA	2.17	0.45
3:L5:1743:A:N1	3:L5:1789:C:O2'	2.48	0.45
3:L5:2361:G:O2'	3:L5:3859:G:O6	2.33	0.45
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.82	0.45
3:L5:3923:A:H2'	3:L5:3924:C:H6	1.80	0.45
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.52	0.45
12:LH:50:LYS:C	12:LH:52:LYS:H	2.25	0.45
14:LJ:101:ASP:OD1	14:LJ:101:ASP:N	2.49	0.45
37:Lh:52:LYS:HA	37:Lh:52:LYS:HD3	1.74	0.45
70:SW:111:MET:SD	70:SW:115:GLU:HG2	2.57	0.45
3:L5:1771:U:H2'	3:L5:1772:C:H6	1.81	0.44
5:L8:84:A:C5	5:L8:88:A:H4'	2.52	0.44
7:LC:298:ILE:HD13	20:LQ:131:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LD:267:ASN:N	8:LD:267:ASN:OD1	2.49	0.44
15:LL:121:ARG:HG3	15:LL:121:ARG:NH1	2.32	0.44
27:LX:64:SER:OG	37:Lh:82:ASP:OD2	2.29	0.44
48:S2:1025:U:H2'	48:S2:1026:C:O4'	2.17	0.44
53:SF:143:PRO:HA	53:SF:146:ARG:HG2	1.99	0.44
57:SJ:158:ASP:OD1	57:SJ:159:PHE:N	2.50	0.44
65:SR:97:GLU:HG2	65:SR:120:THR:CG2	2.46	0.44
79:Sg:206:LEU:HD23	79:Sg:206:LEU:HA	1.79	0.44
1:At:6:G:H22	1:At:67:U:H3	1.65	0.44
3:L5:116:G:H2'	3:L5:117:C:C6	2.52	0.44
3:L5:662:C:H5''	3:L5:663:G:OP1	2.17	0.44
3:L5:1727:U:H2'	3:L5:1728:U:C6	2.53	0.44
3:L5:1893:C:H1'	3:L5:1937:C:O2	2.16	0.44
3:L5:2846:G:O2'	25:LV:19:GLY:O	2.33	0.44
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.82	0.44
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.17	0.44
3:L5:4920:C:H2'	3:L5:4921:C:H6	1.82	0.44
6:LB:107:ALA:HB1	6:LB:202:GLU:HG3	2.00	0.44
11:LG:106:THR:H	11:LG:109:GLU:CD	2.24	0.44
36:Lg:82:MET:HG2	36:Lg:87:VAL:HG23	1.98	0.44
48:S2:797:C:H2'	48:S2:798:G:H8	1.78	0.44
50:SC:74:LYS:HB3	50:SC:269:PHE:CE2	2.52	0.44
55:SH:80:VAL:HG23	55:SH:92:VAL:HG23	1.99	0.44
60:SM:61:TYR:OH	60:SM:108:CYS:HB2	2.17	0.44
67:ST:122:LYS:HB3	67:ST:122:LYS:HE3	1.72	0.44
71:SY:79:LEU:HD12	71:SY:79:LEU:O	2.16	0.44
3:L5:267:G:H2'	3:L5:268:G:C8	2.53	0.44
3:L5:733:A:H2'	3:L5:734:G:O4'	2.17	0.44
3:L5:907:C:H2'	3:L5:908:G:H8	1.83	0.44
3:L5:3641:U:OP2	3:L5:3646:A:N6	2.44	0.44
3:L5:4524:G:N3	6:LB:252:ALA:HB1	2.33	0.44
3:L5:4580:U:O2'	6:LB:182:GLU:OE2	2.23	0.44
3:L5:4670:C:O2'	25:LV:15:ARG:NH2	2.50	0.44
9:LE:149:ILE:HD12	9:LE:271:LEU:HD21	1.98	0.44
13:LI:191:ILE:HG13	13:LI:191:ILE:O	2.16	0.44
22:LS:136:LYS:HB2	22:LS:136:LYS:HE2	1.79	0.44
36:Lg:105:LYS:HD2	36:Lg:106:VAL:N	2.32	0.44
48:S2:921:G:C6	74:Sb:22:LYS:HA	2.52	0.44
48:S2:1220:A:H2'	48:S2:1221:G:O4'	2.17	0.44
60:SM:92:CYS:HA	60:SM:103:VAL:HA	1.98	0.44
66:SS:48:ALA:HB2	66:SS:70:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Sa:26:CYS:SG	73:Sa:28:ARG:HB3	2.57	0.44
3:L5:1244:G:H2'	3:L5:1245:C:C6	2.51	0.44
3:L5:1565:A:C5	3:L5:1566:C:H1'	2.52	0.44
3:L5:2099:G:OP2	10:LF:35:LYS:NZ	2.45	0.44
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.53	0.44
3:L5:4481:U:H2'	3:L5:4482:U:C6	2.53	0.44
8:LD:108:ARG:CZ	8:LD:253:TYR:HB2	2.47	0.44
11:LG:209:SER:HA	11:LG:212:LYS:HG3	1.98	0.44
32:Lc:11:LEU:O	32:Lc:14:ILE:HG22	2.17	0.44
40:Ll:12:PHE:O	40:Ll:16:LYS:HG2	2.18	0.44
41:Lm:106:ARG:HE	41:Lm:106:ARG:HB3	1.64	0.44
48:S2:325:C:H2'	48:S2:326:C:C2	2.53	0.44
48:S2:434:G:OP1	56:SI:23:LYS:HG2	2.17	0.44
48:S2:656:G:H5'	48:S2:662:G:N2	2.33	0.44
48:S2:1256:G:O6	68:SU:65:THR:HG22	2.18	0.44
62:SO:63:LYS:HE2	62:SO:63:LYS:N	2.33	0.44
79:Sg:145:GLU:O	79:Sg:175:LYS:NZ	2.38	0.44
3:L5:1071:C:O2	9:LE:70:LYS:NZ	2.51	0.44
3:L5:2025:A:H4'	3:L5:2026:A:H4'	2.00	0.44
3:L5:2096:G:N2	7:LC:304:ALA:HB1	2.32	0.44
3:L5:4750:G:H2'	3:L5:4751:G:H8	1.83	0.44
12:LH:128:MET:HE2	12:LH:128:MET:HA	1.99	0.44
25:LV:91:LYS:HD3	25:LV:91:LYS:HA	1.79	0.44
43:Lo:23:VAL:HG22	43:Lo:70:LEU:HD23	2.00	0.44
49:SB:83:LYS:HB2	49:SB:83:LYS:HE2	1.65	0.44
50:SC:191:VAL:HG11	50:SC:236:PHE:HA	2.00	0.44
58:SK:14:LEU:HD23	58:SK:21:MET:HE1	2.00	0.44
58:SK:49:MET:HG3	58:SK:69:TRP:CE3	2.53	0.44
64:SQ:72:VAL:HG21	64:SQ:84:ILE:HD11	1.99	0.44
3:L5:2517:A:N3	3:L5:2539:C:O2'	2.49	0.44
3:L5:4744:A:H2'	3:L5:4745:G:O4'	2.17	0.44
3:L5:4954:G:H2'	3:L5:4955:A:H8	1.82	0.44
15:LL:190[B]:ARG:HG2	15:LL:191:LEU:HG	2.00	0.44
48:S2:846:G:C5	52:SE:19:MET:HE3	2.53	0.44
48:S2:1595:U:H2'	48:S2:1596:U:C6	2.53	0.44
60:SM:59:PRO:O	60:SM:62:VAL:HG22	2.17	0.44
71:SY:37:LYS:HA	71:SY:40:ILE:CG2	2.47	0.44
79:Sg:262:GLU:H	79:Sg:262:GLU:HG2	1.71	0.44
80:LA:234:LYS:HG2	80:LA:238:ILE:HG12	1.99	0.44
3:L5:2:G:H2'	3:L5:3:C:C6	2.53	0.44
3:L5:139:G:H2'	3:L5:140:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.83	0.44
3:L5:1481:C:N4	38:Li:4:ARG:HD2	2.32	0.44
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.53	0.44
3:L5:1860:PSU:N1	91:L5:5405:HOH:O	2.33	0.44
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.85	0.44
3:L5:3770:PSU:H2'	3:L5:3771:C:C6	2.53	0.44
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.53	0.44
3:L5:4174:U:H2'	3:L5:4175:G:C8	2.53	0.44
8:LD:232:THR:OG1	8:LD:235:MET:HE1	2.17	0.44
45:Lr:125:MET:N	45:Lr:125:MET:SD	2.90	0.44
48:S2:921:G:C2	74:Sb:22:LYS:HG2	2.53	0.44
48:S2:1101:U:H2'	48:S2:1102:G:C8	2.53	0.44
48:S2:1279:C:H2'	48:S2:1280:G:C8	2.53	0.44
49:SB:94:LYS:HA	49:SB:94:LYS:HD2	1.83	0.44
53:SF:100:ILE:HG23	53:SF:178:ILE:HD11	2.00	0.44
55:SH:160:LYS:HE3	55:SH:191:GLU:HA	2.00	0.44
3:L5:180:C:C4	3:L5:181:C:N4	2.86	0.44
3:L5:1720:C:H2'	3:L5:1721:G:O4'	2.16	0.44
3:L5:2442:G:O2'	3:L5:2512:A:N3	2.47	0.44
3:L5:3848:U:H2'	3:L5:3849:A:H8	1.82	0.44
5:L8:155:C:H2'	5:L8:156:U:O4'	2.17	0.44
8:LD:107:ARG:NH1	8:LD:169:GLY:O	2.45	0.44
16:LM:36:ALA:HB2	16:LM:52:PHE:CZ	2.53	0.44
22:LS:123:SER:O	22:LS:123:SER:OG	2.31	0.44
28:LY:53:ASP:O	28:LY:70:VAL:HG22	2.17	0.44
48:S2:509:OMG:H2'	48:S2:510:G:C8	2.53	0.44
48:S2:554:A:C6	77:Se:98:LYS:HA	2.53	0.44
48:S2:1628:C:H2'	48:S2:1629:C:C6	2.53	0.44
52:SE:252:ARG:HE	52:SE:252:ARG:HB3	1.62	0.44
56:SI:142:SER:O	56:SI:146:GLN:HB2	2.18	0.44
61:SN:46:THR:OG1	61:SN:49:GLN:HG3	2.17	0.44
69:SV:74:LYS:HE3	69:SV:74:LYS:HB2	1.76	0.44
1:At:4:U:H3	1:At:69:G:H22	1.65	0.44
3:L5:134:G:H5''	3:L5:135:G:H3'	1.99	0.44
3:L5:1585:C:N4	87:L5:5371:SPD:H92	2.33	0.44
3:L5:2415:OMU:H1'	3:L5:2415:OMU:HM23	1.51	0.44
3:L5:2885:A:H5''	48:S2:1732:G:H5'	2.00	0.44
3:L5:4253:A:H5'	3:L5:4254:G:C8	2.53	0.44
3:L5:4929:C:O4'	16:LM:118:MET:HE3	2.18	0.44
5:L8:78:G:H2'	5:L8:79:G:C8	2.53	0.44
48:S2:176:U:H2'	48:S2:177:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1497:G:N7	58:SK:25:LYS:HE2	2.32	0.44
66:SS:124:ARG:NH2	66:SS:129:LEU:HB3	2.33	0.44
79:Sg:206:LEU:HD21	79:Sg:227:LEU:HD12	1.98	0.44
3:L5:478:G:H2'	3:L5:479:G:H8	1.82	0.43
3:L5:659:G:C6	3:L5:660:A:C6	3.06	0.43
3:L5:2378:G:N2	3:L5:2381:A:OP2	2.49	0.43
14:LJ:74:VAL:HG11	14:LJ:78:LYS:HG3	1.99	0.43
18:LO:158:GLU:O	18:LO:162:GLU:HG2	2.18	0.43
28:LY:113:LYS:HB3	28:LY:113:LYS:HE2	1.84	0.43
42:Ln:1:MET:HB2	48:S2:1706:G:H5'	2.00	0.43
48:S2:494:C:N4	48:S2:509:OMG:HN22	2.16	0.43
48:S2:671:A:H1'	87:S2:2017:SPD:H71	2.00	0.43
54:SG:44:GLU:OE1	54:SG:44:GLU:N	2.39	0.43
65:SR:29:HIS:HA	65:SR:32:LYS:HE2	2.00	0.43
65:SR:32:LYS:HG3	65:SR:47:ARG:HD3	1.99	0.43
71:SY:82:ALA:O	71:SY:86:GLU:HB3	2.18	0.43
3:L5:679:C:H2'	3:L5:680:G:H8	1.84	0.43
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.53	0.43
3:L5:2459:G:H2'	3:L5:2461:G:OP2	2.18	0.43
3:L5:3771:C:H2'	3:L5:3772:U:O4'	2.17	0.43
3:L5:4551:U:H2'	3:L5:4552:PSU:C6	2.53	0.43
7:LC:163:LYS:HB2	7:LC:166:GLU:HG3	1.98	0.43
10:LF:171:ASP:OD1	10:LF:172:ASN:N	2.51	0.43
12:LH:107:GLU:OE2	12:LH:127:ARG:NH1	2.51	0.43
14:LJ:91:GLU:HG3	14:LJ:93:GLU:HG2	2.00	0.43
26:LW:97:LYS:HD2	26:LW:97:LYS:HA	1.82	0.43
48:S2:223:C:H2'	48:S2:224:A:C8	2.53	0.43
48:S2:1407:U:H1'	48:S2:1442:OMU:O4	2.18	0.43
51:SD:81:GLU:OE2	51:SD:82:GLY:N	2.51	0.43
53:SF:50:PRO:HG2	53:SF:90:VAL:HG22	2.00	0.43
3:L5:911:U:H2'	3:L5:912:G:O4'	2.18	0.43
3:L5:1345:A:H2'	3:L5:1346:C:C6	2.54	0.43
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.53	0.43
3:L5:3724:A2M:HM'3	3:L5:3724:A2M:H1'	1.74	0.43
3:L5:4620:OMU:HM23	3:L5:4620:OMU:H1'	1.83	0.43
3:L5:4862:G:H2'	3:L5:4863:G:C8	2.53	0.43
3:L5:4922:C:H2'	3:L5:4923:C:H6	1.83	0.43
3:L5:4957:C:H2'	3:L5:4958:C:C6	2.53	0.43
3:L5:4968:A:H2'	3:L5:4969:C:C6	2.53	0.43
4:L7:82:G:H2'	4:L7:83:A:C8	2.53	0.43
8:LD:184:ASP:OD2	8:LD:187:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LW:99:GLU:HA	26:LW:102:LYS:HE3	1.99	0.43
67:ST:24:LYS:NZ	67:ST:24:LYS:HB3	2.33	0.43
71:SY:60:PHE:CD1	71:SY:71:GLY:HA3	2.53	0.43
79:Sg:228:TYR:CE2	79:Sg:264:LYS:HG2	2.53	0.43
3:L5:674:G:H2'	3:L5:675:C:C6	2.53	0.43
3:L5:1824:G:H5''	23:LT:35:LYS:HE2	1.99	0.43
3:L5:4136:G:H2'	3:L5:4137:C:C6	2.53	0.43
48:S2:1536:G:H2'	48:S2:1537:A:H8	1.81	0.43
52:SE:18:TRP:HB3	52:SE:20:LEU:HD13	2.00	0.43
52:SE:199:GLU:OE1	52:SE:209:HIS:NE2	2.43	0.43
62:SO:58:GLY:O	62:SO:62:VAL:HG22	2.18	0.43
79:Sg:130:LYS:HG2	79:Sg:141:THR:HB	2.00	0.43
3:L5:260:C:H2'	3:L5:261:G:H8	1.82	0.43
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.53	0.43
3:L5:1452:A:H2'	3:L5:1453:G:O4'	2.19	0.43
3:L5:4635:A:H3'	3:L5:4636:U:H4'	2.00	0.43
12:LH:14:GLU:CD	12:LH:14:GLU:N	2.77	0.43
37:Lh:71:LYS:HB3	37:Lh:71:LYS:NZ	2.34	0.43
48:S2:1468:C:H2'	48:S2:1469:A:C8	2.54	0.43
48:S2:1490:OMG:H5'	48:S2:1490:OMG:H8	1.83	0.43
57:SJ:54:ARG:NH2	57:SJ:58:ARG:HH12	2.17	0.43
62:SO:88:LEU:HD23	62:SO:88:LEU:HA	1.85	0.43
67:ST:116:ASP:OD1	67:ST:117:GLN:NE2	2.51	0.43
2:Et:66:C:O2'	2:Et:67:U:H6	2.02	0.43
3:L5:1210:C:H41	10:LF:66:ARG:CZ	2.32	0.43
3:L5:1771:U:H2'	3:L5:1772:C:C6	2.54	0.43
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.80	0.43
3:L5:4383:U:H2'	3:L5:4384:U:C6	2.53	0.43
5:L8:89:U:H2'	5:L8:90:C:C6	2.53	0.43
9:LE:72:LYS:HD2	31:Lb:119:CYS:HB3	1.99	0.43
13:LI:145:LYS:O	13:LI:149:ILE:HG12	2.18	0.43
15:LL:136:LYS:HB3	15:LL:137:GLY:H	1.52	0.43
48:S2:601:OMG:H1'	48:S2:601:OMG:HM23	1.74	0.43
48:S2:874:G:H2'	48:S2:875:A:H8	1.83	0.43
64:SQ:51:LEU:HD23	64:SQ:51:LEU:HA	1.87	0.43
3:L5:268:G:H2'	3:L5:269:G:C8	2.53	0.43
3:L5:457:G:H2'	3:L5:458:C:C6	2.53	0.43
3:L5:2477:A:H2	3:L5:2478:C:H41	1.67	0.43
3:L5:2580:U:O2'	29:LZ:79:HIS:ND1	2.45	0.43
3:L5:4352:U:P	15:LL:190[B]:ARG:HH22	2.40	0.43
3:L5:4538:G:H2'	3:L5:4539:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4619:U:H2'	3:L5:4620:OMU:C6	2.49	0.43
3:L5:4887:C:H2'	3:L5:4888:U:O4'	2.19	0.43
43:Lo:27:LYS:HB3	43:Lo:27:LYS:HE2	1.57	0.43
48:S2:1069:U:H2'	48:S2:1070:A:C8	2.54	0.43
50:SC:78:LEU:HD12	50:SC:78:LEU:HA	1.85	0.43
55:SH:170:VAL:HG13	55:SH:187:PHE:HB2	2.00	0.43
58:SK:86:PRO:HB2	58:SK:88:GLU:OE1	2.18	0.43
69:SV:23:ILE:C	69:SV:23:ILE:HD12	2.44	0.43
80:LA:75:LEU:HD23	80:LA:75:LEU:HA	1.77	0.43
80:LA:206:PRO:HG3	80:LA:213:GLY:HA3	2.01	0.43
3:L5:1298:C:H2'	3:L5:1299:G:H8	1.84	0.43
3:L5:1907:A:H2'	3:L5:1908:A:C8	2.54	0.43
3:L5:3917:A:H2'	3:L5:3918:G:C8	2.54	0.43
3:L5:4233:A:C4	3:L5:4235:G:N7	2.87	0.43
3:L5:5061:A:H5''	3:L5:5062:G:C8	2.54	0.43
5:L8:141:C:H2'	5:L8:142:U:C6	2.54	0.43
8:LD:83:LEU:HB3	8:LD:88:VAL:HB	2.01	0.43
10:LF:187:MET:HE3	10:LF:187:MET:HB3	1.94	0.43
17:LN:178:HIS:HA	17:LN:181:HIS:NE2	2.33	0.43
28:LY:69:LYS:HE2	28:LY:69:LYS:HB3	1.84	0.43
37:Lh:14:LYS:HB2	37:Lh:14:LYS:HE3	1.76	0.43
48:S2:77:A:H1'	54:SG:176:ILE:HG12	2.01	0.43
55:SH:130:LEU:HD21	55:SH:156:VAL:HG21	2.00	0.43
61:SN:39:LYS:HE2	61:SN:39:LYS:HB3	1.89	0.43
61:SN:43:LYS:NZ	61:SN:43:LYS:HB3	2.34	0.43
61:SN:102:LEU:HD11	61:SN:112:LYS:HA	2.01	0.43
67:ST:27:LYS:HE2	67:ST:27:LYS:HB2	1.69	0.43
79:Sg:178:ASN:ND2	79:Sg:180:ALA:O	2.52	0.43
3:L5:12:A:OP1	87:L8:205:SPD:H21	2.18	0.43
3:L5:657:C:H2'	3:L5:658:C:C6	2.54	0.43
3:L5:1314:C:C2	3:L5:1315:C:C5	3.06	0.43
3:L5:3604:A:H2'	3:L5:3605:C:C6	2.54	0.43
3:L5:4363:A:H5''	43:Lo:36:GLN:HG2	2.01	0.43
16:LM:124:LYS:HB2	16:LM:124:LYS:HE2	1.72	0.43
18:LO:129:LEU:HD12	18:LO:129:LEU:HA	1.88	0.43
25:LV:99:GLU:HG3	26:LW:21:TYR:OH	2.19	0.43
33:Ld:23:ARG:HB3	33:Ld:25:TYR:CE1	2.54	0.43
48:S2:841:G:C8	71:SY:12:PHE:HB3	2.54	0.43
48:S2:1010:G:H2'	48:S2:1011:A:C8	2.53	0.43
48:S2:1322:G:H2'	48:S2:1323:U:H5'	1.99	0.43
48:S2:1616:U:H2'	48:S2:1617:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1740:C:H2'	48:S2:1741:U:C6	2.54	0.43
57:SJ:80:ARG:O	57:SJ:84:ILE:HG12	2.19	0.43
67:ST:122:LYS:HG2	67:ST:123:LEU:N	2.33	0.43
70:SW:3:ARG:HH22	70:SW:28:ARG:NH2	2.17	0.43
3:L5:180:C:H2'	3:L5:181:C:N1	2.34	0.43
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.54	0.43
21:LR:95:TRP:CH2	21:LR:99:MET:HE3	2.53	0.43
26:LW:102:LYS:HE3	26:LW:102:LYS:HB2	1.80	0.43
48:S2:525:A:H2'	48:S2:526:A:C8	2.54	0.43
48:S2:899:U:H2'	48:S2:900:C:O4'	2.19	0.43
48:S2:1391:OMC:HM23	76:Sd:56:ASP:HB3	2.01	0.43
56:SI:46:VAL:HG22	56:SI:48:VAL:HG23	1.99	0.43
3:L5:1756:U:H2'	3:L5:1757:U:H6	1.82	0.42
9:LE:93:THR:O	9:LE:93:THR:OG1	2.29	0.42
13:LI:77:VAL:HG22	13:LI:82:LYS:HA	2.01	0.42
39:Lk:6:GLU:HB2	39:Lk:7:GLU:OE1	2.18	0.42
43:Lo:40:ARG:HA	43:Lo:43[B]:ARG:CZ	2.49	0.42
48:S2:317:C:H5	54:SG:183:ARG:NH2	2.17	0.42
48:S2:689:U:H2'	48:S2:690:G:O4'	2.19	0.42
48:S2:1568:C:H2'	48:S2:1569:A:C8	2.54	0.42
48:S2:1714:U:H2'	48:S2:1715:A:C8	2.54	0.42
51:SD:109:LEU:HD12	51:SD:184:ILE:HD11	2.01	0.42
55:SH:138:GLU:N	55:SH:159:ASP:OD2	2.29	0.42
66:SS:78:LYS:HD3	66:SS:78:LYS:N	2.34	0.42
68:SU:61:LEU:O	68:SU:81:GLN:HA	2.19	0.42
71:SY:37:LYS:HA	71:SY:40:ILE:HG22	2.00	0.42
81:SA:181:GLU:OE2	81:SA:191:ARG:NH1	2.52	0.42
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.81	0.42
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.54	0.42
3:L5:4251:A:H2'	3:L5:4252:C:C6	2.55	0.42
3:L5:4488:A:H4'	3:L5:4489:G:C8	2.54	0.42
7:LC:259:LYS:HE2	7:LC:259:LYS:HB3	1.76	0.42
14:LJ:93:GLU:OE1	14:LJ:173:ILE:HB	2.19	0.42
48:S2:1118:C:H2'	48:S2:1119:A:O4'	2.18	0.42
48:S2:1826:G:H5''	90:S2:2021:HYG:H341	2.01	0.42
49:SB:123:ALA:HB2	49:SB:165:ARG:HG3	2.01	0.42
73:Sa:59:PHE:HB2	73:Sa:62:TYR:HB2	2.01	0.42
73:Sa:60:ASP:OD1	73:Sa:60:ASP:N	2.52	0.42
79:Sg:191:HIS:CD2	79:Sg:195:LEU:HD21	2.54	0.42
79:Sg:246:TYR:CD2	79:Sg:261:LEU:HB2	2.54	0.42
3:L5:1577:G:H5'	3:L5:1578:U:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.85	0.42
3:L5:3744:OMG:HM23	3:L5:3744:OMG:H1'	1.72	0.42
3:L5:4065:G:H2'	3:L5:4066:U:H6	1.84	0.42
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.56	0.42
3:L5:4674:C:H2'	3:L5:4675:U:C6	2.55	0.42
7:LC:208:CYS:SG	7:LC:230:LEU:HD12	2.59	0.42
8:LD:89:LYS:HE3	8:LD:89:LYS:HB2	1.87	0.42
14:LJ:90:ARG:O	14:LJ:91:GLU:HG2	2.19	0.42
21:LR:3:MET:HE3	21:LR:3:MET:HB3	1.93	0.42
22:LS:69:GLU:HG3	22:LS:71:SER:H	1.83	0.42
22:LS:127:MET:HG2	23:LT:153:PRO:O	2.19	0.42
26:LW:105:ARG:HD2	54:SG:150:GLU:O	2.19	0.42
47:Pt:43:A:H2'	47:Pt:44:A:C8	2.54	0.42
48:S2:857:U:H2'	48:S2:858:A:H8	1.68	0.42
52:SE:107:GLY:HA2	52:SE:189:LEU:HG	2.02	0.42
60:SM:42:LEU:HD13	60:SM:68:LEU:HD21	2.01	0.42
62:SO:44:VAL:HG11	62:SO:85:CYS:SG	2.60	0.42
63:SP:18:ARG:NH1	66:SS:88:LYS:O	2.52	0.42
64:SQ:73:LYS:HB3	64:SQ:73:LYS:HE3	1.72	0.42
71:SY:25:ILE:HD11	71:SY:73:GLY:HA3	2.00	0.42
3:L5:456:C:H2'	3:L5:457:G:H8	1.83	0.42
3:L5:1590:C:H5''	3:L5:1591:U:O5'	2.20	0.42
3:L5:2292:C:H2'	3:L5:2293:U:C6	2.54	0.42
3:L5:2602:G:H2'	3:L5:2603:C:H6	1.83	0.42
3:L5:3619:G:H4'	21:LR:79:GLY:O	2.20	0.42
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.54	0.42
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	2.01	0.42
3:L5:4573:G:H2'	3:L5:4574:U:O4'	2.19	0.42
5:L8:106:G:H4'	5:L8:137:A:H5'	2.00	0.42
6:LB:168:MET:HA	6:LB:171:LEU:HD12	2.02	0.42
28:LY:37:GLU:CD	28:LY:37:GLU:N	2.78	0.42
43:Lo:77:CYS:SG	43:Lo:79:SER:HB2	2.60	0.42
48:S2:608:C:H2'	48:S2:609:U:C6	2.55	0.42
48:S2:1115:U:H3'	48:S2:1116:C:C6	2.55	0.42
48:S2:1531:A:H4'	48:S2:1605:G:H4'	2.01	0.42
48:S2:1553:C:H2'	48:S2:1554:C:O4'	2.20	0.42
55:SH:86:LYS:HE3	55:SH:86:LYS:HB2	1.77	0.42
74:Sb:5:LYS:HE3	74:Sb:5:LYS:HB2	1.91	0.42
80:LA:101:VAL:HG22	80:LA:165:VAL:HG22	2.00	0.42
80:LA:150:LEU:HD11	80:LA:156:LYS:HD2	2.02	0.42
3:L5:1364:U:OP2	15:LL:36:ARG:NH2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.34	0.42
3:L5:1786:A:H2'	3:L5:1789:C:C5	2.54	0.42
3:L5:1895:G:H2'	3:L5:1896:A:O4'	2.19	0.42
3:L5:2461:G:H2'	3:L5:2462:C:C6	2.55	0.42
3:L5:2630:U:O4	24:LU:89:LYS:NZ	2.50	0.42
3:L5:2789:A:H1'	40:LI:45:ARG:HH22	1.84	0.42
3:L5:3930:U:H2'	3:L5:3931:C:C6	2.55	0.42
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.62	0.42
3:L5:4220:6MZ:O5'	3:L5:4220:6MZ:H8	2.20	0.42
3:L5:4306:OMU:OP2	20:LQ:159:PRO:HD2	2.20	0.42
3:L5:4406:U:C2	3:L5:4407:G:C8	3.08	0.42
3:L5:4413:C:H2'	3:L5:4414:A:O4'	2.18	0.42
3:L5:4498:OMU:O5'	3:L5:4498:OMU:H6	2.19	0.42
23:LT:102:ARG:HD2	23:LT:102:ARG:HA	1.82	0.42
29:LZ:59:LYS:HB3	29:LZ:59:LYS:HE2	1.71	0.42
48:S2:385:G:H3'	59:SL:136:LYS:HB2	2.00	0.42
48:S2:455:A:H2'	48:S2:456:C:C6	2.54	0.42
48:S2:509:OMG:H2'	48:S2:510:G:H8	1.85	0.42
48:S2:987:A:C6	49:SB:120:MET:HE1	2.55	0.42
50:SC:236:PHE:O	50:SC:240:THR:HG23	2.20	0.42
64:SQ:96:TYR:HD2	64:SQ:104:SER:HB3	1.85	0.42
75:Sc:31:ARG:HE	75:Sc:41:SER:HG	1.64	0.42
80:LA:46:LYS:HD2	80:LA:46:LYS:HA	1.77	0.42
2:Et:25:U:H2'	2:Et:26:G:H8	1.85	0.42
3:L5:489:C:H2'	3:L5:490:C:C6	2.53	0.42
3:L5:1920:C:H3'	3:L5:1921:C:H5''	2.02	0.42
3:L5:2566:G:H2'	3:L5:2567:G:C8	2.53	0.42
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.84	0.42
3:L5:4453:C:H2'	3:L5:4454:G:O4'	2.19	0.42
3:L5:4880:C:H2'	3:L5:4881:U:O4'	2.19	0.42
7:LC:7:LEU:HD22	7:LC:21:ASN:HB3	2.02	0.42
10:LF:143:GLY:HA3	10:LF:240:ILE:HB	2.01	0.42
15:LL:125:ILE:HD11	37:Lh:122:LYS:HG3	2.00	0.42
17:LN:158:HIS:HB3	17:LN:161:MET:HG3	2.01	0.42
23:LT:103:ASP:HA	23:LT:106:LEU:HD12	2.02	0.42
31:Lb:32:LEU:HD13	31:Lb:40:LEU:HD11	2.02	0.42
33:Ld:98:SER:O	33:Ld:101:LYS:NZ	2.53	0.42
48:S2:113:G:O6	48:S2:290:U:H1'	2.20	0.42
48:S2:1315:U:H4'	58:SK:2:LEU:HG	2.01	0.42
50:SC:185:THR:O	50:SC:246:LYS:HD2	2.19	0.42
51:SD:35:SER:HB3	51:SD:97:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SF:197:GLU:O	53:SF:201:LYS:HG3	2.19	0.42
55:SH:100:ILE:HG12	55:SH:125:VAL:HG21	2.01	0.42
59:SL:126:VAL:HG12	59:SL:145:VAL:HG22	2.01	0.42
79:Sg:245:ARG:NH2	79:Sg:312:VAL:HG21	2.35	0.42
3:L5:269:G:H2'	3:L5:270:U:H6	1.85	0.42
3:L5:1247:U:H2'	3:L5:1248:C:H6	1.84	0.42
3:L5:2804:OMC:HM23	3:L5:2804:OMC:H1'	1.85	0.42
3:L5:4128:A:O2'	11:LG:33:GLU:O	2.35	0.42
3:L5:4968:A:H2'	3:L5:4969:C:H6	1.84	0.42
14:LJ:51:SER:HB2	14:LJ:69:ALA:HB3	2.02	0.42
14:LJ:96:LYS:HD2	14:LJ:163:MET:SD	2.60	0.42
26:LW:72:THR:O	26:LW:72:THR:OG1	2.25	0.42
28:LY:2:LYS:HE3	28:LY:2:LYS:HB3	1.65	0.42
48:S2:1678:A2M:HM'3	48:S2:1678:A2M:H1'	1.76	0.42
53:SF:68:ILE:HD12	53:SF:68:ILE:HA	1.90	0.42
56:SI:192:GLY:O	56:SI:196:GLU:HG3	2.19	0.42
60:SM:35:ILE:HD11	60:SM:61:TYR:CZ	2.54	0.42
66:SS:34:LYS:HB2	66:SS:100:ALA:HA	2.02	0.42
73:Sa:64:LEU:HA	73:Sa:65:PRO:HD3	1.94	0.42
83:Lj:39:TYR:CG	83:Lj:40:PRO:HA	2.54	0.42
3:L5:269:G:H2'	3:L5:270:U:C6	2.55	0.42
3:L5:717:U:H2'	3:L5:718:C:C6	2.54	0.42
3:L5:1309:C:H2'	3:L5:1310:C:C6	2.54	0.42
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.54	0.42
3:L5:1802:A:H5''	3:L5:1803:G:H5'	2.01	0.42
3:L5:2019:C:H2'	3:L5:2020:U:C6	2.54	0.42
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.91	0.42
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.20	0.42
3:L5:3718:A2M:H8	3:L5:3718:A2M:O5'	2.19	0.42
6:LB:57:VAL:HG22	6:LB:73:VAL:HG22	2.02	0.42
26:LW:78:PHE:CE2	26:LW:80:ARG:HG2	2.55	0.42
28:LY:91:ASN:OD1	28:LY:93:THR:HG23	2.19	0.42
33:Ld:24:GLU:O	33:Ld:119:THR:HA	2.20	0.42
36:Lg:98:GLU:O	36:Lg:102:ILE:HG13	2.20	0.42
48:S2:841:G:H8	71:SY:12:PHE:HB3	1.85	0.42
48:S2:912:C:C2	48:S2:914:U:H1'	2.55	0.42
48:S2:957:A:OP1	62:SO:59:GLY:HA3	2.19	0.42
48:S2:1188:A:H2'	48:S2:1189:A:O4'	2.20	0.42
49:SB:122:GLU:HG2	49:SB:140:VAL:HG23	2.02	0.42
49:SB:196:ASP:N	49:SB:196:ASP:OD1	2.52	0.42
50:SC:263:LYS:HE2	50:SC:263:LYS:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SI:130:THR:HB	56:SI:133:GLU:CD	2.45	0.42
80:LA:142:GLU:CD	80:LA:142:GLU:H	2.28	0.42
3:L5:1407:C:O2'	3:L5:1408:G:O4'	2.37	0.42
3:L5:1649:U:O2'	87:L5:5374:SPD:N1	2.52	0.42
3:L5:4137:C:H2'	3:L5:4138:C:C6	2.55	0.42
3:L5:4347:G:O2'	3:L5:4348:A:H5'	2.20	0.42
3:L5:4920:C:C2	3:L5:4921:C:C5	3.08	0.42
26:LW:95:ASN:N	26:LW:95:ASN:OD1	2.52	0.42
48:S2:27:A2M:HM'1	48:S2:483:C:H1'	2.02	0.42
48:S2:843:C:H2'	48:S2:844:U:C6	2.55	0.42
48:S2:900:C:H2'	48:S2:901:G:C8	2.55	0.42
48:S2:1478:U:H2'	48:S2:1479:G:C8	2.55	0.42
48:S2:1568:C:P	67:ST:98:SER:HB2	2.60	0.42
50:SC:275:LYS:HB2	50:SC:275:LYS:HE2	1.78	0.42
57:SJ:97:ILE:O	57:SJ:100:LEU:HG	2.20	0.42
60:SM:66:GLU:OE1	60:SM:66:GLU:HA	2.20	0.42
75:Sc:34:PHE:HD2	75:Sc:40:ARG:HB3	1.84	0.42
80:LA:242:ARG:HE	80:LA:242:ARG:HB2	1.70	0.42
3:L5:469:C:H2'	3:L5:470:A:H8	1.85	0.42
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.84	0.42
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.55	0.42
3:L5:2483:G:C6	3:L5:2496:G:C6	3.08	0.42
3:L5:4155:C:H2'	3:L5:4156:G:O4'	2.20	0.42
3:L5:4439:U:H2'	3:L5:4440:G:O4'	2.19	0.42
41:Lm:110:CYS:O	41:Lm:117:HIS:HA	2.20	0.42
48:S2:149:A:H2'	48:S2:150:A:C8	2.55	0.42
48:S2:667:U:H5''	48:S2:1087:A:C5	2.55	0.42
48:S2:847:A:H2	52:SE:248:ILE:HD11	1.85	0.42
48:S2:1374:C:H2'	48:S2:1375:G:O4'	2.20	0.42
48:S2:1438:A:H2'	48:S2:1439:A:H8	1.85	0.42
50:SC:267:GLN:NE2	69:SV:35:ASN:OD1	2.52	0.42
52:SE:62:LYS:HE2	52:SE:62:LYS:HB3	1.82	0.42
60:SM:67:ALA:HB3	78:Sf:114:ILE:HD11	2.02	0.42
61:SN:110:ASP:O	61:SN:114:ARG:HG2	2.20	0.42
66:SS:86:ARG:HD2	66:SS:86:ARG:HA	1.84	0.42
76:Sd:42:CYS:HG	89:Sd:102:ZN:ZN	1.19	0.42
80:LA:71:LYS:HA	80:LA:71:LYS:HD2	1.90	0.42
3:L5:2091:C:H1'	3:L5:2094:G:H1'	2.01	0.41
3:L5:2351:OMC:HM23	7:LC:95:MET:HG3	2.02	0.41
3:L5:4393:G:O4'	3:L5:4447:5MC:HM52	2.19	0.41
4:L7:33:U:H2'	4:L7:34:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LC:350:ARG:HB2	7:LC:350:ARG:HH11	1.84	0.41
9:LE:183:ARG:HA	9:LE:183:ARG:HD2	1.91	0.41
13:LI:139:ARG:NH2	13:LI:195:CYS:HB2	2.34	0.41
48:S2:344:U:H2'	48:S2:345:U:C6	2.55	0.41
55:SH:15:LYS:HB2	55:SH:15:LYS:HE2	1.78	0.41
55:SH:19:PHE:CE2	55:SH:50:GLU:HB2	2.54	0.41
61:SN:23:PRO:HA	74:Sb:84:HIS:HD2	1.84	0.41
1:At:24:G:C6	1:At:25:C:C4	3.08	0.41
3:L5:150:U:OP2	11:LG:200:THR:OG1	2.30	0.41
3:L5:2857:A:H2'	3:L5:2858:A:O4'	2.20	0.41
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.20	0.41
3:L5:4606:G:H2'	3:L5:4607:A:C8	2.55	0.41
5:L8:86:U:H3'	5:L8:87:G:H5'	2.01	0.41
6:LB:92:TYR:HB2	6:LB:159:VAL:HB	2.01	0.41
14:LJ:109:ILE:HD13	14:LJ:109:ILE:HA	1.95	0.41
29:LZ:99:ASP:HB2	29:LZ:102:ARG:HH22	1.85	0.41
37:Lh:12:LYS:HD3	37:Lh:16:GLU:OE2	2.21	0.41
48:S2:1454:A:C8	65:SR:3:ARG:HD3	2.55	0.41
51:SD:23:GLU:O	51:SD:26:THR:OG1	2.34	0.41
57:SJ:108:ARG:NH2	57:SJ:149:VAL:O	2.52	0.41
60:SM:44:LYS:HB3	60:SM:46:GLN:OE1	2.20	0.41
71:SY:42:GLU:O	71:SY:46:LYS:HG2	2.20	0.41
80:LA:145:LYS:HA	80:LA:145:LYS:HD3	1.72	0.41
3:L5:920:C:H2'	3:L5:921:C:C6	2.49	0.41
3:L5:4114:C:H2'	3:L5:4115:G:N3	2.34	0.41
3:L5:4273:A:H2'	3:L5:4274:A:C8	2.56	0.41
3:L5:4327:C:OP1	23:LT:70:HIS:NE2	2.53	0.41
16:LM:104:MET:HE2	16:LM:104:MET:HB2	1.90	0.41
26:LW:95:ASN:C	26:LW:97:LYS:H	2.29	0.41
27:LX:131:ASP:C	27:LX:131:ASP:OD1	2.62	0.41
43:Lo:22:LYS:HB3	43:Lo:22:LYS:HZ2	1.84	0.41
45:Lr:117:ILE:O	45:Lr:121:GLN:HG3	2.20	0.41
48:S2:78:C:OP1	54:SG:159:ARG:NH2	2.53	0.41
48:S2:1372:U:H2'	48:S2:1373:C:O4'	2.20	0.41
52:SE:20:LEU:HD11	52:SE:46:ILE:HD12	2.02	0.41
55:SH:65:PRO:HB2	55:SH:68:GLN:HG2	2.02	0.41
68:SU:48:LEU:HD22	68:SU:93:SER:HB3	2.02	0.41
70:SW:11:LEU:HD12	70:SW:11:LEU:HA	1.87	0.41
75:Sc:60:GLU:OE1	75:Sc:62:GLU:HB2	2.20	0.41
79:Sg:83:TRP:HA	79:Sg:107:ASP:HB3	2.01	0.41
1:At:14:A:C8	1:At:22:G:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:385:A:N3	3:L5:387:G:H5''	2.36	0.41
3:L5:1510:G:H2'	3:L5:1511:U:C6	2.56	0.41
3:L5:1684:A:OP1	30:La:47:LYS:NZ	2.53	0.41
13:LI:39:LYS:HE3	13:LI:39:LYS:HB2	1.85	0.41
15:LL:7:GLY:O	30:La:49:HIS:NE2	2.45	0.41
38:LI:76:ARG:HD3	38:LI:76:ARG:HA	1.85	0.41
40:LI:11:ARG:HE	40:LI:11:ARG:HB3	1.69	0.41
49:SB:225:LEU:O	49:SB:229:MET:HG2	2.20	0.41
55:SH:32:MET:HE2	55:SH:32:MET:HB2	1.96	0.41
55:SH:80:VAL:HG23	55:SH:92:VAL:CG2	2.50	0.41
56:SI:101:ILE:HD12	56:SI:190:LEU:HD11	2.03	0.41
71:SY:49:LYS:HE2	71:SY:49:LYS:HB2	1.84	0.41
3:L5:121:A:H5'	3:L5:122:U:OP2	2.20	0.41
3:L5:169:G:H2'	3:L5:170:C:O4'	2.20	0.41
3:L5:478:G:H2'	3:L5:479:G:C8	2.56	0.41
3:L5:478:G:OP1	45:Lr:66:ARG:NH1	2.50	0.41
3:L5:4571:A2M:H8	3:L5:4571:A2M:O5'	2.20	0.41
3:L5:4611:A:H2'	3:L5:4612:C:H6	1.84	0.41
3:L5:4760:G:H2'	3:L5:4761:G:O4'	2.21	0.41
15:LL:164:GLU:HG3	30:La:100:ILE:HB	2.02	0.41
23:LT:102:ARG:HH21	23:LT:105:PHE:HE2	1.67	0.41
48:S2:381:C:H2'	48:S2:382:C:C6	2.55	0.41
48:S2:1589:A:O3'	67:ST:82:ARG:HD2	2.21	0.41
51:SD:40:ARG:HH21	51:SD:49:ILE:HD11	1.85	0.41
61:SN:25:TRP:CZ3	74:Sb:45:THR:HG21	2.56	0.41
71:SY:36:PRO:O	71:SY:40:ILE:HG22	2.20	0.41
80:LA:92:LYS:HE3	80:LA:92:LYS:HB3	1.83	0.41
3:L5:260:C:C2	3:L5:261:G:C8	3.08	0.41
3:L5:456:C:H2'	3:L5:457:G:C8	2.55	0.41
3:L5:978:G:H2'	3:L5:979:C:C6	2.55	0.41
3:L5:1244:G:H2'	3:L5:1245:C:H6	1.85	0.41
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.56	0.41
3:L5:1326:A2M:HM'3	3:L5:1326:A2M:H1'	1.85	0.41
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.56	0.41
6:LB:229:LYS:HG3	6:LB:272:LYS:HD3	2.03	0.41
7:LC:11:TYR:CZ	7:LC:148:PRO:HB2	2.56	0.41
7:LC:156:ASP:OD2	7:LC:255:SER:OG	2.30	0.41
8:LD:152:ARG:O	8:LD:157:ASN:ND2	2.50	0.41
10:LF:209:TRP:CD1	10:LF:210:PRO:HD2	2.56	0.41
11:LG:48:LYS:HA	11:LG:48:LYS:HD3	1.84	0.41
22:LS:17:LEU:HD11	23:LT:136:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LW:98:PRO:O	26:LW:100:VAL:N	2.53	0.41
28:LY:117:LYS:O	28:LY:120:GLU:HG3	2.21	0.41
48:S2:220:U:H5'	56:SI:177:SER:HB3	2.02	0.41
48:S2:1805:G:H2'	48:S2:1806:A:O4'	2.21	0.41
55:SH:28:LEU:HG	55:SH:32:MET:HE1	2.01	0.41
57:SJ:55:LYS:HB2	57:SJ:55:LYS:HE2	1.81	0.41
57:SJ:88:ASP:OD1	57:SJ:88:ASP:C	2.63	0.41
62:SO:54:CYS:HB2	62:SO:84:ARG:HG2	2.02	0.41
3:L5:179:G:N1	3:L5:258:G:C6	2.88	0.41
3:L5:1346:C:H2'	3:L5:1347:G:H8	1.85	0.41
3:L5:1378:C:H5	15:LL:159:ASN:H	1.67	0.41
3:L5:2499:C:H2'	3:L5:2500:U:H6	1.85	0.41
3:L5:4178:A:H2'	3:L5:4179:G:C8	2.55	0.41
3:L5:4219:A:H2'	3:L5:4220:6MZ:C8	2.51	0.41
5:L8:32:C:H2'	5:L8:33:G:O4'	2.21	0.41
17:LN:104:GLU:HA	17:LN:160:GLU:HG3	2.02	0.41
29:LZ:64:LYS:HE3	29:LZ:64:LYS:HB3	1.94	0.41
30:La:93:ASN:HD21	30:La:97:ALA:H	1.69	0.41
32:Lc:17:ARG:HB3	32:Lc:104:ILE:HD13	2.03	0.41
48:S2:78:C:H5''	48:S2:79:A:OP2	2.20	0.41
48:S2:170:A:H2'	48:S2:171:A:C8	2.56	0.41
48:S2:178:C:H2'	48:S2:179:C:C6	2.55	0.41
48:S2:842:C:H2'	48:S2:843:C:C6	2.56	0.41
48:S2:931:C:H2'	48:S2:932:G:C8	2.55	0.41
48:S2:1416:C:OP1	67:ST:129:ARG:NH1	2.53	0.41
48:S2:1683:C:C2	75:Sc:24:GLN:HG3	2.56	0.41
52:SE:95:THR:HG23	71:SY:16:ARG:HB2	2.02	0.41
53:SF:123:GLU:HG2	53:SF:200:ALA:HB1	2.01	0.41
54:SG:201:LYS:HB3	54:SG:201:LYS:HE3	1.84	0.41
66:SS:34:LYS:HE2	66:SS:34:LYS:HB3	1.80	0.41
1:At:9:A:C4	1:At:45:G:C2	3.08	0.41
2:Et:21:A:C6	2:Et:46:G:H1'	2.56	0.41
3:L5:82:U:H2'	3:L5:83:C:O4'	2.21	0.41
3:L5:175:C:H2'	3:L5:176:G:H8	1.85	0.41
3:L5:178:C:H2'	3:L5:179:G:O4'	2.21	0.41
3:L5:434:A:H2'	3:L5:435:A:O4'	2.20	0.41
3:L5:650:C:H2'	3:L5:651:C:C6	2.55	0.41
3:L5:2519:U:H1'	3:L5:2520:C:C6	2.55	0.41
3:L5:2871:A:H2'	3:L5:2872:C:O4'	2.21	0.41
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.86	0.41
3:L5:3696:C:H2'	3:L5:3697:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3701:OMC:N4	3:L5:3745:U:H2'	2.35	0.41
3:L5:3707:U:H2'	3:L5:3708:C:H6	1.83	0.41
3:L5:4478:G:O2'	3:L5:4602:A:N1	2.50	0.41
6:LB:92:TYR:HB3	6:LB:99:LEU:HD22	2.02	0.41
15:LL:28:GLN:O	15:LL:32:LYS:HG3	2.21	0.41
23:LT:117:LYS:NZ	23:LT:121:GLU:OE2	2.54	0.41
24:LU:111:GLU:HG2	24:LU:113:ARG:HG3	2.00	0.41
48:S2:382:C:H2'	48:S2:383:G:C8	2.56	0.41
48:S2:528:A:H2'	48:S2:529:A:C8	2.56	0.41
48:S2:581:U:H5''	71:SY:66:GLY:N	2.36	0.41
49:SB:76:ASN:OD1	49:SB:76:ASN:N	2.52	0.41
61:SN:83:ASP:OD1	61:SN:83:ASP:N	2.40	0.41
68:SU:32:LEU:HD21	68:SU:87:ARG:HG2	2.03	0.41
81:SA:153:PRO:O	81:SA:154:LEU:HD23	2.21	0.41
81:SA:206:ASP:OD1	81:SA:209:GLU:HG2	2.20	0.41
3:L5:69:A:N1	3:L5:324:A:O2'	2.52	0.41
3:L5:690:C:H2'	3:L5:691:C:C6	2.55	0.41
3:L5:978:G:H2'	3:L5:979:C:H6	1.86	0.41
3:L5:1279:A:O2'	3:L5:1281:G:N7	2.51	0.41
3:L5:1339:U:OP1	30:La:8:THR:OG1	2.34	0.41
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.86	0.41
3:L5:4531:U:O2'	3:L5:4532:PSU:O5'	2.38	0.41
3:L5:4737:G:H2'	3:L5:4738:C:C6	2.55	0.41
3:L5:5066:U:H2'	3:L5:5067:U:C6	2.56	0.41
4:L7:24:C:H2'	4:L7:25:G:O4'	2.21	0.41
5:L8:92:U:H2'	5:L8:93:C:O4'	2.21	0.41
14:LJ:38:LYS:O	14:LJ:42:GLN:HG3	2.21	0.41
15:LL:194:ILE:HD12	15:LL:194:ILE:HA	1.87	0.41
18:LO:183:LYS:HE2	18:LO:183:LYS:HB2	1.74	0.41
23:LT:122:LYS:HA	23:LT:122:LYS:HD2	1.90	0.41
29:LZ:5:MET:HG2	29:LZ:77:TYR:CE1	2.56	0.41
38:Li:16:LYS:HD3	38:Li:16:LYS:HA	1.65	0.41
48:S2:470:G:H2'	48:S2:471:G:C8	2.56	0.41
48:S2:824:C:C2	57:SJ:144:ILE:HG12	2.55	0.41
48:S2:1580:A:O2'	48:S2:1581:C:H5'	2.20	0.41
87:S2:2019:SPD:HN6	87:S2:2019:SPD:H31	1.54	0.41
51:SD:48:ILE:HB	51:SD:86:LEU:HG	2.02	0.41
52:SE:55:ALA:HB1	52:SE:60:GLU:HB3	2.02	0.41
54:SG:193:ALA:O	54:SG:197:GLN:HG3	2.21	0.41
56:SI:4:SER:OG	56:SI:6:ASP:OD2	2.35	0.41
60:SM:68:LEU:HA	60:SM:71:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SZ:92:LEU:HD22	72:SZ:109:TYR:HE1	1.84	0.41
3:L5:134:G:O2'	37:Lh:85:PRO:HG3	2.20	0.41
3:L5:1537:A:H2'	3:L5:1538:U:C6	2.56	0.41
3:L5:1567:U:H2'	3:L5:1568:C:H6	1.86	0.41
3:L5:1613:A:H5'	80:LA:183:GLY:HA2	2.03	0.41
3:L5:1899:G:O2'	34:Le:57:ASN:OD1	2.37	0.41
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.55	0.41
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.83	0.41
3:L5:5052:C:H2'	3:L5:5053:U:O4'	2.20	0.41
12:LH:27:VAL:HG12	12:LH:84:VAL:HG21	2.01	0.41
24:LU:36:ALA:HB1	24:LU:65:ARG:HD2	2.02	0.41
33:Ld:87:ARG:NH1	33:Ld:122:VAL:HG11	2.36	0.41
40:Ll:41:ARG:HA	40:Ll:41:ARG:HD2	1.84	0.41
47:Pt:26:M2G:HM12	47:Pt:44:A:C2	2.49	0.41
48:S2:960:U:H1'	48:S2:963:A:N7	2.35	0.41
48:S2:1410:C:H2'	48:S2:1411:G:C8	2.56	0.41
48:S2:1801:A:H2'	48:S2:1802:C:C6	2.55	0.41
49:SB:38:MET:SD	49:SB:185:VAL:HG11	2.61	0.41
52:SE:160:ILE:HD12	52:SE:169:ILE:HG12	2.03	0.41
52:SE:252:ARG:HH12	57:SJ:75:ASN:HD22	1.69	0.41
57:SJ:112:THR:O	57:SJ:116:LYS:HG2	2.21	0.41
58:SK:18:GLU:C	58:SK:20:VAL:H	2.29	0.41
60:SM:62:VAL:HA	60:SM:65:VAL:HG12	2.02	0.41
62:SO:65:ASP:N	62:SO:65:ASP:OD1	2.54	0.41
75:Sc:9:ILE:HD13	75:Sc:57:THR:HG23	2.03	0.41
75:Sc:14:VAL:HA	75:Sc:32:VAL:HG12	2.02	0.41
79:Sg:17:TRP:HB2	79:Sg:36:ARG:HG3	2.03	0.41
1:At:66:A:C6	1:At:67:U:C4	3.09	0.40
2:Et:49:G:H2'	2:Et:50:A:C8	2.56	0.40
3:L5:687:U:N3	9:LE:95:PRO:HG2	2.36	0.40
3:L5:907:C:H2'	3:L5:908:G:C8	2.56	0.40
3:L5:1076:C:H2'	3:L5:1077:C:H6	1.86	0.40
3:L5:1479:G:H2'	3:L5:1480:C:C6	2.56	0.40
6:LB:385:LYS:O	6:LB:389:MET:HG2	2.21	0.40
7:LC:149:GLU:HG3	45:Lr:72:LYS:HG2	2.02	0.40
8:LD:34:LYS:HE2	23:LT:30:TYR:CZ	2.56	0.40
8:LD:291:GLN:OE1	13:LI:214:SER:HA	2.22	0.40
10:LF:92:VAL:O	10:LF:120:GLY:HA2	2.22	0.40
22:LS:82:LEU:C	22:LS:127:MET:HE2	2.46	0.40
26:LW:110:ARG:NH2	26:LW:111:ALA:HB2	2.36	0.40
33:Ld:44:ARG:HA	33:Ld:44:ARG:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:114:G:O6	48:S2:351:G:H1'	2.21	0.40
48:S2:874:G:H2'	48:S2:875:A:C8	2.57	0.40
48:S2:1088:U:H4'	48:S2:1089:G:OP2	2.21	0.40
48:S2:1145:A:C5	48:S2:1146:C:H1'	2.57	0.40
56:SI:145:ILE:C	56:SI:145:ILE:HD12	2.45	0.40
59:SL:17:PHE:CE1	59:SL:19:ASN:HB2	2.56	0.40
68:SU:78:ASP:OD1	76:Sd:54:LYS:NZ	2.43	0.40
71:SY:29:HIS:HB2	71:SY:32:LYS:HB2	2.03	0.40
79:Sg:72:SER:OG	79:Sg:74:ASP:OD1	2.36	0.40
81:SA:205:ARG:HA	81:SA:209:GLU:OE2	2.21	0.40
3:L5:138:G:H2'	3:L5:139:G:H8	1.86	0.40
3:L5:1412:G:C6	3:L5:1413:C:C4	3.08	0.40
3:L5:1479:G:O2'	3:L5:1480:C:H5'	2.21	0.40
3:L5:1583:A:OP2	87:L5:5371:SPD:N10	2.54	0.40
3:L5:2861:OMC:HM23	3:L5:2861:OMC:H1'	1.94	0.40
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.21	0.40
8:LD:79:TYR:O	8:LD:82:GLU:HG2	2.21	0.40
8:LD:211:LEU:HD23	8:LD:211:LEU:HA	1.88	0.40
11:LG:191:GLY:HA2	11:LG:194:VAL:HG22	2.04	0.40
14:LJ:54:ARG:O	14:LJ:64:ARG:HG3	2.21	0.40
24:LU:41:GLN:O	24:LU:45:GLU:HG2	2.22	0.40
36:Lg:94:ALA:O	36:Lg:98:GLU:HG2	2.21	0.40
48:S2:16:G:H2'	48:S2:17:C:C6	2.56	0.40
48:S2:150:A:H3'	48:S2:151:C:H6	1.86	0.40
48:S2:480:G:H2'	48:S2:481:C:O4'	2.20	0.40
55:SH:80:VAL:O	55:SH:84:GLU:HG3	2.21	0.40
56:SI:111:GLN:C	56:SI:111:GLN:OE1	2.64	0.40
60:SM:31:LEU:HD22	60:SM:111:VAL:HG22	2.02	0.40
61:SN:29:THR:O	61:SN:33:VAL:HG22	2.20	0.40
63:SP:24:GLN:H	63:SP:24:GLN:HG2	1.56	0.40
64:SQ:96:TYR:CD2	64:SQ:104:SER:HB3	2.56	0.40
70:SW:102:ILE:H	70:SW:113:HIS:CD2	2.38	0.40
79:Sg:263:GLY:H	79:Sg:264:LYS:HZ3	1.69	0.40
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.57	0.40
3:L5:2089:G:H1	3:L5:2096:G:N2	2.19	0.40
3:L5:3727:A:H2'	3:L5:3728:A:C8	2.57	0.40
5:L8:14:OMU:HM23	5:L8:14:OMU:H1'	1.59	0.40
9:LE:67:ALA:HA	9:LE:69:TYR:CE1	2.57	0.40
9:LE:205:ASN:OD1	9:LE:205:ASN:C	2.63	0.40
20:LQ:43:PHE:CD2	20:LQ:133:GLY:HA3	2.56	0.40
21:LR:126:LYS:HB3	21:LR:131:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Lk:17:ARG:HH21	39:Lk:19:ASP:CG	2.29	0.40
42:Ln:25:LYS:HE3	42:Ln:25:LYS:HB3	1.76	0.40
48:S2:1181:A:H2'	48:S2:1182:A:C8	2.55	0.40
48:S2:1713:C:H2'	48:S2:1714:U:C6	2.56	0.40
50:SC:70:VAL:HG21	50:SC:93:ILE:HG23	2.03	0.40
55:SH:66:VAL:HG22	55:SH:96:ALA:HB1	2.04	0.40
63:SP:65:LYS:HE2	63:SP:65:LYS:HB3	1.72	0.40
66:SS:60:THR:OG1	66:SS:63:GLU:HG3	2.21	0.40
67:ST:114:GLU:HG2	67:ST:124:THR:HG22	2.03	0.40
79:Sg:279:SER:C	79:Sg:281:ALA:H	2.29	0.40
3:L5:1205:G:H2'	3:L5:1206:C:C6	2.57	0.40
3:L5:1242:G:N3	31:Lb:120:ARG:NH1	2.63	0.40
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.85	0.40
3:L5:2021:G:H2'	3:L5:2021:G:N3	2.37	0.40
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.56	0.40
3:L5:2494:U:H2'	3:L5:2495:U:C6	2.56	0.40
3:L5:4629:U:C2	3:L5:4630:G:C8	3.10	0.40
11:LG:100:HIS:O	11:LG:103:ARG:HD2	2.22	0.40
29:LZ:5:MET:HG2	29:LZ:77:TYR:CZ	2.57	0.40
39:Lk:61:PRO:HA	39:Lk:62:PRO:HD3	1.94	0.40
48:S2:1373:C:O2'	65:SR:10:LYS:NZ	2.54	0.40
48:S2:1442:OMU:HM23	48:S2:1442:OMU:H1'	1.77	0.40
49:SB:138:PHE:O	49:SB:213:ARG:N	2.54	0.40
56:SI:150:ASP:O	56:SI:153:LYS:HB2	2.22	0.40
60:SM:23:LYS:HA	60:SM:23:LYS:HD3	1.79	0.40
60:SM:69:CYS:HB3	60:SM:76:LEU:HD23	2.02	0.40
73:Sa:49:ALA:O	73:Sa:53:ILE:HG12	2.20	0.40
3:L5:222:C:H2'	3:L5:223:G:O4'	2.22	0.40
3:L5:984:C:H2'	3:L5:985:C:H6	1.85	0.40
3:L5:1307:A:H2'	3:L5:1308:C:H6	1.85	0.40
3:L5:2385:U:H2'	3:L5:2386:U:C6	2.56	0.40
3:L5:4220:6MZ:OP2	23:LT:2:THR:N	2.55	0.40
3:L5:4232:U:H4'	3:L5:4233:A:O4'	2.22	0.40
4:L7:92:C:H2'	4:L7:93:G:C8	2.56	0.40
19:LP:84:PRO:HB2	19:LP:87:SER:HB2	2.04	0.40
22:LS:30:MET:HE2	22:LS:30:MET:HB3	1.82	0.40
24:LU:45:GLU:HG2	24:LU:45:GLU:H	1.78	0.40
27:LX:79:PHE:CD1	37:Lh:36:VAL:HG11	2.57	0.40
31:Lb:54:LEU:O	31:Lb:58:GLN:HG2	2.21	0.40
60:SM:116:LYS:HD3	60:SM:116:LYS:HA	1.94	0.40
78:Sf:109:ASP:HB3	78:Sf:113:LYS:HB3	2.03	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	
6	LB	396/403 (98%)	388 (98%)	8 (2%)	0	100	100
7	LC	361/427 (84%)	355 (98%)	6 (2%)	0	100	100
8	LD	292/297 (98%)	287 (98%)	5 (2%)	0	100	100
9	LE	217/288 (75%)	212 (98%)	5 (2%)	0	100	100
10	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
11	LG	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
12	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
13	LI	203/214 (95%)	201 (99%)	2 (1%)	0	100	100
14	LJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
15	LL	205/211 (97%)	201 (98%)	4 (2%)	0	100	100
16	LM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
17	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
18	LO	198/203 (98%)	198 (100%)	0	0	100	100
19	LP	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
20	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
21	LR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
22	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
23	LT	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
24	LU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
25	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
26	LW	101/157 (64%)	95 (94%)	6 (6%)	0	100	100
27	LX	116/156 (74%)	116 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	LY	130/145 (90%)	127 (98%)	3 (2%)	0	100	100
29	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
30	La	144/148 (97%)	141 (98%)	3 (2%)	0	100	100
31	Lb	100/159 (63%)	99 (99%)	1 (1%)	0	100	100
32	Lc	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
33	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
34	Le	127/135 (94%)	127 (100%)	0	0	100	100
35	Lf	108/110 (98%)	108 (100%)	0	0	100	100
36	Lg	110/117 (94%)	110 (100%)	0	0	100	100
37	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
38	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
39	Lk	66/70 (94%)	66 (100%)	0	0	100	100
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
42	Ln	23/25 (92%)	23 (100%)	0	0	100	100
43	Lo	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
44	Lp	88/92 (96%)	84 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
49	SB	217/264 (82%)	210 (97%)	7 (3%)	0	100	100
50	SC	217/293 (74%)	213 (98%)	4 (2%)	0	100	100
51	SD	223/243 (92%)	214 (96%)	9 (4%)	0	100	100
52	SE	257/263 (98%)	249 (97%)	8 (3%)	0	100	100
53	SF	179/204 (88%)	174 (97%)	4 (2%)	1 (1%)	21	32
54	SG	212/249 (85%)	206 (97%)	6 (3%)	0	100	100
55	SH	182/194 (94%)	174 (96%)	8 (4%)	0	100	100
56	SI	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
57	SJ	173/194 (89%)	166 (96%)	7 (4%)	0	100	100
58	SK	93/165 (56%)	90 (97%)	3 (3%)	0	100	100
59	SL	139/158 (88%)	133 (96%)	6 (4%)	0	100	100
60	SM	105/132 (80%)	96 (91%)	9 (9%)	0	100	100
61	SN	148/151 (98%)	147 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	SO	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
63	SP	128/145 (88%)	125 (98%)	3 (2%)	0	100	100
64	SQ	138/146 (94%)	132 (96%)	6 (4%)	0	100	100
65	SR	131/135 (97%)	128 (98%)	3 (2%)	0	100	100
66	SS	146/152 (96%)	139 (95%)	7 (5%)	0	100	100
67	ST	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
68	SU	99/119 (83%)	95 (96%)	4 (4%)	0	100	100
69	SV	81/83 (98%)	81 (100%)	0	0	100	100
70	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
71	SY	119/133 (90%)	111 (93%)	6 (5%)	2 (2%)	7	10
72	SZ	85/125 (68%)	79 (93%)	6 (7%)	0	100	100
73	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
74	Sb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
75	Sc	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
76	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
77	Se	45/133 (34%)	45 (100%)	0	0	100	100
78	Sf	59/156 (38%)	50 (85%)	9 (15%)	0	100	100
79	Sg	310/317 (98%)	297 (96%)	13 (4%)	0	100	100
80	LA	248/257 (96%)	230 (93%)	18 (7%)	0	100	100
81	SA	218/295 (74%)	209 (96%)	9 (4%)	0	100	100
82	SX	137/143 (96%)	132 (96%)	4 (3%)	1 (1%)	18	28
83	Lj	84/97 (87%)	84 (100%)	0	0	100	100
All	All	11153/12762 (87%)	10863 (97%)	286 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
71	SY	30	PRO
71	SY	34	THR
82	SX	124	LYS
53	SF	79	HIS

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	
6	LB	346/348 (99%)	342 (99%)	4 (1%)	63	81
7	LC	302/348 (87%)	301 (100%)	1 (0%)	86	93
8	LD	246/250 (98%)	238 (97%)	8 (3%)	33	55
9	LE	195/252 (77%)	189 (97%)	6 (3%)	35	57
10	LF	191/215 (89%)	190 (100%)	1 (0%)	81	91
11	LG	192/223 (86%)	187 (97%)	5 (3%)	40	63
12	LH	169/171 (99%)	167 (99%)	2 (1%)	63	81
13	LI	175/181 (97%)	168 (96%)	7 (4%)	28	47
14	LJ	143/149 (96%)	139 (97%)	4 (3%)	38	60
15	LL	173/177 (98%)	170 (98%)	3 (2%)	53	74
16	LM	116/161 (72%)	115 (99%)	1 (1%)	70	85
17	LN	171/172 (99%)	169 (99%)	2 (1%)	63	81
18	LO	172/174 (99%)	170 (99%)	2 (1%)	63	81
19	LP	135/163 (83%)	134 (99%)	1 (1%)	76	88
20	LQ	164/165 (99%)	163 (99%)	1 (1%)	78	89
21	LR	146/175 (83%)	144 (99%)	2 (1%)	59	79
22	LS	157/157 (100%)	156 (99%)	1 (1%)	78	89
23	LT	140/140 (100%)	138 (99%)	2 (1%)	59	79
24	LU	89/115 (77%)	86 (97%)	3 (3%)	32	54
25	LV	102/107 (95%)	102 (100%)	0	100	100
26	LW	84/126 (67%)	80 (95%)	4 (5%)	23	40
27	LX	106/133 (80%)	105 (99%)	1 (1%)	70	85
28	LY	122/135 (90%)	121 (99%)	1 (1%)	73	86
29	LZ	117/118 (99%)	115 (98%)	2 (2%)	53	74
30	La	119/120 (99%)	117 (98%)	2 (2%)	53	74
31	Lb	84/125 (67%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Lc	83/97 (86%)	82 (99%)	1 (1%)	63	81
33	Ld	98/110 (89%)	97 (99%)	1 (1%)	68	84
34	Le	115/121 (95%)	113 (98%)	2 (2%)	53	74
35	Lf	88/89 (99%)	88 (100%)	0	100	100
36	Lg	96/100 (96%)	95 (99%)	1 (1%)	68	84
37	Lh	109/110 (99%)	107 (98%)	2 (2%)	51	73
38	Li	86/89 (97%)	82 (95%)	4 (5%)	23	41
39	Lk	63/65 (97%)	61 (97%)	2 (3%)	34	56
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	69
42	Ln	24/24 (100%)	24 (100%)	0	100	100
43	Lo	93/93 (100%)	90 (97%)	3 (3%)	34	56
44	Lp	73/75 (97%)	72 (99%)	1 (1%)	59	79
45	Lr	109/121 (90%)	107 (98%)	2 (2%)	51	73
49	SB	201/231 (87%)	197 (98%)	4 (2%)	48	70
50	SC	185/225 (82%)	179 (97%)	6 (3%)	34	56
51	SD	187/202 (93%)	177 (95%)	10 (5%)	20	36
52	SE	222/225 (99%)	221 (100%)	1 (0%)	81	91
53	SF	154/170 (91%)	152 (99%)	2 (1%)	61	80
54	SG	182/218 (84%)	178 (98%)	4 (2%)	45	67
55	SH	164/174 (94%)	161 (98%)	3 (2%)	51	73
56	SI	178/180 (99%)	175 (98%)	3 (2%)	53	74
57	SJ	147/168 (88%)	144 (98%)	3 (2%)	48	70
58	SK	86/136 (63%)	84 (98%)	2 (2%)	44	66
59	SL	129/142 (91%)	127 (98%)	2 (2%)	55	76
60	SM	69/108 (64%)	63 (91%)	6 (9%)	9	16
61	SN	130/131 (99%)	125 (96%)	5 (4%)	29	49
62	SO	105/119 (88%)	101 (96%)	4 (4%)	29	49
63	SP	116/130 (89%)	113 (97%)	3 (3%)	40	63
64	SQ	116/121 (96%)	112 (97%)	4 (3%)	32	54
65	SR	120/122 (98%)	115 (96%)	5 (4%)	26	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	SS	128/132 (97%)	125 (98%)	3 (2%)	44	66
67	ST	114/115 (99%)	113 (99%)	1 (1%)	70	85
68	SU	93/107 (87%)	89 (96%)	4 (4%)	26	44
69	SV	67/67 (100%)	65 (97%)	2 (3%)	36	58
70	SW	112/113 (99%)	107 (96%)	5 (4%)	24	42
71	SY	106/115 (92%)	102 (96%)	4 (4%)	29	49
72	SZ	75/103 (73%)	74 (99%)	1 (1%)	61	80
73	Sa	86/98 (88%)	84 (98%)	2 (2%)	44	66
74	Sb	75/76 (99%)	72 (96%)	3 (4%)	28	47
75	Sc	56/62 (90%)	54 (96%)	2 (4%)	31	52
76	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	45
77	Se	40/104 (38%)	39 (98%)	1 (2%)	42	64
78	Sf	50/140 (36%)	48 (96%)	2 (4%)	28	47
79	Sg	269/275 (98%)	258 (96%)	11 (4%)	27	46
80	LA	192/198 (97%)	167 (87%)	25 (13%)	4	5
81	SA	181/242 (75%)	176 (97%)	5 (3%)	38	60
82	SX	111/114 (97%)	105 (95%)	6 (5%)	20	35
83	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	79
All	All	9654/10849 (89%)	9421 (98%)	233 (2%)	43	65

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	LB	61	ASP
6	LB	194	LEU
6	LB	362	LYS
6	LB	382	MET
7	LC	170	LEU
8	LD	109	LEU
8	LD	124	GLU
8	LD	126	THR
8	LD	163	LEU
8	LD	187	SER
8	LD	230	SER
8	LD	232	THR
8	LD	242	LYS

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Mol	Chain	Res	Type
9	LE	44	CYS
9	LE	91	THR
9	LE	93	THR
9	LE	106	VAL
9	LE	143	SER
9	LE	198	SER
10	LF	33	LEU
11	LG	43	GLN
11	LG	201	THR
11	LG	222	ILE
11	LG	253	LEU
11	LG	255	LYS
12	LH	51	LYS
12	LH	143	GLU
13	LI	32	ARG
13	LI	48	LEU
13	LI	74	LYS
13	LI	113	THR
13	LI	125	THR
13	LI	197	VAL
13	LI	202	SER
14	LJ	20	LEU
14	LJ	39	VAL
14	LJ	98	ASN
14	LJ	102	THR
15	LL	111	GLN
15	LL	142	GLU
15	LL	164	GLU
16	LM	7	VAL
17	LN	155	VAL
17	LN	169	ARG
18	LO	183	LYS
18	LO	203	VAL
19	LP	2	VAL
20	LQ	82	VAL
21	LR	63	CYS
21	LR	111	GLU
22	LS	48	VAL
23	LT	45	MET
23	LT	76	VAL
24	LU	22	THR
24	LU	33	ILE

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Mol	Chain	Res	Type
24	LU	66	SER
26	LW	4	GLU
26	LW	48	GLN
26	LW	72	THR
26	LW	76	VAL
27	LX	118	ASP
28	LY	46	SER
29	LZ	30	ASP
29	LZ	34	SER
30	La	93	ASN
30	La	119	LYS
32	Lc	106	ARG
33	Ld	119	THR
34	Le	87	VAL
34	Le	117	GLN
36	Lg	43	LYS
37	Lh	44	LEU
37	Lh	97	LYS
38	Li	11	LEU
38	Li	18	THR
38	Li	22	SER
38	Li	81	ILE
39	Lk	23	VAL
39	Lk	30	ASP
41	Lm	82	LEU
43	Lo	27	LYS
43	Lo	79	SER
43	Lo	96	ASP
44	Lp	38	THR
45	Lr	5	LEU
45	Lr	9	VAL
49	SB	9	LEU
49	SB	86	LEU
49	SB	91	VAL
49	SB	232	HIS
50	SC	162	ILE
50	SC	206	SER
50	SC	248	TYR
50	SC	270	THR
50	SC	275	LYS
50	SC	276	THR
51	SD	3	VAL

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Mol	Chain	Res	Type
51	SD	32	ASP
51	SD	53	THR
51	SD	58	VAL
51	SD	72	VAL
51	SD	83	SER
51	SD	93	THR
51	SD	142	LEU
51	SD	179	GLN
51	SD	221	THR
52	SE	19	MET
53	SF	33	ILE
53	SF	34	SER
54	SG	112	VAL
54	SG	127	THR
54	SG	149	LYS
54	SG	184	VAL
55	SH	8	ILE
55	SH	36	LEU
55	SH	83	LEU
56	SI	46	VAL
56	SI	48	VAL
56	SI	119	LEU
57	SJ	104	ASP
57	SJ	112	THR
57	SJ	148	ILE
58	SK	40	VAL
58	SK	90	VAL
59	SL	42	LEU
59	SL	66	VAL
60	SM	14	VAL
60	SM	26	LEU
60	SM	49	LEU
60	SM	54	SER
60	SM	76	LEU
60	SM	110	VAL
61	SN	30	SER
61	SN	53	ILE
61	SN	131	THR
61	SN	140	LYS
61	SN	145	THR
62	SO	26	ASN
62	SO	113	GLN

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Mol	Chain	Res	Type
62	SO	122	SER
62	SO	143	LYS
63	SP	24	GLN
63	SP	130	ARG
63	SP	133	ILE
64	SQ	46	THR
64	SQ	52	LEU
64	SQ	72	VAL
64	SQ	129	SER
65	SR	38	ILE
65	SR	98	VAL
65	SR	99	ASP
65	SR	103	LYS
65	SR	130	THR
66	SS	60	THR
66	SS	116	LYS
66	SS	142	ARG
67	ST	98	SER
68	SU	17	ILE
68	SU	25	THR
68	SU	49	LYS
68	SU	97	ILE
69	SV	23	ILE
69	SV	82	ASN
70	SW	11	LEU
70	SW	30	CYS
70	SW	65	LEU
70	SW	105	THR
70	SW	121	THR
71	SY	26	ASP
71	SY	30	PRO
71	SY	32	LYS
71	SY	85	ASN
72	SZ	58	LEU
73	Sa	46	GLU
73	Sa	60	ASP
74	Sb	61	THR
74	Sb	62	VAL
74	Sb	63	LEU
75	Sc	17	VAL
75	Sc	23	SER
76	Sd	25	SER

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Mol	Chain	Res	Type
76	Sd	36	LEU
77	Se	117	VAL
78	Sf	93	HIS
78	Sf	130	VAL
79	Sg	10	THR
79	Sg	24	THR
79	Sg	50	THR
79	Sg	107	ASP
79	Sg	111	VAL
79	Sg	141	THR
79	Sg	142	VAL
79	Sg	179	LEU
79	Sg	192	THR
79	Sg	303	THR
79	Sg	312	VAL
80	LA	28	ARG
80	LA	32	VAL
80	LA	49	ILE
80	LA	68	ARG
80	LA	75	LEU
80	LA	77	ILE
80	LA	86	GLN
80	LA	92	LYS
80	LA	93	LYS
80	LA	102	LEU
80	LA	142	GLU
80	LA	154	SER
80	LA	159	SER
80	LA	175	ILE
80	LA	179	ILE
80	LA	180	LEU
80	LA	181	LYS
80	LA	208	GLU
80	LA	242	ARG
80	LA	245[A]	ARG
80	LA	245[B]	ARG
80	LA	247	ARG
80	LA	249	THR
80	LA	250	LYS
80	LA	251	THR
81	SA	31	ASP
81	SA	43	SER

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Mol	Chain	Res	Type
81	SA	76	VAL
81	SA	87	VAL
81	SA	151	ASP
82	SX	29	LYS
82	SX	60	LYS
82	SX	61	GLN
82	SX	105	PHE
82	SX	123	VAL
82	SX	137	LYS
83	Lj	36	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
6	LB	289	GLN
6	LB	328	ASN
6	LB	376	HIS
7	LC	21	ASN
7	LC	43	ASN
7	LC	310	HIS
8	LD	191	ASN
8	LD	225	GLN
8	LD	250	ASN
9	LE	266	GLN
9	LE	268	GLN
10	LF	119	ASN
11	LG	100	HIS
11	LG	153	GLN
12	LH	102	ASN
12	LH	116	ASN
12	LH	138	GLN
13	LI	59	GLN
13	LI	73	ASN
14	LJ	65	ASN
16	LM	48	GLN
16	LM	66	HIS
17	LN	87	HIS
18	LO	150	GLN
18	LO	167	HIS
19	LP	56	GLN
19	LP	133	HIS
20	LQ	21	GLN

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Mol	Chain	Res	Type
20	LQ	160	HIS
21	LR	34	ASN
21	LR	40	GLN
27	LX	125	ASN
28	LY	20	ASN
28	LY	72	GLN
28	LY	86	GLN
28	LY	96	HIS
29	LZ	78	ASN
33	Ld	34	HIS
33	Ld	116	ASN
34	Le	52	GLN
35	Lf	20	ASN
35	Lf	99	HIS
36	Lg	112	GLN
37	Lh	30	GLN
38	Li	15	HIS
40	Ll	4	HIS
40	Ll	33	ASN
45	Lr	36	ASN
49	SB	118	GLN
49	SB	179	ASN
50	SC	267	GLN
51	SD	145	GLN
51	SD	179	GLN
51	SD	226	GLN
52	SE	157	ASN
52	SE	197	ASN
54	SG	56	ASN
54	SG	70	HIS
54	SG	81	HIS
54	SG	177	GLN
55	SH	25	GLN
56	SI	7	ASN
56	SI	52	ASN
57	SJ	132	GLN
57	SJ	154	GLN
58	SK	66	HIS
59	SL	94	HIS
61	SN	13	GLN
61	SN	58	HIS
63	SP	137	HIS

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Mol	Chain	Res	Type
65	SR	121	GLN
67	ST	63	HIS
67	ST	83	GLN
67	ST	85	ASN
67	ST	105	GLN
67	ST	117	GLN
67	ST	126	GLN
69	SV	35	ASN
70	SW	70	ASN
71	SY	89	HIS
72	SZ	106	GLN
73	Sa	43	ASN
74	Sb	9	HIS
74	Sb	51	GLN
77	Se	89	GLN
79	Sg	20	GLN
79	Sg	159	ASN
80	LA	22	HIS
83	Lj	66	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	At	66/77 (85%)	25 (37%)	0
2	Et	48/75 (64%)	13 (27%)	0
3	L5	3437/5069 (67%)	425 (12%)	8 (0%)
4	L7	118/120 (98%)	11 (9%)	1 (0%)
46	Mr	6/7 (85%)	2 (33%)	0
47	Pt	70/76 (92%)	19 (27%)	0
48	S2	1607/1869 (85%)	350 (21%)	28 (1%)
5	L8	155/156 (99%)	27 (17%)	2 (1%)
All	All	5507/7449 (73%)	872 (15%)	39 (0%)

All (872) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	At	2	G
1	At	5	G
1	At	7	U
1	At	8	U
1	At	9	A

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Mol	Chain	Res	Type
1	At	10	G
1	At	11	U
1	At	12	U
1	At	18	G
1	At	22	G
1	At	23	A
1	At	30	U
1	At	36	U
1	At	37	A
1	At	38	A
1	At	44	A
1	At	45	G
1	At	46	G
1	At	47	U
1	At	48	C
1	At	54	U
1	At	61	C
1	At	73	A
1	At	74	C
1	At	75	C
2	Et	9	U
2	Et	10	G
2	Et	13	G
2	Et	14	C
2	Et	25	U
2	Et	28	U
2	Et	42	A
2	Et	46	G
2	Et	49	G
2	Et	53	G
2	Et	63	A
2	Et	67	U
2	Et	76	A
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	73	A
3	L5	85	G
3	L5	91	G

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Mol	Chain	Res	Type
3	L5	98	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	122	U
3	L5	132	G
3	L5	134	G
3	L5	136	C
3	L5	141	C
3	L5	142	G
3	L5	159	C
3	L5	171	U
3	L5	172	C
3	L5	179	G
3	L5	180	C
3	L5	181	C
3	L5	200	U
3	L5	209	U
3	L5	210	C
3	L5	218	A
3	L5	219	G
3	L5	233	U
3	L5	234	G
3	L5	253	G
3	L5	257	C
3	L5	266	C
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	387	G
3	L5	408	A
3	L5	410	A
3	L5	412	G
3	L5	413	G
3	L5	432	U
3	L5	440	U
3	L5	451	C
3	L5	453	G

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Mol	Chain	Res	Type
3	L5	454	U
3	L5	461	G
3	L5	464	G
3	L5	467	U
3	L5	483	G
3	L5	484	U
3	L5	485	C
3	L5	489	C
3	L5	509	A
3	L5	510	U
3	L5	663	G
3	L5	669	C
3	L5	670	G
3	L5	686	A
3	L5	692	A
3	L5	696	C
3	L5	697	G
3	L5	704	C
3	L5	705	G
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	740	G
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	929	A
3	L5	932	A
3	L5	933	G
3	L5	936	C
3	L5	943	A
3	L5	944	A
3	L5	945	U
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	964	A
3	L5	965	G
3	L5	966	A
3	L5	968	C

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Mol	Chain	Res	Type
3	L5	969	C
3	L5	1065	G
3	L5	1072	C
3	L5	1094	G
3	L5	1100	U
3	L5	1169	G
3	L5	1170	G
3	L5	1187	G
3	L5	1199	G
3	L5	1210	C
3	L5	1211	G
3	L5	1215	C
3	L5	1216	C
3	L5	1241	C
3	L5	1266	G
3	L5	1270	A
3	L5	1272	C
3	L5	1273	G
3	L5	1279	A
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1302	U
3	L5	1303	A
3	L5	1304	C
3	L5	1313	C
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1387	A
3	L5	1397	A
3	L5	1398	A
3	L5	1403	G
3	L5	1408	G
3	L5	1411	C
3	L5	1420	A
3	L5	1439	C
3	L5	1443	A

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Mol	Chain	Res	Type
3	L5	1444	G
3	L5	1446	C
3	L5	1448	G
3	L5	1498	G
3	L5	1502	G
3	L5	1534	A2M
3	L5	1535	C
3	L5	1547	A
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1614	C
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1638	A
3	L5	1640	C
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1694	C
3	L5	1697	G
3	L5	1698	C
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1707	C
3	L5	1708	G
3	L5	1734	G
3	L5	1750	G
3	L5	1787	A
3	L5	1789	C
3	L5	1804	A
3	L5	1821	G
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G

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Mol	Chain	Res	Type
3	L5	1855	G
3	L5	1869	G
3	L5	1897	A
3	L5	1918	U
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1931	C
3	L5	1932	A
3	L5	1940	G
3	L5	1948	G
3	L5	1966	C
3	L5	2019	C
3	L5	2024	G
3	L5	2025	A
3	L5	2026	A
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2084	C
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2096	G
3	L5	2098	G
3	L5	2099	G
3	L5	2102	G
3	L5	2103	G
3	L5	2106	G
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2314	G
3	L5	2333	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2395	A

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Mol	Chain	Res	Type
3	L5	2397	G
3	L5	2421	G
3	L5	2450	G
3	L5	2453	A
3	L5	2469	C
3	L5	2470	C
3	L5	2471	G
3	L5	2474	G
3	L5	2475	G
3	L5	2478	C
3	L5	2483	G
3	L5	2503	G
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2513	A
3	L5	2519	U
3	L5	2520	C
3	L5	2554	U
3	L5	2573	A
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2601	A
3	L5	2627	C
3	L5	2638	G
3	L5	2647	A
3	L5	2653	C
3	L5	2660	A
3	L5	2662	G
3	L5	2669	C
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2708	U
3	L5	2710	C
3	L5	2711	G
3	L5	2735	G
3	L5	2739	C
3	L5	2743	A
3	L5	2761	U

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Mol	Chain	Res	Type
3	L5	2764	A
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2798	A
3	L5	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2855	G
3	L5	2877	G
3	L5	2899	C
3	L5	2902	G
3	L5	3597	G
3	L5	3615	G
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3648	A
3	L5	3662	A
3	L5	3673	C
3	L5	3712	A
3	L5	3723	A
3	L5	3748	A
3	L5	3753	G
3	L5	3776	G
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3785	A2M
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3851	PSU
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G

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Mol	Chain	Res	Type
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3948	C
3	L5	4076	G
3	L5	4096	C
3	L5	4097	G
3	L5	4098	A
3	L5	4119	C
3	L5	4121	G
3	L5	4122	G
3	L5	4127	A
3	L5	4135	G
3	L5	4150	G
3	L5	4158	C
3	L5	4162	C
3	L5	4163	U
3	L5	4164	C
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4222	G
3	L5	4229	U
3	L5	4233	A
3	L5	4251	A
3	L5	4254	G
3	L5	4266	G
3	L5	4268	A
3	L5	4273	A
3	L5	4281	A
3	L5	4291	G
3	L5	4304	A
3	L5	4305	G
3	L5	4314	C
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A

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Mol	Chain	Res	Type
3	L5	4373	G
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4415	A
3	L5	4422	A
3	L5	4440	G
3	L5	4448	G
3	L5	4464	A
3	L5	4465	U
3	L5	4475	G
3	L5	4500	PSU
3	L5	4501	U
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4524	G
3	L5	4532	PSU
3	L5	4548	A
3	L5	4560	C
3	L5	4567	G
3	L5	4569	PSU
3	L5	4570	G
3	L5	4573	G
3	L5	4575	G
3	L5	4584	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4636	U
3	L5	4637	OMG
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4720	C
3	L5	4730	C

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Mol	Chain	Res	Type
3	L5	4740	G
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4862	G
3	L5	4870	G
3	L5	4871	C
3	L5	4882	U
3	L5	4883	C
3	L5	4895	C
3	L5	4900	C
3	L5	4901	G
3	L5	4903	G
3	L5	4910	G
3	L5	4912	G
3	L5	4913	G
3	L5	4928	C
3	L5	4938	A
3	L5	4943	A
3	L5	4976	U
3	L5	4988	U
3	L5	4993	G
3	L5	5017	G
3	L5	5041	G
3	L5	5050	C
3	L5	5053	U
3	L5	5054	C
3	L5	5055	G
3	L5	5058	A
3	L5	5069	U
4	L7	10	C
4	L7	33	U
4	L7	53	U
4	L7	54	A

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Mol	Chain	Res	Type
4	L7	63	C
4	L7	64	G
4	L7	76	U
4	L7	97	G
4	L7	100	A
4	L7	110	G
4	L7	117	G
5	L8	23	C
5	L8	34	U
5	L8	35	C
5	L8	38	U
5	L8	39	G
5	L8	59	A
5	L8	61	A
5	L8	62	A
5	L8	63	U
5	L8	77	A
5	L8	79	G
5	L8	80	A
5	L8	84	A
5	L8	86	U
5	L8	87	G
5	L8	103	A
5	L8	104	A
5	L8	105	C
5	L8	109	C
5	L8	110	U
5	L8	114	G
5	L8	123	U
5	L8	126	C
5	L8	127	U
5	L8	147	G
5	L8	150	C
5	L8	153	C
46	Mr	5	A
46	Mr	7	C
47	Pt	7	G
47	Pt	8	U
47	Pt	9	1MG
47	Pt	13	C
47	Pt	17	G
47	Pt	18	G

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Mol	Chain	Res	Type
47	Pt	22	A
47	Pt	42	G
47	Pt	46	A
47	Pt	47	U
47	Pt	48	U
47	Pt	49	C
47	Pt	52	G
47	Pt	59	C
47	Pt	63	U
47	Pt	69	G
47	Pt	70	C
47	Pt	74	C
47	Pt	76	A
48	S2	3	C
48	S2	4	C
48	S2	17	C
48	S2	23	G
48	S2	33	G
48	S2	41	G
48	S2	46	A
48	S2	56	G
48	S2	59	U
48	S2	64	A
48	S2	65	C
48	S2	67	C
48	S2	68	A
48	S2	77	A
48	S2	79	A
48	S2	80	G
48	S2	82	G
48	S2	92	A
48	S2	99	A2M
48	S2	103	A
48	S2	110	U
48	S2	113	G
48	S2	115	U
48	S2	122	G
48	S2	126	G
48	S2	127	C
48	S2	129	C
48	S2	142	C
48	S2	143	U

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Mol	Chain	Res	Type
48	S2	147	A
48	S2	155	G
48	S2	160	U
48	S2	162	C
48	S2	163	U
48	S2	168	C
48	S2	173	A
48	S2	175	A
48	S2	184	G
48	S2	204	G
48	S2	205	G
48	S2	207	G
48	S2	212	C
48	S2	213	G
48	S2	214	U
48	S2	215	G
48	S2	295	C
48	S2	302	A
48	S2	309	G
48	S2	312	G
48	S2	313	A
48	S2	319	C
48	S2	323	C
48	S2	324	C
48	S2	327	G
48	S2	328	U
48	S2	335	G
48	S2	347	G
48	S2	351	G
48	S2	362	C
48	S2	364	A
48	S2	368	U
48	S2	369	C
48	S2	370	G
48	S2	377	G
48	S2	385	G
48	S2	386	C
48	S2	391	C
48	S2	400	C
48	S2	407	G
48	S2	409	C
48	S2	417	C

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Mol	Chain	Res	Type
48	S2	428	OMU
48	S2	429	C
48	S2	437	G
48	S2	438	G
48	S2	448	A
48	S2	449	A
48	S2	450	C
48	S2	465	A
48	S2	466	G
48	S2	467	G
48	S2	471	G
48	S2	472	C
48	S2	474	G
48	S2	476	A
48	S2	482	G
48	S2	487	U
48	S2	489	A
48	S2	492	C
48	S2	493	A
48	S2	496	C
48	S2	500	A
48	S2	501	C
48	S2	508	A
48	S2	512	A2M
48	S2	516	A
48	S2	517	OMC
48	S2	518	G
48	S2	523	A
48	S2	525	A
48	S2	532	C
48	S2	533	A
48	S2	534	G
48	S2	552	G
48	S2	553	U
48	S2	554	A
48	S2	555	A
48	S2	559	G
48	S2	563	G
48	S2	564	A
48	S2	569	A
48	S2	576	A2M
48	S2	587	A

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Mol	Chain	Res	Type
48	S2	589	G
48	S2	590	A
48	S2	591	U
48	S2	593	C
48	S2	594	A
48	S2	598	G
48	S2	603	C
48	S2	606	G
48	S2	608	C
48	S2	614	C
48	S2	617	G
48	S2	620	G
48	S2	621	C
48	S2	628	A
48	S2	629	A
48	S2	632	C
48	S2	643	A
48	S2	644	OMG
48	S2	655	A
48	S2	660	C
48	S2	663	C
48	S2	664	A
48	S2	668	A2M
48	S2	669	A
48	S2	670	A
48	S2	671	A
48	S2	672	A
48	S2	673	G
48	S2	683	OMG
48	S2	688	U
48	S2	797	C
48	S2	799	U
48	S2	810	A
48	S2	811	A
48	S2	812	A
48	S2	821	G
48	S2	822	PSU
48	S2	823	U
48	S2	824	C
48	S2	827	A
48	S2	830	A
48	S2	831	G

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Mol	Chain	Res	Type
48	S2	847	A
48	S2	861	A
48	S2	868	G
48	S2	869	A
48	S2	870	A
48	S2	871	U
48	S2	872	A
48	S2	903	A
48	S2	905	C
48	S2	913	A
48	S2	917	U
48	S2	918	PSU
48	S2	919	A
48	S2	920	A
48	S2	922	A
48	S2	930	C
48	S2	933	G
48	S2	943	U
48	S2	971	G
48	S2	977	C
48	S2	985	G
48	S2	990	A
48	S2	992	A
48	S2	1002	U
48	S2	1017	U
48	S2	1023	A
48	S2	1027	A
48	S2	1061	U
48	S2	1062	A
48	S2	1064	C
48	S2	1074	C
48	S2	1080	A
48	S2	1083	A
48	S2	1085	C
48	S2	1087	A
48	S2	1100	A
48	S2	1105	G
48	S2	1107	G
48	S2	1111	U
48	S2	1115	U
48	S2	1121	G
48	S2	1123	C

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Mol	Chain	Res	Type
48	S2	1133	A
48	S2	1138	C
48	S2	1151	G
48	S2	1153	C
48	S2	1154	U
48	S2	1157	G
48	S2	1165	G
48	S2	1166	G
48	S2	1168	G
48	S2	1171	G
48	S2	1183	A
48	S2	1188	A
48	S2	1195	A
48	S2	1200	A
48	S2	1203	G
48	S2	1207	G
48	S2	1208	A
48	S2	1212	G
48	S2	1215	C
48	S2	1221	G
48	S2	1224	G
48	S2	1242	U
48	S2	1243	PSU
48	S2	1251	A
48	S2	1253	A
48	S2	1256	G
48	S2	1257	G
48	S2	1259	A
48	S2	1265	A
48	S2	1271	C
48	S2	1273	C
48	S2	1274	G
48	S2	1275	G
48	S2	1277	C
48	S2	1285	G
48	S2	1286	G
48	S2	1287	A
48	S2	1292	C
48	S2	1301	A
48	S2	1302	G
48	S2	1303	C
48	S2	1308	U

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Mol	Chain	Res	Type
48	S2	1312	G
48	S2	1313	A
48	S2	1314	U
48	S2	1315	U
48	S2	1322	G
48	S2	1324	G
48	S2	1333	U
48	S2	1342	U
48	S2	1345	G
48	S2	1348	G
48	S2	1358	U
48	S2	1363	C
48	S2	1371	U
48	S2	1372	U
48	S2	1373	C
48	S2	1375	G
48	S2	1378	A
48	S2	1382	A
48	S2	1384	C
48	S2	1398	G
48	S2	1401	A
48	S2	1402	A
48	S2	1418	C
48	S2	1422	G
48	S2	1423	C
48	S2	1424	G
48	S2	1428	G
48	S2	1442	OMU
48	S2	1446	A
48	S2	1452	A
48	S2	1454	A
48	S2	1462	U
48	S2	1463	U
48	S2	1466	G
48	S2	1477	U
48	S2	1479	G
48	S2	1480	A
48	S2	1487	A
48	S2	1489	A
48	S2	1490	OMG
48	S2	1494	U
48	S2	1495	G

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Mol	Chain	Res	Type
48	S2	1498	A
48	S2	1506	A
48	S2	1507	G
48	S2	1508	A
48	S2	1509	U
48	S2	1520	G
48	S2	1521	C
48	S2	1522	A
48	S2	1533	A
48	S2	1547	C
48	S2	1548	G
48	S2	1549	U
48	S2	1553	C
48	S2	1556	A
48	S2	1557	C
48	S2	1558	C
48	S2	1560	U
48	S2	1564	C
48	S2	1565	C
48	S2	1578	U
48	S2	1579	A
48	S2	1580	A
48	S2	1585	U
48	S2	1586	U
48	S2	1587	G
48	S2	1588	A
48	S2	1594	A
48	S2	1601	A
48	S2	1602	U
48	S2	1621	U
48	S2	1623	A
48	S2	1639	G7M
48	S2	1641	A
48	S2	1648	G
48	S2	1654	G
48	S2	1661	A
48	S2	1664	A
48	S2	1665	G
48	S2	1671	G
48	S2	1679	A
48	S2	1680	G
48	S2	1683	C

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Mol	Chain	Res	Type
48	S2	1686	G
48	S2	1698	C
48	S2	1700	C
48	S2	1721	U
48	S2	1722	G
48	S2	1727	G
48	S2	1742	C
48	S2	1744	G
48	S2	1745	A
48	S2	1748	G
48	S2	1798	C
48	S2	1800	A
48	S2	1819	A
48	S2	1824	A
48	S2	1826	G
48	S2	1829	G
48	S2	1835	A
48	S2	1836	G
48	S2	1837	G
48	S2	1838	U
48	S2	1849	G
48	S2	1851	MA6
48	S2	1861	G
48	S2	1862	G
48	S2	1863	A
48	S2	1864	U
48	S2	1865	C

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	170	C
3	L5	218	A
3	L5	739	G
3	L5	1410	U
3	L5	1590	C
3	L5	1625	OMG
3	L5	1633	G
3	L5	4699	U
4	L7	109	U
5	L8	83	C
5	L8	94	G

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Mol	Chain	Res	Type
48	S2	3	C
48	S2	64	A
48	S2	214	U
48	S2	293	C
48	S2	312	G
48	S2	500	A
48	S2	563	G
48	S2	593	C
48	S2	620	G
48	S2	628	A
48	S2	670	A
48	S2	861	A
48	S2	868	G
48	S2	1061	U
48	S2	1165	G
48	S2	1253	A
48	S2	1264	C
48	S2	1312	G
48	S2	1344	A
48	S2	1462	U
48	S2	1493	C
48	S2	1586	U
48	S2	1646	C
48	S2	1679	A
48	S2	1700	C
48	S2	1744	G
48	S2	1835	A
48	S2	1837	G

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

216 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
3	PSU	L5	4442	3	18,21,22	4.41	7 (38%)	22,30,33	1.93	6 (27%)
48	A2M	S2	576	48	22,25,26	0.18	0	31,36,39	0.43	0
47	M2G	Pt	26	47	24,27,28	0.41	0	35,40,43	0.48	0
3	OMG	L5	4228	3	23,26,27	2.38	9 (39%)	33,38,41	2.04	10 (30%)
48	PSU	S2	1445	48	18,21,22	0.87	1 (5%)	22,30,33	0.57	0
3	OMU	L5	4227	3	19,22,23	2.97	8 (42%)	26,31,34	1.76	5 (19%)
3	PSU	L5	1536	3	18,21,22	4.39	7 (38%)	22,30,33	1.78	5 (22%)
3	OMC	L5	3869	3	19,22,23	2.90	8 (42%)	26,31,34	0.71	0
3	PSU	L5	3770	3	18,21,22	4.26	8 (44%)	22,30,33	1.83	5 (22%)
48	OMU	S2	172	48	19,22,23	0.22	0	26,31,34	0.58	0
3	OMU	L5	4306	3	19,22,23	2.95	8 (42%)	26,31,34	1.69	5 (19%)
5	OMG	L8	75	5	23,26,27	0.30	0	33,38,41	0.41	0
3	A2M	L5	400	3	22,25,26	3.44	10 (45%)	31,36,39	2.35	10 (32%)
3	UY1	L5	3818	85,3,84	19,22,23	4.01	8 (42%)	22,31,34	1.95	5 (22%)
48	PSU	S2	1625	48	18,21,22	0.85	1 (5%)	22,30,33	0.56	0
48	OMC	S2	1703	48	19,22,23	0.30	0	26,31,34	0.49	0
3	A2M	L5	1871	3,85	22,25,26	3.46	10 (45%)	31,36,39	2.41	10 (32%)
3	A2M	L5	3785	3	22,25,26	3.42	10 (45%)	31,36,39	2.51	11 (35%)
3	OMU	L5	2415	3	19,22,23	2.98	8 (42%)	26,31,34	1.71	4 (15%)
3	OMG	L5	2364	3	23,26,27	2.38	7 (30%)	33,38,41	2.03	10 (30%)
3	UR3	L5	4530	3	19,22,23	2.53	6 (31%)	26,32,35	1.27	1 (3%)
3	OMC	L5	3841	3	19,22,23	2.91	8 (42%)	26,31,34	0.75	0
3	PSU	L5	4689	3	18,21,22	4.38	7 (38%)	22,30,33	1.83	5 (22%)
3	OMC	L5	3808	3	19,22,23	2.88	8 (42%)	26,31,34	0.71	0
3	PSU	L5	5001	3	18,21,22	4.45	7 (38%)	22,30,33	1.70	4 (18%)
48	OMG	S2	644	48	23,26,27	0.28	0	33,38,41	0.47	0
3	PSU	L5	4628	3	18,21,22	4.33	7 (38%)	22,30,33	1.76	5 (22%)
3	OMG	L5	4623	3	23,26,27	2.39	9 (39%)	33,38,41	2.07	10 (30%)
3	OMC	L5	3701	3,84	19,22,23	2.86	8 (42%)	26,31,34	0.81	0
48	PSU	S2	1081	48	18,21,22	0.88	1 (5%)	22,30,33	0.84	1 (4%)
3	PSU	L5	4500	3,84	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
3	OMC	L5	4536	3	19,22,23	2.88	8 (42%)	26,31,34	0.75	0
47	1MG	Pt	9	47	22,26,27	0.58	0	33,39,42	0.61	0
3	OMU	L5	4620	3	19,22,23	2.86	8 (42%)	26,31,34	1.66	5 (19%)
48	A2M	S2	468	48	22,25,26	0.17	0	31,36,39	0.59	0
48	B8N	S2	1248	48	24,29,30	0.41	0	29,42,45	0.50	0
48	OMU	S2	1804	48	19,22,23	0.22	0	26,31,34	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	4AC	S2	1842	48	21,24,25	0.42	0	29,34,37	0.38	0
3	OMG	L5	3627	3	23,26,27	2.38	9 (39%)	33,38,41	2.09	9 (27%)
3	PSU	L5	4420	3	18,21,22	4.48	9 (50%)	22,30,33	1.69	4 (18%)
3	PSU	L5	3695	3,84	18,21,22	4.39	7 (38%)	22,30,33	1.82	5 (22%)
3	PSU	L5	4431	3	18,21,22	4.41	7 (38%)	22,30,33	1.85	5 (22%)
48	PSU	S2	918	48	18,21,22	0.86	1 (5%)	22,30,33	0.90	1 (4%)
3	A2M	L5	1524	3	22,25,26	3.44	10 (45%)	31,36,39	2.47	12 (38%)
3	PSU	L5	3758	3	18,21,22	4.32	7 (38%)	22,30,33	1.78	5 (22%)
3	A2M	L5	3830	3	22,25,26	3.44	10 (45%)	31,36,39	2.38	11 (35%)
3	PSU	L5	4569	3,84	18,21,22	4.43	8 (44%)	22,30,33	1.76	5 (22%)
3	PSU	L5	4353	3,84	18,21,22	4.42	7 (38%)	22,30,33	1.83	5 (22%)
48	PSU	S2	1174	86,84,48	18,21,22	0.88	1 (5%)	22,30,33	0.63	0
3	A2M	L5	398	3	22,25,26	3.44	9 (40%)	31,36,39	2.46	11 (35%)
48	OMU	S2	627	48	19,22,23	0.22	0	26,31,34	0.42	0
3	OMC	L5	2351	3	19,22,23	2.87	8 (42%)	26,31,34	0.81	0
48	PSU	S2	1004	48	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
3	A2M	L5	2363	3,85	22,25,26	3.47	10 (45%)	31,36,39	2.37	10 (32%)
3	OMC	L5	1340	3	19,22,23	2.82	8 (42%)	26,31,34	0.68	0
3	A2M	L5	4590	3	22,25,26	3.47	9 (40%)	31,36,39	2.45	10 (32%)
3	5MC	L5	4447	3,84	18,22,23	3.40	7 (38%)	26,32,35	1.18	1 (3%)
3	A2M	L5	2815	3,85	22,25,26	3.44	10 (45%)	31,36,39	2.38	9 (29%)
48	OMG	S2	683	48	23,26,27	0.30	0	33,38,41	0.43	0
3	PSU	L5	3853	3,85	18,21,22	4.35	7 (38%)	22,30,33	1.73	4 (18%)
3	A2M	L5	3825	3	22,25,26	3.47	10 (45%)	31,36,39	2.36	10 (32%)
48	PSU	S2	866	48	18,21,22	0.86	1 (5%)	22,30,33	0.67	0
48	PSU	S2	1692	48	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
3	OMC	L5	2804	3	19,22,23	2.86	8 (42%)	26,31,34	0.74	0
48	OMG	S2	1447	48	23,26,27	0.30	0	33,38,41	0.42	0
3	PSU	L5	4299	3	18,21,22	4.37	7 (38%)	22,30,33	1.79	5 (22%)
3	PSU	L5	3734	3,84	18,21,22	4.44	7 (38%)	22,30,33	1.94	5 (22%)
3	OMG	L5	4499	3,1	23,26,27	0.33	0	33,38,41	0.48	0
82	HY3	SX	62	82	6,8,9	1.14	0	5,10,12	1.36	1 (20%)
3	PSU	L5	1779	3	18,21,22	4.43	7 (38%)	22,30,33	1.85	5 (22%)
48	A2M	S2	484	48	22,25,26	0.19	0	31,36,39	0.35	0
48	PSU	S2	1056	48	18,21,22	0.90	1 (5%)	22,30,33	0.68	0
48	PSU	S2	1177	48	18,21,22	0.87	1 (5%)	22,30,33	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	406	48	18,21,22	0.87	1 (5%)	22,30,33	0.55	0
80	V5N	LA	216	80	9,11,12	0.55	0	9,14,16	0.91	1 (11%)
3	OMC	L5	2365	3	19,22,23	2.85	8 (42%)	26,31,34	0.70	0
41	M3L	Lm	98	41	10,11,12	0.41	0	9,14,16	0.09	0
48	OMU	S2	121	48	19,22,23	0.21	0	26,31,34	0.51	0
48	OMC	S2	174	85,48	19,22,23	0.26	0	26,31,34	0.47	0
1	MA7	At	58	1	20,24,25	0.51	0	24,35,38	0.64	0
3	A2M	L5	3724	3	22,25,26	3.46	10 (45%)	31,36,39	2.39	10 (32%)
48	PSU	S2	34	48	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
48	A2M	S2	1383	48	22,25,26	0.17	0	31,36,39	0.45	0
5	OMU	L8	14	3,5	19,22,23	0.21	0	26,31,34	0.36	0
48	A2M	S2	99	85,48	22,25,26	0.17	0	31,36,39	0.42	0
48	OMU	S2	354	48	19,22,23	0.21	0	26,31,34	0.68	0
3	OMG	L5	4618	3	23,26,27	2.40	8 (34%)	33,38,41	2.05	10 (30%)
3	PSU	L5	4423	3	18,21,22	4.45	7 (38%)	22,30,33	1.79	5 (22%)
48	OMG	S2	1328	84,48	23,26,27	0.28	0	33,38,41	0.34	0
48	PSU	S2	1243	48	18,21,22	0.91	1 (5%)	22,30,33	1.01	1 (4%)
3	PSU	L5	1862	3	18,21,22	4.38	7 (38%)	22,30,33	1.87	5 (22%)
48	PSU	S2	686	48	18,21,22	0.86	1 (5%)	22,30,33	0.61	0
3	OMU	L5	4498	3,84	19,22,23	2.95	8 (42%)	26,31,34	1.76	5 (19%)
31	MLZ	Lb	5	84,31	8,9,10	0.78	0	4,9,11	0.72	0
3	OMG	L5	2424	3	23,26,27	2.41	8 (34%)	33,38,41	2.02	9 (27%)
3	OMC	L5	1881	3,85	19,22,23	2.89	8 (42%)	26,31,34	0.85	0
3	A2M	L5	3718	3	22,25,26	3.47	9 (40%)	31,36,39	2.25	9 (29%)
3	OMG	L5	1522	3	23,26,27	2.38	9 (39%)	33,38,41	2.11	10 (30%)
3	A2M	L5	1326	3	22,25,26	3.42	10 (45%)	31,36,39	2.42	9 (29%)
3	OMC	L5	2422	3,85	19,22,23	2.89	8 (42%)	26,31,34	0.73	0
48	OMC	S2	517	48	19,22,23	0.28	0	26,31,34	0.43	0
3	A2M	L5	1534	85,3,84	22,25,26	3.46	10 (45%)	31,36,39	2.37	10 (32%)
3	PSU	L5	1782	3	18,21,22	4.43	7 (38%)	22,30,33	1.83	5 (22%)
3	OMC	L5	2824	3	19,22,23	2.91	8 (42%)	26,31,34	0.70	0
3	PSU	L5	4296	3	18,21,22	4.40	7 (38%)	22,30,33	1.83	5 (22%)
3	OMG	L5	4370	3	23,26,27	2.36	8 (34%)	33,38,41	2.10	10 (30%)
48	PSU	S2	1239	48	18,21,22	0.85	1 (5%)	22,30,33	0.57	0
3	PSU	L5	4673	3,84	18,21,22	4.39	7 (38%)	22,30,33	1.82	5 (22%)
3	OMG	L5	4637	3,84	23,26,27	2.37	7 (30%)	33,38,41	2.01	10 (30%)
3	PSU	L5	4293	3	18,21,22	4.33	7 (38%)	22,30,33	1.67	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3920	3,85	18,21,22	4.34	7 (38%)	22,30,33	1.82	5 (22%)
48	G7M	S2	1639	48,47	23,26,27	0.66	1 (4%)	35,39,42	0.53	0
48	MA6	S2	1850	48	23,26,27	0.29	0	34,38,41	0.68	1 (2%)
3	PSU	L5	3637	3,84	18,21,22	4.36	8 (44%)	22,30,33	1.86	4 (18%)
48	OMG	S2	867	48	23,26,27	0.30	0	33,38,41	0.35	0
48	OMC	S2	1391	48	19,22,23	0.28	0	26,31,34	0.46	0
6	HIC	LB	245	6	10,11,12	1.46	1 (10%)	8,14,16	1.07	1 (12%)
3	PSU	L5	4552	3	18,21,22	4.35	7 (38%)	22,30,33	1.82	5 (22%)
48	A2M	S2	512	48	22,25,26	0.18	0	31,36,39	0.54	0
3	PSU	L5	4457	3	18,21,22	4.35	7 (38%)	22,30,33	1.87	5 (22%)
3	PSU	L5	1781	3	18,21,22	4.40	7 (38%)	22,30,33	1.77	5 (22%)
3	A2M	L5	3760	3	22,25,26	3.48	10 (45%)	31,36,39	2.51	13 (41%)
3	A2M	L5	3867	3	22,25,26	3.44	9 (40%)	31,36,39	2.39	9 (29%)
48	A2M	S2	27	85,48	22,25,26	0.17	0	31,36,39	0.44	0
48	A2M	S2	1031	48	22,25,26	0.17	0	31,36,39	0.48	0
48	PSU	S2	573	48	18,21,22	0.83	1 (5%)	22,30,33	0.71	0
46	B8H	Mr	4	47,46	19,22,23	0.23	0	22,32,35	0.31	0
48	OMU	S2	1288	48	19,22,23	0.21	0	26,31,34	0.35	0
48	PSU	S2	822	48	18,21,22	0.88	1 (5%)	22,30,33	0.87	1 (4%)
3	PSU	L5	4521	85,3,84	18,21,22	4.35	7 (38%)	22,30,33	1.85	5 (22%)
47	1MG	Pt	37	84,47	22,26,27	0.47	0	33,39,42	0.95	2 (6%)
43	MLZ	Lo	53	43	8,9,10	0.79	0	4,9,11	0.47	0
3	PSU	L5	4972	3	18,21,22	4.40	7 (38%)	22,30,33	1.80	5 (22%)
3	OMU	L5	3925	3	19,22,23	2.95	8 (42%)	26,31,34	1.79	5 (19%)
48	OMG	S2	436	48	23,26,27	0.29	0	33,38,41	0.42	0
3	OMG	L5	4494	3	23,26,27	2.38	8 (34%)	33,38,41	2.02	10 (30%)
3	PSU	L5	4579	3	18,21,22	4.37	7 (38%)	22,30,33	1.79	5 (22%)
3	OMG	L5	3744	3	23,26,27	2.39	8 (34%)	33,38,41	2.03	10 (30%)
3	OMG	L5	4392	3	23,26,27	2.39	7 (30%)	33,38,41	2.07	10 (30%)
3	PSU	L5	2632	3	18,21,22	4.43	7 (38%)	22,30,33	1.73	4 (18%)
48	OMG	S2	601	48	23,26,27	0.29	0	33,38,41	0.36	0
48	PSU	S2	1232	48	18,21,22	0.88	1 (5%)	22,30,33	0.72	0
48	PSU	S2	649	48	18,21,22	0.86	1 (5%)	22,30,33	0.69	0
48	PSU	S2	1244	48	18,21,22	0.89	1 (5%)	22,30,33	0.71	0
48	PSU	S2	119	48	18,21,22	0.86	1 (5%)	22,30,33	0.57	0
3	PSU	L5	3851	3	18,21,22	4.35	7 (38%)	22,30,33	1.82	5 (22%)
3	PSU	L5	4532	3	18,21,22	4.36	7 (38%)	22,30,33	1.79	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4576	3	18,21,22	4.39	7 (38%)	22,30,33	1.87	5 (22%)
48	OMU	S2	116	48	19,22,23	0.23	0	26,31,34	0.43	0
48	OMC	S2	462	48	19,22,23	0.26	0	26,31,34	0.39	0
48	PSU	S2	651	48	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
3	OMG	L5	3899	3	23,26,27	2.41	9 (39%)	33,38,41	2.11	10 (30%)
3	PSU	L5	1744	3,84	18,21,22	4.37	7 (38%)	22,30,33	1.81	5 (22%)
3	OMG	L5	1316	3,84	23,26,27	2.39	7 (30%)	33,38,41	2.07	10 (30%)
3	PSU	L5	1792	85,3,84	18,21,22	4.35	7 (38%)	22,30,33	1.73	5 (22%)
3	OMG	L5	2876	3	23,26,27	2.42	8 (34%)	33,38,41	2.07	10 (30%)
3	PSU	L5	4403	3	18,21,22	4.34	7 (38%)	22,30,33	1.84	6 (27%)
48	OMU	S2	1442	85,48	19,22,23	0.23	0	26,31,34	0.32	0
48	PSU	S2	814	48	18,21,22	0.88	1 (5%)	22,30,33	0.69	0
3	PSU	L5	1677	3	18,21,22	4.50	8 (44%)	22,30,33	1.90	6 (27%)
48	PSU	S2	966	48	18,21,22	0.87	1 (5%)	22,30,33	0.63	0
3	OMG	L5	3792	3	23,26,27	2.40	8 (34%)	33,38,41	1.96	9 (27%)
48	MA6	S2	1851	48	23,26,27	0.27	0	34,38,41	0.75	1 (2%)
3	1MA	L5	1322	3,85	21,25,26	2.85	6 (28%)	31,37,40	2.86	10 (32%)
3	OMG	L5	4196	3,47	23,26,27	2.35	8 (34%)	33,38,41	2.02	9 (27%)
48	OMG	S2	1490	85,48	23,26,27	0.32	0	33,38,41	0.35	0
48	PSU	S2	36	48	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
3	6MZ	L5	4220	3	22,25,26	2.45	5 (22%)	30,36,39	2.29	11 (36%)
3	OMG	L5	1625	3,84	23,26,27	2.41	8 (34%)	33,38,41	1.99	9 (27%)
3	A2M	L5	4571	3	22,25,26	3.50	10 (45%)	31,36,39	2.36	10 (32%)
5	PSU	L8	69	5	18,21,22	0.85	1 (5%)	22,30,33	0.69	0
48	A2M	S2	668	85,48	22,25,26	0.20	0	31,36,39	0.42	0
48	4AC	S2	1337	48	21,24,25	0.41	0	29,34,37	0.58	0
48	PSU	S2	1367	84,48	18,21,22	0.86	1 (5%)	22,30,33	0.69	0
3	PSU	L5	1860	3	18,21,22	4.39	7 (38%)	22,30,33	1.80	5 (22%)
48	OMG	S2	509	48	23,26,27	0.28	0	33,38,41	0.39	0
3	PSU	L5	4312	3	18,21,22	4.39	7 (38%)	22,30,33	1.88	5 (22%)
3	PSU	L5	4471	3	18,21,22	4.41	7 (38%)	22,30,33	1.81	5 (22%)
48	UY1	S2	1326	85,48	19,22,23	0.19	0	22,31,34	0.34	0
3	OMU	L5	2837	3	19,22,23	2.94	8 (42%)	26,31,34	1.76	4 (15%)
48	PSU	S2	1238	48	18,21,22	0.98	2 (11%)	22,30,33	0.82	0
48	A2M	S2	166	48	22,25,26	0.17	0	31,36,39	0.59	0
48	PSU	S2	109	48	18,21,22	0.86	1 (5%)	22,30,33	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3639	3	18,21,22	4.32	7 (38%)	22,30,33	1.81	5 (22%)
3	A2M	L5	2787	3,85	22,25,26	3.42	10 (45%)	31,36,39	2.39	11 (35%)
3	PSU	L5	3844	3	18,21,22	4.43	7 (38%)	22,30,33	1.77	5 (22%)
3	OMC	L5	4456	3	19,22,23	2.84	8 (42%)	26,31,34	0.72	0
3	PSU	L5	4361	3,84	18,21,22	4.35	7 (38%)	22,30,33	1.78	5 (22%)
3	OMC	L5	2861	3	19,22,23	2.90	8 (42%)	26,31,34	0.70	0
3	A2M	L5	2401	3	22,25,26	3.42	10 (45%)	31,36,39	2.39	10 (32%)
48	PSU	S2	681	48	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
3	PSU	L5	1683	3,84	18,21,22	4.34	7 (38%)	22,30,33	1.84	5 (22%)
3	A2M	L5	4523	3,85	22,25,26	3.43	9 (40%)	31,36,39	2.39	10 (32%)
3	OMC	L5	3887	3	19,22,23	2.89	8 (42%)	26,31,34	0.76	0
48	A2M	S2	159	48	22,25,26	0.17	0	31,36,39	0.35	0
3	PSU	L5	2508	3	18,21,22	4.37	7 (38%)	22,30,33	1.87	5 (22%)
48	PSU	S2	863	48	18,21,22	0.88	1 (5%)	22,30,33	0.54	0
48	PSU	S2	572	48	18,21,22	0.83	1 (5%)	22,30,33	0.65	0
30	V5N	La	39	30	9,11,12	2.86	2 (22%)	9,14,16	1.30	1 (11%)
48	PSU	S2	105	48	18,21,22	0.88	1 (5%)	22,30,33	0.67	0
3	PSU	L5	2839	3	18,21,22	4.36	7 (38%)	22,30,33	1.94	5 (22%)
48	6MZ	S2	1832	85,84,48	22,25,26	0.19	0	30,36,39	0.38	0
48	A2M	S2	1678	48	22,25,26	0.17	0	31,36,39	0.35	0
46	B8H	Mr	6	1,46	19,22,23	0.23	0	22,32,35	0.39	0
48	PSU	S2	218	48	18,21,22	0.85	1 (5%)	22,30,33	0.63	0
48	PSU	S2	93	48	18,21,22	0.88	1 (5%)	22,30,33	0.68	0
48	PSU	S2	815	48	18,21,22	0.84	1 (5%)	22,30,33	0.66	0
3	PSU	L5	3768	3	18,21,22	0.86	1 (5%)	22,30,33	0.64	0
3	PSU	L5	4493	3,84	18,21,22	4.41	7 (38%)	22,30,33	1.81	5 (22%)
48	OMU	S2	428	48	19,22,23	0.21	0	26,31,34	0.38	0
47	1MA	Pt	58	47	21,25,26	4.24	11 (52%)	31,37,40	1.76	6 (19%)
3	PSU	L5	3884	3	18,21,22	4.39	8 (44%)	22,30,33	1.75	4 (18%)
48	PSU	S2	1347	48	18,21,22	0.86	1 (5%)	22,30,33	0.63	0
48	PSU	S2	1643	85,48	18,21,22	0.85	1 (5%)	22,30,33	0.58	0
5	PSU	L8	55	5	18,21,22	0.84	1 (5%)	22,30,33	0.72	0
3	5MC	L5	3782	3,85	18,22,23	3.46	7 (38%)	26,32,35	1.04	2 (7%)

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
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
48	A2M	S2	576	48	-	2/9/27/28	0/3/3/3
47	M2G	Pt	26	47	-	0/11/29/30	0/3/3/3
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
48	OMU	S2	172	48	-	1/9/27/28	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	UY1	L5	3818	85,3,84	-	1/9/27/28	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
48	OMC	S2	1703	48	-	0/9/27/28	0/2/2/2
3	A2M	L5	1871	3,85	-	0/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	3/9/27/28	0/3/3/3
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	2364	3	-	0/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	644	48	-	4/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3701	3,84	-	4/9/27/28	0/2/2/2
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
3	PSU	L5	4500	3,84	-	3/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
47	1MG	Pt	9	47	-	1/7/25/26	0/3/3/3
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
48	A2M	S2	468	48	-	0/9/27/28	0/3/3/3
48	B8N	S2	1248	48	-	2/16/34/35	0/2/2/2
48	OMU	S2	1804	48	-	1/9/27/28	0/2/2/2
48	4AC	S2	1842	48	-	2/11/29/30	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4420	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3,84	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	918	48	-	1/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4569	3,84	-	2/7/25/26	0/2/2/2
3	PSU	L5	4353	3,84	-	0/7/25/26	0/2/2/2
48	PSU	S2	1174	86,84,48	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
48	OMU	S2	627	48	-	2/9/27/28	0/2/2/2
3	OMC	L5	2351	3	-	1/9/27/28	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	3,85	-	1/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	5MC	L5	4447	3,84	-	4/7/25/26	0/2/2/2
3	A2M	L5	2815	3,85	-	3/9/27/28	0/3/3/3
48	OMG	S2	683	48	-	2/9/27/28	0/3/3/3
3	PSU	L5	3853	3,85	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
48	OMG	S2	1447	48	-	2/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3,1	-	0/9/27/28	0/3/3/3
82	HY3	SX	62	82	-	0/1/12/14	0/1/1/1
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
48	A2M	S2	484	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
80	V5N	LA	216	80	-	1/9/10/12	0/1/1/1
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
41	M3L	Lm	98	41	-	3/9/10/12	-
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2
48	OMC	S2	174	85,48	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA7	At	58	1	-	3/7/21/22	0/3/3/3
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	1383	48	-	0/9/27/28	0/3/3/3
5	OMU	L8	14	3,5	-	1/9/27/28	0/2/2/2
48	A2M	S2	99	85,48	-	2/9/27/28	0/3/3/3
48	OMU	S2	354	48	-	0/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	1328	84,48	-	1/9/27/28	0/3/3/3
48	PSU	S2	1243	48	-	3/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3,84	-	0/9/27/28	0/2/2/2
31	MLZ	Lb	5	84,31	-	1/7/8/10	-
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1881	3,85	-	0/9/27/28	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2422	3,85	-	2/9/27/28	0/2/2/2
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
3	A2M	L5	1534	85,3,84	-	2/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
48	PSU	S2	1239	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3,84	-	1/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	3,85	-	0/7/25/26	0/2/2/2
48	G7M	S2	1639	48,47	-	0/7/25/26	0/3/3/3
48	MA6	S2	1850	48	-	0/11/29/30	0/3/3/3
3	PSU	L5	3637	3,84	-	0/7/25/26	0/2/2/2
48	OMG	S2	867	48	-	1/9/27/28	0/3/3/3
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
6	HIC	LB	245	6	-	0/5/6/8	0/1/1/1
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
48	A2M	S2	512	48	-	2/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	3760	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	0/9/27/28	0/3/3/3
48	A2M	S2	27	85,48	-	1/9/27/28	0/3/3/3
48	A2M	S2	1031	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	573	48	-	2/7/25/26	0/2/2/2
46	B8H	Mr	4	47,46	-	2/7/25/26	0/2/2/2
48	OMU	S2	1288	48	-	1/9/27/28	0/2/2/2
48	PSU	S2	822	48	-	2/7/25/26	0/2/2/2
3	PSU	L5	4521	85,3,84	-	0/7/25/26	0/2/2/2
47	1MG	Pt	37	84,47	-	0/7/25/26	0/3/3/3
43	MLZ	Lo	53	43	-	2/7/8/10	-
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
48	OMG	S2	436	48	-	0/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	601	48	-	1/9/27/28	0/3/3/3
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
48	OMC	S2	462	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1744	3,84	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3,84	-	0/9/27/28	0/3/3/3
3	PSU	L5	1792	85,3,84	-	1/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
48	OMU	S2	1442	85,48	-	3/9/27/28	0/2/2/2
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
48	MA6	S2	1851	48	-	3/11/29/30	0/3/3/3
3	1MA	L5	1322	3,85	-	2/7/25/26	0/3/3/3
3	OMG	L5	4196	3,47	-	3/9/27/28	0/3/3/3
48	OMG	S2	1490	85,48	-	3/9/27/28	0/3/3/3
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3,84	-	2/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
48	A2M	S2	668	85,48	-	3/9/27/28	0/3/3/3
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
48	PSU	S2	1367	84,48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
48	OMG	S2	509	48	-	1/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
48	UY1	S2	1326	85,48	-	0/9/27/28	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	166	48	-	0/9/27/28	0/3/3/3
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3,85	-	3/9/27/28	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4361	3,84	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3,84	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,85	-	1/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
48	A2M	S2	159	48	-	0/9/27/28	0/3/3/3
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	572	48	-	2/7/25/26	0/2/2/2
30	V5N	La	39	30	-	1/9/10/12	0/1/1/1
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
48	6MZ	S2	1832	85,84,48	-	2/9/27/28	0/3/3/3
48	A2M	S2	1678	48	-	1/9/27/28	0/3/3/3
46	B8H	Mr	6	1,46	-	0/7/25/26	0/2/2/2
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3,84	-	0/7/25/26	0/2/2/2
48	OMU	S2	428	48	-	6/9/27/28	0/2/2/2
47	1MA	Pt	58	47	-	2/7/25/26	0/3/3/3
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1643	85,48	-	0/7/25/26	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	3,85	-	0/7/25/26	0/2/2/2

All (962) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1677	PSU	C6-C5	11.61	1.48	1.35
3	L5	4423	PSU	C6-C5	11.57	1.48	1.35
3	L5	3844	PSU	C6-C5	11.55	1.48	1.35
3	L5	3884	PSU	C6-C5	11.53	1.48	1.35
3	L5	2632	PSU	C6-C5	11.48	1.48	1.35
3	L5	4420	PSU	C6-C5	11.48	1.48	1.35
3	L5	4569	PSU	C6-C5	11.48	1.48	1.35
3	L5	5001	PSU	C6-C5	11.46	1.48	1.35
3	L5	4296	PSU	C6-C5	11.46	1.48	1.35
3	L5	4431	PSU	C6-C5	11.45	1.48	1.35
3	L5	1782	PSU	C6-C5	11.44	1.48	1.35
3	L5	4471	PSU	C6-C5	11.44	1.48	1.35
3	L5	4353	PSU	C6-C5	11.43	1.48	1.35
3	L5	3637	PSU	C6-C5	11.42	1.48	1.35
3	L5	4673	PSU	C6-C5	11.41	1.48	1.35
3	L5	4493	PSU	C6-C5	11.38	1.48	1.35
3	L5	1683	PSU	C6-C5	11.38	1.48	1.35
3	L5	1779	PSU	C6-C5	11.38	1.48	1.35
3	L5	4972	PSU	C6-C5	11.36	1.48	1.35
3	L5	3695	PSU	C6-C5	11.35	1.48	1.35
3	L5	4576	PSU	C6-C5	11.34	1.48	1.35
3	L5	4312	PSU	C6-C5	11.34	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3734	PSU	C6-C5	11.34	1.48	1.35
3	L5	4689	PSU	C6-C5	11.33	1.48	1.35
3	L5	4442	PSU	C6-C5	11.33	1.48	1.35
3	L5	1862	PSU	C6-C5	11.32	1.48	1.35
3	L5	1744	PSU	C6-C5	11.32	1.48	1.35
3	L5	1781	PSU	C6-C5	11.31	1.48	1.35
3	L5	1860	PSU	C6-C5	11.31	1.48	1.35
3	L5	2839	PSU	C6-C5	11.30	1.48	1.35
3	L5	4361	PSU	C6-C5	11.29	1.48	1.35
3	L5	1536	PSU	C6-C5	11.27	1.48	1.35
3	L5	4293	PSU	C6-C5	11.27	1.48	1.35
3	L5	3853	PSU	C6-C5	11.26	1.48	1.35
3	L5	4552	PSU	C6-C5	11.26	1.48	1.35
3	L5	4299	PSU	C6-C5	11.24	1.48	1.35
3	L5	4521	PSU	C6-C5	11.24	1.48	1.35
3	L5	4579	PSU	C6-C5	11.24	1.48	1.35
3	L5	2508	PSU	C6-C5	11.22	1.48	1.35
3	L5	1792	PSU	C6-C5	11.22	1.48	1.35
3	L5	4457	PSU	C6-C5	11.20	1.48	1.35
3	L5	3851	PSU	C6-C5	11.18	1.48	1.35
3	L5	4532	PSU	C6-C5	11.18	1.48	1.35
3	L5	4403	PSU	C6-C5	11.16	1.48	1.35
3	L5	3920	PSU	C6-C5	11.15	1.48	1.35
3	L5	3639	PSU	C6-C5	11.15	1.48	1.35
3	L5	4628	PSU	C6-C5	11.12	1.48	1.35
3	L5	3770	PSU	C6-C5	10.93	1.48	1.35
3	L5	3758	PSU	C6-C5	10.88	1.48	1.35
3	L5	3818	UY1	C6-C5	10.67	1.47	1.35
3	L5	4220	6MZ	C6-N6	9.75	1.44	1.34
3	L5	1779	PSU	C2-N1	9.65	1.49	1.36
3	L5	5001	PSU	C2-N1	9.59	1.49	1.36
3	L5	3734	PSU	C2-N1	9.52	1.49	1.36
3	L5	4569	PSU	C2-N1	9.52	1.49	1.36
3	L5	1782	PSU	C2-N1	9.51	1.49	1.36
3	L5	4353	PSU	C2-N1	9.50	1.49	1.36
3	L5	4471	PSU	C2-N1	9.48	1.49	1.36
3	L5	1781	PSU	C2-N1	9.48	1.49	1.36
3	L5	3758	PSU	C2-N1	9.47	1.49	1.36
3	L5	4972	PSU	C2-N1	9.47	1.49	1.36
3	L5	1677	PSU	C2-N1	9.47	1.49	1.36
3	L5	2632	PSU	C2-N1	9.46	1.49	1.36
3	L5	4576	PSU	C2-N1	9.46	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1536	PSU	C2-N1	9.45	1.49	1.36
3	L5	4532	PSU	C2-N1	9.45	1.49	1.36
3	L5	4423	PSU	C2-N1	9.43	1.49	1.36
3	L5	4493	PSU	C2-N1	9.42	1.49	1.36
3	L5	1860	PSU	C2-N1	9.40	1.49	1.36
3	L5	1862	PSU	C2-N1	9.40	1.49	1.36
3	L5	3920	PSU	C2-N1	9.40	1.49	1.36
3	L5	3695	PSU	C2-N1	9.40	1.49	1.36
3	L5	4420	PSU	C2-N1	9.39	1.49	1.36
3	L5	4431	PSU	C2-N1	9.39	1.49	1.36
3	L5	4296	PSU	C2-N1	9.39	1.49	1.36
3	L5	3637	PSU	C2-N1	9.36	1.49	1.36
3	L5	2839	PSU	C2-N1	9.36	1.49	1.36
3	L5	2508	PSU	C2-N1	9.36	1.49	1.36
3	L5	4312	PSU	C2-N1	9.35	1.49	1.36
3	L5	3844	PSU	C2-N1	9.35	1.49	1.36
3	L5	4457	PSU	C2-N1	9.35	1.49	1.36
3	L5	4442	PSU	C2-N1	9.34	1.49	1.36
3	L5	4521	PSU	C2-N1	9.30	1.49	1.36
3	L5	1744	PSU	C2-N1	9.30	1.49	1.36
3	L5	4673	PSU	C2-N1	9.30	1.49	1.36
3	L5	4299	PSU	C2-N1	9.29	1.49	1.36
3	L5	1792	PSU	C2-N1	9.29	1.49	1.36
3	L5	3853	PSU	C2-N1	9.29	1.49	1.36
3	L5	4403	PSU	C2-N1	9.28	1.49	1.36
3	L5	4689	PSU	C2-N1	9.27	1.49	1.36
3	L5	4552	PSU	C2-N1	9.27	1.49	1.36
3	L5	4579	PSU	C2-N1	9.25	1.49	1.36
3	L5	3851	PSU	C2-N1	9.24	1.49	1.36
3	L5	4293	PSU	C2-N1	9.24	1.49	1.36
3	L5	3639	PSU	C2-N1	9.24	1.49	1.36
3	L5	3818	UY1	C2-N1	9.23	1.49	1.36
3	L5	3884	PSU	C2-N1	9.23	1.49	1.36
3	L5	4361	PSU	C2-N1	9.20	1.49	1.36
3	L5	4628	PSU	C2-N1	9.14	1.49	1.36
3	L5	1683	PSU	C2-N1	9.06	1.49	1.36
3	L5	4447	5MC	C6-C5	8.97	1.49	1.34
3	L5	3760	A2M	C2'-C1'	-8.96	1.30	1.53
3	L5	4571	A2M	C2'-C1'	-8.95	1.30	1.53
3	L5	3770	PSU	C2-N1	8.91	1.48	1.36
3	L5	3782	5MC	C6-C5	8.89	1.49	1.34
3	L5	3867	A2M	C2'-C1'	-8.85	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3785	A2M	C2'-C1'	-8.84	1.30	1.53
3	L5	2363	A2M	C2'-C1'	-8.83	1.30	1.53
3	L5	3718	A2M	C2'-C1'	-8.82	1.30	1.53
3	L5	1871	A2M	C2'-C1'	-8.79	1.30	1.53
47	Pt	58	1MA	O4'-C1'	8.79	1.62	1.42
3	L5	1534	A2M	C2'-C1'	-8.76	1.30	1.53
3	L5	3830	A2M	C2'-C1'	-8.74	1.30	1.53
3	L5	3825	A2M	C2'-C1'	-8.73	1.30	1.53
3	L5	3724	A2M	C2'-C1'	-8.70	1.30	1.53
3	L5	4590	A2M	C2'-C1'	-8.70	1.30	1.53
3	L5	400	A2M	C2'-C1'	-8.65	1.30	1.53
3	L5	2787	A2M	C2'-C1'	-8.63	1.30	1.53
3	L5	1326	A2M	C2'-C1'	-8.62	1.30	1.53
3	L5	398	A2M	O4'-C1'	8.60	1.62	1.42
3	L5	3724	A2M	O4'-C1'	8.59	1.62	1.42
3	L5	4523	A2M	C2'-C1'	-8.58	1.31	1.53
3	L5	2401	A2M	C2'-C1'	-8.58	1.31	1.53
3	L5	2815	A2M	O4'-C1'	8.58	1.62	1.42
3	L5	4590	A2M	O4'-C1'	8.57	1.62	1.42
3	L5	398	A2M	C2'-C1'	-8.57	1.31	1.53
3	L5	3825	A2M	O4'-C1'	8.55	1.62	1.42
3	L5	3718	A2M	O4'-C1'	8.55	1.62	1.42
3	L5	2815	A2M	C2'-C1'	-8.54	1.31	1.53
3	L5	1871	A2M	O4'-C1'	8.50	1.62	1.42
3	L5	4523	A2M	O4'-C1'	8.49	1.62	1.42
47	Pt	58	1MA	C2-N3	8.49	1.46	1.30
3	L5	3830	A2M	O4'-C1'	8.48	1.62	1.42
3	L5	4571	A2M	O4'-C1'	8.47	1.62	1.42
3	L5	2787	A2M	O4'-C1'	8.47	1.62	1.42
3	L5	1524	A2M	C2'-C1'	-8.44	1.31	1.53
3	L5	2363	A2M	O4'-C1'	8.42	1.61	1.42
3	L5	2401	A2M	O4'-C1'	8.41	1.61	1.42
3	L5	400	A2M	O4'-C1'	8.39	1.61	1.42
3	L5	1534	A2M	O4'-C1'	8.38	1.61	1.42
3	L5	3867	A2M	O4'-C1'	8.31	1.61	1.42
3	L5	1524	A2M	O4'-C1'	8.31	1.61	1.42
3	L5	1326	A2M	O4'-C1'	8.23	1.61	1.42
3	L5	3785	A2M	O4'-C1'	8.13	1.61	1.42
3	L5	3760	A2M	O4'-C1'	7.96	1.60	1.42
47	Pt	58	1MA	C2'-C1'	-7.89	1.28	1.53
3	L5	1322	1MA	C2-N3	7.73	1.45	1.30
3	L5	1677	PSU	C2-N3	7.65	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4420	PSU	C2-N3	7.57	1.50	1.37
3	L5	1322	1MA	C4-N3	7.45	1.51	1.35
3	L5	3734	PSU	C2-N3	7.45	1.50	1.37
3	L5	4442	PSU	C2-N3	7.38	1.50	1.37
3	L5	4423	PSU	C2-N3	7.38	1.50	1.37
3	L5	5001	PSU	C2-N3	7.32	1.50	1.37
3	L5	3844	PSU	C2-N3	7.31	1.50	1.37
3	L5	1782	PSU	C2-N3	7.31	1.50	1.37
3	L5	1779	PSU	C2-N3	7.29	1.50	1.37
3	L5	4353	PSU	C2-N3	7.29	1.50	1.37
3	L5	4689	PSU	C2-N3	7.27	1.50	1.37
3	L5	3695	PSU	C2-N3	7.26	1.50	1.37
3	L5	4299	PSU	C2-N3	7.26	1.49	1.37
3	L5	4431	PSU	C2-N3	7.26	1.49	1.37
3	L5	1744	PSU	C2-N3	7.25	1.49	1.37
3	L5	4403	PSU	C2-N3	7.24	1.49	1.37
3	L5	2508	PSU	C2-N3	7.24	1.49	1.37
3	L5	4493	PSU	C2-N3	7.24	1.49	1.37
3	L5	4312	PSU	C2-N3	7.24	1.49	1.37
3	L5	1781	PSU	C2-N3	7.23	1.49	1.37
3	L5	4579	PSU	C2-N3	7.23	1.49	1.37
3	L5	2632	PSU	C2-N3	7.23	1.49	1.37
3	L5	4673	PSU	C2-N3	7.21	1.49	1.37
3	L5	4361	PSU	C2-N3	7.21	1.49	1.37
3	L5	3851	PSU	C2-N3	7.21	1.49	1.37
3	L5	1862	PSU	C2-N3	7.20	1.49	1.37
3	L5	4628	PSU	C2-N3	7.20	1.49	1.37
3	L5	1860	PSU	C2-N3	7.20	1.49	1.37
3	L5	1683	PSU	C2-N3	7.20	1.49	1.37
3	L5	4972	PSU	C2-N3	7.20	1.49	1.37
3	L5	1536	PSU	C2-N3	7.19	1.49	1.37
3	L5	4296	PSU	C2-N3	7.17	1.49	1.37
3	L5	4457	PSU	C2-N3	7.17	1.49	1.37
3	L5	4576	PSU	C2-N3	7.16	1.49	1.37
3	L5	4552	PSU	C2-N3	7.16	1.49	1.37
3	L5	4569	PSU	C2-N3	7.15	1.49	1.37
3	L5	4471	PSU	C2-N3	7.15	1.49	1.37
3	L5	1792	PSU	C2-N3	7.15	1.49	1.37
3	L5	4521	PSU	C2-N3	7.14	1.49	1.37
3	L5	3884	PSU	C2-N3	7.12	1.49	1.37
3	L5	3920	PSU	C2-N3	7.11	1.49	1.37
3	L5	4532	PSU	C2-N3	7.09	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2839	PSU	C2-N3	7.08	1.49	1.37
3	L5	3758	PSU	C2-N3	7.06	1.49	1.37
3	L5	3639	PSU	C2-N3	7.06	1.49	1.37
3	L5	3853	PSU	C2-N3	7.05	1.49	1.37
30	La	39	V5N	CG-ND1	-7.01	1.31	1.37
47	Pt	58	1MA	C4-N3	7.00	1.50	1.35
3	L5	3818	UY1	C2-N3	7.00	1.49	1.37
3	L5	3770	PSU	C2-N3	6.98	1.49	1.37
3	L5	4293	PSU	C2-N3	6.93	1.49	1.37
3	L5	2415	OMU	C2-N1	6.90	1.49	1.38
3	L5	4227	OMU	C2-N1	6.89	1.49	1.38
3	L5	3925	OMU	C2-N1	6.86	1.49	1.38
3	L5	1524	A2M	O4'-C4'	-6.84	1.29	1.45
3	L5	3637	PSU	C2-N3	6.81	1.49	1.37
3	L5	2837	OMU	C2-N1	6.79	1.49	1.38
3	L5	2415	OMU	C2-N3	6.75	1.50	1.38
3	L5	3760	A2M	O4'-C4'	-6.71	1.30	1.45
3	L5	4498	OMU	C2-N1	6.70	1.49	1.38
3	L5	4306	OMU	C2-N1	6.68	1.49	1.38
3	L5	4571	A2M	O4'-C4'	-6.55	1.30	1.45
3	L5	4227	OMU	C2-N3	6.54	1.49	1.38
3	L5	4590	A2M	O4'-C4'	-6.54	1.30	1.45
3	L5	4498	OMU	C2-N3	6.53	1.49	1.38
3	L5	4620	OMU	C2-N1	6.48	1.48	1.38
3	L5	1534	A2M	O4'-C4'	-6.48	1.30	1.45
3	L5	2837	OMU	C2-N3	6.47	1.49	1.38
3	L5	400	A2M	O4'-C4'	-6.47	1.30	1.45
3	L5	2363	A2M	O4'-C4'	-6.46	1.30	1.45
3	L5	3867	A2M	O4'-C4'	-6.46	1.30	1.45
3	L5	2815	A2M	O4'-C4'	-6.45	1.30	1.45
3	L5	3925	OMU	C2-N3	6.45	1.49	1.38
3	L5	3724	A2M	O4'-C4'	-6.44	1.30	1.45
3	L5	1326	A2M	O4'-C4'	-6.44	1.30	1.45
3	L5	4306	OMU	C2-N3	6.43	1.49	1.38
3	L5	398	A2M	O4'-C4'	-6.42	1.30	1.45
3	L5	4523	A2M	O4'-C4'	-6.37	1.30	1.45
3	L5	1871	A2M	O4'-C4'	-6.37	1.30	1.45
3	L5	3825	A2M	O4'-C4'	-6.37	1.30	1.45
3	L5	2876	OMG	C4-N3	6.35	1.49	1.34
3	L5	4618	OMG	C4-N3	6.35	1.49	1.34
3	L5	2787	A2M	O4'-C4'	-6.34	1.30	1.45
3	L5	4620	OMU	C2-N3	6.32	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2401	A2M	O4'-C4'	-6.31	1.30	1.45
3	L5	3718	A2M	O4'-C4'	-6.29	1.30	1.45
3	L5	3744	OMG	C4-N3	6.28	1.49	1.34
3	L5	3899	OMG	C4-N3	6.27	1.49	1.34
3	L5	3785	A2M	O4'-C4'	-6.26	1.31	1.45
3	L5	1316	OMG	C4-N3	6.25	1.49	1.34
3	L5	3782	5MC	C4-N3	6.25	1.44	1.34
3	L5	3792	OMG	C4-N3	6.25	1.49	1.34
3	L5	1625	OMG	C4-N3	6.24	1.49	1.34
3	L5	2424	OMG	C4-N3	6.24	1.49	1.34
3	L5	3830	A2M	O4'-C4'	-6.24	1.31	1.45
3	L5	3841	OMC	C2-N3	6.18	1.48	1.36
3	L5	4623	OMG	C4-N3	6.17	1.48	1.34
3	L5	4494	OMG	C4-N3	6.16	1.48	1.34
3	L5	4392	OMG	C4-N3	6.16	1.48	1.34
3	L5	3627	OMG	C4-N3	6.15	1.48	1.34
3	L5	4228	OMG	C4-N3	6.14	1.48	1.34
3	L5	1522	OMG	C4-N3	6.14	1.48	1.34
3	L5	4370	OMG	C4-N3	6.12	1.48	1.34
3	L5	2364	OMG	C4-N3	6.12	1.48	1.34
3	L5	4530	UR3	C2-N1	6.12	1.47	1.38
3	L5	4637	OMG	C4-N3	6.12	1.48	1.34
3	L5	3869	OMC	C2-N3	6.11	1.48	1.36
3	L5	3808	OMC	C2-N3	6.08	1.48	1.36
3	L5	2861	OMC	C2-N3	6.06	1.48	1.36
3	L5	2804	OMC	C2-N3	6.06	1.48	1.36
3	L5	2824	OMC	C2-N3	6.05	1.48	1.36
3	L5	1881	OMC	C2-N3	6.01	1.48	1.36
3	L5	2422	OMC	C2-N3	5.99	1.48	1.36
3	L5	4536	OMC	C2-N3	5.97	1.48	1.36
3	L5	2351	OMC	C2-N3	5.97	1.48	1.36
3	L5	3887	OMC	C2-N3	5.96	1.48	1.36
3	L5	2365	OMC	C2-N3	5.95	1.48	1.36
3	L5	4196	OMG	C4-N3	5.94	1.48	1.34
3	L5	3701	OMC	C6-C5	5.92	1.48	1.35
3	L5	3782	5MC	C2-N3	5.92	1.48	1.36
3	L5	2422	OMC	C6-C5	5.89	1.48	1.35
47	Pt	58	1MA	O4'-C4'	-5.88	1.31	1.45
3	L5	3887	OMC	C6-C5	5.88	1.48	1.35
3	L5	4456	OMC	C6-C5	5.87	1.48	1.35
3	L5	1881	OMC	C6-C5	5.87	1.48	1.35
3	L5	2824	OMC	C6-C5	5.86	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1340	OMC	C2-N3	5.85	1.48	1.36
3	L5	4536	OMC	C6-C5	5.82	1.48	1.35
3	L5	2365	OMC	C6-C5	5.82	1.48	1.35
3	L5	4456	OMC	C2-N3	5.81	1.48	1.36
3	L5	4530	UR3	C6-C5	5.80	1.48	1.35
3	L5	2861	OMC	C6-C5	5.79	1.48	1.35
3	L5	3841	OMC	C6-C5	5.78	1.48	1.35
3	L5	1340	OMC	C6-C5	5.78	1.48	1.35
3	L5	3701	OMC	C2-N3	5.77	1.48	1.36
3	L5	4447	5MC	C4-N3	5.75	1.43	1.34
3	L5	2804	OMC	C6-C5	5.75	1.48	1.35
3	L5	3808	OMC	C6-C5	5.74	1.48	1.35
3	L5	3869	OMC	C6-C5	5.74	1.48	1.35
3	L5	4306	OMU	C6-C5	5.70	1.48	1.35
3	L5	2351	OMC	C6-C5	5.66	1.48	1.35
3	L5	4447	5MC	C2-N3	5.61	1.47	1.36
3	L5	4498	OMU	C6-C5	5.56	1.48	1.35
3	L5	4227	OMU	C6-C5	5.54	1.47	1.35
3	L5	2415	OMU	C6-C5	5.52	1.47	1.35
3	L5	2837	OMU	C6-C5	5.51	1.47	1.35
3	L5	3925	OMU	C6-C5	5.48	1.47	1.35
3	L5	2876	OMG	C2-N3	5.48	1.46	1.33
3	L5	4620	OMU	C6-C5	5.45	1.47	1.35
3	L5	2424	OMG	C2-N3	5.42	1.46	1.33
3	L5	4494	OMG	C2-N3	5.40	1.46	1.33
3	L5	4618	OMG	C2-N3	5.36	1.46	1.33
3	L5	1625	OMG	C2-N3	5.36	1.46	1.33
3	L5	3744	OMG	C2-N3	5.36	1.46	1.33
3	L5	1316	OMG	C2-N3	5.34	1.46	1.33
3	L5	4392	OMG	C2-N3	5.33	1.46	1.33
3	L5	4420	PSU	C6-N1	5.32	1.45	1.36
3	L5	3899	OMG	C2-N3	5.32	1.46	1.33
3	L5	4637	OMG	C2-N3	5.32	1.46	1.33
3	L5	1522	OMG	C2-N3	5.29	1.45	1.33
3	L5	3627	OMG	C2-N3	5.29	1.45	1.33
3	L5	4623	OMG	C2-N3	5.29	1.45	1.33
3	L5	2364	OMG	C2-N3	5.27	1.45	1.33
3	L5	5001	PSU	C6-N1	5.27	1.45	1.36
3	L5	3792	OMG	C2-N3	5.26	1.45	1.33
3	L5	2632	PSU	C6-N1	5.24	1.44	1.36
3	L5	4972	PSU	C6-N1	5.24	1.44	1.36
3	L5	1779	PSU	C6-N1	5.21	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1677	PSU	C6-N1	5.21	1.44	1.36
3	L5	4569	PSU	C6-N1	5.19	1.44	1.36
3	L5	1782	PSU	C6-N1	5.19	1.44	1.36
3	L5	4296	PSU	C6-N1	5.19	1.44	1.36
3	L5	1860	PSU	C6-N1	5.18	1.44	1.36
3	L5	1781	PSU	C6-N1	5.18	1.44	1.36
3	L5	4293	PSU	C6-N1	5.18	1.44	1.36
3	L5	4370	OMG	C2-N3	5.18	1.45	1.33
3	L5	4361	PSU	C6-N1	5.17	1.44	1.36
3	L5	3844	PSU	C6-N1	5.17	1.44	1.36
3	L5	1744	PSU	C6-N1	5.17	1.44	1.36
3	L5	2508	PSU	C6-N1	5.16	1.44	1.36
3	L5	4532	PSU	C6-N1	5.16	1.44	1.36
3	L5	4312	PSU	C6-N1	5.16	1.44	1.36
3	L5	3734	PSU	C6-N1	5.16	1.44	1.36
3	L5	3695	PSU	C6-N1	5.15	1.44	1.36
3	L5	4423	PSU	C6-N1	5.14	1.44	1.36
3	L5	4471	PSU	C6-N1	5.14	1.44	1.36
3	L5	4431	PSU	C6-N1	5.13	1.44	1.36
3	L5	3853	PSU	C6-N1	5.13	1.44	1.36
3	L5	4228	OMG	C2-N3	5.13	1.45	1.33
3	L5	4689	PSU	C6-N1	5.13	1.44	1.36
3	L5	4493	PSU	C6-N1	5.12	1.44	1.36
3	L5	3851	PSU	C6-N1	5.12	1.44	1.36
3	L5	4353	PSU	C6-N1	5.11	1.44	1.36
3	L5	1792	PSU	C6-N1	5.11	1.44	1.36
3	L5	4579	PSU	C6-N1	5.10	1.44	1.36
3	L5	4576	PSU	C6-N1	5.10	1.44	1.36
3	L5	3758	PSU	C6-N1	5.08	1.44	1.36
3	L5	4442	PSU	C6-N1	5.08	1.44	1.36
3	L5	4196	OMG	C2-N3	5.08	1.45	1.33
3	L5	4673	PSU	C6-N1	5.07	1.44	1.36
3	L5	3637	PSU	C6-N1	5.07	1.44	1.36
3	L5	1862	PSU	C6-N1	5.07	1.44	1.36
3	L5	4552	PSU	C6-N1	5.06	1.44	1.36
3	L5	3920	PSU	C6-N1	5.05	1.44	1.36
3	L5	3884	PSU	C6-N1	5.03	1.44	1.36
3	L5	4299	PSU	C6-N1	5.03	1.44	1.36
3	L5	4521	PSU	C6-N1	5.03	1.44	1.36
3	L5	1536	PSU	C6-N1	5.02	1.44	1.36
3	L5	3869	OMC	C4-N3	5.01	1.44	1.34
3	L5	4628	PSU	C6-N1	5.00	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4403	PSU	C6-N1	4.99	1.44	1.36
3	L5	2839	PSU	C6-N1	4.95	1.44	1.36
3	L5	3818	UY1	C6-N1	4.93	1.44	1.36
3	L5	3770	PSU	C6-N1	4.93	1.44	1.36
3	L5	1683	PSU	C6-N1	4.93	1.44	1.36
3	L5	2824	OMC	C4-N3	4.92	1.44	1.34
3	L5	4457	PSU	C6-N1	4.92	1.44	1.36
3	L5	2861	OMC	C4-N3	4.90	1.44	1.34
3	L5	3639	PSU	C6-N1	4.90	1.44	1.36
3	L5	3808	OMC	C4-N3	4.90	1.44	1.34
3	L5	2804	OMC	C4-N3	4.89	1.44	1.34
3	L5	4536	OMC	C4-N3	4.85	1.44	1.34
3	L5	2351	OMC	C4-N3	4.85	1.44	1.34
3	L5	3841	OMC	C4-N3	4.80	1.44	1.34
3	L5	1340	OMC	C4-N3	4.80	1.44	1.34
3	L5	2422	OMC	C4-N3	4.78	1.44	1.34
3	L5	3887	OMC	C4-N3	4.77	1.44	1.34
3	L5	1881	OMC	C4-N3	4.75	1.44	1.34
3	L5	2365	OMC	C4-N3	4.73	1.44	1.34
3	L5	2861	OMC	C4-N4	4.70	1.45	1.33
3	L5	3701	OMC	C4-N4	4.70	1.45	1.33
3	L5	3701	OMC	C4-N3	4.69	1.44	1.34
3	L5	3887	OMC	C4-N4	4.68	1.44	1.33
3	L5	2824	OMC	C4-N4	4.68	1.44	1.33
3	L5	3841	OMC	C4-N4	4.67	1.44	1.33
3	L5	4530	UR3	C2-N3	4.67	1.48	1.39
3	L5	4536	OMC	C4-N4	4.65	1.44	1.33
3	L5	2804	OMC	C4-N4	4.65	1.44	1.33
3	L5	2424	OMG	C2-N2	4.64	1.45	1.34
3	L5	3808	OMC	C4-N4	4.64	1.44	1.33
3	L5	1881	OMC	C4-N4	4.63	1.44	1.33
3	L5	3869	OMC	C4-N4	4.62	1.44	1.33
3	L5	3734	PSU	C1'-C5	-4.61	1.39	1.50
3	L5	2351	OMC	C4-N4	4.61	1.44	1.33
3	L5	4456	OMC	C4-N3	4.61	1.43	1.34
3	L5	4228	OMG	C2-N2	4.59	1.45	1.34
3	L5	3770	PSU	C1'-C5	-4.59	1.39	1.50
3	L5	3744	OMG	C2-N2	4.59	1.45	1.34
3	L5	4456	OMC	C4-N4	4.59	1.44	1.33
3	L5	2365	OMC	C4-N4	4.58	1.44	1.33
3	L5	2422	OMC	C4-N4	4.57	1.44	1.33
3	L5	4637	OMG	C2-N2	4.57	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3758	PSU	C1'-C5	-4.56	1.39	1.50
3	L5	4623	OMG	C2-N2	4.56	1.45	1.34
3	L5	2876	OMG	C2-N2	4.56	1.45	1.34
3	L5	1340	OMC	C4-N4	4.55	1.44	1.33
3	L5	3792	OMG	C2-N2	4.54	1.45	1.34
3	L5	4618	OMG	C2-N2	4.54	1.45	1.34
3	L5	1677	PSU	C1'-C5	-4.54	1.39	1.50
3	L5	3627	OMG	C2-N2	4.53	1.45	1.34
3	L5	2364	OMG	C2-N2	4.53	1.45	1.34
3	L5	4494	OMG	C2-N2	4.52	1.44	1.34
3	L5	4392	OMG	C2-N2	4.52	1.44	1.34
3	L5	2839	PSU	C1'-C5	-4.51	1.39	1.50
3	L5	1862	PSU	C1'-C5	-4.51	1.39	1.50
3	L5	4471	PSU	C1'-C5	-4.51	1.39	1.50
3	L5	3637	PSU	C1'-C5	-4.50	1.39	1.50
3	L5	3899	OMG	C2-N2	4.47	1.44	1.34
3	L5	1625	OMG	C2-N2	4.47	1.44	1.34
3	L5	1782	PSU	C1'-C5	-4.46	1.40	1.50
3	L5	1779	PSU	C1'-C5	-4.46	1.40	1.50
3	L5	4493	PSU	C1'-C5	-4.46	1.40	1.50
47	Pt	58	1MA	C2-N1	4.46	1.44	1.35
3	L5	1522	OMG	C2-N2	4.45	1.44	1.34
3	L5	4628	PSU	C1'-C5	-4.44	1.40	1.50
3	L5	2508	PSU	C1'-C5	-4.44	1.40	1.50
3	L5	4299	PSU	C1'-C5	-4.44	1.40	1.50
3	L5	4442	PSU	C1'-C5	-4.44	1.40	1.50
3	L5	4576	PSU	C1'-C5	-4.43	1.40	1.50
3	L5	1781	PSU	C1'-C5	-4.43	1.40	1.50
3	L5	4196	OMG	C2-N2	4.43	1.44	1.34
3	L5	4689	PSU	C1'-C5	-4.42	1.40	1.50
3	L5	3639	PSU	C1'-C5	-4.42	1.40	1.50
3	L5	4431	PSU	C1'-C5	-4.41	1.40	1.50
3	L5	1316	OMG	C2-N2	4.41	1.44	1.34
3	L5	4312	PSU	C1'-C5	-4.40	1.40	1.50
3	L5	1860	PSU	C1'-C5	-4.40	1.40	1.50
3	L5	4552	PSU	C1'-C5	-4.40	1.40	1.50
3	L5	4532	PSU	C1'-C5	-4.40	1.40	1.50
3	L5	1534	A2M	C6-N6	4.40	1.45	1.34
3	L5	4571	A2M	C6-N6	4.39	1.45	1.34
30	La	39	V5N	CD2-NE2	-4.38	1.31	1.37
3	L5	4673	PSU	C1'-C5	-4.38	1.40	1.50
3	L5	3851	PSU	C1'-C5	-4.38	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4521	PSU	C1'-C5	-4.38	1.40	1.50
3	L5	1536	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	398	A2M	C6-N6	4.37	1.45	1.34
3	L5	4457	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	1792	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	4353	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	4579	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	1683	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	400	A2M	C6-N6	4.36	1.45	1.34
3	L5	4569	PSU	C1'-C5	-4.35	1.40	1.50
3	L5	3920	PSU	C1'-C5	-4.35	1.40	1.50
3	L5	4423	PSU	C1'-C5	-4.35	1.40	1.50
3	L5	4403	PSU	C1'-C5	-4.35	1.40	1.50
3	L5	2632	PSU	C1'-C5	-4.35	1.40	1.50
3	L5	4293	PSU	C1'-C5	-4.34	1.40	1.50
3	L5	1524	A2M	C6-N6	4.34	1.45	1.34
3	L5	3695	PSU	C1'-C5	-4.34	1.40	1.50
3	L5	3724	A2M	C6-N6	4.32	1.45	1.34
3	L5	1744	PSU	C1'-C5	-4.32	1.40	1.50
3	L5	2815	A2M	C6-N6	4.32	1.45	1.34
3	L5	3760	A2M	C6-N6	4.32	1.45	1.34
3	L5	4590	A2M	C6-N6	4.32	1.45	1.34
3	L5	3844	PSU	C1'-C5	-4.31	1.40	1.50
3	L5	3830	A2M	C6-N6	4.30	1.44	1.34
3	L5	4972	PSU	C1'-C5	-4.30	1.40	1.50
3	L5	3867	A2M	C6-N6	4.30	1.44	1.34
3	L5	1871	A2M	C6-N6	4.29	1.44	1.34
3	L5	3718	A2M	C6-N6	4.29	1.44	1.34
3	L5	4523	A2M	C6-N6	4.29	1.44	1.34
3	L5	3825	A2M	C6-N6	4.28	1.44	1.34
3	L5	4370	OMG	C2-N2	4.28	1.44	1.34
3	L5	3853	PSU	C1'-C5	-4.28	1.40	1.50
3	L5	4447	5MC	C6-N1	4.27	1.45	1.38
3	L5	2401	A2M	C6-N6	4.27	1.44	1.34
3	L5	2351	OMC	C2-N1	4.27	1.49	1.40
3	L5	5001	PSU	C1'-C5	-4.26	1.40	1.50
3	L5	3884	PSU	C1'-C5	-4.26	1.40	1.50
3	L5	3782	5MC	C6-N1	4.26	1.45	1.38
3	L5	3841	OMC	C2-N1	4.25	1.49	1.40
3	L5	2422	OMC	C2-N1	4.23	1.49	1.40
3	L5	4296	PSU	C1'-C5	-4.23	1.40	1.50
3	L5	2861	OMC	C2-N1	4.22	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2363	A2M	C6-N6	4.21	1.44	1.34
3	L5	4361	PSU	C1'-C5	-4.21	1.40	1.50
3	L5	2787	A2M	C6-N6	4.21	1.44	1.34
3	L5	1326	A2M	C6-N6	4.20	1.44	1.34
3	L5	2824	OMC	C2-N1	4.19	1.49	1.40
3	L5	4447	5MC	C4-N4	4.18	1.45	1.34
3	L5	3869	OMC	C2-N1	4.16	1.49	1.40
3	L5	1881	OMC	C2-N1	4.15	1.49	1.40
3	L5	3782	5MC	C4-N4	4.14	1.44	1.34
3	L5	4420	PSU	C1'-C5	-4.14	1.40	1.50
3	L5	3808	OMC	C2-N1	4.12	1.48	1.40
3	L5	3785	A2M	C6-N6	4.12	1.44	1.34
3	L5	4456	OMC	C2-N1	4.10	1.48	1.40
3	L5	3887	OMC	C2-N1	4.10	1.48	1.40
3	L5	4536	OMC	C2-N1	4.08	1.48	1.40
3	L5	2804	OMC	C2-N1	4.05	1.48	1.40
3	L5	2365	OMC	C2-N1	4.04	1.48	1.40
3	L5	3782	5MC	C2-N1	4.01	1.48	1.40
3	L5	4420	PSU	C4-N3	3.99	1.46	1.38
3	L5	2415	OMU	C4-N3	3.98	1.45	1.38
3	L5	3701	OMC	C2-N1	3.97	1.48	1.40
3	L5	4227	OMU	C4-N3	3.90	1.45	1.38
3	L5	1677	PSU	C4-N3	3.87	1.46	1.38
3	L5	1340	OMC	C2-N1	3.86	1.48	1.40
3	L5	4423	PSU	C4-N3	3.83	1.45	1.38
3	L5	1322	1MA	C5-C6	3.83	1.54	1.43
3	L5	4498	OMU	C4-N3	3.82	1.45	1.38
3	L5	2837	OMU	C4-N3	3.80	1.45	1.38
3	L5	4306	OMU	C4-N3	3.79	1.45	1.38
3	L5	4579	PSU	C4-N3	3.77	1.45	1.38
3	L5	1536	PSU	C4-N3	3.75	1.45	1.38
47	Pt	58	1MA	O3'-C3'	-3.75	1.34	1.43
3	L5	4447	5MC	C2-N1	3.75	1.48	1.40
3	L5	1322	1MA	C2-N1	3.75	1.42	1.35
3	L5	4312	PSU	C4-N3	3.75	1.45	1.38
3	L5	4442	PSU	C4-N3	3.74	1.45	1.38
3	L5	4620	OMU	C4-N3	3.73	1.45	1.38
3	L5	1779	PSU	C4-N3	3.73	1.45	1.38
3	L5	4353	PSU	C4-N3	3.73	1.45	1.38
3	L5	3925	OMU	C4-N3	3.71	1.45	1.38
3	L5	1860	PSU	C4-N3	3.71	1.45	1.38
3	L5	3734	PSU	C4-N3	3.71	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1792	PSU	C4-N3	3.70	1.45	1.38
3	L5	4972	PSU	C4-N3	3.70	1.45	1.38
3	L5	4673	PSU	C4-N3	3.69	1.45	1.38
3	L5	5001	PSU	C4-N3	3.68	1.45	1.38
3	L5	2632	PSU	C4-N3	3.68	1.45	1.38
3	L5	4493	PSU	C4-N3	3.67	1.45	1.38
3	L5	1744	PSU	C4-N3	3.67	1.45	1.38
3	L5	4296	PSU	C4-N3	3.67	1.45	1.38
3	L5	4196	OMG	C5-N7	-3.66	1.32	1.39
3	L5	4628	PSU	C4-N3	3.66	1.45	1.38
3	L5	3853	PSU	C4-N3	3.66	1.45	1.38
3	L5	3884	PSU	C4-N3	3.66	1.45	1.38
3	L5	3844	PSU	C4-N3	3.66	1.45	1.38
3	L5	4431	PSU	C4-N3	3.65	1.45	1.38
3	L5	4552	PSU	C4-N3	3.65	1.45	1.38
3	L5	3851	PSU	C4-N3	3.65	1.45	1.38
3	L5	4299	PSU	C4-N3	3.65	1.45	1.38
3	L5	1781	PSU	C4-N3	3.62	1.45	1.38
3	L5	4457	PSU	C4-N3	3.62	1.45	1.38
3	L5	4293	PSU	C4-N3	3.62	1.45	1.38
3	L5	4532	PSU	C4-N3	3.62	1.45	1.38
3	L5	1782	PSU	C4-N3	3.61	1.45	1.38
3	L5	4361	PSU	C4-N3	3.61	1.45	1.38
3	L5	4403	PSU	C4-N3	3.61	1.45	1.38
3	L5	4689	PSU	C4-N3	3.61	1.45	1.38
3	L5	2508	PSU	C4-N3	3.60	1.45	1.38
3	L5	4370	OMG	C5-N7	-3.60	1.32	1.39
3	L5	4576	PSU	C4-N3	3.59	1.45	1.38
3	L5	4569	PSU	C4-N3	3.59	1.45	1.38
3	L5	1625	OMG	C5-N7	-3.58	1.32	1.39
3	L5	4471	PSU	C4-N3	3.58	1.45	1.38
3	L5	1862	PSU	C4-N3	3.58	1.45	1.38
3	L5	3639	PSU	C4-N3	3.57	1.45	1.38
3	L5	3695	PSU	C4-N3	3.56	1.45	1.38
47	Pt	58	1MA	C5-C6	3.56	1.53	1.43
3	L5	4521	PSU	C4-N3	3.54	1.45	1.38
3	L5	1316	OMG	C5-N7	-3.53	1.32	1.39
3	L5	3792	OMG	C5-N7	-3.52	1.32	1.39
3	L5	2876	OMG	C5-N7	-3.52	1.32	1.39
3	L5	3920	PSU	C4-N3	3.49	1.45	1.38
3	L5	3770	PSU	C4-N3	3.49	1.45	1.38
3	L5	3818	UY1	C4-N3	3.49	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2839	PSU	C4-N3	3.49	1.45	1.38
3	L5	3758	PSU	C4-N3	3.49	1.45	1.38
48	S2	1056	PSU	C6-C5	3.48	1.39	1.35
3	L5	2364	OMG	C5-N7	-3.48	1.32	1.39
3	L5	4392	OMG	C5-N7	-3.48	1.32	1.39
3	L5	1683	PSU	C4-N3	3.47	1.45	1.38
3	L5	4637	OMG	C5-N7	-3.47	1.32	1.39
48	S2	1081	PSU	C6-C5	3.45	1.39	1.35
48	S2	822	PSU	C6-C5	3.45	1.39	1.35
3	L5	4500	PSU	C6-C5	3.43	1.39	1.35
3	L5	3899	OMG	C5-N7	-3.43	1.32	1.39
3	L5	3760	A2M	C5-C4	-3.42	1.32	1.39
48	S2	1238	PSU	C6-C5	3.42	1.39	1.35
48	S2	1232	PSU	C6-C5	3.42	1.39	1.35
48	S2	93	PSU	C6-C5	3.41	1.39	1.35
48	S2	34	PSU	C6-C5	3.41	1.39	1.35
3	L5	1522	OMG	C5-N7	-3.41	1.32	1.39
3	L5	3637	PSU	C4-N3	3.40	1.45	1.38
48	S2	105	PSU	C6-C5	3.40	1.39	1.35
48	S2	1243	PSU	C6-C5	3.40	1.39	1.35
48	S2	406	PSU	C6-C5	3.39	1.39	1.35
3	L5	4623	OMG	C5-N7	-3.39	1.32	1.39
48	S2	1177	PSU	C6-C5	3.39	1.39	1.35
48	S2	1174	PSU	C6-C5	3.38	1.39	1.35
48	S2	1244	PSU	C6-C5	3.38	1.39	1.35
48	S2	863	PSU	C6-C5	3.38	1.39	1.35
3	L5	2424	OMG	C5-N7	-3.37	1.32	1.39
48	S2	814	PSU	C6-C5	3.37	1.39	1.35
48	S2	1692	PSU	C6-C5	3.37	1.39	1.35
48	S2	966	PSU	C6-C5	3.36	1.39	1.35
3	L5	4494	OMG	C5-N7	-3.35	1.32	1.39
48	S2	36	PSU	C6-C5	3.35	1.39	1.35
47	Pt	58	1MA	O2'-C2'	3.35	1.50	1.43
48	S2	1367	PSU	C6-C5	3.34	1.39	1.35
48	S2	119	PSU	C6-C5	3.33	1.39	1.35
48	S2	1004	PSU	C6-C5	3.33	1.39	1.35
48	S2	1445	PSU	C6-C5	3.33	1.39	1.35
48	S2	918	PSU	C6-C5	3.33	1.39	1.35
48	S2	686	PSU	C6-C5	3.33	1.39	1.35
48	S2	681	PSU	C6-C5	3.32	1.39	1.35
48	S2	651	PSU	C6-C5	3.32	1.39	1.35
48	S2	649	PSU	C6-C5	3.32	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3627	OMG	C5-N7	-3.32	1.32	1.39
48	S2	1643	PSU	C6-C5	3.31	1.39	1.35
3	L5	3785	A2M	C5-C4	-3.30	1.32	1.39
48	S2	109	PSU	C6-C5	3.30	1.39	1.35
48	S2	218	PSU	C6-C5	3.30	1.39	1.35
3	L5	3744	OMG	C5-N7	-3.30	1.32	1.39
48	S2	1239	PSU	C6-C5	3.29	1.39	1.35
3	L5	3768	PSU	C6-C5	3.29	1.39	1.35
3	L5	4618	OMG	C5-N7	-3.29	1.32	1.39
48	S2	866	PSU	C6-C5	3.28	1.39	1.35
48	S2	1625	PSU	C6-C5	3.28	1.39	1.35
48	S2	572	PSU	C6-C5	3.28	1.39	1.35
48	S2	1347	PSU	C6-C5	3.27	1.39	1.35
3	L5	4228	OMG	C5-N7	-3.27	1.32	1.39
5	L8	69	PSU	C6-C5	3.26	1.39	1.35
3	L5	4306	OMU	O4-C4	-3.26	1.18	1.24
48	S2	573	PSU	C6-C5	3.25	1.39	1.35
3	L5	1326	A2M	O3'-C3'	-3.25	1.35	1.43
3	L5	3887	OMC	C6-N1	3.25	1.45	1.38
3	L5	3925	OMU	O4-C4	-3.25	1.18	1.24
3	L5	4498	OMU	O4-C4	-3.24	1.18	1.24
5	L8	55	PSU	C6-C5	3.24	1.39	1.35
3	L5	4571	A2M	O3'-C3'	-3.22	1.35	1.43
48	S2	815	PSU	C6-C5	3.21	1.39	1.35
3	L5	4590	A2M	O3'-C3'	-3.20	1.35	1.43
3	L5	2363	A2M	O3'-C3'	-3.19	1.35	1.43
3	L5	3825	A2M	C5-C4	-3.18	1.33	1.39
3	L5	400	A2M	O3'-C3'	-3.18	1.35	1.43
3	L5	3718	A2M	O3'-C3'	-3.17	1.35	1.43
3	L5	4620	OMU	O4-C4	-3.17	1.18	1.24
3	L5	1524	A2M	O3'-C3'	-3.16	1.35	1.43
3	L5	2787	A2M	O3'-C3'	-3.16	1.35	1.43
3	L5	3825	A2M	O3'-C3'	-3.16	1.35	1.43
3	L5	3830	A2M	O3'-C3'	-3.15	1.35	1.43
3	L5	2837	OMU	O4-C4	-3.14	1.18	1.24
3	L5	4227	OMU	O4-C4	-3.14	1.18	1.24
3	L5	1326	A2M	C5-C4	-3.14	1.33	1.39
3	L5	4220	6MZ	C5-C4	-3.13	1.33	1.39
3	L5	3867	A2M	C5-C4	-3.12	1.33	1.39
3	L5	1881	OMC	C6-N1	3.12	1.45	1.38
3	L5	3701	OMC	O2-C2	-3.12	1.17	1.23
3	L5	3867	A2M	O3'-C3'	-3.12	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2363	A2M	C5-C4	-3.12	1.33	1.39
3	L5	1322	1MA	C5-N7	-3.11	1.33	1.39
3	L5	2861	OMC	C6-N1	3.11	1.45	1.38
3	L5	2422	OMC	C6-N1	3.11	1.45	1.38
3	L5	4447	5MC	O2-C2	-3.10	1.18	1.23
3	L5	1871	A2M	O3'-C3'	-3.10	1.35	1.43
3	L5	3841	OMC	C6-N1	3.10	1.45	1.38
3	L5	4536	OMC	C6-N1	3.10	1.45	1.38
3	L5	2365	OMC	C6-N1	3.10	1.45	1.38
3	L5	1534	A2M	C5-C4	-3.09	1.33	1.39
3	L5	2401	A2M	C5-C4	-3.09	1.33	1.39
3	L5	3760	A2M	O3'-C3'	-3.09	1.35	1.43
3	L5	2401	A2M	O3'-C3'	-3.09	1.35	1.43
3	L5	3899	OMG	O6-C6	-3.08	1.17	1.23
3	L5	2351	OMC	C6-N1	3.08	1.45	1.38
3	L5	3841	OMC	O2-C2	-3.08	1.18	1.23
3	L5	2787	A2M	C5-C4	-3.08	1.33	1.39
3	L5	2815	A2M	O3'-C3'	-3.08	1.35	1.43
3	L5	2351	OMC	O2-C2	-3.07	1.18	1.23
3	L5	3830	A2M	C5-C4	-3.07	1.33	1.39
3	L5	4456	OMC	O2-C2	-3.07	1.18	1.23
3	L5	4590	A2M	C5-C4	-3.07	1.33	1.39
3	L5	3869	OMC	O2-C2	-3.07	1.18	1.23
3	L5	2824	OMC	C6-N1	3.06	1.45	1.38
3	L5	2415	OMU	O4-C4	-3.06	1.18	1.24
3	L5	3701	OMC	C6-N1	3.06	1.45	1.38
3	L5	3724	A2M	O3'-C3'	-3.06	1.35	1.43
3	L5	398	A2M	O3'-C3'	-3.05	1.35	1.43
3	L5	4523	A2M	C5-C4	-3.05	1.33	1.39
3	L5	1524	A2M	C5-C4	-3.05	1.33	1.39
3	L5	1881	OMC	O2-C2	-3.05	1.18	1.23
3	L5	4456	OMC	C6-N1	3.04	1.45	1.38
3	L5	2824	OMC	O2-C2	-3.04	1.18	1.23
3	L5	1871	A2M	C5-C4	-3.04	1.33	1.39
3	L5	3869	OMC	C6-N1	3.04	1.45	1.38
3	L5	2815	A2M	C5-C4	-3.03	1.33	1.39
3	L5	3724	A2M	C5-C4	-3.03	1.33	1.39
3	L5	2804	OMC	C6-N1	3.03	1.45	1.38
3	L5	398	A2M	C5-C4	-3.03	1.33	1.39
3	L5	1534	A2M	O3'-C3'	-3.03	1.35	1.43
3	L5	2422	OMC	O2-C2	-3.03	1.18	1.23
3	L5	4523	A2M	O3'-C3'	-3.02	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1340	OMC	O2-C2	-3.02	1.18	1.23
3	L5	4523	A2M	C5-N7	-3.02	1.33	1.39
3	L5	3718	A2M	C5-C4	-3.01	1.33	1.39
3	L5	4571	A2M	C5-C4	-3.01	1.33	1.39
3	L5	3884	PSU	O4-C4	-3.01	1.17	1.23
3	L5	3808	OMC	C6-N1	3.00	1.45	1.38
3	L5	3887	OMC	O2-C2	-2.99	1.18	1.23
3	L5	2365	OMC	O2-C2	-2.98	1.18	1.23
3	L5	3718	A2M	C5-N7	-2.98	1.33	1.39
3	L5	4536	OMC	O2-C2	-2.98	1.18	1.23
3	L5	4196	OMG	O6-C6	-2.98	1.17	1.23
3	L5	1340	OMC	C6-N1	2.98	1.45	1.38
3	L5	1536	PSU	O4-C4	-2.98	1.17	1.23
3	L5	400	A2M	C5-C4	-2.97	1.33	1.39
3	L5	4370	OMG	O6-C6	-2.96	1.18	1.23
3	L5	4521	PSU	O4-C4	-2.95	1.18	1.23
3	L5	2839	PSU	O4-C4	-2.95	1.18	1.23
3	L5	3770	PSU	O4-C4	-2.95	1.18	1.23
3	L5	3785	A2M	O3'-C3'	-2.95	1.36	1.43
3	L5	2804	OMC	O2-C2	-2.95	1.18	1.23
3	L5	3760	A2M	C5-N7	-2.94	1.33	1.39
3	L5	2861	OMC	O2-C2	-2.93	1.18	1.23
3	L5	4689	PSU	O4-C4	-2.92	1.18	1.23
3	L5	4457	PSU	O4-C4	-2.91	1.18	1.23
3	L5	4392	OMG	O6-C6	-2.91	1.18	1.23
3	L5	2787	A2M	C5-N7	-2.91	1.33	1.39
3	L5	3637	PSU	O4-C4	-2.91	1.18	1.23
3	L5	1326	A2M	C5-N7	-2.90	1.33	1.39
3	L5	4361	PSU	O4-C4	-2.90	1.18	1.23
3	L5	4579	PSU	O4-C4	-2.90	1.18	1.23
3	L5	2815	A2M	C5-N7	-2.89	1.33	1.39
3	L5	3808	OMC	O2-C2	-2.89	1.18	1.23
3	L5	1683	PSU	O4-C4	-2.89	1.18	1.23
3	L5	4431	PSU	O4-C4	-2.89	1.18	1.23
3	L5	1522	OMG	O6-C6	-2.89	1.18	1.23
3	L5	4571	A2M	C5-N7	-2.88	1.33	1.39
3	L5	2363	A2M	C5-N7	-2.87	1.33	1.39
3	L5	5001	PSU	O4-C4	-2.87	1.18	1.23
3	L5	3695	PSU	O4-C4	-2.87	1.18	1.23
3	L5	1625	OMG	O6-C6	-2.86	1.18	1.23
3	L5	1316	OMG	O6-C6	-2.86	1.18	1.23
3	L5	3724	A2M	O2'-C2'	2.86	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3825	A2M	C5-N7	-2.86	1.33	1.39
3	L5	4552	PSU	O4-C4	-2.86	1.18	1.23
6	LB	245	HIC	CD2-CG	2.86	1.41	1.36
3	L5	400	A2M	C5-N7	-2.85	1.33	1.39
3	L5	4628	PSU	O4-C4	-2.85	1.18	1.23
3	L5	1871	A2M	C5-N7	-2.85	1.33	1.39
3	L5	3844	PSU	O4-C4	-2.85	1.18	1.23
3	L5	3639	PSU	O4-C4	-2.85	1.18	1.23
3	L5	4296	PSU	O4-C4	-2.85	1.18	1.23
3	L5	4403	PSU	O4-C4	-2.84	1.18	1.23
3	L5	1326	A2M	O2'-C2'	2.84	1.49	1.42
3	L5	1534	A2M	C5-N7	-2.84	1.33	1.39
3	L5	4673	PSU	O4-C4	-2.84	1.18	1.23
3	L5	3792	OMG	O6-C6	-2.83	1.18	1.23
3	L5	4493	PSU	O4-C4	-2.83	1.18	1.23
3	L5	3627	OMG	O6-C6	-2.83	1.18	1.23
3	L5	4569	PSU	O4-C4	-2.83	1.18	1.23
3	L5	4637	OMG	O6-C6	-2.83	1.18	1.23
3	L5	398	A2M	O2'-C2'	2.83	1.49	1.42
3	L5	3782	5MC	O2-C2	-2.83	1.18	1.23
3	L5	4220	6MZ	C5-N7	-2.82	1.33	1.39
3	L5	4423	PSU	O4-C4	-2.82	1.18	1.23
3	L5	2401	A2M	C5-N7	-2.82	1.33	1.39
3	L5	3851	PSU	O4-C4	-2.81	1.18	1.23
3	L5	4623	OMG	O6-C6	-2.81	1.18	1.23
3	L5	3758	PSU	O4-C4	-2.81	1.18	1.23
3	L5	4299	PSU	O4-C4	-2.81	1.18	1.23
3	L5	3867	A2M	C5-N7	-2.81	1.33	1.39
3	L5	2876	OMG	O6-C6	-2.81	1.18	1.23
3	L5	2364	OMG	O6-C6	-2.80	1.18	1.23
3	L5	3785	A2M	C5-N7	-2.80	1.33	1.39
3	L5	1744	PSU	O4-C4	-2.80	1.18	1.23
3	L5	4293	PSU	O4-C4	-2.80	1.18	1.23
3	L5	4228	OMG	O6-C6	-2.79	1.18	1.23
3	L5	4353	PSU	O4-C4	-2.79	1.18	1.23
3	L5	4498	OMU	C6-N1	2.79	1.44	1.38
3	L5	4471	PSU	O4-C4	-2.79	1.18	1.23
3	L5	4590	A2M	O2'-C2'	2.78	1.49	1.42
3	L5	4576	PSU	O4-C4	-2.78	1.18	1.23
3	L5	4571	A2M	O2'-C2'	2.77	1.49	1.42
3	L5	3830	A2M	C5-N7	-2.77	1.33	1.39
3	L5	2632	PSU	O4-C4	-2.77	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4618	OMG	O6-C6	-2.77	1.18	1.23
3	L5	3744	OMG	O6-C6	-2.77	1.18	1.23
3	L5	1792	PSU	O4-C4	-2.77	1.18	1.23
3	L5	3925	OMU	C6-N1	2.77	1.44	1.38
3	L5	3853	PSU	O4-C4	-2.77	1.18	1.23
3	L5	2815	A2M	O2'-C2'	2.77	1.49	1.42
3	L5	3925	OMU	O2-C2	-2.76	1.18	1.23
3	L5	1524	A2M	O2'-C2'	2.76	1.49	1.42
3	L5	2508	PSU	O4-C4	-2.76	1.18	1.23
3	L5	4532	PSU	O4-C4	-2.76	1.18	1.23
3	L5	1782	PSU	O4-C4	-2.76	1.18	1.23
3	L5	3830	A2M	O2'-C2'	2.75	1.49	1.42
3	L5	3718	A2M	O2'-C2'	2.75	1.49	1.42
3	L5	4494	OMG	O6-C6	-2.74	1.18	1.23
3	L5	4442	PSU	O4-C4	-2.74	1.18	1.23
3	L5	4306	OMU	C6-N1	2.74	1.44	1.38
3	L5	4972	PSU	O4-C4	-2.74	1.18	1.23
3	L5	3825	A2M	O2'-C2'	2.74	1.49	1.42
3	L5	1677	PSU	O4-C4	-2.73	1.18	1.23
3	L5	1781	PSU	O4-C4	-2.72	1.18	1.23
3	L5	398	A2M	C5-N7	-2.72	1.33	1.39
3	L5	2415	OMU	C6-N1	2.72	1.44	1.38
3	L5	3920	PSU	O4-C4	-2.72	1.18	1.23
3	L5	1524	A2M	C5-N7	-2.72	1.33	1.39
3	L5	4590	A2M	C5-N7	-2.72	1.33	1.39
3	L5	3734	PSU	O4-C4	-2.72	1.18	1.23
3	L5	3818	UY1	O4-C4	-2.72	1.18	1.23
3	L5	2363	A2M	O2'-C2'	2.72	1.49	1.42
3	L5	4312	PSU	O4-C4	-2.71	1.18	1.23
3	L5	1860	PSU	O4-C4	-2.71	1.18	1.23
3	L5	1862	PSU	O4-C4	-2.71	1.18	1.23
3	L5	2837	OMU	C6-N1	2.69	1.44	1.38
3	L5	1871	A2M	O2'-C2'	2.68	1.49	1.42
3	L5	4523	A2M	O2'-C2'	2.68	1.49	1.42
3	L5	4227	OMU	C6-N1	2.67	1.44	1.38
3	L5	2401	A2M	O2'-C2'	2.67	1.49	1.42
3	L5	400	A2M	O2'-C2'	2.67	1.49	1.42
3	L5	3724	A2M	C5-N7	-2.67	1.34	1.39
3	L5	4530	UR3	C6-N1	2.66	1.44	1.38
3	L5	3785	A2M	O2'-C2'	2.66	1.49	1.42
3	L5	1779	PSU	O4-C4	-2.65	1.18	1.23
3	L5	2787	A2M	O2'-C2'	2.64	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4498	OMU	O2-C2	-2.63	1.18	1.23
3	L5	4420	PSU	O4'-C1'	-2.63	1.40	1.43
3	L5	1534	A2M	O2'-C2'	2.62	1.49	1.42
3	L5	2424	OMG	O6-C6	-2.62	1.18	1.23
3	L5	3867	A2M	O2'-C2'	2.61	1.49	1.42
3	L5	4620	OMU	C6-N1	2.61	1.44	1.38
3	L5	4306	OMU	O2-C2	-2.61	1.18	1.23
3	L5	2837	OMU	O2-C2	-2.59	1.18	1.23
3	L5	4227	OMU	O2-C2	-2.59	1.18	1.23
3	L5	4620	OMU	O2-C2	-2.59	1.18	1.23
47	Pt	58	1MA	C5'-C4'	2.56	1.59	1.51
3	L5	3792	OMG	C2-N1	2.55	1.44	1.37
3	L5	3760	A2M	C8-N9	-2.52	1.33	1.37
3	L5	1322	1MA	C4-N9	-2.51	1.31	1.38
3	L5	4420	PSU	O4-C4	-2.51	1.18	1.23
3	L5	4228	OMG	C2-N1	2.49	1.43	1.37
3	L5	3760	A2M	O2'-C2'	2.48	1.49	1.42
3	L5	2424	OMG	C2-N1	2.48	1.43	1.37
3	L5	2415	OMU	O2-C2	-2.46	1.18	1.23
47	Pt	58	1MA	C5-N7	-2.46	1.34	1.39
3	L5	4392	OMG	C5-C6	2.45	1.53	1.44
3	L5	1522	OMG	C2-N1	2.43	1.43	1.37
3	L5	4623	OMG	C2-N1	2.42	1.43	1.37
3	L5	3701	OMC	C5-C4	2.42	1.48	1.42
3	L5	3744	OMG	C5-C6	2.40	1.53	1.44
3	L5	1625	OMG	C2-N1	2.40	1.43	1.37
3	L5	1534	A2M	C8-N9	-2.40	1.33	1.37
3	L5	3899	OMG	C2-N1	2.39	1.43	1.37
3	L5	4618	OMG	C2-N1	2.39	1.43	1.37
3	L5	2364	OMG	C5-C6	2.39	1.53	1.44
3	L5	3744	OMG	C2-N1	2.38	1.43	1.37
3	L5	4494	OMG	C2-N1	2.38	1.43	1.37
3	L5	2364	OMG	C2-N1	2.38	1.43	1.37
3	L5	1625	OMG	C5-C6	2.37	1.53	1.44
3	L5	4618	OMG	C5-C6	2.37	1.53	1.44
3	L5	2876	OMG	C2-N1	2.37	1.43	1.37
3	L5	3760	A2M	O5'-C5'	-2.37	1.39	1.44
3	L5	2422	OMC	C5-C4	2.37	1.48	1.42
3	L5	4536	OMC	C5-C4	2.36	1.48	1.42
3	L5	3818	UY1	O2-C2	-2.36	1.18	1.23
3	L5	3887	OMC	C5-C4	2.36	1.48	1.42
3	L5	4494	OMG	C5-C6	2.35	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1881	OMC	C5-C4	2.35	1.48	1.42
3	L5	3627	OMG	C2-N1	2.35	1.43	1.37
3	L5	4220	6MZ	C8-N9	-2.34	1.33	1.37
3	L5	4196	OMG	C4-N9	-2.34	1.32	1.38
3	L5	2401	A2M	C8-N9	-2.33	1.33	1.37
48	S2	1639	G7M	C8-N7	2.33	1.37	1.33
3	L5	1316	OMG	C2-N1	2.33	1.43	1.37
3	L5	2824	OMC	C5-C4	2.32	1.48	1.42
3	L5	3627	OMG	C5-C6	2.32	1.53	1.44
3	L5	3718	A2M	C8-N9	-2.32	1.33	1.37
3	L5	2363	A2M	C8-N9	-2.32	1.33	1.37
3	L5	4530	UR3	O2-C2	-2.32	1.18	1.22
3	L5	3825	A2M	C8-N9	-2.32	1.33	1.37
3	L5	3785	A2M	C8-N9	-2.32	1.33	1.37
3	L5	1871	A2M	C8-N9	-2.32	1.33	1.37
3	L5	1522	OMG	C5-C6	2.31	1.53	1.44
3	L5	1316	OMG	C5-C6	2.31	1.53	1.44
3	L5	4228	OMG	C5-C6	2.31	1.53	1.44
3	L5	4637	OMG	C5-C6	2.31	1.53	1.44
3	L5	2815	A2M	C8-N9	-2.31	1.33	1.37
3	L5	2365	OMC	C5-C4	2.31	1.48	1.42
3	L5	400	A2M	C8-N9	-2.31	1.33	1.37
3	L5	2424	OMG	C5-C6	2.31	1.53	1.44
3	L5	2861	OMC	C5-C4	2.31	1.48	1.42
3	L5	4623	OMG	C5-C6	2.31	1.53	1.44
3	L5	3899	OMG	C5-C6	2.30	1.53	1.44
3	L5	4456	OMC	C5-C4	2.30	1.48	1.42
3	L5	4523	A2M	C8-N9	-2.30	1.33	1.37
3	L5	4227	OMU	C5-C4	2.30	1.48	1.43
3	L5	2876	OMG	C5-C6	2.29	1.52	1.44
3	L5	4370	OMG	C5-C6	2.29	1.52	1.44
3	L5	1524	A2M	C8-N9	-2.29	1.33	1.37
3	L5	3808	OMC	C5-C4	2.29	1.48	1.42
3	L5	4637	OMG	C2-N1	2.28	1.43	1.37
3	L5	4530	UR3	O4-C4	-2.28	1.18	1.23
3	L5	4392	OMG	C2-N1	2.28	1.43	1.37
3	L5	1326	A2M	C8-N9	-2.27	1.33	1.37
3	L5	3925	OMU	C5-C4	2.26	1.48	1.43
3	L5	3792	OMG	C5-C6	2.25	1.52	1.44
3	L5	4228	OMG	C4-N9	-2.25	1.32	1.38
3	L5	3724	A2M	C8-N9	-2.25	1.33	1.37
3	L5	4571	A2M	C8-N9	-2.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3841	OMC	C5-C4	2.24	1.48	1.42
3	L5	2837	OMU	C5-C4	2.24	1.48	1.43
3	L5	4306	OMU	C5-C4	2.23	1.48	1.43
3	L5	3869	OMC	C5-C4	2.23	1.48	1.42
3	L5	2351	OMC	C5-C4	2.22	1.48	1.42
3	L5	3867	A2M	C8-N9	-2.22	1.33	1.37
3	L5	1524	A2M	O5'-C5'	-2.22	1.39	1.44
3	L5	400	A2M	O5'-C5'	-2.22	1.39	1.44
3	L5	398	A2M	C8-N9	-2.21	1.33	1.37
3	L5	4590	A2M	C8-N9	-2.21	1.33	1.37
3	L5	1340	OMC	C5-C4	2.19	1.47	1.42
3	L5	3830	A2M	C8-N9	-2.19	1.33	1.37
3	L5	1871	A2M	O5'-C5'	-2.17	1.39	1.44
3	L5	2787	A2M	O5'-C5'	-2.17	1.39	1.44
3	L5	2415	OMU	C5-C4	2.17	1.48	1.43
3	L5	2401	A2M	O5'-C5'	-2.17	1.39	1.44
3	L5	2787	A2M	C8-N9	-2.16	1.33	1.37
3	L5	2363	A2M	O5'-C5'	-2.16	1.39	1.44
3	L5	3785	A2M	O5'-C5'	-2.15	1.39	1.44
3	L5	2424	OMG	C6-N1	2.15	1.42	1.38
3	L5	4370	OMG	C4-N9	-2.14	1.32	1.38
3	L5	3830	A2M	O5'-C5'	-2.13	1.39	1.44
3	L5	3792	OMG	C6-N1	2.13	1.42	1.38
3	L5	4498	OMU	C5-C4	2.13	1.48	1.43
3	L5	1326	A2M	O5'-C5'	-2.13	1.39	1.44
3	L5	4623	OMG	C4-N9	-2.12	1.32	1.38
3	L5	4620	OMU	C5-C4	2.12	1.48	1.43
3	L5	4228	OMG	C6-N1	2.12	1.42	1.38
3	L5	4196	OMG	C2-N1	2.10	1.42	1.37
3	L5	1677	PSU	O4'-C1'	-2.10	1.40	1.43
3	L5	4618	OMG	C6-N1	2.08	1.42	1.38
3	L5	2804	OMC	C5-C4	2.07	1.47	1.42
3	L5	3724	A2M	O5'-C5'	-2.07	1.39	1.44
3	L5	1522	OMG	C6-N1	2.07	1.42	1.38
3	L5	3627	OMG	C6-N1	2.07	1.42	1.38
3	L5	2815	A2M	O5'-C5'	-2.06	1.39	1.44
3	L5	3637	PSU	O2-C2	-2.05	1.19	1.23
3	L5	4569	PSU	O4'-C1'	-2.05	1.41	1.43
48	S2	1238	PSU	C4-C5	-2.05	1.38	1.44
3	L5	3627	OMG	C4-N9	-2.05	1.32	1.38
3	L5	3770	PSU	O2-C2	-2.05	1.19	1.23
3	L5	1522	OMG	C4-N9	-2.04	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1534	A2M	O5'-C5'	-2.04	1.39	1.44
3	L5	4420	PSU	C4-C5	2.04	1.50	1.44
3	L5	4571	A2M	O5'-C5'	-2.04	1.39	1.44
3	L5	1625	OMG	C4-N9	-2.04	1.32	1.38
3	L5	4623	OMG	C6-N1	2.03	1.42	1.38
3	L5	3818	UY1	O4'-C1'	-2.03	1.41	1.43
3	L5	4220	6MZ	C6-N1	-2.03	1.31	1.35
3	L5	3899	OMG	C4-N9	-2.03	1.32	1.38
3	L5	4196	OMG	C5-C6	2.03	1.51	1.44
3	L5	3825	A2M	O5'-C5'	-2.03	1.39	1.44
3	L5	3899	OMG	C6-N1	2.02	1.42	1.38
3	L5	2876	OMG	C6-N1	2.02	1.42	1.38
3	L5	3884	PSU	O2-C2	-2.01	1.19	1.23
3	L5	3744	OMG	C6-N1	2.01	1.42	1.38
3	L5	4370	OMG	C2-N1	2.01	1.42	1.37
3	L5	4494	OMG	C6-N1	2.00	1.42	1.38

All (702) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1322	1MA	C1'-N9-C8	-8.96	101.19	126.70
3	L5	1322	1MA	C1'-N9-C4	8.45	151.61	126.50
3	L5	2876	OMG	C5-C4-N3	-6.00	118.72	128.46
3	L5	1322	1MA	N1-C2-N3	-5.96	118.92	126.00
3	L5	4590	A2M	N3-C2-N1	-5.88	119.40	128.60
3	L5	2787	A2M	C5-C4-N3	-5.76	119.23	126.75
3	L5	1871	A2M	N3-C2-N1	-5.75	119.61	128.60
3	L5	4220	6MZ	N1-C2-N3	-5.74	119.63	128.60
3	L5	1326	A2M	N3-C2-N1	-5.73	119.64	128.60
3	L5	4392	OMG	C5-C4-N3	-5.66	119.28	128.46
3	L5	2815	A2M	N3-C2-N1	-5.63	119.79	128.60
3	L5	2815	A2M	C5-C4-N3	-5.62	119.42	126.75
3	L5	2363	A2M	N3-C2-N1	-5.61	119.83	128.60
3	L5	3760	A2M	C5-C4-N3	-5.60	119.44	126.75
3	L5	3785	A2M	N3-C2-N1	-5.60	119.84	128.60
3	L5	3925	OMU	C4-N3-C2	-5.58	119.21	126.58
3	L5	398	A2M	C5-C4-N3	-5.58	119.47	126.75
3	L5	3744	OMG	C5-C4-N3	-5.58	119.41	128.46
3	L5	4227	OMU	C4-N3-C2	-5.57	119.23	126.58
3	L5	1625	OMG	C5-C4-N3	-5.57	119.43	128.46
3	L5	4370	OMG	C5-C4-N3	-5.56	119.44	128.46
3	L5	3830	A2M	N3-C2-N1	-5.53	119.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	N3-C2-N1	-5.53	119.96	128.60
3	L5	1524	A2M	N3-C2-N1	-5.52	119.96	128.60
3	L5	4637	OMG	C5-C4-N3	-5.52	119.50	128.46
3	L5	3724	A2M	N3-C2-N1	-5.52	119.97	128.60
3	L5	2401	A2M	N3-C2-N1	-5.52	119.97	128.60
3	L5	3825	A2M	N3-C2-N1	-5.51	119.98	128.60
3	L5	2364	OMG	C5-C4-N3	-5.51	119.53	128.46
3	L5	4523	A2M	N3-C2-N1	-5.50	119.99	128.60
3	L5	1316	OMG	C5-C4-N3	-5.49	119.56	128.46
3	L5	3792	OMG	C5-C4-N3	-5.47	119.58	128.46
3	L5	3899	OMG	C5-C4-N3	-5.46	119.61	128.46
3	L5	4494	OMG	C5-C4-N3	-5.45	119.61	128.46
3	L5	4498	OMU	C4-N3-C2	-5.45	119.39	126.58
3	L5	3867	A2M	C5-C4-N3	-5.45	119.64	126.75
3	L5	1524	A2M	C5-C4-N3	-5.45	119.64	126.75
3	L5	4618	OMG	C5-C4-N3	-5.44	119.63	128.46
3	L5	3760	A2M	N3-C2-N1	-5.43	120.11	128.60
3	L5	3724	A2M	C5-C4-N3	-5.43	119.67	126.75
3	L5	3825	A2M	C5-C4-N3	-5.41	119.69	126.75
3	L5	1326	A2M	C5-C4-N3	-5.41	119.69	126.75
3	L5	4571	A2M	N3-C2-N1	-5.41	120.14	128.60
3	L5	3718	A2M	C5-C4-N3	-5.40	119.70	126.75
3	L5	2401	A2M	C5-C4-N3	-5.40	119.71	126.75
3	L5	2837	OMU	C4-N3-C2	-5.39	119.47	126.58
3	L5	400	A2M	C5-C4-N3	-5.37	119.75	126.75
3	L5	1534	A2M	N3-C2-N1	-5.37	120.21	128.60
3	L5	400	A2M	N3-C2-N1	-5.34	120.25	128.60
3	L5	3867	A2M	N3-C2-N1	-5.34	120.25	128.60
3	L5	4590	A2M	C5-C4-N3	-5.33	119.80	126.75
3	L5	398	A2M	N3-C2-N1	-5.32	120.28	128.60
3	L5	4523	A2M	C5-C4-N3	-5.32	119.81	126.75
3	L5	2363	A2M	C5-C4-N3	-5.32	119.81	126.75
3	L5	4196	OMG	C5-C4-N3	-5.30	119.87	128.46
3	L5	3830	A2M	C5-C4-N3	-5.29	119.84	126.75
3	L5	1534	A2M	C5-C4-N3	-5.28	119.86	126.75
3	L5	2415	OMU	C4-N3-C2	-5.26	119.64	126.58
3	L5	3785	A2M	C5-C4-N3	-5.26	119.89	126.75
3	L5	2424	OMG	C5-C4-N3	-5.25	119.95	128.46
3	L5	1522	OMG	C5-C4-N3	-5.22	119.99	128.46
3	L5	1871	A2M	C5-C4-N3	-5.19	119.97	126.75
3	L5	4306	OMU	C4-N3-C2	-5.18	119.74	126.58
3	L5	4571	A2M	C5-C4-N3	-5.16	120.01	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4623	OMG	C5-C4-N3	-5.13	120.13	128.46
3	L5	4590	A2M	N6-C6-N1	-5.10	107.19	118.35
3	L5	3718	A2M	N3-C2-N1	-5.10	120.63	128.60
3	L5	2363	A2M	N6-C6-N1	-5.08	107.22	118.35
3	L5	398	A2M	N6-C6-N1	-5.08	107.23	118.35
3	L5	3627	OMG	C5-C4-N3	-5.02	120.31	128.46
3	L5	3724	A2M	N6-C6-N1	-5.00	107.40	118.35
3	L5	2401	A2M	N6-C6-N1	-4.99	107.42	118.35
3	L5	2839	PSU	C4-N3-C2	-4.98	119.16	126.34
3	L5	4571	A2M	N6-C6-N1	-4.98	107.45	118.35
3	L5	4620	OMU	C4-N3-C2	-4.98	120.02	126.58
3	L5	1326	A2M	N6-C6-N1	-4.97	107.47	118.35
3	L5	1534	A2M	N6-C6-N1	-4.96	107.48	118.35
3	L5	3760	A2M	N6-C6-N1	-4.96	107.49	118.35
3	L5	4220	6MZ	C5-C4-N3	-4.95	120.29	126.75
3	L5	1524	A2M	N6-C6-N1	-4.95	107.51	118.35
3	L5	3830	A2M	N6-C6-N1	-4.94	107.54	118.35
3	L5	3818	UY1	C4-N3-C2	-4.92	119.25	126.34
3	L5	2815	A2M	N6-C6-N1	-4.89	107.63	118.35
3	L5	400	A2M	N6-C6-N1	-4.88	107.66	118.35
3	L5	3867	A2M	N6-C6-N1	-4.88	107.67	118.35
3	L5	3825	A2M	N6-C6-N1	-4.88	107.67	118.35
3	L5	4228	OMG	C5-C4-N3	-4.87	120.55	128.46
3	L5	2787	A2M	N6-C6-N1	-4.87	107.69	118.35
3	L5	1871	A2M	N6-C6-N1	-4.81	107.81	118.35
3	L5	4457	PSU	C4-N3-C2	-4.80	119.42	126.34
3	L5	3785	A2M	N6-C6-N1	-4.80	107.84	118.35
3	L5	3718	A2M	N6-C6-N1	-4.79	107.86	118.35
47	Pt	58	1MA	N1-C2-N3	-4.79	120.31	126.00
3	L5	3770	PSU	C4-N3-C2	-4.78	119.45	126.34
3	L5	4392	OMG	C2-N3-C4	4.75	120.77	112.30
3	L5	4521	PSU	C4-N3-C2	-4.74	119.50	126.34
3	L5	3734	PSU	C4-N3-C2	-4.74	119.51	126.34
3	L5	3637	PSU	C4-N3-C2	-4.74	119.52	126.34
3	L5	4530	UR3	C4-N3-C2	-4.73	120.11	124.56
3	L5	4442	PSU	C4-N3-C2	-4.73	119.53	126.34
3	L5	4576	PSU	C4-N3-C2	-4.70	119.56	126.34
3	L5	3758	PSU	C4-N3-C2	-4.70	119.57	126.34
3	L5	4296	PSU	C4-N3-C2	-4.70	119.57	126.34
3	L5	4431	PSU	C4-N3-C2	-4.68	119.60	126.34
3	L5	4493	PSU	C4-N3-C2	-4.67	119.61	126.34
3	L5	4312	PSU	C4-N3-C2	-4.66	119.62	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2508	PSU	C4-N3-C2	-4.66	119.62	126.34
3	L5	4353	PSU	C4-N3-C2	-4.65	119.63	126.34
3	L5	1536	PSU	C4-N3-C2	-4.65	119.64	126.34
3	L5	3899	OMG	C2-N3-C4	4.64	120.57	112.30
3	L5	1782	PSU	C4-N3-C2	-4.64	119.66	126.34
3	L5	3695	PSU	C4-N3-C2	-4.63	119.67	126.34
3	L5	2876	OMG	C2-N3-C4	4.63	120.54	112.30
3	L5	1862	PSU	C4-N3-C2	-4.62	119.69	126.34
3	L5	3639	PSU	C4-N3-C2	-4.62	119.69	126.34
3	L5	4523	A2M	N6-C6-N1	-4.62	108.24	118.35
3	L5	4972	PSU	C4-N3-C2	-4.61	119.70	126.34
3	L5	4361	PSU	C4-N3-C2	-4.61	119.70	126.34
3	L5	4552	PSU	C4-N3-C2	-4.61	119.70	126.34
3	L5	4403	PSU	C4-N3-C2	-4.60	119.71	126.34
3	L5	4689	PSU	C4-N3-C2	-4.59	119.72	126.34
3	L5	4673	PSU	C4-N3-C2	-4.58	119.74	126.34
3	L5	1779	PSU	C4-N3-C2	-4.58	119.75	126.34
3	L5	4299	PSU	C4-N3-C2	-4.57	119.75	126.34
3	L5	1677	PSU	C4-N3-C2	-4.57	119.76	126.34
3	L5	4579	PSU	C4-N3-C2	-4.56	119.76	126.34
3	L5	4471	PSU	C4-N3-C2	-4.56	119.77	126.34
3	L5	3637	PSU	N1-C2-N3	4.55	120.29	115.13
3	L5	4442	PSU	N1-C2-N3	4.55	120.28	115.13
3	L5	1744	PSU	C4-N3-C2	-4.55	119.79	126.34
3	L5	4370	OMG	C2-N3-C4	4.54	120.39	112.30
3	L5	3884	PSU	C4-N3-C2	-4.54	119.79	126.34
3	L5	2364	OMG	C2-N3-C4	4.53	120.38	112.30
3	L5	1781	PSU	C4-N3-C2	-4.53	119.81	126.34
3	L5	1860	PSU	C4-N3-C2	-4.53	119.82	126.34
3	L5	4618	OMG	C2-N3-C4	4.52	120.34	112.30
3	L5	2839	PSU	N1-C2-N3	4.51	120.24	115.13
3	L5	3851	PSU	C4-N3-C2	-4.51	119.84	126.34
3	L5	3853	PSU	C4-N3-C2	-4.50	119.86	126.34
3	L5	4423	PSU	C4-N3-C2	-4.50	119.86	126.34
3	L5	3792	OMG	C2-N3-C4	4.49	120.30	112.30
3	L5	1792	PSU	C4-N3-C2	-4.49	119.87	126.34
3	L5	1625	OMG	C2-N3-C4	4.46	120.25	112.30
3	L5	4494	OMG	C2-N3-C4	4.45	120.23	112.30
3	L5	1522	OMG	C2-N3-C4	4.44	120.22	112.30
3	L5	3734	PSU	N1-C2-N3	4.44	120.16	115.13
3	L5	1683	PSU	C4-N3-C2	-4.44	119.94	126.34
3	L5	3744	OMG	C2-N3-C4	4.43	120.19	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3785	A2M	N9-C8-N7	-4.43	107.86	113.91
3	L5	4532	PSU	C4-N3-C2	-4.43	119.96	126.34
3	L5	4628	PSU	C4-N3-C2	-4.43	119.96	126.34
3	L5	1316	OMG	C2-N3-C4	4.43	120.19	112.30
3	L5	3760	A2M	N9-C8-N7	-4.42	107.86	113.91
3	L5	1683	PSU	N1-C2-N3	4.42	120.14	115.13
3	L5	5001	PSU	C4-N3-C2	-4.41	119.98	126.34
3	L5	3818	UY1	N1-C2-N3	4.41	120.13	115.13
3	L5	3627	OMG	C1'-N9-C4	-4.41	113.41	126.50
3	L5	4228	OMG	C1'-N9-C4	-4.40	113.43	126.50
3	L5	3627	OMG	C2-N3-C4	4.40	120.13	112.30
3	L5	4569	PSU	C4-N3-C2	-4.40	120.01	126.34
3	L5	1862	PSU	N1-C2-N3	4.39	120.11	115.13
3	L5	4576	PSU	N1-C2-N3	4.39	120.10	115.13
3	L5	3844	PSU	C4-N3-C2	-4.38	120.02	126.34
3	L5	4623	OMG	C2-N3-C4	4.38	120.11	112.30
3	L5	4312	PSU	N1-C2-N3	4.38	120.09	115.13
3	L5	2508	PSU	N1-C2-N3	4.37	120.08	115.13
3	L5	4196	OMG	C2-N3-C4	4.37	120.08	112.30
3	L5	4637	OMG	C2-N3-C4	4.36	120.07	112.30
3	L5	4431	PSU	N1-C2-N3	4.35	120.06	115.13
3	L5	4521	PSU	N1-C2-N3	4.34	120.05	115.13
3	L5	4296	PSU	N1-C2-N3	4.34	120.05	115.13
3	L5	3920	PSU	C4-N3-C2	-4.34	120.09	126.34
3	L5	4673	PSU	N1-C2-N3	4.34	120.04	115.13
3	L5	398	A2M	N9-C8-N7	-4.34	107.98	113.91
3	L5	1677	PSU	N1-C2-N3	4.33	120.04	115.13
3	L5	4293	PSU	C4-N3-C2	-4.32	120.11	126.34
3	L5	3851	PSU	N1-C2-N3	4.31	120.02	115.13
3	L5	4471	PSU	N1-C2-N3	4.30	120.00	115.13
3	L5	2424	OMG	C2-N3-C4	4.30	119.96	112.30
3	L5	4590	A2M	C5-C6-N6	4.30	132.78	123.43
3	L5	3920	PSU	N1-C2-N3	4.29	120.00	115.13
3	L5	3770	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	4447	5MC	C5-C6-N1	-4.28	118.94	123.34
3	L5	4353	PSU	N1-C2-N3	4.28	119.98	115.13
3	L5	4228	OMG	C2-N3-C4	4.28	119.92	112.30
3	L5	1782	PSU	N1-C2-N3	4.27	119.97	115.13
3	L5	4552	PSU	N1-C2-N3	4.27	119.97	115.13
3	L5	4590	A2M	N9-C8-N7	-4.27	108.08	113.91
3	L5	4571	A2M	C5-C6-N6	4.26	132.71	123.43
3	L5	1522	OMG	C1'-N9-C4	-4.25	113.86	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2632	PSU	C4-N3-C2	-4.25	120.21	126.34
3	L5	1744	PSU	N1-C2-N3	4.25	119.94	115.13
3	L5	4457	PSU	N1-C2-N3	4.25	119.94	115.13
3	L5	3724	A2M	C5-C6-N6	4.24	132.66	123.43
3	L5	1524	A2M	N9-C8-N7	-4.24	108.11	113.91
3	L5	1534	A2M	N9-C8-N7	-4.23	108.12	113.91
3	L5	3695	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	4972	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	4493	PSU	N1-C2-N3	4.22	119.92	115.13
3	L5	3724	A2M	N9-C8-N7	-4.22	108.14	113.91
47	Pt	58	1MA	C5-C4-N3	-4.22	120.96	127.26
3	L5	1779	PSU	N1-C2-N3	4.21	119.90	115.13
3	L5	1860	PSU	N1-C2-N3	4.21	119.90	115.13
3	L5	2363	A2M	C5-C6-N6	4.21	132.59	123.43
3	L5	3844	PSU	N1-C2-N3	4.21	119.90	115.13
3	L5	4299	PSU	N1-C2-N3	4.20	119.89	115.13
3	L5	4403	PSU	N1-C2-N3	4.20	119.89	115.13
3	L5	3627	OMG	C1'-N9-C8	4.20	138.66	126.70
3	L5	398	A2M	C5-C6-N6	4.19	132.56	123.43
3	L5	1534	A2M	C5-C6-N6	4.19	132.55	123.43
3	L5	4423	PSU	N1-C2-N3	4.19	119.88	115.13
3	L5	4579	PSU	N1-C2-N3	4.18	119.86	115.13
3	L5	3639	PSU	N1-C2-N3	4.18	119.86	115.13
3	L5	4689	PSU	N1-C2-N3	4.18	119.86	115.13
3	L5	3830	A2M	N9-C8-N7	-4.17	108.21	113.91
3	L5	3830	A2M	C5-C6-N6	4.17	132.50	123.43
3	L5	2401	A2M	C5-C6-N6	4.16	132.49	123.43
3	L5	1781	PSU	N1-C2-N3	4.16	119.84	115.13
3	L5	1326	A2M	N9-C8-N7	-4.16	108.23	113.91
3	L5	4220	6MZ	N9-C8-N7	-4.15	108.23	113.91
3	L5	4361	PSU	N1-C2-N3	4.15	119.83	115.13
3	L5	4569	PSU	N1-C2-N3	4.15	119.83	115.13
3	L5	4420	PSU	C4-N3-C2	-4.15	120.36	126.34
3	L5	4623	OMG	C1'-N9-C4	-4.15	114.19	126.50
3	L5	4628	PSU	N1-C2-N3	4.14	119.83	115.13
3	L5	4571	A2M	N9-C8-N7	-4.14	108.25	113.91
3	L5	400	A2M	C5-C6-N6	4.14	132.44	123.43
3	L5	2401	A2M	N9-C8-N7	-4.14	108.25	113.91
3	L5	4523	A2M	N9-C8-N7	-4.14	108.25	113.91
3	L5	3925	OMU	N3-C2-N1	4.14	120.38	114.89
3	L5	2363	A2M	N9-C8-N7	-4.13	108.27	113.91
3	L5	2632	PSU	N1-C2-N3	4.12	119.80	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1524	A2M	C5-C6-N6	4.12	132.40	123.43
3	L5	3884	PSU	N1-C2-N3	4.12	119.80	115.13
3	L5	3867	A2M	N9-C8-N7	-4.12	108.28	113.91
3	L5	1871	A2M	C5-C6-N6	4.11	132.38	123.43
3	L5	3825	A2M	N9-C8-N7	-4.11	108.29	113.91
3	L5	4532	PSU	N1-C2-N3	4.11	119.79	115.13
3	L5	1326	A2M	C5-C6-N6	4.11	132.37	123.43
3	L5	3853	PSU	N1-C2-N3	4.08	119.75	115.13
3	L5	400	A2M	N9-C8-N7	-4.08	108.34	113.91
3	L5	1871	A2M	N9-C8-N7	-4.06	108.36	113.91
3	L5	4228	OMG	C1'-N9-C8	4.05	138.24	126.70
3	L5	3758	PSU	N1-C2-N3	4.04	119.71	115.13
3	L5	1536	PSU	N1-C2-N3	4.03	119.70	115.13
3	L5	3718	A2M	C5-C6-N6	4.03	132.19	123.43
3	L5	3867	A2M	C5-C6-N6	4.02	132.18	123.43
3	L5	1522	OMG	C1'-N9-C8	4.01	138.11	126.70
3	L5	2815	A2M	C5-C6-N6	4.00	132.14	123.43
3	L5	3825	A2M	C5-C6-N6	3.99	132.11	123.43
3	L5	1792	PSU	N1-C2-N3	3.98	119.64	115.13
3	L5	2424	OMG	C1'-N9-C4	-3.97	114.71	126.50
3	L5	2787	A2M	C5-C6-N6	3.95	132.03	123.43
3	L5	2876	OMG	N9-C4-N3	3.94	133.84	125.94
3	L5	3760	A2M	C5-C6-N6	3.93	131.99	123.43
3	L5	4306	OMU	N3-C2-N1	3.92	120.10	114.89
3	L5	4293	PSU	N1-C2-N3	3.92	119.57	115.13
3	L5	4220	6MZ	C9-N6-C6	-3.90	119.52	122.87
3	L5	2815	A2M	N9-C8-N7	-3.89	108.60	113.91
3	L5	4498	OMU	N3-C2-N1	3.88	120.05	114.89
3	L5	4227	OMU	N3-C2-N1	3.88	120.04	114.89
3	L5	2837	OMU	N3-C2-N1	3.88	120.04	114.89
3	L5	4196	OMG	C1'-N9-C4	-3.88	114.98	126.50
3	L5	5001	PSU	N1-C2-N3	3.85	119.50	115.13
3	L5	4623	OMG	C1'-N9-C8	3.85	137.65	126.70
3	L5	4523	A2M	C5-C6-N6	3.84	131.78	123.43
3	L5	4370	OMG	C1'-N9-C4	-3.83	115.12	126.50
3	L5	2424	OMG	C1'-N9-C8	3.82	137.56	126.70
3	L5	1322	1MA	C2-N3-C4	3.81	119.89	112.41
3	L5	2787	A2M	N9-C8-N7	-3.80	108.72	113.91
3	L5	3899	OMG	C1'-N9-C4	-3.78	115.26	126.50
3	L5	3785	A2M	C5-C6-N6	3.77	131.64	123.43
3	L5	4618	OMG	C1'-N9-C4	-3.77	115.31	126.50
3	L5	2815	A2M	C2-N3-C4	3.76	120.63	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	C2-N3-C4	3.75	120.61	111.75
3	L5	1326	A2M	C2-N3-C4	3.73	120.57	111.75
3	L5	4392	OMG	C1'-N9-C4	-3.73	115.42	126.50
3	L5	4420	PSU	N1-C2-N3	3.73	119.35	115.13
3	L5	1316	OMG	C1'-N9-C4	-3.71	115.48	126.50
3	L5	2415	OMU	N3-C2-N1	3.70	119.80	114.89
3	L5	1524	A2M	C2-N3-C4	3.68	120.44	111.75
3	L5	4637	OMG	C1'-N9-C4	-3.68	115.58	126.50
3	L5	4392	OMG	C1'-N9-C8	3.67	137.15	126.70
3	L5	4220	6MZ	C4-C5-C6	3.66	119.65	116.81
3	L5	4590	A2M	C2-N3-C4	3.66	120.40	111.75
3	L5	3760	A2M	C2-N3-C4	3.65	120.37	111.75
3	L5	4620	OMU	N3-C2-N1	3.65	119.73	114.89
3	L5	3724	A2M	C2-N3-C4	3.64	120.36	111.75
3	L5	3744	OMG	C1'-N9-C4	-3.63	115.73	126.50
3	L5	2401	A2M	C2-N3-C4	3.62	120.29	111.75
3	L5	3825	A2M	C2-N3-C4	3.61	120.29	111.75
3	L5	3785	A2M	C2-N3-C4	3.61	120.27	111.75
3	L5	4494	OMG	C1'-N9-C4	-3.61	115.79	126.50
3	L5	3818	UY1	C6-C5-C4	3.61	120.72	118.20
3	L5	2363	A2M	C2-N3-C4	3.60	120.26	111.75
3	L5	398	A2M	C2-N3-C4	3.60	120.25	111.75
3	L5	4498	OMU	C5-C4-N3	3.60	120.22	114.84
3	L5	3718	A2M	N9-C8-N7	-3.58	109.02	113.91
3	L5	2364	OMG	C1'-N9-C4	-3.57	115.89	126.50
3	L5	4618	OMG	C1'-N9-C8	3.56	136.84	126.70
3	L5	1322	1MA	C5-C4-N3	-3.56	121.95	127.26
3	L5	4523	A2M	C2-N3-C4	3.55	120.15	111.75
3	L5	1871	A2M	C2-N3-C4	3.55	120.14	111.75
3	L5	4196	OMG	C1'-N9-C8	3.55	136.80	126.70
3	L5	3867	A2M	C2-N3-C4	3.55	120.13	111.75
3	L5	4370	OMG	C1'-N9-C8	3.54	136.77	126.70
3	L5	4227	OMU	C5-C4-N3	3.54	120.13	114.84
3	L5	4637	OMG	C1'-N9-C8	3.53	136.74	126.70
3	L5	3899	OMG	N9-C4-N3	3.52	133.00	125.94
3	L5	3830	A2M	C2-N3-C4	3.51	120.05	111.75
3	L5	4220	6MZ	C2-N3-C4	3.51	120.03	111.75
47	Pt	58	1MA	C2-N3-C4	3.50	119.29	112.41
3	L5	3925	OMU	C5-C4-N3	3.50	120.07	114.84
3	L5	400	A2M	C2-N3-C4	3.50	120.01	111.75
3	L5	3744	OMG	C1'-N9-C8	3.48	136.61	126.70
3	L5	1316	OMG	C1'-N9-C8	3.48	136.59	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1534	A2M	C2-N3-C4	3.47	119.95	111.75
3	L5	2364	OMG	C1'-N9-C8	3.46	136.55	126.70
3	L5	4571	A2M	C2-N3-C4	3.45	119.91	111.75
3	L5	2837	OMU	C5-C4-N3	3.45	120.00	114.84
3	L5	2876	OMG	C2-N1-C6	-3.45	118.81	125.10
3	L5	4494	OMG	C1'-N9-C8	3.44	136.49	126.70
47	Pt	58	1MA	N9-C8-N7	-3.44	106.91	113.39
3	L5	1625	OMG	N9-C4-N3	3.44	132.84	125.94
48	S2	918	PSU	C3'-C2'-C1'	3.43	105.63	101.64
3	L5	3782	5MC	C5-C6-N1	-3.42	119.82	123.34
3	L5	3792	OMG	N9-C4-N3	3.41	132.79	125.94
3	L5	4370	OMG	C2-N1-C6	-3.41	118.88	125.10
3	L5	3760	A2M	N3-C4-N9	3.41	132.70	127.08
3	L5	1316	OMG	N9-C4-N3	3.41	132.78	125.94
3	L5	4370	OMG	N9-C4-N3	3.40	132.76	125.94
3	L5	2415	OMU	C5-C4-N3	3.39	119.91	114.84
3	L5	398	A2M	C5-N7-C8	3.39	108.32	103.51
3	L5	4306	OMU	C5-C4-N3	3.37	119.89	114.84
3	L5	3899	OMG	C1'-N9-C8	3.37	136.30	126.70
3	L5	2815	A2M	N3-C4-N9	3.36	132.62	127.08
3	L5	2787	A2M	N3-C4-N9	3.34	132.59	127.08
3	L5	3734	PSU	C6-C5-C4	3.34	120.53	118.20
3	L5	3718	A2M	C2-N3-C4	3.34	119.64	111.75
3	L5	3867	A2M	N3-C4-N9	3.33	132.58	127.08
3	L5	1625	OMG	C1'-N9-C4	-3.33	116.61	126.50
3	L5	4196	OMG	N9-C4-N3	3.32	132.61	125.94
3	L5	4637	OMG	N9-C4-N3	3.32	132.60	125.94
3	L5	1524	A2M	N3-C4-N9	3.30	132.52	127.08
3	L5	4618	OMG	N9-C4-N3	3.30	132.56	125.94
3	L5	4494	OMG	N9-C4-N3	3.29	132.55	125.94
3	L5	3744	OMG	N9-C4-N3	3.29	132.54	125.94
3	L5	4620	OMU	C5-C4-N3	3.29	119.75	114.84
3	L5	4523	A2M	N3-C4-N9	3.28	132.49	127.08
3	L5	4392	OMG	N9-C4-N3	3.28	132.52	125.94
3	L5	3785	A2M	N3-C4-N9	3.25	132.44	127.08
3	L5	2401	A2M	N3-C4-N9	3.25	132.44	127.08
3	L5	1683	PSU	C6-N1-C2	-3.24	119.37	122.68
3	L5	3899	OMG	C2-N1-C6	-3.22	119.23	125.10
3	L5	3744	OMG	C2-N1-C6	-3.22	119.23	125.10
3	L5	1625	OMG	C1'-N9-C8	3.22	135.85	126.70
3	L5	4196	OMG	C2-N1-C6	-3.22	119.23	125.10
3	L5	1534	A2M	C5-N7-C8	3.21	108.07	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2364	OMG	N9-C4-N3	3.20	132.37	125.94
3	L5	2363	A2M	N3-C4-N9	3.19	132.34	127.08
3	L5	3760	A2M	C5-N7-C8	3.18	108.02	103.51
3	L5	1326	A2M	C5-N7-C8	3.17	108.02	103.51
48	S2	822	PSU	C3'-C2'-C1'	3.17	105.33	101.64
3	L5	3825	A2M	N3-C4-N9	3.17	132.30	127.08
3	L5	3718	A2M	N3-C4-N9	3.17	132.30	127.08
3	L5	1524	A2M	C5-N7-C8	3.16	108.00	103.51
3	L5	3920	PSU	C6-N1-C2	-3.16	119.45	122.68
3	L5	2364	OMG	C2-N1-C6	-3.16	119.35	125.10
3	L5	2632	PSU	C6-N1-C2	-3.15	119.46	122.68
3	L5	2424	OMG	N9-C4-N3	3.15	132.27	125.94
3	L5	398	A2M	N3-C4-N9	3.15	132.28	127.08
3	L5	400	A2M	N3-C4-N9	3.15	132.28	127.08
3	L5	1522	OMG	C2-N1-C6	-3.15	119.36	125.10
3	L5	2424	OMG	C2-N1-C6	-3.15	119.36	125.10
3	L5	1625	OMG	C2-N1-C6	-3.13	119.39	125.10
3	L5	3724	A2M	N3-C4-N9	3.13	132.24	127.08
3	L5	3792	OMG	C1'-N9-C4	-3.13	117.22	126.50
3	L5	1326	A2M	N3-C4-N9	3.12	132.23	127.08
3	L5	1677	PSU	C6-N1-C2	-3.12	119.50	122.68
3	L5	4423	PSU	C6-N1-C2	-3.11	119.50	122.68
3	L5	4590	A2M	C5-N7-C8	3.11	107.93	103.51
3	L5	1316	OMG	C2-N1-C6	-3.11	119.43	125.10
3	L5	4590	A2M	N3-C4-N9	3.11	132.20	127.08
3	L5	3785	A2M	O4'-C1'-N9	3.10	114.18	108.06
3	L5	4637	OMG	C2-N1-C6	-3.09	119.46	125.10
3	L5	3724	A2M	C5-N7-C8	3.09	107.90	103.51
3	L5	4523	A2M	C2'-C1'-N9	-3.09	108.33	113.53
3	L5	1522	OMG	N9-C4-N3	3.08	132.13	125.94
3	L5	4442	PSU	C6-N1-C2	-3.08	119.53	122.68
3	L5	4618	OMG	C2-N1-C6	-3.08	119.49	125.10
3	L5	3830	A2M	C5-N7-C8	3.07	107.88	103.51
48	S2	1851	MA6	C2-N1-C6	3.07	119.01	111.75
3	L5	3851	PSU	C6-N1-C2	-3.07	119.54	122.68
48	S2	1850	MA6	C2-N1-C6	3.07	118.99	111.75
3	L5	3825	A2M	C5-N7-C8	3.06	107.86	103.51
3	L5	4392	OMG	C2-N1-C6	-3.06	119.52	125.10
3	L5	2401	A2M	C5-N7-C8	3.06	107.86	103.51
3	L5	4523	A2M	C5-N7-C8	3.06	107.85	103.51
3	L5	400	A2M	C5-N7-C8	3.05	107.85	103.51
3	L5	3844	PSU	C6-N1-C2	-3.04	119.58	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4571	A2M	C5-N7-C8	3.04	107.82	103.51
3	L5	1534	A2M	N3-C4-N9	3.04	132.08	127.08
3	L5	3830	A2M	N3-C4-N9	3.03	132.07	127.08
3	L5	4494	OMG	C2-N1-C6	-3.03	119.58	125.10
3	L5	4623	OMG	N9-C4-N3	3.03	132.02	125.94
3	L5	4220	6MZ	C5-N7-C8	3.02	107.80	103.51
3	L5	1744	PSU	C6-N1-C2	-3.02	119.60	122.68
3	L5	4628	PSU	C6-N1-C2	-3.01	119.60	122.68
3	L5	1871	A2M	C5-N7-C8	3.01	107.79	103.51
3	L5	1871	A2M	N3-C4-N9	3.01	132.05	127.08
3	L5	4228	OMG	C2-N1-C6	-3.01	119.62	125.10
3	L5	3867	A2M	C5-N7-C8	3.00	107.77	103.51
3	L5	4623	OMG	C2-N1-C6	-3.00	119.63	125.10
3	L5	2415	OMU	O4-C4-C5	-3.00	119.88	125.16
3	L5	2363	A2M	C5-N7-C8	2.99	107.76	103.51
3	L5	1779	PSU	C6-C5-C4	2.99	120.29	118.20
3	L5	2787	A2M	C5-N7-C8	2.99	107.75	103.51
3	L5	3792	OMG	C1'-N9-C8	2.98	135.19	126.70
3	L5	3785	A2M	C5-N7-C8	2.98	107.74	103.51
3	L5	3899	OMG	N9-C8-N7	-2.98	107.78	113.39
3	L5	4552	PSU	C6-N1-C2	-2.98	119.64	122.68
3	L5	3734	PSU	C6-N1-C2	-2.97	119.64	122.68
3	L5	4370	OMG	C5-C6-N1	2.97	120.73	113.19
3	L5	4431	PSU	C6-N1-C2	-2.97	119.65	122.68
3	L5	2815	A2M	C5-N7-C8	2.97	107.72	103.51
3	L5	3792	OMG	C2-N1-C6	-2.96	119.70	125.10
3	L5	4689	PSU	C6-N1-C2	-2.96	119.66	122.68
3	L5	3884	PSU	C6-N1-C2	-2.96	119.66	122.68
3	L5	4569	PSU	C6-N1-C2	-2.95	119.67	122.68
3	L5	4623	OMG	N9-C8-N7	-2.95	107.84	113.39
3	L5	1677	PSU	O2-C2-N1	-2.95	119.54	122.79
3	L5	1860	PSU	C6-N1-C2	-2.95	119.67	122.68
3	L5	4579	PSU	C6-N1-C2	-2.95	119.67	122.68
3	L5	1862	PSU	C6-C5-C4	2.94	120.26	118.20
3	L5	4312	PSU	C6-N1-C2	-2.94	119.67	122.68
3	L5	4228	OMG	N9-C8-N7	-2.93	107.87	113.39
3	L5	3785	A2M	C2'-C1'-N9	-2.93	108.60	113.53
3	L5	4673	PSU	C6-N1-C2	-2.93	119.69	122.68
3	L5	2839	PSU	C6-C5-C4	2.92	120.24	118.20
3	L5	4571	A2M	N3-C4-N9	2.92	131.90	127.08
3	L5	4442	PSU	C6-C5-C4	2.92	120.24	118.20
3	L5	4498	OMU	O4-C4-C5	-2.91	120.03	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4471	PSU	C6-N1-C2	-2.91	119.71	122.68
3	L5	3627	OMG	C2-N1-C6	-2.90	119.81	125.10
3	L5	2876	OMG	C1'-N9-C4	-2.90	117.90	126.50
3	L5	3899	OMG	C5-C6-N1	2.90	120.54	113.19
3	L5	2508	PSU	C6-N1-C2	-2.89	119.72	122.68
3	L5	1322	1MA	N9-C8-N7	-2.89	107.94	113.39
3	L5	4972	PSU	C6-N1-C2	-2.89	119.73	122.68
3	L5	2508	PSU	C6-C5-C4	2.88	120.22	118.20
3	L5	4227	OMU	O4-C4-C5	-2.88	120.10	125.16
3	L5	1779	PSU	C6-N1-C2	-2.87	119.75	122.68
3	L5	4370	OMG	N9-C8-N7	-2.87	107.99	113.39
3	L5	3627	OMG	N9-C4-N3	2.87	131.70	125.94
3	L5	3637	PSU	C6-N1-C2	-2.87	119.75	122.68
3	L5	4296	PSU	C6-N1-C2	-2.87	119.75	122.68
3	L5	4576	PSU	C6-N1-C2	-2.87	119.75	122.68
48	S2	1081	PSU	C3'-C2'-C1'	2.86	104.97	101.64
3	L5	4220	6MZ	N3-C4-N9	2.85	131.78	127.08
3	L5	2876	OMG	C5-C6-N1	2.85	120.43	113.19
3	L5	1522	OMG	N9-C8-N7	-2.84	108.04	113.39
3	L5	1782	PSU	C6-N1-C2	-2.84	119.78	122.68
3	L5	4196	OMG	C5-C6-N1	2.83	120.38	113.19
3	L5	4228	OMG	N9-C4-N3	2.83	131.62	125.94
3	L5	1862	PSU	C6-N1-C2	-2.83	119.79	122.68
3	L5	4532	PSU	C6-N1-C2	-2.82	119.80	122.68
3	L5	4403	PSU	C6-N1-C2	-2.81	119.81	122.68
3	L5	1781	PSU	C6-N1-C2	-2.81	119.81	122.68
3	L5	3920	PSU	C6-C5-C4	2.80	120.16	118.20
3	L5	4521	PSU	C6-N1-C2	-2.80	119.82	122.68
3	L5	4576	PSU	C6-C5-C4	2.80	120.16	118.20
3	L5	4353	PSU	C6-N1-C2	-2.80	119.82	122.68
3	L5	4299	PSU	C6-N1-C2	-2.79	119.83	122.68
3	L5	4312	PSU	O2-C2-N1	-2.79	119.72	122.79
3	L5	1522	OMG	C5-C6-N1	2.78	120.26	113.19
3	L5	3695	PSU	C6-N1-C2	-2.77	119.85	122.68
82	SX	62	HY3	O-C-CA	-2.77	117.11	124.83
3	L5	4618	OMG	C5-C6-N1	2.77	120.22	113.19
3	L5	1677	PSU	C6-C5-C4	2.76	120.13	118.20
3	L5	5001	PSU	C6-N1-C2	-2.76	119.86	122.68
3	L5	3627	OMG	N9-C8-N7	-2.75	108.20	113.39
3	L5	4196	OMG	N9-C8-N7	-2.75	108.22	113.39
3	L5	1683	PSU	O2-C2-N1	-2.74	119.77	122.79
3	L5	4293	PSU	C6-N1-C2	-2.74	119.88	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2424	OMG	C5-C6-N1	2.74	120.14	113.19
3	L5	1316	OMG	N9-C8-N7	-2.73	108.24	113.39
3	L5	1316	OMG	C5-C6-N1	2.72	120.11	113.19
3	L5	3853	PSU	C6-N1-C2	-2.72	119.90	122.68
3	L5	4392	OMG	C5-C6-N1	2.72	120.11	113.19
3	L5	3744	OMG	C5-C6-N1	2.72	120.10	113.19
3	L5	4623	OMG	C5-C6-N1	2.72	120.10	113.19
3	L5	2364	OMG	C5-C6-N1	2.72	120.09	113.19
3	L5	1625	OMG	C5-C6-N1	2.71	120.08	113.19
3	L5	4493	PSU	C6-N1-C2	-2.71	119.91	122.68
3	L5	3627	OMG	C5-C6-N1	2.71	120.08	113.19
3	L5	3770	PSU	C6-N1-C2	-2.71	119.91	122.68
3	L5	4618	OMG	N9-C8-N7	-2.71	108.29	113.39
3	L5	4228	OMG	C5-C6-N1	2.71	120.07	113.19
3	L5	2837	OMU	O4-C4-C5	-2.71	120.40	125.16
3	L5	4420	PSU	C6-N1-C2	-2.71	119.92	122.68
3	L5	4457	PSU	C6-C5-C4	2.70	120.09	118.20
3	L5	3760	A2M	O4'-C1'-C2'	-2.70	101.83	106.57
3	L5	4361	PSU	C6-N1-C2	-2.70	119.93	122.68
3	L5	2839	PSU	C6-N1-C2	-2.69	119.93	122.68
3	L5	3695	PSU	C6-C5-C4	2.69	120.08	118.20
3	L5	2876	OMG	O6-C6-C5	-2.69	119.47	126.60
3	L5	3925	OMU	O4-C4-C5	-2.68	120.44	125.16
3	L5	4620	OMU	O4-C4-C5	-2.68	120.45	125.16
3	L5	3899	OMG	O6-C6-C5	-2.68	119.50	126.60
3	L5	4579	PSU	O2-C2-N1	-2.68	119.84	122.79
3	L5	2876	OMG	C1'-N9-C8	2.68	134.31	126.70
3	L5	1782	PSU	C6-C5-C4	2.67	120.07	118.20
3	L5	3639	PSU	C6-N1-C2	-2.67	119.95	122.68
3	L5	1862	PSU	O2-C2-N1	-2.67	119.85	122.79
3	L5	4353	PSU	C6-C5-C4	2.67	120.06	118.20
3	L5	4196	OMG	O6-C6-C5	-2.67	119.53	126.60
3	L5	4442	PSU	O2-C2-N1	-2.66	119.86	122.79
3	L5	1744	PSU	O2-C2-N1	-2.66	119.86	122.79
3	L5	4494	OMG	C5-C6-N1	2.66	119.94	113.19
3	L5	3718	A2M	C5-N7-C8	2.65	107.28	103.51
3	L5	2876	OMG	N9-C8-N7	-2.65	108.40	113.39
3	L5	3744	OMG	N9-C8-N7	-2.65	108.40	113.39
3	L5	4494	OMG	N9-C8-N7	-2.65	108.40	113.39
3	L5	4312	PSU	C6-C5-C4	2.64	120.05	118.20
3	L5	4637	OMG	C5-C6-N1	2.64	119.88	113.19
3	L5	2839	PSU	O2-C2-N1	-2.63	119.89	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4637	OMG	N9-C8-N7	-2.63	108.43	113.39
3	L5	3734	PSU	O2-C2-N1	-2.63	119.90	122.79
3	L5	4392	OMG	N9-C8-N7	-2.62	108.45	113.39
3	L5	4403	PSU	C6-C5-C4	2.62	120.03	118.20
3	L5	4457	PSU	C6-N1-C2	-2.62	120.00	122.68
3	L5	3758	PSU	C6-N1-C2	-2.62	120.01	122.68
3	L5	3818	UY1	C6-N1-C2	-2.61	120.01	122.68
3	L5	3792	OMG	O6-C6-C5	-2.61	119.67	126.60
3	L5	2424	OMG	O6-C6-C5	-2.61	119.67	126.60
80	LA	216	V5N	O-C-CA	-2.61	117.94	124.78
3	L5	4457	PSU	O2-C2-N1	-2.60	119.92	122.79
3	L5	2364	OMG	N9-C8-N7	-2.60	108.49	113.39
3	L5	4299	PSU	C6-C5-C4	2.60	120.01	118.20
3	L5	4471	PSU	C6-C5-C4	2.60	120.01	118.20
3	L5	1625	OMG	O6-C6-C5	-2.59	119.72	126.60
3	L5	3792	OMG	C5-C6-N1	2.59	119.76	113.19
3	L5	3639	PSU	C6-C5-C4	2.59	120.01	118.20
3	L5	2424	OMG	N9-C8-N7	-2.59	108.52	113.39
3	L5	3851	PSU	O2-C2-N1	-2.58	119.95	122.79
3	L5	4306	OMU	O4-C4-C5	-2.57	120.65	125.16
3	L5	1536	PSU	C6-N1-C2	-2.56	120.07	122.68
3	L5	4628	PSU	O2-C2-N1	-2.55	119.98	122.79
3	L5	1871	A2M	C2'-C1'-N9	-2.55	109.23	113.53
48	S2	1243	PSU	C2'-C3'-C4'	-2.55	97.68	102.64
3	L5	4228	OMG	O6-C6-C5	-2.54	119.87	126.60
3	L5	4370	OMG	O6-C6-C5	-2.54	119.87	126.60
3	L5	4521	PSU	C6-C5-C4	2.53	119.97	118.20
3	L5	4623	OMG	O6-C6-C5	-2.53	119.89	126.60
3	L5	4431	PSU	O2-C2-N1	-2.52	120.01	122.79
3	L5	4423	PSU	O2-C2-N1	-2.52	120.02	122.79
3	L5	4673	PSU	C6-C5-C4	2.51	119.95	118.20
3	L5	3770	PSU	O2-C2-N1	-2.50	120.03	122.79
3	L5	1522	OMG	O6-C6-C5	-2.50	119.97	126.60
3	L5	4569	PSU	C6-C5-C4	2.50	119.94	118.20
3	L5	4689	PSU	O2-C2-N1	-2.49	120.04	122.79
3	L5	3639	PSU	O2-C2-N1	-2.49	120.05	122.79
3	L5	3792	OMG	N9-C8-N7	-2.49	108.71	113.39
3	L5	3844	PSU	O2-C2-N1	-2.48	120.06	122.79
3	L5	1536	PSU	O2-C2-N1	-2.48	120.06	122.79
3	L5	1792	PSU	C6-N1-C2	-2.48	120.15	122.68
3	L5	4403	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	4493	PSU	C6-C5-C4	2.46	119.92	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2508	PSU	O2-C2-N1	-2.46	120.09	122.79
3	L5	4618	OMG	O6-C6-C5	-2.45	120.10	126.60
3	L5	1316	OMG	O6-C6-C5	-2.44	120.11	126.60
3	L5	4494	OMG	O6-C6-C5	-2.44	120.11	126.60
3	L5	1625	OMG	N9-C8-N7	-2.44	108.79	113.39
3	L5	4431	PSU	C6-C5-C4	2.44	119.90	118.20
3	L5	4552	PSU	O2-C2-N1	-2.43	120.12	122.79
3	L5	1524	A2M	C4'-O4'-C1'	-2.43	104.12	109.47
3	L5	3637	PSU	C6-C5-C4	2.42	119.89	118.20
3	L5	398	A2M	C4-C5-N7	-2.42	107.67	110.62
3	L5	1779	PSU	O2-C2-N1	-2.42	120.13	122.79
3	L5	4532	PSU	O2-C2-N1	-2.41	120.14	122.79
3	L5	4420	PSU	O2-C2-N1	-2.41	120.14	122.79
3	L5	3718	A2M	C6-C5-C4	2.41	120.42	117.18
3	L5	3851	PSU	C6-C5-C4	2.40	119.88	118.20
3	L5	4673	PSU	O2-C2-N1	-2.40	120.15	122.79
3	L5	4361	PSU	O2-C2-N1	-2.40	120.15	122.79
3	L5	3627	OMG	O6-C6-C5	-2.40	120.24	126.60
3	L5	2364	OMG	O6-C6-C5	-2.39	120.26	126.60
3	L5	4576	PSU	O2-C2-N1	-2.38	120.17	122.79
3	L5	3785	A2M	C4-N9-C8	2.37	108.30	105.73
3	L5	1536	PSU	C6-C5-C4	2.37	119.86	118.20
3	L5	3744	OMG	O6-C6-C5	-2.37	120.32	126.60
3	L5	1781	PSU	C6-C5-C4	2.37	119.85	118.20
3	L5	3818	UY1	O2-C2-N1	-2.36	120.19	122.79
3	L5	4493	PSU	O2-C2-N1	-2.36	120.19	122.79
3	L5	4637	OMG	O6-C6-C5	-2.36	120.35	126.60
3	L5	4296	PSU	C6-C5-C4	2.35	119.84	118.20
3	L5	1860	PSU	C6-C5-C4	2.35	119.84	118.20
3	L5	1860	PSU	O2-C2-N1	-2.35	120.20	122.79
3	L5	1322	1MA	C5-C4-N9	2.35	109.89	105.63
3	L5	4521	PSU	O2-C2-N1	-2.34	120.21	122.79
3	L5	4392	OMG	O6-C6-C5	-2.34	120.39	126.60
3	L5	3760	A2M	C4'-O4'-C1'	-2.33	104.32	109.47
3	L5	1322	1MA	C4-C5-N7	-2.33	107.03	110.72
3	L5	4972	PSU	O2-C2-N1	-2.33	120.22	122.79
3	L5	4353	PSU	O2-C2-N1	-2.32	120.23	122.79
3	L5	4689	PSU	C6-C5-C4	2.32	119.82	118.20
3	L5	3884	PSU	O2-C2-N1	-2.31	120.25	122.79
3	L5	3853	PSU	O2-C2-N1	-2.29	120.27	122.79
3	L5	3770	PSU	C6-C5-C4	2.29	119.80	118.20
3	L5	4552	PSU	C6-C5-C4	2.29	119.80	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3758	PSU	C6-C5-C4	2.28	119.80	118.20
3	L5	1781	PSU	O2-C2-N1	-2.26	120.30	122.79
3	L5	3844	PSU	C6-C5-C4	2.26	119.78	118.20
3	L5	1534	A2M	C4-C5-N7	-2.25	107.88	110.62
3	L5	3782	5MC	CM5-C5-C6	-2.25	119.84	122.85
3	L5	3760	A2M	C6-C5-C4	2.25	120.20	117.18
3	L5	1683	PSU	C6-C5-C4	2.25	119.77	118.20
3	L5	4532	PSU	C6-C5-C4	2.24	119.77	118.20
3	L5	1782	PSU	O2-C2-N1	-2.24	120.32	122.79
3	L5	2787	A2M	C6-C5-C4	2.24	120.19	117.18
3	L5	1792	PSU	C6-C5-C4	2.24	119.76	118.20
3	L5	4471	PSU	O2-C2-N1	-2.23	120.34	122.79
3	L5	398	A2M	C6-C5-C4	2.23	120.18	117.18
3	L5	3867	A2M	C6-C5-C4	2.23	120.17	117.18
3	L5	3920	PSU	O2-C2-N1	-2.22	120.35	122.79
3	L5	4972	PSU	C6-C5-C4	2.22	119.75	118.20
47	Pt	58	1MA	C8-N7-C5	2.21	108.25	104.24
3	L5	4403	PSU	O4'-C1'-C2'	2.20	108.25	105.14
3	L5	4569	PSU	O2-C2-N1	-2.20	120.37	122.79
3	L5	400	A2M	C6-C5-C4	2.19	120.13	117.18
3	L5	3760	A2M	C4-N9-C8	2.19	108.10	105.73
3	L5	2876	OMG	C8-N7-C5	2.19	108.21	104.24
3	L5	1534	A2M	C6-C5-C4	2.19	120.12	117.18
3	L5	4296	PSU	O2-C2-N1	-2.18	120.39	122.79
30	La	39	V5N	O-C-CA	-2.17	119.09	124.78
3	L5	1326	A2M	C4-C5-N7	-2.16	107.98	110.62
3	L5	3724	A2M	C4-C5-N7	-2.16	107.99	110.62
3	L5	5001	PSU	C6-C5-C4	2.15	119.70	118.20
47	Pt	58	1MA	N9-C4-N3	2.15	131.96	126.94
3	L5	4523	A2M	C6-C5-C4	2.15	120.08	117.18
3	L5	4306	OMU	O2-C2-N1	-2.15	119.93	122.79
3	L5	4498	OMU	O2-C2-N1	-2.14	119.94	122.79
3	L5	398	A2M	C5-C4-N9	2.13	108.26	105.78
3	L5	4579	PSU	C6-C5-C4	2.13	119.69	118.20
3	L5	4442	PSU	O4'-C1'-C2'	2.12	108.14	105.14
3	L5	4620	OMU	O2-C2-N1	-2.12	119.97	122.79
3	L5	1677	PSU	O4'-C1'-C2'	2.12	108.14	105.14
3	L5	4571	A2M	C4-C5-N7	-2.12	108.04	110.62
3	L5	1316	OMG	C8-N7-C5	2.12	108.08	104.24
3	L5	3899	OMG	C8-N7-C5	2.12	108.08	104.24
3	L5	4220	6MZ	C4-N9-C1'	-2.12	121.55	126.59
3	L5	1322	1MA	C2'-C1'-N9	2.12	119.22	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3830	A2M	C6-C5-C4	2.11	120.03	117.18
3	L5	4370	OMG	C8-N7-C5	2.11	108.07	104.24
3	L5	4623	OMG	C8-N7-C5	2.11	108.07	104.24
3	L5	4361	PSU	C6-C5-C4	2.11	119.67	118.20
3	L5	3724	A2M	C6-C5-C4	2.11	120.02	117.18
3	L5	4299	PSU	O2-C2-N1	-2.11	120.47	122.79
3	L5	1792	PSU	O2-C2-N1	-2.11	120.47	122.79
3	L5	4590	A2M	C4-C5-N7	-2.10	108.06	110.62
3	L5	4392	OMG	C8-N7-C5	2.10	108.05	104.24
3	L5	1524	A2M	C6-C5-C4	2.10	120.01	117.18
3	L5	400	A2M	C4-C5-N7	-2.10	108.06	110.62
3	L5	3830	A2M	C4-C5-N7	-2.10	108.06	110.62
3	L5	3825	A2M	C6-C5-C4	2.10	120.00	117.18
3	L5	4227	OMU	O2-C2-N1	-2.10	120.00	122.79
3	L5	2632	PSU	O2-C2-N1	-2.09	120.49	122.79
3	L5	1524	A2M	C4-C5-N7	-2.09	108.07	110.62
3	L5	4571	A2M	C6-C5-C4	2.09	119.99	117.18
3	L5	3744	OMG	C8-N7-C5	2.08	108.01	104.24
3	L5	1744	PSU	C6-C5-C4	2.08	119.65	118.20
3	L5	3695	PSU	O2-C2-N1	-2.08	120.50	122.79
3	L5	2815	A2M	C6-C5-C4	2.07	119.97	117.18
3	L5	1524	A2M	C4-N9-C8	2.07	107.97	105.73
3	L5	1522	OMG	C8-N7-C5	2.07	107.98	104.24
3	L5	1322	1MA	C8-N7-C5	2.06	107.97	104.24
3	L5	4220	6MZ	C4-C5-N7	-2.06	108.11	110.62
47	Pt	37	1MG	O2'-C2'-C3'	-2.06	105.16	111.82
3	L5	2787	A2M	C5-C4-N9	2.06	108.17	105.78
3	L5	3825	A2M	C4-C5-N7	-2.06	108.11	110.62
3	L5	4423	PSU	C6-C5-C4	2.05	119.63	118.20
3	L5	2364	OMG	C8-N7-C5	2.05	107.95	104.24
3	L5	2401	A2M	C6-C5-C4	2.05	119.94	117.18
6	LB	245	HIC	CB-CG-CD2	-2.05	124.54	129.81
3	L5	4637	OMG	C8-N7-C5	2.05	107.95	104.24
3	L5	4494	OMG	C8-N7-C5	2.05	107.94	104.24
3	L5	3830	A2M	C2'-C1'-N9	-2.05	110.09	113.53
47	Pt	37	1MG	CM1-N1-C2	-2.04	118.60	120.72
3	L5	1871	A2M	C4-C5-N7	-2.04	108.14	110.62
3	L5	4590	A2M	C4-N9-C8	2.04	107.94	105.73
3	L5	4618	OMG	C8-N7-C5	2.04	107.93	104.24
3	L5	4220	6MZ	C4-N9-C8	2.03	107.93	105.73
3	L5	3760	A2M	C4-C5-N7	-2.03	108.15	110.62
3	L5	3925	OMU	O2-C2-N1	-2.03	120.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	C4-C5-N7	-2.03	108.15	110.62
3	L5	2401	A2M	C4-C5-N7	-2.02	108.15	110.62
3	L5	4293	PSU	O2-C2-N1	-2.02	120.56	122.79
3	L5	4628	PSU	C6-C5-C4	2.02	119.61	118.20
3	L5	3758	PSU	O2-C2-N1	-2.01	120.58	122.79
3	L5	2363	A2M	C6-C5-C4	2.01	119.88	117.18
3	L5	2363	A2M	C4-N9-C8	2.00	107.90	105.73
3	L5	4228	OMG	C8-N7-C5	2.00	107.87	104.24

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	LA	216	V5N	O-C-CA-CB
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	C1'-C2'-O2'-CM'
3	L5	2415	OMU	C1'-C2'-O2'-CM2
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	3744	OMG	C1'-C2'-O2'-CM2
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4523	A2M	C1'-C2'-O2'-CM'
3	L5	4571	A2M	C1'-C2'-O2'-CM'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	4637	OMG	C1'-C2'-O2'-CM2
5	L8	14	OMU	C1'-C2'-O2'-CM2
48	S2	27	A2M	C1'-C2'-O2'-CM'
48	S2	172	OMU	C3'-C2'-O2'-CM2
48	S2	428	OMU	O4'-C4'-C5'-O5'
48	S2	509	OMG	C1'-C2'-O2'-CM2
48	S2	512	A2M	O4'-C4'-C5'-O5'
48	S2	572	PSU	O4'-C1'-C5-C4
48	S2	572	PSU	O4'-C1'-C5-C6
48	S2	573	PSU	O4'-C1'-C5-C4
48	S2	573	PSU	O4'-C1'-C5-C6
48	S2	576	A2M	C3'-C4'-C5'-O5'
48	S2	601	OMG	C1'-C2'-O2'-CM2
48	S2	644	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
48	S2	644	OMG	C1'-C2'-O2'-CM2
48	S2	668	A2M	O4'-C4'-C5'-O5'
48	S2	668	A2M	C3'-C4'-C5'-O5'
48	S2	822	PSU	C3'-C4'-C5'-O5'
48	S2	867	OMG	C1'-C2'-O2'-CM2
48	S2	1243	PSU	O4'-C4'-C5'-O5'
48	S2	1328	OMG	C1'-C2'-O2'-CM2
48	S2	1442	OMU	C1'-C2'-O2'-CM2
48	S2	1490	OMG	C1'-C2'-O2'-CM2
48	S2	1678	A2M	C1'-C2'-O2'-CM'
48	S2	1804	OMU	C1'-C2'-O2'-CM2
48	S2	1832	6MZ	C5-C6-N6-C9
48	S2	1832	6MZ	N1-C6-N6-C9
48	S2	1851	MA6	O4'-C4'-C5'-O5'
48	S2	1851	MA6	C3'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
3	L5	4532	PSU	O4'-C4'-C5'-O5'
48	S2	512	A2M	C3'-C4'-C5'-O5'
48	S2	644	OMG	C3'-C4'-C5'-O5'
48	S2	683	OMG	O4'-C4'-C5'-O5'
48	S2	683	OMG	C3'-C4'-C5'-O5'
48	S2	822	PSU	O4'-C4'-C5'-O5'
48	S2	1243	PSU	C3'-C4'-C5'-O5'
48	S2	1442	OMU	O4'-C4'-C5'-O5'
48	S2	1447	OMG	C3'-C4'-C5'-O5'
3	L5	4532	PSU	C3'-C4'-C5'-O5'
48	S2	428	OMU	C3'-C4'-C5'-O5'
48	S2	576	A2M	O4'-C4'-C5'-O5'
48	S2	428	OMU	C2'-C1'-N1-C6
3	L5	4447	5MC	C2'-C1'-N1-C6
48	S2	428	OMU	C2'-C1'-N1-C2
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4569	PSU	C3'-C4'-C5'-O5'
48	S2	1442	OMU	C3'-C4'-C5'-O5'
3	L5	1781	PSU	C3'-C4'-C5'-O5'
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	3851	PSU	O4'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
48	S2	1447	OMG	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
48	S2	1248	B8N	N34-C33-C34-O36

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Mol	Chain	Res	Type	Atoms
47	Pt	58	1MA	O4'-C4'-C5'-O5'
43	Lo	53	MLZ	CG-CD-CE-NZ
3	L5	4500	PSU	C4'-C5'-O5'-P
3	L5	2422	OMC	C3'-C4'-C5'-O5'
48	S2	1248	B8N	N34-C33-C34-O35
48	S2	1842	4AC	O7-C7-N4-C4
48	S2	1842	4AC	CM7-C7-N4-C4
3	L5	4569	PSU	O4'-C4'-C5'-O5'
48	S2	99	A2M	O4'-C4'-C5'-O5'
48	S2	428	OMU	O4'-C1'-N1-C2
48	S2	428	OMU	O4'-C1'-N1-C6
3	L5	3818	UY1	C4'-C5'-O5'-P
48	S2	1243	PSU	C4'-C5'-O5'-P
3	L5	2787	A2M	C2'-C1'-N9-C4
43	Lo	53	MLZ	CA-CB-CG-CD
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	1625	OMG	C3'-C2'-O2'-CM2
3	L5	2401	A2M	C3'-C2'-O2'-CM'
3	L5	4370	OMG	C3'-C2'-O2'-CM2
48	S2	627	OMU	C3'-C2'-O2'-CM2
3	L5	4447	5MC	O4'-C1'-N1-C6
31	Lb	5	MLZ	N-CA-CB-CG
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	4447	5MC	O4'-C1'-N1-C2
48	S2	1851	MA6	C4'-C5'-O5'-P
41	Lm	98	M3L	CD-CE-NZ-CM3
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	1792	PSU	O4'-C4'-C5'-O5'
3	L5	4196	OMG	O4'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	3844	PSU	C4'-C5'-O5'-P
47	Pt	9	1MG	C4'-C5'-O5'-P
48	S2	1490	OMG	C4'-C5'-O5'-P
30	La	39	V5N	O2-CB-CG-CD2
3	L5	3869	OMC	C3'-C2'-O2'-CM2
3	L5	1534	A2M	O4'-C4'-C5'-O5'
3	L5	1781	PSU	O4'-C4'-C5'-O5'
46	Mr	4	B8H	O4'-C1'-C5-C4
3	L5	2363	A2M	C3'-C2'-O2'-CM'
41	Lm	98	M3L	CD-CE-NZ-CM2

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Mol	Chain	Res	Type	Atoms
3	L5	2787	A2M	O4'-C1'-N9-C8
3	L5	1322	1MA	C2'-C1'-N9-C4
1	At	58	MA7	C4'-C5'-O5'-P
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	4196	OMG	C3'-C4'-C5'-O5'
41	Lm	98	M3L	CD-CE-NZ-CM1
1	At	58	MA7	C2'-C1'-N9-C4
48	S2	627	OMU	C1'-C2'-O2'-CM2
48	S2	668	A2M	C1'-C2'-O2'-CM'
3	L5	1322	1MA	C2'-C1'-N9-C8
1	At	58	MA7	O4'-C4'-C5'-O5'
3	L5	1677	PSU	O4'-C1'-C5-C6
46	Mr	4	B8H	O4'-C1'-C5-C6
3	L5	2815	A2M	C4'-C5'-O5'-P
48	S2	644	OMG	C4'-C5'-O5'-P
48	S2	1081	PSU	C4'-C5'-O5'-P
3	L5	2351	OMC	O4'-C4'-C5'-O5'
47	Pt	58	1MA	C3'-C4'-C5'-O5'
48	S2	99	A2M	C3'-C4'-C5'-O5'
48	S2	1490	OMG	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C2'-C1'-N9-C8
48	S2	918	PSU	C4'-C5'-O5'-P
48	S2	1288	OMU	C2'-C1'-N1-C2

There are no ring outliers.

61 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	576	A2M	1	0
47	Pt	26	M2G	2	0
3	L5	3770	PSU	1	0
3	L5	4306	OMU	1	0
3	L5	3818	UY1	1	0
3	L5	1871	A2M	1	0
3	L5	2415	OMU	4	0
3	L5	2364	OMG	2	0
48	S2	644	OMG	1	0
3	L5	3701	OMC	1	0
3	L5	4536	OMC	1	0
47	Pt	9	1MG	1	0
3	L5	4620	OMU	3	0
3	L5	2351	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2363	A2M	2	0
3	L5	1340	OMC	2	0
3	L5	4447	5MC	2	0
3	L5	2815	A2M	1	0
3	L5	2804	OMC	1	0
3	L5	4299	PSU	3	0
3	L5	4499	OMG	2	0
48	S2	121	OMU	2	0
1	At	58	MA7	1	0
3	L5	3724	A2M	1	0
5	L8	14	OMU	1	0
48	S2	1328	OMG	1	0
3	L5	4498	OMU	1	0
3	L5	3718	A2M	4	0
3	L5	1326	A2M	2	0
3	L5	2422	OMC	1	0
48	S2	1239	PSU	1	0
3	L5	4637	OMG	3	0
48	S2	1639	G7M	1	0
48	S2	867	OMG	1	0
48	S2	1391	OMC	1	0
3	L5	4552	PSU	1	0
3	L5	4457	PSU	1	0
3	L5	3867	A2M	2	0
48	S2	27	A2M	2	0
48	S2	573	PSU	1	0
3	L5	3925	OMU	1	0
3	L5	4579	PSU	1	0
3	L5	3744	OMG	1	0
3	L5	4392	OMG	2	0
3	L5	2632	PSU	1	0
48	S2	601	OMG	1	0
3	L5	4532	PSU	1	0
48	S2	116	OMU	2	0
3	L5	2876	OMG	1	0
48	S2	1442	OMU	2	0
48	S2	1851	MA6	1	0
3	L5	4196	OMG	1	0
48	S2	1490	OMG	1	0
3	L5	4220	6MZ	3	0
3	L5	1625	OMG	2	0
3	L5	4571	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1860	PSU	1	0
48	S2	509	OMG	4	0
3	L5	2861	OMC	2	0
3	L5	4523	A2M	1	0
48	S2	1678	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 447 ligands modelled in this entry, 418 are monoatomic - leaving 29 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	$\# Z > 2$
88	PUT	L5	5379	-	5,5,5	0.22	0	4,4,4	0.19	0
87	SPD	L5	5377	-	9,9,9	0.43	0	8,8,8	0.31	0
90	HYG	S2	2021	84	35,39,39	0.54	1 (2%)	43,60,60	0.88	3 (6%)
88	PUT	L5	5381	-	5,5,5	0.25	0	4,4,4	0.25	0
88	PUT	S2	2018	-	5,5,5	0.15	0	4,4,4	0.20	0
87	SPD	L5	5376	-	9,9,9	0.42	0	8,8,8	0.36	0
87	SPD	L5	5386	-	9,9,9	0.43	0	8,8,8	0.40	0
87	SPD	LN	301	-	9,9,9	0.41	0	8,8,8	0.35	0
87	SPD	L5	5385	-	9,9,9	0.44	0	8,8,8	0.33	0
87	SPD	L8	205	-	9,9,9	0.44	0	8,8,8	0.35	0
87	SPD	S2	2017	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	S2	2016	-	9,9,9	0.17	0	8,8,8	0.20	0
88	PUT	L5	5382	-	5,5,5	0.24	0	4,4,4	0.20	0
88	PUT	L5	5387	-	5,5,5	0.24	0	4,4,4	0.07	0
88	PUT	L5	5384	-	5,5,5	0.23	0	4,4,4	0.17	0
87	SPD	L5	5370	-	9,9,9	0.43	0	8,8,8	0.26	0
88	PUT	L5	5383	-	5,5,5	0.22	0	4,4,4	0.20	0
87	SPD	S2	2014	-	9,9,9	0.43	0	8,8,8	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPD	L5	5374	-	9,9,9	0.41	0	8,8,8	0.41	0
88	PUT	L5	5380	-	5,5,5	0.23	0	4,4,4	0.17	0
87	SPD	L5	5369	-	9,9,9	0.42	0	8,8,8	0.41	0
87	SPD	S2	2019	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	L5	5372	-	9,9,9	0.42	0	8,8,8	0.29	0
87	SPD	L5	5373	-	9,9,9	0.44	0	8,8,8	0.27	0
88	PUT	S2	2020	-	5,5,5	0.16	0	4,4,4	0.25	0
87	SPD	L5	5378	-	9,9,9	0.43	0	8,8,8	0.23	0
87	SPD	S2	2015	-	9,9,9	0.18	0	8,8,8	0.21	0
87	SPD	L5	5375	-	9,9,9	0.44	0	8,8,8	0.42	0
87	SPD	L5	5371	-	9,9,9	0.39	0	8,8,8	0.43	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
88	PUT	L5	5379	-	-	0/3/3/3	-
87	SPD	L5	5377	-	-	0/7/7/7	-
90	HYG	S2	2021	84	1/1/16/17	4/12/87/87	0/4/4/4
88	PUT	L5	5381	-	-	0/3/3/3	-
88	PUT	S2	2018	-	-	2/3/3/3	-
87	SPD	L5	5376	-	-	0/7/7/7	-
87	SPD	L5	5386	-	-	0/7/7/7	-
87	SPD	LN	301	-	-	1/7/7/7	-
87	SPD	L5	5385	-	-	0/7/7/7	-
87	SPD	L8	205	-	-	0/7/7/7	-
87	SPD	S2	2017	-	-	5/7/7/7	-
87	SPD	S2	2016	-	-	3/7/7/7	-
88	PUT	L5	5382	-	-	0/3/3/3	-
88	PUT	L5	5387	-	-	0/3/3/3	-
88	PUT	L5	5384	-	-	0/3/3/3	-
87	SPD	L5	5370	-	-	0/7/7/7	-
88	PUT	L5	5383	-	-	0/3/3/3	-
87	SPD	S2	2014	-	-	0/7/7/7	-
87	SPD	L5	5374	-	-	1/7/7/7	-
88	PUT	L5	5380	-	-	0/3/3/3	-
87	SPD	L5	5369	-	-	0/7/7/7	-
87	SPD	S2	2019	-	-	7/7/7/7	-
87	SPD	L5	5372	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	L5	5373	-	-	0/7/7/7	-
88	PUT	S2	2020	-	-	2/3/3/3	-
87	SPD	L5	5378	-	-	0/7/7/7	-
87	SPD	S2	2015	-	-	6/7/7/7	-
87	SPD	L5	5375	-	-	1/7/7/7	-
87	SPD	L5	5371	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	S2	2021	HYG	O28-C23	2.32	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	S2	2021	HYG	C23-O28-C27	2.12	116.04	112.00
90	S2	2021	HYG	O14-C13-C12	2.06	113.59	109.51
90	S2	2021	HYG	O29-C12-C13	2.01	116.14	110.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
90	S2	2021	HYG	C12

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	S2	2016	SPD	C4-C5-N6-C7
87	S2	2017	SPD	C8-C7-N6-C5
87	S2	2019	SPD	N6-C7-C8-C9
87	S2	2017	SPD	C3-C4-C5-N6
87	S2	2015	SPD	C3-C4-C5-N6
90	S2	2021	HYG	O14-C15-C19-O20
87	S2	2015	SPD	N6-C7-C8-C9
87	S2	2017	SPD	N6-C7-C8-C9
87	S2	2016	SPD	C8-C7-N6-C5
87	S2	2019	SPD	C8-C7-N6-C5
87	S2	2019	SPD	C3-C4-C5-N6
87	S2	2019	SPD	N1-C2-C3-C4
87	S2	2019	SPD	C2-C3-C4-C5
87	S2	2015	SPD	C7-C8-C9-N10

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Mol	Chain	Res	Type	Atoms
87	S2	2016	SPD	C7-C8-C9-N10
87	S2	2017	SPD	C7-C8-C9-N10
90	S2	2021	HYG	C16-C15-C19-O20
88	S2	2020	PUT	C1-C2-C3-C4
87	L5	5375	SPD	C8-C7-N6-C5
88	S2	2018	PUT	C1-C2-C3-C4
90	S2	2021	HYG	O28-C27-C33-C34
88	S2	2018	PUT	N1-C1-C2-C3
87	L5	5371	SPD	N1-C2-C3-C4
87	S2	2015	SPD	C2-C3-C4-C5
87	S2	2019	SPD	C7-C8-C9-N10
87	S2	2015	SPD	C8-C7-N6-C5
87	S2	2017	SPD	C4-C5-N6-C7
87	S2	2019	SPD	C4-C5-N6-C7
90	S2	2021	HYG	C26-C27-C33-C34
87	L5	5374	SPD	C3-C4-C5-N6
87	LN	301	SPD	C4-C5-N6-C7
87	S2	2015	SPD	N1-C2-C3-C4
88	S2	2020	PUT	C2-C3-C4-N2

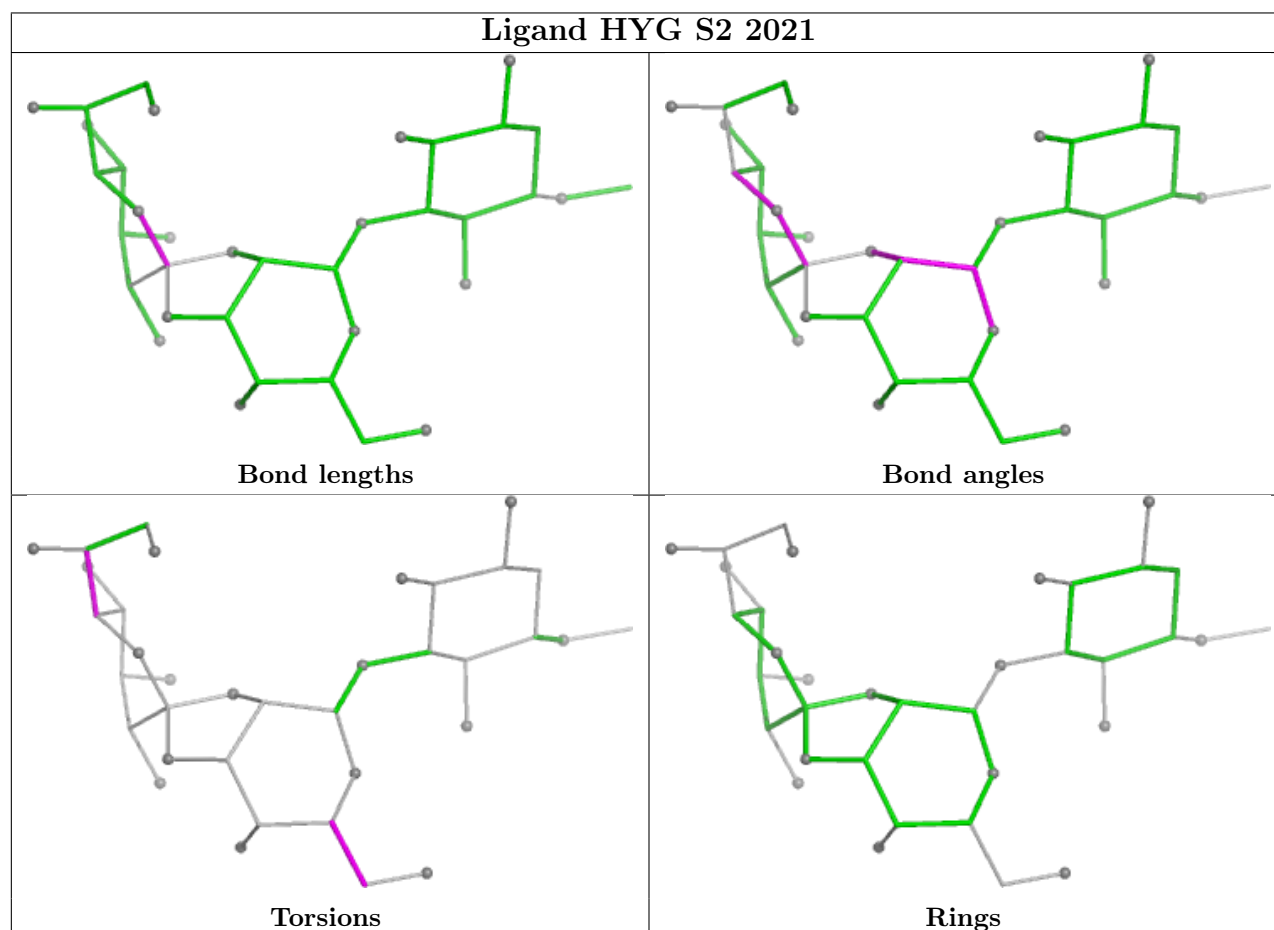
There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	S2	2021	HYG	1	0
88	L5	5381	PUT	1	0
87	L8	205	SPD	1	0
87	S2	2017	SPD	1	0
87	S2	2016	SPD	1	0
88	L5	5387	PUT	1	0
87	L5	5374	SPD	1	0
88	L5	5380	PUT	1	0
87	S2	2019	SPD	1	0
87	L5	5373	SPD	3	0
87	L5	5371	SPD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

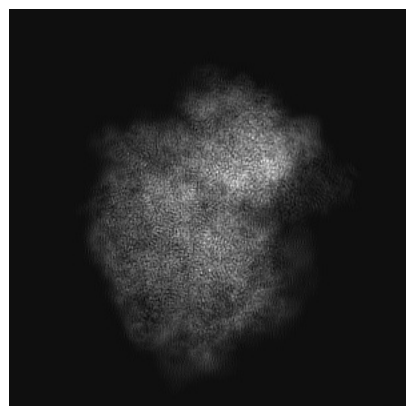
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55083. These allow visual inspection of the internal detail of the map and identification of artifacts.

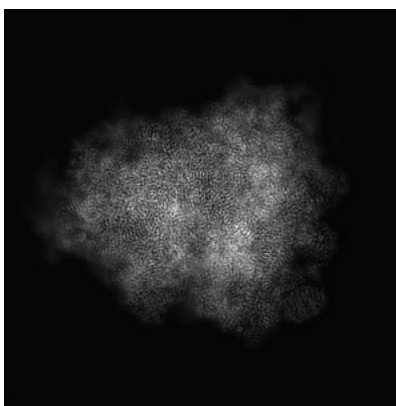
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

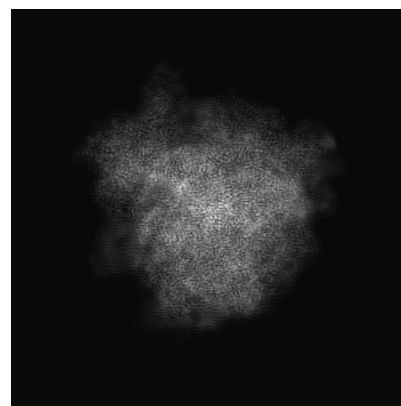
6.1.1 Primary map



X

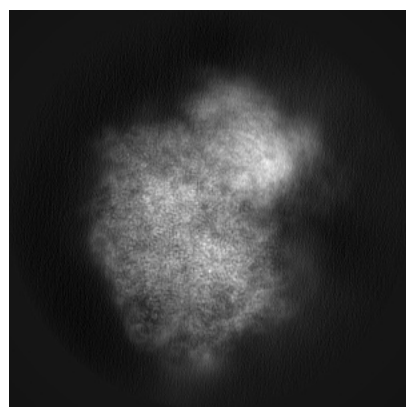


Y

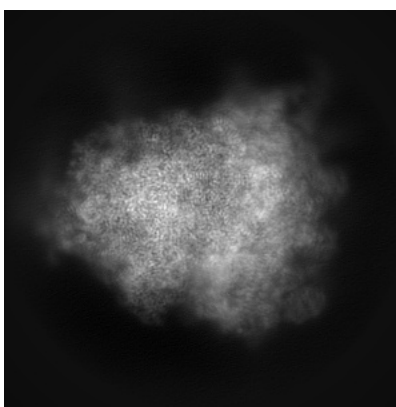


Z

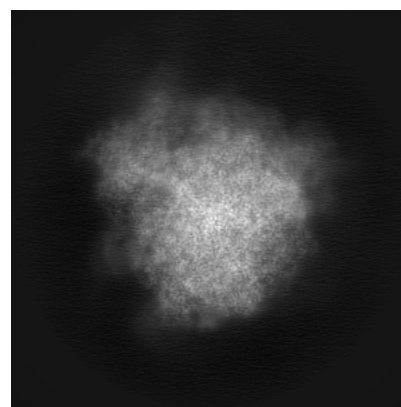
6.1.2 Raw map



X



Y

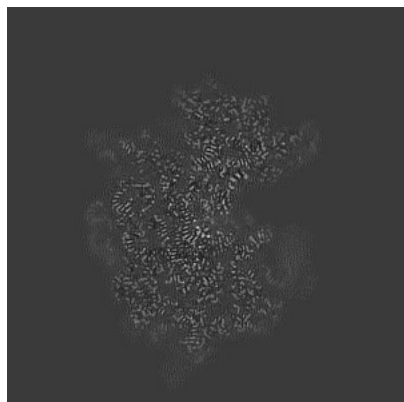


Z

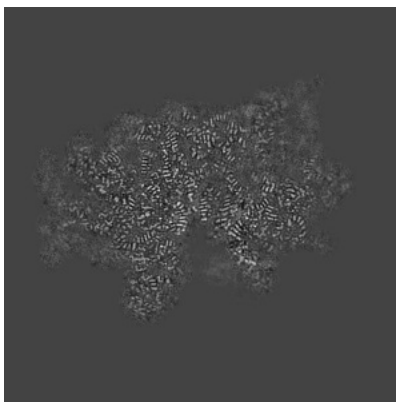
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

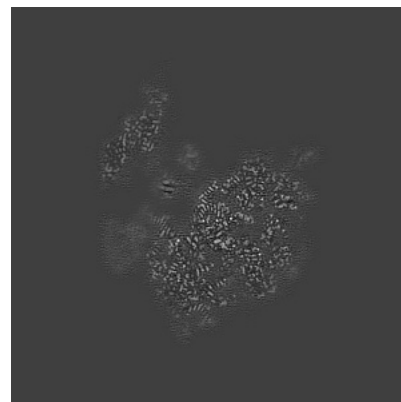
6.2.1 Primary map



X Index: 240

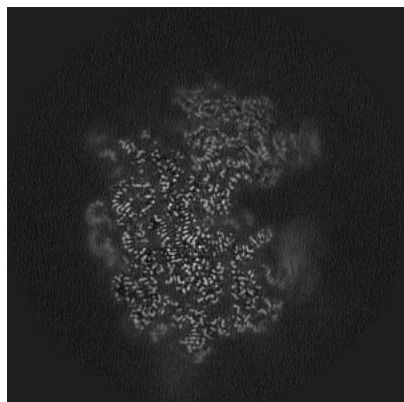


Y Index: 240

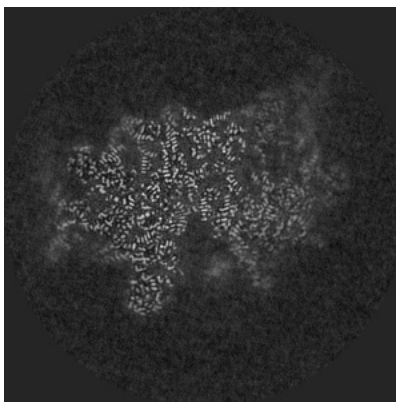


Z Index: 240

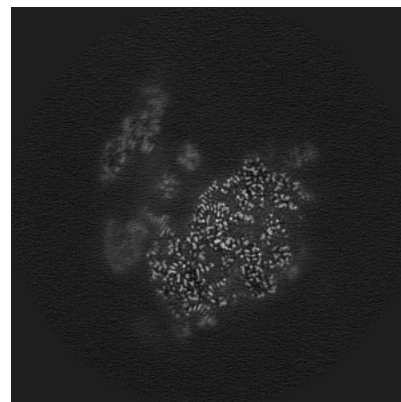
6.2.2 Raw map



X Index: 240



Y Index: 240

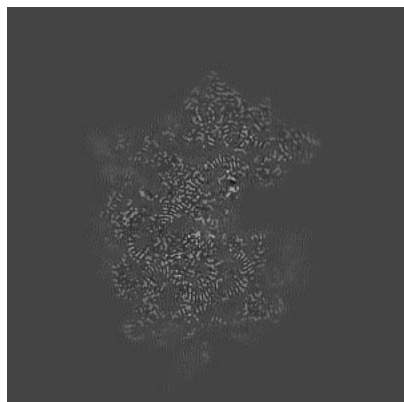


Z Index: 240

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

6.3 Largest variance slices [i](#)

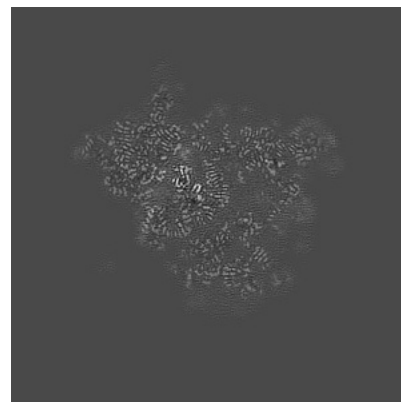
6.3.1 Primary map



X Index: 250

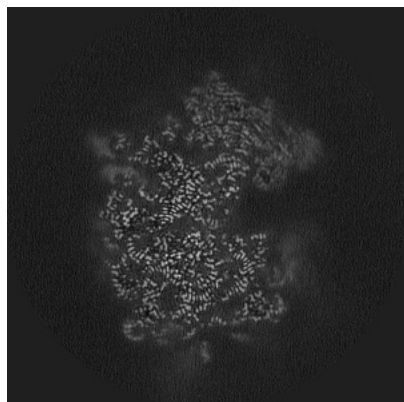


Y Index: 239

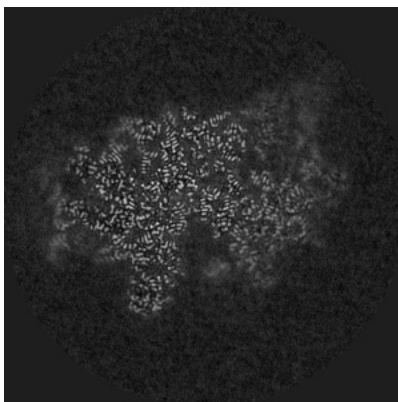


Z Index: 294

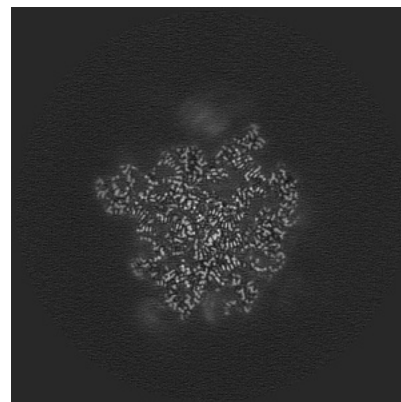
6.3.2 Raw map



X Index: 250



Y Index: 239

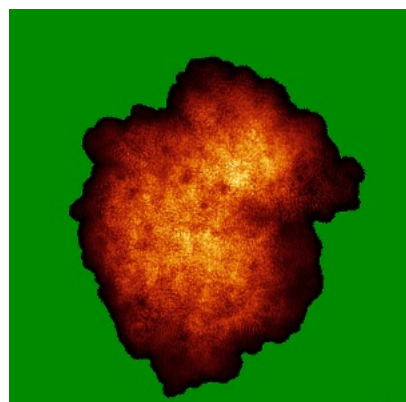


Z Index: 184

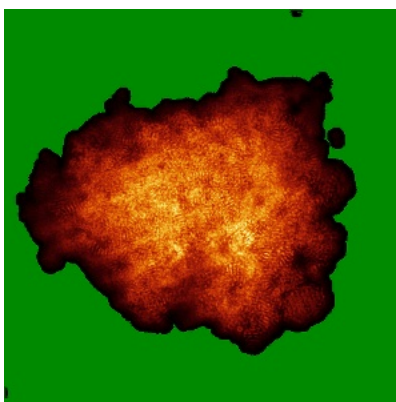
The images above show the largest variance slices of the map in three orthogonal directions.

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

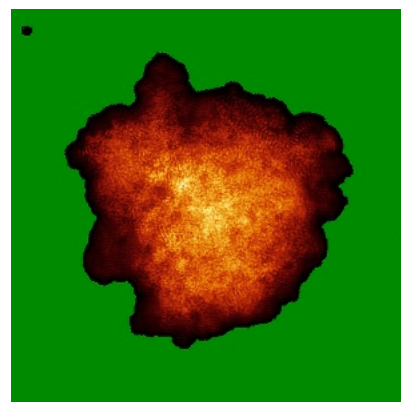
6.4.1 Primary map



X

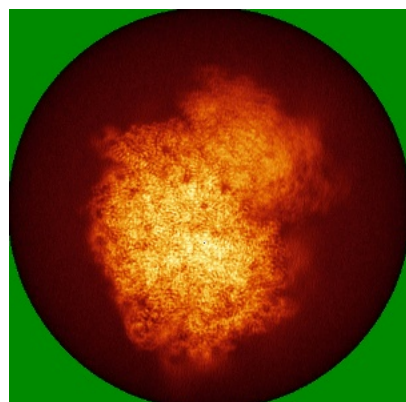


Y

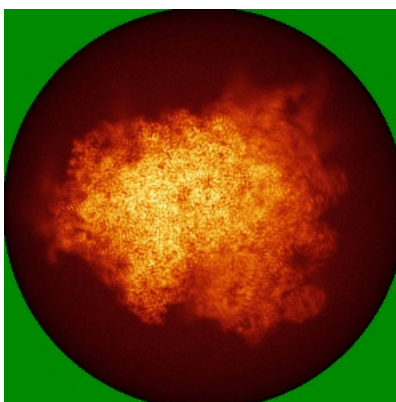


Z

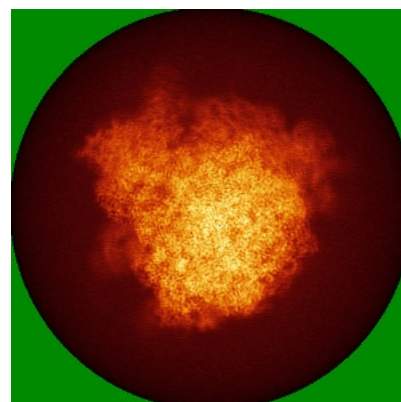
6.4.2 Raw map



X



Y

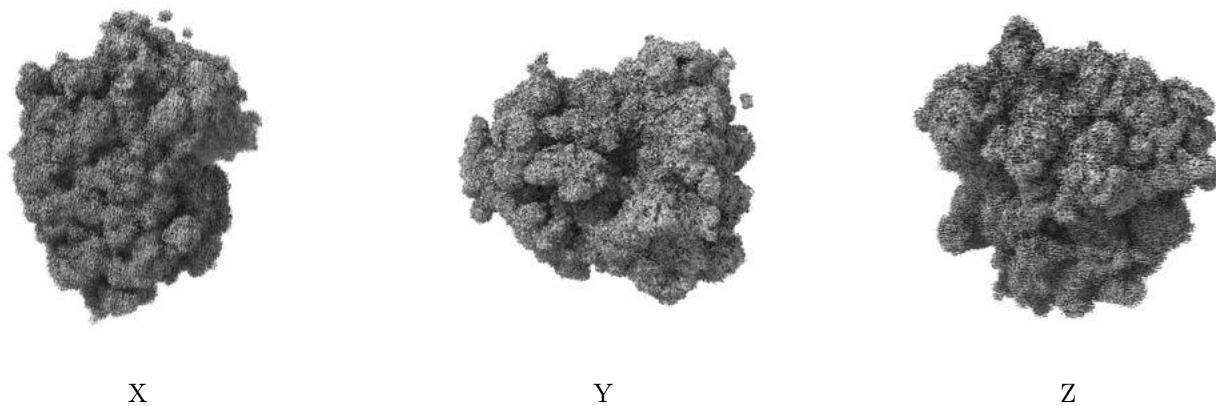


Z

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

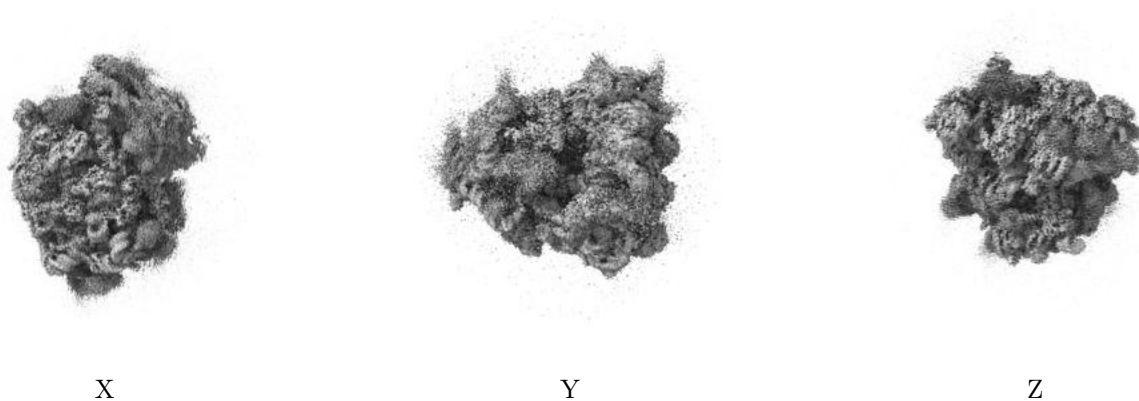
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

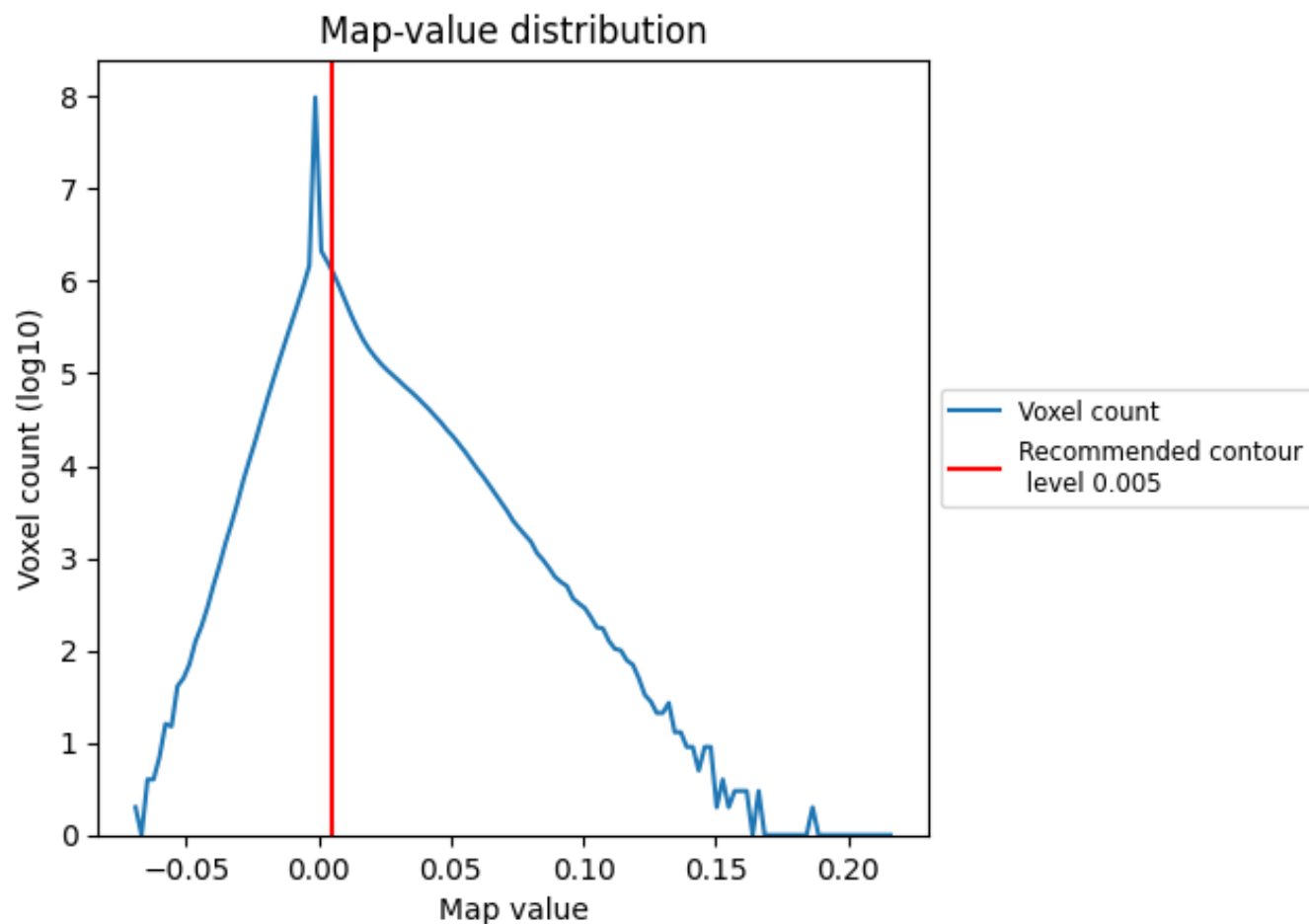
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

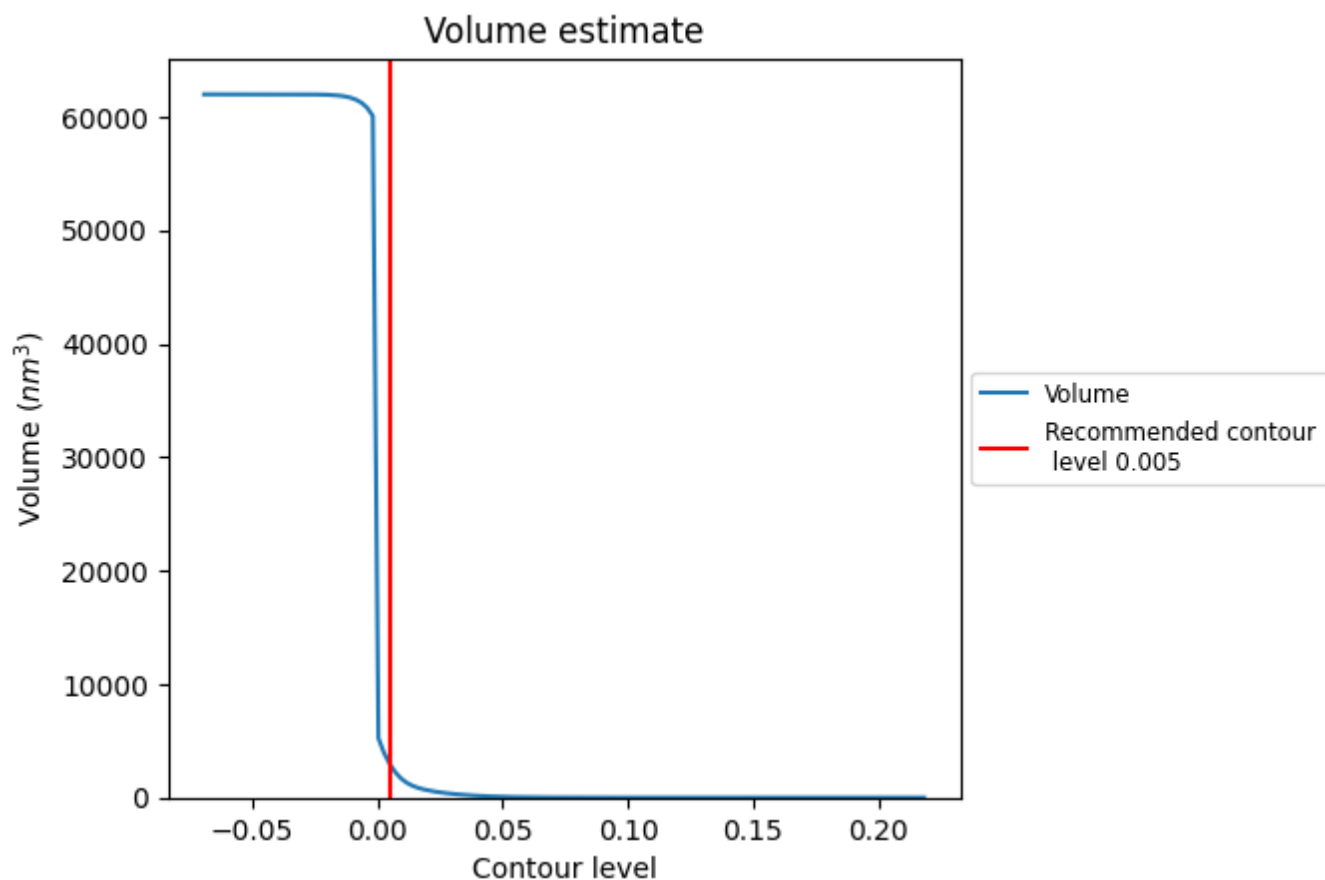
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

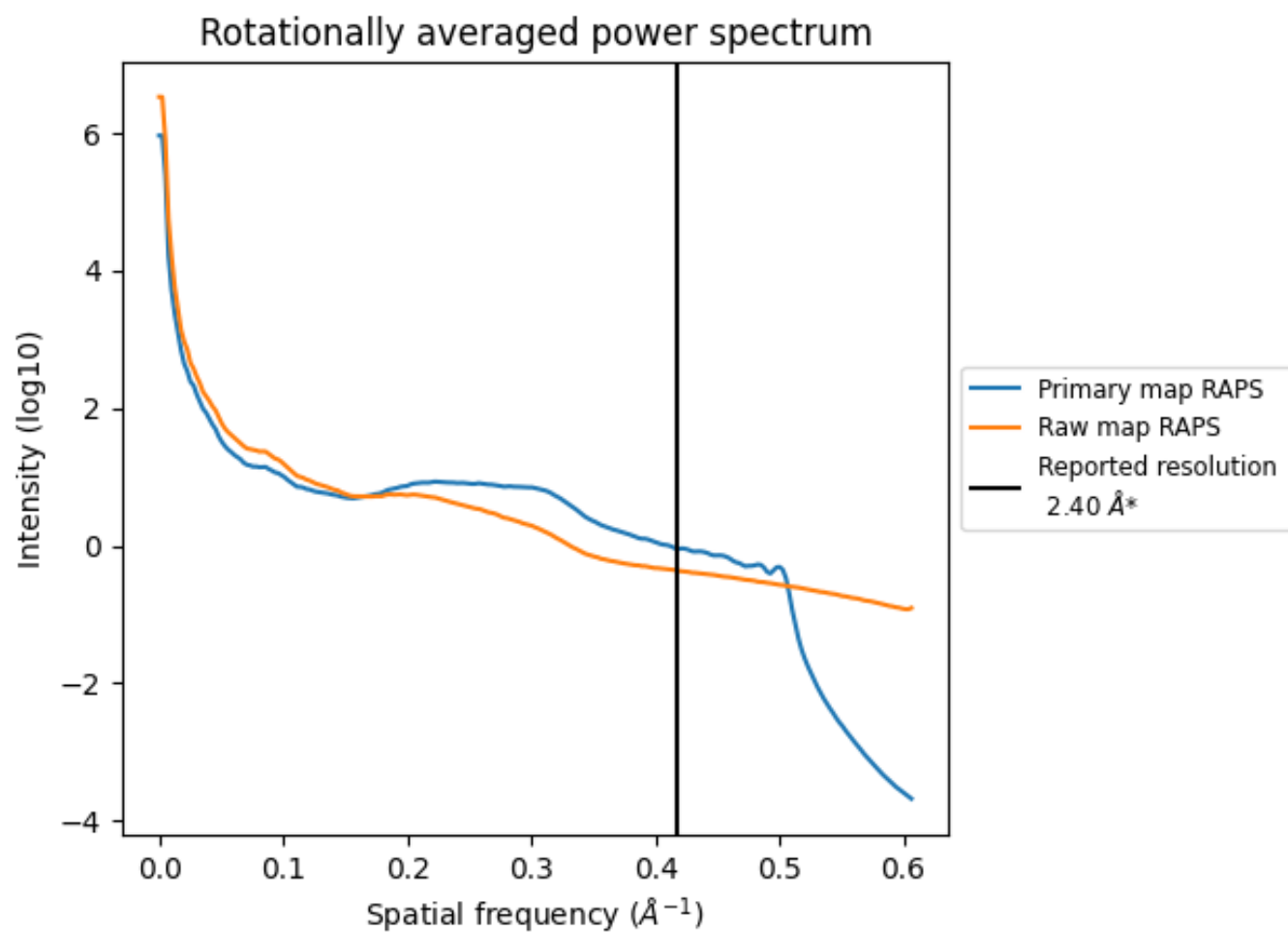
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2960 nm^3 ; this corresponds to an approximate mass of 2674 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 ⓘ

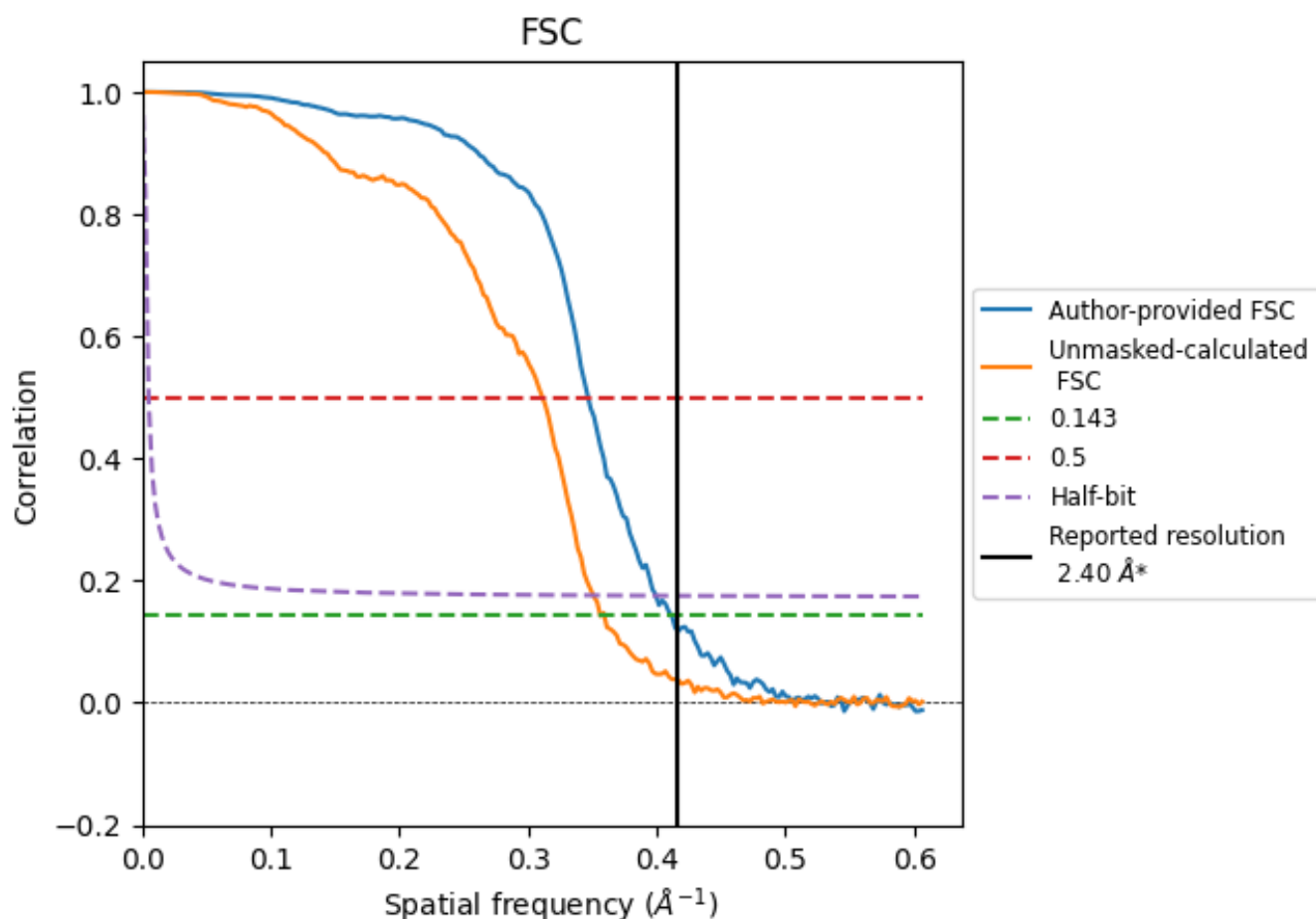


*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

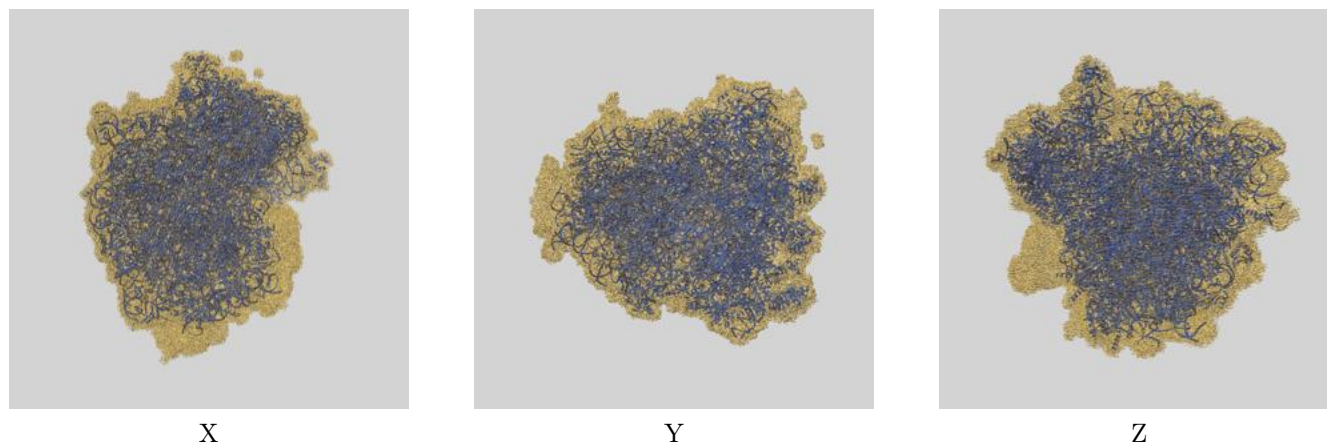
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.43	2.89	2.50
Unmasked-calculated*	2.81	3.21	2.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.81 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

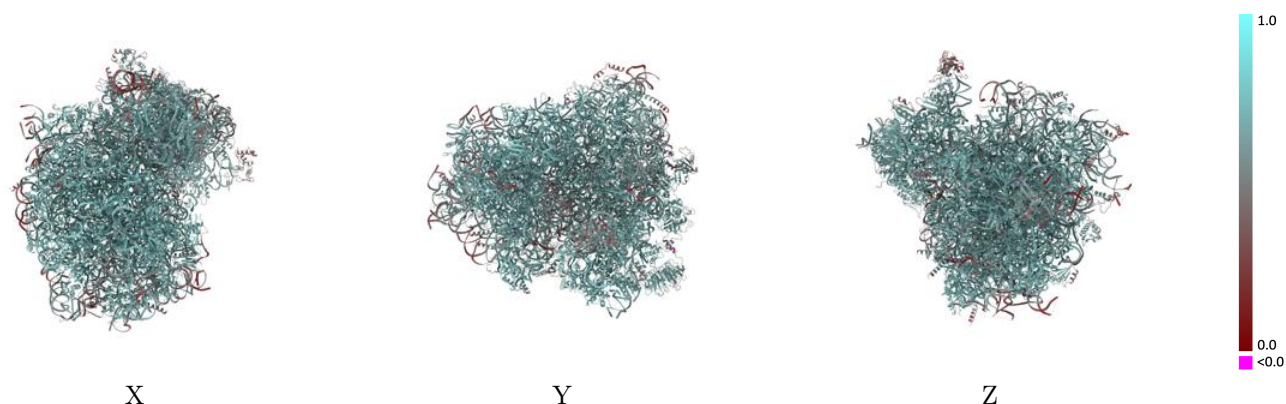
This section contains information regarding the fit between EMDB map EMD-55083 and PDB model 9SPF. Per-residue inclusion information can be found in section [3](#) on page [26](#).

9.1 Map-model overlay [i](#)



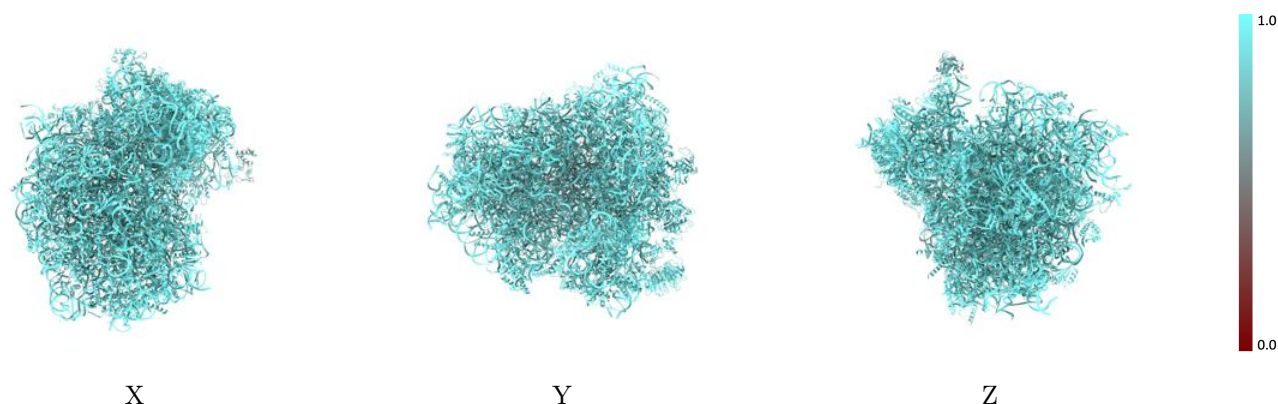
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



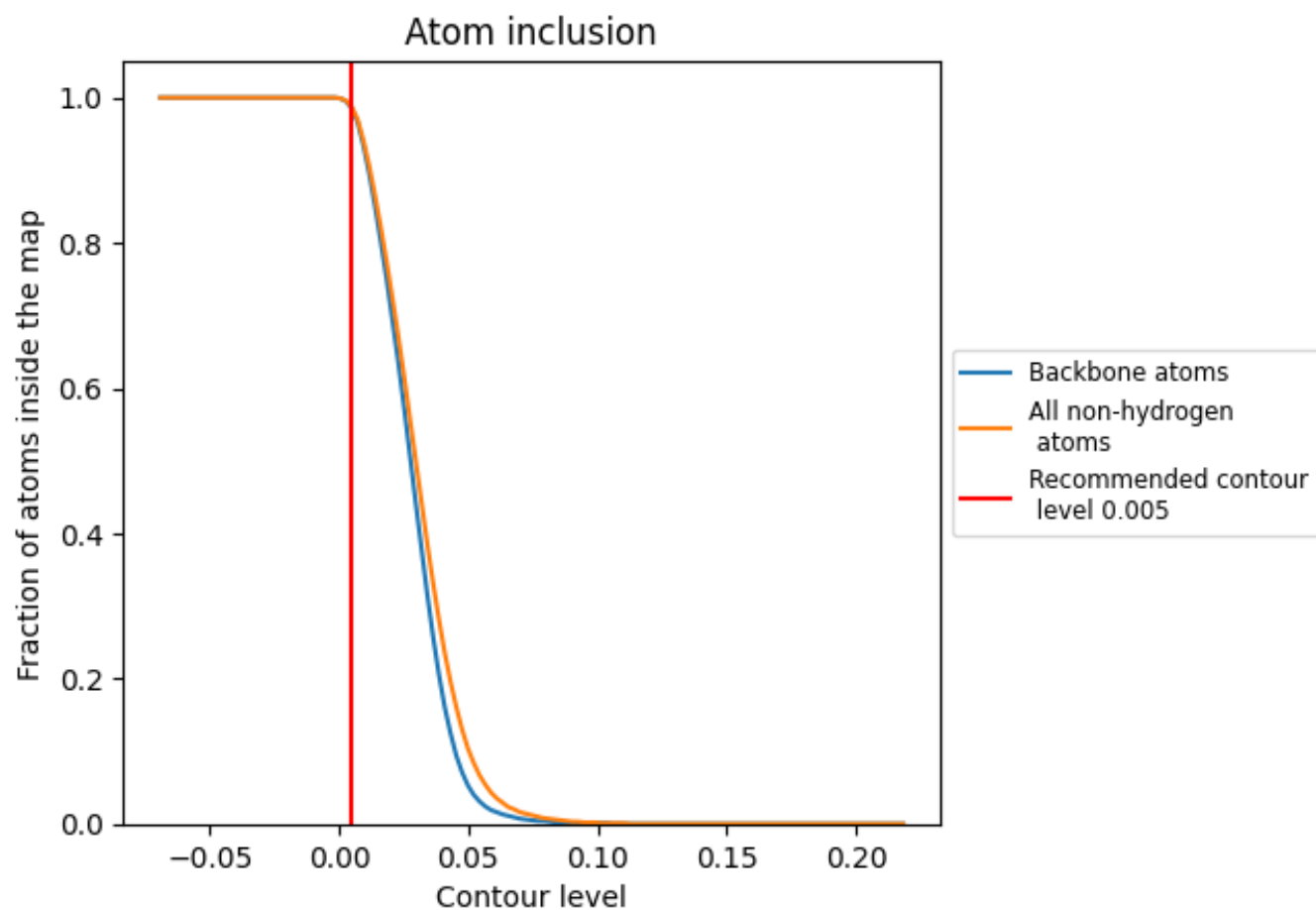
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 98% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9870	 0.6510
At	 0.9670	 0.4410
Et	 0.9690	 0.3890
L5	 0.9880	 0.6520
L7	 1.0000	 0.6890
L8	 0.9910	 0.6620
LA	 0.9970	 0.7250
LB	 0.9920	 0.7110
LC	 0.9940	 0.7150
LD	 0.9870	 0.6580
LE	 0.9950	 0.6600
LF	 0.9980	 0.7230
LG	 0.9780	 0.6430
LH	 0.9900	 0.6770
LI	 0.9960	 0.6890
LJ	 0.9750	 0.5940
LL	 0.9900	 0.6870
LM	 0.9900	 0.6850
LN	 1.0000	 0.7400
LO	 0.9960	 0.7160
LP	 0.9950	 0.7200
LQ	 1.0000	 0.7350
LR	 0.9970	 0.6690
LS	 0.9940	 0.7160
LT	 0.9830	 0.6780
LU	 0.9770	 0.5880
LV	 0.9940	 0.7110
LW	 0.9840	 0.5700
LX	 0.9880	 0.6870
LY	 0.9960	 0.6940
LZ	 0.9940	 0.6630
La	 0.9970	 0.7290
Lb	 0.9880	 0.6370
Lc	 0.9880	 0.6640
Ld	 0.9800	 0.6730



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Chain	Atom inclusion	Q-score
Le	 0.9990	 0.7280
Lf	 0.9950	 0.7350
Lg	 0.9880	 0.6940
Lh	 0.9940	 0.6830
Li	 0.9890	 0.6660
Lj	 1.0000	 0.7350
Lk	 0.9890	 0.6070
Ll	 0.9950	 0.7130
Lm	 0.9930	 0.6970
Ln	 1.0000	 0.6920
Lo	 1.0000	 0.7050
Lp	 0.9960	 0.7110
Lr	 0.9930	 0.7070
Mr	 0.9800	 0.5910
Pt	 0.9880	 0.5690
S2	 0.9920	 0.6400
SA	 0.9830	 0.6460
SB	 0.9890	 0.6300
SC	 0.9910	 0.6480
SD	 0.9710	 0.6210
SE	 0.9910	 0.6340
SF	 0.9940	 0.6850
SG	 0.9750	 0.5890
SH	 0.9300	 0.5380
SI	 0.9660	 0.6220
SJ	 0.9740	 0.5520
SK	 0.9830	 0.6330
SL	 0.9890	 0.6590
SM	 0.7550	 0.3670
SN	 0.9920	 0.6630
SO	 0.9950	 0.6490
SP	 0.9850	 0.6500
SQ	 0.9940	 0.6850
SR	 0.9690	 0.6100
SS	 0.9890	 0.6650
ST	 0.9850	 0.6740
SU	 0.9540	 0.6020
SV	 0.9840	 0.6380
SW	 0.9950	 0.6810
SX	 0.9900	 0.6520
SY	 0.9830	 0.5820
SZ	 0.9560	 0.6040

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Chain	Atom inclusion	Q-score
Sa	 0.9970	 0.6790
Sb	 0.9660	 0.6030
Sc	 0.9830	 0.6330
Sd	 0.9960	 0.6910
Se	 0.9810	 0.5800
Sf	 0.8490	 0.4530
Sg	 0.9690	 0.6070