



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 12:30 am BST

PDB ID : 9SPI / pdb_00009spi
EMDB ID : EMD-55091
Title : CRYO-EM STRUCTURE OF HUMAN 80S RIBOSOME WITH A/P/E-SITE
TRNA AND MRNA CONTAINING URIDINE
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

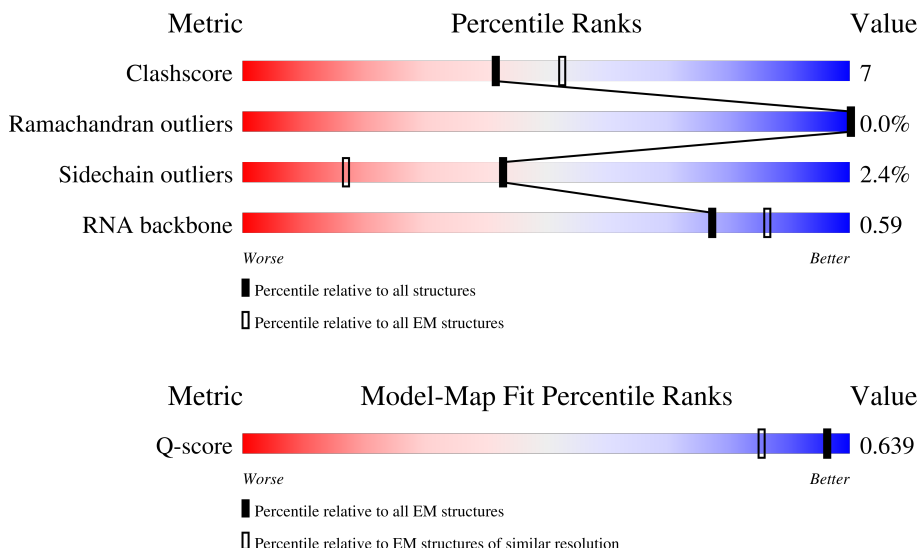
1 Overall quality at a glance

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.



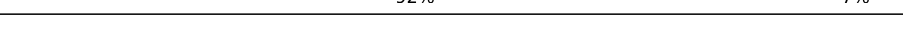
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	 66% 27% 5%
2	Et	75	 43% 24% 5% 28%
3	L5	5069	 42% 22% 33%

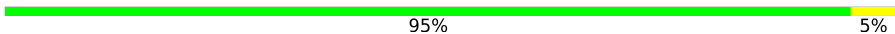
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	257	
7	LB	403	
8	LC	427	
9	LD	297	
10	LE	288	
11	LF	248	
12	LG	266	
13	LH	192	
14	LI	214	
15	LJ	178	
16	LL	211	
17	LM	215	
18	LN	204	
19	LO	203	
20	LP	184	
21	LQ	188	
22	LR	196	
23	LS	176	
24	LT	160	
25	LU	128	
26	LV	140	
27	LW	157	
28	LX	156	

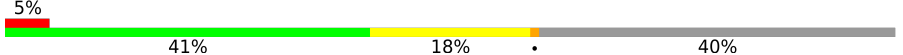
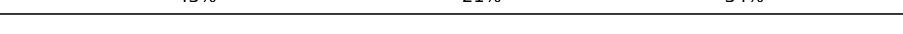
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Mol	Chain	Length	Quality of chain
29	LY	145	
30	LZ	136	
31	La	148	
32	Lb	159	
33	Lc	115	
34	Ld	125	
35	Le	135	
36	Lf	110	
37	Lg	117	
38	Lh	123	
39	Li	105	
40	Lj	97	
41	Lk	70	
42	Ll	51	
43	Lm	128	
44	Ln	25	
45	Lo	106	
46	Lp	92	
47	Lr	137	
48	Mr	7	
49	Pt	76	
50	S2	1869	
51	SA	295	
52	SB	264	
53	SC	293	

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Mol	Chain	Length	Quality of chain
54	SD	243	
55	SE	263	
56	SF	204	
57	SG	249	
58	SH	194	
59	SI	208	
60	SJ	194	
61	SK	165	
62	SL	158	
63	SM	132	
64	SN	151	
65	SO	151	
66	SP	145	
67	SQ	146	
68	SR	135	
69	SS	152	
70	ST	145	
71	SU	119	
72	SV	83	
73	SW	130	
74	SX	143	
75	SY	133	
76	SZ	125	
77	Sa	115	
78	Sb	84	

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Mol	Chain	Length	Quality of chain
79	Sc	69	
80	Sd	56	
81	Se	133	
82	Sf	156	
83	Sg	317	

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	HYG	S2	1944	X	-	-	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 216235 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 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	3413	Total	C	N	O	P	0	0
			73250	32661	13401	23776	3412		

- 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	149	Total	C	N	O	P	0	0
			3177	1418	564	1046	149		

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LA	248	Total	C	N	O	S	1	0
			1907	1194	392	315	6		

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LB	397	Total	C	N	O	S	0	0
			3203	2040	602	547	14		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LC	361	Total	C	N	O	S	0	0
			2873	1808	574	477	14		

- Molecule 9 is a protein called 60S ribosomal protein L5.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	228	Total	C	N	O	S	0	0
			1824	1162	352	306	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called 60S ribosomal protein L10.

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

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LJ	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LL	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

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

- Molecule 20 is a protein called 60S ribosomal protein L17.

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

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called 60S ribosomal protein L22.

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

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	64	Total	C	N	O	S	0	0
			529	338	103	85	3		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

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

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lb	104	Total	C	N	O	S	0	0
			841	523	184	130	4		

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	98	Total	C	N	O	S	0	0
			761	482	134	139	6		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L34.

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

- Molecule 38 is a protein called 60S ribosomal protein L35.

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

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

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

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 46 is a protein called 60S ribosomal protein L37a.

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

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

- Molecule 48 is a RNA chain called Synthetic mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Mr	7	Total	C	N	O	P	0	0
			145	65	23	50	7		

- Molecule 49 is a RNA chain called P site tRNA Arg-ACG.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Pt	72	Total	C	N	O	P	0	0
			1547	692	281	502	72		

- Molecule 50 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	S2	1562	Total	C	N	O	P	0	0
			33424	14950	6020	10893	1561		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SA	214	Total	C	N	O	S	0	0
			1693	1077	297	312	7		

- Molecule 52 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SB	199	Total	C	N	O	S	0	0
			1627	1037	292	285	13		

- Molecule 53 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SC	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 54 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SD	222	Total	C	N	O	S	0	0
			1721	1098	309	307	7		

- Molecule 55 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SE	257	Total	C	N	O	S	0	0
			2041	1305	379	349	8		

- Molecule 56 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SF	180	Total	C	N	O	S	0	0
			1417	890	263	257	7		

- Molecule 57 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SG	205	Total	C	N	O	S	0	0
			1652	1038	329	278	7		

- Molecule 58 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SH	163	Total	C	N	O	S	0	0
			1317	846	243	228			

- Molecule 59 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SI	201	Total	C	N	O	S	0	0
			1651	1035	325	286	5		

- Molecule 60 is a protein called 40S ribosomal protein S9.

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

- Molecule 61 is a protein called 40S ribosomal protein S10.

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

- Molecule 62 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SL	142	Total	C	N	O	S	0	0
			1164	741	220	197	6		

- Molecule 63 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SM	79	Total	C	N	O	S	0	0
			556	353	101	99	3		

- Molecule 64 is a protein called 40S ribosomal protein S13.

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

- Molecule 65 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SO	106	Total	C	N	O	S	0	0
			788	482	156	146	4		

- Molecule 66 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SP	128	Total	C	N	O	S	0	0
			1037	656	195	179	7		

- Molecule 67 is a protein called 40S ribosomal protein S16.

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

- Molecule 68 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SR	127	Total	C	N	O	S	0	0
			1032	648	194	186	4		

- Molecule 69 is a protein called 40S ribosomal protein S18.

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

- Molecule 70 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	ST	140	Total	C	N	O	S	1	0
			1104	697	208	196	3		

- Molecule 71 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SU	95	Total	C	N	O	S	0	0
			755	474	142	135	4		

- Molecule 72 is a protein called 40S ribosomal protein S21.

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

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S23.

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

- Molecule 75 is a protein called 40S ribosomal protein S24.

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

- Molecule 76 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SZ	82	Total	C	N	O	S	0	0
			661	425	123	112	1		

- Molecule 77 is a protein called 40S ribosomal protein S26.

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

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sb	75	Total	C	N	O	S	0	0
			592	372	111	105	4		

- Molecule 79 is a protein called 40S ribosomal protein S28.

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

- Molecule 80 is a protein called 40S ribosomal protein S29.

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

- Molecule 81 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Se	53	Total	C	N	O	S	0	0
			420	258	94	67	1		

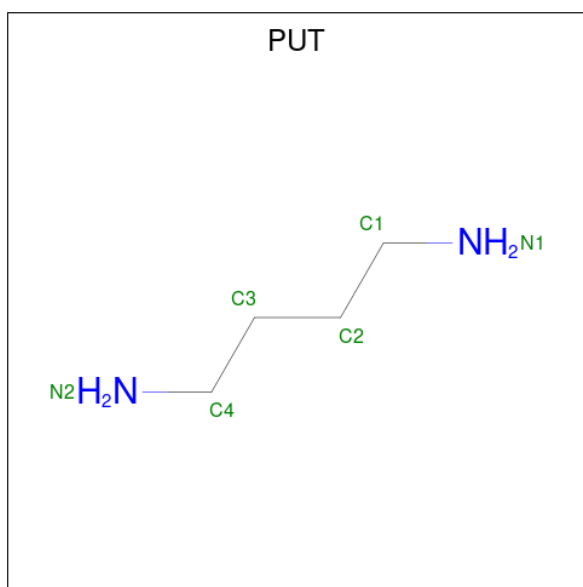
- Molecule 82 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sf	43	Total	C	N	O	S	0	0
			341	217	66	53	5		

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

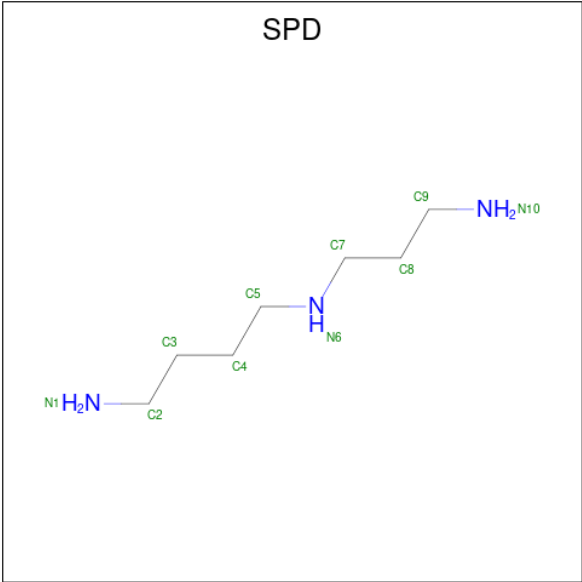
Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sg	282	Total	C	N	O	S	0	0
			2199	1392	386	411	10		

- Molecule 84 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

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



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

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

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	L5	159	Total	Mg	0
			159	159	
86	L7	2	Total	Mg	0
			2	2	
86	L8	3	Total	Mg	0
			3	3	
86	LP	1	Total	Mg	0
			1	1	
86	LR	1	Total	Mg	0
			1	1	
86	S2	29	Total	Mg	0
			29	29	

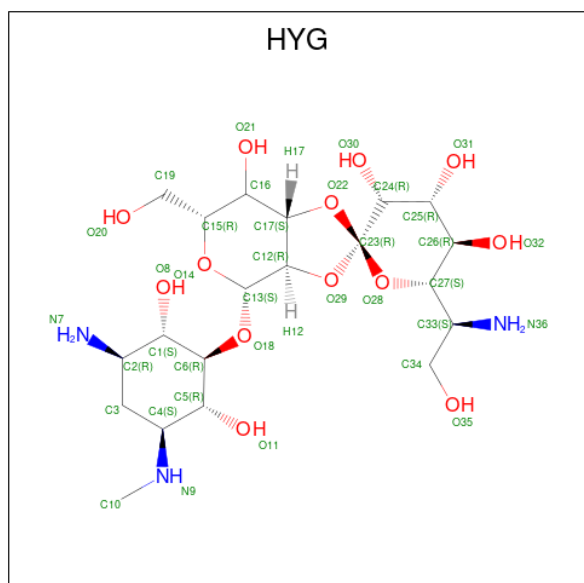
- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
87	L5	60	Total	K	0
			60	60	
87	L8	1	Total	K	0
			1	1	
87	LA	2	Total	K	0
			2	2	
87	LH	1	Total	K	0
			1	1	
87	Lg	1	Total	K	0
			1	1	
87	S2	9	Total	K	0
			9	9	
87	Sd	1	Total	K	0
			1	1	

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 89 is HYGROMYCIN B (CCD ID: HYG) (formula: C₂₀H₃₇N₃O₁₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
90	At	18	Total 18	O 18	0
90	Et	37	Total 37	O 37	0
90	L5	5891	Total 5891	O 5891	0
90	L7	172	Total 172	O 172	0
90	L8	297	Total 297	O 297	0
90	LA	90	Total 90	O 90	0
90	LB	143	Total 143	O 143	0
90	LC	157	Total 157	O 157	0
90	LD	51	Total 51	O 51	0
90	LE	53	Total 53	O 53	0
90	LF	95	Total 95	O 95	0
90	LG	57	Total 57	O 57	0
90	LH	51	Total 51	O 51	0
90	LI	81	Total 81	O 81	0
90	LJ	16	Total 16	O 16	0
90	LL	81	Total 81	O 81	0
90	LM	35	Total 35	O 35	0
90	LN	106	Total 106	O 106	0
90	LO	81	Total 81	O 81	0
90	LP	56	Total 56	O 56	0
90	LQ	89	Total 89	O 89	0
90	LR	72	Total 72	O 72	0

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Mol	Chain	Residues	Atoms		AltConf
90	LS	89	Total 89	O 89	0
90	LT	59	Total 59	O 59	0
90	LU	5	Total 5	O 5	0
90	LV	42	Total 42	O 42	0
90	LW	22	Total 22	O 22	0
90	LX	32	Total 32	O 32	0
90	LY	40	Total 40	O 40	0
90	LZ	27	Total 27	O 27	0
90	La	72	Total 72	O 72	0
90	Lb	30	Total 30	O 30	0
90	Lc	11	Total 11	O 11	0
90	Ld	34	Total 34	O 34	0
90	Le	77	Total 77	O 77	0
90	Lf	52	Total 52	O 52	0
90	Lg	48	Total 48	O 48	0
90	Lh	43	Total 43	O 43	0
90	Li	38	Total 38	O 38	0
90	Lj	53	Total 53	O 53	0
90	Lk	3	Total 3	O 3	0
90	Ll	34	Total 34	O 34	0
90	Lm	21	Total 21	O 21	0

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Mol	Chain	Residues	Atoms		AltConf
90	Ln	18	Total 18	O 18	0
90	Lo	61	Total 61	O 61	0
90	Lp	38	Total 38	O 38	0
90	Lr	53	Total 53	O 53	0
90	Mr	3	Total 3	O 3	0
90	Pt	34	Total 34	O 34	0
90	S2	974	Total 974	O 974	0
90	SA	3	Total 3	O 3	0
90	SC	12	Total 12	O 12	0
90	SD	4	Total 4	O 4	0
90	SE	10	Total 10	O 10	0
90	SF	3	Total 3	O 3	0
90	SG	2	Total 2	O 2	0
90	SH	1	Total 1	O 1	0
90	SI	28	Total 28	O 28	0
90	SJ	7	Total 7	O 7	0
90	SK	1	Total 1	O 1	0
90	SL	29	Total 29	O 29	0
90	SM	3	Total 3	O 3	0
90	SN	14	Total 14	O 14	0
90	SO	7	Total 7	O 7	0

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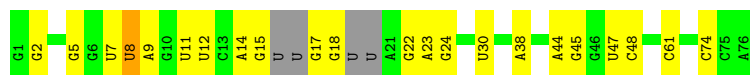
Mol	Chain	Residues	Atoms		AltConf
90	SP	5	Total 5	O 5	0
90	SQ	3	Total 3	O 3	0
90	SR	3	Total 3	O 3	0
90	SS	9	Total 9	O 9	0
90	SU	3	Total 3	O 3	0
90	SV	3	Total 3	O 3	0
90	SW	8	Total 8	O 8	0
90	SX	24	Total 24	O 24	0
90	SY	1	Total 1	O 1	0
90	SZ	1	Total 1	O 1	0
90	Sa	11	Total 11	O 11	0
90	Sb	2	Total 2	O 2	0
90	Sd	4	Total 4	O 4	0
90	Se	3	Total 3	O 3	0

3 Residue-property plots [i](#)

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: tRNA-Ile-AAT-9-1

Chain At:  66% 27% 5%



• Molecule 2: E site tRNA

Chain Et:  43% 24% 5% 28%

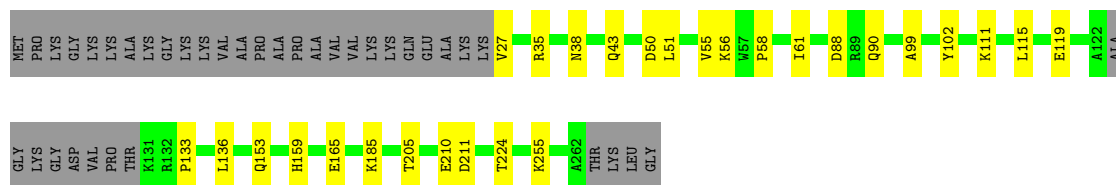








Chain LG:  75% 11% 14%



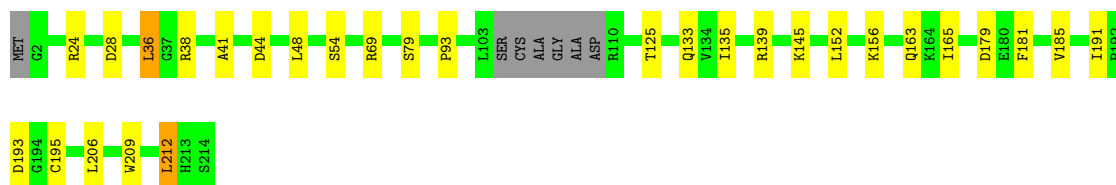
- Molecule 13: 60S ribosomal protein L9

Chain LH:  81% 18% .



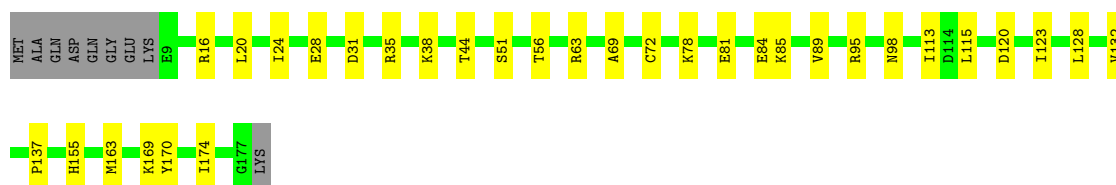
- Molecule 14: 60S ribosomal protein L10

Chain LI:  83% 13% . .



- Molecule 15: 60S ribosomal protein L11

Chain LJ:  77% 18% 5%



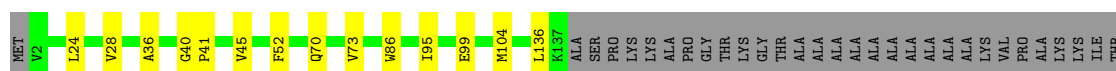
- Molecule 16: Large ribosomal subunit protein eL13

Chain LL:  88% 9% .



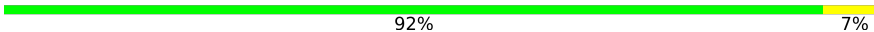
- Molecule 17: 60S ribosomal protein L14

Chain LM:  57% 7% 37%



ALA
ALA
SER
LYS
LYS
LYS
ALA
PRO
PRO
GLN
LYS
VAL
PRO
PRO
ALA
GLN
LYS
ALA
THR
GLY
GLN
LYS
ALA
ALA
PRO
ALA
PRO
LYS
LYS
GLN
LYS
GLY
GLN
LYS
ALA
ALA
PRO
ALA
GLN
LYS
ALA
LYS
SER
GLY
LYS
LYS
ALA

• Molecule 18: 60S ribosomal protein L15

Chain LN:  92% 7%

MET G2 R12 R13 K14 Q15 S16 R20 R24 R25 R26 E104 F138 R143 I151 V155 E160 R169 H178 H181 Y203 R204

• Molecule 19: 60S ribosomal protein L13a

Chain LO:  86% 13%

MET ALA GLU V4 R31 V34 R61 P70 R78 L88 P89 G95 L99 K103 D106 K130 R133 A142 V145 E158 E162 Y168 K172 M175 R176 K179 Q180 A181 V185 H199 V203

• Molecule 20: 60S ribosomal protein L17

Chain LP:  74% 9% 17%

MET V2 R3 Y4 S5 S17 S20 A33 R42 Q54 K55 M63 M64 A98 E99 I117 R126 R135 M140 M148 E154 GLN ILE VAL PRO LYS PRO PRO GLU GLU VAL ALA GLN LYS LYS ILE SER GLN LYS LEU LYS LYS LYS

LEU
MET
ALA
ARG
GLU

• Molecule 21: 60S ribosomal protein L18

Chain LQ:  92% 7%

MET G2 V3 D4 I5 R14 R65 R68 R69 M70 A80 V100 R108 K144 R150 A177 R178 R184 R188

• Molecule 22: 60S ribosomal protein L19

Chain LR:  83% 9% 8%

MET S2 R16 K43 P90 V93 M99 R104 R108 S122 V131 F132 K133 I137 K144 D148 R151 A159 R162 K165 A179 K180 K181 GLU GLU ILE LYS THR LEU SER LYS GLU GLU THR LYS

• Molecule 23: 60S ribosomal protein L18a

Chain LS:  85% 13%

M1 R15 T19 P20 K21 T24 L27 Y28 R29 M30 R43 F47 V48 S49 Q50 E69 K70 S71 K76 W81 M83 R98 D99 L100 T101 T107 Q108 R111 E130 V142 K164 T174 F175 F176

• Molecule 24: 60S ribosomal protein L21

MIT
T2
G6
M31
K35
K43
G51
T68
K83
T84
L85
R92
R102
F105
L106
K107
R108
K117
K120
T124
W125
R142
P148
E157
A160

- | |
|------|
| MET |
| ALA |
| PRO |
| VAL |
| LVS |
| LVS |
| LEU |
| VAL |
| VAL |
| LVS |
| GLY |
| GLY |
| LVS |
| LVS |
| LVS |
| LVS |
| GLN |
| V18 |
| T22 |
| L23 |
| D24 |
| C25 |
| T26 |
| H27 |
| D31 |
| G32 |
| I33 |
| K34 |
| D35 |
| N38 |
| F39 |
| E40 |
| Q41 |
| F42 |
| E45 |
| R46 |
| I47 |
| K48 |
| K52 |
| A53 |
| G54 |
| S65 |
| S66 |
| K67 |
| S68 |
| T73 |
| S74 |
| E75 |
| K80 |
| K89 |
| X90 |
| W99 |
| Y110 |
| Q116 |
| ILE |
| ASN |
| GLN |
| ASP |
| GLU |
| GLU |
| GLU |
| GLU |
| GLU |
| ASP |
| GLU |
| ASP |

- MET SER LYS ARG GLY ARG GLY G8 K13 F14 R15 R48 R89 F95 N108 L128 A140

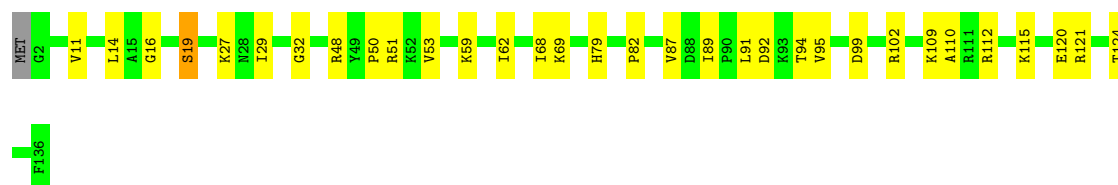
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|-----|
| LYS | LYS | ALA | GLN | ALA | SER | LYS | LYS | THR | ALA | ALA | MET | ALA | LYS | LYS | ALA | LYS | ALA | LYS | ALA | PRO | THR | LYS | LYS | ALA | ALA | LYS | LYS | VAL | VAL | SER | ALA | PRO | ARG | VAL | GLY | GLY | LYS | ARG | | | | | | | | | | |
| M1 | Y11 | Q30 | R44 | S64 | GLU | GLU | ILE | GLN | LYS | LYS | ARG | THR | ARG | ARG | ALA | VAL | LYS | PRE | GLN | ARG | ALA | ILE | THR | GLY | ALA | SER | LEU | ALA | ASP | ILE | MET | ALA | LYS | ARG | ASN | GLN | LYS | PRO | GLU | VAL | ARG | LYS | ALA | ALA | ALA | LYS | GLU | ALA |

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|------|---------|
| VI49 | VI150 | VI151 | VI152 | VI153 | VI154 | VI155 | VI156 | VI157 | VI158 | VI159 | VI160 | VI161 | VI162 | VI163 | VI164 | VI165 | VI166 | VI167 | VI168 | VI169 | VI170 | VI171 | VI172 | VI173 | VI174 | VI175 | VI176 | VI177 | VI178 | VI179 | VI180 | VI181 | VI182 | VI183 | VI184 | VI185 | VI186 | VI187 | VI188 | VI189 | VI190 | VI191 | VI192 | VI193 | VI194 | VI195 | VI196 | VI197 | VI198 | VI199 | VI200 | VI201 | VI202 | VI203 | VI204 | VI205 | VI206 | VI207 | VI208 | VI209 | VI210 | VI211 | VI212 | VI213 | VI214 | VI215 | VI216 | VI217 | VI218 | VI219 | VI220 | VI221 | VI222 | VI223 | VI224 | VI225 | VI226 | VI227 | VI228 | VI229 | VI230 | VI231 | VI232 | VI233 | VI234 | VI235 | VI236 | VI237 | VI238 | VI239 | VI240 | VI241 | VI242 | VI243 | VI244 | VI245 | VI246 | VI247 | VI248 | VI249 | VI250 | VI251 | VI252 | VI253 | VI254 | VI255 | VI256 | VI257 | VI258 | VI259 | VI260 | VI261 | VI262 | VI263 | VI264 | VI265 | VI266 | VI267 | VI268 | VI269 | VI270 | VI271 | VI272 | VI273 | VI274 | VI275 | VI276 | VI277 | VI278 | VI279 | VI280 | VI281 | VI282 | VI283 | VI284 | VI285 | VI286 | VI287 | VI288 | VI289 | VI290 | VI291 | VI292 | VI293 | VI294 | VI295 | VI296 | VI297 | VI298 | VI299 | VI300 | VI301 | VI302 | VI303 | VI304 | VI305 | VI306 | VI307 | VI308 | VI309 | VI310 | VI311 | VI312 | VI313 | VI314 | VI315 | VI316 | VI317 | VI318 | VI319 | VI320 | VI321 | VI322 | VI323 | VI324 | VI325 | VI326 | VI327 | VI328 | VI329 | VI330 | VI331 | VI332 | VI333 | VI334 | VI335 | VI336 | VI337 | VI338 | VI339 | VI340 | VI341 | VI342 | VI343 | VI344 | VI345 | VI346 | VI347 | VI348 | VI349 | VI350 | VI351 | VI352 | VI353 | VI354 | VI355 | VI356 | VI357 | VI358 | VI359 | VI360 | VI361 | VI362 | VI363 | VI364 | VI365 | VI366 | VI367 | VI368 | VI369 | VI370 | VI371 | VI372 | VI373 | VI374 | VI375 | VI376 | VI377 | VI378 | VI379 | VI380 | VI381 | VI382 | VI383 | VI384 | VI385 | VI386 | VI387 | VI388 | VI389 | VI390 | VI391 | VI392 | VI393 | VI394 | VI395 | VI396 | VI397 | VI398 | VI399 | VI400 | VI401 | VI402 | VI403 | VI404 | VI405 | VI406 | VI407 | VI408 | VI409 | VI410 | VI411 | VI412 | VI413 | VI414 | VI415 | VI416 | VI417 | VI418 | VI419 | VI420 | VI421 | VI422 | VI423 | VI424 | VI425 | VI426 | VI427 | VI428 | VI429 | VI430 | VI431 | VI432 | VI433 | VI434 | VI435 | VI436 | VI437 | VI438 | VI439 | VI440 | VI441 | VI442 | VI443 | VI444 | VI445 | VI446 | VI447 | VI448 | VI449 | VI450 | VI451 | VI452 | VI453 | VI454 | VI455 | VI456 | VI457 | VI458 | VI459 | VI460 | VI461 | VI462 | VI463 | VI464 | VI465 | VI466 | VI467 | VI468 | VI469 | VI470 | VI471 | VI472 | VI473 | VI474 | VI475 | VI476 | VI477 | VI478 | VI479 | VI480 | VI481 | VI482 | VI483 | VI484 | VI485 | VI486 | VI487 | VI488 | VI489 | VI490 | VI491 | VI492 | VI493 | VI494 | VI495 | VI496 | VI497 | VI498 | VI499 | VI500 | VI501 | VI502 | VI503 | VI504 | VI505 | VI506 | VI507 | VI508 | VI509 | VI510 | VI511 | VI512 | VI513 | VI514 | VI515 | VI516 | VI517 | VI518 | VI519 | VI520 | VI521 | VI522 | VI523 | VI524 | VI525 | VI526 | VI527 | VI528 | VI529 | VI530 | VI531 | VI532 | VI533 | VI534 | VI535 | VI536 | VI537 | VI538 | VI539 | VI540 | VI541 | VI542 | VI543 | VI544 | VI545 | VI546 | VI547 | VI548 | VI549 | VI550 | VI551 | VI552 | VI553 | VI554 | VI555 | VI556 | VI557 | VI558 | VI559 | VI560 | VI561 | VI562 | VI563 | VI564 | VI565 | VI566 | VI567 | VI568 | VI569 | VI570 | VI571 | VI572 | VI573 | VI574 | VI575 | VI576 | VI577 | VI578 | VI579 | VI580 | VI581 | VI582 | VI583 | VI584 | VI585 | VI586 | VI587 | VI588 | VI589 | VI590 | VI591 | VI592 | VI593 | VI594 | VI595 | VI596 | VI597 | VI598 | VI599 | VI600 | VI601 | VI602 | VI603</ |
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| R#1 | R26 | R27 | R30 | R31 | R45 | R46 | R47 | R48 | Q66 | Q72 | Y81 | Q86 | R89 | T94 | P101 | R108 | D112 | R113 | D114 | I118 | R126 | Q127 | E131 | R132 | GLY | LYS | TYR | LYS | LYS | GLU | GLU | THR | ILE | GLU | LYS | LYS | MET | CIN | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

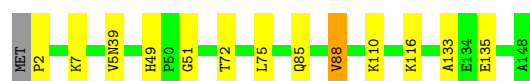
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Chain LZ:  76% 23% ..



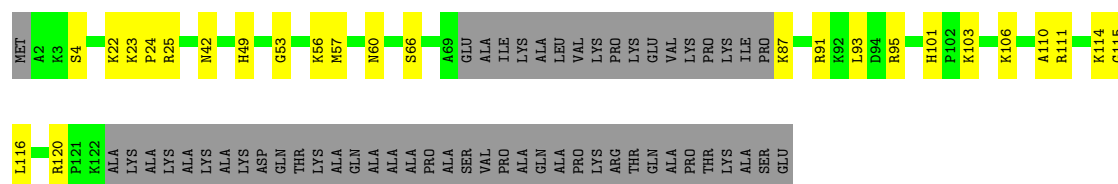
- Molecule 31: Large ribosomal subunit protein uL15

Chain La:  91% 8% ..



- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb:  50% 16% 35%



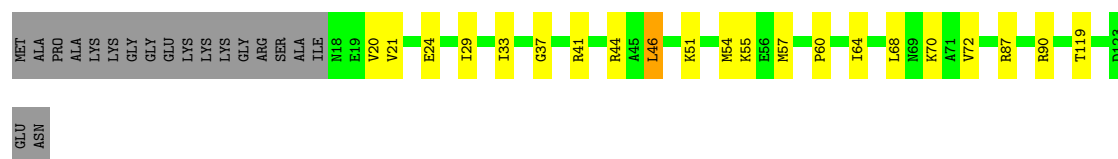
- Molecule 33: 60S ribosomal protein L30

Chain Lc:  73% 12% 15%



- Molecule 34: 60S ribosomal protein L31

Chain Ld:  68% 16% 15%

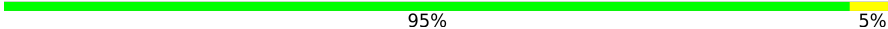


- Molecule 35: 60S ribosomal protein L32

Chain Le:  87% 8% 5%



- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  95% 5%



- Molecule 37: 60S ribosomal protein L34

Chain Lg:  83% 13%



- Molecule 38: 60S ribosomal protein L35

Chain Lh:  81% 18%



- Molecule 39: 60S ribosomal protein L36

Chain Li:  90% 7%



- Molecule 40: Large ribosomal subunit protein eL37

Chain Lj:  79% 9% 11%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  84% 11%



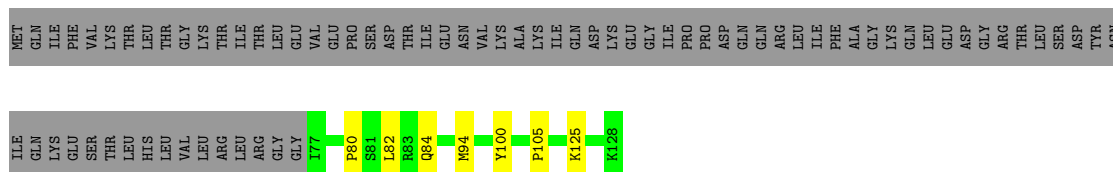
- Molecule 42: 60S ribosomal protein L39

Chain Ll:  78% 18%



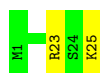
- Molecule 43: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  35% 5% 59%



- Molecule 44: 60S ribosomal protein L41

Chain Ln:  92% 8%



- Molecule 45: Large ribosomal subunit protein eL42

Chain Lo:  85% 14% .



- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  88% 10% .



- Molecule 47: 60S ribosomal protein L28

Chain Lr:  77% 14% 9%



- Molecule 48: Synthetic mRNA

Chain Mr:  71% 29%

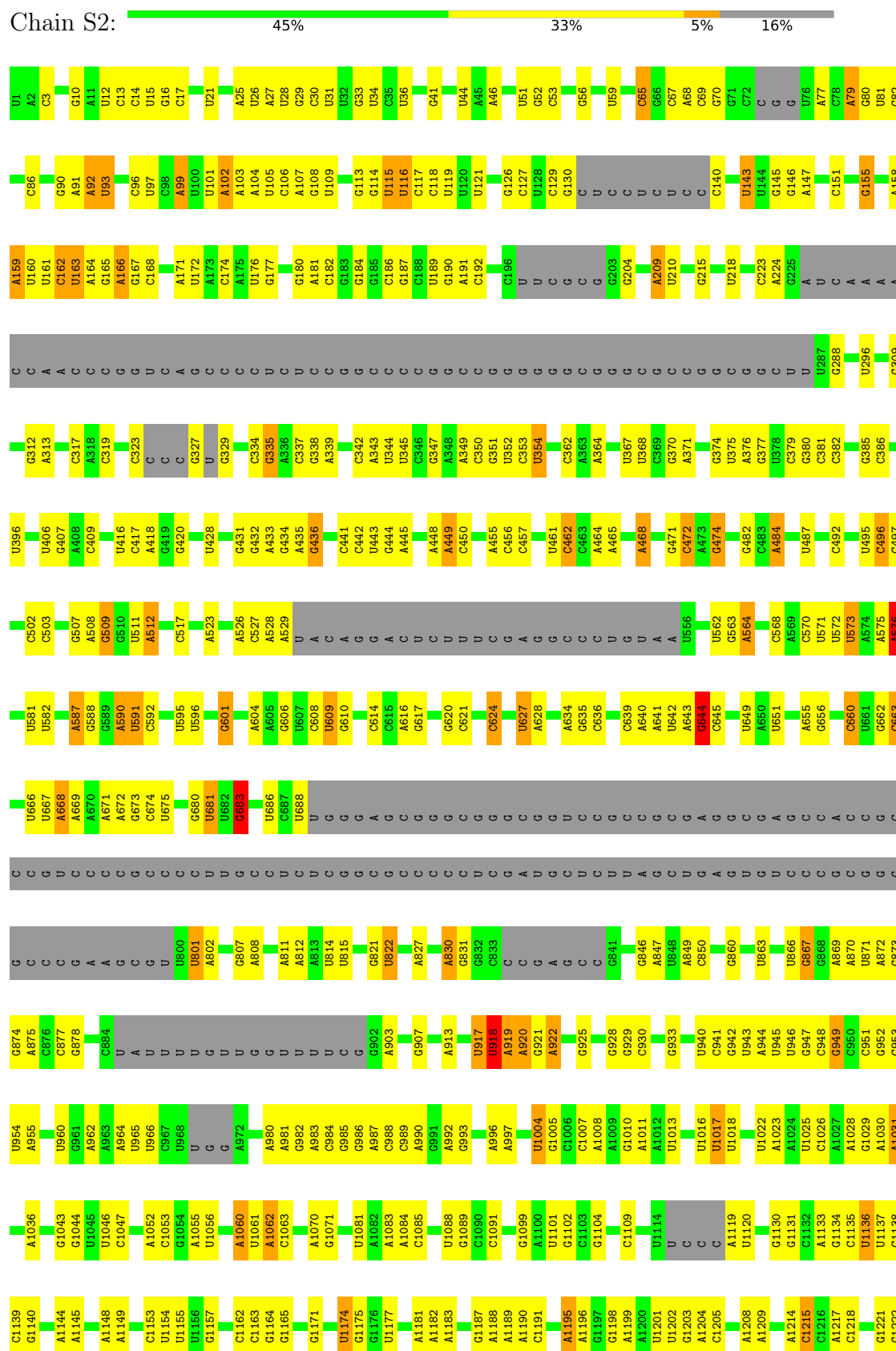


- Molecule 49: P site tRNA Arg-ACG

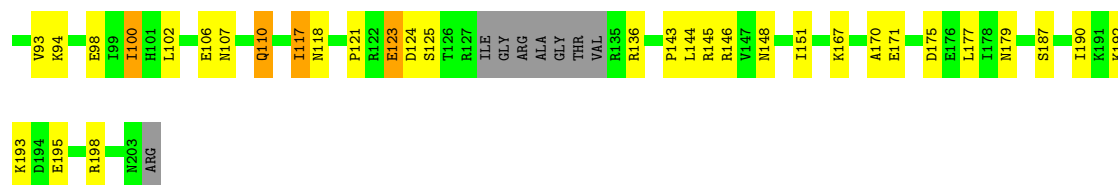
Chain Pt:  76% 16% .. 5%



● Molecule 50: 18S rRNA

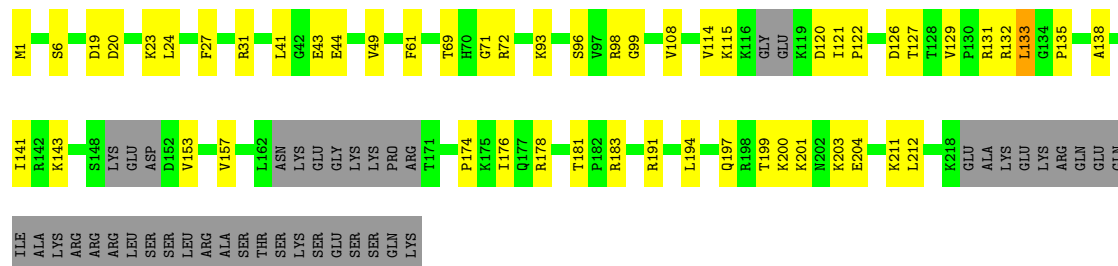






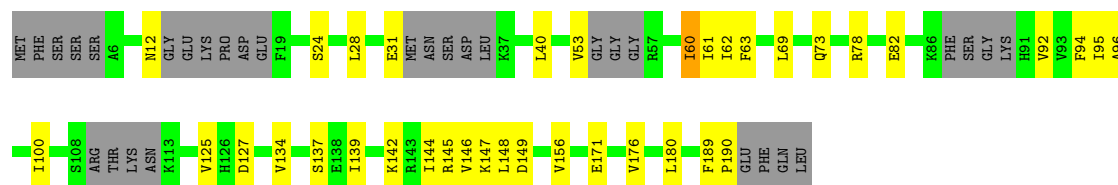
- Molecule 57: 40S ribosomal protein S6

Chain SG:



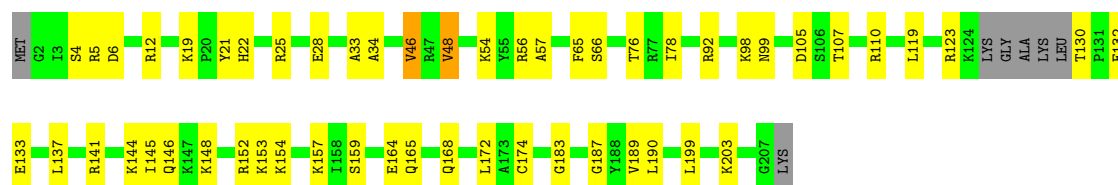
- Molecule 58: 40S ribosomal protein S7

Chain SH:



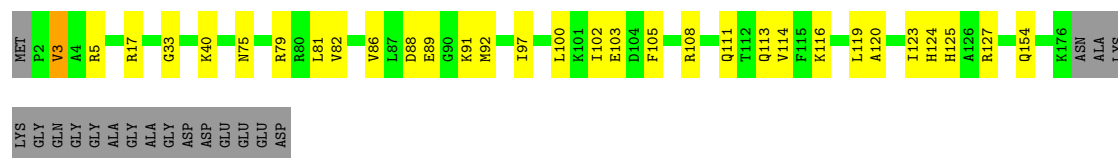
- Molecule 59: 40S ribosomal protein S8

Chain SI:

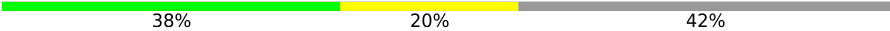


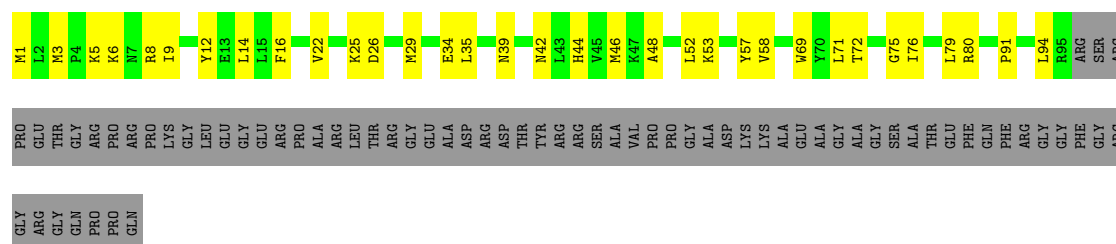
- Molecule 60: 40S ribosomal protein S9

Chain SJ:



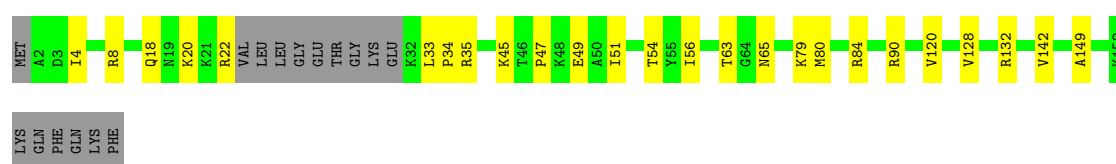
- Molecule 61: 40S ribosomal protein S10

Chain SK:  38% 20% 42%

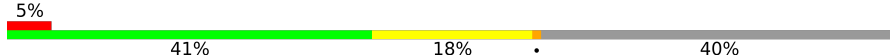


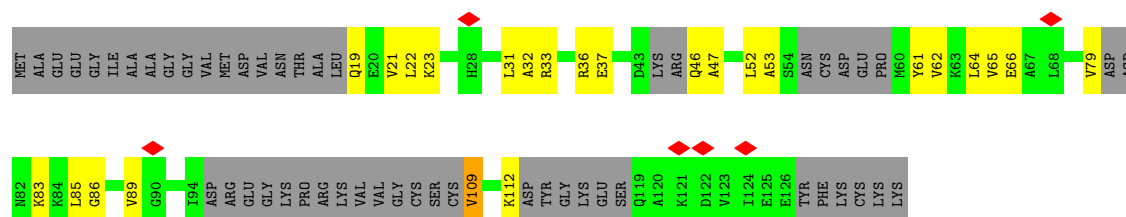
- Molecule 62: 40S ribosomal protein S11

Chain SL:  74% 16% 10%



- Molecule 63: 40S ribosomal protein S12

Chain SM:  5% 41% 18% 40%



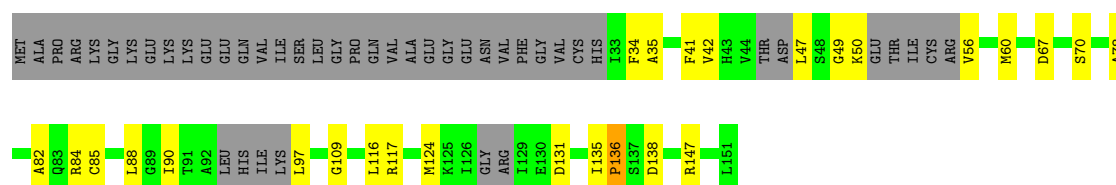
- Molecule 64: 40S ribosomal protein S13

Chain SN:  79% 20% 1%



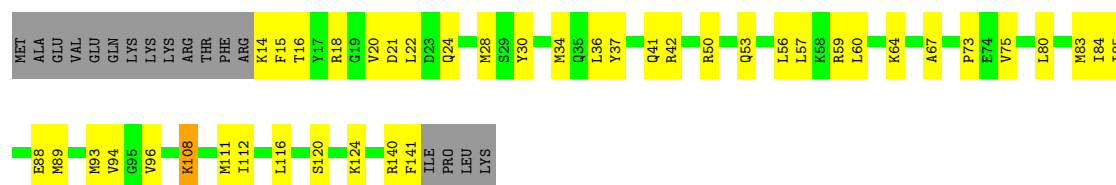
- Molecule 65: 40S ribosomal protein S14

Chain SO:  52% 17% 30%



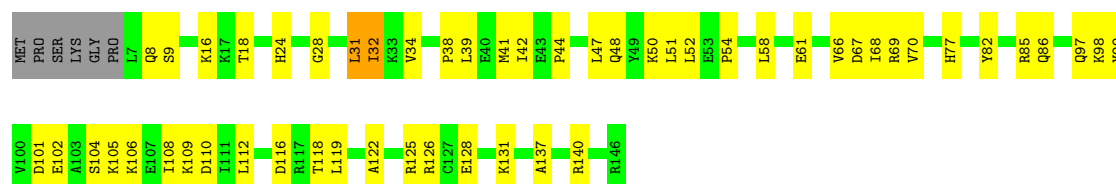
- Molecule 66: 40S ribosomal protein S15

Chain SP:  59% 28% 12%



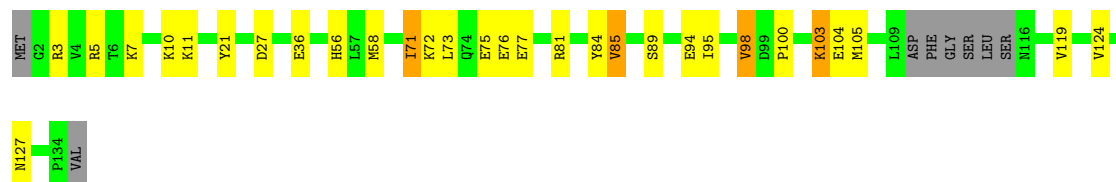
- Molecule 67: 40S ribosomal protein S16

Chain SQ:  60% 35%



- Molecule 68: 40S ribosomal protein S17

Chain SR:  72% 19% 6%



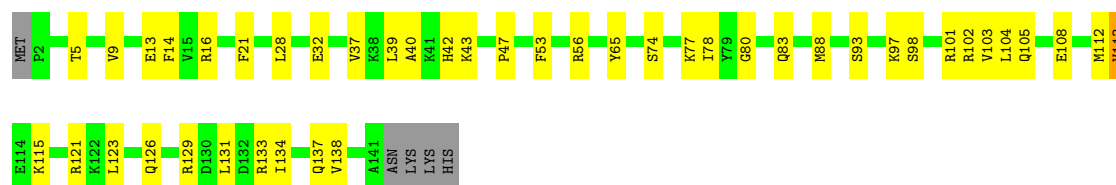
- Molecule 69: 40S ribosomal protein S18

Chain SS:  68% 28%



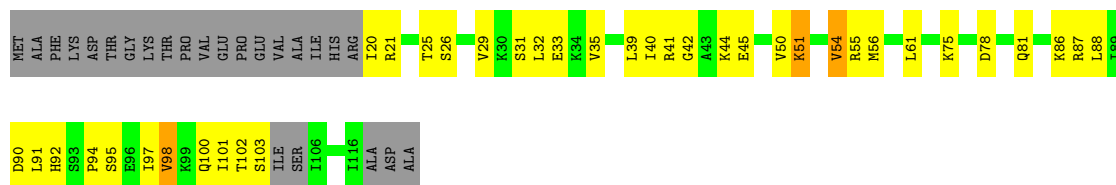
- Molecule 70: 40S ribosomal protein S19

Chain ST:  66% 30%



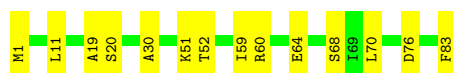
- Molecule 71: 40S ribosomal protein S20

Chain SU:  48% 29% 20%



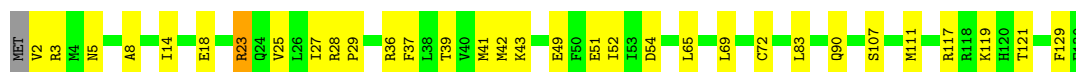
- Molecule 72: 40S ribosomal protein S21

Chain SV:  83% 17%



- Molecule 73: 40S ribosomal protein S15a

Chain SW:  75% 24% ..



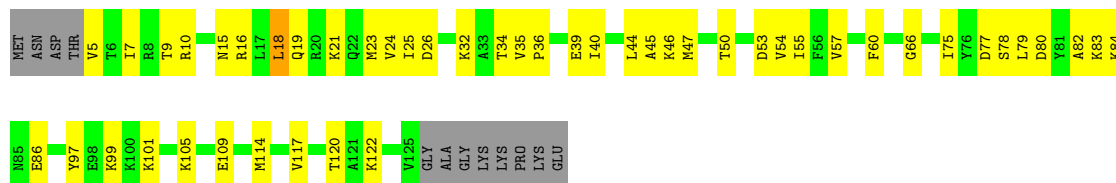
- Molecule 74: 40S ribosomal protein S23

Chain SX:  80% 16% ..



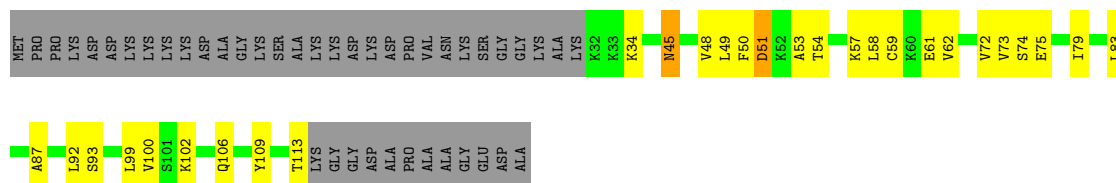
- Molecule 75: 40S ribosomal protein S24

Chain SY:  55% 35% 9%



- Molecule 76: 40S ribosomal protein S25

Chain SZ:  43% 21% 34%



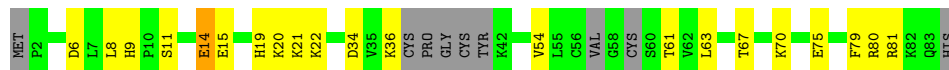
- Molecule 77: 40S ribosomal protein S26

Chain Sa:  75% 10% 14%



- Molecule 78: 40S ribosomal protein S27

Chain Sb:  64% 24% 11%



- Molecule 79: 40S ribosomal protein S28

Chain Sc:  57% 32% 9%



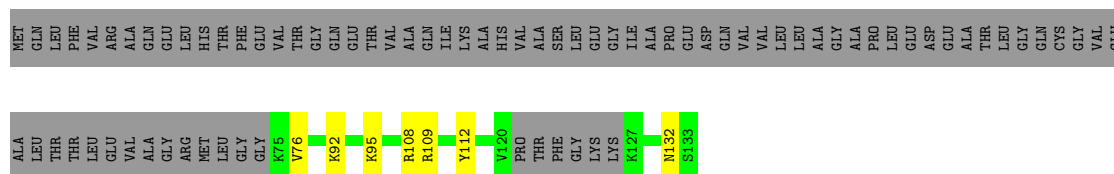
- Molecule 80: 40S ribosomal protein S29

Chain Sd:  73% 23% 4%



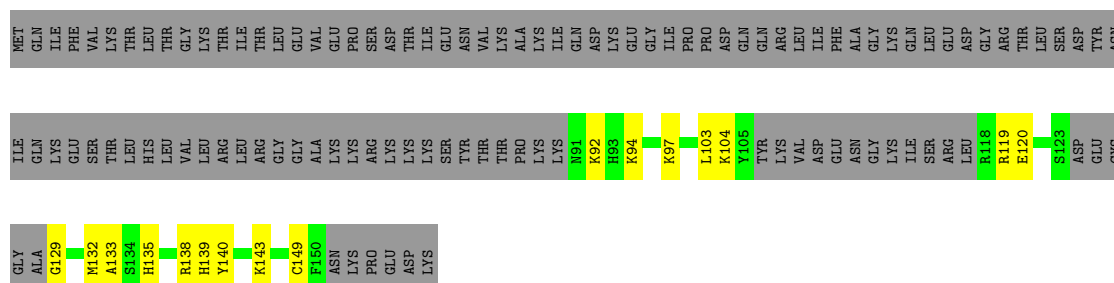
- Molecule 81: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:  35% 5% 60%

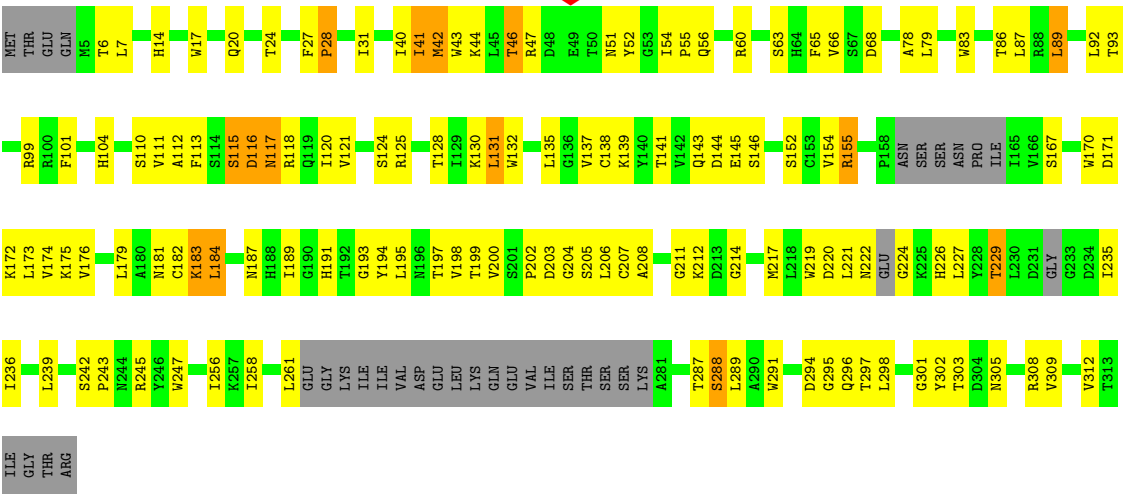


- Molecule 82: Ubiquitin

Chain Sf:  17% 10% 72%



● Molecule 83: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94974	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	0.119	Depositor
Minimum map value	-0.037	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: UR3, K, 4AC, V5N, OMU, SPD, MG, UY1, B8N, HY3, OMC, MA7, 5MC, MLZ, M2G, M3L, A2M, 1MG, PUT, 6MZ, PSU, 1MA, HYG, G7M, MA6, OMG, HIC, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	At	0.70	0/1714	1.00	1/2662 (0.0%)
2	Et	0.11	0/1287	0.27	0/1994
3	L5	0.17	3/78892 (0.0%)	0.30	2/123000 (0.0%)
4	L7	0.13	0/2836	0.26	0/4421
5	L8	0.16	0/3453	0.27	0/5376
6	LA	0.14	0/1935	0.34	0/2592
7	LB	0.12	0/3258	0.30	0/4359
8	LC	0.12	0/2927	0.30	0/3932
9	LD	0.12	0/2430	0.30	0/3254
10	LE	0.13	0/1816	0.29	0/2438
11	LF	0.15	0/1890	0.31	0/2521
12	LG	0.15	0/1855	0.34	1/2501 (0.0%)
13	LH	0.13	0/1537	0.31	0/2066
14	LI	0.13	0/1710	0.30	0/2284
15	LJ	0.13	0/1376	0.35	0/1841
16	LL	0.13	0/1695	0.30	0/2270
17	LM	0.13	0/1142	0.28	0/1527
18	LN	0.14	0/1745	0.33	0/2338
19	LO	0.14	0/1672	0.30	0/2238
20	LP	0.14	0/1279	0.32	0/1716
21	LQ	0.14	0/1536	0.32	0/2052
22	LR	0.13	0/1465	0.28	0/1945
23	LS	0.14	0/1500	0.31	0/2013
24	LT	0.14	0/1334	0.31	0/1781
25	LU	0.15	0/822	0.40	0/1103
26	LV	0.12	0/1002	0.30	0/1345
27	LW	0.13	0/542	0.33	0/722
28	LX	0.12	0/983	0.29	0/1323
29	LY	0.13	0/1115	0.32	0/1484
30	LZ	0.16	0/1130	0.34	0/1507
31	La	0.13	0/1178	0.30	0/1573

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.14	0/843	0.33	0/1111
33	Lc	0.12	0/771	0.28	0/1035
34	Ld	0.14	0/894	0.33	0/1204
35	Le	0.13	0/1082	0.30	0/1443
36	Lf	0.14	0/899	0.30	0/1205
37	Lg	0.12	0/898	0.29	0/1197
38	Lh	0.12	0/1022	0.26	0/1351
39	Li	0.12	0/843	0.31	0/1115
40	Lj	0.13	0/720	0.32	0/952
41	Lk	0.13	0/565	0.33	0/750
42	Ll	0.15	0/453	0.30	0/599
43	Lm	0.12	0/429	0.30	0/571
44	Ln	0.13	0/240	0.25	0/305
45	Lo	0.13	0/881	0.29	0/1161
46	Lp	0.13	0/708	0.30	0/941
47	Lr	0.14	0/1017	0.29	0/1364
48	Mr	0.62	0/160	0.98	0/246
49	Pt	0.71	0/1617	0.96	0/2509
50	S2	0.20	2/35344 (0.0%)	0.33	2/55048 (0.0%)
51	SA	0.15	0/1730	0.36	0/2351
52	SB	0.15	0/1651	0.38	0/2203
53	SC	0.14	0/1726	0.35	0/2332
54	SD	0.22	1/1747 (0.1%)	0.53	4/2350 (0.2%)
55	SE	0.13	0/2083	0.35	0/2805
56	SF	0.15	0/1437	0.42	0/1933
57	SG	0.17	0/1671	0.45	2/2227 (0.1%)
58	SH	0.14	0/1332	0.38	0/1782
59	SI	0.14	0/1679	0.38	0/2239
60	SJ	0.13	0/1446	0.31	0/1937
61	SK	0.16	0/823	0.42	0/1111
62	SL	0.12	0/1184	0.30	0/1583
63	SM	0.13	0/554	0.36	0/743
64	SN	0.12	0/1231	0.28	0/1656
65	SO	0.18	0/793	0.44	1/1056 (0.1%)
66	SP	0.28	0/1057	0.44	0/1414
67	SQ	0.16	0/1133	0.42	0/1517
68	SR	0.13	0/1045	0.36	0/1402
69	SS	0.13	0/1232	0.38	1/1651 (0.1%)
70	ST	0.16	0/1131	0.39	0/1518
71	SU	0.17	0/763	0.42	0/1023
72	SV	0.12	0/643	0.31	0/860
73	SW	0.15	0/1051	0.35	0/1406
74	SX	0.23	0/1096	0.43	0/1461

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SY	0.15	0/1012	0.42	0/1344
76	SZ	0.18	0/669	0.45	0/895
77	Sa	0.14	0/805	0.33	0/1079
78	Sb	0.15	0/600	0.42	0/798
79	Sc	0.15	0/497	0.39	0/666
80	Sd	0.11	0/469	0.32	0/623
81	Se	0.32	0/423	0.48	0/555
82	Sf	0.12	0/347	0.36	0/457
83	Sg	0.77	3/2251 (0.1%)	0.85	6/3062 (0.2%)
All	All	0.20	9/215753 (0.0%)	0.35	20/316324 (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
83	Sg	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	Sg	28	PRO	CG-CD	-25.69	0.63	1.50
83	Sg	28	PRO	CB-CG	12.98	2.14	1.49
83	Sg	28	PRO	N-CD	9.65	1.61	1.47
54	SD	219	PRO	CG-CD	-5.31	1.32	1.50
50	S2	627	OMU	O3'-P	5.21	1.61	1.56
3	L5	3785	A2M	O3'-P	5.17	1.61	1.56
50	S2	484	A2M	O3'-P	5.11	1.61	1.56
3	L5	3830	A2M	O3'-P	5.04	1.61	1.56
3	L5	4523	A2M	O3'-P	5.04	1.61	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	Sg	28	PRO	N-CD-CG	-16.72	78.13	103.20
83	Sg	28	PRO	CA-N-CD	-13.52	93.07	112.00
83	Sg	28	PRO	CB-CG-CD	-12.98	64.57	106.10
54	SD	219	PRO	CA-CB-CG	-11.33	82.98	104.50
54	SD	219	PRO	N-CD-CG	-11.33	86.21	103.20
83	Sg	28	PRO	CA-CB-CG	-11.01	83.59	104.50
83	Sg	28	PRO	N-CA-CB	-9.13	93.66	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SD	219	PRO	N-CA-CB	-7.47	96.66	103.31
57	SG	122	PRO	N-CD-CG	-7.41	92.09	103.20
54	SD	219	PRO	CA-N-CD	-6.44	102.99	112.00
83	Sg	182	CYS	CB-CA-C	-6.41	109.20	116.63
57	SG	122	PRO	CA-N-CD	-6.35	103.12	112.00
50	S2	1824	A	C4'-C3'-O3'	-5.51	104.74	113.00
3	L5	4531	U	C4'-C3'-O3'	5.45	117.57	109.40
69	SS	100	ALA	CB-CA-C	-5.41	109.87	117.23
12	LG	133	PRO	N-CD-CG	-5.40	95.10	103.20
1	At	17	G	C4'-C3'-O3'	5.31	117.36	109.40
65	SO	136	PRO	CA-N-CD	-5.31	104.57	112.00
3	L5	3758	PSU	P-O3'-C3'	5.17	127.96	120.20
50	S2	1084	A	C4'-C3'-O3'	-5.13	105.31	113.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	Sg	155	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	1	0
2	Et	1155	0	593	14	0
3	L5	73250	0	37111	763	0
4	L7	2538	0	1286	20	0
5	L8	3177	0	1613	41	0
6	LA	1907	0	1999	18	0
7	LB	3203	0	3344	29	0
8	LC	2873	0	3046	23	0
9	LD	2385	0	2419	31	0
10	LE	1782	0	1934	26	0
11	LF	1856	0	1981	16	0
12	LG	1824	0	1938	17	0
13	LH	1518	0	1600	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	LI	1672	0	1717	17	0
15	LJ	1353	0	1386	23	0
16	LL	1664	0	1773	15	0
17	LM	1120	0	1187	6	0
18	LN	1700	0	1749	14	0
19	LO	1640	0	1788	18	0
20	LP	1249	0	1276	12	0
21	LQ	1512	0	1628	11	0
22	LR	1449	0	1549	14	0
23	LS	1460	0	1502	16	0
24	LT	1303	0	1379	17	0
25	LU	808	0	831	14	0
26	LV	988	0	1047	6	0
27	LW	529	0	537	3	0
28	LX	966	0	1040	13	0
29	LY	1098	0	1178	12	0
30	LZ	1107	0	1182	23	0
31	La	1162	0	1206	8	0
32	Lb	841	0	912	23	0
33	Lc	761	0	796	9	0
34	Ld	879	0	924	12	0
35	Le	1061	0	1160	8	0
36	Lf	880	0	917	3	0
37	Lg	888	0	977	10	0
38	Lh	1014	0	1148	16	0
39	Li	832	0	917	5	0
40	Lj	705	0	737	8	0
41	Lk	559	0	624	7	0
42	Ll	443	0	483	5	0
43	Lm	432	0	465	5	0
44	Ln	239	0	289	2	0
45	Lo	875	0	941	11	0
46	Lp	698	0	748	7	0
47	Lr	1002	0	1068	14	0
48	Mr	145	0	76	1	0
49	Pt	1547	0	792	4	0
50	S2	33424	0	16927	453	0
51	SA	1693	0	1693	47	0
52	SB	1627	0	1701	35	0
53	SC	1690	0	1777	31	0
54	SD	1721	0	1809	41	0
55	SE	2041	0	2143	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	SF	1417	0	1458	44	0
57	SG	1652	0	1791	33	0
58	SH	1317	0	1409	24	0
59	SI	1651	0	1726	39	0
60	SJ	1424	0	1499	21	0
61	SK	799	0	823	22	0
62	SL	1164	0	1232	16	0
63	SM	556	0	550	15	0
64	SN	1207	0	1294	19	0
65	SO	788	0	813	22	0
66	SP	1037	0	1074	28	0
67	SQ	1116	0	1185	41	0
68	SR	1032	0	1090	20	0
69	SS	1214	0	1275	32	0
70	ST	1104	0	1132	31	0
71	SU	755	0	820	29	0
72	SV	636	0	637	10	0
73	SW	1034	0	1080	23	0
74	SX	1088	0	1149	13	0
75	SY	995	0	1068	34	0
76	SZ	661	0	732	26	0
77	Sa	792	0	841	10	0
78	Sb	592	0	619	13	0
79	Sc	495	0	523	16	0
80	Sd	458	0	448	12	0
81	Se	420	0	463	8	0
82	Sf	341	0	335	15	0
83	Sg	2199	0	2146	76	0
84	L5	36	0	72	2	0
84	S2	12	0	24	3	0
85	L5	140	0	266	9	0
85	LN	10	0	19	0	0
85	S2	30	0	57	0	0
86	L5	159	0	0	0	0
86	L7	2	0	0	0	0
86	L8	3	0	0	0	0
86	LP	1	0	0	0	0
86	LR	1	0	0	0	0
86	S2	29	0	0	0	0
87	L5	60	0	0	0	0
87	L8	1	0	0	0	0
87	LA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LH	1	0	0	0	0
87	Lg	1	0	0	0	0
87	S2	9	0	0	0	0
87	Sd	1	0	0	0	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lm	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	Sa	1	0	0	0	0
88	Sd	1	0	0	0	0
89	S2	36	0	36	1	0
90	At	18	0	0	0	0
90	Et	37	0	0	0	0
90	L5	5891	0	0	9	0
90	L7	172	0	0	0	0
90	L8	297	0	0	0	0
90	LA	90	0	0	0	0
90	LB	143	0	0	0	0
90	LC	157	0	0	2	0
90	LD	51	0	0	1	0
90	LE	53	0	0	1	0
90	LF	95	0	0	1	0
90	LG	57	0	0	1	0
90	LH	51	0	0	0	0
90	LI	81	0	0	0	0
90	LJ	16	0	0	0	0
90	LL	81	0	0	0	0
90	LM	35	0	0	0	0
90	LN	106	0	0	0	0
90	LO	81	0	0	0	0
90	LP	56	0	0	2	0
90	LQ	89	0	0	0	0
90	LR	72	0	0	1	0
90	LS	89	0	0	2	0
90	LT	59	0	0	0	0
90	LU	5	0	0	0	0
90	LV	42	0	0	0	0
90	LW	22	0	0	0	0
90	LX	32	0	0	1	0
90	LY	40	0	0	1	0
90	LZ	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	La	72	0	0	0	0
90	Lb	30	0	0	1	0
90	Lc	11	0	0	0	0
90	Ld	34	0	0	0	0
90	Le	77	0	0	0	0
90	Lf	52	0	0	0	0
90	Lg	48	0	0	0	0
90	Lh	43	0	0	1	0
90	Li	38	0	0	1	0
90	Lj	53	0	0	0	0
90	Lk	3	0	0	0	0
90	Ll	34	0	0	0	0
90	Lm	21	0	0	0	0
90	Ln	18	0	0	0	0
90	Lo	61	0	0	1	0
90	Lp	38	0	0	1	0
90	Lr	53	0	0	1	0
90	Mr	3	0	0	0	0
90	Pt	34	0	0	0	0
90	S2	974	0	0	3	0
90	SA	3	0	0	0	0
90	SC	12	0	0	0	0
90	SD	4	0	0	0	0
90	SE	10	0	0	0	0
90	SF	3	0	0	1	0
90	SG	2	0	0	0	0
90	SH	1	0	0	0	0
90	SI	28	0	0	2	0
90	SJ	7	0	0	0	0
90	SK	1	0	0	0	0
90	SL	29	0	0	2	0
90	SM	3	0	0	0	0
90	SN	14	0	0	0	0
90	SO	7	0	0	0	0
90	SP	5	0	0	0	0
90	SQ	3	0	0	0	0
90	SR	3	0	0	0	0
90	SS	9	0	0	0	0
90	SU	3	0	0	0	0
90	SV	3	0	0	0	0
90	SW	8	0	0	0	0
90	SX	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	SY	1	0	0	0	0
90	SZ	1	0	0	0	0
90	Sa	11	0	0	0	0
90	Sb	2	0	0	0	0
90	Sd	4	0	0	0	0
90	Se	3	0	0	1	0
All	All	216235	0	153322	2426	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 7.

All (2426) 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)
61:SK:91:PRO:HG2	61:SK:94:LEU:HD23	1.52	0.92
76:SZ:45:ASN:O	76:SZ:45:ASN:ND2	2.08	0.85
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.59	0.84
3:L5:4095:G:H1	3:L5:4113:U:H3	1.25	0.82
76:SZ:45:ASN:HD22	76:SZ:45:ASN:C	1.89	0.80
50:S2:928:G:H1	50:S2:1013:U:H3	1.29	0.80
65:SO:117:ARG:HH21	77:Sa:49:ALA:HA	1.47	0.80
3:L5:2364:OMG:N2	3:L5:3858:C:O2	2.12	0.80
50:S2:1536:G:H2'	50:S2:1537:A:H8	1.45	0.79
5:L8:50:C:O2	5:L8:75:OMG:N2	2.15	0.78
50:S2:377:G:H5''	59:SI:98:LYS:HB3	1.67	0.77
15:LJ:31:ASP:OD2	15:LJ:35:ARG:NH2	2.17	0.77
3:L5:4592:C:O2	3:L5:4618:OMG:N2	2.14	0.77
3:L5:3663:A:N6	3:L5:4168:G:O2'	2.18	0.77
76:SZ:48:VAL:HA	76:SZ:83:LEU:HD22	1.65	0.76
3:L5:3944:OMG:HN1	3:L5:4069:U:H3	1.32	0.76
65:SO:56:VAL:N	65:SO:60:MET:SD	2.58	0.76
50:S2:1091:C:HO2'	73:SW:2:VAL:N	1.83	0.76
83:Sg:44:LYS:HB2	83:Sg:56:GLN:HG2	1.67	0.76
70:ST:104:LEU:HD22	70:ST:121:ARG:HG3	1.68	0.74
30:LZ:99:ASP:HB3	30:LZ:102:ARG:HH21	1.52	0.74
3:L5:964:A:H2'	3:L5:965:G:H4'	1.70	0.73
56:SF:71:ARG:NH2	56:SF:148:ASN:OD1	2.21	0.73
24:LT:157:GLU:HG2	24:LT:160:ALA:HB3	1.69	0.73
83:Sg:112:ALA:HB3	83:Sg:121:VAL:HG12	1.69	0.73
34:Ld:57:MET:HE3	34:Ld:90:ARG:HB2	1.69	0.73
50:S2:1536:G:H2'	50:S2:1537:A:C8	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SP:41:GLN:HG3	66:SP:84:ILE:HD12	1.69	0.73
3:L5:4228:OMG:N2	3:L5:4375:C:O2	2.15	0.72
3:L5:2699:C:OP1	22:LR:16:ARG:NH2	2.22	0.72
3:L5:1364:U:OP2	16:LL:36:ARG:NH1	2.22	0.71
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.19	0.71
3:L5:4115:G:N2	3:L5:4115:G:OP2	2.22	0.71
8:LC:140:LYS:HE3	8:LC:245:HIS:HB2	1.71	0.71
79:Sc:18:LEU:HD12	79:Sc:29:GLN:HG2	1.71	0.71
30:LZ:99:ASP:HB3	30:LZ:102:ARG:NH2	2.05	0.71
76:SZ:54:THR:HA	76:SZ:57:LYS:HD3	1.73	0.71
12:LG:153:GLN:NE2	12:LG:205:THR:O	2.23	0.70
3:L5:4546:A:N7	6:LA:215:ASN:ND2	2.40	0.70
50:S2:601:OMG:N2	50:S2:621:C:O2	2.20	0.70
52:SB:128:LYS:HG2	52:SB:134:LEU:HD13	1.72	0.70
67:SQ:58:LEU:HD22	67:SQ:108:ILE:HG22	1.73	0.70
50:S2:1228:A:H2'	50:S2:1229:G:C8	2.26	0.70
57:SG:181:THR:HG22	57:SG:183:ARG:H	1.57	0.70
71:SU:40:ILE:O	71:SU:44:LYS:HG2	1.92	0.70
3:L5:1522:OMG:N2	3:L5:1655:C:O2	2.19	0.69
3:L5:2557:G:H1	3:L5:2570:U:H3	1.39	0.69
3:L5:3938:G:OP2	18:LN:24:ARG:NH1	2.25	0.69
50:S2:1388:A:H61	54:SD:161:GLY:HA3	1.57	0.69
9:LD:217:ASP:HA	9:LD:220:LYS:HE2	1.74	0.69
50:S2:317:C:OP2	57:SG:183:ARG:NH1	2.26	0.69
50:S2:1203:G:H2'	50:S2:1204:A:C8	2.28	0.69
3:L5:4918:C:H2'	3:L5:4919:G:H8	1.58	0.68
29:LY:30:MET:HB3	29:LY:101:PRO:HG3	1.75	0.68
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.58	0.68
55:SE:100:ARG:HG2	55:SE:102:ILE:HG12	1.74	0.68
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.59	0.68
3:L5:2520:C:O2	3:L5:2640:G:N2	2.26	0.68
50:S2:918:PSU:O2'	50:S2:919:A:O4'	2.12	0.68
71:SU:78:ASP:OD1	80:Sd:54:LYS:NZ	2.26	0.68
50:S2:981:A:H2'	50:S2:982:G:C8	2.29	0.68
51:SA:66:VAL:HG21	51:SA:185:MET:HB3	1.75	0.68
23:LS:99:ASP:OD2	23:LS:108:GLN:NE2	2.25	0.68
56:SF:144:LEU:O	56:SF:148:ASN:ND2	2.26	0.68
83:Sg:104:HIS:CD2	83:Sg:130:LYS:HD2	2.29	0.68
52:SB:122:GLU:HG2	52:SB:140:VAL:HG12	1.75	0.68
3:L5:1563:A:N6	50:S2:1028:A:N1	2.42	0.67
50:S2:928:G:H2'	50:S2:929:G:C8	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:433:A:H5''	59:SI:22:HIS:HB3	1.75	0.67
62:SL:65:ASN:O	62:SL:132:ARG:NH1	2.26	0.67
83:Sg:130:LYS:NZ	83:Sg:141:THR:OG1	2.25	0.67
76:SZ:53:ALA:O	76:SZ:57:LYS:HG3	1.94	0.67
70:ST:126:GLN:OE1	70:ST:126:GLN:N	2.22	0.67
74:SX:123:VAL:HG22	74:SX:124:LYS:HG3	1.76	0.67
3:L5:169:G:O2'	16:LL:136:LYS:NZ	2.28	0.67
73:SW:69:LEU:HD11	73:SW:129:PHE:HB2	1.77	0.67
51:SA:33:GLN:NE2	72:SV:64:GLU:OE2	2.28	0.67
22:LR:165:LYS:NZ	50:S2:907:G:OP2	2.28	0.67
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.77	0.66
50:S2:30:C:O2	50:S2:644:OMG:N2	2.19	0.66
50:S2:1588:A:H2'	50:S2:1589:A:C8	2.30	0.66
50:S2:1010:G:H2'	50:S2:1011:A:H8	1.60	0.66
53:SC:102:LEU:HB3	53:SC:130:ILE:HD11	1.77	0.66
61:SK:3:MET:HE1	61:SK:48:ALA:HB2	1.76	0.66
3:L5:143:C:OP1	12:LG:111:LYS:NZ	2.28	0.66
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.31	0.66
3:L5:1418:C:H2'	3:L5:1419:G:O4'	1.95	0.66
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.30	0.66
50:S2:570:C:O2'	75:SY:34:THR:O	2.12	0.66
13:LH:94:SER:HB2	13:LH:142:ASP:HB3	1.76	0.66
50:S2:1413:G:H2'	50:S2:1414:A:H8	1.60	0.66
2:Et:21:A:N6	2:Et:46:G:O2'	2.29	0.66
50:S2:1130:G:OP2	50:S2:1130:G:N2	2.25	0.66
67:SQ:128:GLU:HG2	67:SQ:137:ALA:HB1	1.77	0.66
10:LE:101:ASN:O	10:LE:105:ARG:NH1	2.25	0.66
16:LL:100:PRO:O	39:Li:25:ARG:NH2	2.28	0.66
59:SI:141:ARG:HB3	59:SI:145:ILE:HD11	1.78	0.66
50:S2:1648:G:O6	67:SQ:16:LYS:NZ	2.27	0.66
3:L5:4620:OMU:OP2	3:L5:4670:C:N4	2.28	0.66
3:L5:4910:G:N2	19:LO:106:ASP:O	2.28	0.66
68:SR:100:PRO:O	68:SR:104:GLU:HG3	1.96	0.66
77:Sa:45:VAL:HG11	77:Sa:53:ILE:HG13	1.78	0.66
51:SA:69:GLU:N	51:SA:69:GLU:OE2	2.29	0.65
51:SA:211:GLU:HA	51:SA:214:GLU:HB2	1.79	0.65
7:LB:108:GLU:OE2	7:LB:138:GLN:NE2	2.29	0.65
50:S2:640:A:H2'	50:S2:641:A:C8	2.31	0.65
50:S2:1589:A:N3	50:S2:1653:U:O2'	2.29	0.65
3:L5:2583:C:OP2	37:Lg:76:ARG:NH1	2.29	0.65
60:SJ:114:VAL:HG13	60:SJ:119:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:126:C:H2'	3:L5:127:G:H8	1.62	0.65
3:L5:1245:C:H2'	3:L5:1246:G:H8	1.62	0.65
3:L5:3627:OMG:N2	3:L5:3834:C:O2	2.20	0.65
69:SS:34:LYS:HG2	69:SS:103:LEU:HD23	1.79	0.65
45:Lo:71:GLU:OE2	45:Lo:78:ARG:NH2	2.30	0.65
50:S2:186:C:H2'	50:S2:187:G:H8	1.62	0.65
55:SE:238:LEU:HB2	55:SE:242:LYS:HE3	1.79	0.65
60:SJ:82:VAL:HG21	60:SJ:92:MET:HE1	1.79	0.65
67:SQ:97:GLN:HG3	67:SQ:105:LYS:HE2	1.79	0.65
75:SY:23:MET:SD	75:SY:23:MET:N	2.69	0.65
82:Sf:120:GLU:OE1	82:Sf:129:GLY:N	2.29	0.65
30:LZ:95:VAL:HG13	30:LZ:109:LYS:HG2	1.79	0.65
50:S2:51:U:H2'	50:S2:52:G:H8	1.62	0.65
51:SA:7:VAL:HG13	51:SA:8:LEU:HD22	1.80	0.64
83:Sg:89:LEU:HD21	83:Sg:99:ARG:HB3	1.79	0.64
3:L5:3910:C:O2	3:L5:4392:OMG:N2	2.18	0.64
72:SV:20:SER:HB3	72:SV:59:ILE:HD11	1.79	0.64
3:L5:1279:A:O2'	3:L5:1281:G:N7	2.28	0.64
50:S2:1636:G:OP2	76:SZ:34:LYS:NZ	2.28	0.64
68:SR:7:LYS:HG3	68:SR:11:LYS:HD2	1.78	0.64
83:Sg:44:LYS:N	83:Sg:54:ILE:O	2.31	0.64
3:L5:4734:A:H2'	3:L5:4735:G:C8	2.33	0.64
50:S2:1400:U:O4	50:S2:1401:A:N6	2.31	0.64
83:Sg:220:ASP:O	83:Sg:224:GLY:N	2.31	0.64
7:LB:92:TYR:HB2	7:LB:159:VAL:HB	1.78	0.64
3:L5:280:G:H5''	18:LN:14:LYS:HE2	1.80	0.64
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.32	0.64
42:Ll:9:ILE:HD12	42:Ll:51:LEU:HD11	1.79	0.64
50:S2:1480:A:H5'	67:SQ:131:LYS:HE2	1.80	0.64
65:SO:34:PHE:HB3	65:SO:41:PHE:HB2	1.80	0.64
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.61	0.64
50:S2:1387:G:N1	54:SD:206:ASP:OD2	2.28	0.64
50:S2:1562:C:H2'	50:S2:1563:G:H8	1.63	0.64
67:SQ:104:SER:O	67:SQ:108:ILE:HG12	1.97	0.64
83:Sg:197:THR:HG21	83:Sg:239:LEU:H	1.62	0.64
50:S2:1705:C:H2'	50:S2:1706:G:C8	2.33	0.64
3:L5:2260:C:O2'	47:Lr:99:LYS:NZ	2.31	0.64
50:S2:107:A:H2'	50:S2:108:G:C8	2.33	0.64
50:S2:1587:G:H21	70:ST:77:LYS:HE3	1.63	0.64
3:L5:4455:G:OP1	7:LB:5:LYS:NZ	2.30	0.63
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:181:C:H2'	3:L5:182:G:H8	1.62	0.63
50:S2:189:U:OP1	59:SI:152:ARG:NH2	2.31	0.63
51:SA:76:VAL:HG12	51:SA:123:VAL:HB	1.79	0.63
71:SU:94:PRO:HD2	71:SU:97:ILE:HD11	1.80	0.63
52:SB:173:THR:O	52:SB:177:GLN:HB2	1.97	0.63
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.62	0.63
3:L5:4966:A:H5''	7:LB:128:LYS:HG3	1.81	0.63
3:L5:1903:G:OP1	36:Lf:87:LYS:NZ	2.30	0.63
83:Sg:52:TYR:HD1	83:Sg:309:VAL:HG21	1.63	0.63
50:S2:591:U:H5''	50:S2:592:C:H3'	1.81	0.63
55:SE:112:HIS:NE2	55:SE:237:SER:O	2.29	0.63
83:Sg:43:TRP:HA	83:Sg:55:PRO:HA	1.80	0.63
3:L5:4769:G:OP1	19:LO:176:ARG:NH1	2.31	0.63
60:SJ:113:GLN:OE1	60:SJ:154:GLN:NE2	2.30	0.63
3:L5:173:C:OP1	16:LL:129:ARG:NH2	2.31	0.62
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.35	0.62
53:SC:116:THR:OG1	53:SC:119:GLY:O	2.16	0.62
54:SD:172:VAL:HG22	54:SD:185:LYS:HG2	1.81	0.62
66:SP:30:TYR:O	66:SP:34:MET:HG3	1.99	0.62
3:L5:4618:OMG:H5''	26:LV:15:ARG:HB2	1.81	0.62
28:LX:67:ARG:NH1	90:LX:201:HOH:O	2.31	0.62
55:SE:104:ASP:HB3	55:SE:110:ALA:HB2	1.81	0.62
3:L5:4472:G:O2'	43:Lm:100:TYR:O	2.18	0.62
6:LA:39:GLY:HA2	6:LA:93:LYS:HG3	1.80	0.62
62:SL:35:ARG:HH21	62:SL:63:THR:HG21	1.64	0.62
50:S2:145:G:H2'	50:S2:146:G:C8	2.35	0.62
50:S2:436:OMG:N2	50:S2:457:C:O2	2.19	0.62
50:S2:919:A:OP2	64:SN:64:ARG:NH2	2.30	0.62
50:S2:367:U:H4'	50:S2:371:A:C8	2.35	0.62
75:SY:78:SER:OG	75:SY:80:ASP:OD1	2.17	0.62
50:S2:1255:G:OP1	50:S2:1256:G:O2'	2.13	0.62
55:SE:44:LEU:HD21	55:SE:72:ILE:HD11	1.81	0.62
3:L5:170:C:O2'	3:L5:171:U:OP1	2.17	0.62
3:L5:2091:C:O2	3:L5:2094:G:O2'	2.12	0.62
3:L5:5013:C:N4	3:L5:5029:C:OP1	2.32	0.62
10:LE:99:ASP:OD2	10:LE:100:LYS:NZ	2.29	0.62
50:S2:101:U:H5''	59:SI:19:LYS:HE3	1.82	0.62
66:SP:64:LYS:NZ	66:SP:88:GLU:O	2.32	0.62
3:L5:109:G:OP2	16:LL:74:ARG:NH2	2.29	0.62
3:L5:1405:C:N4	3:L5:1406:G:O6	2.33	0.62
50:S2:951:C:H1'	65:SO:50:LYS:HZ1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LH:92:MET:HE2	13:LH:179:ILE:HG22	1.82	0.61
50:S2:1288:OMU:H3'	82:Sf:97:LYS:NZ	2.14	0.61
4:L7:110:G:OP1	9:LD:270:LYS:NZ	2.33	0.61
3:L5:1238:A:O2'	11:LF:52:GLU:OE1	2.17	0.61
69:SS:92:ASP:HB2	69:SS:94:LYS:HD2	1.82	0.61
74:SX:71:ARG:NH1	74:SX:82:THR:OG1	2.32	0.61
50:S2:1845:A:H2'	50:S2:1846:G:C8	2.36	0.61
63:SM:37:GLU:OE1	63:SM:37:GLU:N	2.31	0.61
50:S2:381:C:H5'	59:SI:48:VAL:HG13	1.83	0.61
50:S2:996:A:H2'	50:S2:997:A:C8	2.35	0.61
50:S2:1521:C:OP2	69:SS:136:THR:OG1	2.13	0.61
50:S2:51:U:H2'	50:S2:52:G:C8	2.36	0.61
52:SB:190:PRO:O	52:SB:195:LYS:NZ	2.33	0.61
3:L5:217:C:H3'	3:L5:218:A:H2'	1.83	0.61
3:L5:294:G:OP2	45:Lo:43[A]:ARG:NH1	2.31	0.61
23:LS:69:GLU:HG3	23:LS:71:SER:H	1.66	0.61
50:S2:573:PSU:N1	50:S2:576:A2M:OP2	2.27	0.61
51:SA:173:LEU:HD11	51:SA:177:MET:HE2	1.83	0.61
56:SF:35:LEU:HD22	56:SF:117:ILE:HD12	1.81	0.61
71:SU:55:ARG:HH11	71:SU:87:ARG:HE	1.47	0.61
3:L5:2899:C:OP1	22:LR:108:ARG:NH2	2.31	0.61
50:S2:1007:C:H2'	50:S2:1008:A:C8	2.35	0.61
3:L5:4095:G:O6	3:L5:4113:U:O4	2.19	0.61
52:SB:68:GLU:HG2	52:SB:85:LYS:HD3	1.83	0.61
3:L5:1293:G:OP2	3:L5:1293:G:N2	2.27	0.60
3:L5:1849:U:H3'	16:LL:5:ARG:HH12	1.65	0.60
3:L5:4397:A:H2'	3:L5:4452:U:O4	2.01	0.60
50:S2:1570:G:N7	70:ST:97:LYS:NZ	2.49	0.60
59:SI:4:SER:OG	59:SI:6:ASP:OD2	2.16	0.60
71:SU:29:VAL:O	71:SU:33:GLU:HG2	2.01	0.60
76:SZ:57:LYS:O	76:SZ:61:GLU:HG2	2.00	0.60
83:Sg:42:MET:O	83:Sg:56:GLN:N	2.22	0.60
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.83	0.60
3:L5:1785:C:OP1	14:LI:133:GLN:NE2	2.34	0.60
23:LS:30:MET:HE1	23:LS:47:PHE:HB3	1.83	0.60
55:SE:107:GLY:HA2	55:SE:189:LEU:HG	1.83	0.60
53:SC:146:GLU:OE1	54:SD:120:TYR:OH	2.17	0.60
3:L5:2414:G:H2'	3:L5:2415:OMU:H6	1.83	0.60
5:L8:102:G:OP2	5:L8:104:A:O2'	2.19	0.60
33:Lc:13:SER:HB2	33:Lc:17:ARG:HH21	1.65	0.60
67:SQ:97:GLN:OE1	83:Sg:60:ARG:NE	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.37	0.60
3:L5:4862:G:H2'	3:L5:4863:G:C8	2.36	0.60
50:S2:925:G:H1	50:S2:1017:U:H3	1.49	0.60
50:S2:948:C:H2'	50:S2:949:G:H8	1.66	0.60
50:S2:989:C:OP2	52:SB:155:TYR:OH	2.18	0.60
50:S2:1291:A:N3	82:Sf:140:TYR:OH	2.29	0.60
50:S2:1606:G:N2	50:S2:1632:G:H1'	2.17	0.60
57:SG:44:GLU:OE2	57:SG:120:ASP:N	2.29	0.60
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.37	0.60
7:LB:220:ILE:HG12	7:LB:278:THR:HG23	1.83	0.60
20:LP:135:ARG:NH2	90:LP:301:HOH:O	2.35	0.60
54:SD:170:THR:HG23	54:SD:187:LYS:HG2	1.84	0.60
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.36	0.59
45:Lo:78:ARG:O	45:Lo:80:LYS:NZ	2.35	0.59
51:SA:80:ARG:NH2	51:SA:165:ASN:O	2.34	0.59
58:SH:148:LEU:HD23	73:SW:42:MET:HE3	1.84	0.59
3:L5:164:G:H2'	3:L5:165:A:H8	1.66	0.59
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.67	0.59
69:SS:67:VAL:HG12	69:SS:71:MET:HE3	1.82	0.59
15:LJ:95:ARG:O	15:LJ:98:ASN:HB2	2.02	0.59
56:SF:145:ARG:HA	56:SF:148:ASN:HD22	1.64	0.59
69:SS:28:PHE:O	69:SS:31:THR:OG1	2.19	0.59
3:L5:164:G:H2'	3:L5:165:A:C8	2.38	0.59
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.37	0.59
3:L5:2756:G:N7	30:LZ:51:ARG:NH2	2.50	0.59
9:LD:62:CYS:HB3	9:LD:105:LEU:HD22	1.84	0.59
15:LJ:56:THR:HG23	15:LJ:63:ARG:HA	1.82	0.59
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	1.85	0.59
50:S2:181:A:OP2	50:S2:182:C:O2'	2.18	0.59
51:SA:198:MET:HE2	68:SR:89:SER:HB2	1.83	0.59
3:L5:3723:A2M:H2'	3:L5:3724:A2M:H8	1.84	0.59
23:LS:19:THR:HG23	23:LS:21:LYS:H	1.66	0.59
50:S2:1303:C:O2	82:Sf:92:LYS:NZ	2.35	0.59
8:LC:163:LYS:HB2	8:LC:166:GLU:HG3	1.84	0.59
14:LI:156:LYS:HD2	14:LI:163:GLN:HB2	1.84	0.59
77:Sa:51:ARG:NH2	79:Sc:39:SER:O	2.33	0.59
63:SM:31:LEU:HB3	63:SM:109:VAL:HG23	1.84	0.59
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.67	0.59
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.37	0.59
10:LE:72:LYS:NZ	32:Lb:115:GLY:O	2.31	0.59
19:LO:158:GLU:O	19:LO:162:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:29:G:H2'	50:S2:30:C:C6	2.38	0.59
52:SB:224:GLU:HB2	52:SB:227:LYS:HE3	1.84	0.59
3:L5:1460:C:H5''	21:LQ:144:LYS:HG2	1.83	0.59
3:L5:4260:U:H2'	3:L5:4261:C:H6	1.68	0.59
12:LG:58:PRO:HD2	12:LG:61:ILE:HD12	1.84	0.59
50:S2:986:G:OP2	50:S2:988:C:N4	2.35	0.59
50:S2:1354:G:N2	50:S2:1357:A:OP2	2.29	0.59
50:S2:1406:G:H2'	50:S2:1407:U:C6	2.38	0.59
33:Lc:28:VAL:HG21	33:Lc:37:MET:HG3	1.85	0.58
50:S2:1404:U:OP1	71:SU:21:ARG:NH2	2.36	0.58
59:SI:92:ARG:NH2	90:SI:302:HOH:O	2.35	0.58
3:L5:74:G:H5'	16:LL:59:VAL:HB	1.85	0.58
3:L5:126:C:H2'	3:L5:127:G:C8	2.38	0.58
3:L5:2809:G:O2'	3:L5:4644:G:OP1	2.21	0.58
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.68	0.58
13:LH:51:LYS:HD3	13:LH:52:LYS:H	1.66	0.58
53:SC:131:GLY:HA3	53:SC:216:MET:HB3	1.83	0.58
62:SL:90:ARG:NH1	90:SL:201:HOH:O	2.34	0.58
66:SP:140:ARG:O	66:SP:141:PHE:C	2.47	0.58
3:L5:1214:C:OP2	32:Lb:91:ARG:NH2	2.36	0.58
29:LY:72:GLN:HB3	29:LY:81:TYR:HB2	1.85	0.58
45:Lo:26:TYR:HB3	45:Lo:67:VAL:HB	1.84	0.58
50:S2:512:A2M:H4'	50:S2:576:A2M:H2	1.86	0.58
50:S2:1261:C:O2	80:Sd:10:HIS:NE2	2.29	0.58
50:S2:1797:U:H2'	50:S2:1798:C:C6	2.38	0.58
83:Sg:214:GLY:HA2	83:Sg:236:ILE:HG13	1.85	0.58
8:LC:189:MET:HE3	8:LC:200:ARG:HB3	1.85	0.58
50:S2:1004:PSU:H2'	50:S2:1005:G:H8	1.69	0.58
51:SA:207:PRO:HA	51:SA:210:ILE:HB	1.84	0.58
70:ST:108:GLU:OE1	70:ST:121:ARG:NH1	2.36	0.58
75:SY:25:ILE:HD13	75:SY:44:LEU:HD11	1.86	0.58
78:Sb:54:VAL:HG13	78:Sb:63:LEU:HB2	1.86	0.58
83:Sg:143:GLN:O	83:Sg:145:GLU:N	2.36	0.58
3:L5:2872:C:H5''	44:Ln:25:LYS:HE3	1.85	0.58
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.37	0.58
3:L5:4892:A:N6	90:L5:5479:HOH:O	2.36	0.58
53:SC:146:GLU:OE1	54:SD:116:ARG:NH1	2.37	0.58
83:Sg:245:ARG:NH2	83:Sg:295:GLY:O	2.36	0.58
3:L5:272:U:H2'	3:L5:273:U:C6	2.38	0.58
50:S2:1055:A:N1	50:S2:1063:C:N4	2.50	0.58
59:SI:123:ARG:NH1	59:SI:133:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SS:15:VAL:HG22	69:SS:68:ILE:HD11	1.85	0.58
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.04	0.58
22:LR:148:ASP:OD1	22:LR:151:ARG:NH2	2.36	0.58
25:LU:48:LYS:HG2	25:LU:53:ALA:HB2	1.85	0.58
71:SU:51:LYS:HB2	71:SU:90:ASP:HB2	1.85	0.58
41:Lk:56:LEU:HA	41:Lk:59:SER:HB3	1.84	0.58
50:S2:656:G:N2	50:S2:663:C:H5''	2.18	0.58
50:S2:1736:G:H2'	50:S2:1737:G:H8	1.69	0.58
3:L5:1355:G:OP1	21:LQ:108:ARG:NH2	2.34	0.58
49:Pt:9:1MG:H2'	49:Pt:11:C:H41	1.68	0.58
2:Et:31:G:H2'	2:Et:32:C:C6	2.39	0.58
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.39	0.58
50:S2:186:C:H2'	50:S2:187:G:C8	2.39	0.58
50:S2:984:C:O2'	65:SO:138:ASP:OD2	2.22	0.58
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.39	0.57
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.69	0.57
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.69	0.57
51:SA:33:GLN:HB3	51:SA:154:LEU:HD12	1.86	0.57
58:SH:171:GLU:OE1	58:SH:171:GLU:N	2.33	0.57
59:SI:12:ARG:NH2	90:SI:301:HOH:O	2.34	0.57
75:SY:79:LEU:O	75:SY:83:LYS:HG2	2.04	0.57
53:SC:79:GLU:N	53:SC:79:GLU:OE2	2.36	0.57
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.39	0.57
11:LF:197:VAL:O	11:LF:201:PHE:HB2	2.04	0.57
50:S2:436:OMG:OP2	50:S2:471:G:O2'	2.22	0.57
62:SL:20:LYS:HE2	62:SL:22:ARG:HG2	1.86	0.57
79:Sc:43:ILE:HG22	79:Sc:65:ALA:HB3	1.84	0.57
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.69	0.57
50:S2:528:A:H2'	50:S2:529:A:C8	2.39	0.57
65:SO:85:CYS:HB2	65:SO:124:MET:HE1	1.86	0.57
13:LH:48:LEU:HD11	13:LH:56:ARG:HE	1.69	0.57
46:Lp:84:ARG:O	46:Lp:88:GLU:HG3	2.04	0.57
50:S2:587:A:H5'	50:S2:592:C:H41	1.68	0.57
3:L5:1201:U:H2'	3:L5:1202:C:C6	2.39	0.57
51:SA:189:ILE:HG21	51:SA:195:TRP:HE1	1.69	0.57
52:SB:35:ALA:HB3	52:SB:42:ARG:HA	1.86	0.57
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.69	0.57
50:S2:455:A:H2'	50:S2:456:C:H6	1.69	0.57
2:Et:21:A:O4'	2:Et:48:C:N4	2.37	0.57
3:L5:679:C:H2'	3:L5:680:G:H8	1.69	0.57
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.04	0.57
3:L5:3944:OMG:N2	3:L5:4069:U:O2	2.29	0.57
3:L5:4918:C:H2'	3:L5:4919:G:C8	2.39	0.57
53:SC:64:THR:OG1	53:SC:90:GLU:OE2	2.23	0.57
3:L5:1751:A:H2'	3:L5:1752:G:H8	1.69	0.57
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.39	0.57
3:L5:4927:G:H5''	3:L5:4928:C:C5	2.39	0.57
10:LE:67:ALA:HA	10:LE:69:TYR:CE2	2.40	0.57
50:S2:140:C:H42	50:S2:313:A:H61	1.52	0.57
50:S2:1595:U:H2'	50:S2:1596:U:C6	2.39	0.57
50:S2:1677:U:H2'	50:S2:1678:A2M:H8	1.87	0.57
52:SB:137:LEU:HG	52:SB:215:VAL:HG22	1.87	0.57
70:ST:108:GLU:OE2	70:ST:115:LYS:NZ	2.37	0.57
71:SU:100:GLN:N	71:SU:100:GLN:OE1	2.37	0.57
3:L5:478:G:OP1	47:Lr:66:ARG:NH1	2.37	0.57
3:L5:4861:G:H2'	3:L5:4862:G:H8	1.70	0.57
50:S2:396:U:OP2	62:SL:79:LYS:NZ	2.30	0.57
62:SL:33:LEU:HD12	62:SL:34:PRO:HD2	1.86	0.57
67:SQ:28:GLY:HA3	67:SQ:67:ASP:HB2	1.85	0.57
70:ST:40:ALA:HB3	70:ST:43:LYS:HG2	1.87	0.57
22:LR:104:ARG:NH2	90:LR:301:HOH:O	2.37	0.56
50:S2:1653:U:H2'	50:S2:1654:G:C8	2.40	0.56
59:SI:119:LEU:HD21	59:SI:153:LYS:HE3	1.86	0.56
60:SJ:103:GLU:H	60:SJ:103:GLU:CD	2.13	0.56
3:L5:711:A:H2'	3:L5:712:C:C6	2.40	0.56
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.20	0.56
66:SP:50:ARG:HB2	66:SP:53:GLN:HE22	1.69	0.56
83:Sg:78:ALA:HB2	83:Sg:92:LEU:HD11	1.87	0.56
83:Sg:115:SER:C	83:Sg:117:ASN:H	2.13	0.56
83:Sg:173:LEU:HD22	83:Sg:189:ILE:HG12	1.87	0.56
3:L5:2800:G:N7	84:L5:5106:PUT:N2	2.52	0.56
3:L5:4474:A:H5''	43:Lm:125:LYS:HG3	1.87	0.56
20:LP:3:ARG:NH2	90:LP:302:HOH:O	2.38	0.56
23:LS:81:TRP:HZ3	23:LS:130:GLU:HG3	1.69	0.56
50:S2:145:G:O6	57:SG:178:ARG:NH2	2.35	0.56
50:S2:948:C:H2'	50:S2:949:G:C8	2.39	0.56
50:S2:1217:A:H2'	50:S2:1218:C:C6	2.40	0.56
50:S2:1373:C:OP1	68:SR:7:LYS:N	2.38	0.56
65:SO:67:ASP:O	65:SO:70:SER:OG	2.20	0.56
3:L5:1952:G:H4'	23:LS:93:MET:HG2	1.88	0.56
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LJ:85:LYS:O	15:LJ:89:VAL:HG23	2.04	0.56
22:LR:159:ALA:O	22:LR:162:ARG:HG2	2.05	0.56
51:SA:53:ARG:HG2	51:SA:53:ARG:HH11	1.70	0.56
52:SB:128:LYS:HE3	52:SB:132:GLY:HA2	1.86	0.56
57:SG:69:THR:HG22	57:SG:71:GLY:H	1.70	0.56
3:L5:153:G:H2'	3:L5:154:G:H8	1.69	0.56
9:LD:232:THR:HG22	9:LD:235:MET:HG2	1.86	0.56
10:LE:180:VAL:HG11	10:LE:258:LEU:HD11	1.86	0.56
17:LM:24:LEU:HD11	17:LM:86:TRP:CG	2.41	0.56
20:LP:33:ALA:HB1	20:LP:117:ILE:HG12	1.87	0.56
50:S2:502:C:H2'	50:S2:503:C:C5	2.41	0.56
55:SE:87:MET:HE3	55:SE:123:LEU:HB2	1.88	0.56
83:Sg:14:HIS:CE1	83:Sg:41:ILE:HG13	2.41	0.56
3:L5:657:C:H2'	3:L5:658:C:C6	2.40	0.56
3:L5:1778:C:H5''	9:LD:5:LYS:HG2	1.86	0.56
12:LG:165:GLU:OE2	18:LN:26:ARG:NH1	2.37	0.56
33:Lc:21:VAL:HG11	33:Lc:96:ILE:HD12	1.86	0.56
50:S2:1036:A:H4'	50:S2:1855:G:N2	2.21	0.56
53:SC:194:ARG:HD3	53:SC:196:ILE:HD11	1.87	0.56
75:SY:45:ALA:O	75:SY:46:LYS:HG2	2.06	0.56
82:Sf:135:HIS:HB2	82:Sf:138:ARG:HG2	1.87	0.56
3:L5:93:G:H2'	3:L5:94:A:C8	2.40	0.56
3:L5:688:U:OP1	10:LE:94:LYS:NZ	2.36	0.56
3:L5:1064:G:H2'	3:L5:1065:G:C8	2.41	0.56
3:L5:1649:U:O2'	85:L5:5112:SPD:N1	2.38	0.56
33:Lc:48:LEU:HD21	33:Lc:60:ILE:HG21	1.86	0.56
50:S2:15:U:H2'	50:S2:16:G:O4'	2.06	0.56
50:S2:1223:A:H5''	56:SF:80:GLY:H	1.71	0.56
52:SB:109:LYS:O	52:SB:113:MET:HG3	2.05	0.56
3:L5:758:G:H5''	13:LH:51:LYS:NZ	2.21	0.56
3:L5:4739:C:H2'	3:L5:4740:G:H5'	1.88	0.56
55:SE:63:LYS:O	55:SE:66:MET:HB3	2.04	0.56
73:SW:69:LEU:HD21	73:SW:72:CYS:HB3	1.86	0.56
3:L5:1459:A:OP1	21:LQ:65:ARG:NH1	2.39	0.56
4:L7:7:G:OP1	9:LD:33:ARG:NH1	2.39	0.56
17:LM:95:ILE:O	17:LM:99:GLU:HG3	2.06	0.56
28:LX:87:MET:O	28:LX:91:GLU:HG2	2.06	0.56
50:S2:455:A:H2'	50:S2:456:C:C6	2.40	0.56
50:S2:1314:U:O2'	61:SK:8:ARG:NH2	2.39	0.56
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.41	0.56
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LC:152:LEU:HD23	8:LC:251:ILE:HG12	1.88	0.56
12:LG:115:LEU:O	12:LG:119:GLU:HG2	2.05	0.56
50:S2:1209:A:O2'	77:Sa:85:ARG:NH1	2.39	0.56
3:L5:300:A:H2'	3:L5:301:G:H8	1.70	0.55
3:L5:1583:A:OP2	85:L5:5109:SPD:N10	2.38	0.55
3:L5:1857:C:H2'	3:L5:1858:A:H8	1.71	0.55
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.41	0.55
50:S2:1174:PSU:H2'	50:S2:1175:G:C8	2.42	0.55
50:S2:1456:G:H2'	50:S2:1457:U:C6	2.41	0.55
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.89	0.55
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.05	0.55
68:SR:72:LYS:O	68:SR:76:GLU:HG2	2.05	0.55
83:Sg:79:LEU:HD22	83:Sg:120:ILE:HD12	1.88	0.55
3:L5:1708:G:OP1	32:Lb:101:HIS:NE2	2.30	0.55
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.71	0.55
30:LZ:89:ILE:HD11	30:LZ:121:ARG:HG2	1.87	0.55
50:S2:12:U:H2'	50:S2:13:C:C6	2.42	0.55
50:S2:115:U:H2'	50:S2:116:OMU:C6	2.36	0.55
3:L5:2672:C:OP1	46:Lp:44:LYS:NZ	2.30	0.55
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.42	0.55
50:S2:987:A:H2'	52:SB:114:VAL:HG11	1.87	0.55
71:SU:42:GLY:HA3	71:SU:101:ILE:HD11	1.88	0.55
3:L5:1419:G:C6	31:La:116:LYS:HD2	2.42	0.55
5:L8:19:C:H2'	5:L8:20:A:C8	2.42	0.55
5:L8:67:U:H2'	5:L8:68:G:H8	1.70	0.55
3:L5:759:G:O3'	13:LH:50:LYS:NZ	2.40	0.55
5:L8:141:C:H2'	5:L8:142:U:C6	2.41	0.55
50:S2:1201:U:H2'	50:S2:1202:U:C6	2.41	0.55
50:S2:1432:U:H2'	50:S2:1438:A:C8	2.41	0.55
3:L5:181:C:H2'	3:L5:182:G:C8	2.40	0.55
3:L5:1564:A:N1	50:S2:1029:G:O2'	2.37	0.55
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.88	0.55
7:LB:383:GLU:OE1	7:LB:383:GLU:N	2.40	0.55
9:LD:261:VAL:HG23	9:LD:263:LYS:H	1.70	0.55
14:LI:181:PHE:O	14:LI:185:VAL:HG23	2.06	0.55
50:S2:1798:C:H2'	50:S2:1799:G:O4'	2.07	0.55
56:SF:124:ASP:OD1	79:Sc:47:LYS:HD2	2.07	0.55
76:SZ:74:SER:HA	76:SZ:79:ILE:HG13	1.89	0.55
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.42	0.55
13:LH:107:GLU:OE1	13:LH:127:ARG:NH1	2.37	0.55
73:SW:28:ARG:HB3	73:SW:29:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:469:C:H2'	3:L5:470:A:H8	1.71	0.55
3:L5:3736:A:H2'	3:L5:3737:A:H8	1.71	0.55
23:LS:71:SER:O	23:LS:76:LYS:NZ	2.40	0.55
25:LU:68:SER:O	25:LU:68:SER:OG	2.25	0.55
29:LY:26:ARG:O	29:LY:30:MET:HG3	2.07	0.55
50:S2:1405:A:H2'	50:S2:1406:G:O4'	2.07	0.55
54:SD:225:GLU:OE1	54:SD:225:GLU:N	2.40	0.55
3:L5:2588:C:OP1	3:L5:2768:C:O2'	2.18	0.54
55:SE:72:ILE:HD13	55:SE:90:ILE:HG12	1.89	0.54
57:SG:135:PRO:HB2	57:SG:141:ILE:HG13	1.89	0.54
75:SY:40:ILE:O	75:SY:44:LEU:HD12	2.07	0.54
3:L5:440:U:H2'	3:L5:441:G:H8	1.72	0.54
3:L5:4927:G:H5''	3:L5:4928:C:H5	1.72	0.54
50:S2:495:U:H2'	50:S2:496:C:O4'	2.07	0.54
50:S2:801:PSU:H2'	50:S2:802:A:H8	1.73	0.54
50:S2:1144:A:H2'	50:S2:1145:A:C8	2.42	0.54
50:S2:1279:C:H2'	50:S2:1280:G:H8	1.71	0.54
55:SE:92:ILE:HD12	55:SE:99:PHE:HE1	1.72	0.54
64:SN:31:ASP:O	64:SN:35:GLU:HG2	2.06	0.54
3:L5:396:A:H2'	3:L5:397:G:C8	2.41	0.54
3:L5:669:C:H5'	47:Lr:68:SER:HB2	1.88	0.54
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.89	0.54
13:LH:103:VAL:HG11	13:LH:144:LEU:HD21	1.89	0.54
50:S2:1289:U:H2'	50:S2:1290:G:C8	2.41	0.54
50:S2:1736:G:H2'	50:S2:1737:G:C8	2.42	0.54
61:SK:26:ASP:HB3	61:SK:29:MET:HG3	1.89	0.54
82:Sf:133:ALA:N	82:Sf:140:TYR:O	2.38	0.54
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.41	0.54
5:L8:102:G:P	40:Lj:20:ARG:HH12	2.31	0.54
58:SH:60:ILE:HB	58:SH:92:VAL:HG22	1.89	0.54
67:SQ:116:ASP:OD1	67:SQ:118:THR:OG1	2.18	0.54
6:LA:101:VAL:HG22	6:LA:165:VAL:HG22	1.88	0.54
50:S2:1155:U:OP1	53:SC:185:THR:OG1	2.21	0.54
57:SG:44:GLU:HG3	57:SG:121:ILE:HD13	1.89	0.54
58:SH:31:GLU:HB3	58:SH:40:LEU:HD23	1.88	0.54
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.43	0.54
3:L5:4862:G:H2'	3:L5:4863:G:H8	1.71	0.54
3:L5:658:C:H2'	3:L5:659:G:C8	2.42	0.54
3:L5:2708:U:H1'	22:LR:43:LYS:HE3	1.90	0.54
4:L7:4:U:H2'	4:L7:5:A:H8	1.73	0.54
29:LY:86:GLN:NE2	90:LY:201:HOH:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lh:101:ASN:ND2	90:Lh:201:HOH:O	2.41	0.54
50:S2:993:G:OP1	50:S2:1131:G:N2	2.36	0.54
55:SE:129:ILE:HD11	55:SE:139:LEU:HD12	1.89	0.54
79:Sc:20:ARG:HD2	79:Sc:28:THR:HG23	1.89	0.54
83:Sg:289:LEU:HD22	83:Sg:298:LEU:HD11	1.90	0.54
3:L5:1:C:H3'	3:L5:2:G:H8	1.71	0.54
3:L5:325:U:H2'	3:L5:326:C:C6	2.43	0.54
3:L5:2303:C:OP1	35:Le:107:ASN:ND2	2.40	0.54
7:LB:165:HIS:HB3	7:LB:180:LEU:HD12	1.90	0.54
42:Ll:20:ASN:ND2	42:Ll:42:ARG:O	2.36	0.54
50:S2:1606:G:H22	50:S2:1632:G:H1'	1.73	0.54
56:SF:89:THR:O	56:SF:93:VAL:HG13	2.08	0.54
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.43	0.54
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.43	0.54
48:Mr:2:C:H42	49:Pt:36:G:H1	1.56	0.54
75:SY:84:LYS:HE2	75:SY:84:LYS:HA	1.89	0.54
79:Sc:38:THR:O	79:Sc:39:SER:OG	2.25	0.54
3:L5:318:A:H2'	3:L5:319:A:C8	2.43	0.54
3:L5:662:C:N4	3:L5:663:G:O6	2.41	0.54
50:S2:21:U:O2	60:SJ:17:ARG:NH2	2.40	0.54
50:S2:377:G:H5'	59:SI:99:ASN:HB2	1.89	0.54
55:SE:124:CYS:HB3	55:SE:141:THR:HB	1.90	0.54
58:SH:78:ARG:O	58:SH:82:GLU:HG2	2.08	0.54
3:L5:1412:G:H2'	3:L5:1413:C:O4'	2.08	0.53
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.43	0.53
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.71	0.53
3:L5:2415:OMU:H2'	3:L5:2416:G:C8	2.43	0.53
50:S2:581:U:H4'	75:SY:66:GLY:HA2	1.90	0.53
3:L5:2079:G:OP2	35:Le:64:LYS:NZ	2.38	0.53
3:L5:2267:U:OP1	47:Lr:37:SER:OG	2.20	0.53
9:LD:53:VAL:HG11	9:LD:159:VAL:HA	1.89	0.53
50:S2:811:A:H2'	50:S2:812:A:C8	2.43	0.53
50:S2:921:G:C2	78:Sb:22:LYS:HG2	2.43	0.53
62:SL:49:GLU:H	62:SL:49:GLU:CD	2.16	0.53
83:Sg:202:PRO:HG3	83:Sg:243:PRO:HA	1.91	0.53
3:L5:318:A:H2'	3:L5:319:A:H8	1.74	0.53
3:L5:478:G:H2'	3:L5:479:G:H8	1.73	0.53
3:L5:1410:U:O2'	32:Lb:49:HIS:NE2	2.30	0.53
73:SW:37:PHE:O	73:SW:41:MET:HG3	2.08	0.53
3:L5:3643:A:OP1	85:L5:5120:SPD:N1	2.41	0.53
7:LB:392:LEU:O	7:LB:396:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:1538:C:H2'	50:S2:1539:U:C6	2.42	0.53
57:SG:194:LEU:HA	57:SG:197:GLN:OE1	2.07	0.53
69:SS:104:ASP:OD1	69:SS:105:ASN:N	2.41	0.53
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.43	0.53
28:LX:82:THR:HG22	28:LX:155:ILE:HG23	1.91	0.53
50:S2:1465:A:OP1	68:SR:56:HIS:NE2	2.41	0.53
51:SA:145:ILE:HG12	51:SA:159:ILE:HB	1.90	0.53
54:SD:216:GLU:OE1	54:SD:216:GLU:N	2.41	0.53
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.44	0.53
4:L7:58:A:H2'	4:L7:59:G:H8	1.74	0.53
19:LO:175:MET:HE2	19:LO:179:LYS:HE2	1.89	0.53
51:SA:50:ASN:OD1	51:SA:53:ARG:HD2	2.07	0.53
56:SF:86:LYS:O	56:SF:90:VAL:HG13	2.09	0.53
57:SG:49:VAL:HB	57:SG:115:LYS:HB3	1.90	0.53
3:L5:4148:C:H5''	30:LZ:59:LYS:NZ	2.24	0.53
30:LZ:120:GLU:O	30:LZ:124:THR:HG23	2.08	0.53
50:S2:379:C:O2	59:SI:5:ARG:NE	2.42	0.53
50:S2:871:U:O2'	50:S2:873:G:OP1	2.26	0.53
50:S2:1801:A:H2'	50:S2:1802:C:C6	2.43	0.53
3:L5:1802:A:O2'	24:LT:108:ARG:NH2	2.42	0.53
3:L5:1834:U:OP1	24:LT:120:LYS:NZ	2.37	0.53
4:L7:12:U:OP2	4:L7:67:C:O2'	2.24	0.53
5:L8:102:G:OP1	40:Lj:20:ARG:NH1	2.41	0.53
50:S2:951:C:H1'	65:SO:50:LYS:NZ	2.23	0.53
59:SI:46:VAL:HG22	59:SI:54:LYS:HB2	1.90	0.53
83:Sg:205:SER:HA	83:Sg:221:LEU:HB2	1.90	0.53
3:L5:453:G:N7	90:L5:5455:HOH:O	2.34	0.53
3:L5:4285:U:OP2	45:Lo:100:LYS:NZ	2.33	0.53
8:LC:71:ARG:NH1	90:LC:502:HOH:O	2.41	0.53
10:LE:250:GLN:NE2	10:LE:254:ASP:OD1	2.42	0.53
16:LL:200:LYS:O	16:LL:204:GLU:HG3	2.09	0.53
26:LV:13:LYS:HD2	26:LV:128:LEU:HD11	1.90	0.53
47:Lr:41:ASN:ND2	90:Lr:202:HOH:O	2.42	0.53
50:S2:1239:PSU:H5'	66:SP:124:LYS:HD2	1.90	0.53
53:SC:65:LYS:HG2	53:SC:273:LEU:HD22	1.91	0.53
64:SN:33:VAL:HA	64:SN:36:GLN:HG3	1.91	0.53
65:SO:47:LEU:HG	65:SO:49:GLY:H	1.74	0.53
3:L5:418:A:C2	5:L8:17:A:H1'	2.43	0.53
3:L5:1433:A:N6	3:L5:1451:G:O2'	2.40	0.53
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.24	0.53
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:468:A2M:OP1	57:SG:96:SER:OG	2.17	0.53
50:S2:1010:G:H2'	50:S2:1011:A:C8	2.42	0.53
50:S2:1829:G:H1'	50:S2:1850:MA6:H2	1.91	0.53
55:SE:153:LEU:O	55:SE:174:LYS:NZ	2.26	0.53
56:SF:143:PRO:HA	56:SF:146:ARG:HG2	1.91	0.53
67:SQ:106:LYS:HG3	67:SQ:110:ASP:OD2	2.09	0.53
70:ST:74:SER:O	70:ST:78:ILE:HG12	2.08	0.53
3:L5:10:A:H2'	3:L5:11:G:C8	2.44	0.52
3:L5:1399:G:H2'	3:L5:1400:G:H8	1.73	0.52
3:L5:2412:A:H2'	3:L5:2413:U:C6	2.44	0.52
4:L7:55:A:H4'	15:LJ:155:HIS:HB2	1.90	0.52
4:L7:110:G:H2'	4:L7:111:C:C6	2.44	0.52
25:LU:75:GLU:N	25:LU:75:GLU:OE2	2.41	0.52
50:S2:1018:U:H5''	64:SN:71:ILE:HD12	1.90	0.52
56:SF:94:LYS:O	56:SF:98:GLU:HG2	2.09	0.52
57:SG:191:ARG:HA	57:SG:194:LEU:HD12	1.91	0.52
3:L5:106:A:H2'	3:L5:107:G:O4'	2.09	0.52
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.43	0.52
3:L5:2318:G:N2	3:L5:2321:G:OP2	2.36	0.52
29:LY:114:ASP:O	29:LY:118:ILE:HG13	2.09	0.52
32:Lb:23:LYS:HG3	32:Lb:24:PRO:HD2	1.90	0.52
50:S2:140:C:O2'	50:S2:143:U:OP1	2.27	0.52
50:S2:1402:A:H1'	71:SU:54:VAL:HG13	1.90	0.52
50:S2:1746:U:OP1	57:SG:31:ARG:NH2	2.42	0.52
52:SB:107:ARG:HH12	65:SO:135:ILE:HD13	1.74	0.52
70:ST:101:ARG:O	70:ST:105:GLN:HG3	2.09	0.52
73:SW:51:GLU:OE1	78:Sb:8:LEU:HD21	2.10	0.52
9:LD:263:LYS:NZ	90:LD:1004:HOH:O	2.41	0.52
50:S2:1536:G:P	56:SF:88:MET:HE1	2.49	0.52
50:S2:1856:C:H2'	50:S2:1857:G:C8	2.44	0.52
57:SG:200:LYS:HG2	57:SG:204:GLU:OE1	2.10	0.52
3:L5:687:U:OP1	10:LE:97:GLY:N	2.38	0.52
3:L5:1082:C:H2'	3:L5:1083:U:O4'	2.10	0.52
37:Lg:49:CYS:SG	37:Lg:85:LYS:NZ	2.82	0.52
50:S2:166:A2M:HM'2	50:S2:167:G:H5'	1.90	0.52
50:S2:1227:G:C2	50:S2:1228:A:C8	2.98	0.52
50:S2:1479:G:H4'	67:SQ:128:GLU:OE1	2.08	0.52
78:Sb:34:ASP:O	78:Sb:79:PHE:HA	2.09	0.52
4:L7:22:A:H2'	4:L7:23:A:C8	2.44	0.52
6:LA:80:GLU:HB2	6:LA:170:ALA:HA	1.90	0.52
50:S2:1228:A:H2'	50:S2:1229:G:H8	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:1845:A:H2'	50:S2:1846:G:H8	1.74	0.52
54:SD:76:ARG:HB2	61:SK:22:VAL:HG11	1.91	0.52
59:SI:76:THR:OG1	59:SI:105:ASP:O	2.23	0.52
67:SQ:39:LEU:HD21	67:SQ:51:LEU:HB3	1.91	0.52
67:SQ:98:LYS:HE3	67:SQ:99:TYR:CZ	2.44	0.52
3:L5:1245:C:H2'	3:L5:1246:G:C8	2.44	0.52
3:L5:1294:A:H1'	3:L5:1295:C:H5	1.74	0.52
3:L5:1298:C:H2'	3:L5:1299:G:H8	1.74	0.52
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.45	0.52
3:L5:1646:A:O2'	40:Lj:49:TRP:O	2.23	0.52
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.75	0.52
3:L5:4148:C:H5''	30:LZ:59:LYS:HZ2	1.75	0.52
4:L7:111:C:H2'	4:L7:112:U:O4'	2.10	0.52
19:LO:61:ARG:HA	19:LO:70:PRO:HD2	1.91	0.52
50:S2:877:C:H2'	50:S2:878:G:C8	2.44	0.52
50:S2:1533:A:H2	50:S2:1536:G:N3	2.08	0.52
57:SG:132:ARG:HG3	57:SG:133:LEU:HD13	1.91	0.52
59:SI:199:LEU:O	59:SI:203:LYS:HG2	2.10	0.52
63:SM:62:VAL:O	63:SM:66:GLU:HG2	2.10	0.52
70:ST:42:HIS:NE2	70:ST:43:LYS:HE2	2.24	0.52
79:Sc:67:ARG:HG2	79:Sc:68:LEU:N	2.23	0.52
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.45	0.52
3:L5:1812:C:H5''	32:Lb:56:LYS:HE3	1.90	0.52
5:L8:96:C:H5''	38:Lh:66:LYS:HD3	1.91	0.52
11:LF:182:TYR:HB3	11:LF:200:ARG:HG3	1.91	0.52
39:Li:43:MET:HE2	39:Li:43:MET:HA	1.91	0.52
50:S2:443:U:H2'	50:S2:444:G:O4'	2.10	0.52
50:S2:1214:A:H2'	50:S2:1217:A:N7	2.24	0.52
50:S2:1712:A:H2'	50:S2:1713:C:C6	2.45	0.52
50:S2:1714:U:H2'	50:S2:1715:A:C8	2.45	0.52
51:SA:44:ASP:OD1	51:SA:44:ASP:N	2.38	0.52
76:SZ:45:ASN:ND2	76:SZ:45:ASN:C	2.63	0.52
3:L5:717:U:H2'	3:L5:718:C:C6	2.45	0.52
3:L5:980:U:H2'	3:L5:981:C:C6	2.44	0.52
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.45	0.52
3:L5:3760:A2M:HM'3	50:S2:1826:G:H1'	1.91	0.52
85:L5:5117:SPD:N1	90:L5:5461:HOH:O	2.34	0.52
19:LO:34:VAL:HG22	19:LO:103:LYS:HB2	1.92	0.52
50:S2:352:U:H2'	50:S2:353:C:C6	2.44	0.52
65:SO:117:ARG:NH2	77:Sa:49:ALA:HA	2.20	0.52
67:SQ:97:GLN:HB2	67:SQ:105:LYS:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1090:G:OP1	24:LT:142:ARG:NH1	2.41	0.52
3:L5:1320:U:O2'	3:L5:1891:A:N1	2.33	0.52
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.45	0.52
30:LZ:27:LYS:HD3	30:LZ:29:ILE:HD11	1.92	0.52
50:S2:656:G:H5'	50:S2:662:G:N2	2.24	0.52
50:S2:874:G:H2'	50:S2:875:A:H8	1.74	0.52
50:S2:982:G:H2'	50:S2:983:A:H8	1.75	0.52
75:SY:5:VAL:HG23	75:SY:32:LYS:HE2	1.92	0.52
3:L5:10:A:H2'	3:L5:11:G:H8	1.73	0.52
3:L5:699:C:H2'	3:L5:700:G:H8	1.75	0.52
3:L5:4137:C:H2'	3:L5:4138:C:C6	2.45	0.52
9:LD:75:VAL:O	9:LD:112:ARG:NH1	2.43	0.52
11:LF:34:ARG:NH1	90:LF:302:HOH:O	2.43	0.52
33:Lc:47:ILE:HB	33:Lc:94:LEU:HG	1.91	0.52
41:Lk:55:LYS:O	41:Lk:58:GLN:NE2	2.42	0.52
51:SA:207:PRO:O	51:SA:211:GLU:HG3	2.10	0.52
54:SD:14:ASP:OD1	54:SD:18:LYS:HD2	2.10	0.52
56:SF:31:ASN:OD1	56:SF:32:ASP:N	2.43	0.52
57:SG:131:ARG:H	57:SG:131:ARG:HD2	1.75	0.52
61:SK:16:PHE:HZ	61:SK:80:ARG:HE	1.57	0.52
70:ST:13:GLU:HA	70:ST:16:ARG:NH1	2.25	0.52
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.44	0.51
3:L5:4538:G:H2'	3:L5:4539:U:C6	2.45	0.51
20:LP:42:ARG:NH2	20:LP:99:GLU:OE2	2.42	0.51
50:S2:575:A:H2'	50:S2:576:A2M:O4'	2.10	0.51
50:S2:1174:PSU:H2'	50:S2:1175:G:H8	1.74	0.51
62:SL:4:ILE:HD11	62:SL:54:THR:HG23	1.91	0.51
83:Sg:44:LYS:HE3	83:Sg:46:THR:HB	1.92	0.51
3:L5:1241:C:O2	32:Lb:120:ARG:HB2	2.10	0.51
3:L5:1262:G:H2'	3:L5:1263:A:H8	1.74	0.51
3:L5:1399:G:H2'	3:L5:1400:G:C8	2.46	0.51
3:L5:2861:OMC:OP2	85:L5:5111:SPD:N10	2.43	0.51
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.76	0.51
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.91	0.51
21:LQ:80:ALA:HB3	21:LQ:100:VAL:HG12	1.92	0.51
25:LU:46:ARG:HH12	25:LU:89:LYS:HE3	1.76	0.51
58:SH:127:ASP:OD1	58:SH:142:LYS:NZ	2.43	0.51
58:SH:145:ARG:HB2	73:SW:51:GLU:OE2	2.10	0.51
66:SP:28:MET:HE1	66:SP:36:LEU:HD11	1.93	0.51
73:SW:14:ILE:HG13	73:SW:27:ILE:HD11	1.92	0.51
3:L5:398:A2M:O5'	3:L5:398:A2M:H8	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:734:G:C2	3:L5:735:G:C8	2.99	0.51
3:L5:1346:C:H2'	3:L5:1347:G:H8	1.75	0.51
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.44	0.51
3:L5:4145:C:H2'	3:L5:4146:G:C8	2.45	0.51
14:LI:152:LEU:HB3	14:LI:165:ILE:HD12	1.91	0.51
50:S2:571:U:O2'	75:SY:60:PHE:O	2.22	0.51
50:S2:1101:U:H2'	50:S2:1102:G:C8	2.45	0.51
50:S2:1551:U:OP1	54:SD:9:ARG:NH1	2.44	0.51
51:SA:15:VAL:O	51:SA:19:LEU:HG	2.09	0.51
56:SF:52:SER:OG	56:SF:70:GLU:OE1	2.26	0.51
66:SP:34:MET:HE3	66:SP:42:ARG:HG3	1.91	0.51
73:SW:18:GLU:OE1	73:SW:69:LEU:HB3	2.10	0.51
80:Sd:25:SER:O	80:Sd:25:SER:OG	2.28	0.51
3:L5:4770:U:H2'	3:L5:4771:C:C5	2.45	0.51
3:L5:4887:C:H2'	3:L5:4888:U:O4'	2.11	0.51
5:L8:67:U:H2'	5:L8:68:G:C8	2.46	0.51
22:LR:133:LYS:HG2	22:LR:137:ILE:HD12	1.91	0.51
50:S2:526:A:H2'	50:S2:527:C:C6	2.45	0.51
50:S2:1374:C:H2'	50:S2:1375:G:O4'	2.10	0.51
50:S2:1454:A:H5''	68:SR:3:ARG:HH11	1.75	0.51
50:S2:1740:C:H2'	50:S2:1741:U:C6	2.45	0.51
3:L5:162:A:H2'	3:L5:163:A:C8	2.45	0.51
3:L5:4145:C:H2'	3:L5:4146:G:H8	1.76	0.51
9:LD:71:GLY:O	9:LD:73:MET:HE2	2.10	0.51
19:LO:4:VAL:HG22	19:LO:31:ARG:HH21	1.74	0.51
30:LZ:29:ILE:HG22	30:LZ:32:GLY:H	1.75	0.51
34:Ld:29:ILE:O	34:Ld:33:ILE:HG12	2.10	0.51
50:S2:1204:A:O2'	50:S2:1700:C:OP2	2.27	0.51
50:S2:1413:G:H2'	50:S2:1414:A:C8	2.41	0.51
50:S2:1854:U:P	65:SO:147:ARG:HH22	2.33	0.51
61:SK:57:TYR:O	61:SK:72:THR:OG1	2.27	0.51
3:L5:1399:G:N2	3:L5:1419:G:H1'	2.26	0.51
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.76	0.51
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.45	0.51
50:S2:1667:U:H2'	50:S2:1668:U:C6	2.45	0.51
56:SF:125:SER:HB2	56:SF:136:ARG:HH21	1.74	0.51
58:SH:28:LEU:O	58:SH:31:GLU:HG2	2.10	0.51
60:SJ:97:ILE:HA	60:SJ:100:LEU:HD13	1.93	0.51
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.46	0.51
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.46	0.51
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:188:LYS:HE3	6:LA:192:LYS:HE3	1.91	0.51
11:LF:71:MET:HA	11:LF:74:MET:HE3	1.91	0.51
21:LQ:178:ARG:HA	21:LQ:184:ARG:O	2.11	0.51
35:Le:82:VAL:O	35:Le:86:GLU:HG2	2.11	0.51
50:S2:639:C:H2'	50:S2:640:A:H8	1.75	0.51
51:SA:123:VAL:HA	51:SA:145:ILE:O	2.11	0.51
51:SA:176:TRP:CH2	51:SA:180:ARG:HD3	2.44	0.51
60:SJ:124:HIS:CE1	81:Se:109:ARG:HD3	2.46	0.51
68:SR:98:VAL:HG12	68:SR:119:VAL:HA	1.91	0.51
83:Sg:124:SER:OG	83:Sg:125:ARG:N	2.43	0.51
3:L5:2848:G:O2'	3:L5:3838:U:O4	2.26	0.51
3:L5:4694:G:OP1	3:L5:4694:G:N2	2.43	0.51
3:L5:4745:G:H1	3:L5:4955:A:H61	1.59	0.51
25:LU:24:ASP:OD1	25:LU:26:THR:HG23	2.11	0.51
47:Lr:26:SER:OG	47:Lr:28:GLU:OE1	2.22	0.51
50:S2:1088:U:H4'	50:S2:1089:G:OP2	2.11	0.51
50:S2:1644:C:H4'	67:SQ:140:ARG:HB2	1.92	0.51
50:S2:1711:U:H2'	50:S2:1712:A:H8	1.76	0.51
57:SG:126:ASP:OD1	57:SG:127:THR:N	2.42	0.51
59:SI:25:ARG:HB2	59:SI:28:GLU:HG3	1.92	0.51
69:SS:15:VAL:HB	69:SS:20:ILE:HD13	1.93	0.51
3:L5:922:C:H2'	3:L5:923:C:H6	1.75	0.51
3:L5:1345:A:H2'	3:L5:1346:C:C6	2.46	0.51
3:L5:3722:G:H2'	3:L5:3723:A2M:H8	1.92	0.51
3:L5:4174:U:H2'	3:L5:4175:G:H8	1.76	0.51
32:Lb:110:ALA:O	32:Lb:114:LYS:HG2	2.10	0.51
38:Lh:6:ALA:O	38:Lh:10:ARG:HG3	2.10	0.51
50:S2:943:U:C2	50:S2:944:A:C8	2.98	0.51
58:SH:146:VAL:O	73:SW:49:GLU:HG2	2.11	0.51
3:L5:1248:C:H2'	3:L5:1249:C:H6	1.76	0.51
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.10	0.51
3:L5:3598:C:H2'	3:L5:3599:A:H8	1.76	0.51
3:L5:4413:C:OP2	85:L5:5110:SPD:N10	2.43	0.51
4:L7:117:G:H5'	9:LD:256:LYS:HD3	1.92	0.51
5:L8:144:U:H2'	5:L8:145:C:C6	2.46	0.51
50:S2:527:C:H2'	50:S2:528:A:H8	1.76	0.51
50:S2:1278:A:H2'	50:S2:1279:C:C6	2.46	0.51
53:SC:105:GLU:HB3	53:SC:216:MET:HE1	1.93	0.51
54:SD:106:ARG:HG3	54:SD:175:VAL:HG22	1.93	0.51
60:SJ:75:ASN:O	60:SJ:79:ARG:HD3	2.10	0.51
63:SM:52:LEU:HD21	63:SM:65:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SM:53:ALA:HB2	63:SM:85:LEU:HD22	1.93	0.51
3:L5:162:A:H2'	3:L5:163:A:H8	1.76	0.50
3:L5:1501:C:O2	21:LQ:68:ARG:NH2	2.45	0.50
50:S2:118:C:H1'	50:S2:445:A:C5	2.45	0.50
50:S2:562:U:H2'	50:S2:563:G:C8	2.46	0.50
50:S2:1672:U:OP1	67:SQ:18:THR:OG1	2.25	0.50
56:SF:80:GLY:HA2	56:SF:83:ASN:CG	2.35	0.50
66:SP:21:ASP:OD2	66:SP:24:GLN:HG2	2.11	0.50
66:SP:67:ALA:HB2	66:SP:73:PRO:HB3	1.93	0.50
3:L5:369:G:N2	3:L5:372:A:OP2	2.39	0.50
3:L5:1727:U:OP1	11:LF:131:ASN:ND2	2.44	0.50
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.47	0.50
24:LT:102:ARG:O	24:LT:106:LEU:HG	2.11	0.50
50:S2:526:A:H2'	50:S2:527:C:H6	1.77	0.50
54:SD:20:GLU:HG2	54:SD:77:PHE:CZ	2.46	0.50
3:L5:137:G:H2'	3:L5:138:G:H8	1.76	0.50
14:LI:48:LEU:HD11	14:LI:145:LYS:HB2	1.91	0.50
17:LM:40:GLY:HA3	17:LM:45:VAL:HB	1.93	0.50
50:S2:102:A:H4'	50:S2:104:A:C8	2.47	0.50
50:S2:1139:C:H2'	50:S2:1140:G:O4'	2.12	0.50
50:S2:1432:U:H2'	50:S2:1438:A:H8	1.75	0.50
56:SF:79:HIS:O	56:SF:81:ARG:N	2.44	0.50
3:L5:1326:A2M:OP2	3:L5:4445:U:O2'	2.26	0.50
3:L5:3786:U:OP1	3:L5:4550:G:O2'	2.23	0.50
3:L5:4137:C:H2'	3:L5:4138:C:H6	1.76	0.50
3:L5:4522:G:O2'	3:L5:4525:C:OP2	2.20	0.50
50:S2:223:C:H2'	50:S2:224:A:C8	2.45	0.50
50:S2:920:A:O2'	50:S2:922:A:OP1	2.19	0.50
50:S2:921:G:C6	78:Sb:22:LYS:HA	2.47	0.50
50:S2:964:A:H2'	50:S2:965:U:C6	2.46	0.50
50:S2:1493:C:O2'	50:S2:1499:U:O4	2.30	0.50
54:SD:44:THR:OG1	54:SD:45:ARG:N	2.44	0.50
55:SE:20:LEU:HD21	55:SE:46:ILE:HD12	1.94	0.50
73:SW:36:ARG:O	73:SW:39:THR:HG22	2.11	0.50
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.26	0.50
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.11	0.50
5:L8:86:U:H3'	5:L8:87:G:H5'	1.94	0.50
17:LM:41:PRO:HG3	17:LM:73:VAL:HG12	1.92	0.50
50:S2:496:C:H2'	50:S2:497:C:H6	1.77	0.50
66:SP:37:TYR:HE2	66:SP:112:ILE:HG22	1.76	0.50
67:SQ:44:PRO:HD3	67:SQ:77:HIS:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sb:11:SER:N	78:Sb:14:GLU:OE2	2.35	0.50
50:S2:165:G:OP2	50:S2:165:G:N2	2.35	0.50
50:S2:1292:C:O2	82:Sf:138:ARG:NH1	2.43	0.50
67:SQ:34:VAL:HG22	67:SQ:70:VAL:HB	1.94	0.50
70:ST:113:VAL:HG12	70:ST:123:LEU:HD12	1.93	0.50
71:SU:98:VAL:O	71:SU:101:ILE:HG22	2.11	0.50
3:L5:7:C:H2'	3:L5:8:U:C6	2.47	0.50
3:L5:1074:G:H2'	3:L5:1075:G:H8	1.77	0.50
9:LD:60:ILE:HB	9:LD:80:ALA:HB2	1.93	0.50
50:S2:1288:OMU:H3'	82:Sf:97:LYS:HZ2	1.76	0.50
63:SM:61:TYR:HA	63:SM:64:LEU:HD23	1.94	0.50
64:SN:115:LEU:O	64:SN:119:GLU:HG3	2.11	0.50
74:SX:40:PRO:HA	74:SX:79:LYS:HD3	1.94	0.50
3:L5:2765:A:H2'	3:L5:2766:A:H8	1.77	0.50
3:L5:4225:G:OP1	14:LI:24:ARG:NH2	2.45	0.50
12:LG:88:ASP:OD1	12:LG:90:GLN:HG2	2.12	0.50
50:S2:159:A2M:O5'	50:S2:159:A2M:H8	2.11	0.50
50:S2:420:G:O2'	50:S2:660:C:N3	2.36	0.50
50:S2:1030:A:H2'	50:S2:1031:A2M:H8	1.93	0.50
50:S2:1199:A:OP1	77:Sa:2:THR:N	2.44	0.50
54:SD:197:LYS:HD2	54:SD:198:ILE:HB	1.94	0.50
70:ST:56:ARG:HG3	70:ST:103:VAL:HG21	1.94	0.50
72:SV:19:ALA:O	73:SW:23:ARG:NH2	2.45	0.50
3:L5:4:G:H2'	3:L5:5:A:H8	1.77	0.50
3:L5:399:G:OP1	20:LP:20:SER:OG	2.21	0.50
3:L5:754:U:O2'	3:L5:755:C:OP1	2.30	0.50
3:L5:2083:C:OP2	21:LQ:14:ARG:NH2	2.41	0.50
3:L5:2652:G:N2	46:Lp:59:SER:O	2.45	0.50
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.46	0.50
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.11	0.50
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.47	0.50
5:L8:32:C:H2'	5:L8:33:G:O4'	2.12	0.50
8:LC:5:ARG:HD2	8:LC:24:LEU:O	2.11	0.50
46:Lp:3:LYS:NZ	90:Lp:201:HOH:O	2.44	0.50
50:S2:380:G:OP1	59:SI:56:ARG:NH2	2.35	0.50
59:SI:34:ALA:HB2	59:SI:56:ARG:HD2	1.93	0.50
73:SW:90:GLN:OE1	73:SW:117:ARG:NH2	2.44	0.50
83:Sg:104:HIS:HD2	83:Sg:130:LYS:HD2	1.76	0.50
83:Sg:120:ILE:HB	83:Sg:132:TRP:HB2	1.93	0.50
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.94	0.49
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LJ:113:ILE:HD11	69:SS:14:ARG:CZ	2.43	0.49
18:LN:138:PHE:HA	18:LN:143:ARG:HD2	1.92	0.49
30:LZ:92:ASP:OD2	30:LZ:94:THR:OG1	2.27	0.49
50:S2:29:G:H2'	50:S2:30:C:H6	1.76	0.49
50:S2:107:A:H2'	50:S2:108:G:H8	1.75	0.49
67:SQ:47:LEU:HD12	67:SQ:50:LYS:HG3	1.92	0.49
83:Sg:242:SER:HB3	83:Sg:247:TRP:HB2	1.94	0.49
3:L5:683:C:H2'	3:L5:684:G:O4'	2.12	0.49
3:L5:1743:A:N1	3:L5:1789:C:O2'	2.44	0.49
6:LA:117:GLU:HG2	6:LA:124:GLY:H	1.77	0.49
12:LG:50:ASP:HB2	28:LX:40:ILE:HD11	1.93	0.49
50:S2:674:C:H2'	50:S2:675:U:C6	2.47	0.49
50:S2:1562:C:H2'	50:S2:1563:G:C8	2.47	0.49
50:S2:1587:G:C5	70:ST:78:ILE:HD11	2.46	0.49
50:S2:1665:G:C8	70:ST:88:MET:HE3	2.47	0.49
54:SD:7:LYS:HD3	71:SU:25:THR:HG21	1.94	0.49
67:SQ:9:SER:HB2	67:SQ:24:HIS:NE2	2.26	0.49
83:Sg:110:SER:HB3	83:Sg:154:VAL:HG22	1.94	0.49
3:L5:286:U:H2'	3:L5:287:U:C6	2.47	0.49
3:L5:1578:U:OP1	3:L5:3637:PSU:O2'	2.29	0.49
3:L5:2634:C:H2'	3:L5:2635:U:H6	1.77	0.49
9:LD:67:ALA:HB1	24:LT:31:MET:HE2	1.94	0.49
50:S2:1299:A:O2'	50:S2:1301:A:OP1	2.30	0.49
50:S2:1491:G:H2'	50:S2:1492:U:C6	2.48	0.49
51:SA:11:LYS:O	51:SA:15:VAL:HG23	2.10	0.49
67:SQ:112:LEU:HD22	67:SQ:119:LEU:HD13	1.93	0.49
78:Sb:67:THR:OG1	78:Sb:70:LYS:O	2.24	0.49
80:Sd:19:ARG:HD2	80:Sd:32:ARG:HD3	1.94	0.49
3:L5:1855:G:OP1	32:Lb:4:SER:HB2	2.12	0.49
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.77	0.49
3:L5:2814:C:H5'	3:L5:2815:A2M:OP2	2.12	0.49
3:L5:4761:G:H2'	3:L5:4762:A:C8	2.48	0.49
32:Lb:87:LYS:NZ	90:Lb:202:HOH:O	2.38	0.49
50:S2:106:C:OP1	50:S2:431:G:O2'	2.27	0.49
50:S2:1497:G:N7	61:SK:25:LYS:NZ	2.45	0.49
3:L5:2:G:H2'	3:L5:3:C:C6	2.47	0.49
3:L5:440:U:H2'	3:L5:441:G:C8	2.48	0.49
3:L5:965:G:H2'	3:L5:2256:C:O2	2.13	0.49
3:L5:2884:G:H2'	3:L5:2885:A:H8	1.77	0.49
3:L5:4173:G:H2'	3:L5:4174:U:C6	2.47	0.49
5:L8:87:G:H8	5:L8:87:G:OP2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:57:VAL:HG22	7:LB:73:VAL:HG22	1.93	0.49
15:LJ:169:LYS:HG2	15:LJ:170:TYR:CE1	2.48	0.49
49:Pt:17:G:C8	49:Pt:58:1MA:HM13	2.48	0.49
50:S2:1406:G:H2'	50:S2:1407:U:H6	1.77	0.49
51:SA:120:ARG:NH1	53:SC:267:GLN:HB2	2.26	0.49
56:SF:121:PRO:HA	56:SF:193:LYS:HD2	1.94	0.49
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.48	0.49
3:L5:4921:C:H2'	3:L5:4922:C:H6	1.77	0.49
10:LE:190:HIS:HB3	10:LE:193:PHE:HD2	1.78	0.49
12:LG:99:ALA:HB1	12:LG:136:LEU:HD11	1.93	0.49
50:S2:942:G:H2'	50:S2:943:U:C6	2.47	0.49
50:S2:1390:U:H2'	50:S2:1391:OMC:C6	2.47	0.49
50:S2:1512:C:H5''	80:Sd:8:TRP:CZ3	2.47	0.49
52:SB:124:HIS:HA	52:SB:137:LEU:O	2.12	0.49
71:SU:100:GLN:O	71:SU:103:SER:OG	2.27	0.49
2:Et:70:G:H2'	2:Et:71:C:C6	2.47	0.49
3:L5:454:U:H2'	3:L5:455:C:C6	2.47	0.49
3:L5:1499:C:OP1	21:LQ:150:ARG:NH2	2.39	0.49
3:L5:3848:U:H2'	3:L5:3849:A:H8	1.77	0.49
56:SF:145:ARG:NH1	90:SF:302:HOH:O	2.43	0.49
3:L5:690:C:OP1	47:Lr:87:ARG:NH1	2.42	0.49
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.78	0.49
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.47	0.49
7:LB:19:ARG:HB2	7:LB:234:ARG:NH2	2.27	0.49
11:LF:241:ASN:O	11:LF:245:ARG:HG2	2.13	0.49
18:LN:24:ARG:HB3	18:LN:24:ARG:CZ	2.43	0.49
23:LS:69:GLU:OE2	23:LS:101:THR:HA	2.13	0.49
50:S2:1215:C:O2'	50:S2:1645:C:OP2	2.29	0.49
56:SF:106:GLU:CD	56:SF:107:ASN:H	2.20	0.49
72:SV:70:LEU:HD21	72:SV:83:PHE:CE2	2.48	0.49
73:SW:3:ARG:HH22	73:SW:28:ARG:HH21	1.60	0.49
28:LX:145:ASP:O	28:LX:149:VAL:HG23	2.13	0.49
50:S2:70:G:H21	50:S2:79:A:H2	1.60	0.49
56:SF:100:ILE:HD11	56:SF:177:LEU:HB2	1.95	0.49
58:SH:69:LEU:HD13	58:SH:96:ALA:HB2	1.94	0.49
66:SP:53:GLN:OE1	66:SP:53:GLN:N	2.35	0.49
70:ST:42:HIS:HB3	70:ST:83:GLN:HB2	1.95	0.49
3:L5:180:C:O5'	3:L5:180:C:H6	1.95	0.49
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.13	0.49
3:L5:3598:C:H2'	3:L5:3599:A:C8	2.48	0.49
5:L8:60:G:O6	5:L8:96:C:O2'	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:234:LYS:HG2	6:LA:238:ILE:HG12	1.95	0.49
7:LB:77:THR:HG21	7:LB:337:VAL:HG22	1.94	0.49
50:S2:609:PSU:H2'	50:S2:610:G:H8	1.77	0.49
50:S2:1203:G:H2'	50:S2:1204:A:H8	1.74	0.49
50:S2:1568:C:H2'	50:S2:1569:A:C8	2.47	0.49
57:SG:1:MET:HG2	57:SG:24:LEU:HD13	1.95	0.49
73:SW:3:ARG:HH22	73:SW:28:ARG:NH2	2.11	0.49
3:L5:408:A:H4'	3:L5:409:G:H3'	1.95	0.48
3:L5:490:C:H2'	3:L5:491:G:C8	2.47	0.48
3:L5:1552:G:O2'	3:L5:1574:G:N2	2.35	0.48
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.48	0.48
4:L7:2:U:H2'	4:L7:3:C:H6	1.77	0.48
41:Lk:9:LYS:O	41:Lk:13:LEU:HD13	2.13	0.48
50:S2:344:U:H2'	50:S2:345:U:C6	2.48	0.48
50:S2:1226:G:N1	50:S2:1639:G7M:OP2	2.42	0.48
51:SA:13:GLU:O	51:SA:17:LYS:HG3	2.13	0.48
52:SB:164:ILE:O	52:SB:168:MET:HG3	2.13	0.48
53:SC:254:ASP:OD2	53:SC:255:LEU:HD12	2.12	0.48
67:SQ:32:ILE:HG22	67:SQ:68:ILE:HB	1.94	0.48
3:L5:23:C:H2'	3:L5:24:G:O4'	2.13	0.48
3:L5:1268:G:N7	32:Lb:111:ARG:NH2	2.44	0.48
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.47	0.48
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.12	0.48
4:L7:58:A:H2'	4:L7:59:G:C8	2.48	0.48
50:S2:96:C:H2'	50:S2:97:U:C6	2.47	0.48
50:S2:1826:G:OP1	89:S2:1944:HYG:H341	2.12	0.48
67:SQ:34:VAL:HB	67:SQ:42:ILE:HD11	1.95	0.48
83:Sg:31:ILE:HG22	83:Sg:43:TRP:HB2	1.95	0.48
3:L5:475:G:H2'	3:L5:476:G:H8	1.78	0.48
3:L5:1087:A:H2'	3:L5:1088:C:C6	2.47	0.48
3:L5:1707:C:H4'	32:Lb:101:HIS:HE1	1.78	0.48
3:L5:2529:A:O2'	3:L5:2531:C:OP2	2.31	0.48
3:L5:3727:A:H2'	3:L5:3728:A:C8	2.48	0.48
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.48	0.48
13:LH:62:GLY:HA2	13:LH:66:GLU:OE2	2.13	0.48
28:LX:79:PHE:CD1	38:Lh:36:VAL:HG21	2.47	0.48
30:LZ:16:GLY:O	30:LZ:19:SER:OG	2.31	0.48
50:S2:1101:U:H2'	50:S2:1102:G:H8	1.78	0.48
50:S2:1388:A:N6	54:SD:161:GLY:HA3	2.27	0.48
59:SI:145:ILE:HA	59:SI:148:LYS:HB3	1.94	0.48
67:SQ:82:TYR:O	67:SQ:85:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:989:U:H3	3:L5:1064:G:H1	1.61	0.48
3:L5:1262:G:H2'	3:L5:1263:A:C8	2.48	0.48
18:LN:104:GLU:HA	18:LN:160:GLU:HG3	1.94	0.48
50:S2:1550:G:H3'	50:S2:1579:A:H61	1.78	0.48
3:L5:469:C:H2'	3:L5:470:A:C8	2.48	0.48
3:L5:2579:G:N2	3:L5:2582:A:OP2	2.39	0.48
3:L5:4342:C:O3'	45:Lo:37:GLY:HA3	2.14	0.48
3:L5:4761:G:H2'	3:L5:4762:A:H8	1.77	0.48
18:LN:24:ARG:NH1	18:LN:24:ARG:HB3	2.29	0.48
50:S2:860:G:H21	73:SW:107:SER:HB3	1.78	0.48
50:S2:1280:G:H2'	50:S2:1281:G:H8	1.76	0.48
60:SJ:111:GLN:NE2	60:SJ:127:ARG:HD2	2.28	0.48
67:SQ:31:LEU:HG	67:SQ:67:ASP:OD2	2.14	0.48
83:Sg:291:TRP:CE2	83:Sg:298:LEU:HD23	2.47	0.48
3:L5:50:C:OP1	16:LL:20:ARG:NH2	2.46	0.48
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.48	0.48
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.49	0.48
3:L5:4861:G:H2'	3:L5:4862:G:C8	2.47	0.48
56:SF:102:LEU:HD23	56:SF:102:LEU:O	2.13	0.48
58:SH:149:ASP:O	73:SW:43:LYS:NZ	2.47	0.48
59:SI:164:GLU:O	59:SI:168:GLN:HG2	2.13	0.48
60:SJ:88:ASP:OD1	60:SJ:89:GLU:N	2.47	0.48
68:SR:127:ASN:OD1	68:SR:127:ASN:N	2.47	0.48
75:SY:101:LYS:HE2	75:SY:101:LYS:HB2	1.58	0.48
3:L5:268:G:H2'	3:L5:269:G:H8	1.79	0.48
3:L5:424:U:H2'	3:L5:425:U:C6	2.49	0.48
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.49	0.48
3:L5:1366:G:N7	16:LL:37:LYS:HE3	2.29	0.48
7:LB:80:GLU:OE1	7:LB:323:TYR:OH	2.26	0.48
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.49	0.48
36:Lf:41:PHE:HE2	36:Lf:110:ILE:HD13	1.79	0.48
50:S2:1442:OMU:HM23	50:S2:1442:OMU:H1'	1.54	0.48
50:S2:1603:G:H4'	69:SS:38:ARG:CZ	2.43	0.48
50:S2:1604:G:OP2	69:SS:38:ARG:NH2	2.39	0.48
53:SC:208:PRO:O	53:SC:212:LYS:HG3	2.13	0.48
58:SH:144:ILE:HB	73:SW:52:ILE:HB	1.95	0.48
64:SN:110:ASP:O	64:SN:114:ARG:HG2	2.12	0.48
79:Sc:32:VAL:HG11	79:Sc:56:LEU:HD12	1.94	0.48
3:L5:2477:A:H2'	3:L5:2478:C:C6	2.48	0.48
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.48	0.48
22:LR:99:MET:HE2	22:LR:99:MET:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:L1:28:ARG:HD3	42:L1:36:ARG:HA	1.94	0.48
50:S2:595:U:H2'	50:S2:596:U:C6	2.49	0.48
50:S2:1279:C:H2'	50:S2:1280:G:C8	2.48	0.48
50:S2:1446:A:O2'	50:S2:1447:OMG:H5''	2.14	0.48
61:SK:57:TYR:HB3	61:SK:75:GLY:HA2	1.96	0.48
69:SS:92:ASP:OD1	69:SS:92:ASP:N	2.37	0.48
79:Sc:36:ASP:OD1	79:Sc:37:ASP:N	2.47	0.48
83:Sg:115:SER:C	83:Sg:117:ASN:N	2.72	0.48
2:Et:49:G:H2'	2:Et:50:A:H8	1.78	0.48
3:L5:1893:C:H1'	3:L5:1937:C:O2	2.14	0.48
3:L5:4220:6MZ:O5'	3:L5:4220:6MZ:H8	2.14	0.48
9:LD:208:MET:HG3	9:LD:223:PHE:CE2	2.49	0.48
14:LI:54:SER:HB2	14:LI:135:ILE:HD11	1.95	0.48
16:LL:198:ARG:O	16:LL:201:GLU:HG3	2.14	0.48
30:LZ:89:ILE:HG22	30:LZ:91:LEU:HG	1.95	0.48
50:S2:1407:U:H2'	50:S2:1408:U:C6	2.49	0.48
61:SK:1:MET:HE1	61:SK:44:HIS:ND1	2.29	0.48
70:ST:14:PHE:CZ	70:ST:131:LEU:HD13	2.49	0.48
75:SY:36:PRO:O	75:SY:40:ILE:HG12	2.13	0.48
3:L5:3603:G:H2'	3:L5:3604:A:C8	2.48	0.48
37:Lg:45:ALA:HB3	37:Lg:82:MET:HE3	1.96	0.48
50:S2:1221:G:H2'	50:S2:1222:G:C8	2.48	0.48
50:S2:1337:4AC:O2	50:S2:1490:OMG:N2	2.26	0.48
50:S2:1805:G:N7	90:S2:2013:HOH:O	2.35	0.48
69:SS:35:GLY:O	69:SS:97:GLN:NE2	2.47	0.48
80:Sd:53:ILE:HD12	80:Sd:55:LEU:HD21	1.96	0.48
83:Sg:7:LEU:HD11	83:Sg:308:ARG:HG2	1.96	0.48
3:L5:1591:U:OP2	3:L5:2856:C:O2'	2.21	0.47
3:L5:1818:G:O2'	3:L5:1820:C:OP2	2.24	0.47
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.49	0.47
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.79	0.47
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.79	0.47
7:LB:128:LYS:O	7:LB:131:THR:OG1	2.28	0.47
14:LI:93:PRO:HB2	14:LI:125:THR:HB	1.95	0.47
15:LJ:84:GLU:HG2	15:LJ:170:TYR:HE2	1.79	0.47
20:LP:55:LYS:HA	20:LP:55:LYS:HD3	1.62	0.47
34:Ld:21:VAL:HG13	34:Ld:57:MET:HE1	1.95	0.47
49:Pt:21:A:H61	49:Pt:46:A:H2'	1.79	0.47
50:S2:1204:A:H2'	50:S2:1205:C:C6	2.48	0.47
50:S2:1534:C:H5''	56:SF:81:ARG:HH22	1.79	0.47
52:SB:100:PHE:CD2	52:SB:185:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SC:144:SER:HB2	53:SC:150:ALA:HB2	1.96	0.47
58:SH:12:ASN:OD1	58:SH:12:ASN:N	2.47	0.47
3:L5:1613:A:H5'	6:LA:183:GLY:HA2	1.97	0.47
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.14	0.47
50:S2:106:C:H2'	50:S2:107:A:H8	1.79	0.47
50:S2:145:G:H2'	50:S2:146:G:H8	1.76	0.47
50:S2:1457:U:H2'	50:S2:1458:G:H8	1.78	0.47
50:S2:1695:A:N6	90:S2:2041:HOH:O	2.40	0.47
55:SE:175:PHE:HE1	55:SE:225:ILE:HG21	1.77	0.47
61:SK:53:LYS:HD2	61:SK:53:LYS:O	2.14	0.47
76:SZ:50:PHE:HB3	76:SZ:54:THR:HB	1.96	0.47
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.49	0.47
3:L5:4940:C:OP1	10:LE:156:ARG:NH2	2.36	0.47
50:S2:1025:U:H2'	50:S2:1026:C:O4'	2.14	0.47
50:S2:1563:G:H2'	50:S2:1564:C:H6	1.80	0.47
50:S2:1690:U:H2'	50:S2:1691:U:C6	2.49	0.47
56:SF:70:GLU:HA	56:SF:73:THR:HG22	1.96	0.47
3:L5:1504:G:H2'	3:L5:1505:C:H6	1.79	0.47
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.49	0.47
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.49	0.47
3:L5:3933:G:H2'	3:L5:3934:G:H8	1.79	0.47
3:L5:4415:A:H2'	3:L5:4416:G:O4'	2.15	0.47
3:L5:4499:OMG:H1'	3:L5:4528:G:N3	2.29	0.47
7:LB:56:ILE:HD13	7:LB:365:LEU:HD22	1.97	0.47
15:LJ:51:SER:HB2	15:LJ:69:ALA:HB3	1.96	0.47
50:S2:1036:A:H4'	50:S2:1855:G:H21	1.79	0.47
50:S2:1136:PSU:H2'	50:S2:1137:U:C6	2.49	0.47
52:SB:138:PHE:O	52:SB:213:ARG:N	2.47	0.47
55:SE:22:LYS:HG3	55:SE:23:LEU:HD23	1.96	0.47
58:SH:95:ILE:HD13	58:SH:180:LEU:HD11	1.95	0.47
68:SR:94:GLU:HG2	68:SR:95:ILE:HG22	1.97	0.47
2:Et:65:C:H2'	2:Et:66:C:H6	1.80	0.47
3:L5:1338:G:H4'	3:L5:1339:U:H6	1.79	0.47
50:S2:683:OMG:N2	50:S2:1022:U:OP2	2.47	0.47
50:S2:1195:A:H2'	50:S2:1196:A:H8	1.80	0.47
79:Sc:34:PHE:CD1	79:Sc:40:ARG:HG2	2.49	0.47
3:L5:3855:C:H2'	3:L5:3856:A:H8	1.79	0.47
5:L8:70:G:H5''	29:LY:27:ARG:CZ	2.43	0.47
14:LI:36:LEU:HD13	14:LI:69:ARG:HH11	1.78	0.47
24:LT:107:LYS:HD2	24:LT:107:LYS:C	2.39	0.47
71:SU:51:LYS:HE2	71:SU:51:LYS:HB3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:52:TYR:CD1	83:Sg:309:VAL:HG21	2.47	0.47
83:Sg:191:HIS:CG	83:Sg:195:LEU:HD21	2.50	0.47
3:L5:679:C:H2'	3:L5:680:G:C8	2.48	0.47
3:L5:2871:A:H2'	3:L5:2872:C:O4'	2.14	0.47
3:L5:3871:A:H2'	3:L5:3872:A:C8	2.49	0.47
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.80	0.47
10:LE:239:LYS:HE3	10:LE:239:LYS:HB3	1.57	0.47
15:LJ:78:LYS:HA	15:LJ:78:LYS:HD2	1.62	0.47
23:LS:81:TRP:CZ3	23:LS:130:GLU:HG3	2.48	0.47
29:LY:108:ARG:HH11	29:LY:108:ARG:HG3	1.79	0.47
50:S2:867:OMG:H4'	62:SL:149:ALA:HB3	1.96	0.47
61:SK:72:THR:O	61:SK:76:ILE:HG13	2.15	0.47
78:Sb:36:LYS:HD2	78:Sb:36:LYS:C	2.40	0.47
83:Sg:68:ASP:OD2	83:Sg:111:VAL:N	2.33	0.47
83:Sg:194:TYR:O	83:Sg:212:LYS:N	2.35	0.47
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.49	0.47
3:L5:2284:G:OP1	31:La:7:LYS:NZ	2.44	0.47
3:L5:2709:C:H5'	22:LR:43:LYS:HD2	1.96	0.47
5:L8:141:C:H2'	5:L8:142:U:H6	1.80	0.47
9:LD:10:LYS:HB2	9:LD:10:LYS:HE3	1.64	0.47
50:S2:379:C:H5'	59:SI:33:ALA:HA	1.97	0.47
50:S2:1171:G:O2'	50:S2:1187:G:O6	2.28	0.47
50:S2:1563:G:H2'	50:S2:1564:C:C6	2.50	0.47
71:SU:41:ARG:HB2	71:SU:41:ARG:NH1	2.30	0.47
83:Sg:89:LEU:HD23	83:Sg:101:PHE:HE2	1.80	0.47
83:Sg:171:ASP:OD1	83:Sg:171:ASP:N	2.48	0.47
3:L5:758:G:H5''	13:LH:51:LYS:HZ3	1.79	0.47
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.50	0.47
3:L5:4077:A:N1	3:L5:4171:C:N4	2.59	0.47
3:L5:4128:A:H1'	12:LG:35:ARG:HB2	1.97	0.47
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.50	0.47
3:L5:4970:C:C2	3:L5:4971:A:C8	3.02	0.47
5:L8:85:U:H5''	5:L8:86:U:H3'	1.96	0.47
25:LU:40:GLU:OE1	25:LU:65:ARG:HB2	2.14	0.47
70:ST:14:PHE:HZ	70:ST:131:LEU:HD13	1.80	0.47
75:SY:55:ILE:HG23	75:SY:75:ILE:HG22	1.97	0.47
3:L5:917:A:H2'	3:L5:918:G:O4'	2.14	0.47
3:L5:982:U:H2'	3:L5:983:C:C6	2.51	0.47
3:L5:1914:C:H4'	19:LO:89:PRO:HD3	1.97	0.47
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.50	0.47
3:L5:2096:G:H21	8:LC:304:ALA:HB1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.50	0.47
8:LC:308:LYS:NZ	90:LC:507:HOH:O	2.48	0.47
11:LF:243:LEU:O	11:LF:247:MET:HG3	2.15	0.47
50:S2:65:C:N3	57:SG:133:LEU:HG	2.30	0.47
50:S2:1633:A:H2'	50:S2:1634:A:C8	2.50	0.47
50:S2:1847:G:O2'	84:S2:1902:PUT:N2	2.48	0.47
56:SF:25:THR:O	56:SF:42:LYS:HG2	2.15	0.47
66:SP:16:THR:HA	66:SP:21:ASP:HA	1.97	0.47
3:L5:2634:C:H2'	3:L5:2635:U:C6	2.50	0.46
3:L5:4873:G:N3	19:LO:175:MET:HG2	2.30	0.46
6:LA:144:LYS:HA	6:LA:144:LYS:HE3	1.98	0.46
15:LJ:85:LYS:NZ	15:LJ:115:LEU:O	2.34	0.46
21:LQ:70:MET:HE3	21:LQ:70:MET:HB3	1.75	0.46
50:S2:680:G:H2'	50:S2:681:PSU:C6	2.50	0.46
50:S2:1119:A:H2'	50:S2:1120:U:C6	2.50	0.46
50:S2:1347:PSU:H2'	50:S2:1348:G:N3	2.29	0.46
50:S2:1566:G:N7	70:ST:101:ARG:NH2	2.63	0.46
50:S2:1854:U:H2'	50:S2:1855:G:H8	1.81	0.46
54:SD:66:ILE:HD11	54:SD:86:LEU:HB3	1.97	0.46
64:SN:146:ALA:HA	64:SN:149:LEU:HD12	1.97	0.46
3:L5:116:G:H2'	3:L5:117:C:C6	2.50	0.46
3:L5:456:C:H2'	3:L5:457:G:C8	2.51	0.46
3:L5:4759:C:H2'	3:L5:4760:G:C8	2.50	0.46
10:LE:56:ARG:O	10:LE:56:ARG:NH1	2.41	0.46
33:Lc:47:ILE:HD12	33:Lc:94:LEU:HD11	1.98	0.46
50:S2:1221:G:O2'	50:S2:1676:U:O2	2.30	0.46
51:SA:24:HIS:HB3	51:SA:51:LEU:HD21	1.97	0.46
51:SA:137:ALA:HB1	51:SA:142:LEU:HB3	1.97	0.46
56:SF:171:GLU:OE1	76:SZ:106:GLN:NE2	2.41	0.46
58:SH:142:LYS:HB3	73:SW:54:ASP:HB3	1.96	0.46
61:SK:71:LEU:HD11	61:SK:79:LEU:HD12	1.98	0.46
70:ST:133:ARG:O	70:ST:137:GLN:HG3	2.16	0.46
75:SY:53:ASP:OD1	75:SY:79:LEU:HD13	2.16	0.46
76:SZ:51:ASP:OD1	76:SZ:51:ASP:N	2.37	0.46
2:Et:10:G:H2'	2:Et:12:C:H41	1.80	0.46
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.16	0.46
3:L5:2569:G:H2'	3:L5:2570:U:C6	2.50	0.46
3:L5:3663:A:N6	3:L5:4168:G:HO2'	2.13	0.46
4:L7:4:U:H2'	4:L7:5:A:C8	2.50	0.46
50:S2:441:C:H2'	50:S2:442:C:C6	2.51	0.46
57:SG:98:ARG:NH1	57:SG:99:GLY:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SI:65:PHE:HA	59:SI:187:GLY:O	2.15	0.46
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.81	0.46
3:L5:2497:C:H2'	3:L5:2498:C:H6	1.81	0.46
3:L5:4392:OMG:HM21	3:L5:4394:A:H2'	1.96	0.46
3:L5:4920:C:H2'	3:L5:4921:C:H6	1.80	0.46
50:S2:641:A:O2'	50:S2:645:C:OP1	2.32	0.46
60:SJ:120:ALA:HB1	60:SJ:125:HIS:HB3	1.98	0.46
61:SK:42:ASN:O	61:SK:46:MET:HG3	2.16	0.46
69:SS:144:ARG:HG3	69:SS:144:ARG:HH11	1.79	0.46
76:SZ:58:LEU:HD12	76:SZ:59:CYS:N	2.31	0.46
83:Sg:195:LEU:HA	83:Sg:211:GLY:HA3	1.97	0.46
3:L5:921:C:H2'	3:L5:922:C:C6	2.51	0.46
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.98	0.46
15:LJ:28:GLU:OE1	15:LJ:28:GLU:N	2.47	0.46
50:S2:1520:G:H5''	50:S2:1521:C:OP2	2.16	0.46
66:SP:56:LEU:HD23	66:SP:83:MET:HG2	1.97	0.46
67:SQ:102:GLU:HA	67:SQ:105:LYS:HB3	1.98	0.46
69:SS:58:GLU:OE1	76:SZ:49:LEU:HD11	2.16	0.46
3:L5:1098:G:H2'	3:L5:1099:C:C6	2.50	0.46
3:L5:1204:C:H2'	3:L5:1205:G:H8	1.80	0.46
3:L5:1359:G:H4'	18:LN:203:TYR:HB2	1.97	0.46
3:L5:2691:U:H2'	3:L5:2692:U:H6	1.79	0.46
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.51	0.46
3:L5:4080:C:H2'	3:L5:4081:G:H8	1.80	0.46
3:L5:4266:G:N3	3:L5:4266:G:H2'	2.30	0.46
4:L7:6:C:H4'	9:LD:52:ILE:HD13	1.98	0.46
5:L8:140:C:H2'	5:L8:141:C:C6	2.51	0.46
50:S2:433:A:H2'	50:S2:434:G:C8	2.50	0.46
50:S2:680:G:H2'	50:S2:681:PSU:H6	1.79	0.46
66:SP:108:LYS:O	66:SP:111:MET:HG2	2.15	0.46
76:SZ:73:VAL:HG12	76:SZ:79:ILE:HD11	1.98	0.46
83:Sg:56:GLN:HA	83:Sg:56:GLN:OE1	2.14	0.46
83:Sg:87:LEU:HB2	83:Sg:101:PHE:HB2	1.98	0.46
3:L5:691:C:H2'	3:L5:692:A:C8	2.50	0.46
3:L5:1472:C:H2'	3:L5:1473:U:C6	2.51	0.46
3:L5:1927:U:OP1	3:L5:1949:U:O2'	2.32	0.46
3:L5:3656:A:H2'	3:L5:3657:U:H6	1.80	0.46
3:L5:4287:G:H2'	3:L5:4288:C:C6	2.50	0.46
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.51	0.46
3:L5:5001:PSU:H5'	7:LB:317:LEU:HD23	1.96	0.46
20:LP:17:SER:HB2	20:LP:98:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LS:98:ARG:HG3	23:LS:142:VAL:HG13	1.98	0.46
30:LZ:14:LEU:HB3	37:Lg:88:ARG:HG3	1.97	0.46
50:S2:1609:C:H5'	69:SS:131:VAL:HG22	1.97	0.46
50:S2:1801:A:H2'	50:S2:1802:C:H6	1.81	0.46
58:SH:100:ILE:HG12	58:SH:125:VAL:HG21	1.98	0.46
77:Sa:41:ILE:HG12	77:Sa:68:TYR:CD2	2.50	0.46
3:L5:1406:G:H2'	3:L5:1407:C:O4'	2.15	0.46
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.51	0.46
3:L5:4438:U:H2'	3:L5:4439:U:O4'	2.16	0.46
4:L7:16:A:H2'	4:L7:17:C:C6	2.50	0.46
5:L8:92:U:H2'	5:L8:93:C:O4'	2.16	0.46
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.97	0.46
7:LB:156:TYR:O	7:LB:158:GLN:NE2	2.49	0.46
9:LD:258:LYS:HE3	9:LD:258:LYS:HB3	1.55	0.46
50:S2:25:A:HO2'	50:S2:26:U:H6	1.61	0.46
50:S2:563:G:O2'	50:S2:564:A:H8	1.99	0.46
50:S2:1311:C:H2'	50:S2:1312:G:O4'	2.16	0.46
50:S2:1692:PSU:H2'	50:S2:1693:G:C8	2.51	0.46
54:SD:22:ASN:O	54:SD:26:THR:OG1	2.27	0.46
79:Sc:14:VAL:HA	79:Sc:32:VAL:HG12	1.98	0.46
3:L5:961:G:O2'	3:L5:963:G:N7	2.49	0.46
3:L5:1344:C:H2'	3:L5:1345:A:H8	1.80	0.46
3:L5:1739:G:H2'	3:L5:1740:C:C6	2.51	0.46
3:L5:2412:A:H2'	3:L5:2413:U:H6	1.79	0.46
3:L5:2505:C:H4'	3:L5:2506:G:O4'	2.15	0.46
3:L5:2517:A:H5'	37:Lg:62:LYS:HD3	1.96	0.46
3:L5:2580:U:O2'	30:LZ:79:HIS:ND1	2.43	0.46
3:L5:3615:G:N3	27:LW:44:ARG:HD3	2.31	0.46
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.51	0.46
90:L5:7374:HOH:O	14:LI:195:CYS:SG	2.61	0.46
11:LF:27:GLU:HA	11:LF:30:ILE:HG22	1.98	0.46
20:LP:94:MET:HG2	20:LP:148:MET:SD	2.56	0.46
50:S2:496:C:H2'	50:S2:497:C:C6	2.51	0.46
50:S2:960:U:O2'	50:S2:962:A:N7	2.30	0.46
50:S2:1587:G:N2	70:ST:77:LYS:HE3	2.30	0.46
50:S2:1839:U:H2'	50:S2:1840:U:C6	2.51	0.46
50:S2:1856:C:H2'	50:S2:1857:G:H8	1.81	0.46
52:SB:185:VAL:O	52:SB:189:ILE:HG13	2.16	0.46
54:SD:20:GLU:HG2	54:SD:77:PHE:HZ	1.81	0.46
54:SD:20:GLU:OE1	54:SD:76:ARG:NH2	2.44	0.46
57:SG:27:PHE:HE2	57:SG:41:LEU:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:302:TYR:OH	83:Sg:308:ARG:HB2	2.15	0.46
3:L5:433:A:H2'	3:L5:434:A:O4'	2.16	0.46
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.51	0.46
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.16	0.46
3:L5:1773:U:H2'	3:L5:1774:C:H6	1.81	0.46
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.81	0.46
3:L5:2415:OMU:HM23	3:L5:2415:OMU:H1'	1.54	0.46
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.80	0.46
5:L8:19:C:H2'	5:L8:20:A:H8	1.81	0.46
5:L8:155:C:H2'	5:L8:156:U:O4'	2.16	0.46
18:LN:178:HIS:HA	18:LN:181:HIS:NE2	2.31	0.46
19:LO:181:ALA:O	19:LO:185:VAL:HG22	2.16	0.46
24:LT:51:GLY:HA3	24:LT:92:ARG:HG3	1.98	0.46
25:LU:99:TRP:HA	25:LU:99:TRP:CE3	2.51	0.46
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.97	0.46
50:S2:980:A:H2'	50:S2:981:A:C8	2.51	0.46
50:S2:1162:C:H2'	50:S2:1163:C:O4'	2.16	0.46
50:S2:1407:U:H2'	50:S2:1408:U:H6	1.81	0.46
53:SC:106:VAL:HG22	53:SC:128:VAL:HG22	1.98	0.46
59:SI:145:ILE:C	59:SI:145:ILE:HD12	2.41	0.46
65:SO:82:ALA:HA	65:SO:124:MET:HE3	1.98	0.46
66:SP:57:LEU:HA	66:SP:60:LEU:HD12	1.99	0.46
70:ST:32:GLU:OE1	70:ST:32:GLU:C	2.59	0.46
3:L5:129:C:H2'	3:L5:130:C:H6	1.81	0.45
3:L5:208:A:C2	3:L5:233:U:H5'	2.51	0.45
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.51	0.45
3:L5:2293:U:H2'	3:L5:2294:G:C8	2.51	0.45
3:L5:4173:G:H2'	3:L5:4174:U:H6	1.80	0.45
3:L5:4708:A:N3	3:L5:4709:U:H5'	2.31	0.45
9:LD:156:GLY:HA2	9:LD:181:PRO:HG3	1.98	0.45
15:LJ:85:LYS:HE3	15:LJ:85:LYS:HB3	1.57	0.45
50:S2:158:A:H2'	50:S2:159:A2M:H8	1.98	0.45
51:SA:189:ILE:HG21	51:SA:195:TRP:NE1	2.31	0.45
52:SB:107:ARG:NH1	65:SO:135:ILE:HD13	2.31	0.45
56:SF:28:VAL:HG12	56:SF:110:GLN:HG2	1.98	0.45
67:SQ:105:LYS:O	67:SQ:109:LYS:HB2	2.17	0.45
83:Sg:217:MET:HE3	83:Sg:219:TRP:CZ2	2.51	0.45
3:L5:223:G:H4'	3:L5:225:G:N7	2.31	0.45
3:L5:1248:C:H2'	3:L5:1249:C:C6	2.50	0.45
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.51	0.45
3:L5:2893:U:H2'	3:L5:2894:A:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LE:238:GLU:OE1	10:LE:238:GLU:N	2.50	0.45
13:LH:137:SER:HB2	13:LH:145:ILE:HD11	1.98	0.45
22:LR:90:PRO:HB2	22:LR:93:VAL:HG23	1.98	0.45
29:LY:31:SER:HA	29:LY:48:PRO:HA	1.97	0.45
30:LZ:68:ILE:O	30:LZ:115:LYS:NZ	2.49	0.45
43:Lm:80:PRO:O	43:Lm:84:GLN:HG3	2.16	0.45
50:S2:1293:A:H1'	82:Sf:138:ARG:CZ	2.45	0.45
51:SA:81:ASN:HA	51:SA:84:GLN:CD	2.41	0.45
52:SB:51:ARG:HE	52:SB:51:ARG:HB3	1.61	0.45
56:SF:68:ILE:HD11	56:SF:151:ILE:HD11	1.98	0.45
75:SY:10:ARG:HE	75:SY:26:ASP:CG	2.24	0.45
79:Sc:34:PHE:HD1	79:Sc:40:ARG:HG2	1.79	0.45
3:L5:387:G:O5'	29:LY:89:LYS:NZ	2.47	0.45
3:L5:1173:G:H2'	3:L5:1174:G:O4'	2.15	0.45
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.50	0.45
3:L5:2706:G:N2	3:L5:2710:C:OP2	2.42	0.45
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.49	0.45
3:L5:4763:U:O2'	23:LS:174:THR:OG1	2.26	0.45
5:L8:66:A:H2'	5:L8:67:U:C6	2.51	0.45
5:L8:89:U:H2'	5:L8:90:C:C6	2.51	0.45
50:S2:191:A:H2'	50:S2:192:C:O4'	2.16	0.45
50:S2:830:A:OP2	50:S2:846:G:N2	2.48	0.45
50:S2:1265:A:H5''	50:S2:1266:C:OP2	2.16	0.45
50:S2:1351:G:O2'	50:S2:1378:A:N1	2.47	0.45
54:SD:55:THR:O	54:SD:58:VAL:HG12	2.17	0.45
55:SE:59:ASP:OD2	55:SE:59:ASP:N	2.50	0.45
57:SG:143:LYS:HE2	57:SG:143:LYS:HB2	1.63	0.45
60:SJ:33:GLY:HA3	81:Se:112:TYR:CG	2.51	0.45
70:ST:9:VAL:HG21	70:ST:138:VAL:HG12	1.97	0.45
71:SU:56:MET:HE2	71:SU:56:MET:HA	1.98	0.45
74:SX:101:LEU:HB3	74:SX:124:LYS:HB2	1.98	0.45
3:L5:181:C:C2	3:L5:182:G:N7	2.84	0.45
3:L5:478:G:H2'	3:L5:479:G:C8	2.50	0.45
3:L5:1344:C:H2'	3:L5:1345:A:C8	2.51	0.45
3:L5:1625:OMG:N1	3:L5:3918:G:OP1	2.47	0.45
3:L5:1786:A:H2'	3:L5:1789:C:C5	2.50	0.45
5:L8:52:A:H5'	42:Ll:21:ARG:HD3	1.98	0.45
26:LV:13:LYS:HE3	26:LV:13:LYS:HB2	1.79	0.45
50:S2:77:A:O2'	57:SG:174:PRO:O	2.33	0.45
50:S2:375:U:H2'	50:S2:376:A:C8	2.51	0.45
52:SB:100:PHE:HZ	52:SB:103:MET:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SI:130:THR:HG22	59:SI:132:GLU:HG2	1.98	0.45
59:SI:154:LYS:HB2	59:SI:154:LYS:HE3	1.78	0.45
69:SS:125:HIS:CD2	69:SS:131:VAL:HG11	2.51	0.45
3:L5:180:C:H2'	3:L5:181:C:C1'	2.46	0.45
3:L5:1241:C:C5	32:Lb:115:GLY:HA2	2.52	0.45
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.16	0.45
3:L5:1743:A:O4'	9:LD:15:ARG:HD2	2.17	0.45
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.99	0.45
3:L5:2376:A:H2'	3:L5:2377:C:C6	2.51	0.45
7:LB:155:LYS:HE2	7:LB:156:TYR:CZ	2.50	0.45
11:LF:164:LYS:HE2	11:LF:164:LYS:HB2	1.66	0.45
13:LH:34:LEU:HD12	13:LH:84:VAL:HG13	1.99	0.45
15:LJ:169:LYS:HG2	15:LJ:170:TYR:CD1	2.52	0.45
18:LN:16:SER:O	18:LN:20:ARG:HB2	2.16	0.45
24:LT:102:ARG:HG2	24:LT:102:ARG:HH11	1.81	0.45
34:Ld:33:ILE:HG22	34:Ld:44:ARG:HG3	1.98	0.45
54:SD:29:LEU:HB3	54:SD:34:TYR:HB2	1.97	0.45
57:SG:43:GLU:N	57:SG:43:GLU:OE2	2.49	0.45
13:LH:85:THR:HG22	13:LH:86:LEU:HG	1.97	0.45
14:LI:48:LEU:O	14:LI:139:ARG:HA	2.17	0.45
50:S2:953:C:H2'	50:S2:954:U:O4'	2.17	0.45
50:S2:1631:U:O4	50:S2:1632:G:N1	2.49	0.45
65:SO:42:VAL:HG11	65:SO:78:ALA:HA	1.98	0.45
70:ST:98:SER:O	70:ST:102:ARG:HG2	2.17	0.45
3:L5:475:G:H2'	3:L5:476:G:C8	2.52	0.45
3:L5:722:G:N7	90:L5:5485:HOH:O	2.36	0.45
3:L5:1475:G:H2'	3:L5:1476:C:C6	2.52	0.45
3:L5:1480:C:O2'	3:L5:1482:G:OP2	2.25	0.45
3:L5:2893:U:H2'	3:L5:2894:A:C8	2.52	0.45
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.32	0.45
3:L5:4934:A:O2'	3:L5:4935:C:O4'	2.27	0.45
3:L5:4965:U:H4'	3:L5:4966:A:H5'	1.99	0.45
25:LU:80:LYS:HE2	25:LU:110:TYR:CZ	2.51	0.45
32:Lb:22:LYS:HB3	32:Lb:22:LYS:HE3	1.84	0.45
34:Ld:37:GLY:O	34:Ld:41:ARG:HG3	2.17	0.45
38:Lh:35:LYS:HA	38:Lh:44:LEU:HD11	1.98	0.45
50:S2:435:A:N6	90:S2:2084:HOH:O	2.50	0.45
50:S2:1259:A:H1'	50:S2:1264:C:H42	1.82	0.45
50:S2:1546:G:N2	50:S2:1670:C:O2	2.45	0.45
51:SA:42:LYS:HB2	51:SA:42:LYS:HE3	1.74	0.45
56:SF:118:ASN:HB3	56:SF:190:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SK:5:LYS:O	61:SK:9:ILE:HG13	2.17	0.45
68:SR:71:ILE:O	68:SR:75:GLU:HG2	2.17	0.45
70:ST:21:PHE:CD1	70:ST:134:ILE:HD11	2.52	0.45
70:ST:65:TYR:HB2	70:ST:123:LEU:HD22	1.98	0.45
83:Sg:207:CYS:HB2	83:Sg:221:LEU:HD21	1.99	0.45
3:L5:62:A:N3	3:L5:77:U:O2'	2.41	0.45
3:L5:669:C:H2'	3:L5:670:G:H8	1.81	0.45
3:L5:3893:C:H2'	3:L5:3894:A:C8	2.52	0.45
3:L5:4085:A:C5	12:LG:56:LYS:HG3	2.51	0.45
5:L8:31:G:H2'	5:L8:32:C:O4'	2.17	0.45
25:LU:35:ASP:HB3	25:LU:38:ASN:OD1	2.17	0.45
29:LY:47:MET:HE3	29:LY:47:MET:HB3	1.87	0.45
30:LZ:53:VAL:HG11	30:LZ:62:ILE:HG23	1.99	0.45
35:Le:78:LEU:HB3	47:Lr:20:ARG:HD3	1.98	0.45
38:Lh:12:LYS:HE3	38:Lh:12:LYS:HB3	1.72	0.45
38:Lh:80:PRO:HD2	38:Lh:83:LEU:HD12	1.97	0.45
50:S2:116:OMU:H2'	50:S2:117:C:C6	2.52	0.45
50:S2:1396:A:O2'	50:S2:1398:G:N7	2.48	0.45
50:S2:1628:C:H2'	50:S2:1629:C:C6	2.51	0.45
55:SE:151:ASP:HB3	55:SE:154:ILE:HG13	1.99	0.45
57:SG:211:LYS:HG2	57:SG:212:LEU:N	2.31	0.45
66:SP:94:VAL:HG11	66:SP:116:LEU:HD21	1.98	0.45
75:SY:57:VAL:HB	75:SY:60:PHE:HE2	1.81	0.45
3:L5:257:C:H2'	3:L5:258:G:C8	2.51	0.45
3:L5:1400:G:H2'	3:L5:1401:C:C6	2.51	0.45
3:L5:4968:A:H2'	3:L5:4969:C:C6	2.52	0.45
8:LC:3:CYS:HB3	8:LC:29:LYS:HE2	1.98	0.45
50:S2:28:U:H2'	50:S2:29:G:H8	1.82	0.45
50:S2:639:C:H2'	50:S2:640:A:C8	2.51	0.45
50:S2:811:A:H2'	50:S2:812:A:H8	1.81	0.45
50:S2:954:U:H2'	50:S2:955:A:C8	2.52	0.45
50:S2:1531:A:H2'	50:S2:1532:C:C6	2.52	0.45
69:SS:120:HIS:CE1	69:SS:124:ARG:HD2	2.52	0.45
3:L5:163:A:H2'	3:L5:164:G:H8	1.82	0.45
3:L5:1094:G:H2'	3:L5:1095:A:C8	2.51	0.45
3:L5:1100:U:H3	3:L5:1195:G:H1	1.64	0.45
3:L5:1174:G:H2'	3:L5:1175:A:H8	1.82	0.45
3:L5:3733:A:H2'	3:L5:3734:PSU:O4'	2.17	0.45
9:LD:179:ARG:HD3	9:LD:179:ARG:HA	1.73	0.45
26:LV:108:ASN:OD1	26:LV:108:ASN:N	2.50	0.45
34:Ld:20:VAL:HA	34:Ld:90:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:442:C:H2'	50:S2:443:U:C6	2.52	0.45
50:S2:449:A:H4'	55:SE:3:ARG:HD3	1.99	0.45
63:SM:32:ALA:HB2	63:SM:112:LYS:HE3	1.99	0.45
63:SM:46:GLN:HB3	63:SM:47:ALA:H	1.58	0.45
64:SN:84:LEU:HD23	64:SN:84:LEU:HA	1.84	0.45
66:SP:80:LEU:HB3	66:SP:83:MET:HB2	1.98	0.45
68:SR:21:TYR:CD1	68:SR:58:MET:HE1	2.52	0.45
82:Sf:132:MET:HE2	82:Sf:132:MET:HB3	1.88	0.45
83:Sg:47:ARG:HA	83:Sg:52:TYR:CD2	2.52	0.45
3:L5:1400:G:H2'	3:L5:1401:C:H6	1.82	0.44
3:L5:1420:A:N6	90:L5:5906:HOH:O	2.50	0.44
7:LB:14:LEU:HD22	7:LB:17:LEU:HD11	2.00	0.44
52:SB:121:ILE:HG12	52:SB:161:VAL:HG13	2.00	0.44
53:SC:80:GLU:H	53:SC:80:GLU:CD	2.25	0.44
58:SH:63:PHE:HA	58:SH:95:ILE:O	2.17	0.44
64:SN:16:LEU:HD23	64:SN:16:LEU:HA	1.85	0.44
69:SS:55:ARG:CZ	76:SZ:48:VAL:HG11	2.47	0.44
71:SU:26:SER:HB3	71:SU:32:LEU:HD13	1.98	0.44
75:SY:45:ALA:C	75:SY:47:MET:H	2.24	0.44
3:L5:19:G:P	38:Lh:93:ARG:HE	2.40	0.44
3:L5:37:U:H2'	3:L5:38:A:O4'	2.17	0.44
3:L5:268:G:H2'	3:L5:269:G:C8	2.53	0.44
3:L5:458:C:OP1	10:LE:114:ARG:HG2	2.18	0.44
3:L5:659:G:H2'	3:L5:660:A:C8	2.51	0.44
3:L5:1509:C:H5''	31:La:2:PRO:HD2	1.99	0.44
3:L5:2621:A:H2'	3:L5:2622:G:C8	2.52	0.44
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.53	0.44
13:LH:17:ASP:OD1	13:LH:28:LYS:HB3	2.16	0.44
28:LX:150:ALA:HA	28:LX:155:ILE:HD12	1.98	0.44
50:S2:1004:PSU:H2'	50:S2:1005:G:C8	2.49	0.44
50:S2:1259:A:H1'	50:S2:1264:C:N4	2.32	0.44
50:S2:1712:A:H2'	50:S2:1713:C:H6	1.81	0.44
54:SD:96:LEU:HD12	54:SD:198:ILE:HG12	1.98	0.44
62:SL:80:MET:HE1	62:SL:120:VAL:HB	1.99	0.44
76:SZ:57:LYS:HB2	76:SZ:57:LYS:HE2	1.81	0.44
3:L5:270:U:H2'	3:L5:271:C:C6	2.52	0.44
3:L5:750:U:H1'	3:L5:917:A:C8	2.53	0.44
3:L5:1338:G:H4'	3:L5:1339:U:C6	2.51	0.44
3:L5:1369:C:OP2	3:L5:1370:G:O2'	2.34	0.44
3:L5:1409:C:H2'	3:L5:1410:U:O4'	2.17	0.44
3:L5:4113:U:H2'	3:L5:4114:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:5028:G:H2'	3:L5:5029:C:C6	2.53	0.44
3:L5:5028:G:H2'	3:L5:5029:C:H6	1.83	0.44
16:LL:170:THR:OG1	16:LL:173:GLU:HG3	2.16	0.44
35:Le:129:LEU:HD23	35:Le:129:LEU:HA	1.87	0.44
40:Lj:39:TYR:CD1	40:Lj:40:PRO:HA	2.52	0.44
50:S2:209:A:H2'	50:S2:210:U:O4'	2.17	0.44
50:S2:952:G:H2'	50:S2:953:C:C6	2.52	0.44
50:S2:1046:U:H2'	50:S2:1047:C:O4'	2.18	0.44
50:S2:1232:PSU:H2'	50:S2:1233:G:C8	2.52	0.44
50:S2:1398:G:H1'	83:Sg:63:SER:HB3	1.99	0.44
53:SC:220:ASP:OD2	53:SC:220:ASP:N	2.51	0.44
55:SE:174:LYS:O	55:SE:179:ASN:ND2	2.50	0.44
56:SF:61:PHE:CE1	79:Sc:49:PRO:HB2	2.51	0.44
57:SG:199:THR:O	57:SG:203:LYS:HG2	2.17	0.44
58:SH:139:ILE:HG23	58:SH:156:VAL:HG13	1.99	0.44
63:SM:22:LEU:HA	63:SM:31:LEU:HD21	1.99	0.44
63:SM:33:ARG:HD2	63:SM:33:ARG:HA	1.73	0.44
75:SY:105:LYS:O	75:SY:109:GLU:HG3	2.16	0.44
83:Sg:116:ASP:C	83:Sg:118:ARG:N	2.74	0.44
3:L5:1074:G:H2'	3:L5:1075:G:C8	2.52	0.44
3:L5:1086:C:H2'	3:L5:1087:A:H8	1.82	0.44
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.17	0.44
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.80	0.44
6:LA:14:SER:OG	6:LA:15:VAL:N	2.50	0.44
19:LO:130:LYS:HB2	19:LO:133:ARG:HG2	1.98	0.44
24:LT:124:THR:OG1	24:LT:125:TRP:N	2.49	0.44
50:S2:160:U:O2'	50:S2:161:U:H3'	2.17	0.44
50:S2:1280:G:H2'	50:S2:1281:G:C8	2.52	0.44
51:SA:176:TRP:CD1	51:SA:199:PRO:HA	2.52	0.44
52:SB:34:LYS:O	52:SB:98:THR:OG1	2.30	0.44
53:SC:252:THR:HB	53:SC:255:LEU:HD13	1.99	0.44
54:SD:75:LYS:HD2	61:SK:22:VAL:HG23	2.00	0.44
66:SP:15:PHE:HD1	66:SP:22:LEU:HB2	1.83	0.44
83:Sg:24:THR:HG23	83:Sg:27:PHE:H	1.82	0.44
2:Et:41:C:O2'	56:SF:198:ARG:NH2	2.51	0.44
2:Et:70:G:H2'	2:Et:71:C:H6	1.82	0.44
3:L5:153:G:H2'	3:L5:154:G:C8	2.50	0.44
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.53	0.44
3:L5:1407:C:H2'	3:L5:1408:G:C5	2.53	0.44
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.53	0.44
3:L5:2884:G:H2'	3:L5:2885:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3930:U:H2'	3:L5:3931:C:C6	2.53	0.44
3:L5:4750:G:H2'	3:L5:4751:G:H8	1.83	0.44
23:LS:29:ARG:HB2	24:LT:148:PRO:HB2	2.00	0.44
25:LU:52:LYS:HB2	25:LU:52:LYS:HE2	1.78	0.44
28:LX:64:SER:HB2	38:Lh:69:LEU:HD13	1.98	0.44
39:Li:30:ARG:NH2	90:Li:203:HOH:O	2.51	0.44
45:Lo:22:LYS:HG3	45:Lo:73:VAL:HG12	1.99	0.44
55:SE:122:LYS:HD2	55:SE:164:LEU:HD11	1.99	0.44
71:SU:56:MET:HB2	71:SU:86:LYS:HB3	1.98	0.44
75:SY:35:VAL:HB	75:SY:40:ILE:HD11	2.00	0.44
3:L5:175:C:H2'	3:L5:176:G:C8	2.52	0.44
3:L5:1259:G:H2'	3:L5:1260:G:C8	2.52	0.44
3:L5:1548:G:O2'	3:L5:2812:A:N3	2.39	0.44
3:L5:4884:G:N7	10:LE:272:ARG:NH2	2.63	0.44
5:L8:6:C:H2'	5:L8:7:U:C6	2.52	0.44
13:LH:95:VAL:HG22	43:Lm:82:LEU:HB3	1.98	0.44
23:LS:43:ARG:NH1	90:LS:208:HOH:O	2.50	0.44
33:Lc:78:ASN:OD1	33:Lc:78:ASN:N	2.50	0.44
40:Lj:67:LEU:HD23	40:Lj:67:LEU:HA	1.83	0.44
50:S2:14:C:H2'	50:S2:15:U:C6	2.53	0.44
50:S2:568:C:H42	50:S2:582:U:H3	1.66	0.44
50:S2:1711:U:H2'	50:S2:1712:A:C8	2.52	0.44
52:SB:71:LEU:HD23	52:SB:79:VAL:HG22	1.98	0.44
52:SB:202:GLN:O	52:SB:202:GLN:HG3	2.17	0.44
57:SG:138:ALA:HA	57:SG:141:ILE:HD12	1.99	0.44
57:SG:153:VAL:O	57:SG:157:VAL:HG23	2.17	0.44
75:SY:46:LYS:HB2	75:SY:46:LYS:HE2	1.78	0.44
83:Sg:183:LYS:HE2	83:Sg:183:LYS:HB2	1.70	0.44
2:Et:69:U:H2'	2:Et:70:G:H8	1.80	0.44
3:L5:223:G:H4'	3:L5:225:G:C8	2.53	0.44
3:L5:445:U:H2'	3:L5:446:C:O4'	2.18	0.44
3:L5:750:U:C2	3:L5:751:G:C8	3.05	0.44
3:L5:1390:G:O2'	85:L5:5113:SPD:N10	2.50	0.44
3:L5:1732:C:H5''	24:LT:43:LYS:HD2	2.00	0.44
3:L5:2065:G:H2'	3:L5:2066:C:O4'	2.18	0.44
3:L5:2267:U:C6	3:L5:2270:G:H4'	2.53	0.44
3:L5:2292:C:H2'	3:L5:2293:U:C6	2.53	0.44
3:L5:3739:C:C2	3:L5:3740:G:C8	3.05	0.44
3:L5:4076:G:N2	90:L5:5575:HOH:O	2.41	0.44
3:L5:4125:C:H2'	3:L5:4126:C:C6	2.52	0.44
3:L5:4638:U:H2'	3:L5:4639:G:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LG:38:ASN:O	12:LG:43:GLN:HB3	2.17	0.44
15:LJ:174:ILE:HG13	15:LJ:174:ILE:O	2.17	0.44
29:LY:127:GLN:O	29:LY:131:GLU:HG2	2.16	0.44
50:S2:1278:A:H2'	50:S2:1279:C:H6	1.82	0.44
52:SB:53:GLN:O	52:SB:56:LYS:N	2.51	0.44
54:SD:138:VAL:HG12	54:SD:142:LEU:HD21	1.99	0.44
57:SG:157:VAL:HG22	57:SG:176:ILE:HD11	1.99	0.44
58:SH:134:VAL:HG23	58:SH:137:SER:O	2.18	0.44
67:SQ:86:GLN:HE22	67:SQ:122:ALA:HA	1.82	0.44
70:ST:129:ARG:HD3	70:ST:133:ARG:HH22	1.82	0.44
74:SX:60:LYS:HD2	74:SX:116:PRO:HB3	1.98	0.44
80:Sd:33:LYS:HE3	80:Sd:34:TYR:CZ	2.53	0.44
3:L5:1076:C:H2'	3:L5:1077:C:H6	1.83	0.44
3:L5:1191:C:H2'	3:L5:1192:C:C6	2.53	0.44
3:L5:1250:C:H2'	3:L5:1251:C:C6	2.53	0.44
3:L5:1346:C:H2'	3:L5:1347:G:C8	2.52	0.44
3:L5:2693:G:H2'	3:L5:2694:G:N2	2.33	0.44
3:L5:3719:A:C4	3:L5:3720:G:C8	3.06	0.44
3:L5:4896:G:H2'	3:L5:4897:G:H8	1.83	0.44
13:LH:56:ARG:NH1	13:LH:58:ASP:OD2	2.51	0.44
23:LS:15:ARG:HB3	23:LS:27:LEU:HD12	2.00	0.44
42:LI:13:LEU:O	42:LI:17:GLN:HG3	2.18	0.44
45:Lo:99:ARG:HB2	45:Lo:102:GLN:HG2	2.00	0.44
50:S2:461:U:H2'	50:S2:462:OMC:H6	1.83	0.44
50:S2:681:PSU:H4'	74:SX:9:THR:HG22	2.00	0.44
50:S2:1804:OMU:H1'	50:S2:1804:OMU:HM23	1.74	0.44
51:SA:198:MET:HG2	51:SA:200:ASP:HB2	2.00	0.44
56:SF:175:ASP:C	56:SF:175:ASP:OD1	2.61	0.44
62:SL:8:ARG:NH1	90:SL:203:HOH:O	2.50	0.44
64:SN:39:LYS:O	64:SN:43:LYS:HG2	2.18	0.44
69:SS:36:VAL:HB	69:SS:40:TYR:HD1	1.82	0.44
82:Sf:119:ARG:N	82:Sf:132:MET:HG3	2.33	0.44
83:Sg:65:PHE:HB2	83:Sg:83:TRP:CG	2.53	0.44
3:L5:175:C:H2'	3:L5:176:G:H8	1.83	0.44
3:L5:1239:C:H5	10:LE:60:SER:HB2	1.83	0.44
3:L5:4392:OMG:H2'	3:L5:4447:5MC:HM51	1.99	0.44
3:L5:4551:U:H2'	3:L5:4552:PSU:C6	2.53	0.44
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.52	0.44
12:LG:210:GLU:CD	12:LG:210:GLU:H	2.25	0.44
23:LS:50:GLN:NE2	90:LS:204:HOH:O	2.47	0.44
28:LX:87:MET:HE2	28:LX:90:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Lo:58:LYS:NZ	90:Lo:305:HOH:O	2.47	0.44
50:S2:99:A2M:HM'3	50:S2:99:A2M:H1'	1.78	0.44
50:S2:349:A:H2'	50:S2:350:C:C6	2.53	0.44
50:S2:634:A:H2'	50:S2:635:G:H8	1.83	0.44
52:SB:180:ASP:O	52:SB:184:VAL:HG13	2.17	0.44
75:SY:117:VAL:O	75:SY:122:LYS:HE3	2.18	0.44
83:Sg:296:GLN:O	83:Sg:312:VAL:HG23	2.17	0.44
3:L5:1569:U:H2'	3:L5:1570:G:C8	2.53	0.43
3:L5:1672:U:H2'	3:L5:1673:U:C6	2.52	0.43
3:L5:2664:G:H4'	3:L5:2677:G:H4'	1.99	0.43
3:L5:2691:U:H2'	3:L5:2692:U:C6	2.53	0.43
3:L5:3933:G:H2'	3:L5:3934:G:C8	2.53	0.43
5:L8:88:A:H2'	5:L8:89:U:O4'	2.18	0.43
6:LA:3:ARG:HG2	6:LA:207:VAL:HG22	2.00	0.43
10:LE:178:PRO:HD2	10:LE:181:LEU:HD12	2.00	0.43
33:Lc:34:THR:HG23	33:Lc:95:ALA:HB2	1.98	0.43
47:Lr:103:ARG:HD2	47:Lr:103:ARG:HA	1.84	0.43
50:S2:1164:G:O2'	50:S2:1165:G:H5'	2.18	0.43
50:S2:1217:A:H2'	50:S2:1218:C:H6	1.82	0.43
53:SC:166:ARG:HH21	72:SV:1:MET:HB2	1.83	0.43
71:SU:20:ILE:HD13	71:SU:20:ILE:HA	1.91	0.43
72:SV:19:ALA:HB2	72:SV:68:SER:OG	2.17	0.43
75:SY:77:ASP:C	75:SY:77:ASP:OD1	2.60	0.43
3:L5:656:C:N3	3:L5:657:C:N4	2.66	0.43
3:L5:2849:A:O2'	3:L5:2855:G:N7	2.41	0.43
3:L5:3932:U:H2'	3:L5:3933:G:H8	1.84	0.43
3:L5:4619:U:H2'	3:L5:4620:OMU:C6	2.47	0.43
4:L7:35:U:O2	4:L7:45:U:O2'	2.31	0.43
10:LE:201:ILE:HG13	10:LE:203:ILE:HG23	1.98	0.43
11:LF:41:MET:HA	11:LF:41:MET:HE3	2.00	0.43
40:Lj:27:TYR:HA	40:Lj:34:CYS:HA	2.00	0.43
50:S2:1387:G:H2'	50:S2:1388:A:O4'	2.18	0.43
50:S2:1457:U:H2'	50:S2:1458:G:C8	2.53	0.43
50:S2:1678:A2M:O2'	50:S2:1679:A:H5'	2.18	0.43
54:SD:127:MET:HG3	54:SD:154:ASP:OD1	2.18	0.43
55:SE:121:TYR:HD1	55:SE:161:GLN:HG3	1.84	0.43
55:SE:184:THR:C	55:SE:189:LEU:HD13	2.43	0.43
60:SJ:111:GLN:OE1	60:SJ:123:ILE:HG12	2.18	0.43
63:SM:36:ARG:HA	63:SM:36:ARG:HD2	1.82	0.43
74:SX:100:VAL:HG12	74:SX:125:VAL:HG22	1.99	0.43
82:Sf:133:ALA:O	82:Sf:139:HIS:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:110:SER:HB2	83:Sg:152:SER:O	2.18	0.43
2:Et:53:G:H2'	2:Et:53:G:N3	2.32	0.43
3:L5:257:C:H2'	3:L5:258:G:H8	1.83	0.43
3:L5:1370:G:O6	8:LC:239:LYS:HE3	2.18	0.43
3:L5:2569:G:H2'	3:L5:2570:U:H6	1.83	0.43
3:L5:3696:C:H2'	3:L5:3697:U:O4'	2.18	0.43
3:L5:4251:A:H2'	3:L5:4252:C:C6	2.53	0.43
3:L5:4306:OMU:H1'	3:L5:4306:OMU:HM23	1.75	0.43
3:L5:4921:C:H2'	3:L5:4922:C:C6	2.53	0.43
13:LH:27:VAL:HG12	13:LH:84:VAL:HG21	1.99	0.43
13:LH:140:GLN:HB3	13:LH:143:GLU:HG3	2.00	0.43
31:La:85:GLN:HA	31:La:88:VAL:HG12	1.99	0.43
36:Lf:106:TYR:HA	36:Lf:107:PRO:C	2.43	0.43
38:Lh:110:LYS:HB2	38:Lh:110:LYS:HE3	1.72	0.43
50:S2:327:G:O2'	50:S2:329:G:H5''	2.18	0.43
50:S2:416:U:H2'	50:S2:417:C:O4'	2.17	0.43
50:S2:929:G:H2'	50:S2:930:C:O4'	2.17	0.43
50:S2:1662:U:O4	50:S2:1663:A:N6	2.51	0.43
67:SQ:128:GLU:HG2	67:SQ:137:ALA:CB	2.47	0.43
75:SY:39:GLU:C	75:SY:39:GLU:OE1	2.61	0.43
78:Sb:80:ARG:HD3	78:Sb:81:ARG:O	2.18	0.43
3:L5:2045:G:O6	3:L5:3870:C:O2'	2.36	0.43
3:L5:3748:A:H5''	6:LA:243:THR:HB	2.01	0.43
3:L5:3893:C:H2'	3:L5:3894:A:H8	1.83	0.43
3:L5:4227:OMU:H1'	3:L5:4227:OMU:HM23	1.78	0.43
3:L5:4459:U:H2'	3:L5:4460:U:H6	1.82	0.43
3:L5:4620:OMU:HM23	3:L5:4620:OMU:H1'	1.79	0.43
3:L5:4919:G:H2'	3:L5:4920:C:H6	1.82	0.43
50:S2:10:G:O2'	53:SC:113:GLN:OE1	2.29	0.43
50:S2:1198:G:H2'	50:S2:1199:A:C8	2.53	0.43
50:S2:1395:C:O2'	50:S2:1396:A:H5'	2.18	0.43
50:S2:1631:U:H5''	69:SS:34:LYS:HG3	2.00	0.43
50:S2:1853:C:O2'	84:S2:1902:PUT:H11	2.18	0.43
54:SD:132:LYS:HB2	54:SD:189:MET:HG3	2.01	0.43
54:SD:133:GLY:HA3	54:SD:156:LEU:O	2.18	0.43
59:SI:174:CYS:HB2	59:SI:190:LEU:HD21	1.99	0.43
65:SO:90:ILE:H	65:SO:90:ILE:HG13	1.67	0.43
68:SR:27:ASP:HB2	83:Sg:17:TRP:HH2	1.84	0.43
76:SZ:50:PHE:CE1	76:SZ:58:LEU:HD21	2.53	0.43
76:SZ:50:PHE:CZ	76:SZ:87:ALA:HB2	2.53	0.43
83:Sg:199:THR:CG2	83:Sg:208:ALA:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:287:THR:N	83:Sg:301:GLY:O	2.29	0.43
3:L5:6:C:H2'	3:L5:7:C:C6	2.54	0.43
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.54	0.43
3:L5:1512:G:H2'	3:L5:1513:U:C6	2.54	0.43
3:L5:1859:C:C4	3:L5:1860:PSU:C2	3.07	0.43
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.53	0.43
3:L5:4770:U:H2'	3:L5:4771:C:C6	2.54	0.43
8:LC:262:GLU:H	8:LC:262:GLU:HG2	1.58	0.43
9:LD:41:LYS:HB2	24:LT:68:THR:O	2.19	0.43
19:LO:89:PRO:O	19:LO:95:GLY:HA3	2.18	0.43
31:La:72:THR:HG22	31:La:110:LYS:HB3	2.00	0.43
32:Lb:116:LEU:HD23	32:Lb:116:LEU:HA	1.83	0.43
46:Lp:38:THR:HA	46:Lp:45:THR:HA	2.01	0.43
50:S2:1195:A:H2'	50:S2:1196:A:C8	2.54	0.43
51:SA:85:ARG:HD3	51:SA:203:PHE:O	2.17	0.43
51:SA:205:ARG:HH21	51:SA:210:ILE:HA	1.84	0.43
67:SQ:24:HIS:O	67:SQ:68:ILE:HA	2.18	0.43
3:L5:1650:A:OP2	85:L5:5112:SPD:H52	2.18	0.43
3:L5:3723:A2M:HM'3	3:L5:3723:A2M:H1'	1.71	0.43
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.53	0.43
3:L5:4684:A:H2'	3:L5:4685:U:O4'	2.19	0.43
7:LB:113:GLU:OE2	7:LB:169:ARG:N	2.45	0.43
9:LD:164:LYS:HA	9:LD:167:VAL:HG22	2.00	0.43
14:LI:206:LEU:HD12	14:LI:209:TRP:HB3	1.99	0.43
19:LO:4:VAL:HG22	19:LO:31:ARG:NH2	2.33	0.43
20:LP:3:ARG:HG2	20:LP:3:ARG:HH11	1.83	0.43
25:LU:42:PHE:CG	25:LU:90:TYR:HD2	2.37	0.43
47:Lr:93:ILE:O	47:Lr:97:ILE:HD12	2.18	0.43
50:S2:1148:A:H4'	50:S2:1149:A:O4'	2.18	0.43
50:S2:1456:G:H2'	50:S2:1457:U:H6	1.83	0.43
50:S2:1841:C:H2'	50:S2:1842:4AC:H6	1.99	0.43
53:SC:77:SER:OG	53:SC:78:LEU:N	2.52	0.43
53:SC:121:ARG:HG3	53:SC:121:ARG:O	2.17	0.43
55:SE:94:LYS:NZ	75:SY:19:GLN:HE21	2.17	0.43
68:SR:77:GLU:OE1	68:SR:81:ARG:NH1	2.49	0.43
69:SS:12:ILE:C	69:SS:13:LEU:HD12	2.43	0.43
69:SS:84:LEU:HD12	69:SS:95:TYR:HB3	2.01	0.43
78:Sb:19:HIS:HD2	78:Sb:21:LYS:H	1.67	0.43
82:Sf:119:ARG:H	82:Sf:132:MET:HG3	1.82	0.43
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.84	0.43
3:L5:3883:U:H2'	3:L5:3884:PSU:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4254:G:H2'	3:L5:4254:G:N3	2.33	0.43
3:L5:4345:C:H2'	3:L5:4346:U:H6	1.83	0.43
4:L7:2:U:H2'	4:L7:3:C:C6	2.54	0.43
5:L8:148:A:H2'	5:L8:149:G:C8	2.53	0.43
50:S2:374:G:H2'	50:S2:375:U:C6	2.53	0.43
50:S2:985:G:O4'	65:SO:138:ASP:OD1	2.37	0.43
50:S2:1017:U:H5'	64:SN:55:ARG:HD3	2.01	0.43
50:S2:1292:C:C2	50:S2:1293:A:C8	3.07	0.43
50:S2:1688:C:H2'	50:S2:1689:C:H6	1.83	0.43
51:SA:118:GLU:HB2	53:SC:65:LYS:HD3	1.99	0.43
53:SC:184:VAL:HG23	53:SC:195:LEU:HB2	2.01	0.43
55:SE:19:MET:HE3	55:SE:19:MET:HB2	1.91	0.43
60:SJ:81:LEU:HD22	60:SJ:86:VAL:HG11	2.00	0.43
65:SO:84:ARG:HH21	65:SO:88:LEU:HD23	1.84	0.43
3:L5:699:C:H2'	3:L5:700:G:C8	2.51	0.43
3:L5:1751:A:H1'	14:LI:193:ASP:OD2	2.19	0.43
3:L5:2306:G:H1'	3:L5:2332:A:N6	2.33	0.43
3:L5:2485:U:H2'	3:L5:2486:G:C8	2.54	0.43
3:L5:2539:C:H2'	3:L5:2540:C:H6	1.81	0.43
3:L5:3770:PSU:H2'	3:L5:3771:C:C6	2.54	0.43
3:L5:4174:U:H2'	3:L5:4175:G:C8	2.52	0.43
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.18	0.43
7:LB:378:ARG:HD3	27:LW:11:TYR:CD2	2.53	0.43
30:LZ:95:VAL:HG12	30:LZ:110:ALA:HA	2.00	0.43
50:S2:342:C:C2	50:S2:343:A:C8	3.07	0.43
50:S2:1134:G:H2'	50:S2:1135:C:H6	1.83	0.43
63:SM:86:GLY:O	63:SM:89:VAL:HG12	2.19	0.43
73:SW:25:VAL:HB	73:SW:65:LEU:HD11	2.01	0.43
73:SW:111:MET:HE1	73:SW:119:LYS:HD3	2.00	0.43
75:SY:15:ASN:HD21	75:SY:18:LEU:HD23	1.83	0.43
83:Sg:172:LYS:HG2	83:Sg:193:GLY:C	2.43	0.43
3:L5:267:G:H2'	3:L5:268:G:H8	1.82	0.43
3:L5:984:C:H2'	3:L5:985:C:H6	1.84	0.43
3:L5:1098:G:H2'	3:L5:1099:C:H6	1.81	0.43
3:L5:1617:G:H1'	3:L5:2513:A:H61	1.83	0.43
3:L5:1858:A:H2'	3:L5:1859:C:H6	1.84	0.43
3:L5:3934:G:H2'	3:L5:3935:C:C6	2.54	0.43
5:L8:142:U:H2'	5:L8:143:G:O4'	2.19	0.43
15:LJ:163:MET:HG2	15:LJ:174:ILE:HG21	2.00	0.43
37:Lg:41:ALA:O	37:Lg:52:ARG:HD3	2.18	0.43
38:Lh:15:GLU:OE2	38:Lh:15:GLU:N	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:1643:PSU:H2'	50:S2:1644:C:C6	2.54	0.43
54:SD:163:PRO:O	54:SD:167:TYR:HB2	2.19	0.43
55:SE:102:ILE:HG21	55:SE:239:PRO:HD3	2.00	0.43
59:SI:144:LYS:HD2	59:SI:144:LYS:HA	1.69	0.43
67:SQ:102:GLU:CD	67:SQ:102:GLU:H	2.27	0.43
68:SR:84:TYR:CD2	68:SR:85:VAL:N	2.87	0.43
76:SZ:50:PHE:HZ	76:SZ:87:ALA:HB2	1.84	0.43
79:Sc:14:VAL:HG13	79:Sc:30:VAL:HB	2.00	0.43
1:At:7:U:H3'	1:At:8:U:H5'	2.00	0.43
3:L5:1689:G:N7	84:L5:5102:PUT:H42	2.33	0.43
3:L5:4743:G:H2'	3:L5:4744:A:H8	1.83	0.43
7:LB:394:LYS:O	7:LB:397:ILE:HG13	2.18	0.43
9:LD:83:LEU:N	9:LD:84:PRO:HD2	2.34	0.43
32:Lb:53:GLY:O	32:Lb:57:MET:HG3	2.19	0.43
34:Ld:24:GLU:HG2	34:Ld:87:ARG:HD3	2.01	0.43
50:S2:53:C:O2'	50:S2:507:G:N7	2.40	0.43
50:S2:158:A:H2'	50:S2:159:A2M:C8	2.49	0.43
50:S2:1404:U:C5	71:SU:88:LEU:HD21	2.54	0.43
50:S2:1716:C:H2'	50:S2:1717:C:H6	1.84	0.43
53:SC:167:ARG:O	72:SV:1:MET:HE1	2.19	0.43
53:SC:209:VAL:HB	53:SC:210:PRO:HD3	1.99	0.43
55:SE:128:LYS:HB3	55:SE:140:VAL:CG1	2.49	0.43
55:SE:233:LYS:HD3	55:SE:233:LYS:HA	1.78	0.43
56:SF:86:LYS:HA	56:SF:89:THR:OG1	2.18	0.43
65:SO:136:PRO:HD2	65:SO:136:PRO:O	2.18	0.43
66:SP:75:VAL:HG12	66:SP:93:MET:HB2	2.00	0.43
71:SU:42:GLY:O	71:SU:45:GLU:HG3	2.18	0.43
77:Sa:60:ASP:C	77:Sa:60:ASP:OD1	2.61	0.43
79:Sc:9:ILE:HG13	79:Sc:59:LEU:HD12	2.00	0.43
3:L5:129:C:H2'	3:L5:130:C:C6	2.54	0.42
3:L5:170:C:HO2'	3:L5:171:U:P	2.41	0.42
3:L5:952:G:H2'	3:L5:953:C:C6	2.54	0.42
3:L5:1266:G:OP1	32:Lb:95:ARG:HD2	2.19	0.42
3:L5:1371:A:N1	5:L8:28:C:O2'	2.52	0.42
3:L5:1392:A:H2'	3:L5:1393:G:C8	2.54	0.42
3:L5:2704:C:H2'	3:L5:2705:G:O4'	2.19	0.42
3:L5:2758:G:O2'	3:L5:2765:A:N3	2.47	0.42
3:L5:4138:C:H2'	3:L5:4139:G:C8	2.54	0.42
3:L5:4734:A:H2'	3:L5:4735:G:H8	1.78	0.42
6:LA:142:GLU:CD	6:LA:142:GLU:H	2.27	0.42
9:LD:237:GLU:OE1	9:LD:241:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LQ:3:VAL:HG12	21:LQ:5:ILE:HG23	2.00	0.42
50:S2:334:C:H2'	50:S2:335:G:O4'	2.19	0.42
50:S2:1043:G:H2'	50:S2:1044:G:O4'	2.19	0.42
50:S2:1099:G:H22	50:S2:1133:A:H2	1.66	0.42
50:S2:1181:A:H2'	50:S2:1182:A:C8	2.54	0.42
52:SB:44:ILE:HD11	52:SB:86:LEU:HD12	2.01	0.42
64:SN:32:ASP:OD2	64:SN:32:ASP:N	2.50	0.42
64:SN:34:LYS:HE3	64:SN:67:THR:HB	2.00	0.42
67:SQ:8:GLN:HB3	67:SQ:99:TYR:CE2	2.54	0.42
83:Sg:139:LYS:HB2	83:Sg:139:LYS:HE2	1.79	0.42
3:L5:1292:C:H2'	3:L5:1293:G:N3	2.34	0.42
3:L5:2758:G:H1'	3:L5:2766:A:H1'	2.01	0.42
3:L5:2898:G:H2'	3:L5:2899:C:C6	2.54	0.42
3:L5:4345:C:H2'	3:L5:4346:U:C6	2.54	0.42
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.85	0.42
3:L5:4917:C:H2'	3:L5:4918:C:C6	2.53	0.42
14:LI:179:ASP:C	14:LI:179:ASP:OD2	2.62	0.42
39:Li:99:LYS:HD3	39:Li:99:LYS:HA	1.69	0.42
41:Lk:30:ASP:OD2	41:Lk:30:ASP:N	2.50	0.42
50:S2:151:C:OP1	75:SY:120:THR:HG23	2.18	0.42
56:SF:167:LYS:HG3	56:SF:171:GLU:OE2	2.19	0.42
66:SP:85:ILE:HA	66:SP:89:MET:HE3	2.01	0.42
69:SS:76:GLN:OE1	69:SS:76:GLN:N	2.35	0.42
83:Sg:40:ILE:HD11	83:Sg:66:VAL:HG11	2.00	0.42
83:Sg:170:TRP:HA	83:Sg:194:TYR:HB2	2.01	0.42
3:L5:425:U:H2'	3:L5:426:A:H8	1.83	0.42
3:L5:655:C:H2'	3:L5:656:C:C6	2.54	0.42
3:L5:732:A:H2'	3:L5:733:A:O4'	2.19	0.42
3:L5:733:A:H2'	3:L5:734:G:O4'	2.19	0.42
3:L5:1440:U:H2'	3:L5:1441:C:C6	2.54	0.42
3:L5:2096:G:N2	8:LC:304:ALA:HB1	2.34	0.42
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.83	0.42
7:LB:113:GLU:HG2	7:LB:178:ALA:HB2	2.02	0.42
12:LG:27:VAL:N	90:LG:306:HOH:O	2.52	0.42
25:LU:45:GLU:HA	25:LU:54:GLY:HA2	2.01	0.42
32:Lb:103:LYS:HA	32:Lb:106:LYS:HE3	2.01	0.42
37:Lg:44:SER:HB2	37:Lg:53:LEU:HD21	2.02	0.42
50:S2:1190:A:H2'	50:S2:1191:C:O4'	2.20	0.42
50:S2:1254:C:H4'	71:SU:75:LYS:HE2	2.01	0.42
50:S2:1380:C:H2'	50:S2:1381:G:O4'	2.19	0.42
50:S2:1511:U:H2'	50:S2:1512:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SK:16:PHE:CE1	61:SK:91:PRO:HD3	2.54	0.42
69:SS:62:ASP:OD1	69:SS:63:GLU:N	2.52	0.42
75:SY:53:ASP:OD2	75:SY:54:VAL:HG13	2.19	0.42
81:Se:95:LYS:H	81:Se:95:LYS:HG2	1.60	0.42
83:Sg:175:LYS:HB3	83:Sg:184:LEU:HD11	2.01	0.42
2:Et:32:C:H2'	2:Et:33:C:C6	2.54	0.42
3:L5:258:G:H2'	3:L5:259:C:C6	2.54	0.42
3:L5:1396:G:O2'	3:L5:1468:C:O2'	2.36	0.42
3:L5:1702:C:H4'	8:LC:308:LYS:HD2	2.02	0.42
3:L5:1779:PSU:H2'	3:L5:1780:A:C8	2.55	0.42
3:L5:1907:A:H2'	3:L5:1908:A:C8	2.54	0.42
3:L5:2485:U:H2'	3:L5:2486:G:H8	1.84	0.42
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.19	0.42
3:L5:4968:A:H2'	3:L5:4969:C:H6	1.83	0.42
5:L8:140:C:H2'	5:L8:141:C:H6	1.84	0.42
7:LB:50:LYS:HB2	7:LB:345:LEU:HD11	2.02	0.42
13:LH:51:LYS:HD3	13:LH:52:LYS:N	2.32	0.42
16:LL:7:GLY:O	31:La:49:HIS:NE2	2.50	0.42
22:LR:144:LYS:HB3	22:LR:144:LYS:HE2	1.91	0.42
28:LX:88:LYS:HE2	28:LX:88:LYS:HB2	1.85	0.42
32:Lb:25:ARG:HD2	32:Lb:25:ARG:HA	1.80	0.42
38:Lh:107:GLN:O	38:Lh:111:GLU:HG3	2.20	0.42
45:Lo:90[B]:HIS:NE2	45:Lo:92:GLU:HG2	2.34	0.42
47:Lr:54:ALA:HA	47:Lr:61:VAL:HG23	2.01	0.42
50:S2:526:A:P	81:Se:109:ARG:HH21	2.42	0.42
50:S2:849:A:H2'	50:S2:850:C:H6	1.85	0.42
50:S2:917:U:H2'	50:S2:918:PSU:C6	2.55	0.42
50:S2:1236:G:H2'	50:S2:1237:C:C6	2.54	0.42
50:S2:1688:C:H2'	50:S2:1689:C:C6	2.54	0.42
51:SA:128:ARG:NH2	51:SA:151:ASP:O	2.53	0.42
55:SE:68:ARG:HB3	55:SE:76:VAL:HG11	2.01	0.42
62:SL:128:VAL:HG12	62:SL:142:VAL:HA	2.00	0.42
66:SP:14:LYS:HD3	66:SP:14:LYS:N	2.34	0.42
68:SR:7:LYS:HD3	68:SR:7:LYS:HA	1.76	0.42
69:SS:4:VAL:HA	76:SZ:50:PHE:O	2.19	0.42
74:SX:46:HIS:CD2	74:SX:103:ALA:HB2	2.55	0.42
83:Sg:51:ASN:C	83:Sg:51:ASN:OD1	2.62	0.42
83:Sg:121:VAL:HG23	83:Sg:131:LEU:HD23	2.00	0.42
3:L5:457:G:H2'	3:L5:458:C:H6	1.84	0.42
3:L5:984:C:H2'	3:L5:985:C:C6	2.54	0.42
3:L5:1064:G:H2'	3:L5:1065:G:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1479:G:H2'	3:L5:1480:C:C6	2.54	0.42
3:L5:3621:A:C8	3:L5:4642:U:H1'	2.55	0.42
3:L5:3664:G:H2'	3:L5:3665:G:C8	2.52	0.42
3:L5:3782:5MC:OP1	44:Ln:23:ARG:NH2	2.46	0.42
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.84	0.42
10:LE:244:GLU:OE1	10:LE:244:GLU:N	2.47	0.42
50:S2:376:A:H2'	50:S2:377:G:O4'	2.19	0.42
50:S2:464:A:H3'	50:S2:465:A:H8	1.83	0.42
50:S2:801:PSU:H2'	50:S2:802:A:C8	2.52	0.42
50:S2:1293:A:H2'	50:S2:1294:G:H8	1.83	0.42
50:S2:1513:C:P	80:Sd:12:ARG:HH22	2.42	0.42
50:S2:1666:C:H2'	50:S2:1667:U:C6	2.54	0.42
51:SA:128:ARG:NH2	51:SA:151:ASP:OD1	2.52	0.42
51:SA:178:LEU:HD12	51:SA:178:LEU:HA	1.90	0.42
53:SC:275:LYS:HG2	53:SC:276:THR:HG23	2.00	0.42
54:SD:16:ILE:HD11	80:Sd:36:LEU:HD23	2.01	0.42
54:SD:214:LYS:HD2	54:SD:214:LYS:HA	1.87	0.42
56:SF:68:ILE:HD12	56:SF:68:ILE:HA	1.82	0.42
58:SH:69:LEU:O	58:SH:73:GLN:HG3	2.19	0.42
65:SO:116:LEU:HG	77:Sa:53:ILE:HD11	2.02	0.42
67:SQ:51:LEU:O	67:SQ:54:PRO:HD2	2.19	0.42
70:ST:28:LEU:HD21	70:ST:53:PHE:CD2	2.55	0.42
71:SU:20:ILE:HB	71:SU:91:LEU:O	2.20	0.42
3:L5:179:G:H2'	3:L5:180:C:C6	2.55	0.42
3:L5:469:C:N3	10:LE:105:ARG:NH2	2.55	0.42
3:L5:672:C:H2'	3:L5:673:C:C6	2.55	0.42
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.84	0.42
3:L5:2089:G:OP2	8:LC:294:LYS:HD3	2.19	0.42
3:L5:2461:G:H5'	18:LN:104:GLU:OE2	2.19	0.42
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.55	0.42
3:L5:2572:C:O2'	30:LZ:112:ARG:NH2	2.52	0.42
3:L5:3724:A2M:H1'	3:L5:3724:A2M:HM'3	1.74	0.42
3:L5:4460:U:H2'	3:L5:4461:C:C6	2.55	0.42
15:LJ:120:ASP:HB3	15:LJ:123:ILE:HG23	2.02	0.42
19:LO:142:ALA:HA	19:LO:145:VAL:HG22	2.02	0.42
50:S2:601:OMG:HM23	50:S2:601:OMG:H1'	1.66	0.42
50:S2:624:C:H6	50:S2:624:C:H5''	1.84	0.42
50:S2:940:U:H2'	50:S2:941:C:C6	2.54	0.42
54:SD:8:LYS:HG2	71:SU:61:LEU:HD21	2.01	0.42
57:SG:201:LYS:HE3	57:SG:201:LYS:HB3	1.83	0.42
59:SI:141:ARG:CB	59:SI:145:ILE:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SQ:101:ASP:OD2	67:SQ:102:GLU:N	2.52	0.42
3:L5:655:C:H5'	8:LC:269:LYS:HD2	2.01	0.42
3:L5:674:G:H2'	3:L5:675:C:C6	2.54	0.42
3:L5:2389:A:H4'	34:Ld:70:LYS:HD2	2.02	0.42
3:L5:4071:U:H2'	3:L5:4072:C:C6	2.54	0.42
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.83	0.42
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.78	0.42
8:LC:316:LYS:HB2	8:LC:324:ILE:HG13	2.02	0.42
11:LF:67:THR:O	11:LF:71:MET:HG2	2.19	0.42
15:LJ:44:THR:HG21	15:LJ:72:CYS:SG	2.59	0.42
19:LO:78:ARG:HD2	19:LO:78:ARG:HA	1.73	0.42
19:LO:88:LEU:HD12	19:LO:99:LEU:HD13	2.02	0.42
20:LP:126:ARG:HB2	20:LP:140:MET:HE1	2.02	0.42
21:LQ:177:ALA:C	31:La:51:GLY:HA2	2.44	0.42
30:LZ:11:VAL:HG12	30:LZ:82:PRO:HA	2.02	0.42
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.54	0.42
50:S2:1070:A:H2'	50:S2:1071:G:O4'	2.20	0.42
50:S2:1474:A:H2'	50:S2:1475:G:C8	2.55	0.42
50:S2:1580:A:O2'	50:S2:1581:C:H5'	2.20	0.42
55:SE:95:THR:O	55:SE:97:GLU:HG2	2.19	0.42
60:SJ:100:LEU:HD23	60:SJ:105:PHE:HE1	1.85	0.42
62:SL:45:LYS:HD2	62:SL:45:LYS:HA	1.73	0.42
63:SM:19:GLN:O	63:SM:23:LYS:HD3	2.19	0.42
67:SQ:38:PRO:HG2	67:SQ:41:MET:HG3	2.00	0.42
67:SQ:48:GLN:O	67:SQ:52:LEU:HD12	2.19	0.42
67:SQ:125:ARG:O	67:SQ:126:ARG:HD3	2.19	0.42
74:SX:48:LYS:HD3	74:SX:99:GLU:OE1	2.19	0.42
80:Sd:30:LEU:HD23	80:Sd:30:LEU:HA	1.89	0.42
83:Sg:52:TYR:CE1	83:Sg:309:VAL:HG11	2.55	0.42
3:L5:457:G:H2'	3:L5:458:C:C6	2.54	0.42
3:L5:487:G:H2'	3:L5:488:G:O4'	2.19	0.42
3:L5:1302:U:H3'	3:L5:1303:A:H5'	2.02	0.42
3:L5:2417:A:C4	3:L5:2418:A:C8	3.07	0.42
3:L5:2467:U:H4'	3:L5:2468:U:H5'	2.02	0.42
3:L5:2613:C:H4'	37:Lg:2:VAL:HG21	2.01	0.42
3:L5:2894:A:H2'	3:L5:2895:A:C8	2.55	0.42
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.19	0.42
3:L5:4456:OMC:H1'	3:L5:4456:OMC:HM23	1.83	0.42
14:LI:38:ARG:HG2	14:LI:41:ALA:HB2	2.01	0.42
16:LL:136:LYS:C	16:LL:138:ASP:H	2.28	0.42
30:LZ:48:ARG:HB3	30:LZ:69:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lh:52:LYS:HA	38:Lh:52:LYS:HD3	1.87	0.42
50:S2:92:A:H4'	50:S2:93:PSU:OP2	2.20	0.42
50:S2:1134:G:H2'	50:S2:1135:C:C6	2.55	0.42
50:S2:1383:A2M:HM'3	50:S2:1383:A2M:H1'	1.88	0.42
50:S2:1661:A:C8	80:Sd:14:PHE:HB2	2.55	0.42
50:S2:1788:A:H2'	50:S2:1789:G:O4'	2.19	0.42
59:SI:21:TYR:CZ	59:SI:22:HIS:HD2	2.38	0.42
62:SL:47:PRO:O	62:SL:51:ILE:HG12	2.20	0.42
64:SN:119:GLU:OE2	64:SN:141:TYR:OH	2.30	0.42
65:SO:97:LEU:O	65:SO:131:ASP:HA	2.19	0.42
66:SP:116:LEU:HD12	66:SP:116:LEU:HA	1.85	0.42
70:ST:39:LEU:HG	70:ST:47:PRO:HG3	2.02	0.42
71:SU:32:LEU:HD21	71:SU:87:ARG:HG2	2.02	0.42
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.54	0.42
3:L5:2633:U:H2'	3:L5:2634:C:H6	1.85	0.42
3:L5:3718:A2M:H2	3:L5:3934:G:C1'	2.50	0.42
3:L5:4120:U:C4	37:Lg:97:ILE:HG12	2.54	0.42
3:L5:4439:U:H2'	3:L5:4440:G:O4'	2.19	0.42
4:L7:23:A:H2'	4:L7:24:C:C6	2.55	0.42
5:L8:5:U:H2'	5:L8:6:C:H6	1.85	0.42
7:LB:74:GLU:OE1	7:LB:285:TYR:OH	2.28	0.42
18:LN:151:ILE:HD12	18:LN:151:ILE:HA	1.87	0.42
22:LR:162:ARG:NH2	50:S2:873:G:C6	2.87	0.42
38:Lh:4:ILE:HG22	38:Lh:56:ARG:HD2	2.02	0.42
50:S2:81:U:H2'	50:S2:82:G:O4'	2.20	0.42
50:S2:176:U:H2'	50:S2:177:G:C8	2.54	0.42
50:S2:666:U:H2'	50:S2:667:U:C6	2.55	0.42
50:S2:1016:U:H5''	64:SN:14:SER:HB3	2.02	0.42
50:S2:1308:U:H2'	50:S2:1309:C:H6	1.85	0.42
50:S2:1454:A:C2	50:S2:1476:A:H1'	2.55	0.42
51:SA:30:LEU:HD11	51:SA:35:GLU:HA	2.02	0.42
69:SS:55:ARG:HB2	69:SS:58:GLU:OE2	2.20	0.42
74:SX:130:LEU:HD23	74:SX:130:LEU:HA	1.90	0.42
75:SY:21:LYS:HD2	75:SY:75:ILE:HD11	2.02	0.42
3:L5:919:C:H2'	3:L5:920:C:H6	1.85	0.42
3:L5:988:C:H2'	3:L5:989:U:C6	2.55	0.42
3:L5:1811:G:H4'	32:Lb:60:ASN:OD1	2.20	0.42
3:L5:2640:G:H2'	3:L5:2641:A:H8	1.84	0.42
5:L8:27:U:H2'	5:L8:28:C:C6	2.55	0.42
5:L8:90:C:H2'	5:L8:91:A:C8	2.54	0.42
7:LB:258:HIS:HA	7:LB:259:PRO:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:380:G:P	59:SI:56:ARG:HH22	2.39	0.42
50:S2:1388:A:C2	54:SD:205:PRO:HG2	2.55	0.42
50:S2:1409:A:H2'	50:S2:1410:C:C6	2.55	0.42
50:S2:1500:G:H2'	50:S2:1501:C:H6	1.85	0.42
50:S2:1725:U:H2'	50:S2:1726:G:H8	1.83	0.42
53:SC:130:ILE:HG22	53:SC:158:ALA:HB1	2.02	0.42
59:SI:57:ALA:HB2	59:SI:183:GLY:HA2	2.02	0.42
59:SI:145:ILE:HD12	59:SI:146:GLN:N	2.35	0.42
62:SL:20:LYS:HE2	62:SL:20:LYS:HB3	1.80	0.42
68:SR:105:MET:HE3	68:SR:105:MET:HB3	1.94	0.42
71:SU:31:SER:O	71:SU:35:VAL:HG23	2.20	0.42
83:Sg:135:LEU:HD23	83:Sg:135:LEU:HA	1.89	0.42
2:Et:49:G:H2'	2:Et:50:A:C8	2.55	0.41
3:L5:247:G:H2'	3:L5:248:C:H6	1.84	0.41
3:L5:1535:C:H2'	3:L5:1536:PSU:O4'	2.20	0.41
3:L5:2094:G:N2	3:L5:2095:A:H2'	2.35	0.41
3:L5:2685:C:H2'	3:L5:2686:G:O4'	2.19	0.41
3:L5:3903:A:H2'	3:L5:3904:G:O4'	2.20	0.41
3:L5:4635:A:O2'	3:L5:4637:OMG:OP1	2.38	0.41
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.20	0.41
5:L8:154:G:H2'	5:L8:155:C:C6	2.55	0.41
43:Lm:94:MET:HG2	43:Lm:105:PRO:HA	2.00	0.41
50:S2:190:G:H1'	50:S2:209:A:H61	1.84	0.41
50:S2:1052:A:H2'	50:S2:1053:C:O4'	2.19	0.41
50:S2:1597:C:H4'	50:S2:1603:G:O6	2.20	0.41
51:SA:148:CYS:HB3	51:SA:152:SER:OG	2.20	0.41
59:SI:157:LYS:HE3	59:SI:157:LYS:HB3	1.88	0.41
63:SM:33:ARG:HD3	63:SM:89:VAL:HG21	2.02	0.41
67:SQ:106:LYS:HE2	67:SQ:106:LYS:HB2	1.74	0.41
83:Sg:20:GLN:HA	83:Sg:288:SER:OG	2.19	0.41
83:Sg:226:HIS:NE2	83:Sg:229:THR:OG1	2.51	0.41
3:L5:63:G:OP1	18:LN:169:ARG:NH2	2.53	0.41
3:L5:295:A:H5'	45:Lo:43[B]:ARG:HH21	1.85	0.41
3:L5:1789:C:H2'	3:L5:1790:U:C6	2.55	0.41
3:L5:2079:G:H2'	3:L5:2080:U:H6	1.85	0.41
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.85	0.41
3:L5:4563:U:C2	3:L5:4564:A:C8	3.07	0.41
9:LD:200:MET:HE3	9:LD:241:LYS:HE3	2.03	0.41
10:LE:119:GLU:OE2	35:Le:93:LYS:HB2	2.19	0.41
17:LM:36:ALA:HB2	17:LM:52:PHE:CE1	2.55	0.41
50:S2:86:C:O2'	50:S2:171:A:N1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:432:G:H2'	50:S2:433:A:C8	2.55	0.41
50:S2:634:A:H2'	50:S2:635:G:C8	2.55	0.41
50:S2:867:OMG:H1'	50:S2:867:OMG:HM23	1.58	0.41
50:S2:1414:A:H2'	50:S2:1415:C:C6	2.55	0.41
50:S2:1422:G:C2	50:S2:1424:G:C5	3.07	0.41
54:SD:140:GLY:O	54:SD:142:LEU:HD12	2.20	0.41
56:SF:49:LEU:HD23	56:SF:49:LEU:HA	1.93	0.41
56:SF:123:GLU:OE2	79:Sc:59:LEU:HB2	2.21	0.41
57:SG:20:ASP:OD1	57:SG:23:LYS:HG3	2.20	0.41
59:SI:172:LEU:HD23	59:SI:172:LEU:HA	1.91	0.41
83:Sg:204:GLY:C	83:Sg:206:LEU:H	2.28	0.41
3:L5:219:G:O6	8:LC:181:LYS:NZ	2.35	0.41
3:L5:364:G:O6	40:Lj:55:ARG:NH2	2.51	0.41
3:L5:680:G:H2'	3:L5:681:G:H8	1.85	0.41
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.55	0.41
3:L5:4208:U:P	24:LT:6:GLY:HA3	2.60	0.41
3:L5:4488:A:H4'	3:L5:4489:G:C8	2.54	0.41
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.55	0.41
3:L5:4772:C:H2'	3:L5:4773:C:H6	1.84	0.41
8:LC:266:THR:O	8:LC:267:TRP:HB2	2.19	0.41
50:S2:445:A:N7	84:S2:1901:PUT:N1	2.68	0.41
50:S2:472:C:O2'	50:S2:474:G:OP1	2.28	0.41
50:S2:523:A:P	60:SJ:127:ARG:HH21	2.43	0.41
50:S2:606:G:H1'	81:Se:132:ASN:HD21	1.84	0.41
50:S2:943:U:H2'	50:S2:944:A:H8	1.85	0.41
51:SA:183:LEU:HD23	51:SA:183:LEU:HA	1.87	0.41
52:SB:131:ASP:HB2	52:SB:180:ASP:HB2	2.03	0.41
54:SD:192:TRP:CZ3	54:SD:194:PRO:HD3	2.55	0.41
58:SH:61:ILE:HD11	58:SH:176:VAL:HG22	2.03	0.41
61:SK:12:TYR:CE1	61:SK:52:LEU:HD11	2.56	0.41
75:SY:55:ILE:HG12	75:SY:75:ILE:HG22	2.03	0.41
78:Sb:11:SER:O	78:Sb:14:GLU:HG2	2.20	0.41
2:Et:69:U:H2'	2:Et:70:G:C8	2.55	0.41
3:L5:447:C:H2'	3:L5:448:G:H8	1.86	0.41
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.84	0.41
3:L5:3807:A:H2'	3:L5:3808:OMC:H6	1.86	0.41
3:L5:4188:U:H2'	3:L5:4189:U:H6	1.86	0.41
3:L5:4263:C:H2'	3:L5:4264:G:O4'	2.19	0.41
3:L5:4406:U:C2	3:L5:4407:G:C8	3.07	0.41
3:L5:4538:G:H2'	3:L5:4539:U:H6	1.82	0.41
11:LF:148:LYS:O	11:LF:152:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LH:41:ILE:HG22	13:LH:43:VAL:HG13	2.02	0.41
15:LJ:20:LEU:HD13	15:LJ:132:VAL:HG22	2.03	0.41
17:LM:104:MET:SD	19:LO:199:HIS:HB3	2.61	0.41
24:LT:83:LYS:HG3	24:LT:85:LEU:CD1	2.50	0.41
33:Lc:20:LEU:HD23	33:Lc:20:LEU:HA	1.86	0.41
47:Lr:90:LEU:HD22	47:Lr:111:ILE:HG23	2.01	0.41
50:S2:31:U:OP1	74:SX:137:LYS:NZ	2.53	0.41
50:S2:461:U:H2'	50:S2:462:OMC:C6	2.55	0.41
50:S2:946:U:C2	50:S2:947:G:C8	3.08	0.41
50:S2:1328:OMG:H1'	50:S2:1328:OMG:HM23	1.84	0.41
50:S2:1377:U:H3'	51:SA:102:ARG:HH22	1.84	0.41
50:S2:1500:G:H2'	50:S2:1501:C:C6	2.56	0.41
52:SB:23:ASP:HA	52:SB:24:PRO:HD2	1.98	0.41
53:SC:132:ASP:CG	53:SC:136:HIS:HB2	2.45	0.41
70:ST:129:ARG:HD3	70:ST:133:ARG:NH2	2.36	0.41
83:Sg:138:CYS:SG	83:Sg:141:THR:OG1	2.75	0.41
3:L5:123:C:H2'	3:L5:124:C:H6	1.85	0.41
3:L5:919:C:H2'	3:L5:920:C:C6	2.56	0.41
3:L5:2293:U:H2'	3:L5:2294:G:H8	1.86	0.41
3:L5:2859:G:H2'	3:L5:2860:C:H6	1.85	0.41
3:L5:3713:U:H2'	3:L5:3714:G:H8	1.86	0.41
3:L5:4772:C:H2'	3:L5:4773:C:C6	2.56	0.41
7:LB:194:LEU:HD13	7:LB:194:LEU:HA	1.85	0.41
8:LC:266:THR:C	8:LC:268:ARG:H	2.29	0.41
41:Lk:9:LYS:HG3	41:Lk:10:ASP:H	1.86	0.41
50:S2:180:G:H2'	50:S2:181:A:C8	2.55	0.41
64:SN:145:THR:O	64:SN:149:LEU:HG	2.19	0.41
72:SV:30:ALA:O	72:SV:60:ARG:HD3	2.20	0.41
82:Sf:103:LEU:C	82:Sf:104:LYS:HD2	2.45	0.41
83:Sg:17:TRP:CD2	83:Sg:303:THR:HG22	2.55	0.41
3:L5:179:G:C2	3:L5:180:C:C4	3.09	0.41
3:L5:272:U:H2'	3:L5:273:U:H6	1.82	0.41
3:L5:922:C:H2'	3:L5:923:C:C6	2.56	0.41
3:L5:2728:U:H2'	3:L5:2729:C:C6	2.55	0.41
3:L5:3799:A:N3	3:L5:4506:C:O2'	2.47	0.41
5:L8:82:A:H5''	38:Lh:3:LYS:HE2	2.02	0.41
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	2.02	0.41
13:LH:93:ARG:HD2	13:LH:143:GLU:HG2	2.01	0.41
47:Lr:52:GLU:HG2	47:Lr:61:VAL:HB	2.02	0.41
50:S2:338:G:H2'	50:S2:339:A:H8	1.85	0.41
52:SB:231:LEU:HA	52:SB:231:LEU:HD23	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SE:11:ARG:HA	55:SE:28:ALA:HB2	2.02	0.41
55:SE:44:LEU:HD23	55:SE:44:LEU:HA	1.81	0.41
55:SE:242:LYS:N	55:SE:242:LYS:HD2	2.36	0.41
56:SF:32:ASP:HB3	56:SF:117:ILE:HD11	2.02	0.41
66:SP:18:ARG:NH1	69:SS:88:LYS:HD2	2.35	0.41
67:SQ:82:TYR:HA	67:SQ:85:ARG:HD3	2.02	0.41
69:SS:47:LYS:HD3	69:SS:47:LYS:HA	1.81	0.41
72:SV:51:LYS:HD3	72:SV:76:ASP:OD2	2.20	0.41
75:SY:97:TYR:HE1	75:SY:99:LYS:HB2	1.85	0.41
3:L5:113:A:H2'	3:L5:114:G:O4'	2.21	0.41
3:L5:4940:C:OP1	10:LE:187:ARG:NH2	2.53	0.41
5:L8:64:U:C2	5:L8:65:A:C8	3.08	0.41
8:LC:211:TYR:OH	8:LC:218:ILE:HD11	2.21	0.41
12:LG:255:LYS:HE2	12:LG:255:LYS:HB2	1.82	0.41
14:LI:212:LEU:HD12	14:LI:212:LEU:HA	1.66	0.41
15:LJ:16:ARG:HD3	15:LJ:137:PRO:HD3	2.01	0.41
41:Lk:7:GLU:HB2	41:Lk:10:ASP:OD1	2.20	0.41
50:S2:375:U:H2'	50:S2:376:A:H8	1.85	0.41
50:S2:1244:PSU:H2'	50:S2:1245:G:H8	1.85	0.41
50:S2:1426:U:OP2	67:SQ:69:ARG:NH2	2.51	0.41
50:S2:1713:C:H2'	50:S2:1714:U:C6	2.56	0.41
58:SH:189:PHE:HA	58:SH:190:PRO:HD2	1.80	0.41
59:SI:65:PHE:CE1	59:SI:78:ILE:HD11	2.56	0.41
59:SI:110:ARG:HH11	59:SI:110:ARG:HG3	1.85	0.41
68:SR:103:LYS:HB2	68:SR:103:LYS:HE2	1.64	0.41
73:SW:5:ASN:HB3	73:SW:8:ALA:HB3	2.02	0.41
74:SX:53:GLU:HG3	74:SX:54:LYS:N	2.35	0.41
3:L5:716:C:OP2	8:LC:320:LYS:NZ	2.54	0.41
3:L5:1554:A:H5'	46:Lp:9:GLY:C	2.46	0.41
3:L5:1730:U:H2'	3:L5:1731:C:H6	1.86	0.41
3:L5:1730:U:H2'	3:L5:1731:C:C6	2.55	0.41
3:L5:2022:C:C4	3:L5:2023:C:C4	3.08	0.41
3:L5:2375:A:H2'	3:L5:2376:A:H8	1.85	0.41
3:L5:2384:U:H2'	3:L5:2385:U:C6	2.55	0.41
3:L5:2876:OMG:N2	90:L5:5521:HOH:O	2.38	0.41
3:L5:4896:G:H2'	3:L5:4897:G:C8	2.56	0.41
9:LD:124:GLU:CD	9:LD:124:GLU:H	2.29	0.41
11:LF:37:PHE:O	11:LF:41:MET:HG2	2.21	0.41
11:LF:131:ASN:OD1	11:LF:134:ARG:NH1	2.53	0.41
13:LH:65:LYS:HD3	13:LH:65:LYS:HA	1.91	0.41
16:LL:162:LYS:HD3	16:LL:163:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LR:162:ARG:NH2	50:S2:873:G:C5	2.89	0.41
28:LX:149:VAL:O	28:LX:153:ILE:HG13	2.20	0.41
34:Ld:46:LEU:HD22	34:Ld:72:VAL:HG11	2.02	0.41
50:S2:511:U:H2'	50:S2:512:A2M:H8	2.03	0.41
50:S2:635:G:H2'	50:S2:636:C:C6	2.56	0.41
50:S2:807:G:H2'	50:S2:808:A:H8	1.86	0.41
51:SA:190:SER:HB3	51:SA:193:HIS:ND1	2.36	0.41
52:SB:164:ILE:HG22	52:SB:168:MET:HE3	2.03	0.41
56:SF:167:LYS:HB3	56:SF:167:LYS:HE2	1.80	0.41
60:SJ:108:ARG:HH22	60:SJ:154:GLN:HE21	1.68	0.41
64:SN:29:THR:O	64:SN:33:VAL:HG12	2.20	0.41
83:Sg:205:SER:HB3	83:Sg:222:ASN:OD1	2.20	0.41
83:Sg:294:ASP:OD1	83:Sg:294:ASP:N	2.46	0.41
3:L5:50:C:C2	3:L5:51:A:C8	3.08	0.41
3:L5:308:G:O6	18:LN:12:ARG:NH1	2.54	0.41
3:L5:667:A:H2'	3:L5:668:C:C6	2.56	0.41
3:L5:1512:G:H2'	3:L5:1513:U:H6	1.85	0.41
3:L5:1577:G:H5'	3:L5:1578:U:H5''	2.01	0.41
3:L5:1590:C:H5''	3:L5:1591:U:O5'	2.21	0.41
3:L5:1802:A:H4'	24:LT:105:PHE:CE1	2.56	0.41
3:L5:1814:C:O2'	32:Lb:42:ASN:OD1	2.28	0.41
3:L5:2080:U:H2'	3:L5:2081:C:C6	2.55	0.41
3:L5:3668:C:H5'	6:LA:8:GLN:O	2.21	0.41
3:L5:4433:G:H2'	3:L5:4434:C:C6	2.55	0.41
3:L5:4531:U:O2'	3:L5:4532:PSU:O5'	2.29	0.41
3:L5:4621:C:OP1	26:LV:48:ARG:HD2	2.21	0.41
3:L5:4642:U:H2'	3:L5:4643:G:C8	2.56	0.41
3:L5:4773:C:H2'	3:L5:4774:C:C6	2.56	0.41
4:L7:57:C:H2'	4:L7:58:A:H8	1.86	0.41
5:L8:40:A:H2'	5:L8:41:A:C8	2.56	0.41
5:L8:65:A:C4	5:L8:66:A:C8	3.08	0.41
6:LA:245[A]:ARG:HA	6:LA:245[A]:ARG:HD2	1.86	0.41
12:LG:51:LEU:O	12:LG:55:VAL:HG23	2.21	0.41
12:LG:102:TYR:OH	12:LG:211:ASP:OD1	2.22	0.41
13:LH:12:ILE:HB	13:LH:53:LYS:HB2	2.03	0.41
23:LS:107:THR:O	23:LS:111:ARG:HG2	2.20	0.41
28:LX:63:LYS:HE2	28:LX:63:LYS:HB2	1.89	0.41
30:LZ:87:VAL:HB	30:LZ:89:ILE:HD13	2.02	0.41
39:Li:23:LYS:H	39:Li:23:LYS:HG3	1.60	0.41
50:S2:90:G:H2'	50:S2:91:A:O4'	2.21	0.41
50:S2:166:A2M:O2'	57:SG:6:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S2:570:C:H4'	75:SY:36:PRO:HG3	2.03	0.41
50:S2:641:A:H2'	50:S2:642:U:O4'	2.20	0.41
50:S2:1060:A:H1'	50:S2:1062:A:N7	2.36	0.41
51:SA:61:ALA:HB1	51:SA:145:ILE:HG21	2.03	0.41
52:SB:133:TYR:HE1	52:SB:220:LYS:HD2	1.85	0.41
53:SC:72:ASP:OD2	53:SC:272:HIS:NE2	2.41	0.41
56:SF:26:ASP:OD2	56:SF:26:ASP:N	2.53	0.41
56:SF:192:LYS:HE2	56:SF:195:GLU:OE2	2.21	0.41
57:SG:61:PHE:CD2	57:SG:72:ARG:HD3	2.56	0.41
57:SG:93:LYS:HE3	57:SG:93:LYS:HB3	1.70	0.41
59:SI:137:LEU:HA	59:SI:137:LEU:HD13	1.87	0.41
59:SI:165:GLN:HA	59:SI:168:GLN:HE21	1.86	0.41
60:SJ:40:LYS:HE3	81:Se:108:ARG:HH21	1.86	0.41
60:SJ:88:ASP:HB3	60:SJ:91:LYS:HD3	2.03	0.41
60:SJ:116:LYS:HD3	60:SJ:116:LYS:HA	1.86	0.41
61:SK:58:VAL:HG21	61:SK:69:TRP:HB3	2.02	0.41
62:SL:56:ILE:O	62:SL:84:ARG:NH2	2.40	0.41
64:SN:87:ASP:OD1	64:SN:87:ASP:N	2.52	0.41
64:SN:130:LYS:HE3	64:SN:139:TRP:HB3	2.03	0.41
71:SU:55:ARG:HH11	71:SU:87:ARG:NE	2.18	0.41
76:SZ:99:LEU:HD11	76:SZ:102:LYS:HD2	2.03	0.41
78:Sb:6:ASP:OD2	78:Sb:9:HIS:HB2	2.20	0.41
3:L5:324:A:H2'	3:L5:325:U:C6	2.56	0.41
3:L5:673:C:H2'	3:L5:674:G:H8	1.86	0.41
3:L5:1205:G:H2'	3:L5:1206:C:H6	1.87	0.41
3:L5:1404:G:H2'	3:L5:1405:C:C6	2.55	0.41
3:L5:2521:G:H2'	3:L5:2522:G:H8	1.86	0.41
3:L5:2521:G:H2'	3:L5:2522:G:C8	2.55	0.41
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.56	0.41
3:L5:4233:A:C8	3:L5:4235:G:C8	3.09	0.41
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.56	0.41
3:L5:4424:A:C4	3:L5:4425:G:C8	3.09	0.41
3:L5:4919:G:H2'	3:L5:4920:C:C6	2.55	0.41
9:LD:211:LEU:HD12	9:LD:223:PHE:HE2	1.85	0.41
14:LI:191:ILE:HD11	14:LI:212:LEU:HD21	2.03	0.41
15:LJ:24:ILE:HG12	15:LJ:128:LEU:HB2	2.03	0.41
29:LY:45:ARG:HB2	29:LY:126:ARG:NH2	2.36	0.41
41:Lk:9:LYS:HG3	41:Lk:10:ASP:N	2.35	0.41
50:S2:114:G:O6	50:S2:351:G:H1'	2.21	0.41
50:S2:1679:A:H2'	56:SF:60:ARG:HD2	2.02	0.41
50:S2:1690:U:H2'	50:S2:1691:U:H6	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SA:16:LEU:HD13	51:SA:16:LEU:HA	1.91	0.41
51:SA:206:ASP:OD2	51:SA:206:ASP:C	2.64	0.41
52:SB:179:ASN:HB3	52:SB:183:GLU:HB3	2.03	0.41
54:SD:10:LYS:HB3	54:SD:10:LYS:HE3	1.66	0.41
54:SD:29:LEU:HD11	54:SD:69:LEU:HD11	2.02	0.41
54:SD:105:LEU:HD22	54:SD:184:ILE:HD13	2.03	0.41
56:SF:40:ALA:HB1	56:SF:45:TYR:CG	2.56	0.41
61:SK:14:LEU:HD21	61:SK:34:GLU:OE1	2.20	0.41
66:SP:83:MET:HE3	66:SP:84:ILE:N	2.36	0.41
75:SY:82:ALA:O	75:SY:86:GLU:CB	2.69	0.41
3:L5:170:C:O2'	3:L5:171:U:P	2.79	0.40
3:L5:260:C:H2'	3:L5:261:G:C8	2.56	0.40
3:L5:1591:U:H5''	3:L5:4527:G:OP1	2.21	0.40
3:L5:2423:A:H2'	3:L5:2424:OMG:C8	2.56	0.40
3:L5:2673:G:H5''	3:L5:2675:G:O4'	2.21	0.40
3:L5:2747:U:H2'	3:L5:2748:C:C6	2.56	0.40
3:L5:2857:A:H2'	3:L5:2858:A:O4'	2.20	0.40
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.86	0.40
3:L5:4571:A2M:H1'	3:L5:4571:A2M:HM'3	1.64	0.40
3:L5:4926:C:H3'	3:L5:4927:G:N2	2.36	0.40
4:L7:33:U:H2'	4:L7:34:C:C6	2.56	0.40
31:La:75:LEU:HD11	31:La:133:ALA:HA	2.03	0.40
50:S2:116:OMU:H6	50:S2:116:OMU:O5'	2.22	0.40
50:S2:945:U:H2'	50:S2:946:U:C6	2.55	0.40
50:S2:1310:U:C2	50:S2:1311:C:C5	3.09	0.40
50:S2:1386:A:H2'	50:S2:1387:G:O4'	2.21	0.40
50:S2:1411:G:H2'	50:S2:1412:C:C6	2.56	0.40
51:SA:178:LEU:O	51:SA:182:VAL:HG12	2.22	0.40
56:SF:170:ALA:HB3	76:SZ:106:GLN:OE1	2.21	0.40
58:SH:145:ARG:HG3	58:SH:147:LYS:HD2	2.03	0.40
61:SK:16:PHE:O	61:SK:91:PRO:HB3	2.21	0.40
61:SK:39:ASN:O	61:SK:39:ASN:ND2	2.54	0.40
66:SP:96:VAL:HB	66:SP:120:SER:HB2	2.03	0.40
68:SR:5:ARG:O	68:SR:10:LYS:NZ	2.54	0.40
71:SU:44:LYS:HD3	71:SU:50:VAL:HG21	2.03	0.40
81:Se:92:LYS:NZ	90:Se:201:HOH:O	2.46	0.40
83:Sg:191:HIS:CD2	83:Sg:195:LEU:HD21	2.55	0.40
3:L5:1097:C:H2'	3:L5:1098:G:H8	1.86	0.40
3:L5:1174:G:H2'	3:L5:1175:A:C8	2.56	0.40
3:L5:1589:C:H2'	3:L5:1590:C:C6	2.56	0.40
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L8:94:G:C5	40:Lj:84:PRO:HD3	2.57	0.40
7:LB:71:GLU:OE1	27:LW:1:MET:N	2.55	0.40
8:LC:60:HIS:HA	8:LC:92:PHE:HE1	1.87	0.40
10:LE:131:LYS:NZ	90:LE:305:HOH:O	2.53	0.40
10:LE:183:ARG:HD2	10:LE:183:ARG:HA	1.78	0.40
12:LG:159:HIS:ND1	12:LG:185:LYS:HA	2.36	0.40
25:LU:27:HIS:ND1	25:LU:27:HIS:N	2.69	0.40
26:LV:89:ARG:HB2	26:LV:95:PHE:CE2	2.56	0.40
28:LX:40:ILE:HD12	28:LX:40:ILE:HA	1.92	0.40
37:Lg:83:CYS:SG	37:Lg:86:CYS:HB2	2.60	0.40
50:S2:155:G:C6	50:S2:164:A:C6	3.09	0.40
50:S2:162:C:H2'	50:S2:163:U:O4'	2.21	0.40
50:S2:874:G:H2'	50:S2:875:A:C8	2.53	0.40
50:S2:1272:C:OP2	82:Sf:94:LYS:NZ	2.35	0.40
50:S2:1868:U:O4	77:Sa:98:PRO:HG2	2.21	0.40
51:SA:31:ASP:N	51:SA:150:THR:O	2.34	0.40
51:SA:213:GLU:OE1	68:SR:84:TYR:CZ	2.74	0.40
55:SE:95:THR:HG22	75:SY:16:ARG:HB2	2.03	0.40
69:SS:113:ARG:O	69:SS:117:ILE:HG12	2.21	0.40
76:SZ:72:VAL:HA	76:SZ:75:GLU:HG2	2.03	0.40
83:Sg:116:ASP:C	83:Sg:118:ARG:H	2.29	0.40
83:Sg:154:VAL:HG12	83:Sg:167:SER:OG	2.21	0.40
3:L5:6:C:H2'	3:L5:7:C:H6	1.86	0.40
3:L5:158:A:N1	3:L5:276:C:O2'	2.49	0.40
3:L5:751:G:H2'	3:L5:752:G:O4'	2.22	0.40
3:L5:1673:U:H2'	3:L5:1674:C:C6	2.56	0.40
3:L5:2379:A:H2'	3:L5:2380:G:O4'	2.21	0.40
3:L5:2639:U:O2'	3:L5:2694:G:O6	2.39	0.40
3:L5:4082:G:N2	90:L5:6031:HOH:O	2.53	0.40
3:L5:4195:G:OP1	3:L5:4221:C:O2'	2.37	0.40
3:L5:4236:G:H2'	3:L5:4237:C:C6	2.56	0.40
3:L5:4323:A:C2	9:LD:146:LEU:HD23	2.56	0.40
3:L5:4413:C:H2'	3:L5:4414:A:O4'	2.20	0.40
3:L5:4750:G:H2'	3:L5:4751:G:C8	2.56	0.40
32:Lb:93:LEU:HD23	32:Lb:93:LEU:HA	1.91	0.40
38:Lh:98:HIS:O	38:Lh:102:LEU:HG	2.22	0.40
50:S2:354:OMU:H1'	50:S2:354:OMU:HM23	1.84	0.40
50:S2:484:A2M:O5'	50:S2:484:A2M:H8	2.22	0.40
50:S2:1189:A:H4'	74:SX:34:THR:HG21	2.04	0.40
56:SF:179:ASN:HB2	56:SF:187:SER:HB3	2.03	0.40
58:SH:62:ILE:HD12	58:SH:94:PHE:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SM:83:LYS:HE2	63:SM:83:LYS:HB3	1.96	0.40
66:SP:53:GLN:H	66:SP:53:GLN:CD	2.26	0.40
66:SP:59:ARG:HE	66:SP:59:ARG:HB3	1.51	0.40
71:SU:81:GLN:NE2	80:Sd:55:LEU:HD12	2.36	0.40
81:Se:95:LYS:HE3	81:Se:95:LYS:HB3	1.85	0.40
3:L5:456:C:H2'	3:L5:457:G:H8	1.85	0.40
3:L5:650:C:H2'	3:L5:651:C:C6	2.57	0.40
3:L5:1241:C:O2'	32:Lb:120:ARG:O	2.32	0.40
3:L5:1249:C:H2'	3:L5:1250:C:C6	2.56	0.40
3:L5:1309:C:H2'	3:L5:1310:C:C6	2.57	0.40
3:L5:1406:G:C6	3:L5:1407:C:N3	2.90	0.40
3:L5:1669:A:H4'	3:L5:1685:G:H22	1.87	0.40
3:L5:1824:G:H5''	24:LT:35:LYS:HE2	2.03	0.40
3:L5:2318:G:OP2	35:Le:14:LYS:NZ	2.55	0.40
3:L5:3841:OMC:HM23	3:L5:3841:OMC:HI'	1.72	0.40
3:L5:4196:OMG:HI'	3:L5:4196:OMG:HM23	1.85	0.40
85:L5:5115:SPD:H51	85:L5:5115:SPD:HN11	1.86	0.40
10:LE:115:TYR:CD1	47:Lr:115:SER:HB3	2.57	0.40
10:LE:153:LEU:HD11	10:LE:195:ILE:HG13	2.03	0.40
15:LJ:35:ARG:HD3	15:LJ:123:ILE:HA	2.02	0.40
15:LJ:38:LYS:HA	15:LJ:38:LYS:HD3	1.98	0.40
50:S2:69:C:H2'	50:S2:70:G:O4'	2.21	0.40
50:S2:1431:G:H2'	50:S2:1432:U:C6	2.57	0.40
50:S2:1444:U:H2'	50:S2:1445:PSU:O4'	2.21	0.40
50:S2:1545:A:H2'	50:S2:1546:G:C8	2.57	0.40
65:SO:35:ALA:O	65:SO:109:GLY:N	2.41	0.40
76:SZ:58:LEU:HA	76:SZ:62:VAL:HG23	2.04	0.40
76:SZ:92:LEU:HD22	76:SZ:109:TYR:HE1	1.86	0.40
83:Sg:27:PHE:HA	83:Sg:28:PRO:HG3	1.72	0.40
3:L5:123:C:H2'	3:L5:124:C:C6	2.56	0.40
3:L5:247:G:H2'	3:L5:248:C:C6	2.56	0.40
3:L5:694:C:H2'	3:L5:695:G:C8	2.57	0.40
3:L5:2876:OMG:C8	46:Lp:16:THR:HG22	2.56	0.40
3:L5:3722:G:H2'	3:L5:3723:A2M:C8	2.52	0.40
3:L5:3923:A:H2'	3:L5:3924:C:H6	1.86	0.40
3:L5:4192:A:H2'	3:L5:4193:C:C6	2.56	0.40
3:L5:4401:G:H2'	3:L5:4402:C:H6	1.86	0.40
3:L5:4994:G:H2'	3:L5:4995:U:C6	2.56	0.40
6:LA:117:GLU:HG2	6:LA:124:GLY:N	2.36	0.40
8:LC:145:GLU:H	8:LC:145:GLU:CD	2.29	0.40
9:LD:79:TYR:O	9:LD:82:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	2.04	0.40
25:LU:23:LEU:HD23	25:LU:110:TYR:HB2	2.04	0.40
34:Ld:46:LEU:HD13	34:Ld:46:LEU:HA	1.96	0.40
34:Ld:54:MET:SD	34:Ld:60:PRO:HA	2.61	0.40
50:S2:337:C:C2	50:S2:338:G:C8	3.09	0.40
50:S2:929:G:N2	50:S2:1104:G:H4'	2.36	0.40
50:S2:1447:OMG:HM23	50:S2:1447:OMG:H1'	1.86	0.40
50:S2:1458:G:H2'	50:S2:1459:G:H8	1.87	0.40
50:S2:1610:G:OP1	69:SS:121:ARG:HD2	2.21	0.40
50:S2:1634:A:H2'	50:S2:1635:C:O4'	2.22	0.40
50:S2:1733:U:H2'	50:S2:1734:G:O4'	2.21	0.40
50:S2:1794:C:H2'	50:S2:1795:G:O4'	2.22	0.40
52:SB:25:PHE:HA	52:SB:28:LYS:HG3	2.02	0.40
54:SD:53:THR:HG21	54:SD:94:ARG:HG2	2.04	0.40
54:SD:64:ARG:HG2	54:SD:68:GLU:OE1	2.22	0.40
60:SJ:3:VAL:HB	60:SJ:5:ARG:HG2	2.03	0.40
67:SQ:58:LEU:HD11	67:SQ:112:LEU:HD11	2.02	0.40
69:SS:5:ILE:H	69:SS:5:ILE:HD12	1.87	0.40
70:ST:80:GLY:HA3	70:ST:93:SER:O	2.22	0.40
72:SV:11:LEU:HD12	72:SV:11:LEU:HA	1.88	0.40
78:Sb:19:HIS:CD2	78:Sb:20:LYS:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
7	LB	394/403 (98%)	388 (98%)	6 (2%)	0	100	100
8	LC	359/427 (84%)	353 (98%)	6 (2%)	0	100	100
9	LD	292/297 (98%)	284 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	LE	217/288 (75%)	210 (97%)	7 (3%)	0	100	100
11	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
12	LG	224/266 (84%)	222 (99%)	2 (1%)	0	100	100
13	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
14	LI	203/214 (95%)	201 (99%)	2 (1%)	0	100	100
15	LJ	167/178 (94%)	165 (99%)	2 (1%)	0	100	100
16	LL	204/211 (97%)	199 (98%)	5 (2%)	0	100	100
17	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
18	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
19	LO	198/203 (98%)	196 (99%)	2 (1%)	0	100	100
20	LP	152/184 (83%)	150 (99%)	2 (1%)	0	100	100
21	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
22	LR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
24	LT	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
25	LU	97/128 (76%)	94 (97%)	3 (3%)	0	100	100
26	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
27	LW	62/157 (40%)	61 (98%)	1 (2%)	0	100	100
28	LX	116/156 (74%)	116 (100%)	0	0	100	100
29	LY	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
30	LZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
31	La	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
32	Lb	99/159 (62%)	97 (98%)	2 (2%)	0	100	100
33	Lc	96/115 (84%)	96 (100%)	0	0	100	100
34	Ld	104/125 (83%)	104 (100%)	0	0	100	100
35	Le	127/135 (94%)	126 (99%)	1 (1%)	0	100	100
36	Lf	108/110 (98%)	108 (100%)	0	0	100	100
37	Lg	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
38	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
40	Lj	84/97 (87%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Lk	66/70 (94%)	66 (100%)	0	0	100	100
42	Ll	48/51 (94%)	48 (100%)	0	0	100	100
43	Lm	50/128 (39%)	50 (100%)	0	0	100	100
44	Ln	23/25 (92%)	23 (100%)	0	0	100	100
45	Lo	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
46	Lp	88/92 (96%)	85 (97%)	3 (3%)	0	100	100
47	Lr	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
51	SA	212/295 (72%)	205 (97%)	7 (3%)	0	100	100
52	SB	191/264 (72%)	185 (97%)	6 (3%)	0	100	100
53	SC	216/293 (74%)	214 (99%)	2 (1%)	0	100	100
54	SD	218/243 (90%)	212 (97%)	6 (3%)	0	100	100
55	SE	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
56	SF	176/204 (86%)	167 (95%)	8 (4%)	1 (1%)	21	32
57	SG	197/249 (79%)	191 (97%)	6 (3%)	0	100	100
58	SH	151/194 (78%)	149 (99%)	2 (1%)	0	100	100
59	SI	197/208 (95%)	194 (98%)	3 (2%)	0	100	100
60	SJ	173/194 (89%)	167 (96%)	6 (4%)	0	100	100
61	SK	93/165 (56%)	89 (96%)	4 (4%)	0	100	100
62	SL	138/158 (87%)	134 (97%)	4 (3%)	0	100	100
63	SM	67/132 (51%)	61 (91%)	6 (9%)	0	100	100
64	SN	148/151 (98%)	148 (100%)	0	0	100	100
65	SO	96/151 (64%)	87 (91%)	9 (9%)	0	100	100
66	SP	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
67	SQ	138/146 (94%)	131 (95%)	7 (5%)	0	100	100
68	SR	123/135 (91%)	121 (98%)	2 (2%)	0	100	100
69	SS	146/152 (96%)	144 (99%)	2 (1%)	0	100	100
70	ST	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
71	SU	91/119 (76%)	86 (94%)	5 (6%)	0	100	100
72	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
73	SW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
74	SX	137/143 (96%)	136 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	SY	119/133 (90%)	116 (98%)	3 (2%)	0	100	100
76	SZ	80/125 (64%)	77 (96%)	3 (4%)	0	100	100
77	Sa	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
78	Sb	68/84 (81%)	66 (97%)	2 (3%)	0	100	100
79	Sc	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
80	Sd	53/56 (95%)	53 (100%)	0	0	100	100
81	Se	49/133 (37%)	48 (98%)	1 (2%)	0	100	100
82	Sf	37/156 (24%)	35 (95%)	2 (5%)	0	100	100
83	Sg	272/317 (86%)	249 (92%)	19 (7%)	4 (2%)	8	12
All	All	10833/12762 (85%)	10592 (98%)	236 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
56	SF	80	GLY
83	Sg	117	ASN
83	Sg	144	ASP
83	Sg	146	SER
83	Sg	184	LEU

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	LA	190/198 (96%)	189 (100%)	1 (0%)	81	91
7	LB	344/348 (99%)	340 (99%)	4 (1%)	63	81
8	LC	300/348 (86%)	296 (99%)	4 (1%)	61	80
9	LD	246/250 (98%)	240 (98%)	6 (2%)	43	65
10	LE	195/252 (77%)	193 (99%)	2 (1%)	68	84
11	LF	191/215 (89%)	190 (100%)	1 (0%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	LG	191/223 (86%)	190 (100%)	1 (0%)	81	91
13	LH	169/171 (99%)	169 (100%)	0	100	100
14	LI	175/181 (97%)	170 (97%)	5 (3%)	37	60
15	LJ	142/149 (95%)	141 (99%)	1 (1%)	76	88
16	LL	172/177 (97%)	171 (99%)	1 (1%)	78	89
17	LM	116/161 (72%)	113 (97%)	3 (3%)	40	63
18	LN	171/172 (99%)	169 (99%)	2 (1%)	63	81
19	LO	172/174 (99%)	172 (100%)	0	100	100
20	LP	135/163 (83%)	133 (98%)	2 (2%)	57	77
21	LQ	164/165 (99%)	164 (100%)	0	100	100
22	LR	146/175 (83%)	144 (99%)	2 (1%)	59	79
23	LS	157/157 (100%)	151 (96%)	6 (4%)	29	49
24	LT	140/140 (100%)	139 (99%)	1 (1%)	76	88
25	LU	89/115 (77%)	80 (90%)	9 (10%)	7	11
26	LV	102/107 (95%)	102 (100%)	0	100	100
27	LW	54/126 (43%)	53 (98%)	1 (2%)	50	71
28	LX	106/133 (80%)	105 (99%)	1 (1%)	70	85
29	LY	122/135 (90%)	119 (98%)	3 (2%)	42	64
30	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	85
31	La	119/120 (99%)	117 (98%)	2 (2%)	53	74
32	Lb	84/125 (67%)	83 (99%)	1 (1%)	63	81
33	Lc	83/97 (86%)	83 (100%)	0	100	100
34	Ld	97/110 (88%)	93 (96%)	4 (4%)	27	46
35	Le	115/121 (95%)	114 (99%)	1 (1%)	70	85
36	Lf	88/89 (99%)	88 (100%)	0	100	100
37	Lg	96/100 (96%)	96 (100%)	0	100	100
38	Lh	109/110 (99%)	109 (100%)	0	100	100
39	Li	86/89 (97%)	84 (98%)	2 (2%)	44	66
40	Lj	73/80 (91%)	73 (100%)	0	100	100
41	Lk	63/65 (97%)	62 (98%)	1 (2%)	55	76
42	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Lm	47/115 (41%)	47 (100%)	0	100	100
44	Ln	24/24 (100%)	24 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	73/75 (97%)	73 (100%)	0	100	100
47	Lr	109/121 (90%)	108 (99%)	1 (1%)	70	85
51	SA	178/243 (73%)	174 (98%)	4 (2%)	45	67
52	SB	182/231 (79%)	178 (98%)	4 (2%)	45	67
53	SC	184/225 (82%)	178 (97%)	6 (3%)	33	55
54	SD	184/202 (91%)	172 (94%)	12 (6%)	15	27
55	SE	220/225 (98%)	217 (99%)	3 (1%)	59	79
56	SF	151/170 (89%)	144 (95%)	7 (5%)	24	41
57	SG	178/218 (82%)	173 (97%)	5 (3%)	38	60
58	SH	146/174 (84%)	143 (98%)	3 (2%)	47	69
59	SI	175/180 (97%)	169 (97%)	6 (3%)	32	54
60	SJ	147/168 (88%)	145 (99%)	2 (1%)	59	79
61	SK	86/136 (63%)	84 (98%)	2 (2%)	44	66
62	SL	128/142 (90%)	127 (99%)	1 (1%)	73	86
63	SM	51/108 (47%)	48 (94%)	3 (6%)	18	31
64	SN	130/131 (99%)	127 (98%)	3 (2%)	44	66
65	SO	81/119 (68%)	81 (100%)	0	100	100
66	SP	112/130 (86%)	110 (98%)	2 (2%)	51	73
67	SQ	116/121 (96%)	112 (97%)	4 (3%)	32	54
68	SR	115/122 (94%)	108 (94%)	7 (6%)	17	30
69	SS	128/132 (97%)	125 (98%)	3 (2%)	44	66
70	ST	112/115 (97%)	108 (96%)	4 (4%)	31	52
71	SU	88/107 (82%)	81 (92%)	7 (8%)	11	19
72	SV	67/67 (100%)	66 (98%)	1 (2%)	57	77
73	SW	112/113 (99%)	109 (97%)	3 (3%)	39	62
74	SX	111/114 (97%)	106 (96%)	5 (4%)	24	42
75	SY	106/115 (92%)	100 (94%)	6 (6%)	18	33
76	SZ	73/103 (71%)	68 (93%)	5 (7%)	14	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	Sa	86/98 (88%)	82 (95%)	4 (5%)	23	41
78	Sb	68/76 (90%)	64 (94%)	4 (6%)	18	31
79	Sc	56/62 (90%)	52 (93%)	4 (7%)	13	23
80	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	69
81	Se	43/104 (41%)	42 (98%)	1 (2%)	44	66
82	Sf	35/140 (25%)	33 (94%)	2 (6%)	18	33
83	Sg	241/275 (88%)	209 (87%)	32 (13%)	4	5
All	All	9450/10850 (87%)	9223 (98%)	227 (2%)	43	65

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	LA	208	GLU
7	LB	69	LYS
7	LB	70	LYS
7	LB	194	LEU
7	LB	306	ASP
8	LC	16	GLU
8	LC	189	MET
8	LC	348	LYS
8	LC	351	VAL
9	LD	56	THR
9	LD	90	VAL
9	LD	117	LYS
9	LD	123	VAL
9	LD	133	GLU
9	LD	134	SER
10	LE	96	VAL
10	LE	274	VAL
11	LF	215	SER
12	LG	224	THR
14	LI	28	ASP
14	LI	36	LEU
14	LI	44	ASP
14	LI	79	SER
14	LI	212	LEU
15	LJ	81	GLU
16	LL	160	VAL
17	LM	28	VAL
17	LM	70	GLN

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Mol	Chain	Res	Type
17	LM	136	LEU
18	LN	151	ILE
18	LN	155	VAL
20	LP	5	SER
20	LP	17	SER
22	LR	122	SER
22	LR	131	VAL
23	LS	19	THR
23	LS	24	THR
23	LS	27	LEU
23	LS	48	VAL
23	LS	50	GLN
23	LS	164	LYS
24	LT	117	LYS
25	LU	18	VAL
25	LU	22	THR
25	LU	27	HIS
25	LU	31	ASP
25	LU	33	ILE
25	LU	38	ASN
25	LU	66	SER
25	LU	68	SER
25	LU	73	THR
27	LW	30	GLN
28	LX	85	SER
29	LY	66	GLN
29	LY	94	THR
29	LY	112	ASP
30	LZ	19	SER
31	La	88	VAL
31	La	135	GLU
32	Lb	66	SER
34	Ld	46	LEU
34	Ld	51	LYS
34	Ld	55	LYS
34	Ld	119	THR
35	Le	87	VAL
39	Li	21	VAL
39	Li	77	VAL
41	Lk	58	GLN
42	Ll	27	ILE
42	Ll	51	LEU

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Mol	Chain	Res	Type
47	Lr	79	ARG
51	SA	7	VAL
51	SA	82	THR
51	SA	140	VAL
51	SA	192	GLU
52	SB	60	ASP
52	SB	98	THR
52	SB	127	VAL
52	SB	178	THR
53	SC	63	VAL
53	SC	69	LEU
53	SC	75	ILE
53	SC	162	ILE
53	SC	245	SER
53	SC	270	THR
54	SD	26	THR
54	SD	32	ASP
54	SD	35	SER
54	SD	38	GLU
54	SD	41	VAL
54	SD	46	THR
54	SD	49	ILE
54	SD	51	LEU
54	SD	84	VAL
54	SD	149	SER
54	SD	150	MET
54	SD	219	PRO
55	SE	91	SER
55	SE	133	THR
55	SE	162	ILE
56	SF	33	ILE
56	SF	72	LEU
56	SF	89	THR
56	SF	100	ILE
56	SF	110	GLN
56	SF	117	ILE
56	SF	123	GLU
57	SG	19	ASP
57	SG	108	VAL
57	SG	114	VAL
57	SG	129	VAL
57	SG	133	LEU

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Mol	Chain	Res	Type
58	SH	24	SER
58	SH	53	VAL
58	SH	60	ILE
59	SI	46	VAL
59	SI	48	VAL
59	SI	66	SER
59	SI	107	THR
59	SI	159	SER
59	SI	189	VAL
60	SJ	3	VAL
60	SJ	102	ILE
61	SK	6	LYS
61	SK	35	LEU
62	SL	18	GLN
63	SM	21	VAL
63	SM	79	VAL
63	SM	109	VAL
64	SN	69	ASN
64	SN	131	THR
64	SN	150	VAL
66	SP	20	VAL
66	SP	108	LYS
67	SQ	31	LEU
67	SQ	32	ILE
67	SQ	61	GLU
67	SQ	66	VAL
68	SR	36	GLU
68	SR	71	ILE
68	SR	73	LEU
68	SR	85	VAL
68	SR	98	VAL
68	SR	103	LYS
68	SR	124	VAL
69	SS	18	THR
69	SS	36	VAL
69	SS	111	LEU
70	ST	5	THR
70	ST	37	VAL
70	ST	112	MET
70	ST	113	VAL
71	SU	39	LEU
71	SU	51	LYS

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Mol	Chain	Res	Type
71	SU	54	VAL
71	SU	92	HIS
71	SU	95	SER
71	SU	98	VAL
71	SU	102	THR
72	SV	52	THR
73	SW	23	ARG
73	SW	83	LEU
73	SW	121	THR
74	SX	26	GLN
74	SX	53	GLU
74	SX	55	VAL
74	SX	105	PHE
74	SX	123	VAL
75	SY	7	ILE
75	SY	9	THR
75	SY	18	LEU
75	SY	24	VAL
75	SY	50	THR
75	SY	114	MET
76	SZ	45	ASN
76	SZ	51	ASP
76	SZ	93	SER
76	SZ	100	VAL
76	SZ	113	THR
77	Sa	30	VAL
77	Sa	45	VAL
77	Sa	54	SER
77	Sa	69	VAL
78	Sb	14	GLU
78	Sb	15	GLU
78	Sb	61	THR
78	Sb	75	GLU
79	Sc	13	ARG
79	Sc	28	THR
79	Sc	38	THR
79	Sc	50	VAL
80	Sd	25	SER
81	Se	76	VAL
82	Sf	143	LYS
82	Sf	149	CYS
83	Sg	6	THR

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Mol	Chain	Res	Type
83	Sg	41	ILE
83	Sg	42	MET
83	Sg	46	THR
83	Sg	86	THR
83	Sg	89	LEU
83	Sg	93	THR
83	Sg	113	PHE
83	Sg	115	SER
83	Sg	116	ASP
83	Sg	128	THR
83	Sg	131	LEU
83	Sg	137	VAL
83	Sg	155	ARG
83	Sg	174	VAL
83	Sg	176	VAL
83	Sg	179	LEU
83	Sg	181	ASN
83	Sg	183	LYS
83	Sg	187	ASN
83	Sg	198	VAL
83	Sg	200	VAL
83	Sg	203	ASP
83	Sg	227	LEU
83	Sg	229	THR
83	Sg	235	ILE
83	Sg	256	ILE
83	Sg	258	ILE
83	Sg	261	LEU
83	Sg	288	SER
83	Sg	297	THR
83	Sg	305	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
6	LA	97	ASN
6	LA	140	ASN
7	LB	376	HIS
8	LC	38	ASN
8	LC	43	ASN
8	LC	187	GLN
8	LC	329	ASN

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Mol	Chain	Res	Type
9	LD	198	HIS
9	LD	202	GLN
9	LD	244	HIS
11	LF	63	GLN
11	LF	119	ASN
11	LF	126	ASN
12	LG	64	GLN
12	LG	66	GLN
12	LG	90	GLN
12	LG	100	HIS
12	LG	141	ASN
12	LG	159	HIS
12	LG	206	GLN
12	LG	208	ASN
12	LG	225	ASN
13	LH	98	HIS
14	LI	59	GLN
14	LI	130	HIS
14	LI	177	ASN
15	LJ	98	ASN
15	LJ	104	ASN
16	LL	19	GLN
16	LL	115	GLN
17	LM	75	GLN
17	LM	131	GLN
18	LN	201	HIS
19	LO	26	GLN
20	LP	21	ASN
20	LP	28	ASN
20	LP	56	GLN
20	LP	133	HIS
21	LQ	7	HIS
22	LR	40	GLN
23	LS	125	GLN
24	LT	144	ASN
26	LV	27	ASN
27	LW	50	ASN
28	LX	151	ASN
29	LY	18	HIS
30	LZ	132	GLN
31	La	89	ASN
33	Lc	73	HIS

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Mol	Chain	Res	Type
34	Ld	116	ASN
35	Le	52	GLN
35	Le	117	GLN
36	Lf	20	ASN
38	Lh	20	GLN
41	Lk	28	ASN
43	Lm	117	HIS
47	Lr	85	ASN
51	SA	141	ASN
52	SB	40	ASN
52	SB	118	GLN
54	SD	159	HIS
54	SD	165	ASN
56	SF	74	ASN
56	SF	165	ASN
57	SG	155	GLN
60	SJ	113	GLN
60	SJ	140	GLN
60	SJ	154	GLN
61	SK	39	ASN
64	SN	13	GLN
64	SN	105	ASN
65	SO	103	ASN
68	SR	83	ASN
69	SS	73	ASN
70	ST	42	HIS
70	ST	63	HIS
70	ST	137	GLN
71	SU	81	GLN
73	SW	24	GLN
74	SX	23	HIS
77	Sa	8	ASN
78	Sb	29	ASN
79	Sc	29	GLN
83	Sg	14	HIS
83	Sg	26	GLN
83	Sg	178	ASN
83	Sg	187	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	At	66/77 (85%)	20 (30%)	0
2	Et	48/75 (64%)	9 (18%)	0
3	L5	3370/5069 (66%)	394 (11%)	9 (0%)
4	L7	118/120 (98%)	7 (5%)	0
48	Mr	6/7 (85%)	1 (16%)	0
49	Pt	66/76 (86%)	7 (10%)	0
5	L8	146/156 (93%)	12 (8%)	0
50	S2	1539/1869 (82%)	200 (12%)	2 (0%)
All	All	5359/7449 (71%)	650 (12%)	11 (0%)

All (650) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	At	2	G
1	At	5	G
1	At	8	U
1	At	9	A
1	At	11	U
1	At	12	U
1	At	14	A
1	At	15	G
1	At	18	G
1	At	22	G
1	At	23	A
1	At	24	G
1	At	30	U
1	At	38	A
1	At	44	A
1	At	45	G
1	At	47	U
1	At	48	C
1	At	61	C
1	At	74	C
2	Et	10	G
2	Et	14	C
2	Et	22	G
2	Et	32	C
2	Et	46	G
2	Et	53	G
2	Et	54	A
2	Et	63	A
2	Et	76	A
3	L5	39	A

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Mol	Chain	Res	Type
3	L5	42	A
3	L5	48	G
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	70	A
3	L5	73	A
3	L5	85	G
3	L5	91	G
3	L5	98	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	132	G
3	L5	141	C
3	L5	143	C
3	L5	159	C
3	L5	171	U
3	L5	172	C
3	L5	179	G
3	L5	181	C
3	L5	200	U
3	L5	209	U
3	L5	210	C
3	L5	216	C
3	L5	218	A
3	L5	219	G
3	L5	234	G
3	L5	253	G
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	410	A
3	L5	412	G
3	L5	413	G
3	L5	440	U

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Mol	Chain	Res	Type
3	L5	451	C
3	L5	453	G
3	L5	454	U
3	L5	461	G
3	L5	467	U
3	L5	484	U
3	L5	485	C
3	L5	487	G
3	L5	489	C
3	L5	491	G
3	L5	509	A
3	L5	510	U
3	L5	659	G
3	L5	662	C
3	L5	663	G
3	L5	669	C
3	L5	686	A
3	L5	692	A
3	L5	704	C
3	L5	731	G
3	L5	742	G
3	L5	755	C
3	L5	913	U
3	L5	915	A
3	L5	917	A
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	943	A
3	L5	945	U
3	L5	956	A
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	1070	G
3	L5	1072	C
3	L5	1094	G
3	L5	1168	G

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Mol	Chain	Res	Type
3	L5	1170	G
3	L5	1183	C
3	L5	1210	C
3	L5	1211	G
3	L5	1215	C
3	L5	1216	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	1408	G
3	L5	1410	U
3	L5	1411	C
3	L5	1413	C
3	L5	1439	C
3	L5	1445	U
3	L5	1446	C
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

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Mol	Chain	Res	Type
3	L5	1582	PSU
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	1641	G
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	1704	C
3	L5	1707	C
3	L5	1708	G
3	L5	1721	G
3	L5	1722	C
3	L5	1734	G
3	L5	1750	G
3	L5	1785	C
3	L5	1787	A
3	L5	1789	C
3	L5	1804	A
3	L5	1822	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A
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

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Mol	Chain	Res	Type
3	L5	1925	G
3	L5	1931	C
3	L5	1932	A
3	L5	1948	G
3	L5	2019	C
3	L5	2024	G
3	L5	2026	A
3	L5	2028	C
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2069	A
3	L5	2084	C
3	L5	2092	G
3	L5	2095	A
3	L5	2096	G
3	L5	2098	G
3	L5	2261	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	2364	OMG
3	L5	2395	A
3	L5	2397	G
3	L5	2417	A
3	L5	2421	G
3	L5	2450	G
3	L5	2453	A
3	L5	2470	C
3	L5	2471	G
3	L5	2474	G
3	L5	2483	G
3	L5	2505	C
3	L5	2513	A
3	L5	2519	U
3	L5	2520	C

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Mol	Chain	Res	Type
3	L5	2529	A
3	L5	2554	U
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2601	A
3	L5	2627	C
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	2705	G
3	L5	2706	G
3	L5	2711	G
3	L5	2712	G
3	L5	2735	G
3	L5	2739	C
3	L5	2743	A
3	L5	2761	U
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	2897	G
3	L5	2899	C
3	L5	2902	G
3	L5	3615	G
3	L5	3617	G
3	L5	3618	C
3	L5	3626	G

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Mol	Chain	Res	Type
3	L5	3635	A
3	L5	3644	U
3	L5	3648	A
3	L5	3662	A
3	L5	3673	C
3	L5	3710	G
3	L5	3712	A
3	L5	3748	A
3	L5	3753	G
3	L5	3754	G
3	L5	3776	G
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3818	UY1
3	L5	3819	G
3	L5	3838	U
3	L5	3840	U
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
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	3944	OMG
3	L5	4076	G
3	L5	4098	A
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4135	G
3	L5	4150	G
3	L5	4151	G
3	L5	4158	C
3	L5	4162	C
3	L5	4163	U

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Mol	Chain	Res	Type
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	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4380	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4415	A
3	L5	4420	PSU
3	L5	4422	A
3	L5	4440	G
3	L5	4448	G
3	L5	4453	C
3	L5	4464	A
3	L5	4465	U
3	L5	4475	G
3	L5	4476	C
3	L5	4512	U

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Mol	Chain	Res	Type
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	4584	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
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
3	L5	4740	G
3	L5	4743	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	4772	C
3	L5	4775	C
3	L5	4865	C
3	L5	4870	G
3	L5	4871	C
3	L5	4883	C
3	L5	4895	C
3	L5	4902	C
3	L5	4903	G
3	L5	4910	G
3	L5	4911	A

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Mol	Chain	Res	Type
3	L5	4912	G
3	L5	4914	C
3	L5	4935	C
3	L5	4938	A
3	L5	4943	A
3	L5	4976	U
3	L5	4988	U
3	L5	4994	G
3	L5	5017	G
3	L5	5041	G
3	L5	5050	C
3	L5	5053	U
3	L5	5061	A
3	L5	5062	G
3	L5	5069	U
4	L7	7	G
4	L7	33	U
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	100	A
4	L7	110	G
5	L8	34	U
5	L8	35	C
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	87	G
5	L8	103	A
5	L8	105	C
5	L8	110	U
5	L8	111	U
5	L8	114	G
5	L8	147	G
48	Mr	5	A
49	Pt	9	1MG
49	Pt	13	C
49	Pt	46	A
49	Pt	59	C
49	Pt	61	C
49	Pt	74	C
49	Pt	75	C

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Mol	Chain	Res	Type
50	S2	3	C
50	S2	17	C
50	S2	33	G
50	S2	41	G
50	S2	44	U
50	S2	46	A
50	S2	56	G
50	S2	59	U
50	S2	65	C
50	S2	67	C
50	S2	68	A
50	S2	79	A
50	S2	80	G
50	S2	92	A
50	S2	102	A
50	S2	103	A
50	S2	113	G
50	S2	115	U
50	S2	126	G
50	S2	127	C
50	S2	129	C
50	S2	130	G
50	S2	143	U
50	S2	147	A
50	S2	155	G
50	S2	162	C
50	S2	163	U
50	S2	168	C
50	S2	184	G
50	S2	204	G
50	S2	209	A
50	S2	215	G
50	S2	288	G
50	S2	309	G
50	S2	312	G
50	S2	319	C
50	S2	323	C
50	S2	335	G
50	S2	347	G
50	S2	362	C
50	S2	364	A
50	S2	368	U

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Mol	Chain	Res	Type
50	S2	370	G
50	S2	382	C
50	S2	385	G
50	S2	386	C
50	S2	407	G
50	S2	409	C
50	S2	418	A
50	S2	448	A
50	S2	449	A
50	S2	450	C
50	S2	472	C
50	S2	474	G
50	S2	482	G
50	S2	487	U
50	S2	492	C
50	S2	496	C
50	S2	508	A
50	S2	509	OMG
50	S2	564	A
50	S2	576	A2M
50	S2	587	A
50	S2	588	G
50	S2	590	A2M
50	S2	591	U
50	S2	604	A
50	S2	608	C
50	S2	614	C
50	S2	616	A
50	S2	617	G
50	S2	620	G
50	S2	624	C
50	S2	627	OMU
50	S2	628	A
50	S2	643	A
50	S2	644	OMG
50	S2	655	A
50	S2	660	C
50	S2	663	C
50	S2	668	A2M
50	S2	669	A
50	S2	671	A
50	S2	672	A

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Mol	Chain	Res	Type
50	S2	673	G
50	S2	683	OMG
50	S2	688	U
50	S2	821	G
50	S2	822	PSU
50	S2	827	A
50	S2	830	A
50	S2	831	G
50	S2	847	A
50	S2	869	A
50	S2	870	A
50	S2	872	A
50	S2	903	A
50	S2	913	A
50	S2	917	U
50	S2	918	PSU
50	S2	919	A
50	S2	920	A
50	S2	922	A
50	S2	933	G
50	S2	949	G
50	S2	990	A
50	S2	992	A
50	S2	1017	U
50	S2	1023	A
50	S2	1060	A
50	S2	1061	U
50	S2	1062	A
50	S2	1083	A
50	S2	1085	C
50	S2	1109	C
50	S2	1138	C
50	S2	1153	C
50	S2	1154	U
50	S2	1157	G
50	S2	1183	A
50	S2	1188	A
50	S2	1195	A
50	S2	1208	A
50	S2	1215	C
50	S2	1224	G
50	S2	1242	U

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Mol	Chain	Res	Type
50	S2	1243	PSU
50	S2	1251	A
50	S2	1253	A
50	S2	1256	G
50	S2	1257	G
50	S2	1259	A
50	S2	1265	A
50	S2	1274	G
50	S2	1275	G
50	S2	1308	U
50	S2	1313	A
50	S2	1315	U
50	S2	1324	G
50	S2	1331	C
50	S2	1342	U
50	S2	1345	G
50	S2	1348	G
50	S2	1358	U
50	S2	1371	U
50	S2	1372	U
50	S2	1373	C
50	S2	1378	A
50	S2	1402	A
50	S2	1406	G
50	S2	1422	G
50	S2	1429	G
50	S2	1439	A
50	S2	1442	OMU
50	S2	1447	OMG
50	S2	1454	A
50	S2	1455	A
50	S2	1466	G
50	S2	1489	A
50	S2	1490	OMG
50	S2	1498	A
50	S2	1520	G
50	S2	1521	C
50	S2	1533	A
50	S2	1535	U
50	S2	1536	G
50	S2	1564	C
50	S2	1580	A

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Mol	Chain	Res	Type
50	S2	1585	U
50	S2	1586	U
50	S2	1587	G
50	S2	1588	A
50	S2	1601	A
50	S2	1602	U
50	S2	1621	U
50	S2	1623	A
50	S2	1648	G
50	S2	1654	G
50	S2	1661	A
50	S2	1664	A
50	S2	1665	G
50	S2	1671	G
50	S2	1698	C
50	S2	1721	U
50	S2	1722	G
50	S2	1744	G
50	S2	1823	A
50	S2	1824	A
50	S2	1825	A
50	S2	1826	G
50	S2	1835	A
50	S2	1837	G
50	S2	1838	U
50	S2	1849	G
50	S2	1851	MA6
50	S2	1861	G
50	S2	1862	G
50	S2	1863	A
50	S2	1864	U
50	S2	1865	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	170	C
3	L5	218	A
3	L5	754	U
3	L5	1590	C
3	L5	1633	G
3	L5	1677	PSU

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Mol	Chain	Res	Type
3	L5	4475	G
3	L5	4699	U
3	L5	4913	G
50	S2	918	PSU
50	S2	1344	A

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

228 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
50	PSU	S2	119	50	18,21,22	4.50	8 (44%)	22,30,33	1.64	3 (13%)
3	PSU	L5	3768	3	18,21,22	4.49	7 (38%)	22,30,33	1.75	5 (22%)
50	PSU	S2	573	50	18,21,22	4.51	8 (44%)	22,30,33	1.71	5 (22%)
3	PSU	L5	4296	3	18,21,22	4.46	7 (38%)	22,30,33	1.78	5 (22%)
3	A2M	L5	3723	3	22,25,26	3.43	9 (40%)	31,36,39	2.37	10 (32%)
3	OMG	L5	4637	87,3	23,26,27	2.40	9 (39%)	33,38,41	2.47	11 (33%)
50	A2M	S2	99	86,50	22,25,26	3.43	10 (45%)	31,36,39	2.36	12 (38%)
50	OMC	S2	462	50	19,22,23	3.01	8 (42%)	26,31,34	0.71	0
3	PSU	L5	3764	87,3	18,21,22	4.49	7 (38%)	22,30,33	1.76	5 (22%)
3	A2M	L5	3825	3	22,25,26	3.44	9 (40%)	31,36,39	2.35	10 (32%)
50	PSU	S2	105	50	18,21,22	4.48	7 (38%)	22,30,33	1.82	5 (22%)
50	OMG	S2	1328	50	23,26,27	0.30	0	33,38,41	0.37	0
3	OMC	L5	2861	3	19,22,23	3.00	8 (42%)	26,31,34	0.76	0
50	PSU	S2	651	50	18,21,22	4.50	7 (38%)	22,30,33	1.80	5 (22%)
3	PSU	L5	4552	3	18,21,22	4.44	7 (38%)	22,30,33	1.73	5 (22%)
3	OMC	L5	2824	3	19,22,23	2.97	8 (42%)	26,31,34	0.78	0
3	OMU	L5	3925	3	19,22,23	3.03	8 (42%)	26,31,34	1.74	5 (19%)
50	PSU	S2	572	50	18,21,22	4.49	8 (44%)	22,30,33	1.66	4 (18%)
50	OMU	S2	121	50	19,22,23	3.04	8 (42%)	26,31,34	1.70	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4636	3	18,21,22	4.48	8 (44%)	22,30,33	1.79	6 (27%)
50	OMC	S2	517	50	19,22,23	2.99	8 (42%)	26,31,34	0.74	0
3	PSU	L5	3920	3,86	18,21,22	4.43	7 (38%)	22,30,33	1.80	5 (22%)
50	OMG	S2	683	50	23,26,27	2.45	9 (39%)	33,38,41	2.56	10 (30%)
3	OMC	L5	4536	3	19,22,23	2.97	8 (42%)	26,31,34	0.77	0
3	A2M	L5	3830	3	22,25,26	3.41	8 (36%)	31,36,39	2.41	11 (35%)
50	OMU	S2	1804	50	19,22,23	3.07	8 (42%)	26,31,34	1.71	4 (15%)
50	PSU	S2	866	50	18,21,22	4.55	7 (38%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4442	3	18,21,22	4.48	7 (38%)	22,30,33	1.82	6 (27%)
3	OMG	L5	4623	3	23,26,27	2.38	9 (39%)	33,38,41	2.39	11 (33%)
50	PSU	S2	681	50	18,21,22	4.45	7 (38%)	22,30,33	1.77	5 (22%)
50	PSU	S2	1243	50	18,21,22	4.50	7 (38%)	22,30,33	1.71	4 (18%)
50	MA6	S2	1850	50	23,26,27	1.41	4 (17%)	34,38,41	2.95	12 (35%)
74	HY3	SX	62	87,74	6,8,9	1.23	0	5,10,12	2.06	2 (40%)
3	PSU	L5	4689	3	18,21,22	4.44	7 (38%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3637	87,3	18,21,22	4.45	7 (38%)	22,30,33	1.82	4 (18%)
3	OMC	L5	3841	3	19,22,23	2.95	8 (42%)	26,31,34	0.71	0
50	MA6	S2	1851	50	23,26,27	1.40	5 (21%)	34,38,41	3.07	13 (38%)
50	A2M	S2	576	50	22,25,26	3.40	9 (40%)	31,36,39	2.40	12 (38%)
5	PSU	L8	55	5	18,21,22	4.46	7 (38%)	22,30,33	1.75	5 (22%)
50	PSU	S2	1232	50	18,21,22	4.52	7 (38%)	22,30,33	1.78	5 (22%)
45	MLZ	Lo	53	45	8,9,10	0.73	0	4,9,11	0.58	0
3	A2M	L5	3718	3	22,25,26	3.42	9 (40%)	31,36,39	2.25	11 (35%)
50	PSU	S2	1136	50	18,21,22	4.50	7 (38%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4521	3,86	18,21,22	4.48	7 (38%)	22,30,33	1.85	6 (27%)
50	PSU	S2	686	50	18,21,22	4.56	7 (38%)	22,30,33	1.82	5 (22%)
50	PSU	S2	1174	50	18,21,22	4.47	7 (38%)	22,30,33	1.71	5 (22%)
50	OMC	S2	1391	50	19,22,23	2.98	8 (42%)	26,31,34	0.69	0
50	A2M	S2	1031	50	22,25,26	3.42	9 (40%)	31,36,39	2.36	10 (32%)
50	A2M	S2	668	86,50	22,25,26	3.40	10 (45%)	31,36,39	2.40	11 (35%)
31	V5N	La	39	31	9,11,12	2.62	2 (22%)	9,14,16	1.30	1 (11%)
3	PSU	L5	1782	3	18,21,22	4.47	7 (38%)	22,30,33	1.82	5 (22%)
3	OMG	L5	3792	3	23,26,27	2.39	9 (39%)	33,38,41	2.48	10 (30%)
50	PSU	S2	1056	50	18,21,22	4.46	7 (38%)	22,30,33	1.82	5 (22%)
50	OMG	S2	867	50	23,26,27	2.44	9 (39%)	33,38,41	2.60	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4312	3	18,21,22	4.49	7 (38%)	22,30,33	1.74	5 (22%)
3	PSU	L5	1792	3	18,21,22	4.47	7 (38%)	22,30,33	1.75	5 (22%)
3	OMC	L5	2351	3	19,22,23	2.96	8 (42%)	26,31,34	0.79	0
3	PSU	L5	2843	3	18,21,22	4.48	7 (38%)	22,30,33	1.77	4 (18%)
3	PSU	L5	3734	3	18,21,22	4.52	7 (38%)	22,30,33	1.82	6 (27%)
3	OMG	L5	4494	3	23,26,27	2.38	9 (39%)	33,38,41	2.45	11 (33%)
3	PSU	L5	4532	3	18,21,22	4.47	7 (38%)	22,30,33	1.75	5 (22%)
7	HIC	LB	245	7	10,11,12	1.52	1 (10%)	8,14,16	1.03	0
3	PSU	L5	1781	3	18,21,22	4.49	7 (38%)	22,30,33	1.71	5 (22%)
3	PSU	L5	4576	3	18,21,22	4.47	7 (38%)	22,30,33	1.81	5 (22%)
3	OMU	L5	4306	3	19,22,23	3.01	8 (42%)	26,31,34	1.69	5 (19%)
3	OMU	L5	4620	3	19,22,23	2.99	8 (42%)	26,31,34	1.62	5 (19%)
50	PSU	S2	1445	50	18,21,22	4.52	7 (38%)	22,30,33	1.82	6 (27%)
50	A2M	S2	512	50	22,25,26	3.41	9 (40%)	31,36,39	2.43	11 (35%)
3	PSU	L5	3844	3	18,21,22	4.45	7 (38%)	22,30,33	1.70	4 (18%)
50	OMG	S2	644	50	23,26,27	2.41	9 (39%)	33,38,41	2.51	10 (30%)
3	OMC	L5	2365	3	19,22,23	2.96	8 (42%)	26,31,34	0.71	0
3	UY1	L5	3818	87,3	19,22,23	0.18	0	22,31,34	0.40	0
3	PSU	L5	4361	3	18,21,22	4.45	7 (38%)	22,30,33	1.74	5 (22%)
43	M3L	Lm	98	43	10,11,12	0.51	0	9,14,16	0.48	0
3	OMG	L5	4196	3,49	23,26,27	2.41	9 (39%)	33,38,41	2.55	10 (30%)
3	OMC	L5	1881	3,86	19,22,23	2.96	8 (42%)	26,31,34	0.79	0
3	PSU	L5	4403	3	18,21,22	4.41	7 (38%)	22,30,33	1.89	6 (27%)
3	PSU	L5	4471	3	18,21,22	4.46	7 (38%)	22,30,33	1.71	5 (22%)
3	A2M	L5	4523	3,86	22,25,26	3.40	8 (36%)	31,36,39	2.42	11 (35%)
3	OMC	L5	3887	3	19,22,23	2.97	8 (42%)	26,31,34	0.74	0
5	PSU	L8	69	5	18,21,22	4.51	8 (44%)	22,30,33	1.86	6 (27%)
50	OMC	S2	174	50	19,22,23	3.02	8 (42%)	26,31,34	0.74	0
50	OMU	S2	428	50	19,22,23	3.04	8 (42%)	26,31,34	1.77	5 (19%)
50	PSU	S2	918	50	18,21,22	4.56	8 (44%)	22,30,33	1.89	5 (22%)
3	OMG	L5	3744	3	23,26,27	2.39	9 (39%)	33,38,41	2.47	11 (33%)
50	OMU	S2	627	50	19,22,23	0.26	0	26,31,34	0.45	0
50	PSU	S2	609	50	18,21,22	4.52	7 (38%)	22,30,33	1.81	5 (22%)
3	PSU	L5	2508	3	18,21,22	4.49	7 (38%)	22,30,33	1.73	5 (22%)
3	OMU	L5	4227	3	19,22,23	3.07	8 (42%)	26,31,34	1.76	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	PSU	S2	649	50	18,21,22	4.48	7 (38%)	22,30,33	1.81	5 (22%)
3	PSU	L5	3851	3	18,21,22	4.45	7 (38%)	22,30,33	1.79	6 (27%)
50	PSU	S2	1244	50	18,21,22	4.49	7 (38%)	22,30,33	1.76	5 (22%)
50	A2M	S2	27	50	22,25,26	3.40	9 (40%)	31,36,39	2.40	11 (35%)
3	OMG	L5	3627	3	23,26,27	2.39	9 (39%)	33,38,41	2.37	13 (39%)
50	PSU	S2	815	50	18,21,22	4.51	7 (38%)	22,30,33	1.77	5 (22%)
50	A2M	S2	468	50	22,25,26	3.43	8 (36%)	31,36,39	2.40	12 (38%)
3	OMC	L5	1340	3	19,22,23	2.92	8 (42%)	26,31,34	0.70	0
50	G7M	S2	1639	50,49	23,26,27	2.62	8 (34%)	35,39,42	2.56	11 (31%)
50	A2M	S2	1383	50	22,25,26	3.42	8 (36%)	31,36,39	2.44	11 (35%)
3	PSU	L5	4293	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
3	PSU	L5	4972	3	18,21,22	4.47	7 (38%)	22,30,33	1.73	5 (22%)
50	PSU	S2	296	50	18,21,22	4.52	7 (38%)	22,30,33	1.79	5 (22%)
3	PSU	L5	1744	87,3	18,21,22	4.46	7 (38%)	22,30,33	1.80	5 (22%)
49	M2G	Pt	26	49	24,27,28	0.55	0	35,40,43	0.75	1 (2%)
3	OMC	L5	2422	3,86	19,22,23	2.98	8 (42%)	26,31,34	0.76	0
3	A2M	L5	3785	3	22,25,26	3.36	9 (40%)	31,36,39	2.51	12 (38%)
3	OMU	L5	2837	3	19,22,23	3.01	8 (42%)	26,31,34	1.74	5 (19%)
50	PSU	S2	218	50	18,21,22	4.50	7 (38%)	22,30,33	1.71	4 (18%)
3	OMG	L5	4228	3	23,26,27	2.37	9 (39%)	33,38,41	2.36	12 (36%)
50	4AC	S2	1337	50	21,24,25	3.43	10 (47%)	29,34,37	1.02	2 (6%)
3	A2M	L5	2787	3	22,25,26	3.41	10 (45%)	31,36,39	2.37	11 (35%)
3	PSU	L5	4299	3	18,21,22	4.50	7 (38%)	22,30,33	1.79	5 (22%)
50	PSU	S2	1643	50	18,21,22	4.52	7 (38%)	22,30,33	1.81	6 (27%)
3	OMU	L5	4498	3	19,22,23	3.04	8 (42%)	26,31,34	1.72	5 (19%)
50	OMU	S2	354	50	19,22,23	3.03	8 (42%)	26,31,34	1.75	5 (19%)
50	PSU	S2	863	50	18,21,22	4.53	7 (38%)	22,30,33	1.81	5 (22%)
3	OMG	L5	2876	3	23,26,27	2.41	9 (39%)	33,38,41	2.65	10 (30%)
3	A2M	L5	2363	3,86	22,25,26	3.43	9 (40%)	31,36,39	2.34	10 (32%)
3	PSU	L5	4420	3	18,21,22	4.49	9 (50%)	22,30,33	1.69	4 (18%)
3	OMC	L5	4456	3	19,22,23	2.98	8 (42%)	26,31,34	0.75	0
3	PSU	L5	3729	3	18,21,22	4.49	7 (38%)	22,30,33	1.70	5 (22%)
1	MA7	At	58	1	20,24,25	0.54	0	24,35,38	0.75	0
3	PSU	L5	4431	3	18,21,22	4.47	7 (38%)	22,30,33	1.79	5 (22%)
50	PSU	S2	109	50	18,21,22	4.49	7 (38%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	PSU	S2	966	50	18,21,22	4.53	7 (38%)	22,30,33	1.85	5 (22%)
50	OMU	S2	1442	50	19,22,23	3.08	8 (42%)	26,31,34	1.66	4 (15%)
50	4AC	S2	1842	50	21,24,25	3.45	9 (42%)	29,34,37	1.06	3 (10%)
3	OMG	L5	3944	3	23,26,27	2.44	9 (39%)	33,38,41	2.54	10 (30%)
50	PSU	S2	1692	50	18,21,22	4.47	7 (38%)	22,30,33	1.78	5 (22%)
3	A2M	L5	1871	3,86	22,25,26	3.44	9 (40%)	31,36,39	2.39	11 (35%)
3	A2M	L5	1326	3	22,25,26	3.43	9 (40%)	31,36,39	2.36	10 (32%)
3	PSU	L5	1862	3	18,21,22	4.50	7 (38%)	22,30,33	1.79	5 (22%)
50	A2M	S2	590	50	22,25,26	3.40	9 (40%)	31,36,39	2.47	12 (38%)
3	PSU	L5	1860	3	18,21,22	4.43	7 (38%)	22,30,33	1.79	5 (22%)
50	OMU	S2	172	50	19,22,23	3.06	8 (42%)	26,31,34	1.74	5 (19%)
3	A2M	L5	398	3	22,25,26	3.41	9 (40%)	31,36,39	2.35	10 (32%)
3	OMG	L5	3899	3,86	23,26,27	2.37	9 (39%)	33,38,41	2.37	13 (39%)
3	A2M	L5	4590	3	22,25,26	3.42	9 (40%)	31,36,39	2.40	10 (32%)
3	PSU	L5	3695	87,3	18,21,22	4.49	7 (38%)	22,30,33	1.90	6 (27%)
50	PSU	S2	822	50	18,21,22	4.55	8 (44%)	22,30,33	1.79	6 (27%)
50	PSU	S2	406	50	18,21,22	4.50	7 (38%)	22,30,33	1.84	5 (22%)
3	A2M	L5	3760	3	22,25,26	0.20	0	31,36,39	0.58	0
3	6MZ	L5	4220	3	22,25,26	2.50	4 (18%)	30,36,39	2.24	9 (30%)
50	PSU	S2	801	50	18,21,22	4.53	7 (38%)	22,30,33	1.82	5 (22%)
3	OMG	L5	4392	3	23,26,27	2.35	9 (39%)	33,38,41	2.36	10 (30%)
6	V5N	LA	216	6	9,11,12	2.61	2 (22%)	9,14,16	1.23	0
50	PSU	S2	1367	50	18,21,22	4.55	7 (38%)	22,30,33	1.85	5 (22%)
3	PSU	L5	3884	3	18,21,22	4.46	7 (38%)	22,30,33	1.79	5 (22%)
3	5MC	L5	4447	3	18,22,23	3.54	7 (38%)	26,32,35	1.07	1 (3%)
3	PSU	L5	5001	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
3	UR3	L5	4530	87,3	19,22,23	2.75	8 (42%)	26,32,35	1.31	2 (7%)
3	PSU	L5	3762	3	18,21,22	4.48	7 (38%)	22,30,33	1.79	5 (22%)
50	OMG	S2	601	50	23,26,27	2.37	9 (39%)	33,38,41	2.48	11 (33%)
3	PSU	L5	4500	3	18,21,22	4.49	7 (38%)	22,30,33	1.87	5 (22%)
3	PSU	L5	1582	3	18,21,22	4.45	7 (38%)	22,30,33	1.74	5 (22%)
3	OMG	L5	2424	3	23,26,27	2.43	8 (34%)	33,38,41	2.58	9 (27%)
50	OMG	S2	1447	50	23,26,27	2.45	9 (39%)	33,38,41	2.58	10 (30%)
50	PSU	S2	1238	50	18,21,22	4.52	7 (38%)	22,30,33	1.85	5 (22%)
50	PSU	S2	814	50	18,21,22	4.47	7 (38%)	22,30,33	1.73	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	2364	3	23,26,27	2.35	9 (39%)	33,38,41	2.39	12 (36%)
3	OMG	L5	4499	1,3	23,26,27	2.40	9 (39%)	33,38,41	2.46	10 (30%)
49	1MA	Pt	58	49	21,25,26	0.37	0	31,37,40	0.68	0
3	PSU	L5	2632	3	18,21,22	4.50	7 (38%)	22,30,33	1.74	5 (22%)
3	OMC	L5	2804	3	19,22,23	2.98	8 (42%)	26,31,34	0.70	0
3	A2M	L5	2815	3	22,25,26	3.41	10 (45%)	31,36,39	2.40	10 (32%)
50	A2M	S2	166	50	22,25,26	3.44	9 (40%)	31,36,39	2.43	11 (35%)
50	B8N	S2	1248	50	24,29,30	3.15	8 (33%)	29,42,45	1.73	5 (17%)
3	PSU	L5	4423	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
50	OMG	S2	1490	86,50	23,26,27	2.38	9 (39%)	33,38,41	2.39	11 (33%)
3	PSU	L5	4628	3	18,21,22	4.50	7 (38%)	22,30,33	1.88	5 (22%)
50	PSU	S2	93	50	18,21,22	4.52	7 (38%)	22,30,33	1.68	4 (18%)
3	PSU	L5	3770	3	18,21,22	4.48	7 (38%)	22,30,33	1.80	5 (22%)
3	A2M	L5	3867	3	22,25,26	3.44	10 (45%)	31,36,39	2.37	11 (35%)
3	PSU	L5	3853	3,86	18,21,22	4.45	7 (38%)	22,30,33	1.79	5 (22%)
50	PSU	S2	1081	50	18,21,22	0.93	1 (5%)	22,30,33	0.89	1 (4%)
3	PSU	L5	2839	3	18,21,22	4.48	7 (38%)	22,30,33	1.75	5 (22%)
50	PSU	S2	1004	50	18,21,22	4.54	7 (38%)	22,30,33	1.77	5 (22%)
3	OMG	L5	1522	3	23,26,27	2.38	9 (39%)	33,38,41	2.40	11 (33%)
3	5MC	L5	3782	3,86	18,22,23	3.51	7 (38%)	26,32,35	1.04	2 (7%)
3	PSU	L5	4457	3	18,21,22	4.46	7 (38%)	22,30,33	1.74	5 (22%)
3	PSU	L5	4493	3	18,21,22	4.47	7 (38%)	22,30,33	1.75	5 (22%)
50	OMG	S2	436	50	23,26,27	2.41	9 (39%)	33,38,41	2.47	12 (36%)
50	A2M	S2	159	50	22,25,26	3.43	9 (40%)	31,36,39	2.36	10 (32%)
3	OMC	L5	3808	3	19,22,23	2.93	8 (42%)	26,31,34	0.73	0
3	OMG	L5	4618	3	23,26,27	2.38	9 (39%)	33,38,41	2.39	13 (39%)
50	UY1	S2	1326	50	19,22,23	0.17	0	22,31,34	0.31	0
50	PSU	S2	1239	50	18,21,22	4.53	7 (38%)	22,30,33	1.77	5 (22%)
3	A2M	L5	400	3	22,25,26	3.43	9 (40%)	31,36,39	2.36	10 (32%)
50	PSU	S2	1625	50	18,21,22	4.55	7 (38%)	22,30,33	1.75	5 (22%)
3	PSU	L5	4673	3	18,21,22	4.46	7 (38%)	22,30,33	1.76	5 (22%)
50	PSU	S2	1347	50	18,21,22	4.51	7 (38%)	22,30,33	1.80	5 (22%)
32	MLZ	Lb	5	32	8,9,10	0.76	0	4,9,11	0.61	0
3	OMC	L5	3701	87,3	19,22,23	2.95	8 (42%)	26,31,34	0.73	0
3	PSU	L5	5010	3	18,21,22	4.48	7 (38%)	22,30,33	1.83	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	OMC	S2	1703	50	19,22,23	0.30	0	26,31,34	0.49	0
50	OMU	S2	116	50	19,22,23	3.02	8 (42%)	26,31,34	1.67	4 (15%)
3	A2M	L5	1534	3,86	22,25,26	3.42	9 (40%)	31,36,39	2.36	11 (35%)
3	PSU	L5	4353	3	18,21,22	4.47	7 (38%)	22,30,33	1.76	5 (22%)
50	A2M	S2	484	50	22,25,26	3.38	9 (40%)	31,36,39	2.39	10 (32%)
3	A2M	L5	1524	3	22,25,26	3.41	9 (40%)	31,36,39	2.43	12 (38%)
5	OMU	L8	14	5,3	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
50	PSU	S2	34	50	18,21,22	4.52	7 (38%)	22,30,33	1.79	5 (22%)
3	OMU	L5	2415	3	19,22,23	3.05	8 (42%)	26,31,34	1.70	5 (19%)
3	PSU	L5	3639	3	18,21,22	4.47	7 (38%)	22,30,33	1.81	6 (27%)
3	PSU	L5	4569	3	18,21,22	4.48	7 (38%)	22,30,33	1.72	5 (22%)
3	1MA	L5	1322	3,86	21,25,26	2.89	6 (28%)	31,37,40	2.90	8 (25%)
3	OMG	L5	1316	3	23,26,27	2.40	9 (39%)	33,38,41	2.42	11 (33%)
3	OMC	L5	3869	3	19,22,23	2.96	8 (42%)	26,31,34	0.74	0
49	1MG	Pt	37	49	22,26,27	0.54	0	33,39,42	0.71	1 (3%)
50	PSU	S2	36	50	18,21,22	4.51	7 (38%)	22,30,33	1.79	5 (22%)
3	A2M	L5	3724	3	22,25,26	3.44	9 (40%)	31,36,39	2.35	10 (32%)
3	PSU	L5	4579	3	18,21,22	4.44	7 (38%)	22,30,33	1.76	5 (22%)
50	OMU	S2	1288	50	19,22,23	3.08	8 (42%)	26,31,34	1.62	5 (19%)
3	PSU	L5	1536	3	18,21,22	4.45	7 (38%)	22,30,33	1.81	5 (22%)
3	PSU	L5	1779	3	18,21,22	4.50	7 (38%)	22,30,33	1.78	5 (22%)
3	PSU	L5	3758	3	18,21,22	4.52	7 (38%)	22,30,33	1.81	5 (22%)
49	1MG	Pt	9	49	22,26,27	0.60	0	33,39,42	0.73	1 (3%)
50	6MZ	S2	1832	86,50	22,25,26	0.14	0	30,36,39	0.40	0
3	A2M	L5	4571	3	22,25,26	3.46	9 (40%)	31,36,39	2.37	11 (35%)
3	PSU	L5	1677	3	18,21,22	4.54	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	L5	1683	87,3	18,21,22	4.50	7 (38%)	22,30,33	1.75	5 (22%)
3	OMG	L5	1625	87,3	23,26,27	2.39	9 (39%)	33,38,41	2.50	10 (30%)
3	OMG	L5	4370	3	23,26,27	2.38	9 (39%)	33,38,41	2.46	10 (30%)
3	A2M	L5	2401	3	22,25,26	3.40	9 (40%)	31,36,39	2.34	9 (29%)
50	OMG	S2	509	50	23,26,27	2.40	9 (39%)	33,38,41	2.51	10 (30%)
50	A2M	S2	1678	50	22,25,26	3.46	9 (40%)	31,36,39	2.43	11 (35%)
5	OMG	L8	75	5	23,26,27	2.39	9 (39%)	33,38,41	2.44	12 (36%)
50	PSU	S2	1177	50	18,21,22	4.50	7 (38%)	22,30,33	1.83	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PSU	S2	119	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	573	50	-	2/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4637	87,3	-	3/9/27/28	0/3/3/3
50	A2M	S2	99	86,50	-	2/9/27/28	0/3/3/3
50	OMC	S2	462	50	-	1/9/27/28	0/2/2/2
3	PSU	L5	3764	87,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	105	50	-	0/7/25/26	0/2/2/2
50	OMG	S2	1328	50	-	1/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	651	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	572	50	-	2/7/25/26	0/2/2/2
50	OMU	S2	121	50	-	0/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
50	OMC	S2	517	50	-	0/9/27/28	0/2/2/2
3	PSU	L5	3920	3,86	-	0/7/25/26	0/2/2/2
50	OMG	S2	683	50	-	2/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
50	OMU	S2	1804	50	-	1/9/27/28	0/2/2/2
50	PSU	S2	866	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	681	50	-	0/7/25/26	0/2/2/2
50	PSU	S2	1243	50	-	5/7/25/26	0/2/2/2
50	MA6	S2	1850	50	-	0/11/29/30	0/3/3/3
74	HY3	SX	62	87,74	-	1/1/12/14	0/1/1/1
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	87,3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
50	MA6	S2	1851	50	-	3/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A2M	S2	576	50	-	2/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
50	PSU	S2	1232	50	-	0/7/25/26	0/2/2/2
45	MLZ	Lo	53	45	-	0/7/8/10	-
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	1136	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	3,86	-	0/7/25/26	0/2/2/2
50	PSU	S2	686	50	-	0/7/25/26	0/2/2/2
50	PSU	S2	1174	50	-	0/7/25/26	0/2/2/2
50	OMC	S2	1391	50	-	0/9/27/28	0/2/2/2
50	A2M	S2	1031	50	-	0/9/27/28	0/3/3/3
50	A2M	S2	668	86,50	-	5/9/27/28	0/3/3/3
31	V5N	La	39	31	-	1/9/10/12	0/1/1/1
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	1056	50	-	0/7/25/26	0/2/2/2
50	OMG	S2	867	50	-	1/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	2/7/25/26	0/2/2/2
7	HIC	LB	245	7	-	0/5/6/8	0/1/1/1
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	1445	50	-	0/7/25/26	0/2/2/2
50	A2M	S2	512	50	-	2/9/27/28	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
50	OMG	S2	644	50	-	4/9/27/28	0/3/3/3
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	UY1	L5	3818	87,3	-	4/9/27/28	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
43	M3L	Lm	98	43	-	2/9/10/12	-
3	OMG	L5	4196	3,49	-	0/9/27/28	0/3/3/3
3	OMC	L5	1881	3,86	-	0/9/27/28	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,86	-	0/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
50	OMC	S2	174	50	-	0/9/27/28	0/2/2/2
50	OMU	S2	428	50	-	6/9/27/28	0/2/2/2
50	PSU	S2	918	50	-	2/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
50	OMU	S2	627	50	-	0/9/27/28	0/2/2/2
50	PSU	S2	609	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	1/9/27/28	0/2/2/2
50	PSU	S2	649	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	2/7/25/26	0/2/2/2
50	PSU	S2	1244	50	-	0/7/25/26	0/2/2/2
50	A2M	S2	27	50	-	1/9/27/28	0/3/3/3
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	815	50	-	0/7/25/26	0/2/2/2
50	A2M	S2	468	50	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
50	G7M	S2	1639	50,49	-	0/7/25/26	0/3/3/3
50	A2M	S2	1383	50	-	2/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	296	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
49	M2G	Pt	26	49	-	0/11/29/30	0/3/3/3
3	OMC	L5	2422	3,86	-	2/9/27/28	0/2/2/2
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
50	PSU	S2	218	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
50	4AC	S2	1337	50	-	0/11/29/30	0/2/2/2
3	A2M	L5	2787	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	1643	50	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
50	OMU	S2	354	50	-	0/9/27/28	0/2/2/2
50	PSU	S2	863	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	3,86	-	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	-	2/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
1	MA7	At	58	1	-	1/7/21/22	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	109	50	-	0/7/25/26	0/2/2/2
50	PSU	S2	966	50	-	0/7/25/26	0/2/2/2
50	OMU	S2	1442	50	-	3/9/27/28	0/2/2/2
50	4AC	S2	1842	50	-	0/11/29/30	0/2/2/2
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
50	PSU	S2	1692	50	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	3,86	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
50	A2M	S2	590	50	-	4/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
50	OMU	S2	172	50	-	0/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	3899	3,86	-	0/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3695	87,3	-	0/7/25/26	0/2/2/2
50	PSU	S2	822	50	-	2/7/25/26	0/2/2/2
50	PSU	S2	406	50	-	0/7/25/26	0/2/2/2
3	A2M	L5	3760	3	-	0/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	801	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
6	V5N	LA	216	6	-	1/9/10/12	0/1/1/1
50	PSU	S2	1367	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
50	OMG	S2	601	50	-	1/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
50	OMG	S2	1447	50	-	2/9/27/28	0/3/3/3
50	PSU	S2	1238	50	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PSU	S2	814	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4499	1,3	-	0/9/27/28	0/3/3/3
49	1MA	Pt	58	49	-	2/7/25/26	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2815	3	-	3/9/27/28	0/3/3/3
50	A2M	S2	166	50	-	0/9/27/28	0/3/3/3
50	B8N	S2	1248	50	-	2/16/34/35	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
50	OMG	S2	1490	86,50	-	3/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	93	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3853	3,86	-	0/7/25/26	0/2/2/2
50	PSU	S2	1081	50	-	1/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	1004	50	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	3782	3,86	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
50	OMG	S2	436	50	-	0/9/27/28	0/3/3/3
50	A2M	S2	159	50	-	0/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
50	UY1	S2	1326	50	-	2/9/27/28	0/2/2/2
50	PSU	S2	1239	50	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
50	PSU	S2	1625	50	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
50	PSU	S2	1347	50	-	0/7/25/26	0/2/2/2
32	MLZ	Lb	5	32	-	2/7/8/10	-
3	OMC	L5	3701	87,3	-	4/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
50	OMC	S2	1703	50	-	0/9/27/28	0/2/2/2
50	OMU	S2	116	50	-	2/9/27/28	0/2/2/2
3	A2M	L5	1534	3,86	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
50	A2M	S2	484	50	-	0/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
5	OMU	L8	14	5,3	-	1/9/27/28	0/2/2/2
50	PSU	S2	34	50	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	0/7/25/26	0/2/2/2
3	1MA	L5	1322	3,86	-	1/7/25/26	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
49	1MG	Pt	37	49	-	0/7/25/26	0/3/3/3
50	PSU	S2	36	50	-	0/7/25/26	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
50	OMU	S2	1288	50	-	1/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
49	1MG	Pt	9	49	-	1/7/25/26	0/3/3/3
50	6MZ	S2	1832	86,50	-	1/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	87,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
50	OMG	S2	509	50	-	2/9/27/28	0/3/3/3
50	A2M	S2	1678	50	-	1/9/27/28	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
50	PSU	S2	1177	50	-	0/7/25/26	0/2/2/2

All (1630) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	1625	PSU	C6-C5	11.83	1.49	1.35
50	S2	1232	PSU	C6-C5	11.82	1.49	1.35
50	S2	93	PSU	C6-C5	11.81	1.49	1.35
3	L5	1683	PSU	C6-C5	11.80	1.49	1.35
50	S2	686	PSU	C6-C5	11.77	1.49	1.35
50	S2	1367	PSU	C6-C5	11.76	1.49	1.35
3	L5	1862	PSU	C6-C5	11.75	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	866	PSU	C6-C5	11.74	1.49	1.35
3	L5	4628	PSU	C6-C5	11.74	1.49	1.35
3	L5	3729	PSU	C6-C5	11.73	1.49	1.35
50	S2	1004	PSU	C6-C5	11.73	1.49	1.35
3	L5	4569	PSU	C6-C5	11.72	1.49	1.35
50	S2	1239	PSU	C6-C5	11.71	1.49	1.35
50	S2	573	PSU	C6-C5	11.71	1.48	1.35
3	L5	1779	PSU	C6-C5	11.71	1.48	1.35
50	S2	822	PSU	C6-C5	11.71	1.48	1.35
50	S2	296	PSU	C6-C5	11.69	1.48	1.35
50	S2	649	PSU	C6-C5	11.69	1.48	1.35
50	S2	801	PSU	C6-C5	11.69	1.48	1.35
50	S2	119	PSU	C6-C5	11.69	1.48	1.35
50	S2	218	PSU	C6-C5	11.68	1.48	1.35
3	L5	1677	PSU	C6-C5	11.68	1.48	1.35
50	S2	1238	PSU	C6-C5	11.68	1.48	1.35
50	S2	572	PSU	C6-C5	11.67	1.48	1.35
3	L5	2843	PSU	C6-C5	11.67	1.48	1.35
3	L5	4423	PSU	C6-C5	11.67	1.48	1.35
50	S2	34	PSU	C6-C5	11.67	1.48	1.35
50	S2	863	PSU	C6-C5	11.67	1.48	1.35
3	L5	1781	PSU	C6-C5	11.67	1.48	1.35
3	L5	2632	PSU	C6-C5	11.67	1.48	1.35
3	L5	2839	PSU	C6-C5	11.67	1.48	1.35
50	S2	1445	PSU	C6-C5	11.67	1.48	1.35
3	L5	5010	PSU	C6-C5	11.66	1.48	1.35
50	S2	815	PSU	C6-C5	11.66	1.48	1.35
50	S2	1643	PSU	C6-C5	11.66	1.48	1.35
50	S2	609	PSU	C6-C5	11.66	1.48	1.35
50	S2	966	PSU	C6-C5	11.66	1.48	1.35
3	L5	4293	PSU	C6-C5	11.66	1.48	1.35
50	S2	36	PSU	C6-C5	11.66	1.48	1.35
5	L8	69	PSU	C6-C5	11.65	1.48	1.35
50	S2	1347	PSU	C6-C5	11.65	1.48	1.35
3	L5	3762	PSU	C6-C5	11.65	1.48	1.35
3	L5	3768	PSU	C6-C5	11.65	1.48	1.35
3	L5	3844	PSU	C6-C5	11.65	1.48	1.35
3	L5	4636	PSU	C6-C5	11.65	1.48	1.35
50	S2	1243	PSU	C6-C5	11.65	1.48	1.35
3	L5	4500	PSU	C6-C5	11.64	1.48	1.35
3	L5	4312	PSU	C6-C5	11.63	1.48	1.35
3	L5	3734	PSU	C6-C5	11.63	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	406	PSU	C6-C5	11.63	1.48	1.35
3	L5	3758	PSU	C6-C5	11.62	1.48	1.35
50	S2	1244	PSU	C6-C5	11.62	1.48	1.35
3	L5	4299	PSU	C6-C5	11.61	1.48	1.35
3	L5	4532	PSU	C6-C5	11.60	1.48	1.35
3	L5	3764	PSU	C6-C5	11.60	1.48	1.35
3	L5	3637	PSU	C6-C5	11.60	1.48	1.35
3	L5	4673	PSU	C6-C5	11.60	1.48	1.35
3	L5	4521	PSU	C6-C5	11.59	1.48	1.35
50	S2	651	PSU	C6-C5	11.59	1.48	1.35
3	L5	4493	PSU	C6-C5	11.58	1.48	1.35
50	S2	1174	PSU	C6-C5	11.58	1.48	1.35
3	L5	1536	PSU	C6-C5	11.58	1.48	1.35
3	L5	1782	PSU	C6-C5	11.58	1.48	1.35
50	S2	1177	PSU	C6-C5	11.58	1.48	1.35
3	L5	4420	PSU	C6-C5	11.58	1.48	1.35
50	S2	814	PSU	C6-C5	11.58	1.48	1.35
50	S2	105	PSU	C6-C5	11.57	1.48	1.35
3	L5	4431	PSU	C6-C5	11.56	1.48	1.35
3	L5	3695	PSU	C6-C5	11.56	1.48	1.35
3	L5	3884	PSU	C6-C5	11.55	1.48	1.35
3	L5	4552	PSU	C6-C5	11.55	1.48	1.35
3	L5	4353	PSU	C6-C5	11.55	1.48	1.35
3	L5	4471	PSU	C6-C5	11.55	1.48	1.35
3	L5	4972	PSU	C6-C5	11.55	1.48	1.35
3	L5	5001	PSU	C6-C5	11.54	1.48	1.35
50	S2	918	PSU	C6-C5	11.54	1.48	1.35
50	S2	1136	PSU	C6-C5	11.54	1.48	1.35
3	L5	4296	PSU	C6-C5	11.54	1.48	1.35
3	L5	2508	PSU	C6-C5	11.54	1.48	1.35
3	L5	4361	PSU	C6-C5	11.53	1.48	1.35
3	L5	3770	PSU	C6-C5	11.53	1.48	1.35
3	L5	4457	PSU	C6-C5	11.53	1.48	1.35
3	L5	3920	PSU	C6-C5	11.53	1.48	1.35
50	S2	1692	PSU	C6-C5	11.52	1.48	1.35
50	S2	109	PSU	C6-C5	11.51	1.48	1.35
3	L5	1582	PSU	C6-C5	11.51	1.48	1.35
3	L5	4442	PSU	C6-C5	11.50	1.48	1.35
50	S2	681	PSU	C6-C5	11.50	1.48	1.35
5	L8	55	PSU	C6-C5	11.50	1.48	1.35
3	L5	3639	PSU	C6-C5	11.49	1.48	1.35
3	L5	3851	PSU	C6-C5	11.49	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3853	PSU	C6-C5	11.46	1.48	1.35
3	L5	4689	PSU	C6-C5	11.46	1.48	1.35
3	L5	4579	PSU	C6-C5	11.46	1.48	1.35
3	L5	1792	PSU	C6-C5	11.45	1.48	1.35
3	L5	1744	PSU	C6-C5	11.44	1.48	1.35
3	L5	4576	PSU	C6-C5	11.44	1.48	1.35
3	L5	1860	PSU	C6-C5	11.42	1.48	1.35
50	S2	1056	PSU	C6-C5	11.39	1.48	1.35
3	L5	4403	PSU	C6-C5	11.20	1.48	1.35
3	L5	4220	6MZ	C6-N6	10.26	1.45	1.34
50	S2	1367	PSU	C2-N1	9.94	1.50	1.36
50	S2	866	PSU	C2-N1	9.86	1.50	1.36
50	S2	686	PSU	C2-N1	9.83	1.50	1.36
50	S2	801	PSU	C2-N1	9.83	1.50	1.36
50	S2	966	PSU	C2-N1	9.80	1.50	1.36
50	S2	1004	PSU	C2-N1	9.78	1.50	1.36
3	L5	3758	PSU	C2-N1	9.78	1.50	1.36
50	S2	573	PSU	C2-N1	9.77	1.50	1.36
50	S2	109	PSU	C2-N1	9.76	1.49	1.36
50	S2	822	PSU	C2-N1	9.76	1.49	1.36
3	L5	4299	PSU	C2-N1	9.76	1.49	1.36
50	S2	815	PSU	C2-N1	9.76	1.49	1.36
50	S2	34	PSU	C2-N1	9.75	1.49	1.36
50	S2	863	PSU	C2-N1	9.75	1.49	1.36
50	S2	651	PSU	C2-N1	9.75	1.49	1.36
50	S2	1177	PSU	C2-N1	9.74	1.49	1.36
50	S2	93	PSU	C2-N1	9.73	1.49	1.36
50	S2	1239	PSU	C2-N1	9.73	1.49	1.36
50	S2	1625	PSU	C2-N1	9.73	1.49	1.36
50	S2	1445	PSU	C2-N1	9.73	1.49	1.36
3	L5	3734	PSU	C2-N1	9.72	1.49	1.36
50	S2	36	PSU	C2-N1	9.72	1.49	1.36
3	L5	1862	PSU	C2-N1	9.72	1.49	1.36
50	S2	406	PSU	C2-N1	9.71	1.49	1.36
50	S2	1243	PSU	C2-N1	9.71	1.49	1.36
50	S2	296	PSU	C2-N1	9.71	1.49	1.36
50	S2	918	PSU	C2-N1	9.70	1.49	1.36
3	L5	3695	PSU	C2-N1	9.70	1.49	1.36
50	S2	572	PSU	C2-N1	9.69	1.49	1.36
3	L5	1781	PSU	C2-N1	9.69	1.49	1.36
3	L5	4972	PSU	C2-N1	9.69	1.49	1.36
50	S2	1347	PSU	C2-N1	9.69	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2508	PSU	C2-N1	9.68	1.49	1.36
50	S2	1056	PSU	C2-N1	9.67	1.49	1.36
50	S2	609	PSU	C2-N1	9.67	1.49	1.36
50	S2	1643	PSU	C2-N1	9.67	1.49	1.36
50	S2	119	PSU	C2-N1	9.67	1.49	1.36
50	S2	1238	PSU	C2-N1	9.66	1.49	1.36
3	L5	4576	PSU	C2-N1	9.66	1.49	1.36
3	L5	3770	PSU	C2-N1	9.66	1.49	1.36
50	S2	1692	PSU	C2-N1	9.66	1.49	1.36
3	L5	3764	PSU	C2-N1	9.66	1.49	1.36
3	L5	4353	PSU	C2-N1	9.65	1.49	1.36
50	S2	105	PSU	C2-N1	9.65	1.49	1.36
3	L5	2632	PSU	C2-N1	9.64	1.49	1.36
3	L5	3639	PSU	C2-N1	9.64	1.49	1.36
50	S2	1136	PSU	C2-N1	9.64	1.49	1.36
5	L8	55	PSU	C2-N1	9.63	1.49	1.36
3	L5	1792	PSU	C2-N1	9.63	1.49	1.36
3	L5	1779	PSU	C2-N1	9.63	1.49	1.36
3	L5	4442	PSU	C2-N1	9.63	1.49	1.36
3	L5	2843	PSU	C2-N1	9.63	1.49	1.36
3	L5	4296	PSU	C2-N1	9.62	1.49	1.36
3	L5	4521	PSU	C2-N1	9.62	1.49	1.36
50	S2	1244	PSU	C2-N1	9.62	1.49	1.36
3	L5	4532	PSU	C2-N1	9.62	1.49	1.36
3	L5	5001	PSU	C2-N1	9.62	1.49	1.36
3	L5	4457	PSU	C2-N1	9.61	1.49	1.36
3	L5	4431	PSU	C2-N1	9.61	1.49	1.36
3	L5	4312	PSU	C2-N1	9.61	1.49	1.36
3	L5	1677	PSU	C2-N1	9.61	1.49	1.36
50	S2	218	PSU	C2-N1	9.61	1.49	1.36
5	L8	69	PSU	C2-N1	9.60	1.49	1.36
3	L5	4628	PSU	C2-N1	9.59	1.49	1.36
3	L5	1744	PSU	C2-N1	9.59	1.49	1.36
3	L5	4569	PSU	C2-N1	9.59	1.49	1.36
3	L5	4493	PSU	C2-N1	9.59	1.49	1.36
3	L5	3637	PSU	C2-N1	9.58	1.49	1.36
3	L5	1683	PSU	C2-N1	9.58	1.49	1.36
3	L5	3768	PSU	C2-N1	9.58	1.49	1.36
3	L5	1860	PSU	C2-N1	9.58	1.49	1.36
3	L5	4500	PSU	C2-N1	9.57	1.49	1.36
50	S2	814	PSU	C2-N1	9.57	1.49	1.36
3	L5	4471	PSU	C2-N1	9.56	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	681	PSU	C2-N1	9.56	1.49	1.36
50	S2	1232	PSU	C2-N1	9.56	1.49	1.36
3	L5	3853	PSU	C2-N1	9.55	1.49	1.36
3	L5	4636	PSU	C2-N1	9.55	1.49	1.36
3	L5	1782	PSU	C2-N1	9.55	1.49	1.36
3	L5	1536	PSU	C2-N1	9.54	1.49	1.36
3	L5	4361	PSU	C2-N1	9.54	1.49	1.36
3	L5	4420	PSU	C2-N1	9.54	1.49	1.36
50	S2	649	PSU	C2-N1	9.53	1.49	1.36
3	L5	2839	PSU	C2-N1	9.53	1.49	1.36
3	L5	5010	PSU	C2-N1	9.53	1.49	1.36
3	L5	3729	PSU	C2-N1	9.53	1.49	1.36
3	L5	4423	PSU	C2-N1	9.53	1.49	1.36
50	S2	1174	PSU	C2-N1	9.52	1.49	1.36
3	L5	3851	PSU	C2-N1	9.50	1.49	1.36
3	L5	4403	PSU	C2-N1	9.50	1.49	1.36
3	L5	4689	PSU	C2-N1	9.48	1.49	1.36
3	L5	3762	PSU	C2-N1	9.48	1.49	1.36
3	L5	4552	PSU	C2-N1	9.48	1.49	1.36
3	L5	4673	PSU	C2-N1	9.48	1.49	1.36
3	L5	4579	PSU	C2-N1	9.48	1.49	1.36
3	L5	3884	PSU	C2-N1	9.48	1.49	1.36
3	L5	1582	PSU	C2-N1	9.47	1.49	1.36
3	L5	3844	PSU	C2-N1	9.45	1.49	1.36
3	L5	3920	PSU	C2-N1	9.44	1.49	1.36
3	L5	4293	PSU	C2-N1	9.40	1.49	1.36
3	L5	4447	5MC	C6-C5	9.25	1.49	1.34
3	L5	3782	5MC	C6-C5	9.05	1.49	1.34
50	S2	166	A2M	O4'-C1'	8.79	1.62	1.42
3	L5	3867	A2M	C2'-C1'	-8.78	1.30	1.53
50	S2	1383	A2M	O4'-C1'	8.78	1.62	1.42
3	L5	398	A2M	O4'-C1'	8.77	1.62	1.42
3	L5	4571	A2M	C2'-C1'	-8.76	1.30	1.53
50	S2	1678	A2M	C2'-C1'	-8.73	1.30	1.53
3	L5	1326	A2M	C2'-C1'	-8.72	1.30	1.53
3	L5	3785	A2M	C2'-C1'	-8.71	1.30	1.53
3	L5	4523	A2M	O4'-C1'	8.71	1.62	1.42
50	S2	99	A2M	O4'-C1'	8.70	1.62	1.42
3	L5	2815	A2M	O4'-C1'	8.69	1.62	1.42
50	S2	512	A2M	O4'-C1'	8.69	1.62	1.42
3	L5	1534	A2M	O4'-C1'	8.67	1.62	1.42
3	L5	3825	A2M	C2'-C1'	-8.67	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4590	A2M	O4'-C1'	8.67	1.62	1.42
3	L5	1871	A2M	C2'-C1'	-8.66	1.30	1.53
3	L5	1871	A2M	O4'-C1'	8.66	1.62	1.42
3	L5	4571	A2M	O4'-C1'	8.66	1.62	1.42
50	S2	468	A2M	O4'-C1'	8.65	1.62	1.42
3	L5	400	A2M	O4'-C1'	8.65	1.62	1.42
3	L5	3724	A2M	C2'-C1'	-8.64	1.30	1.53
3	L5	3723	A2M	O4'-C1'	8.64	1.62	1.42
3	L5	3718	A2M	O4'-C1'	8.64	1.62	1.42
50	S2	576	A2M	C2'-C1'	-8.63	1.30	1.53
3	L5	3830	A2M	O4'-C1'	8.63	1.62	1.42
50	S2	1678	A2M	O4'-C1'	8.63	1.62	1.42
50	S2	159	A2M	O4'-C1'	8.63	1.62	1.42
3	L5	3830	A2M	C2'-C1'	-8.62	1.30	1.53
50	S2	99	A2M	C2'-C1'	-8.62	1.30	1.53
50	S2	166	A2M	C2'-C1'	-8.62	1.30	1.53
3	L5	2787	A2M	O4'-C1'	8.62	1.62	1.42
50	S2	1031	A2M	C2'-C1'	-8.61	1.30	1.53
50	S2	27	A2M	C2'-C1'	-8.61	1.30	1.53
50	S2	159	A2M	C2'-C1'	-8.61	1.30	1.53
50	S2	468	A2M	C2'-C1'	-8.61	1.30	1.53
3	L5	2363	A2M	C2'-C1'	-8.60	1.30	1.53
3	L5	2363	A2M	O4'-C1'	8.60	1.62	1.42
3	L5	3825	A2M	O4'-C1'	8.59	1.62	1.42
50	S2	27	A2M	O4'-C1'	8.59	1.62	1.42
3	L5	4590	A2M	C2'-C1'	-8.59	1.31	1.53
3	L5	3724	A2M	O4'-C1'	8.58	1.62	1.42
50	S2	590	A2M	O4'-C1'	8.58	1.62	1.42
3	L5	400	A2M	C2'-C1'	-8.57	1.31	1.53
50	S2	1031	A2M	O4'-C1'	8.56	1.62	1.42
3	L5	2401	A2M	C2'-C1'	-8.56	1.31	1.53
3	L5	3723	A2M	C2'-C1'	-8.56	1.31	1.53
3	L5	2401	A2M	O4'-C1'	8.55	1.62	1.42
50	S2	1383	A2M	C2'-C1'	-8.55	1.31	1.53
50	S2	576	A2M	O4'-C1'	8.54	1.62	1.42
3	L5	1326	A2M	O4'-C1'	8.52	1.62	1.42
3	L5	4523	A2M	C2'-C1'	-8.51	1.31	1.53
3	L5	2787	A2M	C2'-C1'	-8.51	1.31	1.53
3	L5	3867	A2M	O4'-C1'	8.51	1.62	1.42
3	L5	3718	A2M	C2'-C1'	-8.50	1.31	1.53
50	S2	484	A2M	O4'-C1'	8.49	1.62	1.42
3	L5	1534	A2M	C2'-C1'	-8.48	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	512	A2M	C2'-C1'	-8.47	1.31	1.53
3	L5	2815	A2M	C2'-C1'	-8.47	1.31	1.53
3	L5	398	A2M	C2'-C1'	-8.46	1.31	1.53
3	L5	1524	A2M	O4'-C1'	8.45	1.62	1.42
50	S2	484	A2M	C2'-C1'	-8.44	1.31	1.53
50	S2	668	A2M	C2'-C1'	-8.36	1.31	1.53
3	L5	1524	A2M	C2'-C1'	-8.36	1.31	1.53
50	S2	590	A2M	C2'-C1'	-8.35	1.31	1.53
50	S2	668	A2M	O4'-C1'	8.33	1.61	1.42
3	L5	3785	A2M	O4'-C1'	8.23	1.61	1.42
3	L5	1322	1MA	C2-N3	7.95	1.45	1.30
50	S2	1248	B8N	C6-N1	7.81	1.55	1.36
50	S2	918	PSU	C2-N3	7.71	1.50	1.37
50	S2	1136	PSU	C2-N3	7.69	1.50	1.37
50	S2	686	PSU	C2-N3	7.68	1.50	1.37
3	L5	1677	PSU	C2-N3	7.68	1.50	1.37
50	S2	296	PSU	C2-N3	7.67	1.50	1.37
50	S2	218	PSU	C2-N3	7.66	1.50	1.37
50	S2	609	PSU	C2-N3	7.66	1.50	1.37
50	S2	1643	PSU	C2-N3	7.63	1.50	1.37
50	S2	1004	PSU	C2-N3	7.63	1.50	1.37
50	S2	34	PSU	C2-N3	7.63	1.50	1.37
50	S2	1445	PSU	C2-N3	7.63	1.50	1.37
50	S2	1232	PSU	C2-N3	7.62	1.50	1.37
50	S2	822	PSU	C2-N3	7.62	1.50	1.37
3	L5	3762	PSU	C2-N3	7.61	1.50	1.37
3	L5	4500	PSU	C2-N3	7.61	1.50	1.37
50	S2	863	PSU	C2-N3	7.61	1.50	1.37
50	S2	1625	PSU	C2-N3	7.61	1.50	1.37
50	S2	866	PSU	C2-N3	7.60	1.50	1.37
3	L5	1322	1MA	C4-N3	7.60	1.51	1.35
3	L5	3758	PSU	C2-N3	7.59	1.50	1.37
50	S2	1239	PSU	C2-N3	7.59	1.50	1.37
50	S2	1244	PSU	C2-N3	7.58	1.50	1.37
50	S2	1248	B8N	C4-N3	-7.58	1.26	1.40
50	S2	1238	PSU	C2-N3	7.58	1.50	1.37
3	L5	5010	PSU	C2-N3	7.57	1.50	1.37
50	S2	801	PSU	C2-N3	7.57	1.50	1.37
50	S2	815	PSU	C2-N3	7.57	1.50	1.37
5	L8	69	PSU	C2-N3	7.56	1.50	1.37
50	S2	814	PSU	C2-N3	7.56	1.50	1.37
50	S2	109	PSU	C2-N3	7.55	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3734	PSU	C2-N3	7.55	1.50	1.37
3	L5	3884	PSU	C2-N3	7.54	1.50	1.37
3	L5	3768	PSU	C2-N3	7.54	1.50	1.37
50	S2	966	PSU	C2-N3	7.54	1.50	1.37
3	L5	4420	PSU	C2-N3	7.54	1.50	1.37
50	S2	1174	PSU	C2-N3	7.54	1.50	1.37
3	L5	3729	PSU	C2-N3	7.53	1.50	1.37
3	L5	4628	PSU	C2-N3	7.52	1.50	1.37
3	L5	4293	PSU	C2-N3	7.52	1.50	1.37
3	L5	2632	PSU	C2-N3	7.52	1.50	1.37
50	S2	573	PSU	C2-N3	7.52	1.50	1.37
3	L5	4689	PSU	C2-N3	7.52	1.50	1.37
3	L5	1779	PSU	C2-N3	7.52	1.50	1.37
50	S2	651	PSU	C2-N3	7.52	1.50	1.37
3	L5	3770	PSU	C2-N3	7.51	1.50	1.37
3	L5	4576	PSU	C2-N3	7.51	1.50	1.37
3	L5	3764	PSU	C2-N3	7.51	1.50	1.37
3	L5	1792	PSU	C2-N3	7.50	1.50	1.37
50	S2	1367	PSU	C2-N3	7.50	1.50	1.37
3	L5	4442	PSU	C2-N3	7.50	1.50	1.37
50	S2	406	PSU	C2-N3	7.50	1.50	1.37
50	S2	1347	PSU	C2-N3	7.50	1.50	1.37
50	S2	649	PSU	C2-N3	7.49	1.50	1.37
50	S2	119	PSU	C2-N3	7.49	1.50	1.37
3	L5	1782	PSU	C2-N3	7.48	1.50	1.37
3	L5	2839	PSU	C2-N3	7.47	1.50	1.37
50	S2	105	PSU	C2-N3	7.47	1.50	1.37
50	S2	1056	PSU	C2-N3	7.47	1.50	1.37
3	L5	5001	PSU	C2-N3	7.47	1.50	1.37
3	L5	1744	PSU	C2-N3	7.47	1.50	1.37
50	S2	1692	PSU	C2-N3	7.46	1.50	1.37
3	L5	1683	PSU	C2-N3	7.46	1.50	1.37
3	L5	2508	PSU	C2-N3	7.45	1.50	1.37
3	L5	4431	PSU	C2-N3	7.45	1.50	1.37
3	L5	4579	PSU	C2-N3	7.45	1.50	1.37
3	L5	4312	PSU	C2-N3	7.45	1.50	1.37
50	S2	1243	PSU	C2-N3	7.45	1.50	1.37
3	L5	4423	PSU	C2-N3	7.45	1.50	1.37
3	L5	1582	PSU	C2-N3	7.44	1.50	1.37
50	S2	36	PSU	C2-N3	7.44	1.50	1.37
50	S2	1177	PSU	C2-N3	7.44	1.50	1.37
3	L5	3639	PSU	C2-N3	7.44	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4493	PSU	C2-N3	7.42	1.50	1.37
50	S2	681	PSU	C2-N3	7.42	1.50	1.37
3	L5	4361	PSU	C2-N3	7.42	1.50	1.37
3	L5	3695	PSU	C2-N3	7.42	1.50	1.37
3	L5	4353	PSU	C2-N3	7.42	1.50	1.37
3	L5	3851	PSU	C2-N3	7.42	1.50	1.37
3	L5	4521	PSU	C2-N3	7.41	1.50	1.37
3	L5	4673	PSU	C2-N3	7.41	1.50	1.37
3	L5	4403	PSU	C2-N3	7.41	1.50	1.37
3	L5	3853	PSU	C2-N3	7.41	1.50	1.37
3	L5	4972	PSU	C2-N3	7.41	1.50	1.37
3	L5	4532	PSU	C2-N3	7.40	1.50	1.37
3	L5	1862	PSU	C2-N3	7.40	1.50	1.37
3	L5	4471	PSU	C2-N3	7.40	1.50	1.37
3	L5	4636	PSU	C2-N3	7.40	1.50	1.37
3	L5	1781	PSU	C2-N3	7.40	1.50	1.37
3	L5	1860	PSU	C2-N3	7.39	1.50	1.37
3	L5	3844	PSU	C2-N3	7.39	1.50	1.37
3	L5	4299	PSU	C2-N3	7.39	1.50	1.37
50	S2	93	PSU	C2-N3	7.38	1.50	1.37
5	L8	55	PSU	C2-N3	7.38	1.50	1.37
3	L5	3920	PSU	C2-N3	7.38	1.50	1.37
3	L5	4296	PSU	C2-N3	7.37	1.50	1.37
3	L5	1536	PSU	C2-N3	7.37	1.50	1.37
3	L5	4457	PSU	C2-N3	7.36	1.50	1.37
3	L5	2843	PSU	C2-N3	7.36	1.50	1.37
3	L5	4552	PSU	C2-N3	7.35	1.50	1.37
3	L5	4569	PSU	C2-N3	7.34	1.50	1.37
50	S2	572	PSU	C2-N3	7.33	1.50	1.37
3	L5	3637	PSU	C2-N3	7.26	1.49	1.37
50	S2	1442	OMU	C2-N1	7.25	1.50	1.38
3	L5	4227	OMU	C2-N1	7.22	1.50	1.38
3	L5	2415	OMU	C2-N1	7.16	1.49	1.38
50	S2	1804	OMU	C2-N1	7.15	1.49	1.38
50	S2	1288	OMU	C2-N1	7.12	1.49	1.38
50	S2	172	OMU	C2-N1	7.06	1.49	1.38
50	S2	354	OMU	C2-N1	7.03	1.49	1.38
50	S2	121	OMU	C2-N1	7.03	1.49	1.38
50	S2	116	OMU	C2-N1	7.00	1.49	1.38
3	L5	3925	OMU	C2-N1	6.98	1.49	1.38
3	L5	2837	OMU	C2-N1	6.97	1.49	1.38
3	L5	4530	UR3	C2-N1	6.96	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	1288	OMU	C2-N3	6.96	1.50	1.38
50	S2	172	OMU	C2-N3	6.95	1.50	1.38
50	S2	1442	OMU	C2-N3	6.95	1.50	1.38
50	S2	428	OMU	C2-N1	6.93	1.49	1.38
3	L5	4498	OMU	C2-N1	6.92	1.49	1.38
5	L8	14	OMU	C2-N1	6.89	1.49	1.38
3	L5	4306	OMU	C2-N1	6.89	1.49	1.38
50	S2	116	OMU	C2-N3	6.88	1.50	1.38
50	S2	1804	OMU	C2-N3	6.87	1.50	1.38
3	L5	4227	OMU	C2-N3	6.85	1.50	1.38
50	S2	1842	4AC	C4-N3	6.83	1.44	1.32
3	L5	4498	OMU	C2-N3	6.81	1.50	1.38
50	S2	354	OMU	C2-N3	6.80	1.50	1.38
3	L5	4620	OMU	C2-N1	6.79	1.49	1.38
50	S2	121	OMU	C2-N3	6.79	1.50	1.38
50	S2	428	OMU	C2-N3	6.77	1.50	1.38
3	L5	3925	OMU	C2-N3	6.76	1.50	1.38
3	L5	2415	OMU	C2-N3	6.75	1.50	1.38
5	L8	14	OMU	C2-N3	6.73	1.50	1.38
3	L5	4306	OMU	C2-N3	6.70	1.49	1.38
3	L5	2837	OMU	C2-N3	6.70	1.49	1.38
3	L5	4620	OMU	C2-N3	6.67	1.49	1.38
50	S2	1337	4AC	C6-C5	6.66	1.50	1.35
3	L5	1524	A2M	O4'-C4'	-6.63	1.30	1.45
50	S2	668	A2M	O4'-C4'	-6.57	1.30	1.45
50	S2	1337	4AC	C4-N3	6.56	1.44	1.32
50	S2	1678	A2M	O4'-C4'	-6.55	1.30	1.45
50	S2	590	A2M	O4'-C4'	-6.52	1.30	1.45
50	S2	683	OMG	C4-N3	6.42	1.49	1.34
50	S2	867	OMG	C4-N3	6.42	1.49	1.34
50	S2	1842	4AC	C6-C5	6.42	1.50	1.35
50	S2	1447	OMG	C4-N3	6.40	1.49	1.34
3	L5	3944	OMG	C4-N3	6.39	1.49	1.34
3	L5	3724	A2M	O4'-C4'	-6.38	1.30	1.45
3	L5	2424	OMG	C4-N3	6.38	1.49	1.34
50	S2	1639	G7M	C4-N3	6.36	1.49	1.34
3	L5	2363	A2M	O4'-C4'	-6.36	1.30	1.45
3	L5	1534	A2M	O4'-C4'	-6.36	1.30	1.45
50	S2	174	OMC	C2-N3	6.36	1.49	1.36
3	L5	2861	OMC	C2-N3	6.35	1.49	1.36
3	L5	3867	A2M	O4'-C4'	-6.33	1.30	1.45
6	LA	216	V5N	CG-ND1	-6.33	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3723	A2M	O4'-C4'	-6.32	1.30	1.45
3	L5	4571	A2M	O4'-C4'	-6.32	1.30	1.45
50	S2	1031	A2M	O4'-C4'	-6.32	1.30	1.45
50	S2	517	OMC	C2-N3	6.32	1.49	1.36
3	L5	1326	A2M	O4'-C4'	-6.31	1.30	1.45
50	S2	1248	B8N	C6-C5	6.31	1.43	1.34
3	L5	400	A2M	O4'-C4'	-6.31	1.30	1.45
50	S2	462	OMC	C2-N3	6.30	1.49	1.36
3	L5	2804	OMC	C2-N3	6.30	1.49	1.36
3	L5	2876	OMG	C4-N3	6.29	1.49	1.34
50	S2	468	A2M	O4'-C4'	-6.29	1.30	1.45
50	S2	484	A2M	O4'-C4'	-6.29	1.30	1.45
3	L5	2815	A2M	O4'-C4'	-6.28	1.31	1.45
3	L5	4590	A2M	O4'-C4'	-6.28	1.31	1.45
3	L5	3825	A2M	O4'-C4'	-6.27	1.31	1.45
50	S2	1391	OMC	C2-N3	6.27	1.49	1.36
3	L5	4536	OMC	C2-N3	6.27	1.49	1.36
50	S2	509	OMG	C4-N3	6.27	1.49	1.34
3	L5	3782	5MC	C4-N3	6.26	1.44	1.34
3	L5	1871	A2M	O4'-C4'	-6.25	1.31	1.45
50	S2	512	A2M	O4'-C4'	-6.25	1.31	1.45
50	S2	99	A2M	O4'-C4'	-6.24	1.31	1.45
3	L5	4196	OMG	C4-N3	6.24	1.49	1.34
3	L5	2422	OMC	C2-N3	6.23	1.49	1.36
31	La	39	V5N	CG-ND1	-6.23	1.31	1.37
50	S2	27	A2M	O4'-C4'	-6.23	1.31	1.45
3	L5	4456	OMC	C2-N3	6.23	1.49	1.36
50	S2	159	A2M	O4'-C4'	-6.22	1.31	1.45
50	S2	166	A2M	O4'-C4'	-6.22	1.31	1.45
3	L5	1316	OMG	C4-N3	6.22	1.49	1.34
3	L5	2824	OMC	C2-N3	6.22	1.49	1.36
3	L5	4637	OMG	C4-N3	6.22	1.49	1.34
50	S2	644	OMG	C4-N3	6.22	1.49	1.34
3	L5	3869	OMC	C2-N3	6.22	1.49	1.36
3	L5	3792	OMG	C4-N3	6.22	1.49	1.34
3	L5	4523	A2M	O4'-C4'	-6.21	1.31	1.45
50	S2	436	OMG	C4-N3	6.21	1.49	1.34
3	L5	3887	OMC	C2-N3	6.21	1.48	1.36
3	L5	2365	OMC	C2-N3	6.21	1.48	1.36
50	S2	576	A2M	O4'-C4'	-6.20	1.31	1.45
3	L5	4370	OMG	C4-N3	6.19	1.49	1.34
3	L5	3718	A2M	O4'-C4'	-6.18	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	1490	OMG	C4-N3	6.17	1.48	1.34
3	L5	2787	A2M	O4'-C4'	-6.17	1.31	1.45
50	S2	1383	A2M	O4'-C4'	-6.17	1.31	1.45
3	L5	1881	OMC	C2-N3	6.16	1.48	1.36
3	L5	3744	OMG	C4-N3	6.16	1.48	1.34
3	L5	1340	OMC	C2-N3	6.16	1.48	1.36
3	L5	4494	OMG	C4-N3	6.15	1.48	1.34
3	L5	3830	A2M	O4'-C4'	-6.15	1.31	1.45
3	L5	1625	OMG	C4-N3	6.15	1.48	1.34
3	L5	2401	A2M	O4'-C4'	-6.15	1.31	1.45
3	L5	3808	OMC	C2-N3	6.14	1.48	1.36
3	L5	4499	OMG	C4-N3	6.14	1.48	1.34
3	L5	3841	OMC	C2-N3	6.14	1.48	1.36
3	L5	4447	5MC	C4-N3	6.13	1.44	1.34
3	L5	398	A2M	O4'-C4'	-6.13	1.31	1.45
3	L5	1522	OMG	C4-N3	6.12	1.48	1.34
3	L5	2351	OMC	C2-N3	6.12	1.48	1.36
3	L5	4623	OMG	C4-N3	6.11	1.48	1.34
3	L5	3701	OMC	C2-N3	6.11	1.48	1.36
3	L5	3627	OMG	C4-N3	6.10	1.48	1.34
5	L8	75	OMG	C4-N3	6.10	1.48	1.34
3	L5	2422	OMC	C6-C5	6.09	1.49	1.35
3	L5	4530	UR3	C6-C5	6.06	1.49	1.35
50	S2	601	OMG	C4-N3	6.06	1.48	1.34
3	L5	3899	OMG	C4-N3	6.05	1.48	1.34
50	S2	1842	4AC	C7-N4	6.05	1.48	1.37
3	L5	3785	A2M	O4'-C4'	-6.05	1.31	1.45
50	S2	462	OMC	C6-C5	6.05	1.49	1.35
50	S2	174	OMC	C6-C5	6.03	1.49	1.35
3	L5	4618	OMG	C4-N3	6.03	1.48	1.34
50	S2	1248	B8N	C2-N1	6.01	1.57	1.39
3	L5	2861	OMC	C6-C5	6.00	1.49	1.35
50	S2	1337	4AC	C7-N4	6.00	1.48	1.37
3	L5	1881	OMC	C6-C5	6.00	1.49	1.35
3	L5	3701	OMC	C6-C5	5.99	1.49	1.35
3	L5	4392	OMG	C4-N3	5.99	1.48	1.34
3	L5	2351	OMC	C6-C5	5.98	1.49	1.35
3	L5	4228	OMG	C4-N3	5.98	1.48	1.34
50	S2	1391	OMC	C6-C5	5.98	1.48	1.35
3	L5	2365	OMC	C6-C5	5.97	1.48	1.35
3	L5	4536	OMC	C6-C5	5.97	1.48	1.35
3	L5	3887	OMC	C6-C5	5.96	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4456	OMC	C6-C5	5.95	1.48	1.35
3	L5	2804	OMC	C6-C5	5.95	1.48	1.35
3	L5	3782	5MC	C2-N3	5.95	1.48	1.36
50	S2	517	OMC	C6-C5	5.94	1.48	1.35
3	L5	2364	OMG	C4-N3	5.93	1.48	1.34
3	L5	3869	OMC	C6-C5	5.92	1.48	1.35
3	L5	4447	5MC	C2-N3	5.92	1.48	1.36
3	L5	3841	OMC	C6-C5	5.90	1.48	1.35
3	L5	3808	OMC	C6-C5	5.87	1.48	1.35
3	L5	1340	OMC	C6-C5	5.87	1.48	1.35
3	L5	2824	OMC	C6-C5	5.86	1.48	1.35
50	S2	1842	4AC	C2-N3	5.83	1.48	1.36
50	S2	428	OMU	C6-C5	5.80	1.48	1.35
3	L5	4227	OMU	C6-C5	5.77	1.48	1.35
50	S2	121	OMU	C6-C5	5.77	1.48	1.35
50	S2	1288	OMU	C6-C5	5.75	1.48	1.35
50	S2	172	OMU	C6-C5	5.75	1.48	1.35
50	S2	1804	OMU	C6-C5	5.74	1.48	1.35
3	L5	4620	OMU	C6-C5	5.73	1.48	1.35
3	L5	2837	OMU	C6-C5	5.72	1.48	1.35
3	L5	2415	OMU	C6-C5	5.72	1.48	1.35
3	L5	4498	OMU	C6-C5	5.68	1.48	1.35
3	L5	3925	OMU	C6-C5	5.68	1.48	1.35
50	S2	1337	4AC	C2-N3	5.68	1.47	1.36
50	S2	354	OMU	C6-C5	5.67	1.48	1.35
3	L5	4306	OMU	C6-C5	5.66	1.48	1.35
50	S2	1442	OMU	C6-C5	5.63	1.48	1.35
50	S2	116	OMU	C6-C5	5.60	1.48	1.35
5	L8	14	OMU	C6-C5	5.58	1.48	1.35
50	S2	867	OMG	C2-N3	5.53	1.46	1.33
3	L5	3944	OMG	C2-N3	5.52	1.46	1.33
50	S2	1447	OMG	C2-N3	5.52	1.46	1.33
50	S2	1639	G7M	C2-N3	5.49	1.46	1.33
50	S2	1367	PSU	C6-N1	5.49	1.45	1.36
3	L5	2424	OMG	C2-N3	5.48	1.46	1.33
50	S2	36	PSU	C6-N1	5.48	1.45	1.36
50	S2	119	PSU	C6-N1	5.47	1.45	1.36
50	S2	801	PSU	C6-N1	5.47	1.45	1.36
50	S2	93	PSU	C6-N1	5.46	1.45	1.36
50	S2	686	PSU	C6-N1	5.45	1.45	1.36
50	S2	1625	PSU	C6-N1	5.45	1.45	1.36
50	S2	1692	PSU	C6-N1	5.45	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	866	PSU	C6-N1	5.45	1.45	1.36
50	S2	1004	PSU	C6-N1	5.44	1.45	1.36
50	S2	683	OMG	C2-N3	5.44	1.46	1.33
50	S2	1177	PSU	C6-N1	5.44	1.45	1.36
50	S2	572	PSU	C6-N1	5.43	1.45	1.36
50	S2	1243	PSU	C6-N1	5.42	1.45	1.36
50	S2	509	OMG	C2-N3	5.42	1.46	1.33
50	S2	822	PSU	C6-N1	5.42	1.45	1.36
50	S2	1232	PSU	C6-N1	5.42	1.45	1.36
50	S2	863	PSU	C6-N1	5.41	1.45	1.36
50	S2	1347	PSU	C6-N1	5.41	1.45	1.36
50	S2	1136	PSU	C6-N1	5.41	1.45	1.36
50	S2	966	PSU	C6-N1	5.41	1.45	1.36
3	L5	3768	PSU	C6-N1	5.41	1.45	1.36
3	L5	3758	PSU	C6-N1	5.41	1.45	1.36
3	L5	3734	PSU	C6-N1	5.40	1.45	1.36
3	L5	1792	PSU	C6-N1	5.40	1.45	1.36
3	L5	2876	OMG	C2-N3	5.39	1.46	1.33
50	S2	105	PSU	C6-N1	5.39	1.45	1.36
50	S2	573	PSU	C6-N1	5.38	1.45	1.36
3	L5	2508	PSU	C6-N1	5.38	1.45	1.36
50	S2	406	PSU	C6-N1	5.38	1.45	1.36
3	L5	4312	PSU	C6-N1	5.37	1.45	1.36
3	L5	2843	PSU	C6-N1	5.36	1.45	1.36
50	S2	109	PSU	C6-N1	5.36	1.45	1.36
50	S2	1056	PSU	C6-N1	5.36	1.45	1.36
3	L5	2632	PSU	C6-N1	5.36	1.45	1.36
3	L5	3764	PSU	C6-N1	5.36	1.45	1.36
3	L5	4196	OMG	C2-N3	5.35	1.46	1.33
3	L5	4299	PSU	C6-N1	5.35	1.45	1.36
3	L5	4530	UR3	C2-N3	5.35	1.49	1.39
50	S2	609	PSU	C6-N1	5.35	1.45	1.36
50	S2	1643	PSU	C6-N1	5.35	1.45	1.36
3	L5	4296	PSU	C6-N1	5.35	1.45	1.36
3	L5	3637	PSU	C6-N1	5.34	1.45	1.36
50	S2	1445	PSU	C6-N1	5.34	1.45	1.36
3	L5	3770	PSU	C6-N1	5.34	1.45	1.36
50	S2	1244	PSU	C6-N1	5.34	1.45	1.36
3	L5	4636	PSU	C6-N1	5.34	1.45	1.36
50	S2	296	PSU	C6-N1	5.34	1.45	1.36
50	S2	218	PSU	C6-N1	5.34	1.45	1.36
3	L5	2839	PSU	C6-N1	5.33	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	1239	PSU	C6-N1	5.33	1.45	1.36
3	L5	1625	OMG	C2-N3	5.32	1.46	1.33
3	L5	4972	PSU	C6-N1	5.32	1.45	1.36
3	L5	1781	PSU	C6-N1	5.32	1.45	1.36
50	S2	815	PSU	C6-N1	5.32	1.45	1.36
50	S2	651	PSU	C6-N1	5.31	1.45	1.36
3	L5	5001	PSU	C6-N1	5.31	1.45	1.36
3	L5	1779	PSU	C6-N1	5.31	1.45	1.36
3	L5	4576	PSU	C6-N1	5.31	1.45	1.36
3	L5	4457	PSU	C6-N1	5.31	1.45	1.36
3	L5	3695	PSU	C6-N1	5.30	1.45	1.36
50	S2	1238	PSU	C6-N1	5.30	1.45	1.36
3	L5	1862	PSU	C6-N1	5.30	1.45	1.36
3	L5	1582	PSU	C6-N1	5.30	1.45	1.36
50	S2	34	PSU	C6-N1	5.30	1.45	1.36
3	L5	1744	PSU	C6-N1	5.30	1.45	1.36
3	L5	4353	PSU	C6-N1	5.30	1.45	1.36
5	L8	55	PSU	C6-N1	5.30	1.45	1.36
3	L5	4420	PSU	C6-N1	5.29	1.45	1.36
3	L5	3639	PSU	C6-N1	5.29	1.45	1.36
50	S2	644	OMG	C2-N3	5.29	1.45	1.33
50	S2	1174	PSU	C6-N1	5.29	1.45	1.36
3	L5	4532	PSU	C6-N1	5.28	1.45	1.36
50	S2	918	PSU	C6-N1	5.28	1.45	1.36
3	L5	3792	OMG	C2-N3	5.28	1.45	1.33
3	L5	4521	PSU	C6-N1	5.27	1.45	1.36
3	L5	4673	PSU	C6-N1	5.27	1.45	1.36
3	L5	4569	PSU	C6-N1	5.27	1.45	1.36
3	L5	3729	PSU	C6-N1	5.26	1.45	1.36
3	L5	3853	PSU	C6-N1	5.26	1.45	1.36
3	L5	4442	PSU	C6-N1	5.25	1.45	1.36
3	L5	1677	PSU	C6-N1	5.25	1.45	1.36
50	S2	436	OMG	C2-N3	5.25	1.45	1.33
3	L5	4552	PSU	C6-N1	5.25	1.44	1.36
3	L5	4637	OMG	C2-N3	5.25	1.45	1.33
50	S2	814	PSU	C6-N1	5.25	1.44	1.36
5	L8	69	PSU	C6-N1	5.25	1.44	1.36
3	L5	4628	PSU	C6-N1	5.24	1.44	1.36
3	L5	3884	PSU	C6-N1	5.24	1.44	1.36
3	L5	4471	PSU	C6-N1	5.24	1.44	1.36
50	S2	649	PSU	C6-N1	5.23	1.44	1.36
3	L5	4293	PSU	C6-N1	5.23	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	681	PSU	C6-N1	5.23	1.44	1.36
3	L5	3851	PSU	C6-N1	5.23	1.44	1.36
3	L5	4423	PSU	C6-N1	5.23	1.44	1.36
50	S2	1490	OMG	C2-N3	5.23	1.45	1.33
3	L5	1782	PSU	C6-N1	5.23	1.44	1.36
3	L5	4499	OMG	C2-N3	5.22	1.45	1.33
3	L5	3844	PSU	C6-N1	5.22	1.44	1.36
3	L5	4370	OMG	C2-N3	5.22	1.45	1.33
3	L5	1316	OMG	C2-N3	5.22	1.45	1.33
50	S2	174	OMC	C4-N3	5.22	1.45	1.34
3	L5	4493	PSU	C6-N1	5.22	1.44	1.36
3	L5	1860	PSU	C6-N1	5.21	1.44	1.36
3	L5	4431	PSU	C6-N1	5.21	1.44	1.36
3	L5	4579	PSU	C6-N1	5.21	1.44	1.36
3	L5	5010	PSU	C6-N1	5.21	1.44	1.36
3	L5	4500	PSU	C6-N1	5.20	1.44	1.36
3	L5	1683	PSU	C6-N1	5.20	1.44	1.36
3	L5	4494	OMG	C2-N3	5.19	1.45	1.33
3	L5	3920	PSU	C6-N1	5.19	1.44	1.36
50	S2	517	OMC	C4-N3	5.18	1.44	1.34
3	L5	3762	PSU	C6-N1	5.18	1.44	1.36
3	L5	3744	OMG	C2-N3	5.16	1.45	1.33
3	L5	4361	PSU	C6-N1	5.16	1.44	1.36
5	L8	75	OMG	C2-N3	5.16	1.45	1.33
3	L5	1536	PSU	C6-N1	5.15	1.44	1.36
3	L5	4403	PSU	C6-N1	5.14	1.44	1.36
3	L5	1522	OMG	C2-N3	5.14	1.45	1.33
3	L5	2804	OMC	C4-N3	5.13	1.44	1.34
50	S2	1391	OMC	C4-N3	5.13	1.44	1.34
3	L5	4689	PSU	C6-N1	5.12	1.44	1.36
3	L5	3869	OMC	C4-N3	5.11	1.44	1.34
50	S2	462	OMC	C4-N3	5.10	1.44	1.34
50	S2	601	OMG	C2-N3	5.09	1.45	1.33
3	L5	3627	OMG	C2-N3	5.09	1.45	1.33
3	L5	3887	OMC	C4-N3	5.09	1.44	1.34
3	L5	4623	OMG	C2-N3	5.09	1.45	1.33
3	L5	2824	OMC	C4-N3	5.07	1.44	1.34
3	L5	1881	OMC	C4-N3	5.07	1.44	1.34
3	L5	3701	OMC	C4-N3	5.07	1.44	1.34
3	L5	4456	OMC	C4-N3	5.05	1.44	1.34
3	L5	2861	OMC	C4-N3	5.05	1.44	1.34
3	L5	4536	OMC	C4-N3	5.04	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3841	OMC	C4-N3	5.03	1.44	1.34
3	L5	4392	OMG	C2-N3	5.03	1.45	1.33
3	L5	3899	OMG	C2-N3	5.01	1.45	1.33
3	L5	4618	OMG	C2-N3	5.00	1.45	1.33
3	L5	1340	OMC	C4-N3	4.99	1.44	1.34
3	L5	2365	OMC	C4-N3	4.99	1.44	1.34
3	L5	4228	OMG	C2-N3	4.98	1.45	1.33
3	L5	2364	OMG	C2-N3	4.97	1.45	1.33
3	L5	3808	OMC	C4-N3	4.97	1.44	1.34
3	L5	2422	OMC	C4-N3	4.95	1.44	1.34
3	L5	2351	OMC	C4-N3	4.95	1.44	1.34
50	S2	1639	G7M	C2-N2	4.90	1.45	1.34
50	S2	1391	OMC	C4-N4	4.89	1.45	1.33
50	S2	462	OMC	C4-N4	4.84	1.45	1.33
3	L5	3887	OMC	C4-N4	4.83	1.45	1.33
3	L5	2861	OMC	C4-N4	4.81	1.45	1.33
50	S2	174	OMC	C4-N4	4.79	1.45	1.33
3	L5	2422	OMC	C4-N4	4.78	1.45	1.33
3	L5	1340	OMC	C4-N4	4.78	1.45	1.33
3	L5	2365	OMC	C4-N4	4.77	1.45	1.33
3	L5	3841	OMC	C4-N4	4.77	1.45	1.33
3	L5	2824	OMC	C4-N4	4.76	1.45	1.33
50	S2	683	OMG	C2-N2	4.76	1.45	1.34
3	L5	4456	OMC	C4-N4	4.76	1.45	1.33
3	L5	3808	OMC	C4-N4	4.75	1.45	1.33
3	L5	2351	OMC	C4-N4	4.75	1.45	1.33
50	S2	1447	OMG	C2-N2	4.75	1.45	1.34
3	L5	3869	OMC	C4-N4	4.74	1.45	1.33
3	L5	2804	OMC	C4-N4	4.74	1.45	1.33
50	S2	517	OMC	C4-N4	4.73	1.45	1.33
3	L5	4536	OMC	C4-N4	4.72	1.45	1.33
3	L5	3944	OMG	C2-N2	4.72	1.45	1.34
3	L5	3701	OMC	C4-N4	4.71	1.45	1.33
3	L5	1881	OMC	C4-N4	4.70	1.45	1.33
50	S2	867	OMG	C2-N2	4.70	1.45	1.34
3	L5	4499	OMG	C2-N2	4.68	1.45	1.34
3	L5	2424	OMG	C2-N2	4.67	1.45	1.34
3	L5	3792	OMG	C2-N2	4.66	1.45	1.34
50	S2	1490	OMG	C2-N2	4.64	1.45	1.34
3	L5	3744	OMG	C2-N2	4.63	1.45	1.34
50	S2	1639	G7M	C5-N7	-4.62	1.33	1.39
3	L5	4196	OMG	C2-N2	4.62	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	644	OMG	C2-N2	4.62	1.45	1.34
50	S2	436	OMG	C2-N2	4.62	1.45	1.34
5	L8	75	OMG	C2-N2	4.61	1.45	1.34
3	L5	2876	OMG	C2-N2	4.60	1.45	1.34
3	L5	3627	OMG	C2-N2	4.59	1.45	1.34
50	S2	468	A2M	C6-N6	4.59	1.45	1.34
3	L5	4637	OMG	C2-N2	4.58	1.45	1.34
50	S2	1337	4AC	C5-C4	4.57	1.50	1.40
3	L5	4447	5MC	C6-N1	4.57	1.45	1.38
3	L5	4494	OMG	C2-N2	4.57	1.45	1.34
3	L5	1316	OMG	C2-N2	4.56	1.45	1.34
3	L5	1625	OMG	C2-N2	4.56	1.45	1.34
50	S2	1842	4AC	C5-C4	4.55	1.50	1.40
3	L5	4618	OMG	C2-N2	4.55	1.45	1.34
50	S2	601	OMG	C2-N2	4.53	1.45	1.34
3	L5	3782	5MC	C6-N1	4.52	1.45	1.38
3	L5	4370	OMG	C2-N2	4.52	1.44	1.34
50	S2	484	A2M	C6-N6	4.52	1.45	1.34
3	L5	4623	OMG	C2-N2	4.52	1.44	1.34
3	L5	3899	OMG	C2-N2	4.52	1.44	1.34
50	S2	1678	A2M	C6-N6	4.51	1.45	1.34
3	L5	398	A2M	C6-N6	4.51	1.45	1.34
50	S2	1383	A2M	C6-N6	4.51	1.45	1.34
3	L5	4228	OMG	C2-N2	4.51	1.44	1.34
50	S2	159	A2M	C6-N6	4.50	1.45	1.34
3	L5	3723	A2M	C6-N6	4.50	1.45	1.34
50	S2	509	OMG	C2-N2	4.50	1.44	1.34
3	L5	1871	A2M	C6-N6	4.50	1.45	1.34
50	S2	512	A2M	C6-N6	4.49	1.45	1.34
50	S2	668	A2M	C6-N6	4.49	1.45	1.34
50	S2	590	A2M	C6-N6	4.49	1.45	1.34
3	L5	2364	OMG	C2-N2	4.49	1.44	1.34
50	S2	576	A2M	C6-N6	4.49	1.45	1.34
50	S2	918	PSU	C1'-C5	-4.48	1.39	1.50
50	S2	166	A2M	C6-N6	4.48	1.45	1.34
50	S2	462	OMC	C2-N1	4.48	1.49	1.40
50	S2	517	OMC	C2-N1	4.48	1.49	1.40
3	L5	3718	A2M	C6-N6	4.48	1.45	1.34
3	L5	1522	OMG	C2-N2	4.48	1.44	1.34
3	L5	4571	A2M	C6-N6	4.48	1.45	1.34
3	L5	1534	A2M	C6-N6	4.47	1.45	1.34
3	L5	4590	A2M	C6-N6	4.47	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4392	OMG	C2-N2	4.47	1.44	1.34
3	L5	2363	A2M	C6-N6	4.46	1.45	1.34
3	L5	2401	A2M	C6-N6	4.46	1.45	1.34
3	L5	2787	A2M	C6-N6	4.46	1.45	1.34
3	L5	2824	OMC	C2-N1	4.46	1.49	1.40
3	L5	2815	A2M	C6-N6	4.46	1.45	1.34
3	L5	400	A2M	C6-N6	4.45	1.45	1.34
50	S2	99	A2M	C6-N6	4.45	1.45	1.34
3	L5	1524	A2M	C6-N6	4.45	1.45	1.34
3	L5	3867	A2M	C6-N6	4.44	1.45	1.34
3	L5	4456	OMC	C2-N1	4.44	1.49	1.40
3	L5	3825	A2M	C6-N6	4.43	1.45	1.34
3	L5	3724	A2M	C6-N6	4.43	1.45	1.34
50	S2	27	A2M	C6-N6	4.43	1.45	1.34
50	S2	649	PSU	C1'-C5	-4.42	1.40	1.50
3	L5	2861	OMC	C2-N1	4.42	1.49	1.40
50	S2	1031	A2M	C6-N6	4.42	1.45	1.34
50	S2	1238	PSU	C1'-C5	-4.41	1.40	1.50
3	L5	1326	A2M	C6-N6	4.40	1.45	1.34
3	L5	3830	A2M	C6-N6	4.40	1.45	1.34
3	L5	2351	OMC	C2-N1	4.40	1.49	1.40
3	L5	4403	PSU	C1'-C5	-4.40	1.40	1.50
3	L5	4532	PSU	C1'-C5	-4.40	1.40	1.50
3	L5	2839	PSU	C1'-C5	-4.39	1.40	1.50
3	L5	2422	OMC	C2-N1	4.39	1.49	1.40
3	L5	4431	PSU	C1'-C5	-4.38	1.40	1.50
50	S2	966	PSU	C1'-C5	-4.38	1.40	1.50
50	S2	1177	PSU	C1'-C5	-4.38	1.40	1.50
50	S2	174	OMC	C2-N1	4.38	1.49	1.40
3	L5	4523	A2M	C6-N6	4.37	1.45	1.34
50	S2	296	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	3637	PSU	C1'-C5	-4.37	1.40	1.50
3	L5	1862	PSU	C1'-C5	-4.36	1.40	1.50
3	L5	1782	PSU	C1'-C5	-4.36	1.40	1.50
3	L5	4521	PSU	C1'-C5	-4.36	1.40	1.50
3	L5	4500	PSU	C1'-C5	-4.35	1.40	1.50
50	S2	651	PSU	C1'-C5	-4.35	1.40	1.50
5	L8	69	PSU	C1'-C5	-4.35	1.40	1.50
3	L5	4536	OMC	C2-N1	4.35	1.49	1.40
3	L5	3851	PSU	C1'-C5	-4.34	1.40	1.50
50	S2	1445	PSU	C1'-C5	-4.34	1.40	1.50
3	L5	4293	PSU	C1'-C5	-4.34	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3695	PSU	C1'-C5	-4.34	1.40	1.50
50	S2	863	PSU	C1'-C5	-4.34	1.40	1.50
3	L5	4423	PSU	C1'-C5	-4.33	1.40	1.50
3	L5	4493	PSU	C1'-C5	-4.33	1.40	1.50
50	S2	1842	4AC	O2-C2	-4.33	1.15	1.23
50	S2	1842	4AC	C2-N1	4.33	1.49	1.40
3	L5	4299	PSU	C1'-C5	-4.32	1.40	1.50
3	L5	3785	A2M	C6-N6	4.32	1.45	1.34
50	S2	681	PSU	C1'-C5	-4.32	1.40	1.50
3	L5	4552	PSU	C1'-C5	-4.32	1.40	1.50
3	L5	4442	PSU	C1'-C5	-4.31	1.40	1.50
3	L5	3887	OMC	C2-N1	4.31	1.49	1.40
3	L5	2843	PSU	C1'-C5	-4.31	1.40	1.50
3	L5	4673	PSU	C1'-C5	-4.31	1.40	1.50
3	L5	1744	PSU	C1'-C5	-4.31	1.40	1.50
3	L5	1582	PSU	C1'-C5	-4.31	1.40	1.50
3	L5	2804	OMC	C2-N1	4.31	1.49	1.40
50	S2	1056	PSU	C1'-C5	-4.30	1.40	1.50
50	S2	1244	PSU	C1'-C5	-4.30	1.40	1.50
50	S2	1625	PSU	C1'-C5	-4.30	1.40	1.50
3	L5	3729	PSU	C1'-C5	-4.30	1.40	1.50
50	S2	801	PSU	C1'-C5	-4.30	1.40	1.50
3	L5	3853	PSU	C1'-C5	-4.30	1.40	1.50
3	L5	4579	PSU	C1'-C5	-4.30	1.40	1.50
3	L5	3808	OMC	C2-N1	4.30	1.49	1.40
50	S2	1643	PSU	C1'-C5	-4.30	1.40	1.50
3	L5	3768	PSU	C1'-C5	-4.30	1.40	1.50
3	L5	4689	PSU	C1'-C5	-4.29	1.40	1.50
50	S2	1288	OMU	C4-N3	4.29	1.46	1.38
50	S2	609	PSU	C1'-C5	-4.29	1.40	1.50
50	S2	1391	OMC	C2-N1	4.29	1.49	1.40
50	S2	1367	PSU	C1'-C5	-4.29	1.40	1.50
3	L5	3841	OMC	C2-N1	4.29	1.49	1.40
3	L5	4628	PSU	C1'-C5	-4.29	1.40	1.50
3	L5	1779	PSU	C1'-C5	-4.29	1.40	1.50
50	S2	866	PSU	C1'-C5	-4.29	1.40	1.50
3	L5	3639	PSU	C1'-C5	-4.28	1.40	1.50
3	L5	1781	PSU	C1'-C5	-4.28	1.40	1.50
3	L5	3869	OMC	C2-N1	4.28	1.49	1.40
3	L5	4447	5MC	C4-N4	4.28	1.45	1.34
3	L5	1683	PSU	C1'-C5	-4.28	1.40	1.50
3	L5	3758	PSU	C1'-C5	-4.27	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4361	PSU	C1'-C5	-4.27	1.40	1.50
3	L5	3734	PSU	C1'-C5	-4.27	1.40	1.50
50	S2	686	PSU	C1'-C5	-4.27	1.40	1.50
50	S2	1136	PSU	C1'-C5	-4.27	1.40	1.50
50	S2	105	PSU	C1'-C5	-4.27	1.40	1.50
50	S2	1239	PSU	C1'-C5	-4.27	1.40	1.50
3	L5	3884	PSU	C1'-C5	-4.26	1.40	1.50
3	L5	1677	PSU	C1'-C5	-4.26	1.40	1.50
3	L5	3762	PSU	C1'-C5	-4.26	1.40	1.50
3	L5	4353	PSU	C1'-C5	-4.26	1.40	1.50
50	S2	36	PSU	C1'-C5	-4.26	1.40	1.50
5	L8	55	PSU	C1'-C5	-4.25	1.40	1.50
3	L5	2365	OMC	C2-N1	4.25	1.49	1.40
3	L5	3770	PSU	C1'-C5	-4.25	1.40	1.50
50	S2	34	PSU	C1'-C5	-4.25	1.40	1.50
3	L5	2508	PSU	C1'-C5	-4.25	1.40	1.50
3	L5	4576	PSU	C1'-C5	-4.25	1.40	1.50
50	S2	406	PSU	C1'-C5	-4.24	1.40	1.50
3	L5	1881	OMC	C2-N1	4.24	1.49	1.40
3	L5	4972	PSU	C1'-C5	-4.24	1.40	1.50
50	S2	1232	PSU	C1'-C5	-4.24	1.40	1.50
50	S2	1347	PSU	C1'-C5	-4.24	1.40	1.50
3	L5	1792	PSU	C1'-C5	-4.24	1.40	1.50
50	S2	1337	4AC	O2-C2	-4.23	1.15	1.23
50	S2	109	PSU	C1'-C5	-4.23	1.40	1.50
3	L5	3782	5MC	C4-N4	4.23	1.45	1.34
3	L5	3920	PSU	C1'-C5	-4.23	1.40	1.50
50	S2	1004	PSU	C1'-C5	-4.23	1.40	1.50
3	L5	1860	PSU	C1'-C5	-4.23	1.40	1.50
50	S2	1442	OMU	C4-N3	4.23	1.46	1.38
50	S2	815	PSU	C1'-C5	-4.23	1.40	1.50
3	L5	2632	PSU	C1'-C5	-4.23	1.40	1.50
50	S2	93	PSU	C1'-C5	-4.23	1.40	1.50
50	S2	1174	PSU	C1'-C5	-4.22	1.40	1.50
50	S2	172	OMU	C4-N3	4.22	1.46	1.38
3	L5	4471	PSU	C1'-C5	-4.22	1.40	1.50
50	S2	822	PSU	C1'-C5	-4.22	1.40	1.50
3	L5	1340	OMC	C2-N1	4.21	1.49	1.40
3	L5	4296	PSU	C1'-C5	-4.20	1.40	1.50
3	L5	5001	PSU	C1'-C5	-4.20	1.40	1.50
3	L5	1536	PSU	C1'-C5	-4.20	1.40	1.50
3	L5	4312	PSU	C1'-C5	-4.19	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4636	PSU	C1'-C5	-4.19	1.40	1.50
3	L5	3701	OMC	C2-N1	4.19	1.49	1.40
50	S2	116	OMU	C4-N3	4.18	1.46	1.38
50	S2	814	PSU	C1'-C5	-4.17	1.40	1.50
3	L5	5010	PSU	C1'-C5	-4.17	1.40	1.50
50	S2	1692	PSU	C1'-C5	-4.17	1.40	1.50
50	S2	354	OMU	C4-N3	4.17	1.46	1.38
3	L5	3844	PSU	C1'-C5	-4.16	1.40	1.50
3	L5	3782	5MC	C2-N1	4.16	1.49	1.40
50	S2	1804	OMU	C4-N3	4.15	1.46	1.38
50	S2	1337	4AC	C2-N1	4.15	1.49	1.40
3	L5	3764	PSU	C1'-C5	-4.15	1.40	1.50
31	La	39	V5N	CD2-NE2	-4.14	1.31	1.37
3	L5	4498	OMU	C4-N3	4.14	1.46	1.38
3	L5	4457	PSU	C1'-C5	-4.14	1.40	1.50
3	L5	4569	PSU	C1'-C5	-4.13	1.40	1.50
50	S2	428	OMU	C4-N3	4.12	1.45	1.38
50	S2	121	OMU	C4-N3	4.10	1.45	1.38
5	L8	14	OMU	C4-N3	4.10	1.45	1.38
50	S2	1243	PSU	C1'-C5	-4.09	1.40	1.50
3	L5	2415	OMU	C4-N3	4.08	1.45	1.38
3	L5	4227	OMU	C4-N3	4.08	1.45	1.38
50	S2	918	PSU	C4-N3	4.08	1.46	1.38
3	L5	4306	OMU	C4-N3	4.06	1.45	1.38
50	S2	218	PSU	C4-N3	4.06	1.46	1.38
50	S2	573	PSU	C1'-C5	-4.05	1.40	1.50
3	L5	3925	OMU	C4-N3	4.04	1.45	1.38
3	L5	2837	OMU	C4-N3	4.03	1.45	1.38
50	S2	1643	PSU	C4-N3	4.03	1.46	1.38
50	S2	822	PSU	C4-N3	4.02	1.46	1.38
6	LA	216	V5N	CD2-NE2	-4.02	1.31	1.37
3	L5	4447	5MC	C2-N1	4.01	1.48	1.40
50	S2	609	PSU	C4-N3	4.00	1.46	1.38
50	S2	218	PSU	C1'-C5	-4.00	1.41	1.50
50	S2	119	PSU	C4-N3	3.99	1.46	1.38
3	L5	4420	PSU	C1'-C5	-3.99	1.41	1.50
50	S2	1136	PSU	C4-N3	3.99	1.46	1.38
50	S2	1004	PSU	C4-N3	3.98	1.46	1.38
3	L5	4420	PSU	C4-N3	3.98	1.46	1.38
50	S2	686	PSU	C4-N3	3.98	1.46	1.38
50	S2	119	PSU	C1'-C5	-3.98	1.41	1.50
50	S2	1239	PSU	C4-N3	3.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4293	PSU	C4-N3	3.97	1.46	1.38
50	S2	814	PSU	C4-N3	3.96	1.46	1.38
3	L5	4620	OMU	C4-N3	3.96	1.45	1.38
50	S2	815	PSU	C4-N3	3.96	1.46	1.38
3	L5	3758	PSU	C4-N3	3.96	1.46	1.38
50	S2	866	PSU	C4-N3	3.96	1.46	1.38
3	L5	3762	PSU	C4-N3	3.95	1.46	1.38
50	S2	651	PSU	C4-N3	3.95	1.46	1.38
50	S2	1232	PSU	C4-N3	3.95	1.46	1.38
3	L5	1322	1MA	C2-N1	3.95	1.43	1.35
3	L5	3734	PSU	C4-N3	3.95	1.46	1.38
50	S2	1625	PSU	C4-N3	3.94	1.46	1.38
3	L5	3770	PSU	C4-N3	3.94	1.46	1.38
3	L5	1677	PSU	C4-N3	3.93	1.46	1.38
50	S2	1244	PSU	C4-N3	3.93	1.46	1.38
50	S2	1347	PSU	C4-N3	3.92	1.46	1.38
50	S2	966	PSU	C4-N3	3.92	1.46	1.38
50	S2	1445	PSU	C4-N3	3.92	1.46	1.38
50	S2	1174	PSU	C4-N3	3.92	1.46	1.38
5	L8	69	PSU	C4-N3	3.92	1.46	1.38
3	L5	4442	PSU	C4-N3	3.91	1.46	1.38
3	L5	4500	PSU	C4-N3	3.91	1.46	1.38
50	S2	34	PSU	C4-N3	3.91	1.46	1.38
3	L5	4312	PSU	C4-N3	3.91	1.46	1.38
50	S2	1243	PSU	C4-N3	3.91	1.46	1.38
50	S2	1337	4AC	C4-N4	3.91	1.45	1.39
3	L5	4423	PSU	C4-N3	3.91	1.46	1.38
3	L5	4576	PSU	C4-N3	3.91	1.46	1.38
3	L5	1792	PSU	C4-N3	3.91	1.46	1.38
3	L5	2632	PSU	C4-N3	3.91	1.46	1.38
3	L5	4569	PSU	C4-N3	3.90	1.46	1.38
3	L5	5010	PSU	C4-N3	3.90	1.46	1.38
3	L5	4361	PSU	C4-N3	3.90	1.46	1.38
50	S2	1692	PSU	C4-N3	3.90	1.46	1.38
3	L5	2508	PSU	C4-N3	3.89	1.46	1.38
50	S2	1238	PSU	C4-N3	3.89	1.46	1.38
50	S2	573	PSU	C4-N3	3.89	1.46	1.38
50	S2	681	PSU	C4-N3	3.89	1.46	1.38
50	S2	406	PSU	C4-N3	3.89	1.46	1.38
3	L5	1779	PSU	C4-N3	3.88	1.46	1.38
50	S2	801	PSU	C4-N3	3.88	1.46	1.38
50	S2	109	PSU	C4-N3	3.88	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1782	PSU	C4-N3	3.88	1.46	1.38
50	S2	93	PSU	C4-N3	3.87	1.46	1.38
50	S2	296	PSU	C4-N3	3.87	1.46	1.38
50	S2	863	PSU	C4-N3	3.87	1.46	1.38
3	L5	4457	PSU	C4-N3	3.87	1.46	1.38
50	S2	572	PSU	C1'-C5	-3.87	1.41	1.50
3	L5	1536	PSU	C4-N3	3.87	1.46	1.38
3	L5	1860	PSU	C4-N3	3.86	1.46	1.38
3	L5	5001	PSU	C4-N3	3.86	1.46	1.38
3	L5	4353	PSU	C4-N3	3.86	1.46	1.38
50	S2	36	PSU	C4-N3	3.86	1.46	1.38
3	L5	3768	PSU	C4-N3	3.86	1.46	1.38
50	S2	1367	PSU	C4-N3	3.86	1.46	1.38
3	L5	1744	PSU	C4-N3	3.86	1.46	1.38
3	L5	4673	PSU	C4-N3	3.86	1.46	1.38
50	S2	572	PSU	C4-N3	3.86	1.46	1.38
50	S2	1056	PSU	C4-N3	3.85	1.46	1.38
3	L5	1582	PSU	C4-N3	3.85	1.46	1.38
3	L5	4296	PSU	C4-N3	3.85	1.46	1.38
3	L5	3695	PSU	C4-N3	3.85	1.46	1.38
50	S2	1177	PSU	C4-N3	3.85	1.46	1.38
3	L5	3764	PSU	C4-N3	3.84	1.46	1.38
3	L5	4299	PSU	C4-N3	3.84	1.46	1.38
3	L5	1322	1MA	C5-C6	3.84	1.54	1.43
3	L5	4689	PSU	C4-N3	3.84	1.46	1.38
3	L5	3729	PSU	C4-N3	3.84	1.46	1.38
5	L8	55	PSU	C4-N3	3.83	1.46	1.38
3	L5	3920	PSU	C4-N3	3.83	1.46	1.38
3	L5	1683	PSU	C4-N3	3.83	1.45	1.38
3	L5	1862	PSU	C4-N3	3.83	1.45	1.38
3	L5	4579	PSU	C4-N3	3.83	1.45	1.38
50	S2	649	PSU	C4-N3	3.82	1.45	1.38
3	L5	3639	PSU	C4-N3	3.82	1.45	1.38
3	L5	3884	PSU	C4-N3	3.82	1.45	1.38
3	L5	4972	PSU	C4-N3	3.81	1.45	1.38
3	L5	3844	PSU	C4-N3	3.81	1.45	1.38
50	S2	1639	G7M	C5-C6	3.81	1.54	1.43
3	L5	4493	PSU	C4-N3	3.81	1.45	1.38
3	L5	3851	PSU	C4-N3	3.81	1.45	1.38
3	L5	4521	PSU	C4-N3	3.81	1.45	1.38
3	L5	4628	PSU	C4-N3	3.81	1.45	1.38
50	S2	105	PSU	C4-N3	3.80	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4403	PSU	C4-N3	3.80	1.45	1.38
50	S2	1842	4AC	C4-N4	3.80	1.45	1.39
3	L5	3853	PSU	C4-N3	3.80	1.45	1.38
3	L5	4532	PSU	C4-N3	3.80	1.45	1.38
3	L5	4471	PSU	C4-N3	3.78	1.45	1.38
3	L5	4636	PSU	C4-N3	3.78	1.45	1.38
3	L5	1781	PSU	C4-N3	3.77	1.45	1.38
3	L5	4552	PSU	C4-N3	3.76	1.45	1.38
3	L5	4431	PSU	C4-N3	3.76	1.45	1.38
3	L5	2839	PSU	C4-N3	3.73	1.45	1.38
50	S2	1248	B8N	C1'-C5	3.68	1.58	1.50
3	L5	2843	PSU	C4-N3	3.68	1.45	1.38
50	S2	1850	MA6	C6-N6	3.64	1.47	1.36
50	S2	1851	MA6	C6-N6	3.58	1.47	1.36
3	L5	3637	PSU	C4-N3	3.55	1.45	1.38
50	S2	1081	PSU	C6-C5	3.45	1.39	1.35
50	S2	1337	4AC	C6-N1	3.43	1.46	1.38
50	S2	1842	4AC	C6-N1	3.35	1.46	1.38
3	L5	2351	OMC	C6-N1	3.30	1.46	1.38
3	L5	2365	OMC	C6-N1	3.29	1.45	1.38
50	S2	462	OMC	C6-N1	3.29	1.45	1.38
50	S2	174	OMC	C6-N1	3.28	1.45	1.38
3	L5	3869	OMC	C6-N1	3.26	1.45	1.38
3	L5	3887	OMC	C6-N1	3.23	1.45	1.38
3	L5	4536	OMC	C6-N1	3.23	1.45	1.38
3	L5	3701	OMC	C6-N1	3.23	1.45	1.38
3	L5	3841	OMC	C6-N1	3.23	1.45	1.38
3	L5	1881	OMC	C6-N1	3.22	1.45	1.38
3	L5	2861	OMC	C6-N1	3.22	1.45	1.38
3	L5	2422	OMC	C6-N1	3.22	1.45	1.38
3	L5	2824	OMC	C6-N1	3.22	1.45	1.38
50	S2	517	OMC	C6-N1	3.22	1.45	1.38
50	S2	1391	OMC	C6-N1	3.22	1.45	1.38
3	L5	4456	OMC	C6-N1	3.21	1.45	1.38
3	L5	2804	OMC	C6-N1	3.19	1.45	1.38
3	L5	1322	1MA	C5-N7	-3.17	1.32	1.39
5	L8	14	OMU	O4-C4	-3.16	1.18	1.24
3	L5	1340	OMC	C6-N1	3.15	1.45	1.38
3	L5	1326	A2M	O3'-C3'	-3.15	1.35	1.43
3	L5	3808	OMC	C6-N1	3.14	1.45	1.38
3	L5	400	A2M	O3'-C3'	-3.13	1.35	1.43
3	L5	3867	A2M	O3'-C3'	-3.13	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4306	OMU	O4-C4	-3.12	1.18	1.24
3	L5	2787	A2M	O3'-C3'	-3.12	1.35	1.43
3	L5	2424	OMG	C5-N7	-3.11	1.33	1.39
3	L5	3825	A2M	O3'-C3'	-3.11	1.35	1.43
3	L5	4571	A2M	O3'-C3'	-3.11	1.35	1.43
50	S2	159	A2M	O3'-C3'	-3.08	1.35	1.43
3	L5	4498	OMU	O4-C4	-3.08	1.18	1.24
50	S2	1288	OMU	C6-N1	3.06	1.45	1.38
3	L5	2815	A2M	O3'-C3'	-3.06	1.35	1.43
3	L5	3718	A2M	O3'-C3'	-3.06	1.35	1.43
50	S2	1678	A2M	O3'-C3'	-3.05	1.35	1.43
3	L5	4620	OMU	O4-C4	-3.05	1.18	1.24
3	L5	3925	OMU	O4-C4	-3.05	1.18	1.24
3	L5	3724	A2M	O3'-C3'	-3.05	1.35	1.43
3	L5	1524	A2M	O3'-C3'	-3.04	1.35	1.43
3	L5	3830	A2M	O3'-C3'	-3.03	1.35	1.43
50	S2	1383	A2M	O3'-C3'	-3.01	1.35	1.43
3	L5	398	A2M	O3'-C3'	-3.01	1.35	1.43
3	L5	2363	A2M	O3'-C3'	-3.01	1.35	1.43
50	S2	166	A2M	O3'-C3'	-3.00	1.35	1.43
3	L5	4530	UR3	C6-N1	3.00	1.45	1.38
50	S2	468	A2M	O3'-C3'	-3.00	1.35	1.43
50	S2	428	OMU	O4-C4	-3.00	1.18	1.24
50	S2	512	A2M	O3'-C3'	-3.00	1.35	1.43
3	L5	4590	A2M	O3'-C3'	-2.99	1.35	1.43
3	L5	2837	OMU	O4-C4	-2.99	1.18	1.24
3	L5	3944	OMG	C5-N7	-2.98	1.33	1.39
3	L5	4227	OMU	O4-C4	-2.98	1.18	1.24
50	S2	354	OMU	O4-C4	-2.98	1.18	1.24
3	L5	2415	OMU	O4-C4	-2.97	1.18	1.24
50	S2	590	A2M	O3'-C3'	-2.97	1.36	1.43
3	L5	2876	OMG	C5-N7	-2.97	1.33	1.39
7	LB	245	HIC	CD2-CG	2.97	1.41	1.36
3	L5	3841	OMC	O2-C2	-2.96	1.18	1.23
3	L5	4494	OMG	C5-N7	-2.96	1.33	1.39
50	S2	1804	OMU	O4-C4	-2.96	1.18	1.24
3	L5	1871	A2M	O3'-C3'	-2.96	1.36	1.43
3	L5	4523	A2M	O3'-C3'	-2.96	1.36	1.43
50	S2	576	A2M	O3'-C3'	-2.96	1.36	1.43
3	L5	3925	OMU	C6-N1	2.96	1.45	1.38
50	S2	1442	OMU	C6-N1	2.95	1.45	1.38
3	L5	2415	OMU	C6-N1	2.95	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4196	OMG	C5-N7	-2.95	1.33	1.39
3	L5	398	A2M	O2'-C2'	2.95	1.50	1.42
3	L5	4498	OMU	C6-N1	2.94	1.45	1.38
50	S2	1243	PSU	O4-C4	-2.94	1.18	1.23
3	L5	3723	A2M	O3'-C3'	-2.94	1.36	1.43
50	S2	116	OMU	O4-C4	-2.94	1.18	1.24
50	S2	428	OMU	C6-N1	2.93	1.45	1.38
3	L5	3785	A2M	C5-C4	-2.93	1.33	1.39
3	L5	2815	A2M	O2'-C2'	2.93	1.50	1.42
3	L5	3825	A2M	C5-C4	-2.92	1.33	1.39
3	L5	3724	A2M	O2'-C2'	2.92	1.50	1.42
50	S2	121	OMU	O4-C4	-2.92	1.18	1.24
3	L5	3792	OMG	C5-N7	-2.92	1.33	1.39
50	S2	99	A2M	O3'-C3'	-2.92	1.36	1.43
50	S2	1031	A2M	O3'-C3'	-2.92	1.36	1.43
3	L5	4571	A2M	O2'-C2'	2.92	1.50	1.42
50	S2	1490	OMG	C5-N7	-2.91	1.33	1.39
3	L5	2401	A2M	C5-C4	-2.91	1.33	1.39
50	S2	172	OMU	O4-C4	-2.91	1.18	1.24
3	L5	2843	PSU	O4-C4	-2.91	1.18	1.23
50	S2	27	A2M	O3'-C3'	-2.91	1.36	1.43
3	L5	1881	OMC	O2-C2	-2.91	1.18	1.23
50	S2	590	A2M	O2'-C2'	2.91	1.50	1.42
3	L5	1625	OMG	C5-N7	-2.90	1.33	1.39
3	L5	1871	A2M	C5-C4	-2.90	1.33	1.39
50	S2	1804	OMU	C6-N1	2.90	1.45	1.38
50	S2	121	OMU	C6-N1	2.90	1.45	1.38
50	S2	668	A2M	O3'-C3'	-2.90	1.36	1.43
50	S2	668	A2M	C5-C4	-2.89	1.33	1.39
3	L5	2401	A2M	O3'-C3'	-2.89	1.36	1.43
3	L5	3723	A2M	C5-C4	-2.89	1.33	1.39
50	S2	1447	OMG	C5-N7	-2.89	1.33	1.39
3	L5	4306	OMU	C6-N1	2.88	1.44	1.38
3	L5	1326	A2M	O2'-C2'	2.88	1.50	1.42
50	S2	509	OMG	C5-N7	-2.88	1.33	1.39
50	S2	1031	A2M	C5-C4	-2.88	1.33	1.39
3	L5	2804	OMC	O2-C2	-2.87	1.18	1.23
3	L5	4227	OMU	C6-N1	2.87	1.44	1.38
3	L5	2363	A2M	C5-C4	-2.87	1.33	1.39
3	L5	2861	OMC	O2-C2	-2.87	1.18	1.23
3	L5	2422	OMC	O2-C2	-2.87	1.18	1.23
3	L5	4499	OMG	C5-N7	-2.87	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3701	OMC	O2-C2	-2.87	1.18	1.23
3	L5	2837	OMU	C6-N1	2.87	1.44	1.38
3	L5	4220	6MZ	C5-C4	-2.86	1.33	1.39
50	S2	1442	OMU	O4-C4	-2.86	1.18	1.24
3	L5	1534	A2M	O3'-C3'	-2.86	1.36	1.43
3	L5	4523	A2M	C5-C4	-2.86	1.33	1.39
50	S2	484	A2M	O2'-C2'	2.86	1.49	1.42
3	L5	1316	OMG	C5-N7	-2.86	1.33	1.39
3	L5	3723	A2M	O2'-C2'	2.86	1.49	1.42
3	L5	3884	PSU	O4-C4	-2.85	1.18	1.23
3	L5	3718	A2M	O2'-C2'	2.85	1.49	1.42
3	L5	2824	OMC	O2-C2	-2.85	1.18	1.23
50	S2	354	OMU	C6-N1	2.85	1.44	1.38
3	L5	4620	OMU	C6-N1	2.85	1.44	1.38
50	S2	683	OMG	C5-N7	-2.85	1.33	1.39
50	S2	668	A2M	O2'-C2'	2.85	1.49	1.42
3	L5	1524	A2M	C5-C4	-2.85	1.33	1.39
3	L5	3724	A2M	C5-C4	-2.85	1.33	1.39
50	S2	601	OMG	C5-N7	-2.85	1.33	1.39
50	S2	436	OMG	C5-N7	-2.85	1.33	1.39
3	L5	1536	PSU	O4-C4	-2.85	1.18	1.23
3	L5	4590	A2M	O2'-C2'	2.85	1.49	1.42
3	L5	2365	OMC	O2-C2	-2.85	1.18	1.23
50	S2	1288	OMU	O4-C4	-2.84	1.19	1.24
50	S2	159	A2M	O2'-C2'	2.84	1.49	1.42
3	L5	2351	OMC	O2-C2	-2.84	1.18	1.23
3	L5	4536	OMC	O2-C2	-2.84	1.18	1.23
50	S2	644	OMG	C5-N7	-2.84	1.33	1.39
50	S2	166	A2M	O2'-C2'	2.84	1.49	1.42
3	L5	1326	A2M	C5-C4	-2.84	1.33	1.39
50	S2	1031	A2M	O2'-C2'	2.84	1.49	1.42
3	L5	3825	A2M	O2'-C2'	2.83	1.49	1.42
50	S2	867	OMG	C5-N7	-2.83	1.33	1.39
3	L5	400	A2M	C5-C4	-2.83	1.33	1.39
3	L5	4571	A2M	C5-C4	-2.83	1.33	1.39
3	L5	1524	A2M	O2'-C2'	2.83	1.49	1.42
3	L5	3808	OMC	O2-C2	-2.83	1.18	1.23
3	L5	4456	OMC	O2-C2	-2.83	1.18	1.23
3	L5	3830	A2M	O2'-C2'	2.83	1.49	1.42
3	L5	1534	A2M	O2'-C2'	2.82	1.49	1.42
50	S2	172	OMU	C6-N1	2.82	1.44	1.38
50	S2	468	A2M	C5-C4	-2.82	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	1383	A2M	O2'-C2'	2.82	1.49	1.42
3	L5	3830	A2M	C5-C4	-2.82	1.33	1.39
3	L5	2401	A2M	O2'-C2'	2.82	1.49	1.42
3	L5	4447	5MC	O2-C2	-2.81	1.18	1.23
3	L5	3744	OMG	C2-N1	2.81	1.44	1.37
3	L5	4590	A2M	C5-C4	-2.81	1.33	1.39
3	L5	1871	A2M	O2'-C2'	2.81	1.49	1.42
5	L8	14	OMU	C6-N1	2.81	1.44	1.38
3	L5	2787	A2M	C5-C4	-2.81	1.33	1.39
50	S2	576	A2M	O2'-C2'	2.81	1.49	1.42
3	L5	3639	PSU	O4-C4	-2.81	1.18	1.23
3	L5	1534	A2M	C5-C4	-2.81	1.33	1.39
3	L5	3867	A2M	O2'-C2'	2.81	1.49	1.42
50	S2	644	OMG	C2-N1	2.81	1.44	1.37
50	S2	1678	A2M	O2'-C2'	2.80	1.49	1.42
50	S2	683	OMG	C2-N1	2.80	1.44	1.37
3	L5	4370	OMG	C5-N7	-2.80	1.33	1.39
3	L5	3785	A2M	O3'-C3'	-2.80	1.36	1.43
50	S2	99	A2M	O2'-C2'	2.80	1.49	1.42
50	S2	572	PSU	O4-C4	-2.80	1.18	1.23
50	S2	576	A2M	C5-C4	-2.80	1.33	1.39
3	L5	4523	A2M	O2'-C2'	2.80	1.49	1.42
3	L5	4228	OMG	C2-N1	2.80	1.44	1.37
3	L5	400	A2M	O2'-C2'	2.79	1.49	1.42
3	L5	1625	OMG	C2-N1	2.79	1.44	1.37
3	L5	1683	PSU	O4-C4	-2.79	1.18	1.23
3	L5	3944	OMG	C2-N1	2.79	1.44	1.37
3	L5	4623	OMG	C5-N7	-2.79	1.33	1.39
50	S2	166	A2M	C5-C4	-2.79	1.33	1.39
3	L5	4618	OMG	C2-N1	2.79	1.44	1.37
3	L5	5001	PSU	O4-C4	-2.79	1.18	1.23
50	S2	601	OMG	C2-N1	2.79	1.44	1.37
5	L8	75	OMG	C2-N1	2.79	1.44	1.37
3	L5	2363	A2M	O2'-C2'	2.79	1.49	1.42
3	L5	1522	OMG	C5-N7	-2.78	1.33	1.39
50	S2	174	OMC	O2-C2	-2.78	1.18	1.23
3	L5	3718	A2M	C5-N7	-2.78	1.33	1.39
3	L5	4457	PSU	O4-C4	-2.78	1.18	1.23
50	S2	512	A2M	O2'-C2'	2.78	1.49	1.42
50	S2	1447	OMG	C2-N1	2.77	1.44	1.37
50	S2	99	A2M	C5-C4	-2.77	1.33	1.39
3	L5	4521	PSU	O4-C4	-2.77	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	27	A2M	O2'-C2'	2.77	1.49	1.42
3	L5	4637	OMG	C5-N7	-2.77	1.33	1.39
3	L5	4293	PSU	O4-C4	-2.77	1.18	1.23
50	S2	517	OMC	O2-C2	-2.77	1.18	1.23
3	L5	4392	OMG	C2-N1	2.76	1.44	1.37
3	L5	1340	OMC	O2-C2	-2.76	1.18	1.23
3	L5	4392	OMG	C5-N7	-2.76	1.33	1.39
50	S2	468	A2M	O2'-C2'	2.76	1.49	1.42
50	S2	436	OMG	C2-N1	2.76	1.44	1.37
5	L8	75	OMG	C5-N7	-2.76	1.33	1.39
3	L5	3744	OMG	C5-N7	-2.76	1.33	1.39
5	L8	55	PSU	O4-C4	-2.75	1.18	1.23
50	S2	159	A2M	C5-C4	-2.75	1.33	1.39
50	S2	863	PSU	O4-C4	-2.75	1.18	1.23
50	S2	484	A2M	O3'-C3'	-2.75	1.36	1.43
3	L5	4296	PSU	O4-C4	-2.75	1.18	1.23
3	L5	3869	OMC	O2-C2	-2.75	1.18	1.23
50	S2	27	A2M	C5-C4	-2.75	1.33	1.39
3	L5	2364	OMG	C2-N1	2.75	1.44	1.37
3	L5	4361	PSU	O4-C4	-2.75	1.18	1.23
50	S2	462	OMC	O2-C2	-2.75	1.18	1.23
3	L5	4403	PSU	O4-C4	-2.75	1.18	1.23
3	L5	3782	5MC	O2-C2	-2.74	1.18	1.23
50	S2	867	OMG	C2-N1	2.74	1.44	1.37
3	L5	3899	OMG	C5-N7	-2.74	1.33	1.39
3	L5	4471	PSU	O4-C4	-2.74	1.18	1.23
3	L5	3627	OMG	C2-N1	2.74	1.44	1.37
3	L5	3695	PSU	O4-C4	-2.74	1.18	1.23
50	S2	1383	A2M	C5-C4	-2.73	1.33	1.39
3	L5	1522	OMG	C2-N1	2.73	1.44	1.37
3	L5	4623	OMG	C2-N1	2.73	1.44	1.37
3	L5	4494	OMG	C2-N1	2.73	1.44	1.37
3	L5	3785	A2M	O2'-C2'	2.72	1.49	1.42
3	L5	3867	A2M	C5-C4	-2.72	1.33	1.39
3	L5	2876	OMG	C2-N1	2.72	1.44	1.37
3	L5	4370	OMG	C2-N1	2.72	1.44	1.37
3	L5	3844	PSU	O4-C4	-2.72	1.18	1.23
50	S2	116	OMU	C6-N1	2.72	1.44	1.38
3	L5	2787	A2M	O2'-C2'	2.72	1.49	1.42
3	L5	4579	PSU	O4-C4	-2.72	1.18	1.23
3	L5	2424	OMG	C2-N1	2.72	1.44	1.37
3	L5	4353	PSU	O4-C4	-2.72	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3887	OMC	O2-C2	-2.72	1.18	1.23
3	L5	1316	OMG	C2-N1	2.72	1.44	1.37
50	S2	1850	MA6	C5-C4	-2.72	1.33	1.39
3	L5	4499	OMG	C2-N1	2.71	1.44	1.37
3	L5	4636	PSU	O4-C4	-2.71	1.18	1.23
50	S2	1639	G7M	C2-N1	2.71	1.44	1.37
50	S2	590	A2M	C5-C4	-2.71	1.33	1.39
3	L5	3899	OMG	C2-N1	2.71	1.44	1.37
50	S2	36	PSU	O4-C4	-2.71	1.18	1.23
3	L5	4312	PSU	O4-C4	-2.71	1.18	1.23
50	S2	1851	MA6	C5-C4	-2.71	1.33	1.39
3	L5	2787	A2M	C5-N7	-2.71	1.33	1.39
3	L5	4689	PSU	O4-C4	-2.71	1.18	1.23
50	S2	484	A2M	C5-C4	-2.71	1.34	1.39
3	L5	3853	PSU	O4-C4	-2.71	1.18	1.23
50	S2	918	PSU	O4'-C1'	-2.71	1.40	1.43
3	L5	3734	PSU	O4-C4	-2.70	1.18	1.23
50	S2	509	OMG	O6-C6	-2.70	1.18	1.23
3	L5	4552	PSU	O4-C4	-2.70	1.18	1.23
3	L5	2364	OMG	C5-N7	-2.70	1.33	1.39
3	L5	1744	PSU	O4-C4	-2.70	1.18	1.23
50	S2	1391	OMC	O2-C2	-2.70	1.18	1.23
3	L5	4623	OMG	O6-C6	-2.70	1.18	1.23
3	L5	4493	PSU	O4-C4	-2.70	1.18	1.23
3	L5	4196	OMG	C2-N1	2.69	1.44	1.37
3	L5	1316	OMG	O6-C6	-2.69	1.18	1.23
3	L5	2508	PSU	O4-C4	-2.69	1.18	1.23
3	L5	4228	OMG	C5-N7	-2.69	1.33	1.39
3	L5	4673	PSU	O4-C4	-2.69	1.18	1.23
3	L5	3920	PSU	O4-C4	-2.69	1.18	1.23
3	L5	4628	PSU	O4-C4	-2.69	1.18	1.23
3	L5	3851	PSU	O4-C4	-2.69	1.18	1.23
3	L5	4299	PSU	O4-C4	-2.69	1.18	1.23
3	L5	3718	A2M	C5-C4	-2.69	1.34	1.39
50	S2	681	PSU	O4-C4	-2.68	1.18	1.23
50	S2	686	PSU	O4-C4	-2.68	1.18	1.23
3	L5	1792	PSU	O4-C4	-2.68	1.18	1.23
3	L5	3637	PSU	O4-C4	-2.68	1.18	1.23
50	S2	1239	PSU	O4-C4	-2.68	1.18	1.23
3	L5	4220	6MZ	C5-N7	-2.68	1.34	1.39
5	L8	69	PSU	O4-C4	-2.68	1.18	1.23
50	S2	1490	OMG	C2-N1	2.67	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	398	A2M	C5-N7	-2.67	1.34	1.39
3	L5	1860	PSU	O4-C4	-2.67	1.18	1.23
3	L5	4228	OMG	C4-N9	-2.67	1.31	1.38
3	L5	2364	OMG	O6-C6	-2.67	1.18	1.23
3	L5	4196	OMG	O6-C6	-2.67	1.18	1.23
3	L5	3729	PSU	O4-C4	-2.67	1.18	1.23
3	L5	1677	PSU	O4'-C1'	-2.67	1.40	1.43
3	L5	3899	OMG	O6-C6	-2.67	1.18	1.23
3	L5	4637	OMG	O6-C6	-2.67	1.18	1.23
50	S2	1678	A2M	C5-C4	-2.67	1.34	1.39
50	S2	406	PSU	O4-C4	-2.67	1.18	1.23
3	L5	4392	OMG	O6-C6	-2.67	1.18	1.23
3	L5	4637	OMG	C2-N1	2.67	1.44	1.37
3	L5	4618	OMG	C5-N7	-2.67	1.33	1.39
3	L5	2815	A2M	C5-C4	-2.67	1.34	1.39
3	L5	4431	PSU	O4-C4	-2.67	1.18	1.23
50	S2	1238	PSU	O4-C4	-2.66	1.18	1.23
3	L5	1779	PSU	O4-C4	-2.66	1.18	1.23
3	L5	3792	OMG	C2-N1	2.66	1.44	1.37
3	L5	1782	PSU	O4-C4	-2.66	1.18	1.23
3	L5	2839	PSU	O4-C4	-2.66	1.18	1.23
3	L5	398	A2M	C5-C4	-2.66	1.34	1.39
3	L5	4972	PSU	O4-C4	-2.66	1.18	1.23
50	S2	1347	PSU	O4-C4	-2.66	1.18	1.23
3	L5	3768	PSU	O4-C4	-2.66	1.18	1.23
3	L5	4494	OMG	O6-C6	-2.66	1.18	1.23
3	L5	4618	OMG	O6-C6	-2.66	1.18	1.23
50	S2	159	A2M	C5-N7	-2.66	1.34	1.39
50	S2	109	PSU	O4-C4	-2.66	1.18	1.23
3	L5	1582	PSU	O4-C4	-2.65	1.18	1.23
3	L5	4569	PSU	O4-C4	-2.65	1.18	1.23
3	L5	1781	PSU	O4-C4	-2.65	1.18	1.23
3	L5	4228	OMG	C6-N1	2.65	1.43	1.38
3	L5	5010	PSU	O4-C4	-2.65	1.18	1.23
3	L5	3770	PSU	O4-C4	-2.65	1.18	1.23
3	L5	1522	OMG	O6-C6	-2.64	1.18	1.23
3	L5	4228	OMG	O6-C6	-2.64	1.18	1.23
3	L5	3627	OMG	C5-N7	-2.64	1.34	1.39
50	S2	1177	PSU	O4-C4	-2.64	1.18	1.23
3	L5	4370	OMG	O6-C6	-2.63	1.18	1.23
3	L5	1871	A2M	C5-N7	-2.63	1.34	1.39
50	S2	512	A2M	C5-C4	-2.63	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3899	OMG	C4-N9	-2.63	1.31	1.38
50	S2	822	PSU	O4-C4	-2.63	1.18	1.23
3	L5	4442	PSU	O4-C4	-2.62	1.18	1.23
50	S2	99	A2M	C5-N7	-2.62	1.34	1.39
50	S2	1625	PSU	O4-C4	-2.62	1.18	1.23
3	L5	4618	OMG	C5-C6	2.62	1.54	1.44
50	S2	644	OMG	O6-C6	-2.62	1.18	1.23
3	L5	4618	OMG	C6-N1	2.62	1.43	1.38
3	L5	1524	A2M	C5-N7	-2.62	1.34	1.39
50	S2	668	A2M	C5-N7	-2.62	1.34	1.39
3	L5	3867	A2M	C5-N7	-2.61	1.34	1.39
3	L5	4500	PSU	O4-C4	-2.61	1.18	1.23
3	L5	3627	OMG	O6-C6	-2.61	1.18	1.23
3	L5	3830	A2M	C5-N7	-2.61	1.34	1.39
50	S2	814	PSU	O4-C4	-2.61	1.18	1.23
50	S2	1174	PSU	O4-C4	-2.61	1.18	1.23
3	L5	1677	PSU	O4-C4	-2.61	1.18	1.23
3	L5	3764	PSU	O4-C4	-2.61	1.18	1.23
50	S2	1056	PSU	O4-C4	-2.61	1.18	1.23
50	S2	1244	PSU	O4-C4	-2.61	1.18	1.23
50	S2	966	PSU	O4-C4	-2.61	1.18	1.23
3	L5	1625	OMG	O6-C6	-2.61	1.18	1.23
3	L5	4499	OMG	O6-C6	-2.60	1.18	1.23
3	L5	3758	PSU	O4-C4	-2.60	1.18	1.23
3	L5	2364	OMG	C5-C6	2.60	1.54	1.44
3	L5	2815	A2M	C5-N7	-2.60	1.34	1.39
50	S2	573	PSU	O4-C4	-2.59	1.18	1.23
3	L5	4576	PSU	O4-C4	-2.59	1.18	1.23
50	S2	815	PSU	O4-C4	-2.59	1.18	1.23
3	L5	4618	OMG	C4-N9	-2.59	1.31	1.38
3	L5	1326	A2M	C5-N7	-2.59	1.34	1.39
50	S2	509	OMG	C2-N1	2.59	1.44	1.37
50	S2	436	OMG	O6-C6	-2.59	1.18	1.23
3	L5	1862	PSU	O4-C4	-2.59	1.18	1.23
3	L5	4532	PSU	O4-C4	-2.59	1.18	1.23
50	S2	218	PSU	O4-C4	-2.59	1.18	1.23
50	S2	601	OMG	O6-C6	-2.59	1.18	1.23
3	L5	4423	PSU	O4-C4	-2.59	1.18	1.23
50	S2	1232	PSU	O4-C4	-2.58	1.18	1.23
50	S2	1445	PSU	O4-C4	-2.58	1.18	1.23
3	L5	3627	OMG	C6-N1	2.58	1.43	1.38
50	S2	1367	PSU	O4-C4	-2.58	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4228	OMG	C5-C6	2.58	1.54	1.44
50	S2	105	PSU	O4-C4	-2.58	1.18	1.23
50	S2	1136	PSU	O4-C4	-2.58	1.18	1.23
50	S2	866	PSU	O4-C4	-2.58	1.18	1.23
50	S2	1678	A2M	C5-N7	-2.58	1.34	1.39
50	S2	1643	PSU	O4-C4	-2.58	1.18	1.23
3	L5	2363	A2M	C5-N7	-2.58	1.34	1.39
5	L8	75	OMG	O6-C6	-2.58	1.18	1.23
50	S2	649	PSU	O4-C4	-2.58	1.18	1.23
50	S2	644	OMG	C6-N1	2.58	1.43	1.38
3	L5	3744	OMG	O6-C6	-2.57	1.18	1.23
50	S2	93	PSU	O4-C4	-2.57	1.18	1.23
50	S2	119	PSU	O4-C4	-2.57	1.18	1.23
3	L5	2401	A2M	C5-N7	-2.57	1.34	1.39
5	L8	75	OMG	C5-C6	2.57	1.53	1.44
3	L5	3792	OMG	O6-C6	-2.57	1.18	1.23
50	S2	1639	G7M	C6-N1	2.57	1.43	1.38
3	L5	3627	OMG	C5-C6	2.57	1.53	1.44
3	L5	1522	OMG	C5-C6	2.57	1.53	1.44
3	L5	4637	OMG	C5-C6	2.57	1.53	1.44
50	S2	296	PSU	O4-C4	-2.57	1.18	1.23
3	L5	400	A2M	C5-N7	-2.57	1.34	1.39
3	L5	1534	A2M	C5-N7	-2.57	1.34	1.39
3	L5	3825	A2M	C5-N7	-2.56	1.34	1.39
50	S2	1692	PSU	O4-C4	-2.56	1.18	1.23
50	S2	1031	A2M	C5-N7	-2.56	1.34	1.39
50	S2	436	OMG	C6-N1	2.56	1.43	1.38
50	S2	683	OMG	C6-N1	2.56	1.43	1.38
50	S2	609	PSU	O4-C4	-2.56	1.18	1.23
3	L5	2424	OMG	O6-C6	-2.56	1.18	1.23
3	L5	3762	PSU	O4-C4	-2.56	1.18	1.23
50	S2	651	PSU	O4-C4	-2.56	1.18	1.23
50	S2	509	OMG	C5-C6	2.55	1.53	1.44
50	S2	512	A2M	C5-N7	-2.55	1.34	1.39
50	S2	683	OMG	O6-C6	-2.55	1.18	1.23
50	S2	644	OMG	C5-C6	2.55	1.53	1.44
50	S2	174	OMC	C5-C4	2.55	1.48	1.42
3	L5	3744	OMG	C6-N1	2.55	1.43	1.38
50	S2	436	OMG	C5-C6	2.54	1.53	1.44
3	L5	4420	PSU	O4-C4	-2.54	1.18	1.23
50	S2	918	PSU	O4-C4	-2.54	1.18	1.23
3	L5	4623	OMG	C5-C6	2.54	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	34	PSU	O4-C4	-2.54	1.18	1.23
5	L8	75	OMG	C6-N1	2.54	1.43	1.38
3	L5	2364	OMG	C4-N9	-2.54	1.31	1.38
3	L5	4571	A2M	C5-N7	-2.54	1.34	1.39
50	S2	801	PSU	O4-C4	-2.53	1.18	1.23
3	L5	3899	OMG	C5-C6	2.53	1.53	1.44
50	S2	1447	OMG	O6-C6	-2.52	1.18	1.23
50	S2	1383	A2M	C5-N7	-2.52	1.34	1.39
3	L5	4392	OMG	C5-C6	2.52	1.53	1.44
3	L5	2632	PSU	O4-C4	-2.52	1.18	1.23
3	L5	4523	A2M	C5-N7	-2.52	1.34	1.39
50	S2	484	A2M	C5-N7	-2.52	1.34	1.39
3	L5	3701	OMC	C5-C4	2.52	1.48	1.42
3	L5	4494	OMG	C5-C6	2.51	1.53	1.44
3	L5	4499	OMG	C5-C6	2.51	1.53	1.44
50	S2	428	OMU	C5-C4	2.51	1.49	1.43
3	L5	3744	OMG	C5-C6	2.51	1.53	1.44
3	L5	3724	A2M	C5-N7	-2.51	1.34	1.39
50	S2	27	A2M	C5-N7	-2.51	1.34	1.39
50	S2	166	A2M	C5-N7	-2.51	1.34	1.39
50	S2	1447	OMG	C5-C6	2.51	1.53	1.44
3	L5	2364	OMG	C6-N1	2.51	1.43	1.38
3	L5	4590	A2M	C5-N7	-2.50	1.34	1.39
3	L5	3627	OMG	C4-N9	-2.50	1.31	1.38
3	L5	2876	OMG	C5-C6	2.50	1.53	1.44
50	S2	601	OMG	C6-N1	2.50	1.43	1.38
3	L5	2876	OMG	O6-C6	-2.50	1.18	1.23
3	L5	3723	A2M	C5-N7	-2.50	1.34	1.39
50	S2	1447	OMG	C6-N1	2.50	1.43	1.38
3	L5	3899	OMG	C6-N1	2.50	1.43	1.38
3	L5	3944	OMG	C6-N1	2.50	1.43	1.38
3	L5	4306	OMU	O2-C2	-2.50	1.18	1.23
3	L5	3944	OMG	O6-C6	-2.49	1.18	1.23
3	L5	1316	OMG	C5-C6	2.49	1.53	1.44
3	L5	4498	OMU	O2-C2	-2.49	1.18	1.23
3	L5	1625	OMG	C5-C6	2.49	1.53	1.44
50	S2	1490	OMG	C5-C6	2.49	1.53	1.44
50	S2	601	OMG	C5-C6	2.49	1.53	1.44
50	S2	1490	OMG	O6-C6	-2.49	1.18	1.23
50	S2	867	OMG	C5-C6	2.49	1.53	1.44
3	L5	4370	OMG	C5-C6	2.49	1.53	1.44
50	S2	867	OMG	C6-N1	2.48	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2424	OMG	C5-C6	2.48	1.53	1.44
50	S2	1850	MA6	C5-N7	-2.48	1.34	1.39
50	S2	576	A2M	C5-N7	-2.48	1.34	1.39
3	L5	4196	OMG	C5-C6	2.48	1.53	1.44
3	L5	4623	OMG	C6-N1	2.47	1.43	1.38
50	S2	683	OMG	C5-C6	2.47	1.53	1.44
3	L5	4623	OMG	C4-N9	-2.47	1.31	1.38
50	S2	590	A2M	C5-N7	-2.47	1.34	1.39
50	S2	1004	PSU	O4-C4	-2.46	1.18	1.23
3	L5	4499	OMG	C6-N1	2.46	1.43	1.38
3	L5	3925	OMU	O2-C2	-2.46	1.18	1.23
3	L5	1522	OMG	C4-N9	-2.46	1.31	1.38
3	L5	4392	OMG	C4-N9	-2.46	1.31	1.38
50	S2	468	A2M	C5-N7	-2.46	1.34	1.39
3	L5	2365	OMC	C5-C4	2.45	1.48	1.42
3	L5	3887	OMC	C5-C4	2.45	1.48	1.42
50	S2	462	OMC	C5-C4	2.45	1.48	1.42
3	L5	4392	OMG	C6-N1	2.45	1.43	1.38
3	L5	3944	OMG	C5-C6	2.45	1.53	1.44
3	L5	4456	OMC	C5-C4	2.45	1.48	1.42
3	L5	4420	PSU	O4'-C1'	-2.45	1.40	1.43
50	S2	867	OMG	O6-C6	-2.45	1.18	1.23
50	S2	1639	G7M	O6-C6	-2.44	1.18	1.23
3	L5	4227	OMU	C5-C4	2.44	1.49	1.43
3	L5	3792	OMG	C5-C6	2.44	1.53	1.44
3	L5	1881	OMC	C5-C4	2.44	1.48	1.42
50	S2	517	OMC	C5-C4	2.43	1.48	1.42
3	L5	3785	A2M	C5-N7	-2.43	1.34	1.39
3	L5	2422	OMC	C5-C4	2.42	1.48	1.42
3	L5	1322	1MA	C4-N9	-2.42	1.31	1.38
3	L5	3869	OMC	C5-C4	2.42	1.48	1.42
3	L5	4370	OMG	C6-N1	2.41	1.43	1.38
50	S2	1804	OMU	C5-C4	2.41	1.49	1.43
3	L5	2351	OMC	C5-C4	2.41	1.48	1.42
3	L5	4620	OMU	O2-C2	-2.41	1.18	1.23
3	L5	1625	OMG	C6-N1	2.41	1.43	1.38
3	L5	2861	OMC	C5-C4	2.40	1.48	1.42
50	S2	1391	OMC	C5-C4	2.40	1.48	1.42
3	L5	2824	OMC	C5-C4	2.40	1.48	1.42
3	L5	4227	OMU	O2-C2	-2.39	1.18	1.23
50	S2	1851	MA6	C5-N7	-2.39	1.34	1.39
50	S2	1288	OMU	C5-C4	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S2	172	OMU	C5-C4	2.39	1.48	1.43
3	L5	1522	OMG	C6-N1	2.39	1.43	1.38
3	L5	3925	OMU	C5-C4	2.39	1.48	1.43
50	S2	1442	OMU	C5-C4	2.39	1.48	1.43
3	L5	4536	OMC	C5-C4	2.38	1.48	1.42
50	S2	601	OMG	C4-N9	-2.38	1.31	1.38
3	L5	2804	OMC	C5-C4	2.38	1.48	1.42
3	L5	2424	OMG	C6-N1	2.37	1.43	1.38
3	L5	2415	OMU	O2-C2	-2.37	1.18	1.23
5	L8	14	OMU	O2-C2	-2.37	1.18	1.23
3	L5	3808	OMC	C5-C4	2.37	1.48	1.42
3	L5	3841	OMC	C5-C4	2.36	1.48	1.42
50	S2	121	OMU	C5-C4	2.36	1.48	1.43
3	L5	1316	OMG	C4-N9	-2.36	1.31	1.38
3	L5	2837	OMU	C5-C4	2.36	1.48	1.43
50	S2	1490	OMG	C6-N1	2.36	1.43	1.38
50	S2	354	OMU	O2-C2	-2.35	1.18	1.23
3	L5	3718	A2M	C8-N9	-2.35	1.33	1.37
5	L8	75	OMG	C4-N9	-2.35	1.31	1.38
3	L5	4498	OMU	C5-C4	2.35	1.48	1.43
3	L5	4494	OMG	C6-N1	2.35	1.43	1.38
3	L5	4637	OMG	C6-N1	2.34	1.43	1.38
3	L5	1316	OMG	C6-N1	2.34	1.43	1.38
50	S2	428	OMU	O2-C2	-2.34	1.18	1.23
3	L5	4196	OMG	C6-N1	2.34	1.43	1.38
50	S2	354	OMU	C5-C4	2.34	1.48	1.43
50	S2	1248	B8N	O2-C2	-2.33	1.18	1.22
3	L5	2876	OMG	C6-N1	2.33	1.43	1.38
3	L5	4499	OMG	C4-N9	-2.33	1.32	1.38
50	S2	1804	OMU	O2-C2	-2.33	1.18	1.23
50	S2	1490	OMG	C4-N9	-2.32	1.32	1.38
50	S2	1248	B8N	O4-C4	-2.32	1.18	1.23
3	L5	2837	OMU	O2-C2	-2.32	1.18	1.23
3	L5	3744	OMG	C4-N9	-2.32	1.32	1.38
3	L5	4370	OMG	C4-N9	-2.32	1.32	1.38
5	L8	14	OMU	C5-C4	2.31	1.48	1.43
3	L5	1625	OMG	C4-N9	-2.31	1.32	1.38
3	L5	4620	OMU	C5-C4	2.30	1.48	1.43
50	S2	509	OMG	C6-N1	2.30	1.43	1.38
3	L5	3792	OMG	C6-N1	2.29	1.43	1.38
50	S2	121	OMU	O2-C2	-2.29	1.18	1.23
3	L5	4494	OMG	C4-N9	-2.29	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2415	OMU	C5-C4	2.28	1.48	1.43
50	S2	116	OMU	O2-C2	-2.28	1.18	1.23
3	L5	3792	OMG	C4-N9	-2.28	1.32	1.38
3	L5	4306	OMU	C5-C4	2.28	1.48	1.43
50	S2	1442	OMU	O2-C2	-2.26	1.18	1.23
50	S2	436	OMG	C4-N9	-2.26	1.32	1.38
3	L5	1340	OMC	C5-C4	2.26	1.48	1.42
3	L5	4530	UR3	C5-C4	2.25	1.49	1.43
50	S2	116	OMU	C5-C4	2.25	1.48	1.43
50	S2	172	OMU	O2-C2	-2.24	1.19	1.23
3	L5	4637	OMG	C4-N9	-2.23	1.32	1.38
50	S2	1288	OMU	O2-C2	-2.22	1.19	1.23
50	S2	644	OMG	C4-N9	-2.21	1.32	1.38
3	L5	1534	A2M	C8-N9	-2.21	1.33	1.37
3	L5	4196	OMG	C4-N9	-2.18	1.32	1.38
3	L5	2876	OMG	C4-N9	-2.18	1.32	1.38
50	S2	590	A2M	C8-N9	-2.18	1.33	1.37
3	L5	4590	A2M	C8-N9	-2.16	1.33	1.37
50	S2	159	A2M	C8-N9	-2.15	1.33	1.37
3	L5	1524	A2M	C8-N9	-2.15	1.33	1.37
3	L5	4220	6MZ	C8-N9	-2.15	1.33	1.37
50	S2	683	OMG	C4-N9	-2.15	1.32	1.38
3	L5	4571	A2M	C8-N9	-2.14	1.33	1.37
3	L5	3723	A2M	C8-N9	-2.13	1.33	1.37
3	L5	2815	A2M	C8-N9	-2.13	1.33	1.37
3	L5	3825	A2M	C8-N9	-2.12	1.33	1.37
50	S2	509	OMG	C4-N9	-2.12	1.32	1.38
50	S2	99	A2M	C8-N9	-2.12	1.33	1.37
3	L5	3724	A2M	C8-N9	-2.11	1.33	1.37
50	S2	668	A2M	C8-N9	-2.11	1.33	1.37
3	L5	3785	A2M	C8-N9	-2.10	1.33	1.37
3	L5	3867	A2M	C8-N9	-2.10	1.33	1.37
3	L5	4530	UR3	O4-C4	-2.10	1.19	1.23
3	L5	2363	A2M	C8-N9	-2.09	1.33	1.37
50	S2	1851	MA6	C10-N6	2.09	1.50	1.45
50	S2	1031	A2M	C8-N9	-2.09	1.33	1.37
5	L8	69	PSU	O4'-C1'	-2.08	1.41	1.43
3	L5	4420	PSU	C4-C5	2.08	1.50	1.44
3	L5	2787	A2M	C8-N9	-2.08	1.33	1.37
50	S2	119	PSU	C4-C5	2.07	1.50	1.44
3	L5	400	A2M	C8-N9	-2.07	1.33	1.37
50	S2	822	PSU	O4'-C1'	-2.07	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4530	UR3	O2-C2	-2.06	1.18	1.22
50	S2	1678	A2M	C8-N9	-2.06	1.33	1.37
50	S2	1447	OMG	C4-N9	-2.06	1.32	1.38
3	L5	1326	A2M	C8-N9	-2.06	1.33	1.37
50	S2	99	A2M	O5'-C5'	-2.05	1.39	1.44
3	L5	398	A2M	C8-N9	-2.05	1.33	1.37
50	S2	484	A2M	C8-N9	-2.05	1.33	1.37
50	S2	576	A2M	C8-N9	-2.05	1.33	1.37
50	S2	512	A2M	C8-N9	-2.05	1.33	1.37
50	S2	1337	4AC	CM7-C7	2.05	1.54	1.50
50	S2	166	A2M	C8-N9	-2.04	1.33	1.37
3	L5	4636	PSU	C4-C5	2.04	1.50	1.44
50	S2	27	A2M	C8-N9	-2.04	1.33	1.37
50	S2	573	PSU	C4-C5	2.04	1.50	1.44
50	S2	1248	B8N	C2-N3	2.04	1.42	1.38
3	L5	4530	UR3	C4-N3	2.04	1.45	1.40
50	S2	1850	MA6	C10-N6	2.03	1.50	1.45
3	L5	1871	A2M	O5'-C5'	-2.03	1.39	1.44
50	S2	867	OMG	C4-N9	-2.03	1.32	1.38
50	S2	668	A2M	O5'-C5'	-2.02	1.39	1.44
3	L5	2787	A2M	O5'-C5'	-2.02	1.39	1.44
50	S2	1851	MA6	C4-N9	-2.02	1.33	1.37
3	L5	3867	A2M	O5'-C5'	-2.02	1.39	1.44
3	L5	3944	OMG	C4-N9	-2.02	1.32	1.38
3	L5	2401	A2M	C8-N9	-2.02	1.33	1.37
50	S2	572	PSU	C4-C5	2.01	1.49	1.44
3	L5	2815	A2M	O5'-C5'	-2.00	1.39	1.44

All (1320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	1851	MA6	N1-C6-N6	-11.53	104.48	117.08
50	S2	1850	MA6	N1-C6-N6	-10.70	105.39	117.08
3	L5	1322	1MA	C1'-N9-C8	-9.31	100.21	126.70
3	L5	1322	1MA	C1'-N9-C4	8.98	153.18	126.50
3	L5	2876	OMG	C1'-N9-C8	-8.63	102.14	126.70
50	S2	867	OMG	C1'-N9-C8	-8.06	103.75	126.70
3	L5	2424	OMG	C1'-N9-C8	-8.04	103.82	126.70
50	S2	1447	OMG	C1'-N9-C8	-7.95	104.06	126.70
3	L5	4196	OMG	C1'-N9-C8	-7.94	104.08	126.70
3	L5	3944	OMG	C1'-N9-C8	-7.91	104.18	126.70
3	L5	3792	OMG	C1'-N9-C8	-7.84	104.38	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	683	OMG	C1'-N9-C8	-7.77	104.56	126.70
3	L5	1625	OMG	C1'-N9-C8	-7.77	104.58	126.70
50	S2	601	OMG	C1'-N9-C8	-7.66	104.89	126.70
50	S2	509	OMG	C1'-N9-C8	-7.61	105.03	126.70
50	S2	1639	G7M	C1'-N9-C4	7.60	149.08	126.50
50	S2	1639	G7M	C1'-N9-C8	-7.54	101.27	126.74
50	S2	644	OMG	C1'-N9-C8	-7.50	105.34	126.70
3	L5	4370	OMG	C1'-N9-C8	-7.45	105.48	126.70
3	L5	4499	OMG	C1'-N9-C8	-7.45	105.50	126.70
50	S2	1490	OMG	C1'-N9-C8	-7.42	105.56	126.70
3	L5	3744	OMG	C1'-N9-C8	-7.38	105.70	126.70
3	L5	2876	OMG	C1'-N9-C4	7.34	148.30	126.50
3	L5	4637	OMG	C1'-N9-C8	-7.31	105.89	126.70
3	L5	2424	OMG	C1'-N9-C4	7.30	148.18	126.50
3	L5	4494	OMG	C1'-N9-C8	-7.27	106.00	126.70
50	S2	436	OMG	C1'-N9-C8	-7.25	106.06	126.70
5	L8	75	OMG	C1'-N9-C8	-7.13	106.41	126.70
3	L5	1316	OMG	C1'-N9-C8	-7.09	106.51	126.70
3	L5	1522	OMG	C1'-N9-C8	-7.06	106.59	126.70
3	L5	4392	OMG	C1'-N9-C8	-7.03	106.69	126.70
3	L5	4623	OMG	C1'-N9-C8	-6.93	106.96	126.70
3	L5	3944	OMG	C1'-N9-C4	6.90	147.00	126.50
3	L5	2364	OMG	C1'-N9-C8	-6.85	107.18	126.70
3	L5	4196	OMG	C1'-N9-C4	6.85	146.85	126.50
50	S2	867	OMG	C1'-N9-C4	6.85	146.84	126.50
50	S2	1447	OMG	C1'-N9-C4	6.84	146.82	126.50
3	L5	3899	OMG	C1'-N9-C8	-6.68	107.67	126.70
3	L5	1625	OMG	C1'-N9-C4	6.68	146.34	126.50
3	L5	4618	OMG	C1'-N9-C8	-6.67	107.70	126.70
3	L5	3792	OMG	C1'-N9-C4	6.65	146.25	126.50
50	S2	601	OMG	C1'-N9-C4	6.63	146.19	126.50
50	S2	509	OMG	C1'-N9-C4	6.58	146.06	126.50
50	S2	683	OMG	C1'-N9-C4	6.53	145.91	126.50
3	L5	4228	OMG	C1'-N9-C8	-6.52	108.13	126.70
3	L5	3627	OMG	C1'-N9-C8	-6.49	108.22	126.70
50	S2	644	OMG	C1'-N9-C4	6.41	145.53	126.50
3	L5	4499	OMG	C1'-N9-C4	6.38	145.44	126.50
3	L5	4494	OMG	C1'-N9-C4	6.37	145.42	126.50
3	L5	4370	OMG	C1'-N9-C4	6.37	145.41	126.50
50	S2	1490	OMG	C1'-N9-C4	6.32	145.29	126.50
3	L5	3744	OMG	C1'-N9-C4	6.24	145.02	126.50
50	S2	436	OMG	C1'-N9-C4	6.18	144.86	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4637	OMG	C1'-N9-C4	6.15	144.76	126.50
5	L8	75	OMG	C1'-N9-C4	6.04	144.44	126.50
3	L5	4392	OMG	C1'-N9-C4	5.99	144.31	126.50
3	L5	1522	OMG	C1'-N9-C4	5.99	144.29	126.50
50	S2	1851	MA6	C5-C6-N6	5.98	135.71	125.30
3	L5	1316	OMG	C1'-N9-C4	5.90	144.03	126.50
3	L5	4623	OMG	C1'-N9-C4	5.86	143.91	126.50
50	S2	590	A2M	C5-C4-N3	-5.79	119.20	126.75
3	L5	4590	A2M	N3-C2-N1	-5.75	119.61	128.60
50	S2	512	A2M	N3-C2-N1	-5.75	119.61	128.60
3	L5	2815	A2M	C5-C4-N3	-5.72	119.29	126.75
3	L5	1322	1MA	N1-C2-N3	-5.71	119.21	126.00
3	L5	2364	OMG	C1'-N9-C4	5.69	143.41	126.50
3	L5	1871	A2M	N3-C2-N1	-5.65	119.77	128.60
3	L5	2363	A2M	N3-C2-N1	-5.64	119.77	128.60
3	L5	3724	A2M	N3-C2-N1	-5.63	119.79	128.60
3	L5	1326	A2M	N3-C2-N1	-5.61	119.83	128.60
50	S2	1031	A2M	N3-C2-N1	-5.61	119.83	128.60
3	L5	2401	A2M	N3-C2-N1	-5.60	119.83	128.60
50	S2	1851	MA6	N1-C2-N3	-5.60	119.84	128.60
50	S2	166	A2M	N3-C2-N1	-5.60	119.85	128.60
3	L5	3830	A2M	N3-C2-N1	-5.58	119.87	128.60
50	S2	1850	MA6	C5-C6-N6	5.58	135.02	125.30
3	L5	400	A2M	N3-C2-N1	-5.57	119.89	128.60
50	S2	668	A2M	N3-C2-N1	-5.56	119.90	128.60
3	L5	4220	6MZ	N1-C2-N3	-5.55	119.91	128.60
3	L5	4523	A2M	N3-C2-N1	-5.55	119.92	128.60
3	L5	398	A2M	C5-C4-N3	-5.55	119.51	126.75
50	S2	428	OMU	C4-N3-C2	-5.54	119.27	126.58
50	S2	1678	A2M	C5-C4-N3	-5.54	119.52	126.75
50	S2	159	A2M	N3-C2-N1	-5.52	119.97	128.60
3	L5	4618	OMG	C1'-N9-C4	5.51	142.87	126.50
3	L5	3785	A2M	N3-C2-N1	-5.51	119.99	128.60
50	S2	1850	MA6	N1-C2-N3	-5.49	120.01	128.60
3	L5	3723	A2M	N3-C2-N1	-5.49	120.01	128.60
50	S2	512	A2M	C5-C4-N3	-5.49	119.59	126.75
3	L5	2787	A2M	C5-C4-N3	-5.49	119.59	126.75
50	S2	27	A2M	N3-C2-N1	-5.48	120.03	128.60
3	L5	3899	OMG	C1'-N9-C4	5.47	142.76	126.50
3	L5	3867	A2M	C5-C4-N3	-5.47	119.61	126.75
50	S2	590	A2M	N3-C2-N1	-5.47	120.05	128.60
50	S2	468	A2M	N3-C2-N1	-5.47	120.05	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2815	A2M	N3-C2-N1	-5.46	120.06	128.60
50	S2	1383	A2M	N3-C2-N1	-5.45	120.07	128.60
50	S2	1678	A2M	N3-C2-N1	-5.45	120.07	128.60
50	S2	99	A2M	N3-C2-N1	-5.44	120.09	128.60
3	L5	1534	A2M	N3-C2-N1	-5.44	120.09	128.60
3	L5	3825	A2M	N3-C2-N1	-5.42	120.12	128.60
50	S2	27	A2M	C5-C4-N3	-5.42	119.68	126.75
50	S2	99	A2M	C5-C4-N3	-5.42	119.68	126.75
3	L5	4227	OMU	C4-N3-C2	-5.41	119.44	126.58
50	S2	484	A2M	N3-C2-N1	-5.39	120.16	128.60
3	L5	1524	A2M	N3-C2-N1	-5.38	120.18	128.60
3	L5	4571	A2M	N3-C2-N1	-5.37	120.20	128.60
3	L5	3925	OMU	C4-N3-C2	-5.36	119.51	126.58
3	L5	3718	A2M	C5-C4-N3	-5.36	119.76	126.75
50	S2	1383	A2M	C5-C4-N3	-5.36	119.76	126.75
3	L5	2787	A2M	N3-C2-N1	-5.36	120.22	128.60
3	L5	3830	A2M	C5-C4-N3	-5.35	119.77	126.75
5	L8	14	OMU	C4-N3-C2	-5.35	119.52	126.58
50	S2	166	A2M	C5-C4-N3	-5.35	119.77	126.75
50	S2	484	A2M	C5-C4-N3	-5.34	119.78	126.75
3	L5	4523	A2M	C5-C4-N3	-5.33	119.79	126.75
3	L5	398	A2M	N3-C2-N1	-5.33	120.26	128.60
50	S2	576	A2M	N3-C2-N1	-5.33	120.26	128.60
3	L5	4498	OMU	C4-N3-C2	-5.33	119.55	126.58
50	S2	576	A2M	C5-C4-N3	-5.31	119.82	126.75
3	L5	3825	A2M	C5-C4-N3	-5.31	119.82	126.75
3	L5	2837	OMU	C4-N3-C2	-5.30	119.59	126.58
50	S2	172	OMU	C4-N3-C2	-5.29	119.60	126.58
3	L5	4571	A2M	C5-C4-N3	-5.29	119.85	126.75
3	L5	4228	OMG	C1'-N9-C4	5.29	142.20	126.50
3	L5	1524	A2M	C5-C4-N3	-5.28	119.86	126.75
3	L5	3627	OMG	C1'-N9-C4	5.28	142.18	126.50
50	S2	468	A2M	C5-C4-N3	-5.27	119.88	126.75
50	S2	354	OMU	C4-N3-C2	-5.26	119.64	126.58
3	L5	3723	A2M	C5-C4-N3	-5.24	119.92	126.75
3	L5	3785	A2M	C5-C4-N3	-5.23	119.92	126.75
3	L5	1326	A2M	C5-C4-N3	-5.23	119.93	126.75
50	S2	1804	OMU	C4-N3-C2	-5.22	119.70	126.58
3	L5	3867	A2M	N3-C2-N1	-5.21	120.45	128.60
3	L5	4590	A2M	C5-C4-N3	-5.20	119.96	126.75
3	L5	4306	OMU	C4-N3-C2	-5.19	119.73	126.58
3	L5	2363	A2M	C5-C4-N3	-5.19	119.97	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1534	A2M	C5-C4-N3	-5.19	119.98	126.75
50	S2	159	A2M	C5-C4-N3	-5.18	120.00	126.75
3	L5	400	A2M	C5-C4-N3	-5.17	120.01	126.75
3	L5	2401	A2M	C5-C4-N3	-5.17	120.01	126.75
3	L5	4220	6MZ	C5-C4-N3	-5.16	120.02	126.75
50	S2	1248	B8N	C5-C4-N3	5.15	125.72	116.17
50	S2	1031	A2M	C5-C4-N3	-5.15	120.03	126.75
3	L5	3724	A2M	C5-C4-N3	-5.15	120.03	126.75
3	L5	2424	OMG	C5-C4-N3	-5.13	120.14	128.46
50	S2	668	A2M	C5-C4-N3	-5.13	120.06	126.75
50	S2	121	OMU	C4-N3-C2	-5.11	119.83	126.58
50	S2	1442	OMU	C4-N3-C2	-5.08	119.89	126.58
3	L5	2415	OMU	C4-N3-C2	-5.06	119.91	126.58
50	S2	1850	MA6	C5-C4-N3	-5.05	120.16	126.75
50	S2	116	OMU	C4-N3-C2	-4.99	120.00	126.58
3	L5	3785	A2M	N6-C6-N1	-4.96	107.48	118.35
3	L5	1871	A2M	C5-C4-N3	-4.94	120.30	126.75
3	L5	4590	A2M	N6-C6-N1	-4.93	107.56	118.35
50	S2	1851	MA6	C5-C4-N3	-4.91	120.34	126.75
50	S2	166	A2M	N6-C6-N1	-4.90	107.62	118.35
3	L5	1534	A2M	N6-C6-N1	-4.90	107.62	118.35
50	S2	27	A2M	N6-C6-N1	-4.89	107.64	118.35
3	L5	1326	A2M	N6-C6-N1	-4.87	107.69	118.35
50	S2	576	A2M	N6-C6-N1	-4.86	107.71	118.35
50	S2	1288	OMU	C4-N3-C2	-4.85	120.18	126.58
50	S2	1383	A2M	N6-C6-N1	-4.84	107.75	118.35
3	L5	4571	A2M	N6-C6-N1	-4.84	107.75	118.35
50	S2	484	A2M	N6-C6-N1	-4.83	107.78	118.35
3	L5	2815	A2M	N6-C6-N1	-4.83	107.78	118.35
50	S2	468	A2M	N6-C6-N1	-4.83	107.78	118.35
3	L5	4620	OMU	C4-N3-C2	-4.83	120.21	126.58
50	S2	590	A2M	N6-C6-N1	-4.82	107.79	118.35
50	S2	668	A2M	N6-C6-N1	-4.82	107.79	118.35
50	S2	1447	OMG	C5-C4-N3	-4.82	120.64	128.46
3	L5	398	A2M	N6-C6-N1	-4.82	107.80	118.35
3	L5	2401	A2M	N6-C6-N1	-4.82	107.80	118.35
50	S2	1031	A2M	N6-C6-N1	-4.82	107.80	118.35
3	L5	3724	A2M	N6-C6-N1	-4.82	107.81	118.35
3	L5	4530	UR3	C4-N3-C2	-4.81	120.04	124.56
3	L5	4523	A2M	N6-C6-N1	-4.81	107.83	118.35
3	L5	3718	A2M	N3-C2-N1	-4.81	121.08	128.60
3	L5	3830	A2M	N6-C6-N1	-4.80	107.83	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3718	A2M	N6-C6-N1	-4.80	107.84	118.35
50	S2	867	OMG	C5-C4-N3	-4.79	120.69	128.46
3	L5	400	A2M	N6-C6-N1	-4.79	107.86	118.35
50	S2	159	A2M	N6-C6-N1	-4.79	107.86	118.35
50	S2	512	A2M	N6-C6-N1	-4.77	107.91	118.35
3	L5	3944	OMG	C5-C4-N3	-4.77	120.73	128.46
3	L5	1524	A2M	N6-C6-N1	-4.76	107.92	118.35
3	L5	2363	A2M	N6-C6-N1	-4.76	107.92	118.35
50	S2	1678	A2M	N6-C6-N1	-4.76	107.92	118.35
3	L5	4628	PSU	C4-N3-C2	-4.76	119.48	126.34
3	L5	3723	A2M	N6-C6-N1	-4.76	107.93	118.35
50	S2	509	OMG	C5-C4-N3	-4.75	120.75	128.46
3	L5	1871	A2M	N6-C6-N1	-4.75	107.96	118.35
3	L5	1536	PSU	C4-N3-C2	-4.74	119.50	126.34
3	L5	3825	A2M	N6-C6-N1	-4.74	107.97	118.35
3	L5	2843	PSU	C4-N3-C2	-4.71	119.55	126.34
3	L5	2787	A2M	N6-C6-N1	-4.71	108.03	118.35
3	L5	4196	OMG	C5-C4-N3	-4.71	120.82	128.46
3	L5	3867	A2M	N6-C6-N1	-4.71	108.04	118.35
3	L5	3695	PSU	C4-N3-C2	-4.70	119.56	126.34
50	S2	683	OMG	C5-C4-N3	-4.68	120.86	128.46
3	L5	2876	OMG	C5-C4-N3	-4.68	120.86	128.46
50	S2	686	PSU	C4-N3-C2	-4.67	119.62	126.34
50	S2	99	A2M	N6-C6-N1	-4.66	108.16	118.35
3	L5	4296	PSU	C4-N3-C2	-4.65	119.64	126.34
50	S2	406	PSU	C4-N3-C2	-4.65	119.64	126.34
50	S2	801	PSU	C4-N3-C2	-4.65	119.64	126.34
50	S2	1177	PSU	C4-N3-C2	-4.64	119.66	126.34
3	L5	3639	PSU	C4-N3-C2	-4.63	119.67	126.34
3	L5	3758	PSU	C4-N3-C2	-4.62	119.68	126.34
3	L5	3884	PSU	C4-N3-C2	-4.62	119.68	126.34
50	S2	863	PSU	C4-N3-C2	-4.62	119.68	126.34
3	L5	1782	PSU	C4-N3-C2	-4.62	119.69	126.34
50	S2	1056	PSU	C4-N3-C2	-4.61	119.69	126.34
50	S2	609	PSU	C4-N3-C2	-4.60	119.70	126.34
50	S2	1238	PSU	C4-N3-C2	-4.60	119.71	126.34
3	L5	4494	OMG	C5-C4-N3	-4.60	121.00	128.46
3	L5	5010	PSU	C4-N3-C2	-4.60	119.71	126.34
3	L5	5001	PSU	C4-N3-C2	-4.60	119.72	126.34
50	S2	1445	PSU	C4-N3-C2	-4.59	119.72	126.34
50	S2	966	PSU	C4-N3-C2	-4.59	119.73	126.34
3	L5	3734	PSU	C4-N3-C2	-4.58	119.73	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4521	PSU	C4-N3-C2	-4.58	119.74	126.34
50	S2	649	PSU	C4-N3-C2	-4.58	119.74	126.34
50	S2	36	PSU	C4-N3-C2	-4.57	119.75	126.34
3	L5	4500	PSU	C4-N3-C2	-4.57	119.76	126.34
50	S2	1347	PSU	C4-N3-C2	-4.57	119.76	126.34
3	L5	3770	PSU	C4-N3-C2	-4.56	119.77	126.34
3	L5	4403	PSU	C4-N3-C2	-4.56	119.77	126.34
50	S2	105	PSU	C4-N3-C2	-4.56	119.77	126.34
5	L8	55	PSU	C4-N3-C2	-4.55	119.79	126.34
50	S2	644	OMG	C5-C4-N3	-4.55	121.09	128.46
3	L5	3853	PSU	C4-N3-C2	-4.54	119.79	126.34
3	L5	4457	PSU	C4-N3-C2	-4.54	119.79	126.34
3	L5	4299	PSU	C4-N3-C2	-4.54	119.80	126.34
50	S2	866	PSU	C4-N3-C2	-4.53	119.81	126.34
3	L5	4423	PSU	C4-N3-C2	-4.53	119.81	126.34
50	S2	296	PSU	C4-N3-C2	-4.53	119.81	126.34
50	S2	815	PSU	C4-N3-C2	-4.53	119.82	126.34
50	S2	1639	G7M	C2-N3-C4	4.52	120.36	112.30
50	S2	1136	PSU	C4-N3-C2	-4.52	119.83	126.34
3	L5	4361	PSU	C4-N3-C2	-4.52	119.83	126.34
50	S2	814	PSU	C4-N3-C2	-4.51	119.84	126.34
3	L5	4689	PSU	C4-N3-C2	-4.51	119.85	126.34
3	L5	4972	PSU	C4-N3-C2	-4.50	119.85	126.34
50	S2	1367	PSU	C4-N3-C2	-4.50	119.85	126.34
3	L5	1862	PSU	C4-N3-C2	-4.50	119.85	126.34
50	S2	651	PSU	C4-N3-C2	-4.50	119.85	126.34
3	L5	4353	PSU	C4-N3-C2	-4.50	119.85	126.34
3	L5	3637	PSU	C4-N3-C2	-4.50	119.86	126.34
3	L5	1625	OMG	C5-C4-N3	-4.49	121.17	128.46
50	S2	109	PSU	C4-N3-C2	-4.49	119.86	126.34
50	S2	918	PSU	C4-N3-C2	-4.49	119.86	126.34
3	L5	4576	PSU	C4-N3-C2	-4.48	119.88	126.34
3	L5	4493	PSU	C4-N3-C2	-4.48	119.88	126.34
50	S2	1239	PSU	C4-N3-C2	-4.48	119.89	126.34
3	L5	4431	PSU	C4-N3-C2	-4.48	119.89	126.34
50	S2	436	OMG	C5-C4-N3	-4.48	121.20	128.46
3	L5	1860	PSU	C4-N3-C2	-4.47	119.90	126.34
3	L5	4370	OMG	C5-C4-N3	-4.47	121.22	128.46
50	S2	34	PSU	C4-N3-C2	-4.46	119.91	126.34
3	L5	1779	PSU	C4-N3-C2	-4.46	119.91	126.34
3	L5	3920	PSU	C4-N3-C2	-4.46	119.91	126.34
50	S2	1851	MA6	N9-C8-N7	-4.46	107.81	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2508	PSU	C4-N3-C2	-4.46	119.92	126.34
50	S2	1625	PSU	C4-N3-C2	-4.46	119.92	126.34
3	L5	1744	PSU	C4-N3-C2	-4.45	119.92	126.34
3	L5	4293	PSU	C4-N3-C2	-4.45	119.92	126.34
50	S2	1243	PSU	C4-N3-C2	-4.45	119.93	126.34
3	L5	4628	PSU	N1-C2-N3	4.44	120.16	115.13
50	S2	1232	PSU	C4-N3-C2	-4.43	119.95	126.34
50	S2	1244	PSU	C4-N3-C2	-4.42	119.96	126.34
3	L5	3851	PSU	C4-N3-C2	-4.42	119.97	126.34
3	L5	4637	OMG	C5-C4-N3	-4.42	121.29	128.46
3	L5	3768	PSU	C4-N3-C2	-4.42	119.97	126.34
3	L5	4499	OMG	C5-C4-N3	-4.42	121.30	128.46
3	L5	4673	PSU	C4-N3-C2	-4.41	119.98	126.34
50	S2	1004	PSU	C4-N3-C2	-4.41	119.99	126.34
3	L5	4312	PSU	C4-N3-C2	-4.41	119.99	126.34
50	S2	822	PSU	C4-N3-C2	-4.40	119.99	126.34
50	S2	1692	PSU	C4-N3-C2	-4.40	119.99	126.34
50	S2	681	PSU	C4-N3-C2	-4.40	119.99	126.34
3	L5	1582	PSU	C4-N3-C2	-4.40	120.00	126.34
3	L5	4442	PSU	C4-N3-C2	-4.40	120.00	126.34
5	L8	69	PSU	C4-N3-C2	-4.40	120.00	126.34
3	L5	4532	PSU	C4-N3-C2	-4.40	120.00	126.34
3	L5	4420	PSU	C4-N3-C2	-4.39	120.01	126.34
50	S2	1850	MA6	N9-C8-N7	-4.39	107.91	113.91
50	S2	573	PSU	C4-N3-C2	-4.39	120.01	126.34
3	L5	3764	PSU	C4-N3-C2	-4.39	120.02	126.34
3	L5	3762	PSU	C4-N3-C2	-4.39	120.02	126.34
3	L5	1792	PSU	C4-N3-C2	-4.38	120.02	126.34
3	L5	3637	PSU	N1-C2-N3	4.38	120.10	115.13
3	L5	3785	A2M	N9-C8-N7	-4.38	107.92	113.91
3	L5	1683	PSU	C4-N3-C2	-4.37	120.04	126.34
3	L5	4579	PSU	C4-N3-C2	-4.37	120.04	126.34
3	L5	1781	PSU	C4-N3-C2	-4.37	120.04	126.34
50	S2	468	A2M	N9-C8-N7	-4.37	107.94	113.91
3	L5	4403	PSU	N1-C2-N3	4.35	120.06	115.13
3	L5	2632	PSU	C4-N3-C2	-4.35	120.07	126.34
3	L5	4471	PSU	C4-N3-C2	-4.35	120.07	126.34
50	S2	1031	A2M	N9-C8-N7	-4.35	107.96	113.91
3	L5	1524	A2M	N9-C8-N7	-4.35	107.97	113.91
50	S2	601	OMG	C5-C4-N3	-4.35	121.41	128.46
50	S2	166	A2M	N9-C8-N7	-4.34	107.97	113.91
50	S2	668	A2M	N9-C8-N7	-4.34	107.98	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2839	PSU	C4-N3-C2	-4.34	120.09	126.34
50	S2	93	PSU	C4-N3-C2	-4.33	120.10	126.34
3	L5	4552	PSU	C4-N3-C2	-4.33	120.10	126.34
3	L5	4500	PSU	N1-C2-N3	4.33	120.04	115.13
3	L5	1677	PSU	C4-N3-C2	-4.32	120.12	126.34
3	L5	3723	A2M	N9-C8-N7	-4.32	108.01	113.91
3	L5	4569	PSU	C4-N3-C2	-4.32	120.12	126.34
50	S2	1643	PSU	C4-N3-C2	-4.31	120.12	126.34
5	L8	75	OMG	C5-C4-N3	-4.31	121.47	128.46
3	L5	4636	PSU	C4-N3-C2	-4.31	120.14	126.34
50	S2	1367	PSU	N1-C2-N3	4.30	120.00	115.13
3	L5	4571	A2M	N9-C8-N7	-4.30	108.03	113.91
3	L5	3744	OMG	C5-C4-N3	-4.30	121.48	128.46
50	S2	572	PSU	C4-N3-C2	-4.30	120.15	126.34
3	L5	3695	PSU	N1-C2-N3	4.30	120.00	115.13
5	L8	75	OMG	C2-N3-C4	4.30	119.95	112.30
3	L5	4689	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	4636	PSU	N1-C2-N3	4.28	119.98	115.13
3	L5	1677	PSU	N1-C2-N3	4.28	119.98	115.13
3	L5	1326	A2M	N9-C8-N7	-4.28	108.06	113.91
3	L5	3792	OMG	C5-C4-N3	-4.28	121.52	128.46
3	L5	1871	A2M	N9-C8-N7	-4.28	108.06	113.91
50	S2	1174	PSU	C4-N3-C2	-4.28	120.18	126.34
50	S2	1248	B8N	C4-N3-C2	-4.27	120.05	125.46
50	S2	218	PSU	C4-N3-C2	-4.27	120.18	126.34
50	S2	867	OMG	C2-N3-C4	4.27	119.91	112.30
3	L5	3762	PSU	N1-C2-N3	4.27	119.96	115.13
50	S2	105	PSU	N1-C2-N3	4.26	119.96	115.13
50	S2	576	A2M	N9-C8-N7	-4.26	108.08	113.91
3	L5	4196	OMG	C2-N3-C4	4.26	119.89	112.30
3	L5	5010	PSU	N1-C2-N3	4.26	119.96	115.13
3	L5	2424	OMG	C2-N3-C4	4.26	119.88	112.30
50	S2	683	OMG	C2-N3-C4	4.26	119.88	112.30
50	S2	1238	PSU	N1-C2-N3	4.26	119.95	115.13
3	L5	1316	OMG	C5-C4-N3	-4.25	121.56	128.46
50	S2	644	OMG	C2-N3-C4	4.25	119.88	112.30
50	S2	406	PSU	N1-C2-N3	4.25	119.94	115.13
3	L5	3724	A2M	N9-C8-N7	-4.25	108.11	113.91
3	L5	3844	PSU	C4-N3-C2	-4.25	120.22	126.34
3	L5	3825	A2M	N9-C8-N7	-4.24	108.11	113.91
50	S2	1678	A2M	N9-C8-N7	-4.24	108.11	113.91
50	S2	649	PSU	N1-C2-N3	4.24	119.93	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1782	PSU	N1-C2-N3	4.24	119.93	115.13
3	L5	3729	PSU	C4-N3-C2	-4.23	120.24	126.34
3	L5	2363	A2M	N9-C8-N7	-4.23	108.12	113.91
3	L5	3744	OMG	C2-N3-C4	4.23	119.84	112.30
50	S2	436	OMG	C2-N3-C4	4.23	119.84	112.30
50	S2	966	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	400	A2M	N9-C8-N7	-4.22	108.14	113.91
50	S2	119	PSU	C4-N3-C2	-4.22	120.26	126.34
3	L5	3920	PSU	N1-C2-N3	4.22	119.91	115.13
50	S2	1177	PSU	N1-C2-N3	4.22	119.91	115.13
3	L5	4494	OMG	C2-N3-C4	4.22	119.82	112.30
50	S2	27	A2M	N9-C8-N7	-4.21	108.15	113.91
3	L5	2401	A2M	N9-C8-N7	-4.21	108.15	113.91
3	L5	3853	PSU	N1-C2-N3	4.21	119.90	115.13
3	L5	4521	PSU	N1-C2-N3	4.21	119.90	115.13
50	S2	1447	OMG	C2-N3-C4	4.21	119.80	112.30
3	L5	4637	OMG	C2-N3-C4	4.21	119.80	112.30
3	L5	3830	A2M	N9-C8-N7	-4.20	108.16	113.91
50	S2	99	A2M	N9-C8-N7	-4.20	108.16	113.91
3	L5	4618	OMG	C2-N3-C4	4.20	119.78	112.30
50	S2	918	PSU	N1-C2-N3	4.20	119.89	115.13
50	S2	1383	A2M	N9-C8-N7	-4.20	108.17	113.91
3	L5	4576	PSU	N1-C2-N3	4.20	119.89	115.13
3	L5	4590	A2M	C5-C6-N6	4.19	132.56	123.43
50	S2	866	PSU	N1-C2-N3	4.19	119.88	115.13
3	L5	1534	A2M	N9-C8-N7	-4.19	108.18	113.91
3	L5	1862	PSU	N1-C2-N3	4.19	119.88	115.13
3	L5	1534	A2M	C5-C6-N6	4.19	132.55	123.43
50	S2	1347	PSU	N1-C2-N3	4.19	119.88	115.13
3	L5	4590	A2M	N9-C8-N7	-4.19	108.19	113.91
3	L5	3851	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	3770	PSU	N1-C2-N3	4.17	119.85	115.13
3	L5	2364	OMG	C2-N3-C4	4.17	119.72	112.30
3	L5	1860	PSU	N1-C2-N3	4.17	119.85	115.13
3	L5	4523	A2M	N9-C8-N7	-4.16	108.22	113.91
3	L5	1522	OMG	C5-C4-N3	-4.16	121.70	128.46
3	L5	4299	PSU	N1-C2-N3	4.16	119.85	115.13
3	L5	1744	PSU	N1-C2-N3	4.16	119.85	115.13
50	S2	1056	PSU	N1-C2-N3	4.16	119.85	115.13
5	L8	69	PSU	N1-C2-N3	4.16	119.84	115.13
3	L5	1625	OMG	C2-N3-C4	4.16	119.71	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4431	PSU	N1-C2-N3	4.16	119.84	115.13
3	L5	4499	OMG	C2-N3-C4	4.16	119.71	112.30
3	L5	4296	PSU	N1-C2-N3	4.16	119.84	115.13
50	S2	681	PSU	N1-C2-N3	4.15	119.83	115.13
3	L5	1316	OMG	C2-N3-C4	4.15	119.69	112.30
3	L5	4370	OMG	C2-N3-C4	4.15	119.69	112.30
3	L5	3627	OMG	C2-N3-C4	4.15	119.69	112.30
50	S2	509	OMG	C2-N3-C4	4.15	119.69	112.30
50	S2	512	A2M	N9-C8-N7	-4.14	108.25	113.91
3	L5	3718	A2M	C5-C6-N6	4.14	132.44	123.43
50	S2	801	PSU	N1-C2-N3	4.14	119.82	115.13
3	L5	3867	A2M	N9-C8-N7	-4.14	108.25	113.91
50	S2	651	PSU	N1-C2-N3	4.14	119.82	115.13
3	L5	3734	PSU	N1-C2-N3	4.14	119.82	115.13
3	L5	4673	PSU	N1-C2-N3	4.14	119.81	115.13
3	L5	1536	PSU	N1-C2-N3	4.13	119.81	115.13
50	S2	609	PSU	N1-C2-N3	4.13	119.81	115.13
50	S2	576	A2M	C5-C6-N6	4.13	132.42	123.43
50	S2	34	PSU	N1-C2-N3	4.13	119.81	115.13
50	S2	686	PSU	N1-C2-N3	4.13	119.81	115.13
3	L5	1779	PSU	N1-C2-N3	4.13	119.80	115.13
50	S2	484	A2M	N9-C8-N7	-4.12	108.27	113.91
3	L5	4442	PSU	N1-C2-N3	4.12	119.80	115.13
3	L5	4220	6MZ	N9-C8-N7	-4.12	108.28	113.91
3	L5	4227	OMU	N3-C2-N1	4.12	120.36	114.89
3	L5	2787	A2M	N9-C8-N7	-4.12	108.28	113.91
3	L5	4623	OMG	C2-N3-C4	4.12	119.64	112.30
3	L5	1326	A2M	C5-C6-N6	4.12	132.39	123.43
50	S2	1136	PSU	N1-C2-N3	4.11	119.79	115.13
3	L5	3764	PSU	N1-C2-N3	4.11	119.79	115.13
3	L5	3884	PSU	N1-C2-N3	4.11	119.79	115.13
3	L5	4623	OMG	C5-C4-N3	-4.11	121.79	128.46
3	L5	1683	PSU	N1-C2-N3	4.11	119.79	115.13
3	L5	4579	PSU	N1-C2-N3	4.11	119.78	115.13
50	S2	109	PSU	N1-C2-N3	4.11	119.78	115.13
50	S2	1692	PSU	N1-C2-N3	4.11	119.78	115.13
50	S2	36	PSU	N1-C2-N3	4.11	119.78	115.13
50	S2	1643	PSU	N1-C2-N3	4.10	119.78	115.13
3	L5	3724	A2M	C5-C6-N6	4.10	132.35	123.43
3	L5	4493	PSU	N1-C2-N3	4.10	119.77	115.13
50	S2	1445	PSU	N1-C2-N3	4.10	119.77	115.13
3	L5	2876	OMG	C2-N3-C4	4.09	119.59	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4569	PSU	N1-C2-N3	4.09	119.76	115.13
50	S2	166	A2M	C5-C6-N6	4.09	132.33	123.43
3	L5	5001	PSU	N1-C2-N3	4.08	119.76	115.13
3	L5	4423	PSU	N1-C2-N3	4.08	119.76	115.13
3	L5	4220	6MZ	C4-C5-C6	4.08	119.97	116.81
50	S2	863	PSU	N1-C2-N3	4.08	119.75	115.13
3	L5	3899	OMG	C2-N3-C4	4.08	119.57	112.30
50	S2	668	A2M	C5-C6-N6	4.08	132.31	123.43
50	S2	601	OMG	C2-N3-C4	4.08	119.56	112.30
3	L5	4293	PSU	N1-C2-N3	4.08	119.75	115.13
50	S2	822	PSU	N1-C2-N3	4.08	119.75	115.13
50	S2	1490	OMG	C5-C4-N3	-4.07	121.85	128.46
3	L5	3758	PSU	N1-C2-N3	4.07	119.74	115.13
50	S2	1004	PSU	N1-C2-N3	4.07	119.74	115.13
50	S2	1383	A2M	C5-C6-N6	4.06	132.27	123.43
50	S2	590	A2M	N9-C8-N7	-4.06	108.36	113.91
3	L5	4392	OMG	C2-N3-C4	4.06	119.54	112.30
50	S2	159	A2M	N9-C8-N7	-4.06	108.36	113.91
50	S2	1239	PSU	N1-C2-N3	4.06	119.73	115.13
3	L5	1522	OMG	C2-N3-C4	4.05	119.52	112.30
3	L5	3944	OMG	C2-N3-C4	4.05	119.52	112.30
50	S2	296	PSU	N1-C2-N3	4.05	119.72	115.13
50	S2	1232	PSU	N1-C2-N3	4.05	119.72	115.13
3	L5	4532	PSU	N1-C2-N3	4.05	119.71	115.13
3	L5	2632	PSU	N1-C2-N3	4.04	119.71	115.13
3	L5	2843	PSU	N1-C2-N3	4.04	119.71	115.13
3	L5	1871	A2M	C5-C6-N6	4.04	132.22	123.43
3	L5	398	A2M	C5-C6-N6	4.04	132.22	123.43
3	L5	4353	PSU	N1-C2-N3	4.04	119.70	115.13
50	S2	159	A2M	C5-C6-N6	4.04	132.21	123.43
3	L5	3844	PSU	N1-C2-N3	4.03	119.70	115.13
3	L5	3792	OMG	C2-N3-C4	4.03	119.48	112.30
3	L5	4228	OMG	C2-N3-C4	4.03	119.48	112.30
3	L5	4471	PSU	N1-C2-N3	4.03	119.70	115.13
50	S2	815	PSU	N1-C2-N3	4.03	119.70	115.13
3	L5	4571	A2M	C5-C6-N6	4.03	132.20	123.43
3	L5	1582	PSU	N1-C2-N3	4.03	119.70	115.13
3	L5	2401	A2M	C5-C6-N6	4.03	132.20	123.43
50	S2	484	A2M	C5-C6-N6	4.03	132.20	123.43
50	S2	27	A2M	C5-C6-N6	4.03	132.19	123.43
5	L8	55	PSU	N1-C2-N3	4.03	119.69	115.13
3	L5	2363	A2M	C5-C6-N6	4.02	132.19	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	400	A2M	C5-C6-N6	4.02	132.18	123.43
3	L5	4972	PSU	N1-C2-N3	4.02	119.69	115.13
3	L5	3768	PSU	N1-C2-N3	4.02	119.68	115.13
50	S2	468	A2M	C5-C6-N6	4.02	132.17	123.43
50	S2	1244	PSU	N1-C2-N3	4.02	119.68	115.13
3	L5	2364	OMG	C5-C4-N3	-4.01	121.95	128.46
3	L5	2839	PSU	N1-C2-N3	4.01	119.68	115.13
3	L5	1781	PSU	N1-C2-N3	4.01	119.67	115.13
3	L5	2815	A2M	C5-C6-N6	4.01	132.15	123.43
3	L5	3830	A2M	C5-C6-N6	4.01	132.15	123.43
50	S2	814	PSU	N1-C2-N3	4.01	119.67	115.13
3	L5	1792	PSU	N1-C2-N3	4.01	119.67	115.13
3	L5	4312	PSU	N1-C2-N3	4.01	119.67	115.13
3	L5	4523	A2M	C5-C6-N6	4.00	132.14	123.43
50	S2	1639	G7M	C5-C4-N3	-4.00	120.48	128.15
50	S2	1031	A2M	C5-C6-N6	3.99	132.12	123.43
50	S2	1625	PSU	N1-C2-N3	3.99	119.66	115.13
3	L5	3785	A2M	C5-C6-N6	3.99	132.12	123.43
3	L5	2787	A2M	C5-C6-N6	3.99	132.12	123.43
50	S2	1639	G7M	C5-C6-N1	3.99	120.13	111.79
3	L5	4361	PSU	N1-C2-N3	3.99	119.65	115.13
3	L5	3627	OMG	C5-C4-N3	-3.99	121.99	128.46
3	L5	3867	A2M	C5-C6-N6	3.98	132.09	123.43
3	L5	4552	PSU	N1-C2-N3	3.98	119.64	115.13
50	S2	1490	OMG	C2-N3-C4	3.97	119.38	112.30
3	L5	4392	OMG	C5-C4-N3	-3.96	122.03	128.46
3	L5	4618	OMG	C5-C4-N3	-3.96	122.03	128.46
3	L5	1524	A2M	C5-C6-N6	3.96	132.05	123.43
3	L5	4457	PSU	N1-C2-N3	3.96	119.61	115.13
50	S2	1174	PSU	N1-C2-N3	3.96	119.61	115.13
50	S2	1243	PSU	N1-C2-N3	3.95	119.61	115.13
3	L5	2837	OMU	N3-C2-N1	3.94	120.12	114.89
3	L5	3925	OMU	N3-C2-N1	3.93	120.11	114.89
50	S2	428	OMU	N3-C2-N1	3.93	120.11	114.89
3	L5	2508	PSU	N1-C2-N3	3.93	119.58	115.13
3	L5	2815	A2M	N9-C8-N7	-3.93	108.54	113.91
50	S2	512	A2M	C5-C6-N6	3.93	131.97	123.43
50	S2	93	PSU	N1-C2-N3	3.92	119.58	115.13
50	S2	218	PSU	N1-C2-N3	3.92	119.58	115.13
50	S2	590	A2M	C5-C6-N6	3.92	131.97	123.43
3	L5	398	A2M	N9-C8-N7	-3.92	108.55	113.91
50	S2	573	PSU	N1-C2-N3	3.92	119.57	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3899	OMG	C5-C4-N3	-3.92	122.11	128.46
3	L5	3723	A2M	C5-C6-N6	3.91	131.94	123.43
3	L5	3729	PSU	N1-C2-N3	3.91	119.56	115.13
50	S2	1678	A2M	C5-C6-N6	3.90	131.92	123.43
3	L5	3825	A2M	C5-C6-N6	3.90	131.92	123.43
3	L5	4498	OMU	N3-C2-N1	3.89	120.06	114.89
50	S2	121	OMU	N3-C2-N1	3.86	120.02	114.89
50	S2	1804	OMU	N3-C2-N1	3.85	120.00	114.89
50	S2	99	A2M	C5-C6-N6	3.85	131.81	123.43
3	L5	4228	OMG	N9-C8-N7	-3.84	106.15	113.39
50	S2	119	PSU	N1-C2-N3	3.84	119.48	115.13
3	L5	1322	1MA	C5-C4-N3	-3.82	121.56	127.26
3	L5	4420	PSU	N1-C2-N3	3.80	119.44	115.13
3	L5	4228	OMG	C5-C4-N3	-3.80	122.30	128.46
50	S2	354	OMU	N3-C2-N1	3.80	119.93	114.89
50	S2	572	PSU	N1-C2-N3	3.79	119.43	115.13
3	L5	4447	5MC	C5-C6-N1	-3.76	119.47	123.34
50	S2	172	OMU	N3-C2-N1	3.76	119.88	114.89
3	L5	3627	OMG	N9-C8-N7	-3.73	106.37	113.39
3	L5	2415	OMU	N3-C2-N1	3.72	119.83	114.89
3	L5	1322	1MA	C2-N3-C4	3.72	119.72	112.41
50	S2	590	A2M	C2-N3-C4	3.72	120.53	111.75
50	S2	590	A2M	N3-C4-N9	3.71	133.20	127.08
3	L5	2815	A2M	C2-N3-C4	3.71	120.51	111.75
3	L5	4306	OMU	N3-C2-N1	3.71	119.81	114.89
3	L5	4618	OMG	N9-C8-N7	-3.70	106.42	113.39
50	S2	512	A2M	C2-N3-C4	3.70	120.49	111.75
50	S2	1850	MA6	C4-C5-C6	3.68	120.00	115.88
50	S2	166	A2M	C2-N3-C4	3.66	120.39	111.75
3	L5	2364	OMG	N9-C8-N7	-3.66	106.50	113.39
50	S2	1678	A2M	C2-N3-C4	3.65	120.39	111.75
3	L5	3899	OMG	N9-C8-N7	-3.65	106.51	113.39
5	L8	14	OMU	C5-C4-N3	3.62	120.26	114.84
50	S2	1851	MA6	C2-N1-C6	3.62	120.29	111.75
3	L5	4590	A2M	C2-N3-C4	3.60	120.27	111.75
3	L5	3830	A2M	C2-N3-C4	3.60	120.25	111.75
50	S2	27	A2M	C2-N3-C4	3.60	120.24	111.75
3	L5	2363	A2M	C2-N3-C4	3.59	120.23	111.75
3	L5	4523	A2M	C2-N3-C4	3.59	120.23	111.75
50	S2	116	OMU	N3-C2-N1	3.59	119.65	114.89
3	L5	398	A2M	C2-N3-C4	3.58	120.21	111.75
3	L5	2401	A2M	C2-N3-C4	3.58	120.20	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3785	A2M	C2-N3-C4	3.57	120.20	111.75
50	S2	1850	MA6	C2-N1-C6	3.57	120.19	111.75
50	S2	484	A2M	C2-N3-C4	3.57	120.18	111.75
50	S2	1031	A2M	C2-N3-C4	3.57	120.18	111.75
3	L5	4620	OMU	N3-C2-N1	3.56	119.62	114.89
5	L8	14	OMU	N3-C2-N1	3.56	119.61	114.89
50	S2	1851	MA6	C2-N3-C4	3.56	120.15	111.75
3	L5	1326	A2M	C2-N3-C4	3.56	120.15	111.75
50	S2	99	A2M	C2-N3-C4	3.55	120.15	111.75
3	L5	3723	A2M	C2-N3-C4	3.55	120.15	111.75
50	S2	1383	A2M	C2-N3-C4	3.55	120.15	111.75
3	L5	400	A2M	C2-N3-C4	3.54	120.12	111.75
3	L5	2787	A2M	C2-N3-C4	3.54	120.12	111.75
50	S2	468	A2M	C2-N3-C4	3.54	120.12	111.75
3	L5	3825	A2M	C2-N3-C4	3.53	120.10	111.75
3	L5	3724	A2M	C2-N3-C4	3.53	120.09	111.75
50	S2	1442	OMU	N3-C2-N1	3.53	119.57	114.89
3	L5	2815	A2M	N3-C4-N9	3.52	132.88	127.08
3	L5	4637	OMG	N9-C8-N7	-3.52	106.77	113.39
3	L5	1316	OMG	N9-C8-N7	-3.52	106.77	113.39
50	S2	668	A2M	C2-N3-C4	3.51	120.05	111.75
3	L5	3744	OMG	N9-C8-N7	-3.51	106.78	113.39
50	S2	1850	MA6	C2-N3-C4	3.51	120.04	111.75
50	S2	576	A2M	C2-N3-C4	3.51	120.04	111.75
3	L5	1524	A2M	C2-N3-C4	3.50	120.03	111.75
3	L5	1534	A2M	C2-N3-C4	3.50	120.03	111.75
3	L5	4571	A2M	C2-N3-C4	3.50	120.02	111.75
50	S2	683	OMG	N9-C8-N7	-3.50	106.81	113.39
49	Pt	26	M2G	N1-C2-N2	3.50	121.01	118.04
50	S2	1288	OMU	N3-C2-N1	3.49	119.52	114.89
3	L5	4220	6MZ	C2-N3-C4	3.48	119.97	111.75
50	S2	512	A2M	N3-C4-N9	3.48	132.81	127.08
50	S2	159	A2M	C2-N3-C4	3.47	119.96	111.75
3	L5	2876	OMG	N9-C8-N7	-3.46	106.87	113.39
3	L5	4498	OMU	C5-C4-N3	3.46	120.02	114.84
3	L5	3867	A2M	C2-N3-C4	3.46	119.93	111.75
3	L5	1871	A2M	C2-N3-C4	3.46	119.93	111.75
5	L8	75	OMG	N9-C8-N7	-3.46	106.87	113.39
50	S2	428	OMU	C5-C4-N3	3.46	120.01	114.84
50	S2	436	OMG	N9-C8-N7	-3.45	106.89	113.39
50	S2	644	OMG	N9-C8-N7	-3.45	106.90	113.39
50	S2	1639	G7M	O6-C6-C5	-3.44	120.30	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3792	OMG	N9-C8-N7	-3.44	106.91	113.39
3	L5	4306	OMU	C5-C4-N3	3.43	119.98	114.84
3	L5	3718	A2M	N9-C8-N7	-3.43	109.22	113.91
3	L5	4623	OMG	N9-C8-N7	-3.43	106.94	113.39
50	S2	867	OMG	N9-C8-N7	-3.42	106.96	113.39
3	L5	1522	OMG	N9-C8-N7	-3.41	106.97	113.39
3	L5	4392	OMG	N9-C8-N7	-3.39	107.00	113.39
3	L5	3782	5MC	C5-C6-N1	-3.39	119.85	123.34
3	L5	3925	OMU	C5-C4-N3	3.38	119.90	114.84
50	S2	1490	OMG	N9-C8-N7	-3.37	107.04	113.39
3	L5	4370	OMG	N9-C8-N7	-3.37	107.04	113.39
50	S2	1678	A2M	N3-C4-N9	3.37	132.63	127.08
50	S2	1447	OMG	N9-C8-N7	-3.36	107.05	113.39
3	L5	2415	OMU	C5-C4-N3	3.36	119.86	114.84
3	L5	3867	A2M	N3-C4-N9	3.35	132.61	127.08
3	L5	4499	OMG	N9-C8-N7	-3.35	107.08	113.39
50	S2	1442	OMU	C5-C4-N3	3.35	119.85	114.84
3	L5	4689	PSU	C6-N1-C2	-3.34	119.26	122.68
50	S2	172	OMU	C5-C4-N3	3.33	119.82	114.84
3	L5	3762	PSU	C6-N1-C2	-3.32	119.28	122.68
3	L5	1677	PSU	C6-N1-C2	-3.32	119.29	122.68
50	S2	99	A2M	N3-C4-N9	3.31	132.54	127.08
3	L5	1625	OMG	N9-C8-N7	-3.30	107.18	113.39
50	S2	1851	MA6	C4-C5-C6	3.29	119.56	115.88
3	L5	2787	A2M	C5-N7-C8	3.29	108.19	103.51
50	S2	354	OMU	C5-C4-N3	3.29	119.76	114.84
3	L5	4227	OMU	C5-C4-N3	3.28	119.75	114.84
50	S2	601	OMG	N9-C8-N7	-3.28	107.21	113.39
3	L5	2837	OMU	C5-C4-N3	3.28	119.74	114.84
50	S2	1639	G7M	N9-C4-N3	3.27	132.50	125.94
50	S2	121	OMU	C5-C4-N3	3.27	119.73	114.84
50	S2	1804	OMU	C5-C4-N3	3.27	119.73	114.84
50	S2	509	OMG	N9-C8-N7	-3.27	107.24	113.39
3	L5	3825	A2M	N3-C4-N9	3.26	132.45	127.08
50	S2	27	A2M	N3-C4-N9	3.26	132.45	127.08
3	L5	4620	OMU	C5-C4-N3	3.25	119.71	114.84
3	L5	398	A2M	N3-C4-N9	3.25	132.43	127.08
50	S2	681	PSU	C6-N1-C2	-3.24	119.36	122.68
3	L5	4196	OMG	N9-C8-N7	-3.24	107.28	113.39
3	L5	1524	A2M	C5-N7-C8	3.24	108.11	103.51
50	S2	1288	OMU	C5-C4-N3	3.24	119.68	114.84
50	S2	166	A2M	C5-N7-C8	3.23	108.10	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3718	A2M	C2-N3-C4	3.23	119.38	111.75
74	SX	62	HY3	C5-C4-C3	-3.22	98.83	103.74
50	S2	1851	MA6	C5-N7-C8	3.22	108.08	103.51
50	S2	668	A2M	C5-N7-C8	3.22	108.08	103.51
50	S2	1678	A2M	C5-N7-C8	3.21	108.06	103.51
50	S2	116	OMU	C5-C4-N3	3.20	119.63	114.84
3	L5	3830	A2M	N3-C4-N9	3.20	132.35	127.08
3	L5	4636	PSU	C6-N1-C2	-3.20	119.41	122.68
3	L5	4571	A2M	N3-C4-N9	3.19	132.34	127.08
3	L5	1524	A2M	N3-C4-N9	3.19	132.34	127.08
3	L5	5010	PSU	C6-N1-C2	-3.19	119.42	122.68
3	L5	1326	A2M	C5-N7-C8	3.19	108.04	103.51
50	S2	1383	A2M	N3-C4-N9	3.18	132.33	127.08
3	L5	1534	A2M	C5-N7-C8	3.18	108.03	103.51
3	L5	3830	A2M	C5-N7-C8	3.18	108.03	103.51
50	S2	1850	MA6	C5-N7-C8	3.18	108.03	103.51
3	L5	4571	A2M	C5-N7-C8	3.18	108.02	103.51
50	S2	918	PSU	C6-N1-C2	-3.18	119.44	122.68
50	S2	166	A2M	N3-C4-N9	3.16	132.30	127.08
50	S2	576	A2M	C5-N7-C8	3.16	108.00	103.51
50	S2	27	A2M	C5-N7-C8	3.16	108.00	103.51
3	L5	3764	PSU	C6-N1-C2	-3.15	119.46	122.68
50	S2	468	A2M	C5-N7-C8	3.15	107.98	103.51
3	L5	4523	A2M	N3-C4-N9	3.15	132.27	127.08
50	S2	576	A2M	N3-C4-N9	3.15	132.27	127.08
50	S2	1383	A2M	C5-N7-C8	3.15	107.98	103.51
3	L5	3944	OMG	N9-C8-N7	-3.14	107.47	113.39
3	L5	3851	PSU	C6-N1-C2	-3.14	119.47	122.68
3	L5	3785	A2M	O4'-C1'-N9	3.14	114.25	108.06
50	S2	590	A2M	C5-N7-C8	3.14	107.96	103.51
3	L5	3637	PSU	C6-N1-C2	-3.13	119.48	122.68
3	L5	4494	OMG	N9-C8-N7	-3.13	107.49	113.39
3	L5	4576	PSU	C6-N1-C2	-3.13	119.48	122.68
3	L5	2787	A2M	N3-C4-N9	3.13	132.24	127.08
3	L5	4590	A2M	N3-C4-N9	3.13	132.24	127.08
5	L8	69	PSU	C6-N1-C2	-3.12	119.49	122.68
50	S2	1367	PSU	C6-N1-C2	-3.12	119.49	122.68
3	L5	3785	A2M	C5-N7-C8	3.12	107.94	103.51
50	S2	484	A2M	C5-N7-C8	3.12	107.94	103.51
3	L5	4403	PSU	C6-N1-C2	-3.12	119.49	122.68
50	S2	99	A2M	C5-N7-C8	3.12	107.94	103.51
3	L5	4500	PSU	C6-N1-C2	-3.12	119.50	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1326	A2M	N3-C4-N9	3.11	132.22	127.08
3	L5	2363	A2M	C5-N7-C8	3.11	107.93	103.51
3	L5	3723	A2M	N3-C4-N9	3.11	132.21	127.08
3	L5	4628	PSU	C6-N1-C2	-3.11	119.50	122.68
3	L5	3867	A2M	C5-N7-C8	3.11	107.93	103.51
3	L5	2815	A2M	C5-N7-C8	3.11	107.93	103.51
3	L5	3724	A2M	N3-C4-N9	3.11	132.21	127.08
50	S2	1031	A2M	N3-C4-N9	3.11	132.20	127.08
3	L5	3723	A2M	C5-N7-C8	3.11	107.92	103.51
3	L5	398	A2M	C5-N7-C8	3.11	107.92	103.51
50	S2	468	A2M	N3-C4-N9	3.11	132.20	127.08
50	S2	1643	PSU	C6-N1-C2	-3.10	119.51	122.68
3	L5	3844	PSU	C6-N1-C2	-3.09	119.52	122.68
50	S2	159	A2M	N3-C4-N9	3.09	132.18	127.08
3	L5	2401	A2M	C5-N7-C8	3.09	107.90	103.51
3	L5	4590	A2M	C5-N7-C8	3.09	107.90	103.51
50	S2	484	A2M	N3-C4-N9	3.09	132.17	127.08
50	S2	218	PSU	C6-N1-C2	-3.09	119.53	122.68
50	S2	1639	G7M	CN7-N7-C5	3.08	130.59	126.77
3	L5	1871	A2M	C5-N7-C8	3.07	107.88	103.51
3	L5	4523	A2M	C5-N7-C8	3.07	107.87	103.51
3	L5	4579	PSU	C6-N1-C2	-3.07	119.54	122.68
50	S2	1031	A2M	C5-N7-C8	3.07	107.87	103.51
3	L5	2363	A2M	N3-C4-N9	3.07	132.14	127.08
3	L5	1860	PSU	C6-N1-C2	-3.07	119.55	122.68
3	L5	3785	A2M	N3-C4-N9	3.06	132.13	127.08
3	L5	4220	6MZ	N3-C4-N9	3.06	132.13	127.08
3	L5	2424	OMG	N9-C4-N3	3.06	132.09	125.94
3	L5	1683	PSU	C6-N1-C2	-3.06	119.56	122.68
3	L5	4442	PSU	C6-N1-C2	-3.05	119.56	122.68
3	L5	3825	A2M	C5-N7-C8	3.05	107.85	103.51
50	S2	1692	PSU	C6-N1-C2	-3.05	119.56	122.68
50	S2	1174	PSU	C6-N1-C2	-3.05	119.57	122.68
3	L5	400	A2M	N3-C4-N9	3.05	132.10	127.08
3	L5	1744	PSU	C6-N1-C2	-3.04	119.57	122.68
50	S2	509	OMG	C2-N1-C6	-3.04	119.55	125.10
3	L5	3729	PSU	C6-N1-C2	-3.04	119.58	122.68
3	L5	4569	PSU	C6-N1-C2	-3.04	119.58	122.68
3	L5	4673	PSU	C6-N1-C2	-3.03	119.58	122.68
3	L5	3724	A2M	C5-N7-C8	3.03	107.82	103.51
50	S2	1004	PSU	C6-N1-C2	-3.03	119.58	122.68
5	L8	14	OMU	O4-C4-C5	-3.03	119.83	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	867	OMG	N9-C4-N3	3.03	132.02	125.94
3	L5	4220	6MZ	C5-N7-C8	3.03	107.81	103.51
3	L5	2876	OMG	N9-C4-N3	3.02	132.01	125.94
3	L5	2424	OMG	C2-N1-C6	-3.02	119.59	125.10
3	L5	2401	A2M	N3-C4-N9	3.02	132.05	127.08
50	S2	644	OMG	C2-N1-C6	-3.01	119.61	125.10
3	L5	1862	PSU	C6-N1-C2	-3.01	119.61	122.68
3	L5	3853	PSU	C6-N1-C2	-3.01	119.61	122.68
3	L5	400	A2M	C5-N7-C8	3.01	107.78	103.51
50	S2	512	A2M	C5-N7-C8	3.01	107.78	103.51
3	L5	3718	A2M	N3-C4-N9	3.00	132.03	127.08
50	S2	1136	PSU	C6-N1-C2	-3.00	119.61	122.68
50	S2	159	A2M	C5-N7-C8	3.00	107.77	103.51
50	S2	1232	PSU	C6-N1-C2	-3.00	119.62	122.68
50	S2	866	PSU	C6-N1-C2	-3.00	119.62	122.68
50	S2	116	OMU	O4-C4-C5	-2.99	119.90	125.16
50	S2	1442	OMU	O4-C4-C5	-2.99	119.90	125.16
50	S2	406	PSU	C6-N1-C2	-2.99	119.63	122.68
50	S2	1447	OMG	C2-N1-C6	-2.98	119.66	125.10
3	L5	1779	PSU	C6-N1-C2	-2.98	119.63	122.68
50	S2	651	PSU	C6-N1-C2	-2.97	119.64	122.68
50	S2	822	PSU	C6-N1-C2	-2.97	119.65	122.68
3	L5	3944	OMG	N9-C4-N3	2.97	131.90	125.94
74	SX	62	HY3	O-C-CA	-2.97	116.56	124.83
50	S2	109	PSU	C6-N1-C2	-2.97	119.65	122.68
50	S2	649	PSU	C6-N1-C2	-2.96	119.65	122.68
50	S2	34	PSU	C6-N1-C2	-2.96	119.66	122.68
3	L5	4431	PSU	C6-N1-C2	-2.96	119.66	122.68
3	L5	4471	PSU	C6-N1-C2	-2.95	119.66	122.68
3	L5	4293	PSU	C6-N1-C2	-2.95	119.66	122.68
3	L5	2632	PSU	C6-N1-C2	-2.95	119.67	122.68
50	S2	1239	PSU	C6-N1-C2	-2.95	119.67	122.68
3	L5	1782	PSU	C6-N1-C2	-2.94	119.67	122.68
3	L5	3770	PSU	C6-N1-C2	-2.94	119.67	122.68
50	S2	966	PSU	C6-N1-C2	-2.94	119.68	122.68
3	L5	1871	A2M	C2'-C1'-N9	-2.94	108.58	113.53
50	S2	683	OMG	N9-C4-N3	2.94	131.83	125.94
3	L5	3695	PSU	C6-C5-C4	2.93	120.25	118.20
50	S2	683	OMG	C2-N1-C6	-2.93	119.75	125.10
3	L5	4494	OMG	C2-N1-C6	-2.93	119.76	125.10
50	S2	601	OMG	C2-N1-C6	-2.93	119.77	125.10
50	S2	1447	OMG	N9-C4-N3	2.92	131.81	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3920	PSU	C6-N1-C2	-2.92	119.70	122.68
50	S2	172	OMU	O4-C4-C5	-2.92	120.03	125.16
50	S2	867	OMG	C2-N1-C6	-2.92	119.78	125.10
50	S2	105	PSU	C6-N1-C2	-2.92	119.70	122.68
3	L5	4196	OMG	C2-N1-C6	-2.91	119.78	125.10
50	S2	436	OMG	C2-N1-C6	-2.91	119.78	125.10
3	L5	4521	PSU	C6-N1-C2	-2.91	119.70	122.68
3	L5	1625	OMG	C2-N1-C6	-2.91	119.79	125.10
50	S2	354	OMU	O4-C4-C5	-2.91	120.04	125.16
50	S2	1238	PSU	C6-C5-C4	2.91	120.23	118.20
3	L5	1534	A2M	N3-C4-N9	2.91	131.88	127.08
3	L5	2415	OMU	O4-C4-C5	-2.90	120.05	125.16
50	S2	1244	PSU	C6-N1-C2	-2.90	119.71	122.68
3	L5	2839	PSU	C6-N1-C2	-2.90	119.72	122.68
3	L5	3734	PSU	C6-N1-C2	-2.90	119.72	122.68
50	S2	668	A2M	N3-C4-N9	2.90	131.86	127.08
3	L5	1582	PSU	C6-N1-C2	-2.90	119.72	122.68
3	L5	3884	PSU	C6-N1-C2	-2.90	119.72	122.68
50	S2	1850	MA6	N3-C4-N9	2.90	131.86	127.08
3	L5	1792	PSU	C6-N1-C2	-2.89	119.73	122.68
3	L5	3639	PSU	C6-N1-C2	-2.89	119.73	122.68
50	S2	1248	B8N	N3-C2-N1	2.89	120.84	116.76
50	S2	119	PSU	C6-N1-C2	-2.89	119.73	122.68
3	L5	2364	OMG	C2-N1-C6	-2.88	119.84	125.10
3	L5	4299	PSU	C6-N1-C2	-2.88	119.73	122.68
3	L5	4552	PSU	C6-N1-C2	-2.88	119.74	122.68
50	S2	1288	OMU	O4-C4-C5	-2.88	120.10	125.16
3	L5	4637	OMG	C2-N1-C6	-2.88	119.85	125.10
50	S2	1367	PSU	C6-C5-C4	2.87	120.21	118.20
50	S2	1177	PSU	C6-N1-C2	-2.87	119.75	122.68
3	L5	4370	OMG	C2-N1-C6	-2.87	119.87	125.10
50	S2	966	PSU	C6-C5-C4	2.87	120.20	118.20
3	L5	3744	OMG	C2-N1-C6	-2.86	119.88	125.10
3	L5	4228	OMG	C2-N1-C6	-2.86	119.88	125.10
3	L5	4499	OMG	C2-N1-C6	-2.86	119.88	125.10
50	S2	572	PSU	C6-N1-C2	-2.86	119.76	122.68
50	S2	1347	PSU	C6-N1-C2	-2.86	119.76	122.68
50	S2	1243	PSU	C6-N1-C2	-2.86	119.76	122.68
3	L5	4306	OMU	O4-C4-C5	-2.86	120.14	125.16
50	S2	36	PSU	C6-N1-C2	-2.86	119.76	122.68
3	L5	4498	OMU	O4-C4-C5	-2.86	120.14	125.16
50	S2	1383	A2M	C2'-C1'-N9	-2.86	108.72	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4196	OMG	N9-C4-N3	2.86	131.67	125.94
50	S2	1639	G7M	C2-N1-C6	-2.85	119.90	125.10
3	L5	2876	OMG	C2-N1-C6	-2.85	119.90	125.10
50	S2	121	OMU	O4-C4-C5	-2.85	120.15	125.16
50	S2	1056	PSU	C6-N1-C2	-2.85	119.77	122.68
50	S2	1238	PSU	C6-N1-C2	-2.84	119.77	122.68
5	L8	75	OMG	C2-N1-C6	-2.84	119.91	125.10
50	S2	1081	PSU	C3'-C2'-C1'	2.84	104.95	101.64
3	L5	1871	A2M	N3-C4-N9	2.84	131.77	127.08
3	L5	3695	PSU	C6-N1-C2	-2.84	119.78	122.68
3	L5	1781	PSU	C6-N1-C2	-2.84	119.78	122.68
50	S2	609	PSU	C6-N1-C2	-2.83	119.79	122.68
50	S2	428	OMU	O4-C4-C5	-2.83	120.18	125.16
3	L5	5001	PSU	C6-N1-C2	-2.83	119.79	122.68
50	S2	296	PSU	C6-N1-C2	-2.83	119.79	122.68
3	L5	3944	OMG	C2-N1-C6	-2.83	119.94	125.10
50	S2	686	PSU	C6-N1-C2	-2.83	119.79	122.68
3	L5	4618	OMG	C2-N1-C6	-2.82	119.95	125.10
50	S2	1804	OMU	O4-C4-C5	-2.82	120.20	125.16
3	L5	4623	OMG	C2-N1-C6	-2.82	119.97	125.10
3	L5	3768	PSU	C6-N1-C2	-2.81	119.81	122.68
3	L5	4493	PSU	C6-N1-C2	-2.81	119.81	122.68
3	L5	4423	PSU	C6-N1-C2	-2.81	119.81	122.68
3	L5	4227	OMU	O4-C4-C5	-2.80	120.24	125.16
3	L5	1522	OMG	C2-N1-C6	-2.79	120.01	125.10
3	L5	4403	PSU	C6-C5-C4	2.79	120.15	118.20
3	L5	4312	PSU	C6-N1-C2	-2.79	119.83	122.68
3	L5	4500	PSU	O2-C2-N1	-2.79	119.72	122.79
3	L5	3899	OMG	C2-N1-C6	-2.79	120.02	125.10
3	L5	3762	PSU	O2-C2-N1	-2.78	119.73	122.79
3	L5	3627	OMG	C2-N1-C6	-2.78	120.03	125.10
50	S2	1625	PSU	C6-N1-C2	-2.78	119.84	122.68
50	S2	863	PSU	C6-N1-C2	-2.77	119.85	122.68
3	L5	4972	PSU	C6-N1-C2	-2.77	119.85	122.68
50	S2	918	PSU	C6-C5-C4	2.77	120.13	118.20
50	S2	509	OMG	N9-C4-N3	2.76	131.49	125.94
50	S2	814	PSU	C6-N1-C2	-2.76	119.86	122.68
3	L5	4392	OMG	C2-N1-C6	-2.76	120.07	125.10
50	S2	1445	PSU	C6-N1-C2	-2.76	119.86	122.68
50	S2	512	A2M	C2'-C1'-N9	-2.76	108.89	113.53
5	L8	55	PSU	C6-N1-C2	-2.75	119.87	122.68
3	L5	3718	A2M	C5-N7-C8	2.75	107.41	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	93	PSU	C6-N1-C2	-2.75	119.88	122.68
50	S2	1445	PSU	C6-C5-C4	2.74	120.11	118.20
3	L5	2424	OMG	N9-C8-N7	-2.74	108.23	113.39
3	L5	4637	OMG	C5-C6-N1	2.74	120.15	113.19
50	S2	1136	PSU	O2-C2-N1	-2.74	119.78	122.79
3	L5	4532	PSU	C6-N1-C2	-2.74	119.89	122.68
3	L5	4500	PSU	C6-C5-C4	2.73	120.11	118.20
50	S2	801	PSU	C6-N1-C2	-2.73	119.89	122.68
3	L5	3925	OMU	O4-C4-C5	-2.73	120.36	125.16
3	L5	1316	OMG	C2-N1-C6	-2.73	120.12	125.10
50	S2	509	OMG	C5-C6-N1	2.73	120.12	113.19
50	S2	866	PSU	C6-C5-C4	2.73	120.10	118.20
50	S2	867	OMG	C5-C6-N1	2.72	120.11	113.19
50	S2	683	OMG	C5-C6-N1	2.72	120.11	113.19
3	L5	2837	OMU	O4-C4-C5	-2.72	120.39	125.16
3	L5	4296	PSU	C6-N1-C2	-2.71	119.91	122.68
3	L5	3758	PSU	C6-C5-C4	2.71	120.09	118.20
3	L5	5010	PSU	O2-C2-N1	-2.71	119.81	122.79
50	S2	644	OMG	C5-C6-N1	2.71	120.06	113.19
3	L5	4196	OMG	C5-C6-N1	2.70	120.05	113.19
3	L5	2508	PSU	C6-N1-C2	-2.70	119.92	122.68
3	L5	3758	PSU	C6-N1-C2	-2.70	119.92	122.68
3	L5	4353	PSU	C6-N1-C2	-2.70	119.92	122.68
3	L5	3744	OMG	C5-C6-N1	2.69	120.03	113.19
3	L5	1316	OMG	C5-C6-N1	2.69	120.01	113.19
50	S2	1447	OMG	C5-C6-N1	2.68	120.01	113.19
3	L5	3627	OMG	C5-C6-N1	2.68	120.00	113.19
3	L5	3899	OMG	C5-C6-N1	2.68	120.00	113.19
50	S2	573	PSU	C6-N1-C2	-2.68	119.94	122.68
5	L8	75	OMG	C5-C6-N1	2.68	119.99	113.19
3	L5	2364	OMG	C5-C6-N1	2.68	119.98	113.19
50	S2	436	OMG	C5-C6-N1	2.68	119.98	113.19
3	L5	4623	OMG	C5-C6-N1	2.67	119.98	113.19
5	L8	69	PSU	C6-C5-C4	2.67	120.07	118.20
3	L5	1536	PSU	C6-N1-C2	-2.67	119.95	122.68
3	L5	4457	PSU	C6-N1-C2	-2.67	119.95	122.68
50	S2	815	PSU	C6-N1-C2	-2.67	119.95	122.68
3	L5	1625	OMG	C5-C6-N1	2.67	119.97	113.19
3	L5	4618	OMG	C5-C6-N1	2.67	119.97	113.19
3	L5	4523	A2M	C2'-C1'-N9	-2.67	109.04	113.53
3	L5	4494	OMG	C5-C6-N1	2.66	119.94	113.19
3	L5	4521	PSU	C6-C5-C4	2.66	120.06	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4228	OMG	C5-C6-N1	2.66	119.93	113.19
3	L5	1860	PSU	O2-C2-N1	-2.65	119.87	122.79
50	S2	651	PSU	O2-C2-N1	-2.65	119.87	122.79
3	L5	4370	OMG	C5-C6-N1	2.65	119.91	113.19
50	S2	1851	MA6	N3-C4-N9	2.64	131.44	127.08
3	L5	4499	OMG	C5-C6-N1	2.64	119.90	113.19
3	L5	3830	A2M	C2'-C1'-N9	-2.64	109.09	113.53
50	S2	918	PSU	O2-C2-N1	-2.64	119.89	122.79
50	S2	1056	PSU	C6-C5-C4	2.63	120.04	118.20
50	S2	801	PSU	C6-C5-C4	2.63	120.04	118.20
3	L5	2424	OMG	C5-C6-N1	2.63	119.86	113.19
3	L5	4442	PSU	C6-C5-C4	2.63	120.03	118.20
50	S2	576	A2M	C2'-C1'-N9	-2.62	109.11	113.53
3	L5	1677	PSU	O2-C2-N1	-2.62	119.90	122.79
3	L5	2843	PSU	C6-N1-C2	-2.62	120.00	122.68
3	L5	1522	OMG	C5-C6-N1	2.62	119.85	113.19
3	L5	4392	OMG	C5-C6-N1	2.62	119.83	113.19
3	L5	1625	OMG	N9-C4-N3	2.62	131.19	125.94
3	L5	4620	OMU	O4-C4-C5	-2.61	120.56	125.16
50	S2	1248	B8N	O4-C4-N3	-2.61	115.54	119.98
3	L5	4689	PSU	O2-C2-N1	-2.61	119.92	122.79
50	S2	296	PSU	C6-C5-C4	2.61	120.02	118.20
50	S2	105	PSU	C6-C5-C4	2.61	120.02	118.20
50	S2	863	PSU	C6-C5-C4	2.61	120.02	118.20
3	L5	4361	PSU	C6-N1-C2	-2.61	120.02	122.68
50	S2	1842	4AC	C6-C5-C4	2.60	120.15	116.96
3	L5	4628	PSU	O2-C2-N1	-2.60	119.92	122.79
50	S2	1643	PSU	O2-C2-N1	-2.60	119.93	122.79
50	S2	601	OMG	C5-C6-N1	2.60	119.80	113.19
3	L5	1744	PSU	O2-C2-N1	-2.60	119.93	122.79
3	L5	4403	PSU	O2-C2-N1	-2.60	119.93	122.79
3	L5	2876	OMG	C5-C6-N1	2.60	119.78	113.19
50	S2	1232	PSU	O2-C2-N1	-2.59	119.94	122.79
50	S2	1643	PSU	C6-C5-C4	2.59	120.01	118.20
50	S2	609	PSU	O2-C2-N1	-2.59	119.94	122.79
3	L5	4228	OMG	N2-C2-N1	2.59	122.23	116.71
50	S2	1239	PSU	O2-C2-N1	-2.59	119.94	122.79
50	S2	1136	PSU	C6-C5-C4	2.59	120.01	118.20
50	S2	109	PSU	C6-C5-C4	2.58	120.00	118.20
50	S2	406	PSU	C6-C5-C4	2.57	120.00	118.20
3	L5	1779	PSU	O2-C2-N1	-2.57	119.96	122.79
3	L5	4618	OMG	N2-C2-N1	2.56	122.17	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1536	PSU	O2-C2-N1	-2.56	119.98	122.79
3	L5	2839	PSU	C6-C5-C4	2.56	119.98	118.20
5	L8	69	PSU	O2-C2-N1	-2.55	119.98	122.79
50	S2	1177	PSU	C6-C5-C4	2.55	119.98	118.20
3	L5	4576	PSU	O2-C2-N1	-2.55	119.99	122.79
50	S2	815	PSU	C6-C5-C4	2.55	119.98	118.20
3	L5	3920	PSU	C6-C5-C4	2.54	119.97	118.20
50	S2	34	PSU	C6-C5-C4	2.54	119.97	118.20
3	L5	3792	OMG	N9-C4-N3	2.54	131.04	125.94
50	S2	609	PSU	C6-C5-C4	2.54	119.97	118.20
50	S2	644	OMG	N9-C4-N3	2.53	131.03	125.94
3	L5	3944	OMG	C5-C6-N1	2.53	119.63	113.19
50	S2	686	PSU	C6-C5-C4	2.53	119.97	118.20
3	L5	3734	PSU	C6-C5-C4	2.53	119.96	118.20
3	L5	3944	OMG	O6-C6-C5	-2.52	119.91	126.60
50	S2	649	PSU	O2-C2-N1	-2.52	120.02	122.79
50	S2	296	PSU	O2-C2-N1	-2.51	120.03	122.79
3	L5	3792	OMG	C5-C6-N1	2.51	119.56	113.19
50	S2	683	OMG	O6-C6-C5	-2.51	119.95	126.60
50	S2	867	OMG	O6-C6-C5	-2.50	119.96	126.60
3	L5	2364	OMG	N2-C2-N1	2.50	122.04	116.71
3	L5	1322	1MA	N9-C8-N7	-2.50	108.68	113.39
3	L5	3920	PSU	O2-C2-N1	-2.49	120.04	122.79
3	L5	3792	OMG	C2-N1-C6	-2.49	120.55	125.10
50	S2	651	PSU	C6-C5-C4	2.49	119.94	118.20
3	L5	3718	A2M	C6-C5-C4	2.49	120.53	117.18
50	S2	1244	PSU	C6-C5-C4	2.49	119.94	118.20
3	L5	1782	PSU	O2-C2-N1	-2.49	120.05	122.79
3	L5	4220	6MZ	C9-N6-C6	-2.49	120.73	122.87
50	S2	1447	OMG	O6-C6-C5	-2.48	120.01	126.60
50	S2	1004	PSU	C6-C5-C4	2.48	119.93	118.20
3	L5	4370	OMG	N9-C4-N3	2.48	130.91	125.94
3	L5	4494	OMG	N9-C4-N3	2.48	130.91	125.94
50	S2	1639	G7M	CN7-N7-C8	-2.48	121.02	124.84
3	L5	4431	PSU	O2-C2-N1	-2.48	120.06	122.79
3	L5	1744	PSU	C6-C5-C4	2.48	119.93	118.20
3	L5	1782	PSU	C6-C5-C4	2.47	119.93	118.20
50	S2	822	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	4312	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	4353	PSU	C6-C5-C4	2.47	119.92	118.20
3	L5	2632	PSU	O2-C2-N1	-2.46	120.08	122.79
3	L5	4423	PSU	O2-C2-N1	-2.46	120.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1677	PSU	C6-C5-C4	2.46	119.92	118.20
3	L5	4637	OMG	N9-C4-N3	2.46	130.88	125.94
50	S2	109	PSU	O2-C2-N1	-2.46	120.08	122.79
3	L5	3884	PSU	O2-C2-N1	-2.46	120.08	122.79
50	S2	1347	PSU	C6-C5-C4	2.46	119.92	118.20
3	L5	4361	PSU	O2-C2-N1	-2.46	120.09	122.79
3	L5	2424	OMG	O6-C6-C5	-2.45	120.10	126.60
3	L5	4673	PSU	O2-C2-N1	-2.45	120.10	122.79
50	S2	1238	PSU	O2-C2-N1	-2.44	120.10	122.79
50	S2	1692	PSU	C6-C5-C4	2.44	119.91	118.20
3	L5	4196	OMG	O6-C6-C5	-2.44	120.12	126.60
3	L5	1316	OMG	N9-C4-N3	2.44	130.84	125.94
3	L5	4420	PSU	C6-N1-C2	-2.44	120.19	122.68
3	L5	3770	PSU	C6-C5-C4	2.44	119.90	118.20
3	L5	2415	OMU	C1'-N1-C2	2.44	121.98	117.57
3	L5	4579	PSU	O2-C2-N1	-2.43	120.11	122.79
50	S2	36	PSU	C6-C5-C4	2.43	119.90	118.20
49	Pt	9	1MG	CM1-N1-C2	-2.43	118.20	120.72
3	L5	3899	OMG	N2-C2-N1	2.42	121.88	116.71
3	L5	4499	OMG	O6-C6-C5	-2.42	120.17	126.60
5	L8	69	PSU	O4'-C1'-C2'	2.42	108.56	105.14
3	L5	3734	PSU	O2-C2-N1	-2.42	120.12	122.79
3	L5	4228	OMG	C8-N7-C5	2.42	108.62	104.24
3	L5	4521	PSU	O2-C2-N1	-2.42	120.12	122.79
3	L5	3744	OMG	O6-C6-C5	-2.42	120.18	126.60
3	L5	4499	OMG	N9-C4-N3	2.42	130.79	125.94
50	S2	1842	4AC	N4-C4-N3	2.42	117.91	113.85
3	L5	3768	PSU	C6-C5-C4	2.42	119.89	118.20
50	S2	218	PSU	O2-C2-N1	-2.42	120.13	122.79
50	S2	644	OMG	O6-C6-C5	-2.41	120.20	126.60
50	S2	34	PSU	O2-C2-N1	-2.41	120.14	122.79
50	S2	815	PSU	O2-C2-N1	-2.41	120.14	122.79
3	L5	4293	PSU	O2-C2-N1	-2.41	120.14	122.79
3	L5	3851	PSU	C6-C5-C4	2.41	119.88	118.20
3	L5	4299	PSU	C6-C5-C4	2.41	119.88	118.20
50	S2	436	OMG	N9-C4-N3	2.40	130.76	125.94
3	L5	4442	PSU	O2-C2-N1	-2.40	120.14	122.79
50	S2	1445	PSU	O2-C2-N1	-2.40	120.15	122.79
50	S2	1056	PSU	O2-C2-N1	-2.40	120.15	122.79
3	L5	4431	PSU	C6-C5-C4	2.40	119.88	118.20
50	S2	1490	OMG	C5-C6-N1	2.39	119.27	113.19
50	S2	166	A2M	C2'-C1'-N9	-2.39	109.51	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	814	PSU	O2-C2-N1	-2.39	120.16	122.79
50	S2	1625	PSU	C6-C5-C4	2.39	119.87	118.20
3	L5	1524	A2M	C4'-O4'-C1'	-2.39	104.20	109.47
3	L5	1625	OMG	O6-C6-C5	-2.39	120.27	126.60
50	S2	1337	4AC	C6-C5-C4	2.38	119.88	116.96
3	L5	4618	OMG	C8-N7-C5	2.38	108.55	104.24
3	L5	2364	OMG	C8-N7-C5	2.38	108.55	104.24
3	L5	3695	PSU	O2-C2-N1	-2.38	120.18	122.79
50	S2	1244	PSU	O2-C2-N1	-2.38	120.18	122.79
50	S2	1692	PSU	O2-C2-N1	-2.38	120.18	122.79
3	L5	3853	PSU	O2-C2-N1	-2.37	120.18	122.79
50	S2	573	PSU	O2-C2-N1	-2.37	120.18	122.79
3	L5	1683	PSU	O2-C2-N1	-2.37	120.18	122.79
5	L8	75	OMG	O6-C6-C5	-2.37	120.32	126.60
3	L5	3627	OMG	C8-N7-C5	2.37	108.53	104.24
3	L5	4576	PSU	C6-C5-C4	2.37	119.85	118.20
3	L5	4637	OMG	C8-N7-C5	2.37	108.52	104.24
3	L5	3627	OMG	N2-C2-N1	2.37	121.75	116.71
3	L5	3639	PSU	O2-C2-N1	-2.37	120.19	122.79
50	S2	406	PSU	O2-C2-N1	-2.36	120.19	122.79
3	L5	4493	PSU	O2-C2-N1	-2.36	120.19	122.79
3	L5	4442	PSU	O4'-C1'-C2'	2.36	108.47	105.14
3	L5	4370	OMG	O6-C6-C5	-2.36	120.34	126.60
50	S2	863	PSU	O2-C2-N1	-2.36	120.19	122.79
3	L5	1582	PSU	O2-C2-N1	-2.36	120.20	122.79
3	L5	3770	PSU	O2-C2-N1	-2.36	120.20	122.79
50	S2	966	PSU	O2-C2-N1	-2.35	120.20	122.79
50	S2	1174	PSU	O2-C2-N1	-2.35	120.20	122.79
3	L5	4623	OMG	O6-C6-C5	-2.35	120.38	126.60
3	L5	4628	PSU	C6-C5-C4	2.34	119.84	118.20
3	L5	3867	A2M	C6-C5-C4	2.34	120.33	117.18
3	L5	1779	PSU	C6-C5-C4	2.34	119.84	118.20
3	L5	1862	PSU	C6-C5-C4	2.34	119.84	118.20
3	L5	4532	PSU	C6-C5-C4	2.34	119.84	118.20
3	L5	4636	PSU	O2-C2-N1	-2.34	120.21	122.79
50	S2	822	PSU	C6-C5-C4	2.34	119.83	118.20
50	S2	681	PSU	O2-C2-N1	-2.34	120.22	122.79
50	S2	1177	PSU	O2-C2-N1	-2.34	120.22	122.79
3	L5	4392	OMG	N2-C2-N1	2.34	121.69	116.71
50	S2	436	OMG	C8-N7-C5	2.34	108.47	104.24
3	L5	4494	OMG	O6-C6-C5	-2.34	120.40	126.60
3	L5	2787	A2M	C4-C5-N7	-2.34	107.77	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4353	PSU	O2-C2-N1	-2.34	120.22	122.79
50	S2	601	OMG	O6-C6-C5	-2.34	120.40	126.60
3	L5	2787	A2M	C6-C5-C4	2.33	120.32	117.18
3	L5	2876	OMG	O6-C6-C5	-2.33	120.41	126.60
50	S2	1851	MA6	C4-C5-N7	-2.33	107.78	110.62
3	L5	4392	OMG	O6-C6-C5	-2.33	120.42	126.60
3	L5	1316	OMG	O6-C6-C5	-2.33	120.42	126.60
50	S2	644	OMG	C8-N7-C5	2.33	108.45	104.24
50	S2	436	OMG	O6-C6-C5	-2.33	120.42	126.60
3	L5	3627	OMG	C2'-C1'-N9	-2.32	109.71	114.22
3	L5	3744	OMG	N9-C4-N3	2.32	130.60	125.94
50	S2	866	PSU	O2-C2-N1	-2.32	120.23	122.79
3	L5	2876	OMG	C8-N7-C5	2.32	108.44	104.24
3	L5	3729	PSU	O2-C2-N1	-2.32	120.24	122.79
3	L5	1522	OMG	O6-C6-C5	-2.32	120.46	126.60
5	L8	75	OMG	N2-C2-N1	2.31	121.64	116.71
3	L5	1862	PSU	O2-C2-N1	-2.31	120.25	122.79
31	La	39	V5N	O-C-CA	-2.31	118.73	124.78
3	L5	4457	PSU	O2-C2-N1	-2.31	120.25	122.79
50	S2	686	PSU	O2-C2-N1	-2.31	120.25	122.79
50	S2	867	OMG	C8-N7-C5	2.31	108.42	104.24
3	L5	1322	1MA	C5-C4-N9	2.31	109.81	105.63
3	L5	1534	A2M	C4-C5-N7	-2.31	107.81	110.62
50	S2	590	A2M	C6-C5-C4	2.30	120.28	117.18
3	L5	3768	PSU	O2-C2-N1	-2.30	120.25	122.79
3	L5	3639	PSU	C6-C5-C4	2.30	119.81	118.20
50	S2	1447	OMG	C8-N7-C5	2.30	108.41	104.24
3	L5	3758	PSU	O2-C2-N1	-2.30	120.26	122.79
3	L5	3792	OMG	O6-C6-C5	-2.30	120.50	126.60
3	L5	3899	OMG	O6-C6-C5	-2.30	120.51	126.60
50	S2	1031	A2M	C4-N9-C8	2.30	108.22	105.73
50	S2	1490	OMG	C2-N1-C6	-2.30	120.91	125.10
5	L8	75	OMG	C8-N7-C5	2.29	108.39	104.24
3	L5	4618	OMG	O6-C6-C5	-2.29	120.52	126.60
3	L5	3627	OMG	O6-C6-C5	-2.29	120.52	126.60
3	L5	3744	OMG	C8-N7-C5	2.29	108.39	104.24
3	L5	4403	PSU	O4'-C1'-C2'	2.29	108.37	105.14
50	S2	601	OMG	N2-C2-N1	2.29	121.58	116.71
3	L5	3853	PSU	C6-C5-C4	2.29	119.80	118.20
3	L5	4579	PSU	C6-C5-C4	2.29	119.80	118.20
50	S2	428	OMU	O2-C2-N1	-2.29	119.75	122.79
3	L5	3899	OMG	C8-N7-C5	2.29	108.38	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4228	OMG	O6-C6-C5	-2.28	120.54	126.60
49	Pt	37	1MG	CM1-N1-C2	-2.28	118.36	120.72
3	L5	4420	PSU	O2-C2-N1	-2.28	120.28	122.79
50	S2	601	OMG	N9-C4-N3	2.28	130.51	125.94
50	S2	683	OMG	C8-N7-C5	2.28	108.36	104.24
3	L5	3785	A2M	C4-N9-C8	2.27	108.19	105.73
3	L5	3764	PSU	O2-C2-N1	-2.27	120.29	122.79
3	L5	4623	OMG	N2-C2-N1	2.27	121.54	116.71
50	S2	1337	4AC	C5-C4-N3	-2.27	118.94	122.59
3	L5	3844	PSU	O2-C2-N1	-2.27	120.30	122.79
3	L5	4299	PSU	O2-C2-N1	-2.27	120.30	122.79
3	L5	3637	PSU	C6-C5-C4	2.26	119.78	118.20
3	L5	4312	PSU	C6-C5-C4	2.26	119.78	118.20
50	S2	1643	PSU	O4'-C1'-C2'	2.26	108.33	105.14
3	L5	3925	OMU	O2-C2-N1	-2.26	119.78	122.79
50	S2	105	PSU	O2-C2-N1	-2.26	120.30	122.79
3	L5	1792	PSU	O2-C2-N1	-2.26	120.31	122.79
3	L5	4618	OMG	C4-C5-N7	-2.26	107.15	110.72
5	L8	75	OMG	N9-C4-N3	2.25	130.46	125.94
50	S2	801	PSU	O2-C2-N1	-2.25	120.31	122.79
50	S2	1004	PSU	O2-C2-N1	-2.25	120.31	122.79
50	S2	468	A2M	C2'-C1'-N9	-2.25	109.74	113.53
3	L5	1316	OMG	C8-N7-C5	2.25	108.31	104.24
3	L5	3744	OMG	N2-C2-N1	2.25	121.50	116.71
3	L5	4552	PSU	C6-C5-C4	2.25	119.77	118.20
3	L5	4296	PSU	O2-C2-N1	-2.25	120.32	122.79
3	L5	2508	PSU	O2-C2-N1	-2.24	120.32	122.79
3	L5	2815	A2M	C6-C5-C4	2.24	120.19	117.18
50	S2	1625	PSU	O2-C2-N1	-2.24	120.33	122.79
3	L5	1792	PSU	C6-C5-C4	2.24	119.76	118.20
3	L5	4293	PSU	C6-C5-C4	2.24	119.76	118.20
50	S2	1347	PSU	O2-C2-N1	-2.24	120.33	122.79
50	S2	1490	OMG	N9-C4-N3	2.24	130.43	125.94
50	S2	668	A2M	C4-C5-N7	-2.24	107.89	110.62
3	L5	4498	OMU	O2-C2-N1	-2.24	119.81	122.79
3	L5	3723	A2M	C4-N9-C8	2.24	108.15	105.73
3	L5	2364	OMG	O6-C6-C5	-2.24	120.67	126.60
3	L5	1522	OMG	N2-C2-N1	2.23	121.47	116.71
3	L5	5001	PSU	O2-C2-N1	-2.23	120.33	122.79
3	L5	2364	OMG	C4-C5-N7	-2.23	107.19	110.72
3	L5	4689	PSU	C6-C5-C4	2.23	119.76	118.20
5	L8	55	PSU	O2-C2-N1	-2.23	120.34	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	509	OMG	C8-N7-C5	2.22	108.27	104.24
3	L5	4637	OMG	O6-C6-C5	-2.22	120.70	126.60
50	S2	1850	MA6	C4-N9-C8	2.22	108.14	105.73
3	L5	3792	OMG	C8-N7-C5	2.22	108.26	104.24
3	L5	1781	PSU	C6-C5-C4	2.22	119.75	118.20
3	L5	3724	A2M	C4-N9-C8	2.21	108.13	105.73
3	L5	4370	OMG	C8-N7-C5	2.21	108.24	104.24
3	L5	4493	PSU	C6-C5-C4	2.21	119.74	118.20
3	L5	4571	A2M	C4-N9-C8	2.21	108.12	105.73
50	S2	484	A2M	C4-C5-N7	-2.21	107.93	110.62
50	S2	468	A2M	C4-N9-C8	2.21	108.12	105.73
3	L5	4499	OMG	C8-N7-C5	2.20	108.23	104.24
3	L5	398	A2M	C6-C5-C4	2.20	120.15	117.18
3	L5	3851	PSU	O2-C2-N1	-2.20	120.36	122.79
50	S2	649	PSU	C6-C5-C4	2.20	119.74	118.20
3	L5	4471	PSU	O2-C2-N1	-2.20	120.37	122.79
3	L5	4618	OMG	C6-C5-N7	2.20	134.34	130.25
3	L5	4636	PSU	C6-C5-C4	2.20	119.73	118.20
3	L5	4623	OMG	C8-N7-C5	2.20	108.22	104.24
3	L5	1860	PSU	C6-C5-C4	2.20	119.73	118.20
3	L5	3785	A2M	C2'-C1'-N9	-2.19	109.84	113.53
3	L5	4530	UR3	C6-N1-C2	-2.19	119.82	121.79
50	S2	1850	MA6	C4-C5-N7	-2.19	107.95	110.62
3	L5	1524	A2M	C4-N9-C8	2.19	108.10	105.73
3	L5	4228	OMG	C4-C5-N7	-2.19	107.25	110.72
50	S2	1851	MA6	C4-N9-C8	2.19	108.10	105.73
50	S2	121	OMU	O2-C2-N1	-2.19	119.88	122.79
3	L5	1522	OMG	C8-N7-C5	2.19	108.20	104.24
50	S2	1490	OMG	O6-C6-C5	-2.18	120.81	126.60
50	S2	166	A2M	C4-C5-N7	-2.18	107.96	110.62
50	S2	509	OMG	O6-C6-C5	-2.18	120.82	126.60
3	L5	3825	A2M	C4-N9-C8	2.18	108.09	105.73
3	L5	3695	PSU	O4'-C1'-C2'	2.18	108.21	105.14
3	L5	4569	PSU	C6-C5-C4	2.18	119.72	118.20
3	L5	4228	OMG	C6-C5-N7	2.17	134.29	130.25
3	L5	2508	PSU	C6-C5-C4	2.17	119.72	118.20
3	L5	4423	PSU	C6-C5-C4	2.17	119.72	118.20
50	S2	99	A2M	C6-C5-C4	2.17	120.10	117.18
3	L5	1625	OMG	C8-N7-C5	2.17	108.16	104.24
3	L5	4532	PSU	O2-C2-N1	-2.17	120.41	122.79
3	L5	1322	1MA	C4-C5-N7	-2.16	107.30	110.72
50	S2	1239	PSU	C6-C5-C4	2.16	119.71	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	1490	OMG	C8-N7-C5	2.16	108.15	104.24
3	L5	398	A2M	C4-C5-N7	-2.16	107.99	110.62
50	S2	572	PSU	O4'-C1'-C2'	2.16	108.19	105.14
50	S2	1678	A2M	C6-C5-C4	2.16	120.08	117.18
3	L5	1582	PSU	C6-C5-C4	2.16	119.70	118.20
3	L5	3944	OMG	C8-N7-C5	2.16	108.14	104.24
50	S2	576	A2M	C4-C5-N7	-2.15	107.99	110.62
3	L5	3785	A2M	C4-C5-N7	-2.15	108.00	110.62
50	S2	512	A2M	C4-N9-C8	2.15	108.06	105.73
3	L5	4552	PSU	O2-C2-N1	-2.15	120.42	122.79
50	S2	1243	PSU	O2-C2-N1	-2.15	120.42	122.79
50	S2	1678	A2M	C4-C5-N7	-2.15	108.00	110.62
3	L5	4521	PSU	O4'-C1'-C2'	2.15	108.17	105.14
3	L5	3782	5MC	CM5-C5-C6	-2.15	119.98	122.85
50	S2	36	PSU	O2-C2-N1	-2.15	120.43	122.79
50	S2	1367	PSU	O2-C2-N1	-2.15	120.43	122.79
3	L5	4196	OMG	C8-N7-C5	2.15	108.13	104.24
3	L5	2364	OMG	C6-C5-N7	2.15	134.24	130.25
50	S2	1842	4AC	C5-C4-N3	-2.15	119.14	122.59
50	S2	668	A2M	C3'-C2'-C1'	2.14	106.92	102.89
3	L5	4392	OMG	C8-N7-C5	2.14	108.11	104.24
3	L5	1326	A2M	C4-C5-N7	-2.14	108.01	110.62
3	L5	4618	OMG	C2'-C1'-N9	-2.14	110.07	114.22
50	S2	27	A2M	C4-C5-N7	-2.14	108.02	110.62
3	L5	4571	A2M	C4-C5-N7	-2.13	108.02	110.62
3	L5	1524	A2M	C4-C5-N7	-2.13	108.02	110.62
50	S2	601	OMG	C8-N7-C5	2.13	108.10	104.24
3	L5	4494	OMG	N2-C2-N1	2.13	121.25	116.71
50	S2	166	A2M	C4-N9-C8	2.13	108.03	105.73
3	L5	2632	PSU	C6-C5-C4	2.12	119.68	118.20
3	L5	1326	A2M	C4-N9-C8	2.12	108.03	105.73
50	S2	576	A2M	C6-C5-C4	2.12	120.04	117.18
3	L5	4590	A2M	C4-N9-C8	2.12	108.03	105.73
50	S2	1639	G7M	N9-C8-N7	-2.12	106.97	112.21
3	L5	3718	A2M	C4-C5-N7	-2.12	108.04	110.62
50	S2	468	A2M	C4-C5-N7	-2.12	108.04	110.62
3	L5	1683	PSU	C6-C5-C4	2.12	119.68	118.20
50	S2	1383	A2M	C6-C5-C4	2.12	120.03	117.18
3	L5	4571	A2M	C6-C5-C4	2.11	120.03	117.18
3	L5	400	A2M	C4-N9-C8	2.11	108.02	105.73
3	L5	3627	OMG	C4-C5-N7	-2.11	107.38	110.72
3	L5	3723	A2M	C4-C5-N7	-2.11	108.05	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4296	PSU	C6-C5-C4	2.11	119.67	118.20
3	L5	4494	OMG	C8-N7-C5	2.10	108.05	104.24
50	S2	1383	A2M	C4-C5-N7	-2.10	108.06	110.62
3	L5	1524	A2M	C6-C5-C4	2.10	120.01	117.18
50	S2	576	A2M	C4-N9-C8	2.10	108.00	105.73
3	L5	4972	PSU	C6-C5-C4	2.10	119.67	118.20
3	L5	4361	PSU	C6-C5-C4	2.10	119.67	118.20
50	S2	484	A2M	C6-C5-C4	2.10	120.00	117.18
50	S2	354	OMU	O2-C2-N1	-2.10	120.00	122.79
3	L5	1536	PSU	C6-C5-C4	2.09	119.66	118.20
50	S2	1851	MA6	C5-C4-N9	2.09	108.22	105.78
3	L5	2815	A2M	C4-C5-N7	-2.09	108.07	110.62
3	L5	4569	PSU	O2-C2-N1	-2.09	120.49	122.79
3	L5	3851	PSU	O4'-C1'-C2'	2.09	108.09	105.14
3	L5	2363	A2M	C4-C5-N7	-2.09	108.07	110.62
50	S2	822	PSU	O4'-C1'-C2'	2.09	108.09	105.14
50	S2	99	A2M	C4-N9-C8	2.09	107.99	105.73
50	S2	93	PSU	O2-C2-N1	-2.08	120.50	122.79
3	L5	2363	A2M	C4-N9-C8	2.08	107.99	105.73
3	L5	3825	A2M	C6-C5-C4	2.08	119.98	117.18
3	L5	3718	A2M	C5-C4-N9	2.08	108.20	105.78
50	S2	172	OMU	O2-C2-N1	-2.08	120.02	122.79
5	L8	55	PSU	C6-C5-C4	2.08	119.65	118.20
3	L5	4590	A2M	C4-C5-N7	-2.08	108.09	110.62
3	L5	1781	PSU	O2-C2-N1	-2.08	120.50	122.79
3	L5	2839	PSU	O2-C2-N1	-2.08	120.50	122.79
3	L5	3762	PSU	C6-C5-C4	2.08	119.65	118.20
50	S2	681	PSU	C6-C5-C4	2.08	119.65	118.20
50	S2	27	A2M	C6-C5-C4	2.08	119.97	117.18
3	L5	3867	A2M	C4-C5-N7	-2.08	108.09	110.62
3	L5	1871	A2M	C4-N9-C8	2.08	107.98	105.73
3	L5	4972	PSU	O2-C2-N1	-2.07	120.51	122.79
3	L5	1522	OMG	N9-C4-N3	2.07	130.10	125.94
3	L5	3830	A2M	C4-C5-N7	-2.07	108.09	110.62
3	L5	4523	A2M	C6-C5-C4	2.07	119.97	117.18
3	L5	3830	A2M	C6-C5-C4	2.07	119.97	117.18
3	L5	2837	OMU	O2-C2-N1	-2.07	120.04	122.79
3	L5	1534	A2M	C6-C5-C4	2.07	119.96	117.18
50	S2	27	A2M	C4-N9-C8	2.07	107.97	105.73
50	S2	1678	A2M	C4-N9-C8	2.07	107.97	105.73
5	L8	14	OMU	O2-C2-N1	-2.06	120.04	122.79
50	S2	668	A2M	C4-N9-C8	2.06	107.96	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	S2	590	A2M	C4'-O4'-C1'	-2.06	104.93	109.47
50	S2	1248	B8N	O4'-C1'-C2'	2.06	108.05	105.14
3	L5	3729	PSU	C6-C5-C4	2.06	119.64	118.20
3	L5	3899	OMG	C4-C5-N7	-2.06	107.47	110.72
3	L5	2401	A2M	C4-C5-N7	-2.05	108.12	110.62
3	L5	2787	A2M	C5-C4-N9	2.05	108.17	105.78
3	L5	4623	OMG	N9-C4-N3	2.05	130.06	125.94
3	L5	4306	OMU	O2-C2-N1	-2.05	120.06	122.79
50	S2	1174	PSU	C6-C5-C4	2.05	119.63	118.20
3	L5	3627	OMG	C6-C5-N7	2.05	134.06	130.25
3	L5	3884	PSU	C6-C5-C4	2.05	119.63	118.20
3	L5	4523	A2M	C4-C5-N7	-2.05	108.13	110.62
3	L5	3867	A2M	C4-N9-C8	2.05	107.94	105.73
50	S2	159	A2M	C6-C5-C4	2.05	119.93	117.18
50	S2	99	A2M	C4-C5-N7	-2.05	108.13	110.62
3	L5	2843	PSU	C6-C5-C4	2.04	119.63	118.20
3	L5	4636	PSU	O4'-C1'-C2'	2.04	108.03	105.14
3	L5	4673	PSU	C6-C5-C4	2.04	119.63	118.20
50	S2	1490	OMG	N1-C2-N3	-2.04	119.52	123.32
3	L5	3899	OMG	C6-C5-N7	2.04	134.04	130.25
50	S2	1232	PSU	C6-C5-C4	2.04	119.62	118.20
3	L5	1534	A2M	C5-C4-N9	2.03	108.14	105.78
50	S2	590	A2M	C4-C5-N7	-2.03	108.15	110.62
50	S2	590	A2M	C4-N9-C8	2.03	107.92	105.73
3	L5	1871	A2M	C4-C5-N7	-2.03	108.15	110.62
3	L5	3724	A2M	C6-C5-C4	2.03	119.91	117.18
5	L8	75	OMG	C4-C5-N7	-2.02	107.52	110.72
3	L5	3734	PSU	O4'-C1'-C2'	2.02	108.00	105.14
50	S2	1288	OMU	C1'-N1-C2	2.02	121.23	117.57
50	S2	468	A2M	C6-C5-C4	2.02	119.90	117.18
3	L5	5001	PSU	C6-C5-C4	2.02	119.61	118.20
3	L5	4457	PSU	O4'-C1'-C2'	2.02	107.99	105.14
50	S2	512	A2M	C6-C5-C4	2.01	119.89	117.18
3	L5	1316	OMG	C2'-C1'-N9	-2.01	110.31	114.22
50	S2	436	OMG	N2-C2-N1	2.01	121.00	116.71
3	L5	400	A2M	C4-C5-N7	-2.01	108.17	110.62
3	L5	3899	OMG	C2'-C1'-N9	-2.01	110.32	114.22
3	L5	4220	6MZ	C4-C5-N7	-2.01	108.17	110.62
50	S2	159	A2M	C4-C5-N7	-2.01	108.17	110.62
3	L5	4637	OMG	C4-C5-N7	-2.01	107.54	110.72
50	S2	436	OMG	C4-C5-N7	-2.01	107.55	110.72
50	S2	1445	PSU	O4'-C1'-C2'	2.01	107.97	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3764	PSU	C6-C5-C4	2.01	119.60	118.20
3	L5	4471	PSU	C6-C5-C4	2.00	119.60	118.20
50	S2	99	A2M	C2'-C1'-N9	-2.00	110.16	113.53
50	S2	1031	A2M	C4-C5-N7	-2.00	108.18	110.62
3	L5	3639	PSU	O4'-C1'-C2'	2.00	107.97	105.14
3	L5	4620	OMU	O2-C2-N1	-2.00	120.13	122.79
50	S2	573	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	LA	216	V5N	O-C-CA-CB
32	Lb	5	MLZ	N-CA-CB-CG
32	Lb	5	MLZ	C-CA-CB-CG
43	Lm	98	M3L	C-CA-CB-CG
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	1582	PSU	C3'-C4'-C5'-O5'
3	L5	1582	PSU	O4'-C4'-C5'-O5'
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	2824	OMC	C1'-C2'-O2'-CM2
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3808	OMC	C1'-C2'-O2'-CM2
3	L5	3841	OMC	C1'-C2'-O2'-CM2
3	L5	3944	OMG	O4'-C4'-C5'-O5'
3	L5	3944	OMG	C3'-C4'-C5'-O5'
3	L5	4306	OMU	C1'-C2'-O2'-CM2
3	L5	4420	PSU	C3'-C4'-C5'-O5'
3	L5	4420	PSU	O4'-C4'-C5'-O5'
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
50	S2	27	A2M	C1'-C2'-O2'-CM'
50	S2	99	A2M	C1'-C2'-O2'-CM'
50	S2	116	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
50	S2	462	OMC	C1'-C2'-O2'-CM2
50	S2	572	PSU	O4'-C1'-C5-C4
50	S2	572	PSU	O4'-C1'-C5-C6
50	S2	573	PSU	O4'-C1'-C5-C4
50	S2	573	PSU	O4'-C1'-C5-C6
50	S2	576	A2M	C3'-C4'-C5'-O5'
50	S2	601	OMG	C1'-C2'-O2'-CM2
50	S2	644	OMG	O4'-C4'-C5'-O5'
50	S2	644	OMG	C1'-C2'-O2'-CM2
50	S2	668	A2M	C1'-C2'-O2'-CM'
50	S2	683	OMG	O4'-C4'-C5'-O5'
50	S2	822	PSU	C3'-C4'-C5'-O5'
50	S2	822	PSU	O4'-C4'-C5'-O5'
50	S2	867	OMG	C1'-C2'-O2'-CM2
50	S2	1243	PSU	C2'-C1'-C5-C4
50	S2	1243	PSU	O4'-C1'-C5-C4
50	S2	1243	PSU	O4'-C1'-C5-C6
50	S2	1248	B8N	C31-C32-C33-N34
50	S2	1326	UY1	C2'-C1'-C5-C4
50	S2	1442	OMU	C1'-C2'-O2'-CM2
50	S2	1447	OMG	C3'-C4'-C5'-O5'
50	S2	1804	OMU	C1'-C2'-O2'-CM2
50	S2	1851	MA6	O4'-C4'-C5'-O5'
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
3	L5	3818	UY1	C3'-C4'-C5'-O5'
3	L5	3818	UY1	O4'-C4'-C5'-O5'
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	4637	OMG	O4'-C4'-C5'-O5'
50	S2	590	A2M	O4'-C4'-C5'-O5'
50	S2	590	A2M	C3'-C4'-C5'-O5'
50	S2	644	OMG	C3'-C4'-C5'-O5'
50	S2	668	A2M	O4'-C4'-C5'-O5'
50	S2	668	A2M	C3'-C4'-C5'-O5'
50	S2	683	OMG	C3'-C4'-C5'-O5'
50	S2	1243	PSU	C3'-C4'-C5'-O5'
50	S2	1243	PSU	O4'-C4'-C5'-O5'
50	S2	1442	OMU	C3'-C4'-C5'-O5'
50	S2	1442	OMU	O4'-C4'-C5'-O5'
50	S2	1490	OMG	O4'-C4'-C5'-O5'
50	S2	1851	MA6	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	4532	PSU	O4'-C4'-C5'-O5'
3	L5	4618	OMG	O4'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
50	S2	509	OMG	O4'-C4'-C5'-O5'
50	S2	576	A2M	O4'-C4'-C5'-O5'
50	S2	1447	OMG	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C4
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	1534	A2M	C3'-C2'-O2'-CM'
50	S2	512	A2M	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
50	S2	428	OMU	C2'-C1'-N1-C6
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	3818	UY1	C4'-C5'-O5'-P
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	3867	A2M	C3'-C4'-C5'-O5'
3	L5	4532	PSU	C3'-C4'-C5'-O5'
3	L5	4618	OMG	C3'-C4'-C5'-O5'
50	S2	428	OMU	O4'-C4'-C5'-O5'
50	S2	428	OMU	C3'-C4'-C5'-O5'
50	S2	99	A2M	O4'-C4'-C5'-O5'
43	Lm	98	M3L	CG-CD-CE-NZ
3	L5	4227	OMU	C1'-C2'-O2'-CM2
50	S2	1383	A2M	C1'-C2'-O2'-CM'
3	L5	4500	PSU	C4'-C5'-O5'-P
3	L5	2401	A2M	C3'-C4'-C5'-O5'
50	S2	1490	OMG	C3'-C4'-C5'-O5'
50	S2	1248	B8N	C31-C32-C33-C34
50	S2	668	A2M	C2'-C1'-N9-C8
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C6
50	S2	428	OMU	O4'-C1'-N1-C6
1	At	58	MA7	C4'-C5'-O5'-P
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
49	Pt	9	1MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
50	S2	428	OMU	C2'-C1'-N1-C2
50	S2	644	OMG	C4'-C5'-O5'-P
50	S2	1081	PSU	C4'-C5'-O5'-P
50	S2	1490	OMG	C4'-C5'-O5'-P
31	La	39	V5N	O2-CB-CG-CD2
3	L5	3729	PSU	O4'-C4'-C5'-O5'
50	S2	116	OMU	C3'-C2'-O2'-CM2
49	Pt	58	1MA	C2'-C1'-N9-C8
3	L5	2815	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
50	S2	590	A2M	C4'-C5'-O5'-P
50	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	4636	PSU	O4'-C4'-C5'-O5'
50	S2	509	OMG	C3'-C4'-C5'-O5'
49	Pt	58	1MA	C2'-C1'-N9-C4
3	L5	2351	OMC	O4'-C4'-C5'-O5'
50	S2	428	OMU	O4'-C1'-N1-C2
50	S2	918	PSU	O4'-C1'-C5-C4
50	S2	1326	UY1	O4'-C1'-C5-C4
3	L5	2401	A2M	C3'-C2'-O2'-CM'
50	S2	1832	6MZ	N1-C6-N6-C9
3	L5	1524	A2M	O4'-C1'-N9-C8
3	L5	398	A2M	O4'-C4'-C5'-O5'
50	S2	1383	A2M	C3'-C4'-C5'-O5'
50	S2	590	A2M	O4'-C1'-N9-C8
50	S2	512	A2M	C3'-C4'-C5'-O5'
50	S2	1328	OMG	C1'-C2'-O2'-CM2
50	S2	1678	A2M	C1'-C2'-O2'-CM'
3	L5	4494	OMG	C3'-C2'-O2'-CM2
50	S2	668	A2M	O4'-C1'-N9-C8
3	L5	1781	PSU	O4'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
74	SX	62	HY3	O-C-CA-C3
3	L5	3818	UY1	O4'-C1'-C5-C6
50	S2	918	PSU	O4'-C1'-C5-C6
3	L5	2787	A2M	O4'-C1'-N9-C8
3	L5	1534	A2M	O4'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
50	S2	1288	OMU	C2'-C1'-N1-C2
3	L5	2351	OMC	C2'-C1'-N1-C2
3	L5	1322	1MA	C2'-C1'-N9-C8

There are no ring outliers.

101 monomers are involved in 140 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	S2	573	PSU	1	0
3	L5	3723	A2M	4	0
3	L5	4637	OMG	2	0
50	S2	99	A2M	1	0
50	S2	462	OMC	2	0
50	S2	1328	OMG	1	0
3	L5	2861	OMC	1	0
3	L5	4552	PSU	1	0
3	L5	3925	OMU	1	0
50	S2	683	OMG	1	0
3	L5	4536	OMC	1	0
50	S2	1804	OMU	1	0
50	S2	681	PSU	3	0
50	S2	1850	MA6	1	0
3	L5	4689	PSU	1	0
3	L5	3637	PSU	1	0
3	L5	3841	OMC	1	0
50	S2	576	A2M	3	0
50	S2	1232	PSU	1	0
3	L5	3718	A2M	4	0
50	S2	1136	PSU	1	0
50	S2	1174	PSU	2	0
50	S2	1391	OMC	1	0
50	S2	1031	A2M	1	0
50	S2	867	OMG	2	0
3	L5	2351	OMC	1	0
3	L5	3734	PSU	1	0
3	L5	4532	PSU	1	0
3	L5	4306	OMU	1	0
3	L5	4620	OMU	4	0
50	S2	1445	PSU	1	0
50	S2	512	A2M	2	0
50	S2	644	OMG	1	0
3	L5	4196	OMG	1	0
50	S2	918	PSU	2	0
50	S2	609	PSU	1	0
3	L5	4227	OMU	1	0
50	S2	1244	PSU	1	0
3	L5	3627	OMG	1	0
50	S2	468	A2M	1	0
3	L5	1340	OMC	1	0
50	S2	1639	G7M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	S2	1383	A2M	1	0
3	L5	4228	OMG	1	0
50	S2	1337	4AC	1	0
50	S2	1643	PSU	1	0
50	S2	354	OMU	1	0
3	L5	2876	OMG	3	0
3	L5	2363	A2M	1	0
3	L5	4456	OMC	1	0
50	S2	1442	OMU	1	0
50	S2	1842	4AC	1	0
3	L5	3944	OMG	2	0
50	S2	1692	PSU	1	0
3	L5	1871	A2M	1	0
3	L5	1326	A2M	1	0
3	L5	1860	PSU	1	0
3	L5	398	A2M	2	0
3	L5	3760	A2M	1	0
3	L5	4220	6MZ	1	0
50	S2	801	PSU	2	0
3	L5	4392	OMG	3	0
3	L5	3884	PSU	1	0
3	L5	4447	5MC	1	0
3	L5	5001	PSU	2	0
50	S2	601	OMG	2	0
3	L5	2424	OMG	1	0
50	S2	1447	OMG	2	0
3	L5	2364	OMG	1	0
3	L5	4499	OMG	1	0
49	Pt	58	1MA	1	0
3	L5	2815	A2M	1	0
50	S2	166	A2M	2	0
50	S2	1490	OMG	1	0
50	S2	93	PSU	1	0
3	L5	3770	PSU	1	0
3	L5	3867	A2M	2	0
50	S2	1004	PSU	2	0
3	L5	1522	OMG	1	0
3	L5	3782	5MC	1	0
3	L5	4457	PSU	1	0
50	S2	436	OMG	2	0
50	S2	159	A2M	3	0
3	L5	3808	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4618	OMG	2	0
50	S2	1239	PSU	1	0
50	S2	1347	PSU	1	0
50	S2	116	OMU	3	0
50	S2	484	A2M	1	0
3	L5	2415	OMU	3	0
3	L5	3724	A2M	2	0
3	L5	4579	PSU	2	0
50	S2	1288	OMU	2	0
3	L5	1536	PSU	1	0
3	L5	1779	PSU	1	0
49	Pt	9	1MG	1	0
3	L5	4571	A2M	1	0
3	L5	1683	PSU	1	0
3	L5	1625	OMG	1	0
50	S2	1678	A2M	2	0
5	L8	75	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 304 ligands modelled in this entry, 277 are monoatomic - leaving 27 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	$\# Z > 2$
84	PUT	S2	1902	-	5,5,5	0.25	0	4,4,4	0.16	0
84	PUT	L5	5101	-	5,5,5	0.24	0	4,4,4	0.17	0
84	PUT	L5	5106	-	5,5,5	0.23	0	4,4,4	0.20	0
85	SPD	L5	5109	-	9,9,9	0.43	0	8,8,8	0.31	0
84	PUT	L5	5103	-	5,5,5	0.24	0	4,4,4	0.19	0
85	SPD	L5	5112	-	9,9,9	0.43	0	8,8,8	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	SPD	L5	5114	-	9,9,9	0.44	0	8,8,8	0.25	0
85	SPD	L5	5120	-	9,9,9	0.43	0	8,8,8	0.30	0
85	SPD	LN	301	-	9,9,9	0.43	0	8,8,8	0.28	0
85	SPD	S2	1905	-	9,9,9	0.43	0	8,8,8	0.29	0
85	SPD	L5	5107	-	9,9,9	0.43	0	8,8,8	0.38	0
85	SPD	L5	5118	-	9,9,9	0.44	0	8,8,8	0.32	0
84	PUT	L5	5104	-	5,5,5	0.24	0	4,4,4	0.18	0
85	SPD	L5	5111	-	9,9,9	0.45	0	8,8,8	0.30	0
85	SPD	L5	5116	-	9,9,9	0.44	0	8,8,8	0.28	0
84	PUT	S2	1901	-	5,5,5	0.23	0	4,4,4	0.16	0
85	SPD	L5	5108	-	9,9,9	0.44	0	8,8,8	0.23	0
85	SPD	L5	5119	-	9,9,9	0.44	0	8,8,8	0.25	0
84	PUT	L5	5102	-	5,5,5	0.24	0	4,4,4	0.17	0
85	SPD	L5	5113	-	9,9,9	0.43	0	8,8,8	0.41	0
85	SPD	S2	1903	-	9,9,9	0.44	0	8,8,8	0.27	0
85	SPD	S2	1904	-	9,9,9	0.15	0	8,8,8	0.09	0
89	HYG	S2	1944	87	35,39,39	0.46	0	43,60,60	1.56	2 (4%)
85	SPD	L5	5110	-	9,9,9	0.43	0	8,8,8	0.27	0
85	SPD	L5	5117	-	9,9,9	0.44	0	8,8,8	0.26	0
85	SPD	L5	5115	-	9,9,9	0.44	0	8,8,8	0.31	0
84	PUT	L5	5105	-	5,5,5	0.24	0	4,4,4	0.17	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
84	PUT	S2	1902	-	-	0/3/3/3	-
84	PUT	L5	5101	-	-	0/3/3/3	-
84	PUT	L5	5106	-	-	0/3/3/3	-
85	SPD	L5	5109	-	-	2/7/7/7	-
84	PUT	L5	5103	-	-	0/3/3/3	-
85	SPD	L5	5112	-	-	1/7/7/7	-
85	SPD	L5	5114	-	-	0/7/7/7	-
85	SPD	L5	5120	-	-	0/7/7/7	-
85	SPD	LN	301	-	-	0/7/7/7	-
85	SPD	S2	1905	-	-	0/7/7/7	-
85	SPD	L5	5107	-	-	0/7/7/7	-
85	SPD	L5	5118	-	-	0/7/7/7	-
84	PUT	L5	5104	-	-	0/3/3/3	-
85	SPD	L5	5111	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	L5	5116	-	-	0/7/7/7	-
84	PUT	S2	1901	-	-	0/3/3/3	-
85	SPD	L5	5108	-	-	0/7/7/7	-
85	SPD	L5	5119	-	-	0/7/7/7	-
84	PUT	L5	5102	-	-	0/3/3/3	-
85	SPD	L5	5113	-	-	0/7/7/7	-
85	SPD	S2	1903	-	-	0/7/7/7	-
85	SPD	S2	1904	-	-	2/7/7/7	-
89	HYG	S2	1944	87	1/1/16/17	6/12/87/87	0/4/4/4
85	SPD	L5	5110	-	-	0/7/7/7	-
85	SPD	L5	5117	-	-	0/7/7/7	-
85	SPD	L5	5115	-	-	0/7/7/7	-
84	PUT	L5	5105	-	-	0/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	S2	1944	HYG	O29-C12-C13	9.08	134.69	110.86
89	S2	1944	HYG	C23-O28-C27	2.36	116.50	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
89	S2	1944	HYG	C12

All (11) torsion outliers are listed below:

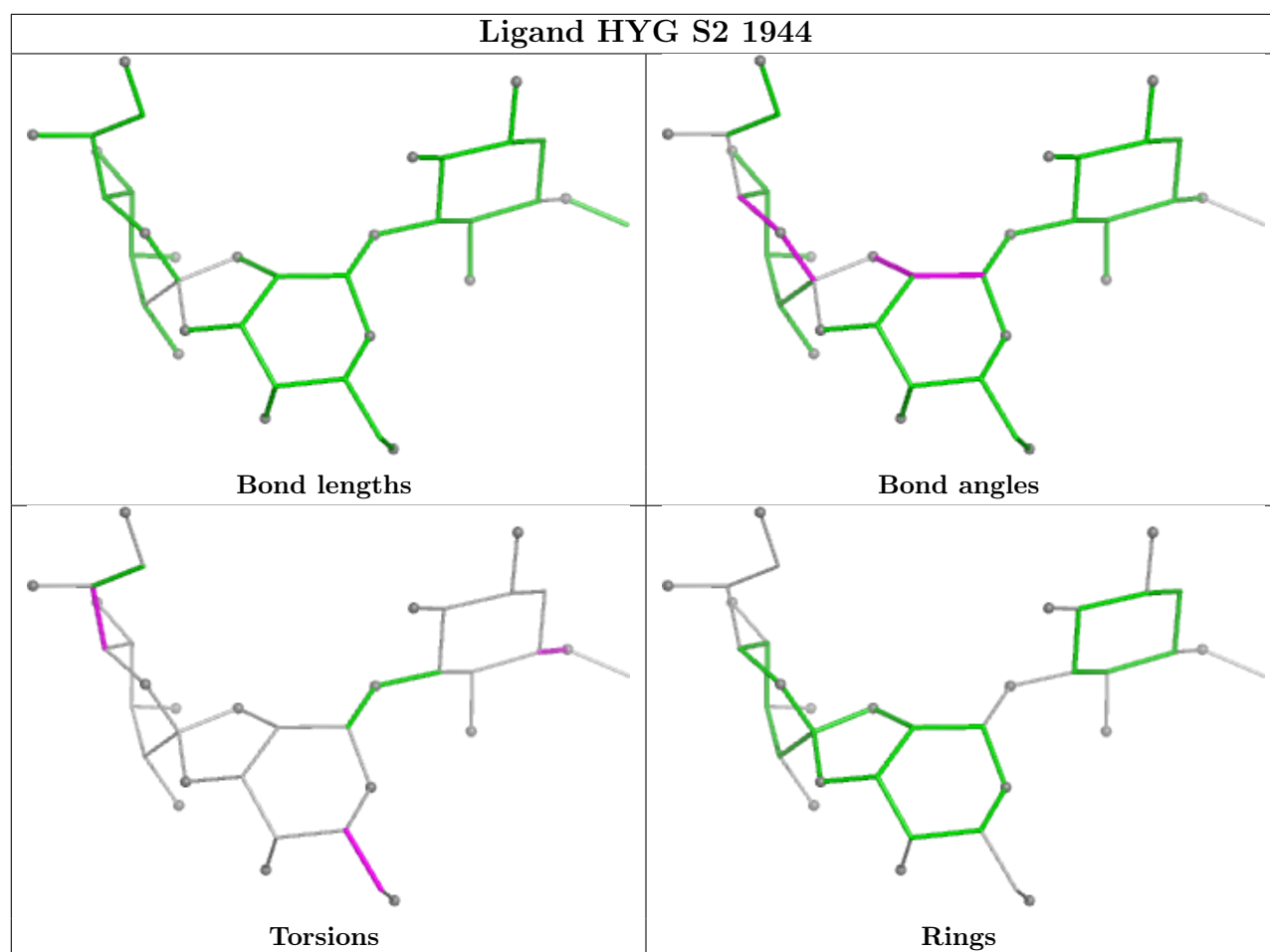
Mol	Chain	Res	Type	Atoms
89	S2	1944	HYG	C5-C4-N9-C10
89	S2	1944	HYG	C26-C27-C33-C34
89	S2	1944	HYG	O28-C27-C33-C34
85	S2	1904	SPD	N6-C7-C8-C9
89	S2	1944	HYG	C16-C15-C19-O20
89	S2	1944	HYG	O14-C15-C19-O20
85	L5	5109	SPD	C2-C3-C4-C5
85	L5	5112	SPD	N1-C2-C3-C4
89	S2	1944	HYG	C3-C4-N9-C10
85	S2	1904	SPD	N1-C2-C3-C4
85	L5	5109	SPD	N1-C2-C3-C4

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	S2	1902	PUT	2	0
84	L5	5106	PUT	1	0
85	L5	5109	SPD	1	0
85	L5	5112	SPD	2	0
85	L5	5120	SPD	1	0
85	L5	5111	SPD	1	0
84	S2	1901	PUT	1	0
84	L5	5102	PUT	1	0
85	L5	5113	SPD	1	0
89	S2	1944	HYG	1	0
85	L5	5110	SPD	1	0
85	L5	5117	SPD	1	0
85	L5	5115	SPD	1	0

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



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.

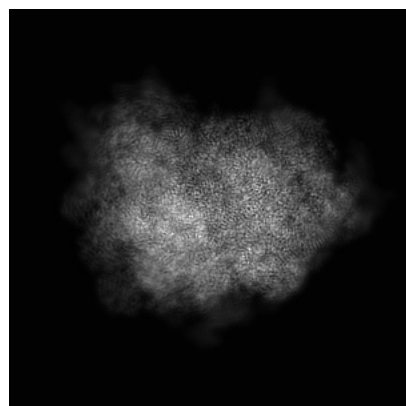
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55091. These allow visual inspection of the internal detail of the map and identification of artifacts.

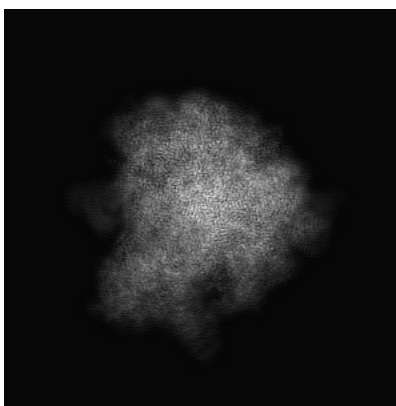
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

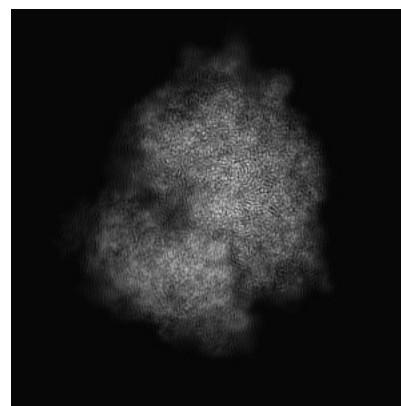
6.1.1 Primary map



X

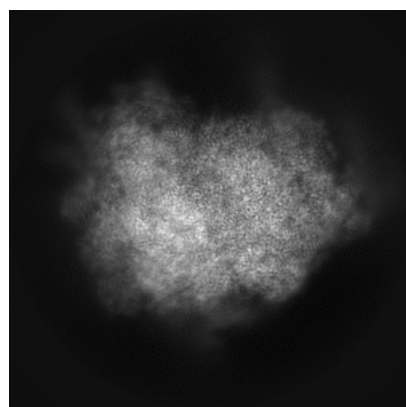


Y

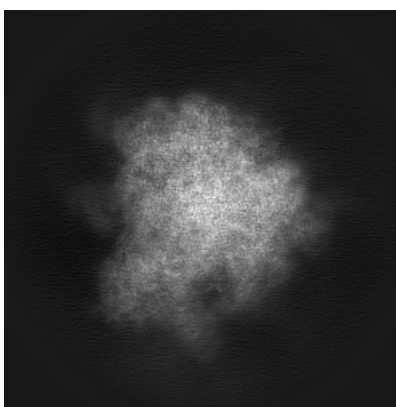


Z

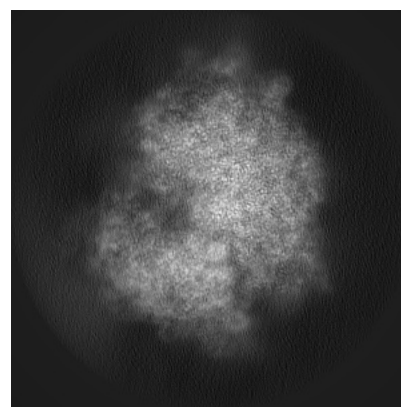
6.1.2 Raw map



X



Y

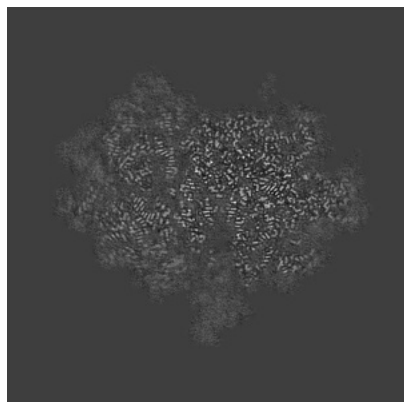


Z

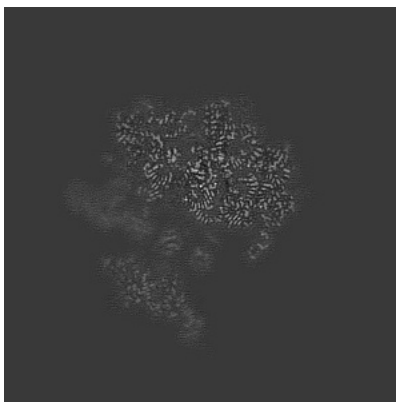
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

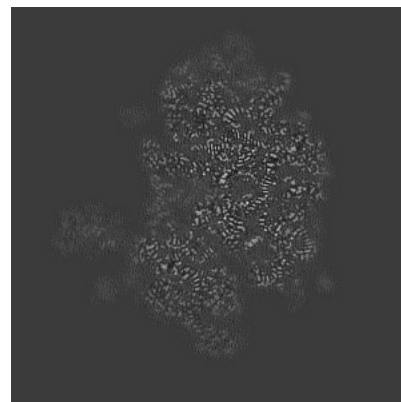
6.2.1 Primary map



X Index: 240

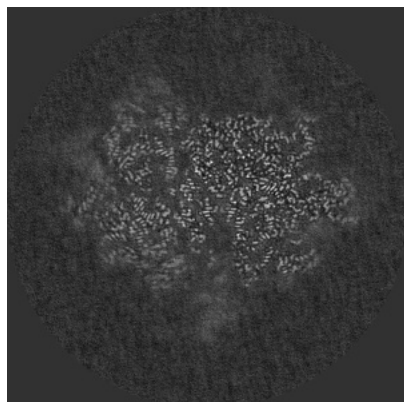


Y Index: 240

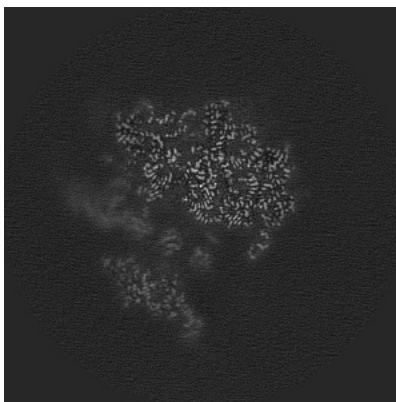


Z Index: 240

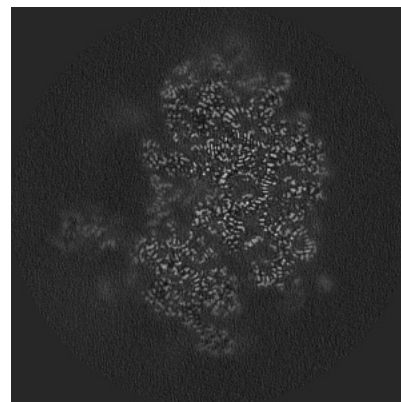
6.2.2 Raw map



X Index: 240



Y Index: 240

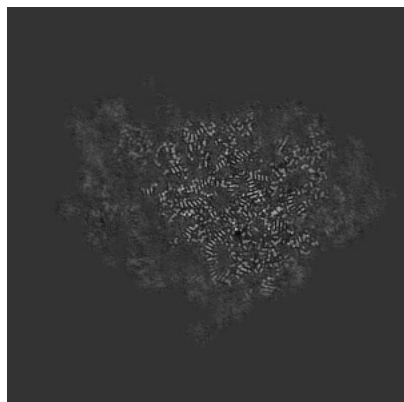


Z Index: 240

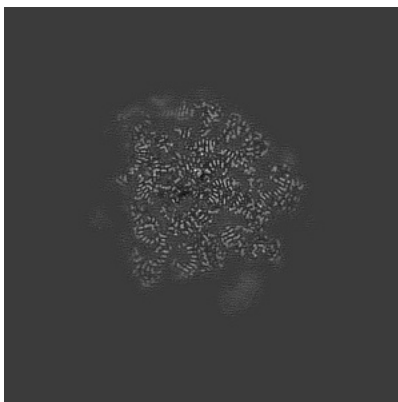
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

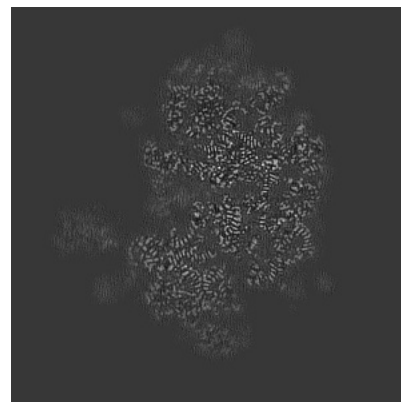
6.3.1 Primary map



X Index: 268

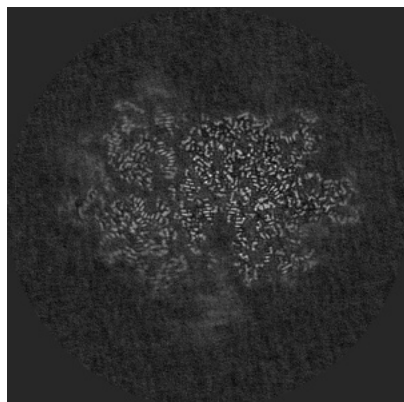


Y Index: 293

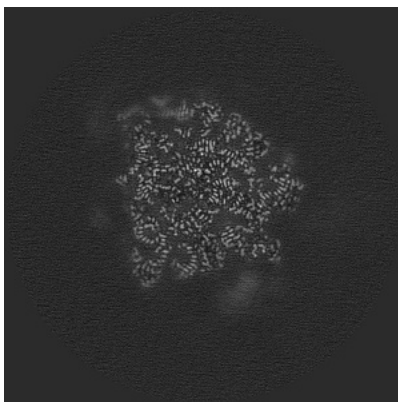


Z Index: 243

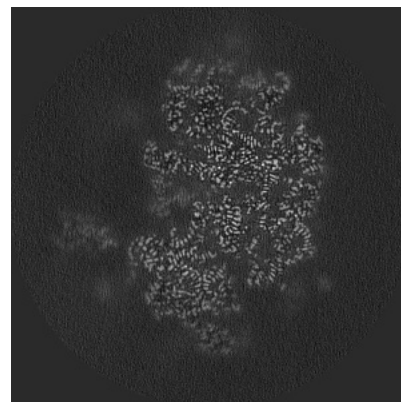
6.3.2 Raw map



X Index: 241



Y Index: 293

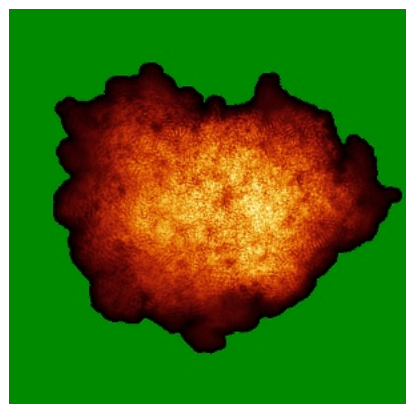


Z Index: 243

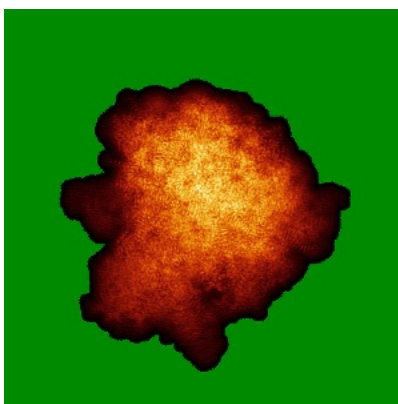
The images above show the largest variance slices of the map in three orthogonal directions.

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

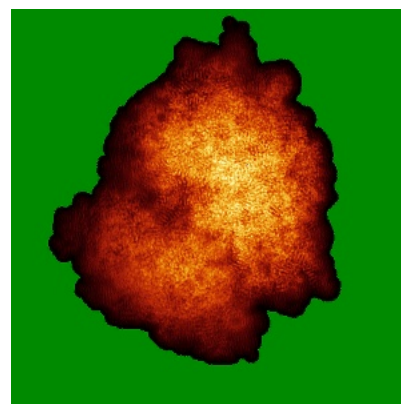
6.4.1 Primary map



X

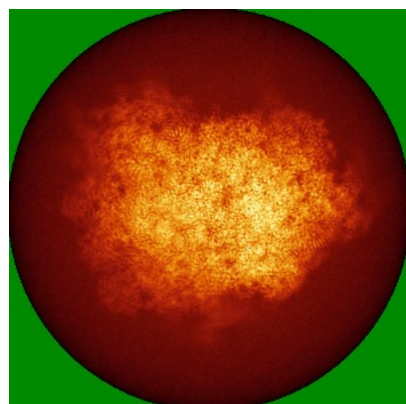


Y

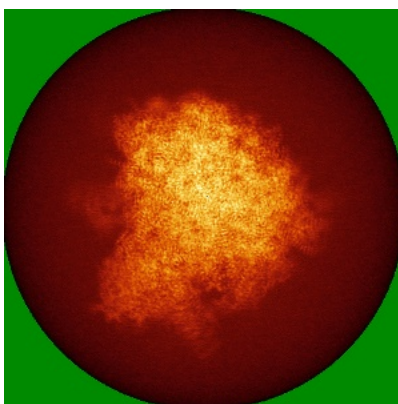


Z

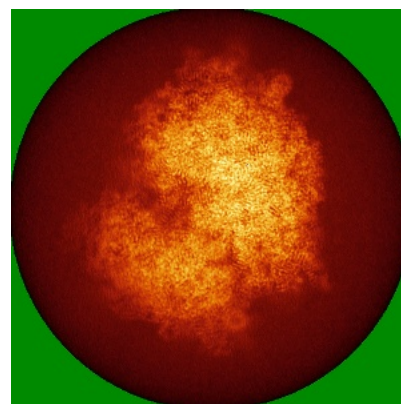
6.4.2 Raw map



X



Y

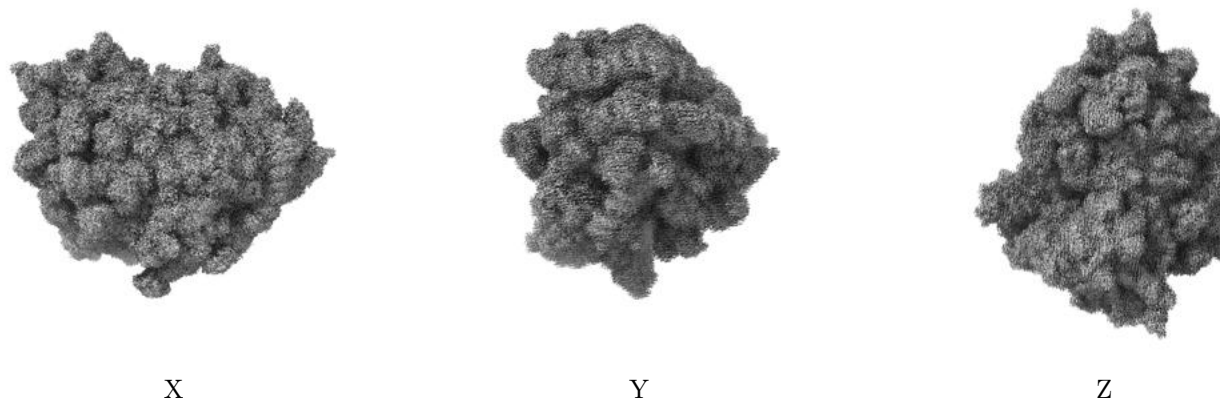


Z

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.

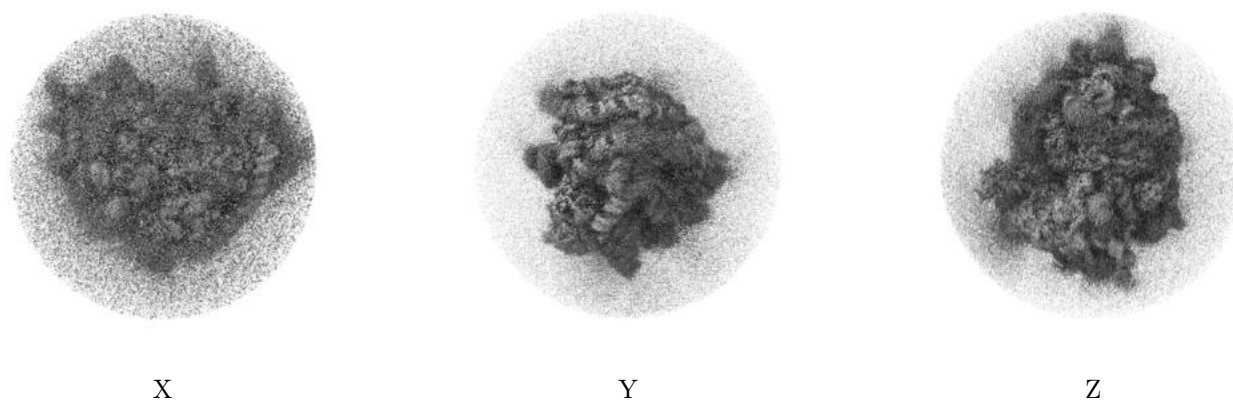
6.5 Orthogonal surface views [i](#)

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.

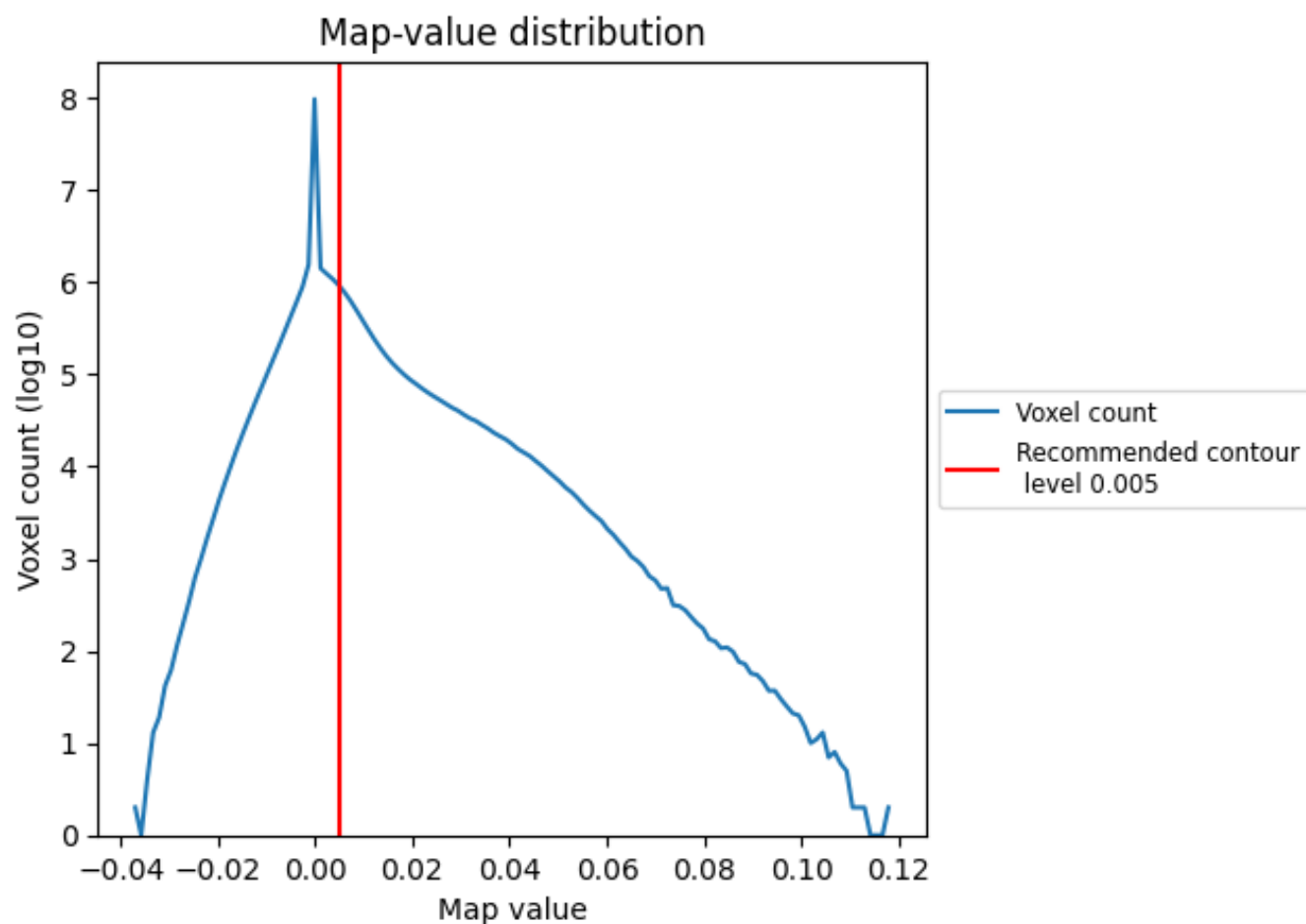
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

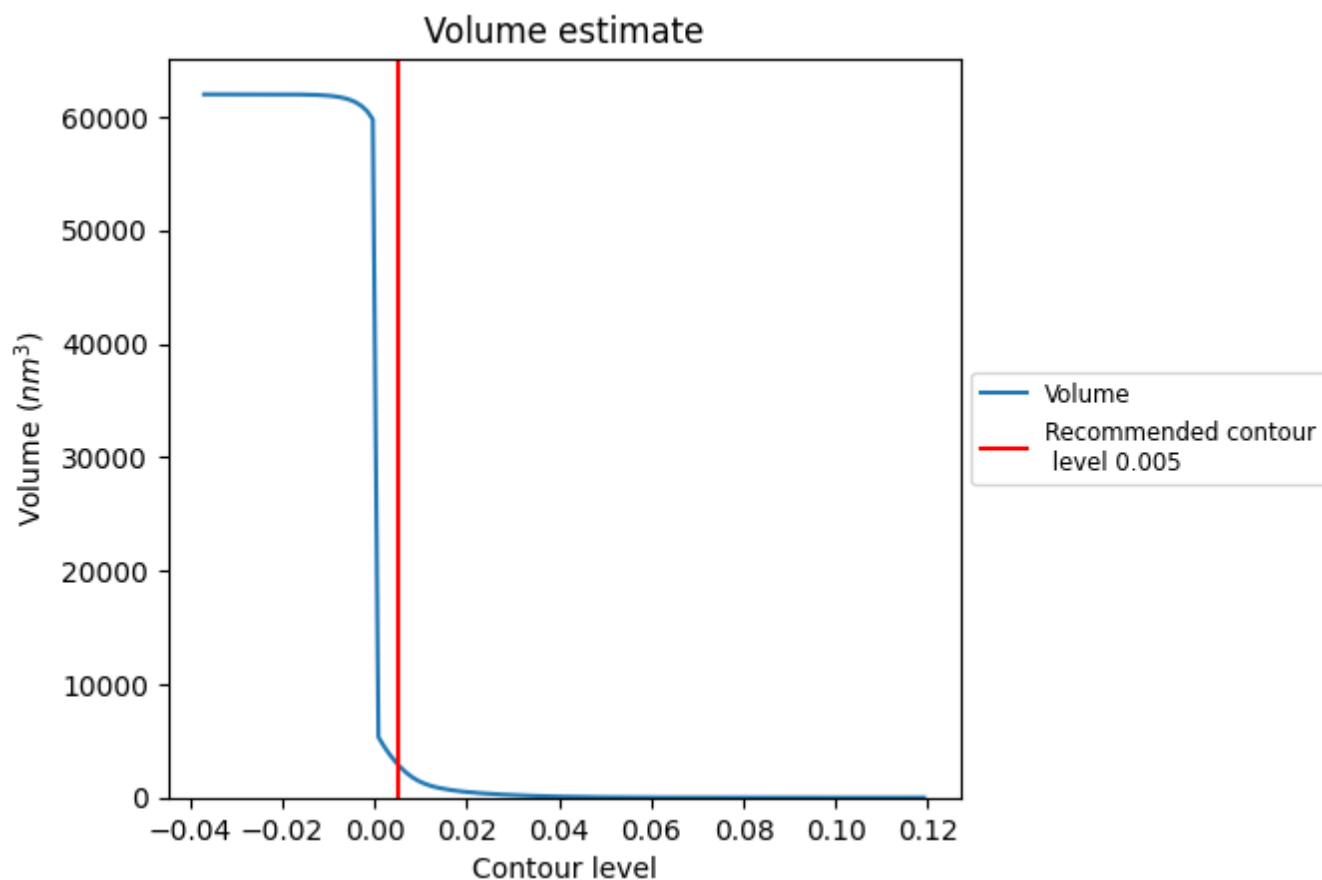
This section contains the results of statistical analysis of the map.

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.

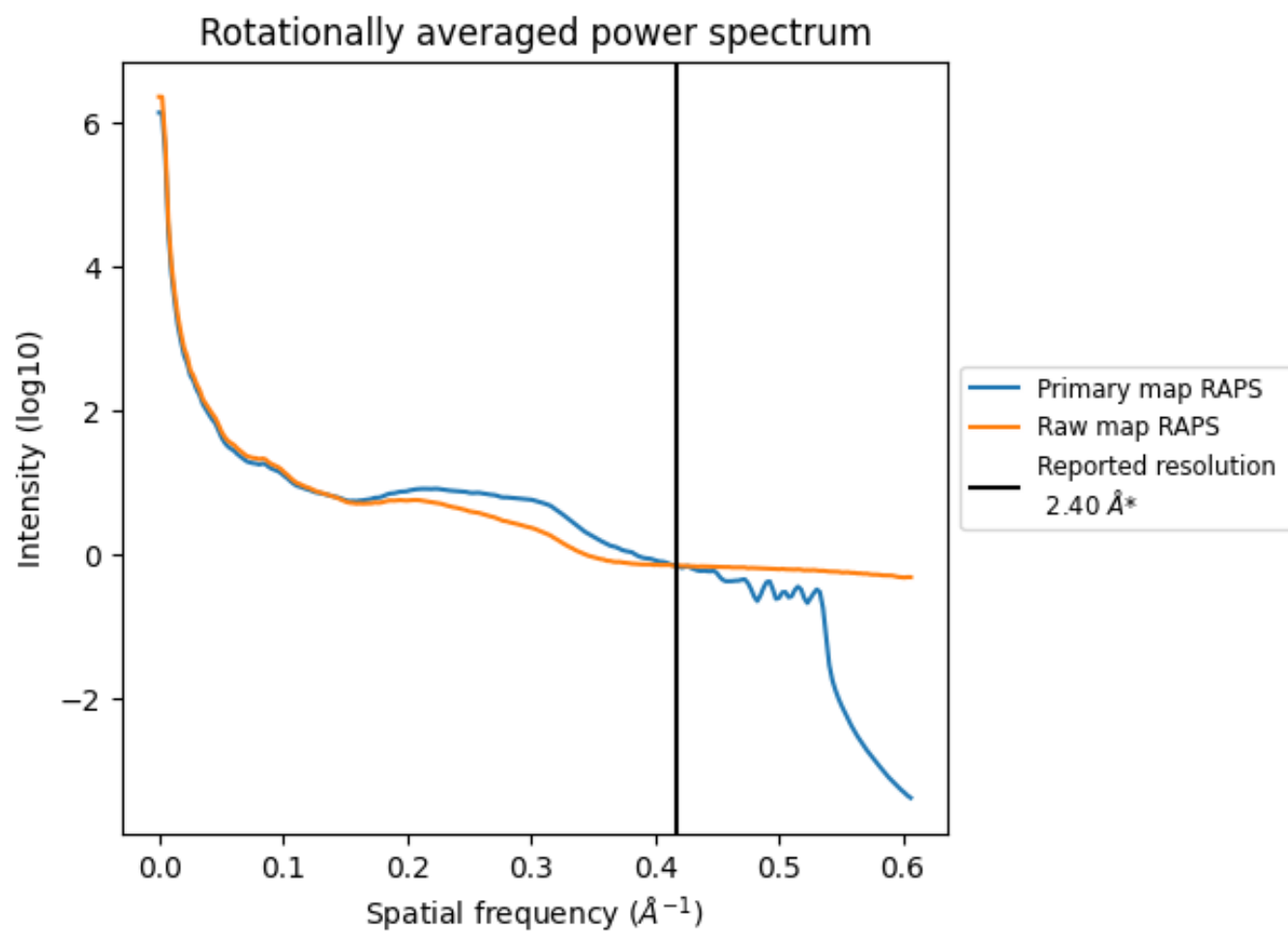
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2936 nm^3 ; this corresponds to an approximate mass of 2653 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 ⓘ

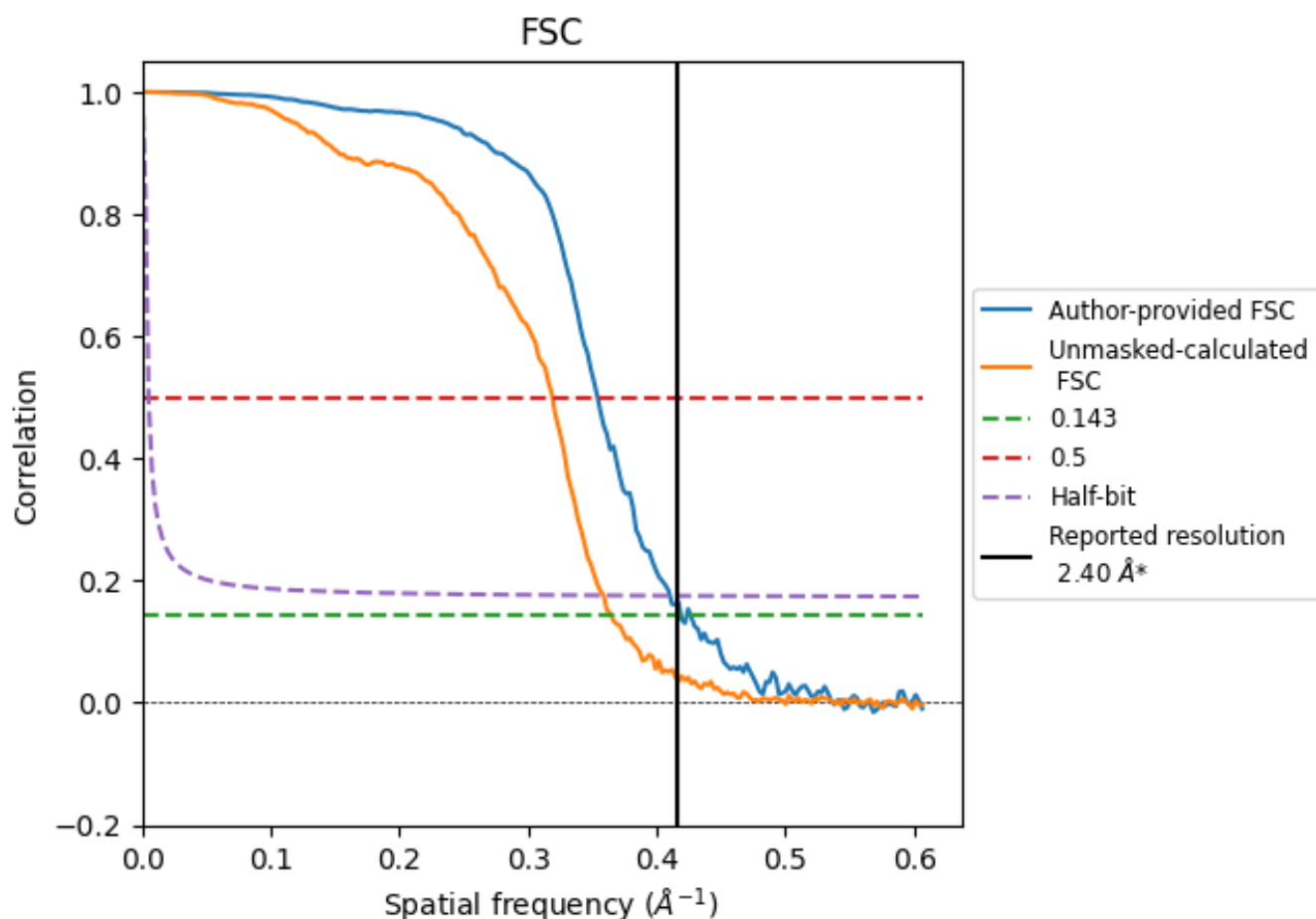


*Reported resolution corresponds to spatial frequency of $0.417 \text{ \AA}^{-1}$

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](#)

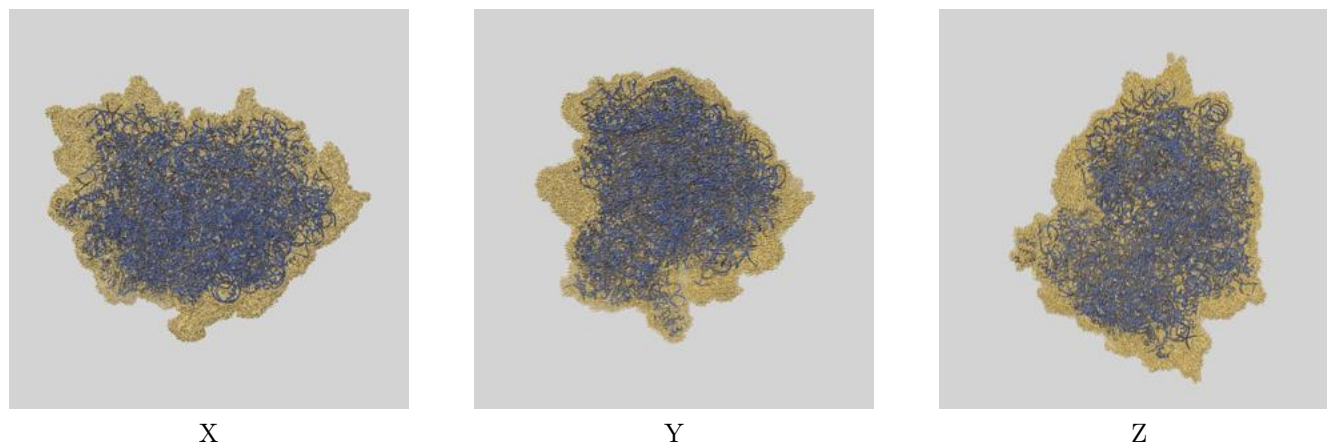
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.39	2.82	2.44
Unmasked-calculated*	2.74	3.14	2.79

*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 2.74 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

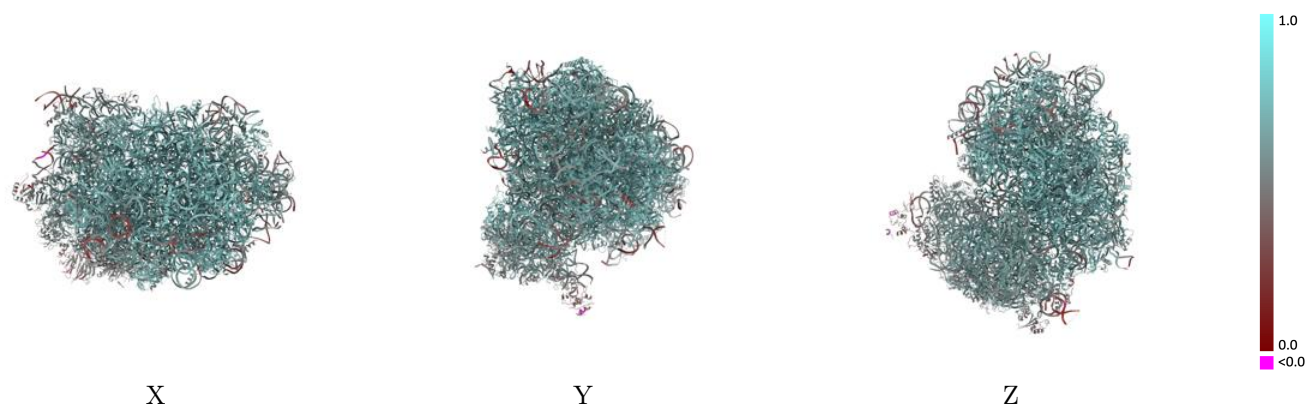
This section contains information regarding the fit between EMDB map EMD-55091 and PDB model 9SPI. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



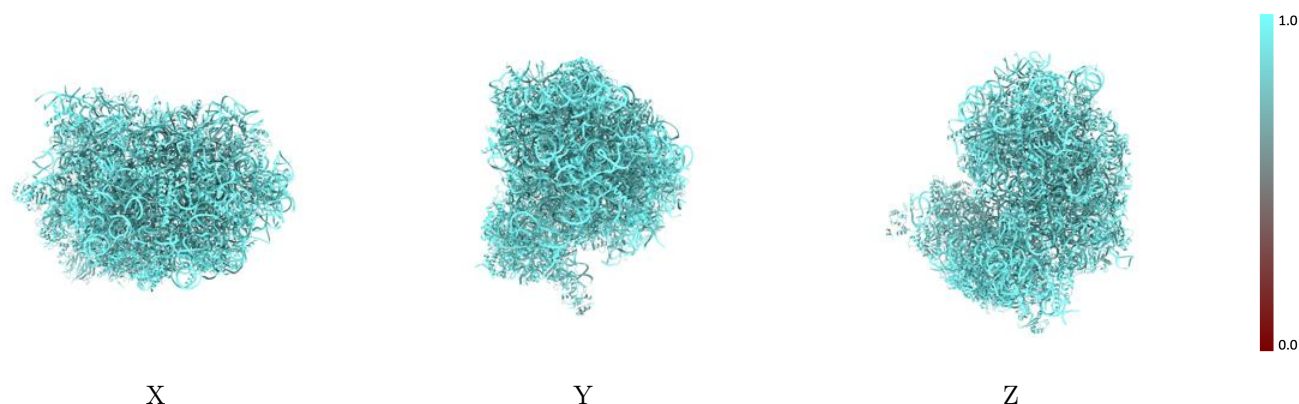
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



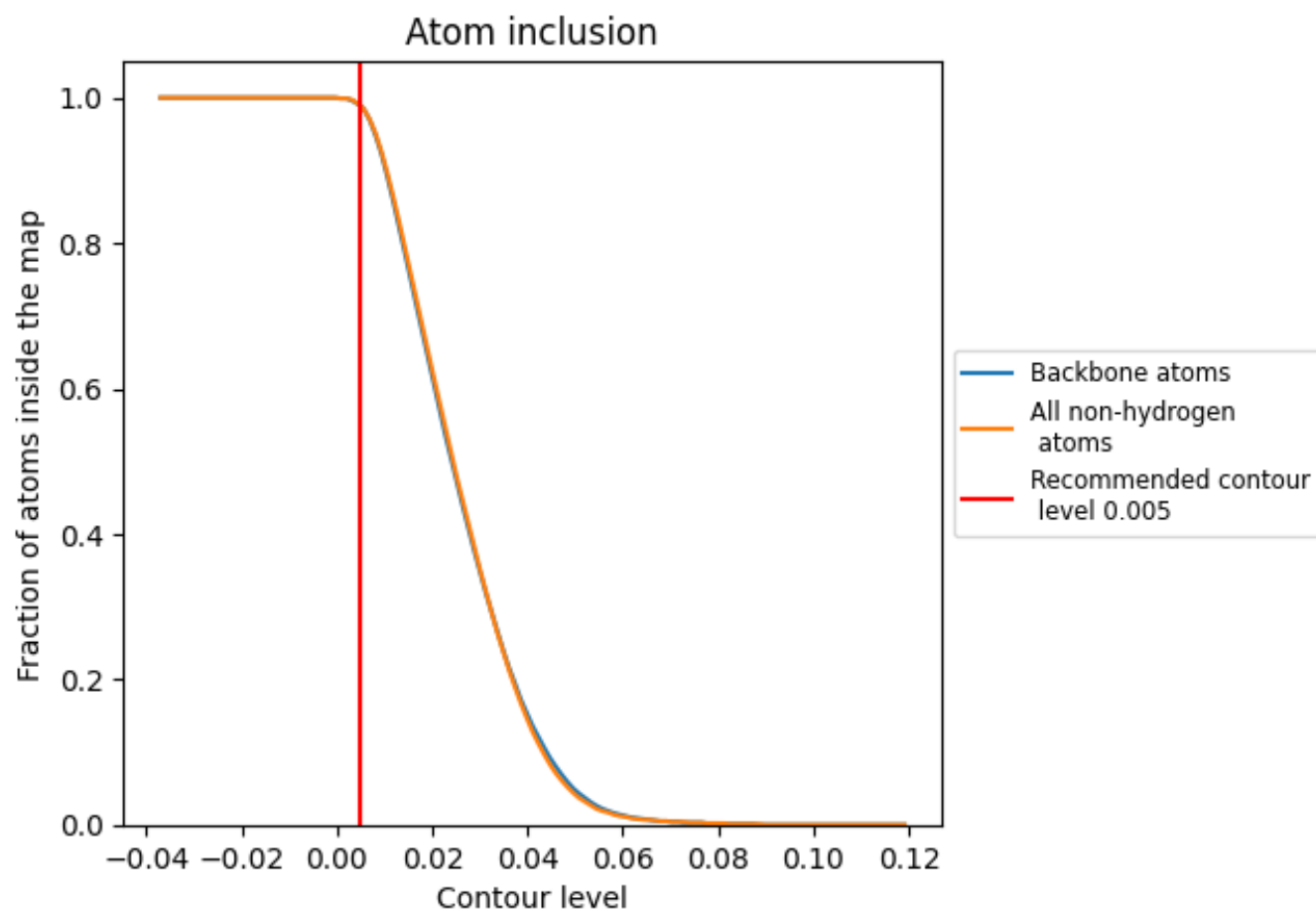
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9890	 0.6390
At	 0.9700	 0.4980
Et	 0.9620	 0.3690
L5	 0.9940	 0.6590
L7	 1.0000	 0.6730
L8	 0.9980	 0.6830
LA	 1.0000	 0.7340
LB	 0.9970	 0.7180
LC	 0.9960	 0.7120
LD	 0.9920	 0.6570
LE	 0.9940	 0.6590
LF	 0.9940	 0.7170
LG	 0.9890	 0.6570
LH	 0.9950	 0.6800
LI	 0.9960	 0.6920
LJ	 0.9880	 0.5980
LL	 0.9910	 0.6880
LM	 0.9990	 0.6930
LN	 0.9990	 0.7370
LO	 0.9940	 0.7160
LP	 0.9980	 0.7210
LQ	 0.9990	 0.7320
LR	 0.9900	 0.6780
LS	 0.9990	 0.7160
LT	 0.9920	 0.6790
LU	 0.9810	 0.6060
LV	 0.9990	 0.7180
LW	 0.9980	 0.6970
LX	 0.9950	 0.6960
LY	 0.9960	 0.6950
LZ	 0.9980	 0.6760
La	 0.9960	 0.7280
Lb	 0.9900	 0.6500
Lc	 0.9930	 0.6750
Ld	 0.9870	 0.6930



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Chain	Atom inclusion	Q-score
Le	 0.9980	 0.7290
Lf	 0.9990	 0.7320
Lg	 0.9870	 0.6990
Lh	 0.9960	 0.6830
Li	 0.9950	 0.6740
Lj	 1.0000	 0.7350
Lk	 0.9850	 0.6320
Ll	 1.0000	 0.7100
Lm	 0.9980	 0.6990
Ln	 0.9950	 0.6920
Lo	 0.9990	 0.7060
Lp	 0.9960	 0.7120
Lr	 0.9990	 0.7040
Mr	 0.9930	 0.6510
Pt	 0.9790	 0.5270
S2	 0.9940	 0.6130
SA	 0.9730	 0.5510
SB	 0.9620	 0.5170
SC	 0.9860	 0.6320
SD	 0.9670	 0.5520
SE	 0.9940	 0.6000
SF	 0.9810	 0.5560
SG	 0.9770	 0.5610
SH	 0.9540	 0.5010
SI	 0.9810	 0.6150
SJ	 0.9890	 0.6060
SK	 0.9570	 0.5110
SL	 0.9860	 0.6530
SM	 0.7680	 0.3500
SN	 0.9830	 0.6040
SO	 0.9730	 0.5380
SP	 0.9720	 0.5440
SQ	 0.9860	 0.5650
SR	 0.9590	 0.5180
SS	 0.9760	 0.5580
ST	 0.9770	 0.5500
SU	 0.9540	 0.5210
SV	 0.9810	 0.5790
SW	 0.9910	 0.6460
SX	 0.9970	 0.6840
SY	 0.9810	 0.5640
SZ	 0.9460	 0.5070

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Chain	Atom inclusion	Q-score
Sa	 0.9840	 0.6080
Sb	 0.9760	 0.5400
Sc	 0.9600	 0.5290
Sd	 0.9840	 0.6080
Se	 0.9830	 0.5910
Sf	 0.8770	 0.3860
Sg	 0.9230	 0.4070