



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:22 AM UTC

PDB ID : 9FQZ / pdb_00009fqz
EMDB ID : EMD-50673
Title : CRYO-EM STRUCTURE OF HCT15 POLYSOMES BOUND TO EEF2, EBP1, AND SERBP1
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2024-06-17
Resolution : 2.85 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:

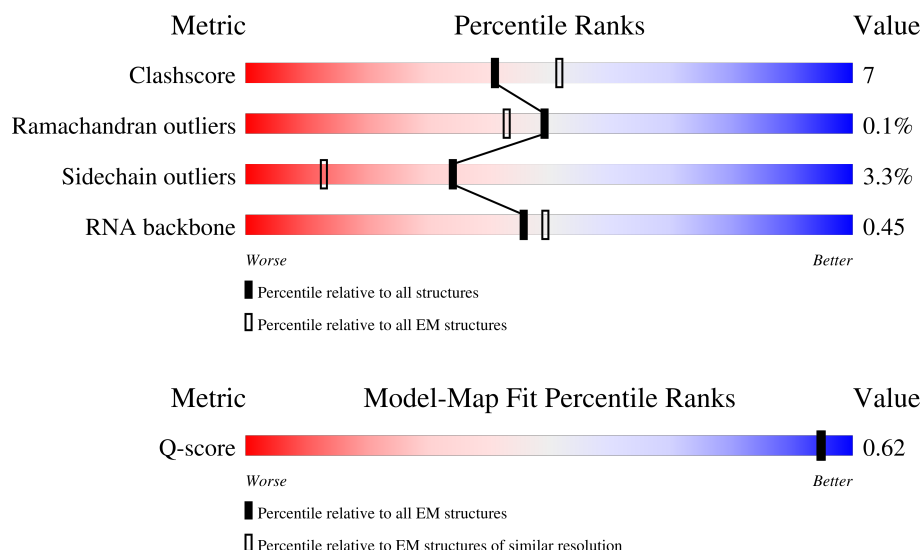
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.85 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.











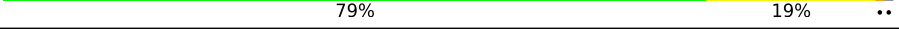

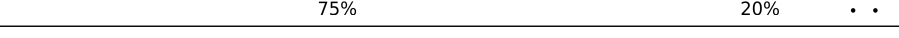
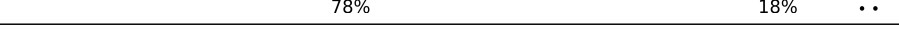

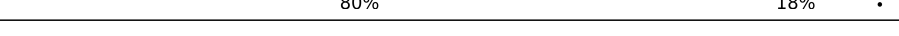


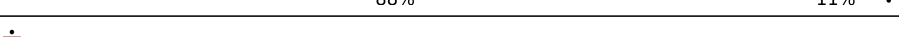

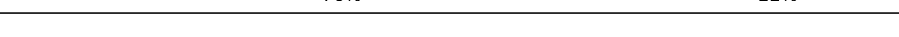






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	CB	858	
2	CC	85	
3	CD	402	


























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Mol	Chain	Length	Quality of chain
4	L8	156	
5	LA	257	
6	LB	403	
7	LC	427	
8	LD	297	
9	LE	288	
10	LF	248	
11	LG	266	
12	LH	192	
13	LI	214	
14	LJ	178	
15	LL	211	
16	LM	215	
17	LN	204	
18	LO	203	
19	LP	184	
20	LQ	188	
21	LR	196	
22	LS	176	
23	LT	160	
24	LU	128	
25	LV	140	
26	LW	157	
27	LX	156	
28	LY	145	





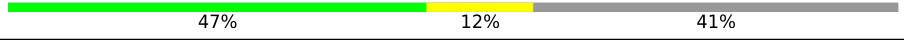

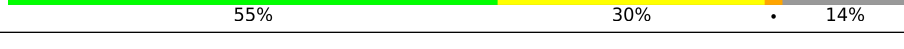
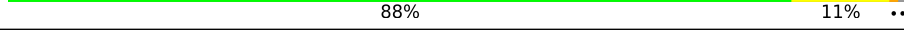
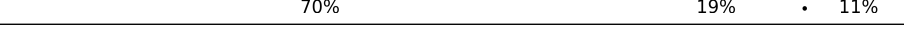
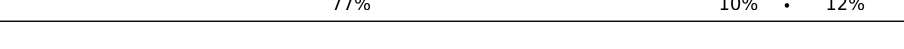
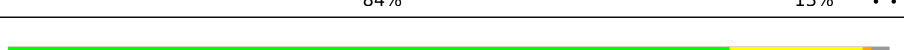

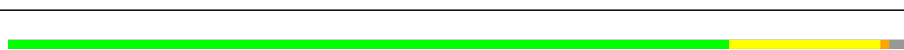

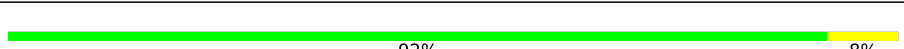



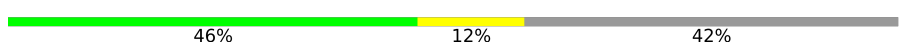

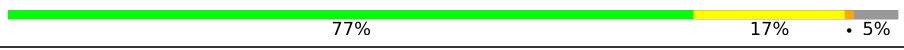
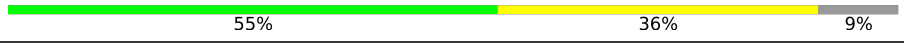



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Mol	Chain	Length	Quality of chain
29	LZ	136	
30	La	148	
31	Lb	159	
32	Lc	115	
33	Ld	125	
34	Le	135	
35	Lf	110	
36	Lg	117	
37	Lh	123	
38	Li	105	
39	Lj	97	
40	Lk	70	
41	Ll	51	
42	Lm	128	
43	Ln	25	
44	Lo	106	
45	Lp	92	
46	Lr	137	
47	S2	1871	
48	SA	295	
49	SB	264	
50	SC	293	
51	SD	243	
52	SE	263	
53	SF	204	

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

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Mol	Chain	Length	Quality of chain
79	Sf	156	
80	Sg	317	
81	L5	5069	
82	L7	120	
83	Lq	317	
84	CA	394	

2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 216008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CB	819	Total	C	N	O	S	0	0
			6379	4059	1091	1186	43		

- Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CC	22	Total	C	N	O	P	0	0
			470	210	84	154	22		

- Molecule 3 is a protein called Isoform 2 of SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CD	72	Total	C	N	O	S	0	0
			585	352	114	118	1		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L8	155	Total	C	N	O	P	0	0
			3296	1473	583	1086	154		

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LA	247	Total	C	N	O	S	1	0
			1896	1188	389	313	6		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LB	399	Total	C	N	O	S	0	0
			3220	2050	605	551	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	364	Total	C	N	O	S	0	0
			2895	1822	578	480	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD	292	Total	C	N	O	S	0	0
			2375	1501	434	426	14		

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	225	Total	C	N	O	S	0	0
			1800	1159	342	295	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LF	225	Total	C	N	O	S	1	0
			1880	1208	362	301	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	227	Total	C	N	O	S	0	0
			1838	1173	354	307	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	203	Total	C	N	O	S	0	0
			1642	1042	315	270	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	49	CYS	GLY	conflict	UNP Q96L21

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	170	Total	C	N	O	S	0	0
			1367	864	254	243	6		

- Molecule 15 is a protein called 60S ribosomal protein L13.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	137	Total	C	N	O	S	0	0
			1125	722	216	180	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	201	Total	C	N	O	S	0	0
			1649	1063	321	260	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LP	158	Total	C	N	O	S	0	0
			1282	803	248	222	9		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LS	175	Total	C	N	O	S	0	0
			1452	925	283	234	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	158	Total	C	N	O	S	0	0
			1292	820	251	215	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	100	Total	C	N	O	S	0	0
			817	523	143	149	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LW	113	Total	C	N	O	S	1	0
			935	586	192	152	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LX	120	Total	C	N	O	S	1	0
			994	636	188	169	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		

- Molecule 30 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	La	147	Total	C	N	O	S	0	0
			1161	736	237	185	3		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lb	105	Total	C	N	O	S	0	0
			853	529	187	133	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lc	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lf	110	Total	C	N	O	S	0	0
			881	558	175	145	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lg	113	Total	C	N	O	S	0	0
			897	560	185	146	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Li	102	Total	C	N	O	S	1	0
			843	527	181	130	5		

- Molecule 39 is a protein called 60S ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lm	52	Total	C	N	O	S	0	0
			425	263	89	67	6		

- Molecule 43 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 44 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lo	104	Total	C	N	O	S	1	0
			861	539	177	139	6		

- Molecule 45 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lp	91	Total	C	N	O	S	0	0
			704	443	135	119	7		

- Molecule 46 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lr	126	Total	C	N	O	S	0	0
			1007	625	208	169	5		

- Molecule 47 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S2	1598	Total	C	N	O	P	0	0
			34174	15280	6142	11155	1597		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SA	215	Total	C	N	O	S	0	0
			1700	1080	298	314	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	226	Total	C	N	O	S	0	0
			1757	1120	316	314	7		

- Molecule 52 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SE	260	Total	C	N	O	S	0	0
			2065	1319	384	354	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	184	Total	C	N	O	S	0	0
			1463	915	276	265	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SG	235	Total	C	N	O	S	0	0
			1909	1191	385	326	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
55	SH	185	Total	C	N	O		
			1466	936	273	257	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	205	Total	C	N	O	S		
			1678	1053	330	290	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SJ	180	Total	C	N	O	S		
			1499	955	300	242	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SK	97	Total	C	N	O	S		
			816	533	144	133	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SL	145	Total	C	N	O	S		
			1189	759	223	201	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SM	113	Total	C	N	O	S		
			864	545	149	163	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SN	150	Total	C	N	O	S		
			1208	773	229	205	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SO	135	Total	C	N	O	S	0	0
			1007	617	198	186	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SP	128	Total	C	N	O	S	0	0
			1054	669	200	178	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SQ	142	Total	C	N	O	S	0	0
			1117	712	210	192	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	142	Total	C	N	O	S	0	0
			1103	691	212	197	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SW	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 71 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SX	141	Total	C	N	O	S	0	0
			1094	691	218	182	3		

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SY	123	Total	C	N	O	S	0	0
			1006	637	197	167	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sa	101	Total	C	N	O	S	1	0
			813	504	171	133	5		

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sb	80	Total	C	N	O	S	0	0
			634	398	118	112	6		

- Molecule 76 is a protein called 40S ribosomal protein S28.

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

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sd	55	Total	C	N	O	S	0	0
			454	285	94	72	3		

- Molecule 78 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Se	52	Total	C	N	O	S	0	0
			414	253	93	67	1		

- Molecule 79 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sf	65	Total	C	N	O	S	0	0
			528	333	100	89	6		

- Molecule 80 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sg	313	Total	C	N	O	S	0	0
			2434	1535	424	465	10		

- Molecule 81 is a RNA chain called LSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	L5	3475	Total	C	N	O	P	0	0
			74592	33254	13663	24201	3474		

- Molecule 82 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	L7	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

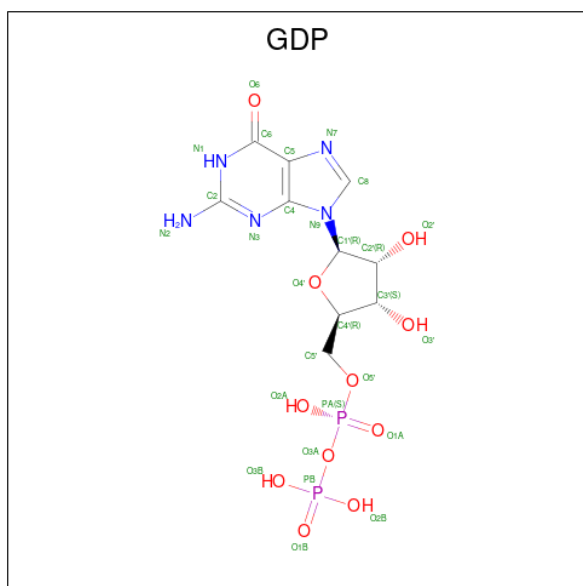
- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Lq	199	Total	C	N	O	S	0	0
			1529	973	266	281	9		

- Molecule 84 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CA	15	Total	C	N	O	S	1	0
			115	72	22	19	2		

- Molecule 85 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
85	CB	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

Mol	Chain	Residues	Atoms		AltConf
86	CB	1	Total	Mg	0
			1	1	
86	L8	2	Total	Mg	0
			2	2	
86	LB	1	Total	Mg	0
			1	1	
86	LC	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	LI	1	Total 1	Mg 1	0
86	Lg	1	Total 1	Mg 1	0
86	Lj	1	Total 1	Mg 1	0
86	S2	60	Total 60	Mg 60	0
86	SX	1	Total 1	Mg 1	0
86	Sd	1	Total 1	Mg 1	0
86	L5	198	Total 198	Mg 198	0
86	L7	3	Total 3	Mg 3	0

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

Mol	Chain	Residues	Atoms		AltConf
87	L8	3	Total 3	K 3	0
87	LA	1	Total 1	K 1	0
87	LI	1	Total 1	K 1	0
87	LN	1	Total 1	K 1	0
87	LP	1	Total 1	K 1	0
87	LV	1	Total 1	K 1	0
87	Le	1	Total 1	K 1	0
87	Lf	1	Total 1	K 1	0
87	S2	17	Total 17	K 17	0
87	Sa	1	Total 1	K 1	0
87	L5	74	Total 74	K 74	0

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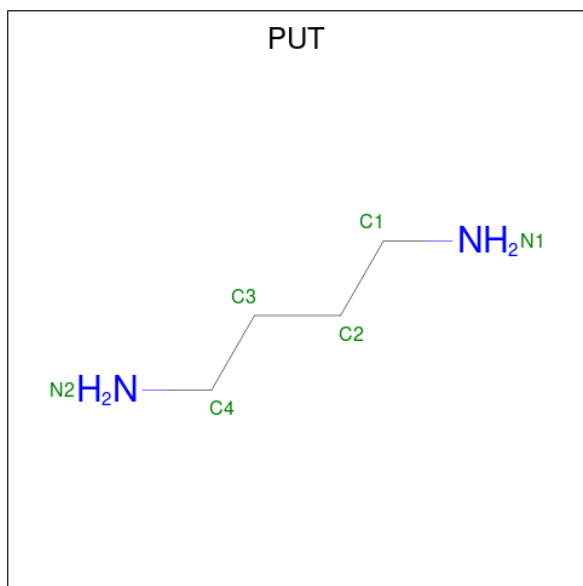
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Mol	Chain	Residues	Atoms		AltConf
87	L7	2	Total	K	0
			2	2	

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

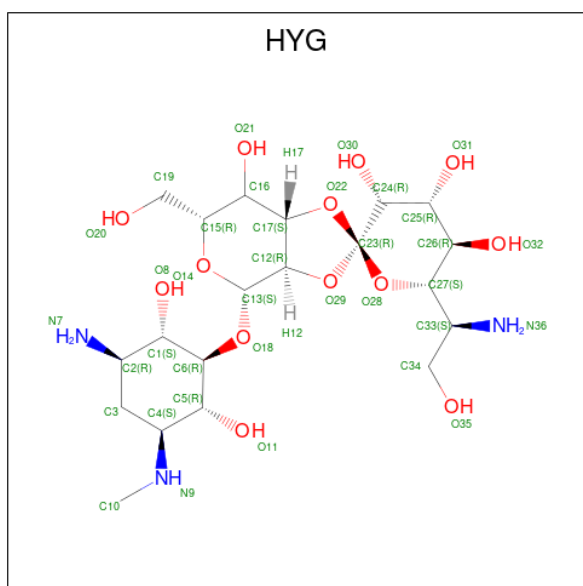
Mol	Chain	Residues	Atoms		AltConf
88	Lg	1	Total	Zn	0
			1	1	
88	Lj	1	Total	Zn	0
			1	1	
88	Lm	1	Total	Zn	0
			1	1	
88	Lo	1	Total	Zn	0
			1	1	
88	Lp	1	Total	Zn	0
			1	1	
88	Sa	1	Total	Zn	0
			1	1	
88	Sd	1	Total	Zn	0
			1	1	
88	Sf	1	Total	Zn	0
			1	1	

- Molecule 89 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



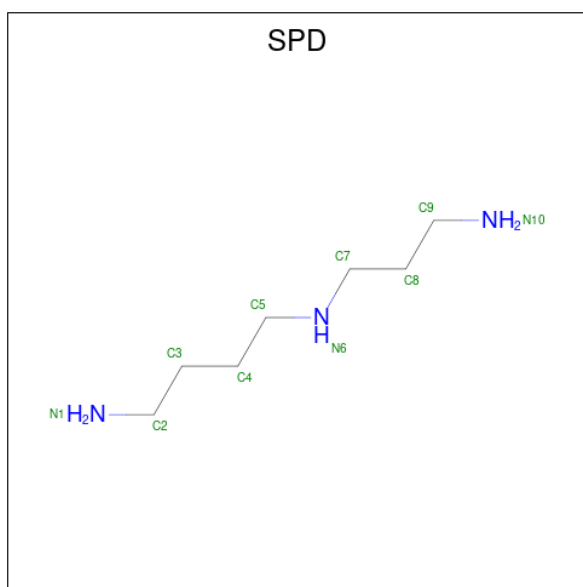
[illegible]

- Molecule 90 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



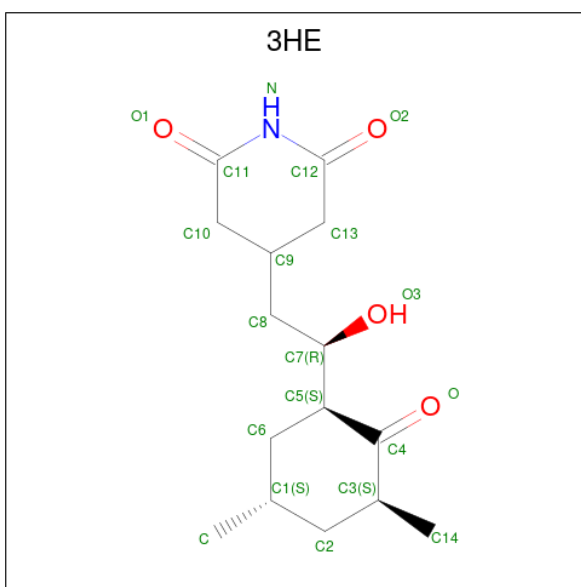
Mol	Chain	Residues	Atoms				AltConf
90	S2	1	Total	C	N	O	0
			36	20	3	13	

- Molecule 91 is SPERMIDINE (CCD ID: SPD) (formula: $\text{C}_7\text{H}_{19}\text{N}_3$).



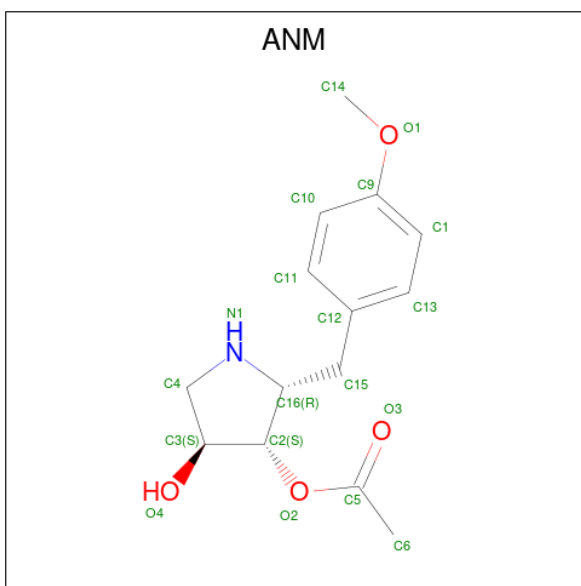
Mol	Chain	Residues	Atoms			AltConf
91	L5	1	Total	C	N	0
			10	7	3	
91	L5	1	Total	C	N	0
			10	7	3	
91	L5	1	Total	C	N	0
			10	7	3	
91	L5	1	Total	C	N	0
			10	7	3	
91	L5	1	Total	C	N	0
			10	7	3	
91	L5	1	Total	C	N	0
			10	7	3	
91	L5	1	Total	C	N	0
			10	7	3	

- Molecule 92 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄).



Mol	Chain	Residues	Atoms				AltConf
92	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 93 is ANISOMYCIN (CCD ID: ANM) (formula: $C_{14}H_{19}NO_4$).



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

- Molecule 94 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
94	L5	1	Total	Na	0
			1	1	

- Molecule 95 is water.

Mol	Chain	Residues	Atoms		AltConf
95	CB	1	Total	O	0
			1	1	
95	L8	7	Total	O	0
			7	7	
95	LA	6	Total	O	0
			6	6	
95	LB	5	Total	O	0
			5	5	
95	LC	4	Total	O	0
			4	4	
95	LF	2	Total	O	0
			2	2	
95	LH	1	Total	O	0
			1	1	
95	LN	3	Total	O	0
			3	3	
95	LO	1	Total	O	0
			1	1	
95	LP	2	Total	O	0
			2	2	
95	LQ	1	Total	O	0
			1	1	
95	LS	1	Total	O	0
			1	1	
95	LT	1	Total	O	0
			1	1	
95	LV	1	Total	O	0
			1	1	
95	La	2	Total	O	0
			2	2	
95	Lc	1	Total	O	0
			1	1	
95	Le	5	Total	O	0
			5	5	
95	Lf	2	Total	O	0
			2	2	
95	Lg	1	Total	O	0
			1	1	

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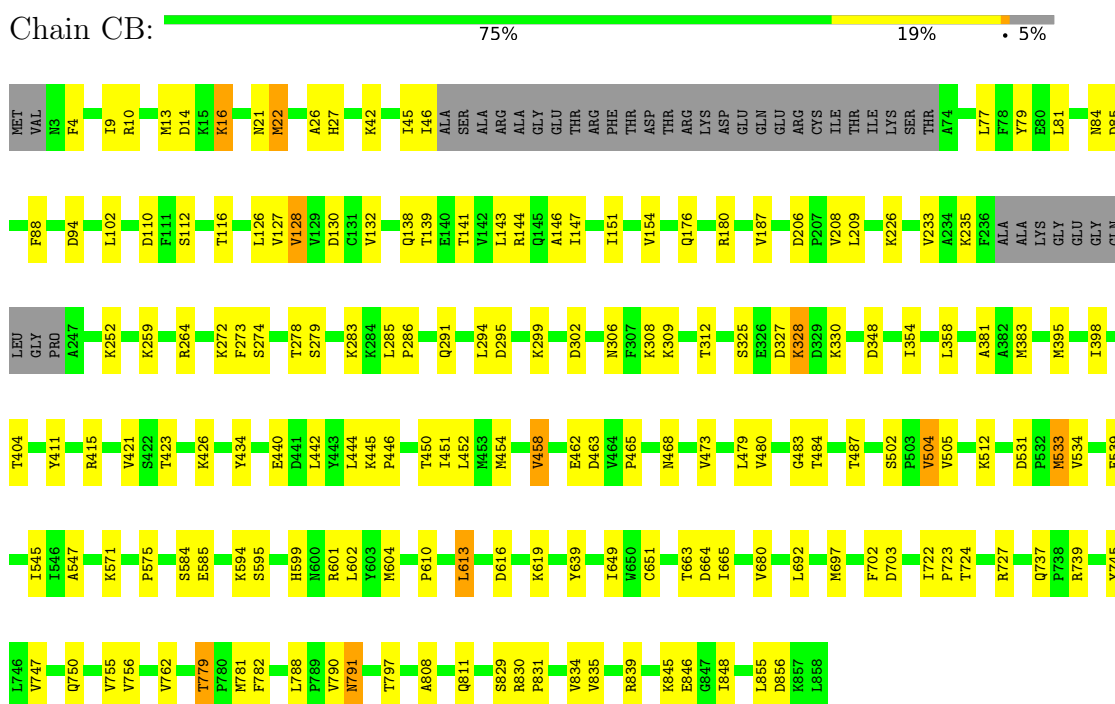
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Mol	Chain	Residues	Atoms		AltConf
95	Lj	1	Total 1	O 1	0
95	Lo	1	Total 1	O 1	0
95	Lp	3	Total 3	O 3	0
95	S2	78	Total 78	O 78	0
95	SF	1	Total 1	O 1	0
95	SL	1	Total 1	O 1	0
95	SN	1	Total 1	O 1	0
95	L5	263	Total 263	O 263	0
95	L7	2	Total 2	O 2	0

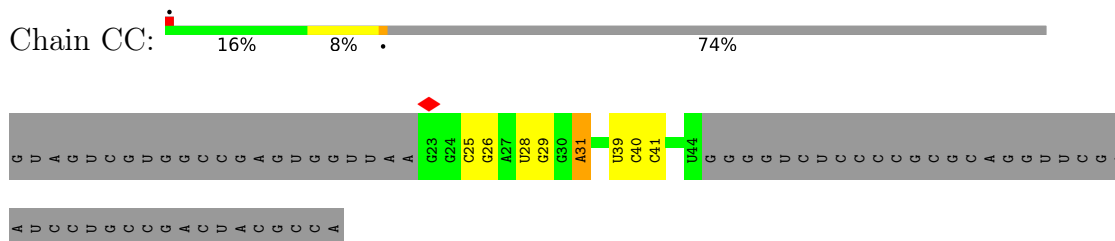
3 Residue-property plots

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

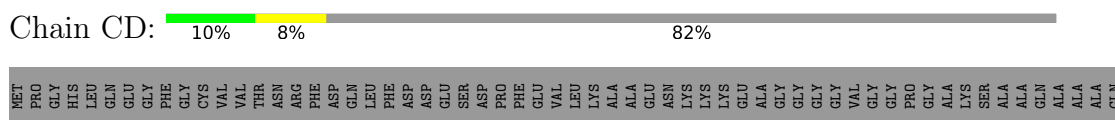
• Molecule 1: Elongation factor 2



• Molecule 2: tRNA

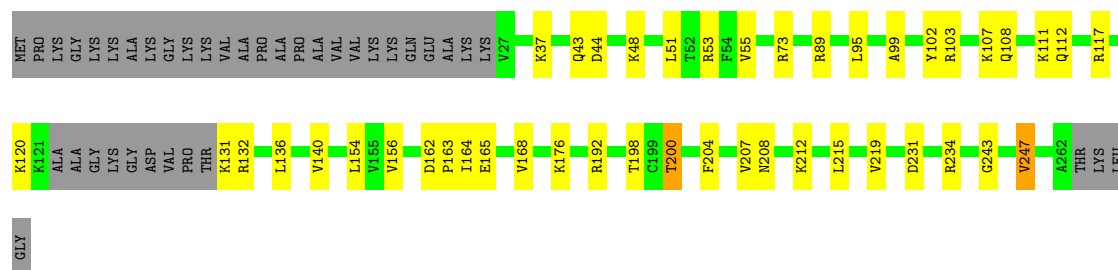


• Molecule 3: Isoform 2 of SERPINE1 mRNA-binding protein 1




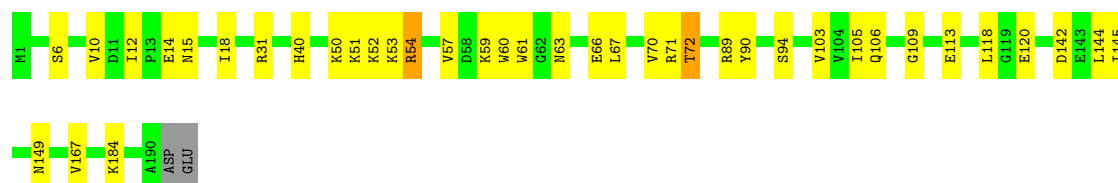
- Molecule 11: 60S ribosomal protein L7a

Chain LG:  69% 16% 15%



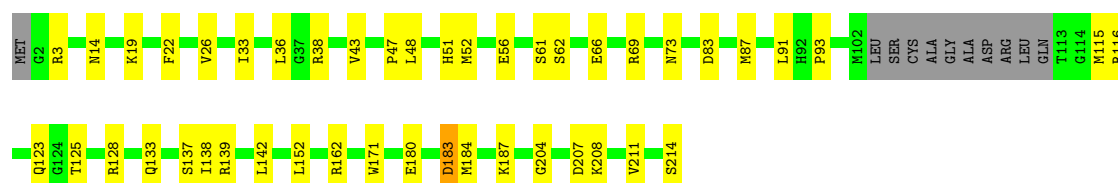
- Molecule 12: 60S ribosomal protein L9

Chain LH:  79% 19% ..




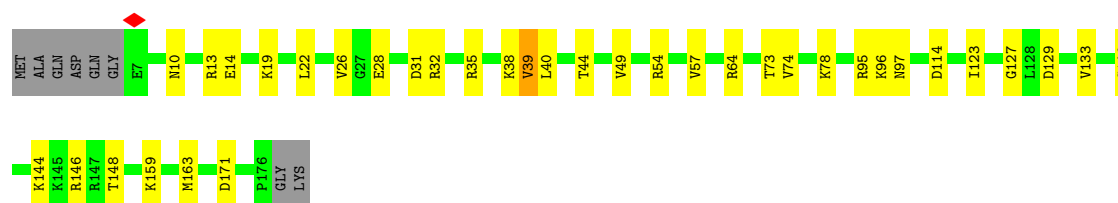
- Molecule 13: 60S ribosomal protein L10-like

Chain LI:  74% 21% 5%




- Molecule 14: 60S ribosomal protein L11

Chain LJ:  75% 20% ..



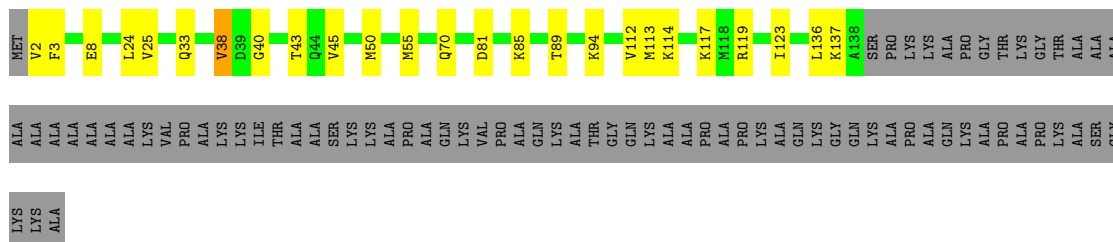
- Molecule 15: 60S ribosomal protein L13

Chain LL:  78% 18% ..

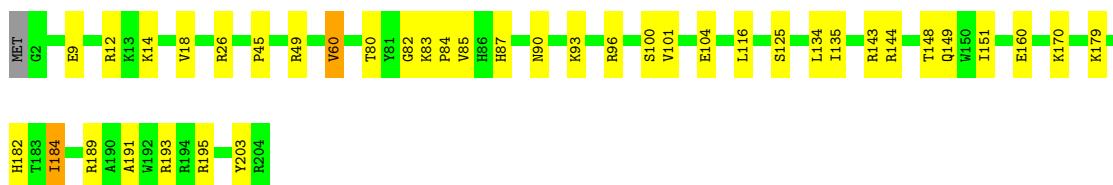
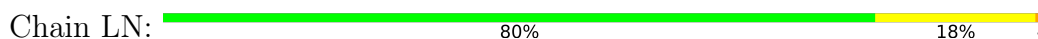




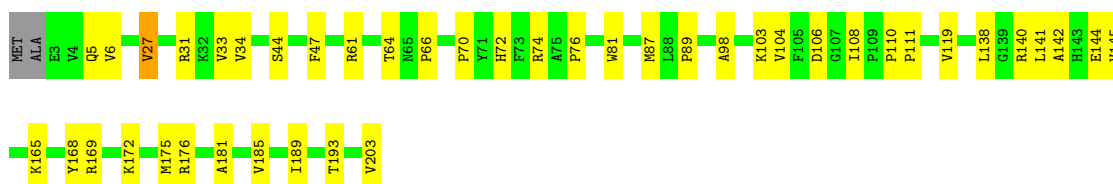
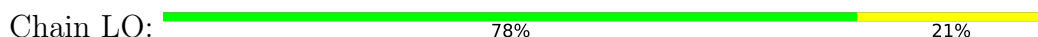
- Molecule 16: 60S ribosomal protein L14



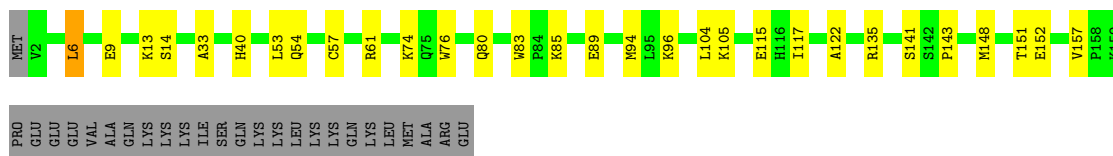
- Molecule 17: 60S ribosomal protein L15



- Molecule 18: 60S ribosomal protein L13a



- Molecule 19: 60S ribosomal protein L17

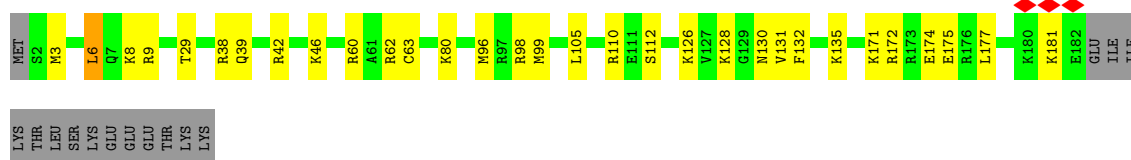
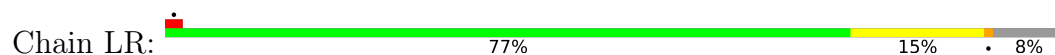


- Molecule 20: 60S ribosomal protein L18

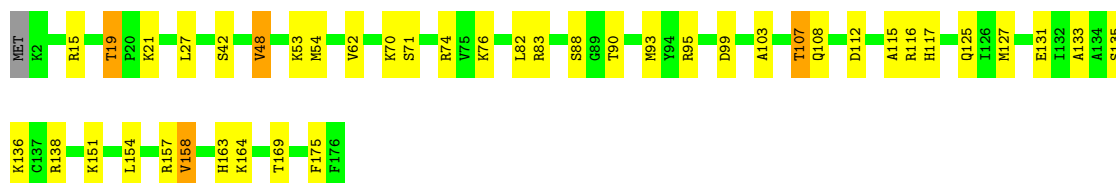
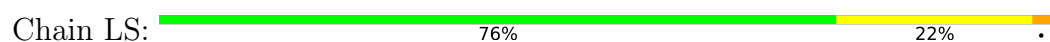




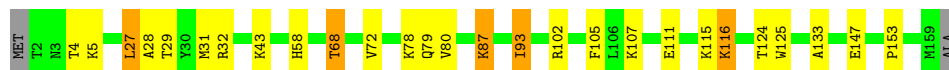
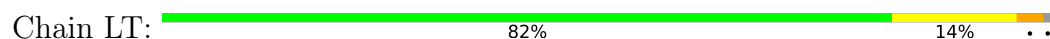
- Molecule 21: 60S ribosomal protein L19



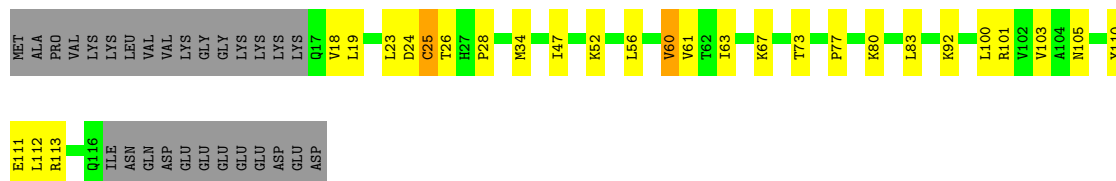
- Molecule 22: 60S ribosomal protein L18a



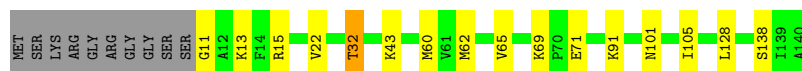
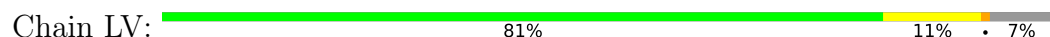
- Molecule 23: 60S ribosomal protein L21



- Molecule 24: 60S ribosomal protein L22

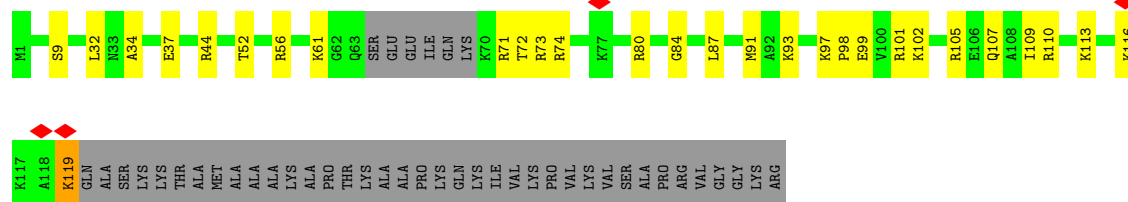


- Molecule 25: 60S ribosomal protein L23



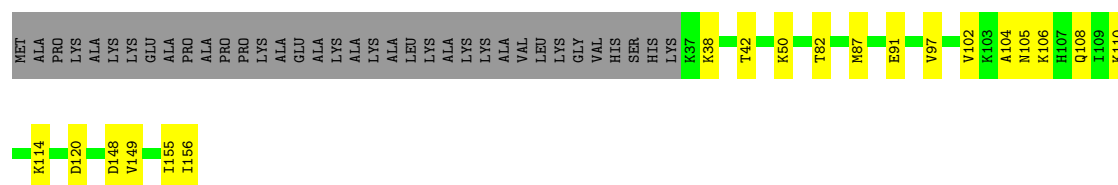
- Molecule 26: 60S ribosomal protein L24

Chain LW: 



- Molecule 27: 60S ribosomal protein L23a

Chain LX: 




- Molecule 28: 60S ribosomal protein L26

Chain LY: 




- Molecule 29: 60S ribosomal protein L27

Chain LZ: 



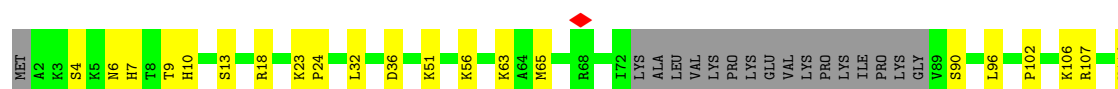
- Molecule 30: 60S ribosomal protein L27a

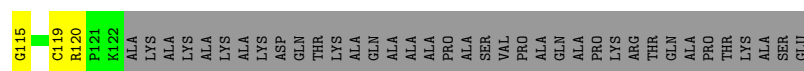
Chain La: 



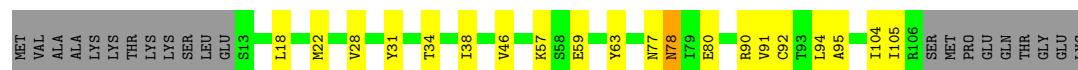
- Molecule 31: 60S ribosomal protein L29

Chain Lb: 

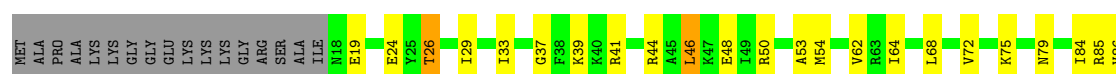




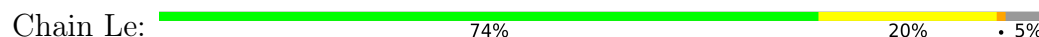
- Molecule 32: 60S ribosomal protein L30



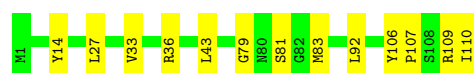
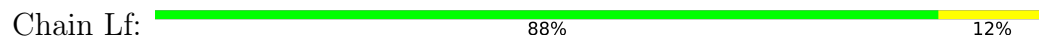
- Molecule 33: 60S ribosomal protein L31



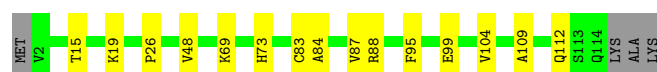
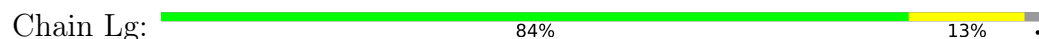
- Molecule 34: 60S ribosomal protein L32



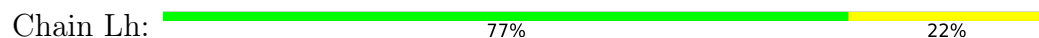
- Molecule 35: 60S ribosomal protein L35a




- Molecule 36: 60S ribosomal protein L34



- Molecule 37: 60S ribosomal protein L35




- Molecule 38: 60S ribosomal protein L36

Chain Li:  82% 15% .



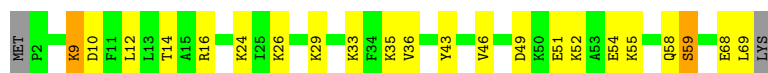
- Molecule 39: 60S ribosomal protein L37

Chain Lj:  74% 14% 11%




- Molecule 40: 60S ribosomal protein L38

Chain Lk:  66% 29% . .




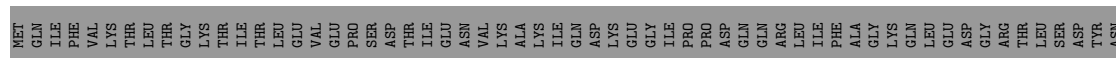
- Molecule 41: 60S ribosomal protein L39

Chain Ll:  86% 12% .




- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain Lm:  32% 9% 59%




- Molecule 43: 60S ribosomal protein L41

Chain Ln:  76% 20% .



- Molecule 44: 60S ribosomal protein L36a

Chain Lo:  84% 13% . .



- C C G C G C G C G C G A G C G C G A G C C C C C C C C C C C C C C D D U D U D C C746
C748

G1846	C	C1363	G1280	A1195	G1089	A998	A913	G	U
G1849	C	U1364	G1281	U1201	C1090	G999	A918	C	C
A1850	A	G1365	A1282	U1202	A1093	A1000	U918	C	U
A1851	C	G1366	C1283	A1204	C1094	A1001	G841	G	U
C1852	C	U1371	G1286	A1208	C1098	G1005	G842	C	A
G1857	C	U1372	A1287	A1209	G1099	C1006	U844	C	G
G1858	C	C1373	U1288	C1213	G1102	C1007	A920	C	U
A1859	C	C1374	U1289	U1201	G1109	A1008	G925	C	U
A1860	U	G1375	G1290	C1214	G1102	A1009	G928	C	G
G1861	G	A1376	A1291	C1215	G1109	G1010	G929	C	A
G1862	C	U1377	C1292	C1216	C1109	A1011	G850	C	G
A1863	C	A1378	A1293	A1217	U1115	A1012	C853	C	U
G1864	C	G1447	G1294	C1218	C1116	A1013	A854	C	U
A1865	G	A1448	A1295	G1224	C1117	U1016	U857	C	C
A1866	A	U1382	A1301	G1227	C1118	U1017	G860	C	C
U1867	C	A1383	G1302	A1228	G1121	U1018	U940	C	G
B8N1870	C	A1388	C1303	G1229	A1122	C1019	G942	C	G
A1871	C	C1389	U1304	C1230	C1123	A1020	U943	C	G
		C1391	C1305	C1231	C1124	U1021	A869	C	G
		C1395	U1308	U1232	G1129	A1022	A870	C	G
		A1396	C1309	G1233	A1133	A1023	A871	C	G
		U1387	G1312	U1238	C1135	U1024	A872	C	C
		U1462	A1313	U1242	C1138	A1031	A873	C	C
		U1463	U1314	U1243	C1139	G1037	G874	C	G
		C1471	U1315	U1244	C1140	U1038	A875	C	A
		G1473	C1316	U1245	A1144	U1039	G878	C	A
		A1474	G1320	A1246	A1145	G1044	C879	C	A
		G1475	G1321	G	A1146	U1045	G880	C	C
		U1476	G1322	A1247	C1147	A1046	G881	C	G
		U1477	A1405	A1247	A1148	G1047	U882	C	U799
		A1480	G1406	G	C1153	G1048	C883	C	U800
		A1486	U1407	A1249	U1154	A1056	U884	C	U801
		A1487	U1408	A1250	U1155	A1060	U	C	U804
		A1488	C1412	A1251	U1156	U1061	U	C	U805
		A1489	C1415	C1252	U1157	A1062	U	C	U806
		G1490	C1416	A1253	U1158	U1063	U	C	U807
		U1494	C1417	A1258	G1164	A1064	U	C	A808
		G1495	C	A1259	G1165	U1065	U	C	A809
		U1496	C	A1260	U1174	U1066	U	C	A810
		G1497	C	U1263	G1175	G1067	U	C	A811
		A1498	A	C1264	U1176	U1068	U	C	U815
		U1499	C	G1270	U1177	A1069	U	C	A816
		G1500	C	C1271	U1178	A1070	U	C	G821
		C1501	G1424	U1272	U1179	A1071	U	C	U822
		U1508	G1425	C1273	A1182	A1080	U	C	U823
		U1509	U1426	G1274	A1183	G991	U	C	C824
		A1508	U1509	G1275	U1189	A1083	A	C	A830
		A1509	G1510	A1276	A1190	A1084	C905	C	C833
		C1512	U1511	C1277	A1194	C1085	U906	C	C834
		U1594	C	A1278		U1088	G907	C	C
				C1279			G908	C	A
							G909	C	A

• Molecule 48: 40S ribosomal protein SA

Chain SA:  58% 15% 27%



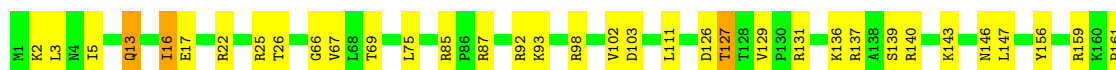
- Molecule 53: 40S ribosomal protein S5

Chain SF: 70% 20% 10%



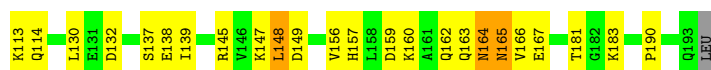
- Molecule 54: 40S ribosomal protein S6

Chain SG: 74% 19% 6%



- Molecule 55: 40S ribosomal protein S7

Chain SH: 69% 25% 5%



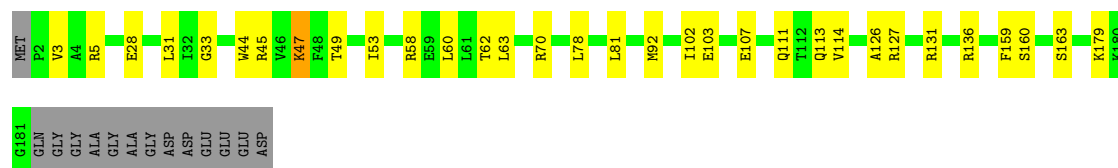
- Molecule 56: 40S ribosomal protein S8

Chain SI: 75% 23% 2%

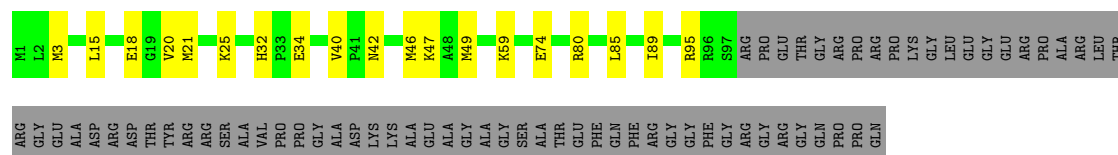


- Molecule 57: 40S ribosomal protein S9

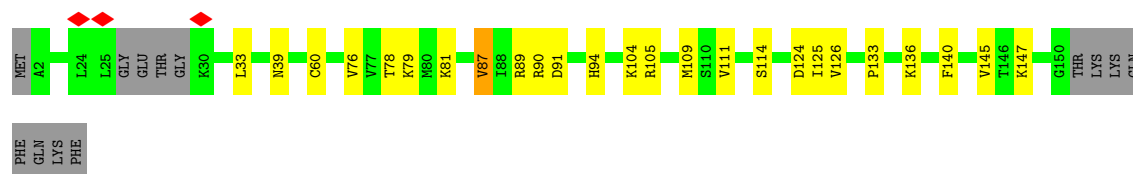
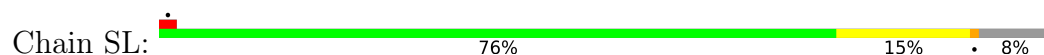
Chain SJ: 76% 16% 7%



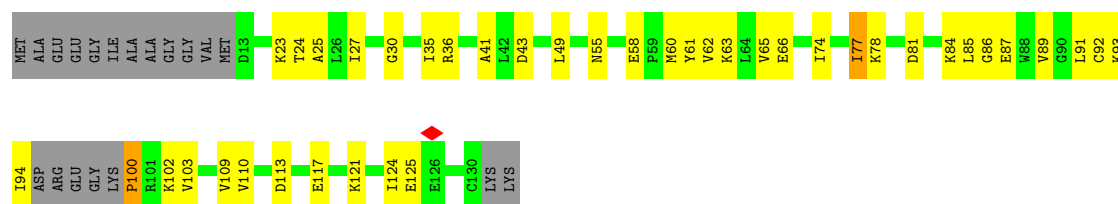
- Molecule 58: 40S ribosomal protein S10



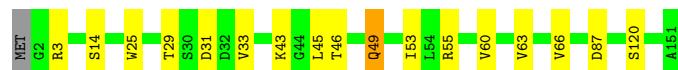
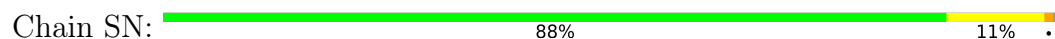
- Molecule 59: 40S ribosomal protein S11



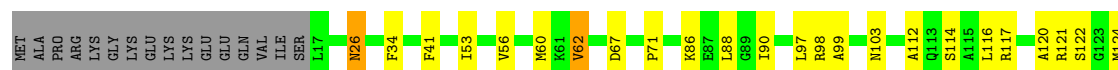
- Molecule 60: 40S ribosomal protein S12

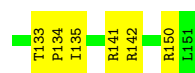


- Molecule 61: 40S ribosomal protein S13



- Molecule 62: 40S ribosomal protein S14





- Molecule 63: 40S ribosomal protein S15

Chain SP: 77% 10% 12%



- Molecule 64: 40S ribosomal protein S16

Chain SQ: 84% 13% 3%



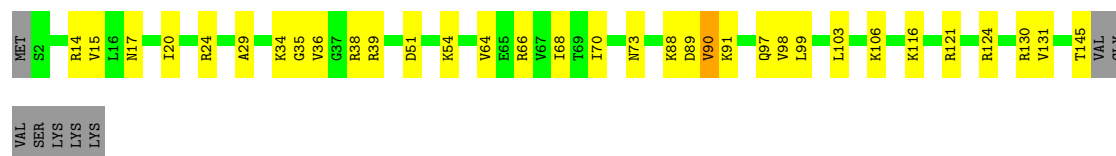
- Molecule 65: 40S ribosomal protein S17

Chain SR: 81% 15% 4%



- Molecule 66: 40S ribosomal protein S18

Chain SS: 73% 21% 6%



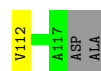
- Molecule 67: 40S ribosomal protein S19

Chain ST: 81% 17% 2%




- Molecule 68: 40S ribosomal protein S20

Chain SU: 62% 22% 16%



- Molecule 75: 40S ribosomal protein S27

Chain Sb:  77% 17% 5%




- Molecule 76: 40S ribosomal protein S28

Chain Sc:  55% 36% 9%



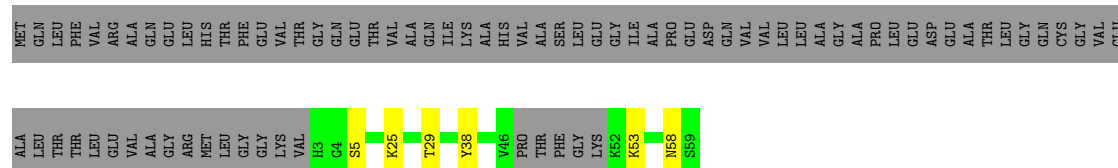
- Molecule 77: 40S ribosomal protein S29

Chain Sd:  84% 14% 2%



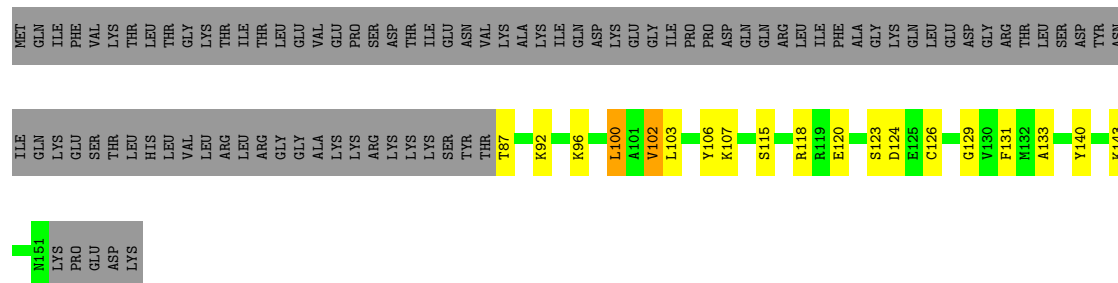
- Molecule 78: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

Chain Se:  35% 5% 61%



- Molecule 79: Ubiquitin

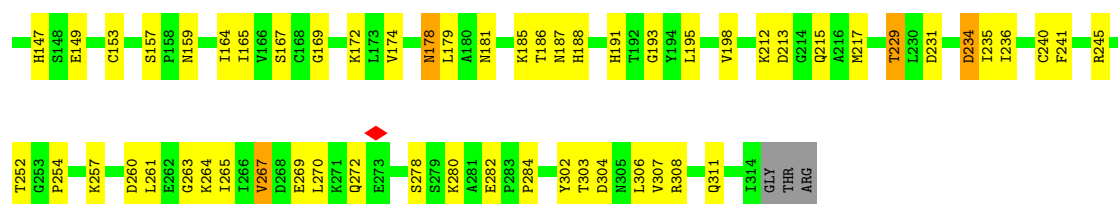
Chain Sf:  29% 11% 58%



- Molecule 80: Receptor of activated protein C kinase 1

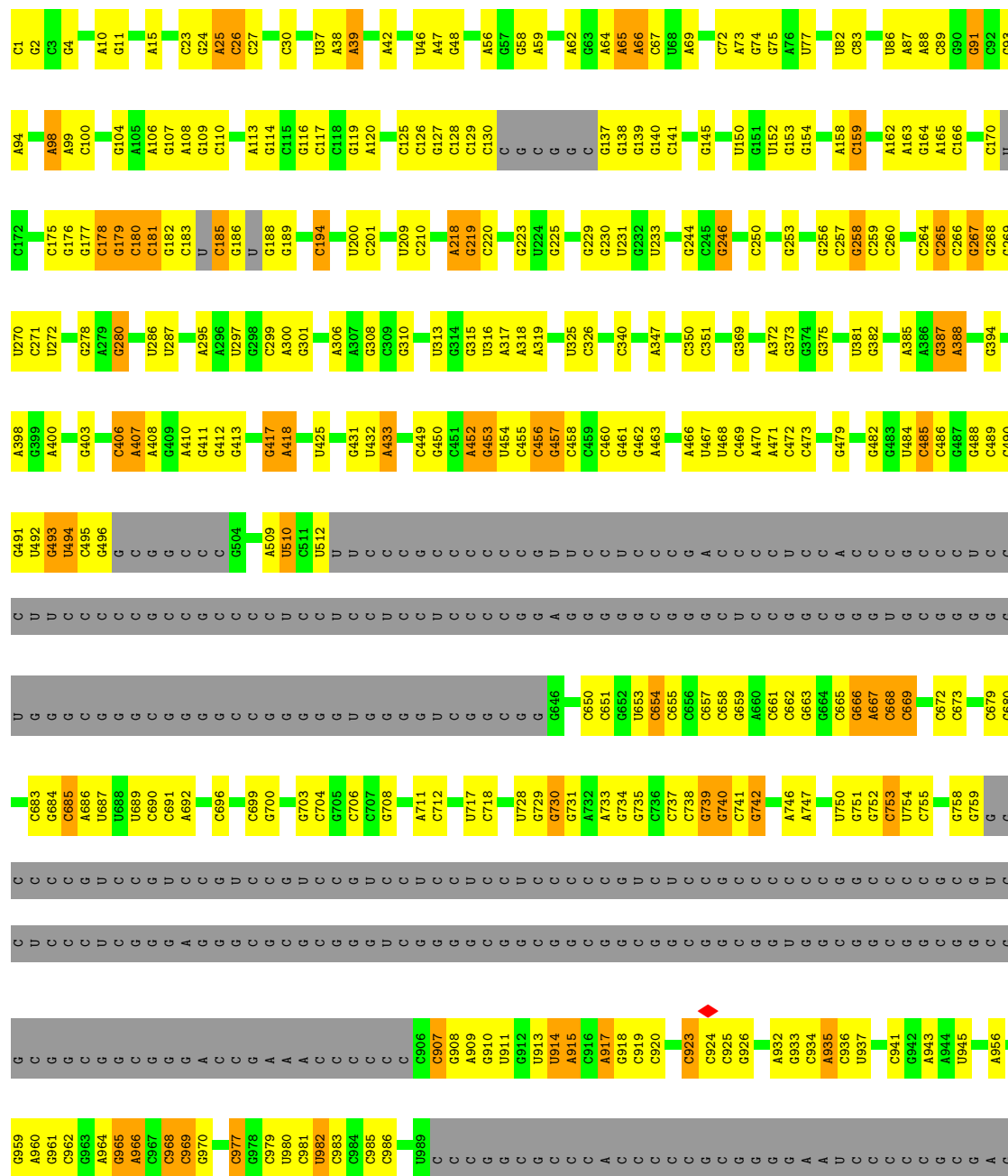
Chain Sg:  70% 28% 2%





• Molecule 81: LSU rRNA

Chain L5: 38% 24% 6% 31%







G4975	U4881	G4647	C4747	G4647	C4560	G4478	A4376	C4281	C4177	C4096	G	G	G3897	C3809
U4976	U4882	A4648	U4748	A4648	C4561	G4479	G4377	A4281	G4183	G4097	C	C	A3901	C3810
A4979	C4883	G4649	C4749	G4649	U4563	U4481	A4378	G4291	G4184	A4098	C	C	G	C3811
C4980	C4889	U4656	G4750	U4657	A4564	U4482	A4379	U4291	C	G4099	C	C	G	C3812
A4982	C4894	U4657	G4751	U4657	G4567	U4483	C4387	U4292	G4187	A3906	C	C	G	A3813
U4985	C4895	G4681	C4752	G4681	A4568	C4486	A4388	U4293	U4188	G3907	C	C	G	U3814
G4986	C4896	C4670	U4758	C4670	A4569	A4487	C4389	U4299	U4189	A3908	C	C	G	A3817
C4987	C4897	C4671	C4759	C4671	G4570	A4488	A4390	U4300	U4190	C3909	C	C	G	DY13818
U4988	C4900	C4672	G4760	U4673	A4571	G4489	G4391	U4301	G4191	C3910	C	C	G	C3819
U	G4901	U4674	G4761	U4674	G4572	U4494	G4392	U4302	U4194	U3912	C	C	G	U3912
C	C4910	C4674	C4761	C4674	U4576	G4495	A4394	A4304	G4195	U3915	C	C	G	G3823
U4991	A4911	G4680	A4764	G4680	U4577	U4498	A4397	G4305	G4196	C	C	C	G	A3824
G4992	G4912	A4681	G4765	A4681	G4578	G4499	C4398	G4306	G4197	G3918	C	C	G	A3825
G4993	G4913	G4682	G4766	G4682	U4579	U4501	U4399	U4312	U4202	C3919	C	C	G	A3830
G4994	G4914	G4683	G4767	G4683	U4580	U4502	G4400	A4313	U4208	U3920	C	C	G	C3834
U4995	C4919	A4684	U4770	A4684	U4581	C4504	G4401	C4314	A4208	C	C	C	G	C3834
U5001	G4919	U4685	C4771	U4685	A4584	C4505	G4402	G4322	A4214	A3923	C	C	G	U3838
U5002	C4921	G4686	C4772	G4686	C4585	C4506	U4403	G4323	G4225	C3924	C	C	G	G3839
U5003	C4922	C4687	C4773	C4687	A4585	A4507	U4404	A4325	A4220	U3925	C	C	G	U3840
U5004	C4923	C4688	C4774	C4688	A4589	C4508	G4405	A4326	A4219	A3928	C	C	G	C3841
G5005	C4924	U4689	C4775	U4689	U4591	U4512	U4406	G4328	G4221	G3929	C	C	G	A3845
U5006	G4925	A4691	C4776	G4690	C4592	A4513	G4407	G4329	G4222	U3930	C	C	G	C3846
U5007	C4926	A4692	C	G4691	C4593	G4514	C4413	G4330	G4223	C3931	C	C	G	U3847
C5008	G4927	U4693	C	U4692	C4594	G4515	A4414	G4331	G4224	U3932	C	C	G	A3849
G5009	C4928	U4694	C	U4693	C4595	G4516	C4415	C4332	G4225	G3933	C	C	G	G3850
U5010	C4929	U4695	C	U4694	C4596	G4517	C4416	C4333	U4227	G3934	C	C	G	U3851
A5011	G4934	A4700	C	U4695	C4597	A4518	A4422	U4334	G4228	A3935	C	C	G	C3852
G5012	C4935	A4701	C	U4696	C4598	G4519	U4423	G4335	U4229	A3936	C	C	G	A3856
C5013	C4936	U4702	C	U4697	C4599	G4520	C4426	C4336	C	C3937	C	C	G	G3857
A5014	C4937	U4703	C	U4698	C4600	A4521	U4427	C4337	A4233	G3938	C	C	G	C3858
G5015	C4938	C4710	C	U4699	C4601	G4522	U4428	C4338	A4234	A3942	C	C	G	A3861
A5016	C4939	C4711	C	U4700	C4602	G4523	G4431	U4339	G4236	A3943	C	C	G	A3862
G5017	C4940	C4712	C	U4701	C4603	G4524	C4432	U4340	G4237	G3944	C	C	G	A3867
U5022	C4941	A4717	C	U4702	C4604	G4525	C4433	G4341	A4251	A3945	C	C	G	C3868
C5023	C4942	G4718	C	U4703	C4605	U4530	U4442	C4342	G4254	G3946	C	C	G	C3869
C5024	C4943	G4719	C	U4704	C4606	U4531	U4443	C4343	C	A	C	C	G	C3870
C5025	C4944	C	C	U4705	C4607	U4532	G4448	U4344	U4076	A	C	C	G	G3873
C5026	C4945	A4723	C	U4706	C4608	G4536	G4449	U4346	U4077	C	C	C	G	G3874
C5027	C4946	A4724	C	U4707	C4609	C4537	C4456	G4347	A4072	C	C	C	G	A3877
G5028	A4954	C4730	C	U4708	C4610	G4538	U4457	A4348	A4073	C	C	C	G	C3878
C5029	A4955	G4731	C	U4709	C4611	U4539	C4458	C4349	C4258	A	C	C	G	C3879
U5030	C4957	G4732	C	U4710	C4612	G4540	U4459	C4350	C4259	G	C	C	G	C3880
G5031	C4958	C4733	C	U4711	C4613	G4541	U4460	U4353	U4260	G	C	C	G	C3881
C5032	U4959	A4734	C	U4712	C4614	G4542	C4461	U4354	A4077	C	C	C	G	G3882
G5033	C4960	G4735	C	U4713	C4615	U4544	C4462	U4355	G4084	C	C	C	G	C3883
A5034	C4961	C4736	C	U4714	C4616	G4545	C4463	U4356	C4088	C	C	C	G	A3884
G5041	C4962	C4737	C	U4715	C4617	C4546	U4464	G4357	G4089	C	C	C	G	A3885
A5042	A4966	C4738	C	U4716	C4618	G4547	U4465	A4358	C4171	C	C	C	G	A3886
A5043	A4967	G4740	C	U4717	C4619	C4548	C4466	C4359	A4273	C	C	C	G	C3887
A5044	A4968	C4741	C	U4718	C4620	G4549	C4467	C4360	G4092	C	C	C	G	U3892
U5047	C4970	G4742	C	U4719	C4621	U4551	U4471	U4372	G4093	C	C	C	G	C3893
C5047	C4971	C4743	C	U4720	C4622	G4552	C4472	U4373	G4094	C	C	C	G	C3894
U5050	U4972	A4744	C	U4721	C4623	U4553	A4473	U4374	G4095	C	C	C	G	A
C5050	C4974	C4746	C	U4722	C4624	U4554	G4475	C4375						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	546553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	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	0.157	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	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: GDP, OMU, PSU, K, UY1, PUT, ANM, OMC, A2M, OMG, 6MZ, 5MC, 4AC, B8N, NA, 3HE, MG, ZN, MA6, UR3, HYG, SPD

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	CB	0.24	0/6505	0.38	0/8787
2	CC	0.12	0/525	0.23	0/816
3	CD	0.18	0/594	0.31	0/788
4	L8	0.26	0/3608	0.36	0/5619
5	LA	0.23	0/1934	0.42	0/2593
6	LB	0.20	0/3288	0.37	0/4400
7	LC	0.21	0/2949	0.36	0/3960
8	LD	0.17	0/2420	0.32	0/3240
9	LE	0.18	0/1834	0.36	0/2460
10	LF	0.21	0/1915	0.34	0/2553
11	LG	0.19	0/1869	0.36	0/2515
12	LH	0.20	0/1537	0.36	0/2066
13	LI	0.19	0/1681	0.32	0/2246
14	LJ	0.17	0/1390	0.37	0/1859
15	LL	0.25	0/1695	0.54	1/2270 (0.0%)
16	LM	0.19	0/1147	0.35	0/1534
17	LN	0.22	0/1745	0.36	0/2338
18	LO	0.22	0/1681	0.36	0/2250
19	LP	0.20	0/1309	0.37	0/1757
20	LQ	0.21	0/1536	0.35	0/2052
21	LR	0.19	0/1533	0.33	0/2025
22	LS	0.21	0/1492	0.37	0/2003
23	LT	0.19	0/1320	0.35	0/1763
24	LU	0.16	0/831	0.40	0/1115
25	LV	0.21	0/986	0.35	0/1324
26	LW	0.18	0/949	0.39	0/1256
27	LX	0.19	0/1012	0.35	0/1360
28	LY	0.19	0/1132	0.35	0/1504
29	LZ	0.18	0/1129	0.31	0/1507
30	La	0.20	0/1190	0.31	0/1591
31	Lb	0.19	0/866	0.36	0/1143

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.21	0/742	0.36	0/996
33	Ld	0.19	0/903	0.36	0/1216
34	Le	0.22	0/1071	0.35	0/1429
35	Lf	0.21	0/900	0.34	0/1205
36	Lg	0.19	0/907	0.32	0/1209
37	Lh	0.18	0/1023	0.33	0/1351
38	Li	0.17	0/854	0.32	0/1129
39	Lj	0.22	0/720	0.40	0/952
40	Lk	0.19	0/565	0.31	0/750
41	Ll	0.20	0/454	0.35	0/599
42	Lm	0.17	0/431	0.32	0/571
43	Ln	0.27	0/231	0.50	0/294
44	Lo	0.20	0/875	0.34	0/1155
45	Lp	0.24	0/714	0.36	0/948
46	Lr	0.20	0/1022	0.33	0/1371
47	S2	0.27	1/36887 (0.0%)	0.34	1/57466 (0.0%)
48	SA	0.16	0/1737	0.32	0/2360
49	SB	0.17	0/1756	0.32	0/2350
50	SC	0.18	0/1744	0.35	0/2357
51	SD	0.21	0/1785	0.37	0/2404
52	SE	0.17	0/2107	0.33	0/2836
53	SF	0.18	0/1484	0.38	0/1994
54	SG	0.16	0/1932	0.34	0/2571
55	SH	0.42	1/1488 (0.1%)	0.73	4/1995 (0.2%)
56	SI	0.19	0/1707	0.35	0/2278
57	SJ	0.16	0/1524	0.30	0/2035
58	SK	0.17	0/840	0.38	0/1133
59	SL	0.17	0/1209	0.28	0/1617
60	SM	0.21	0/873	0.50	1/1175 (0.1%)
61	SN	0.19	0/1232	0.31	0/1656
62	SO	0.18	0/1020	0.34	0/1368
63	SP	0.19	0/1074	0.33	0/1434
64	SQ	0.17	0/1135	0.36	0/1522
65	SR	0.19	0/1082	0.36	0/1452
66	SS	0.16	0/1208	0.33	0/1618
67	ST	0.17	0/1122	0.34	0/1504
68	SU	0.17	0/805	0.37	0/1081
69	SV	0.15	0/643	0.25	0/860
70	SW	0.19	0/1050	0.34	0/1405
71	SX	0.20	0/1112	0.34	0/1485
72	SY	0.16	0/1023	0.33	0/1359
73	SZ	0.15	0/580	0.30	0/780
74	Sa	0.20	0/826	0.39	0/1107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sb	0.16	0/647	0.38	0/865
76	Sc	0.18	0/497	0.35	0/666
77	Sd	0.19	0/465	0.34	0/617
78	Se	0.20	0/417	0.39	0/545
79	Sf	0.17	0/539	0.41	0/716
80	Sg	0.16	0/2491	0.37	0/3392
81	L5	0.27	1/81104 (0.0%)	0.34	0/126490
82	L7	0.24	0/2839	0.28	0/4425
83	Lq	0.15	0/1553	0.36	0/2097
84	CA	0.19	0/115	0.42	0/151
All	All	0.24	3/226666 (0.0%)	0.35	7/331035 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	SH	11	PRO	CG-CD	-13.57	1.04	1.50
81	L5	3785	A2M	O3'-P	5.21	1.61	1.56
47	S2	27	A2M	O3'-P	5.20	1.61	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	SH	11	PRO	N-CD-CG	-19.56	73.86	103.20
55	SH	11	PRO	CA-CB-CG	-17.10	72.02	104.50
15	LL	134	PRO	CA-N-CD	-12.75	94.15	112.00
55	SH	11	PRO	N-CA-CB	-11.10	95.10	102.65
60	SM	100	PRO	N-CD-CG	-7.57	91.85	103.20
55	SH	11	PRO	CA-N-CD	-5.88	103.77	112.00
47	S2	968	U	O3'-P-O5'	-5.18	96.22	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CB	6379	0	6451	102	0
2	CC	470	0	237	5	0
3	CD	585	0	547	22	0
4	L8	3296	0	1677	56	0
5	LA	1896	0	1987	34	0
6	LB	3220	0	3362	59	0
7	LC	2895	0	3076	36	0
8	LD	2375	0	2409	37	0
9	LE	1800	0	1960	39	0
10	LF	1880	0	2008	30	0
11	LG	1838	0	1979	32	0
12	LH	1518	0	1601	26	0
13	LI	1642	0	1680	28	0
14	LJ	1367	0	1402	20	0
15	LL	1664	0	1773	33	0
16	LM	1125	0	1192	17	0
17	LN	1700	0	1749	27	0
18	LO	1649	0	1794	25	0
19	LP	1282	0	1317	17	0
20	LQ	1512	0	1628	16	0
21	LR	1517	0	1670	20	0
22	LS	1452	0	1490	24	0
23	LT	1292	0	1361	19	0
24	LU	817	0	839	19	0
25	LV	972	0	1034	10	0
26	LW	935	0	995	21	0
27	LX	994	0	1072	12	0
28	LY	1115	0	1205	21	0
29	LZ	1106	0	1182	18	0
30	La	1161	0	1213	19	0
31	Lb	853	0	921	20	0
32	Lc	732	0	769	10	0
33	Ld	888	0	930	16	0
34	Le	1053	0	1147	19	0
35	Lf	881	0	917	6	0
36	Lg	897	0	985	10	0
37	Lh	1015	0	1148	17	0
38	Li	843	0	929	12	0
39	Lj	705	0	737	10	0
40	Lk	559	0	624	15	0
41	Ll	444	0	483	4	0
42	Lm	425	0	454	7	0
43	Ln	230	0	276	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Lo	861	0	926	11	0
45	Lp	704	0	750	9	0
46	Lr	1007	0	1073	11	0
47	S2	34174	0	17301	419	0
48	SA	1700	0	1701	29	0
49	SB	1729	0	1803	19	0
50	SC	1707	0	1791	22	0
51	SD	1757	0	1853	36	0
52	SE	2065	0	2169	32	0
53	SF	1463	0	1511	24	0
54	SG	1909	0	2073	39	0
55	SH	1466	0	1532	36	0
56	SI	1678	0	1758	34	0
57	SJ	1499	0	1618	18	0
58	SK	816	0	841	15	0
59	SL	1189	0	1262	15	0
60	SM	864	0	879	28	0
61	SN	1208	0	1294	14	0
62	SO	1007	0	1032	20	0
63	SP	1054	0	1108	14	0
64	SQ	1117	0	1180	15	0
65	SR	1068	0	1121	15	0
66	SS	1190	0	1249	22	0
67	ST	1103	0	1133	20	0
68	SU	795	0	862	18	0
69	SV	636	0	637	4	0
70	SW	1033	0	1077	9	0
71	SX	1094	0	1161	9	0
72	SY	1006	0	1078	15	0
73	SZ	574	0	627	8	0
74	Sa	813	0	857	26	0
75	Sb	634	0	652	12	0
76	Sc	495	0	523	13	0
77	Sd	454	0	442	7	0
78	Se	414	0	454	5	0
79	Sf	528	0	533	13	0
80	Sg	2434	0	2387	52	0
81	L5	74592	0	37762	813	0
82	L7	2541	0	1285	11	0
83	Lq	1529	0	1584	39	0
84	CA	115	0	124	2	0
85	CB	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	CB	1	0	0	0	0
86	L5	198	0	0	0	0
86	L7	3	0	0	0	0
86	L8	2	0	0	0	0
86	LB	1	0	0	0	0
86	LC	1	0	0	0	0
86	LI	1	0	0	0	0
86	Lg	1	0	0	0	0
86	Lj	1	0	0	0	0
86	S2	60	0	0	0	0
86	SX	1	0	0	0	0
86	Sd	1	0	0	0	0
87	L5	74	0	0	0	0
87	L7	2	0	0	0	0
87	L8	3	0	0	0	0
87	LA	1	0	0	0	0
87	LI	1	0	0	0	0
87	LN	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lf	1	0	0	0	0
87	S2	17	0	0	0	0
87	Sa	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
88	Sf	1	0	0	0	0
89	L5	36	0	72	5	0
89	S2	6	0	12	1	0
90	S2	36	0	37	0	0
91	L5	80	0	152	4	0
92	L5	20	0	23	2	0
93	L5	19	0	19	1	0
94	L5	1	0	0	0	0
95	CB	1	0	0	0	0
95	L5	263	0	0	2	0
95	L7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	L8	7	0	0	0	0
95	LA	6	0	0	1	0
95	LB	5	0	0	0	0
95	LC	4	0	0	0	0
95	LF	2	0	0	0	0
95	LH	1	0	0	0	0
95	LN	3	0	0	0	0
95	LO	1	0	0	0	0
95	LP	2	0	0	0	0
95	LQ	1	0	0	0	0
95	LS	1	0	0	0	0
95	LT	1	0	0	0	0
95	LV	1	0	0	0	0
95	La	2	0	0	0	0
95	Lc	1	0	0	0	0
95	Le	5	0	0	0	0
95	Lf	2	0	0	0	0
95	Lg	1	0	0	0	0
95	Lj	1	0	0	0	0
95	Lo	1	0	0	0	0
95	Lp	3	0	0	0	0
95	S2	78	0	0	0	0
95	SF	1	0	0	0	0
95	SL	1	0	0	0	0
95	SN	1	0	0	0	0
All	All	216008	0	163540	2571	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 (2571) 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)
55:SH:10:LYS:HZ3	55:SH:20:GLU:HB3	1.33	0.93
81:L5:181:C:H2'	81:L5:182:G:H8	1.35	0.89
81:L5:181:C:H2'	81:L5:182:G:C8	2.08	0.89
81:L5:4894:A:H3'	81:L5:4895:C:H5'	1.56	0.87
47:S2:563:G:H1	47:S2:592:C:H5	1.24	0.86
30:La:26:ARG:NH2	81:L5:1656:U:OP2	2.09	0.85
15:LL:63:THR:HG22	15:LL:65:ARG:H	1.40	0.85
15:LL:63:THR:HG21	30:La:66:ASN:HB3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:2847:G:H1	81:L5:3841:OMC:H5	1.27	0.82
1:CB:21:ASN:HD22	1:CB:415:ARG:HH11	1.26	0.81
81:L5:2364:OMG:N2	81:L5:3858:C:O2	2.12	0.81
1:CB:595:SER:HA	1:CB:724:THR:HG21	1.63	0.81
65:SR:23:ARG:NH1	80:Sg:149:GLU:OE2	2.12	0.81
1:CB:26:ALA:HB2	1:CB:128:VAL:HG13	1.61	0.80
30:La:86:THR:HG22	81:L5:510:U:H5'	1.63	0.79
80:Sg:87:LEU:HB2	80:Sg:101:PHE:HB2	1.64	0.79
81:L5:3910:C:O2	81:L5:4392:OMG:N2	2.14	0.79
81:L5:2611:A:H5'	81:L5:2688:G:H4'	1.63	0.79
81:L5:5025:C:H2'	81:L5:5028:G:H1'	1.63	0.78
81:L5:1270:A:H8	81:L5:2106:G:H21	1.29	0.78
60:SM:25:ALA:HB1	60:SM:30:GLY:HA3	1.65	0.78
18:LO:47:PHE:HZ	18:LO:144:GLU:HG3	1.48	0.78
12:LH:71:ARG:HG2	81:L5:4691:A:H4'	1.64	0.77
26:LW:80:ARG:NH2	47:S2:167:G:O2'	2.18	0.77
81:L5:2658:G:N2	81:L5:2676:A:OP2	2.18	0.77
47:S2:1328:OMG:N2	47:S2:1501:C:O2	2.16	0.76
81:L5:4228:OMG:N2	81:L5:4375:C:O2	2.15	0.76
47:S2:1228:A:H2'	47:S2:1229:G:C8	2.20	0.76
47:S2:1281:G:H1	47:S2:1316:C:H5	1.32	0.76
51:SD:216:GLU:OE2	51:SD:216:GLU:N	2.18	0.76
81:L5:2297:G:OP2	91:L5:5107:SPD:N1	2.19	0.76
28:LY:121:ARG:NH1	81:L5:194:C:O2	2.18	0.75
54:SG:22:ARG:HA	54:SG:25:ARG:HE	1.51	0.75
4:L8:82:A:OP2	37:Lh:2:ALA:N	2.20	0.75
17:LN:60:VAL:HG22	17:LN:134:LEU:HB2	1.68	0.75
8:LD:286:SER:HB3	81:L5:1178:G:H2'	1.69	0.75
47:S2:1703:OMC:H5	47:S2:1871:6MZ:H6	1.35	0.75
62:SO:86:LYS:NZ	62:SO:122:SER:O	2.17	0.75
64:SQ:53:GLU:OE2	64:SQ:85:ARG:NH1	2.20	0.74
13:LI:14:ASN:O	13:LI:128:ARG:NH2	2.21	0.74
15:LL:132:SER:O	15:LL:134:PRO:HD2	1.87	0.74
81:L5:4092:G:H3'	81:L5:4093:G:H21	1.52	0.74
63:SP:110:GLU:OE2	63:SP:110:GLU:N	2.20	0.74
81:L5:2469:C:H5	81:L5:2471:G:H1	1.32	0.74
10:LF:220:MET:HE2	10:LF:223:LYS:HB2	1.70	0.74
19:LP:135:ARG:NH2	81:L5:1596:U:O2'	2.20	0.74
55:SH:163:GLN:O	55:SH:167:GLU:HB2	1.88	0.74
81:L5:495:C:H2'	81:L5:496:G:C8	2.23	0.73
79:Sf:107:LYS:HE2	79:Sf:107:LYS:HA	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:3627:OMG:N2	81:L5:3834:C:O2	2.14	0.73
83:Lq:39:GLN:HG2	83:Lq:107:VAL:HG11	1.70	0.73
16:LM:119:ARG:HE	18:LO:193:THR:HG22	1.52	0.73
83:Lq:190:GLN:O	83:Lq:191:GLN:NE2	2.17	0.73
81:L5:4623:OMG:N2	81:L5:4674:C:O2	2.18	0.73
47:S2:1536:G:H2'	47:S2:1537:A:H8	1.54	0.72
56:SI:76:THR:OG1	56:SI:105:ASP:OD1	2.05	0.72
56:SI:89:GLU:OE2	56:SI:92:ARG:NH1	2.22	0.72
44:Lo:98:LYS:HE3	81:L5:4233:A:H4'	1.71	0.72
60:SM:121:LYS:NZ	60:SM:125:GLU:OE1	2.22	0.72
10:LF:219:GLY:O	10:LF:246:ARG:NH2	2.22	0.72
56:SI:34:ALA:HB2	56:SI:56:ARG:HD3	1.70	0.72
81:L5:1316:OMG:N2	81:L5:1327:C:O2	2.16	0.72
51:SD:4:GLN:OE1	51:SD:4:GLN:N	2.22	0.72
9:LE:59:ARG:NH2	81:L5:977:C:OP2	2.23	0.71
13:LI:36:LEU:HD21	13:LI:69:ARG:HH11	1.55	0.71
46:Lr:32:LEU:HD23	46:Lr:113:ARG:HD3	1.71	0.71
80:Sg:257:LYS:NZ	80:Sg:269:GLU:OE2	2.23	0.71
47:S2:317:C:OP2	54:SG:183:ARG:NH2	2.24	0.71
14:LJ:31:ASP:OD1	14:LJ:35:ARG:NH1	2.24	0.71
17:LN:125:SER:HB2	81:L5:3937:C:H1'	1.73	0.71
55:SH:10:LYS:NZ	55:SH:20:GLU:HB3	2.06	0.71
60:SM:94:ILE:HG22	60:SM:100:PRO:HA	1.72	0.70
60:SM:55:ASN:HD21	60:SM:81:ASP:HA	1.55	0.70
8:LD:41:LYS:NZ	23:LT:32:ARG:O	2.23	0.70
39:Lj:20:ARG:NH2	39:Lj:39:TYR:OH	2.25	0.70
51:SD:75:LYS:NZ	58:SK:18:GLU:OE2	2.23	0.70
60:SM:62:VAL:O	60:SM:66:GLU:HG2	1.92	0.70
6:LB:2:SER:N	81:L5:4517:A:N7	2.39	0.70
29:LZ:17:ARG:NH1	81:L5:2578:G:N7	2.38	0.70
81:L5:4592:C:O2	81:L5:4618:OMG:N2	2.20	0.70
47:S2:801:U:O4	55:SH:106:ARG:NH2	2.24	0.69
5:LA:215:ASN:ND2	81:L5:4546:A:N7	2.39	0.69
5:LA:21:LYS:HD3	81:L5:1541:C:H5''	1.74	0.69
58:SK:15:LEU:HD22	58:SK:49:MET:HE1	1.73	0.69
4:L8:17:A:H61	81:L5:417:G:H1'	1.55	0.69
75:Sb:30:SER:HB3	75:Sb:49:HIS:HD2	1.57	0.69
10:LF:105:VAL:HG13	10:LF:136:VAL:HG12	1.74	0.69
81:L5:4107:G:H2'	81:L5:4108:G:C8	2.28	0.69
47:S2:1536:G:H2'	47:S2:1537:A:C8	2.28	0.69
54:SG:164:LYS:HG2	54:SG:167:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CD:295:ARG:NH2	60:SM:113:ASP:OD2	2.26	0.69
74:Sa:2:THR:HG23	74:Sa:3:LYS:H	1.58	0.69
28:LY:31:SER:HA	28:LY:48:PRO:HA	1.74	0.68
59:SL:124:ASP:OD2	59:SL:147:LYS:NZ	2.26	0.68
55:SH:10:LYS:HE3	55:SH:45:ILE:HG13	1.75	0.68
47:S2:1598:G:O2'	73:SZ:80:ARG:O	2.12	0.68
75:Sb:59:CYS:SG	75:Sb:60:SER:N	2.66	0.68
9:LE:188:ARG:NH2	81:L5:4941:G:OP2	2.25	0.68
45:Lp:36:LYS:HD3	45:Lp:48:LYS:HG3	1.75	0.68
27:LX:114:LYS:NZ	27:LX:120:ASP:OD1	2.26	0.68
81:L5:1082:C:O2'	81:L5:1083:U:O5'	2.11	0.68
31:Lb:23:LYS:HG3	31:Lb:24:PRO:HD2	1.75	0.68
81:L5:138:G:H2'	81:L5:139:G:H8	1.59	0.68
54:SG:162:LEU:HD11	54:SG:172:LYS:HD2	1.75	0.68
81:L5:4638:U:H5	81:L5:4661:G:H1	1.40	0.68
47:S2:1156:U:OP1	70:SW:71:LYS:NZ	2.27	0.68
61:SN:46:THR:H	61:SN:49:GLN:HE21	1.42	0.68
47:S2:683:OMG:N2	47:S2:1022:U:OP2	2.22	0.68
1:CB:187:VAL:HG21	83:Lq:135:THR:HG21	1.75	0.67
66:SS:15:VAL:HG13	66:SS:68:ILE:HD11	1.76	0.67
23:LT:5:LYS:HD3	81:L5:4302:U:H4'	1.76	0.67
58:SK:80:ARG:NH1	58:SK:89:ILE:O	2.26	0.67
47:S2:1217:A:H2'	47:S2:1218:C:H6	1.59	0.67
11:LG:176:LYS:HD2	38:Li:43:MET:HE1	1.77	0.67
28:LY:10:ASP:HB3	28:LY:13:LYS:HB2	1.77	0.67
81:L5:982:U:H2'	81:L5:983:C:C6	2.30	0.67
25:LV:15:ARG:NH2	81:L5:4672:A:OP1	2.27	0.67
9:LE:101:ASN:ND2	81:L5:685:C:OP1	2.28	0.67
51:SD:16:ILE:HD11	77:Sd:36:LEU:HD23	1.76	0.66
11:LG:162:ASP:HB2	11:LG:163:PRO:HD3	1.76	0.66
47:S2:1228:A:H2'	47:S2:1229:G:H8	1.60	0.66
5:LA:20:VAL:HA	5:LA:23:ARG:HG3	1.78	0.66
13:LI:183:ASP:O	13:LI:187:LYS:HG3	1.96	0.66
20:LQ:173:LYS:NZ	81:L5:88:A:N7	2.44	0.66
1:CB:791:ASN:OD1	1:CB:791:ASN:N	2.21	0.66
19:LP:96:LYS:HE3	81:L5:394:G:H5'	1.78	0.66
38:Li:2:ALA:N	38:Li:5:TYR:HH	1.93	0.66
81:L5:1365:C:H3'	81:L5:1366:G:H5''	1.77	0.66
81:L5:4775:C:H6	81:L5:4859:C:H42	1.42	0.66
6:LB:358:ARG:NH2	81:L5:4617:G:OP2	2.28	0.66
7:LC:143:ARG:NH1	7:LC:145:GLU:OE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LM:40:GLY:HA3	16:LM:45:VAL:HB	1.78	0.66
81:L5:4342:C:O2	81:L5:4370:OMG:N2	2.16	0.66
1:CB:440:GLU:OE1	71:SX:142:ARG:NH2	2.29	0.66
81:L5:907:C:H2'	81:L5:908:G:H8	1.61	0.66
81:L5:1522:OMG:N2	81:L5:1655:C:O2	2.15	0.66
65:SR:62:GLN:NE2	80:Sg:282:GLU:OE2	2.28	0.66
52:SE:97:GLU:OE1	52:SE:113:ARG:NH1	2.29	0.66
1:CB:512:LYS:HG2	1:CB:571:LYS:HG3	1.78	0.65
30:La:2:PRO:HD2	81:L5:1509:C:H5''	1.78	0.65
55:SH:98:ARG:NH1	55:SH:132:ASP:OD2	2.28	0.65
47:S2:107:A:H2'	47:S2:108:G:C8	2.32	0.65
81:L5:964:A:H2'	81:L5:965:G:H4'	1.78	0.65
81:L5:1654:G:N2	81:L5:1678:C:OP1	2.29	0.65
1:CB:13:MET:HE1	1:CB:452:LEU:HD11	1.78	0.65
26:LW:80:ARG:NH1	54:SG:129:VAL:O	2.30	0.65
47:S2:171:A:H5'	54:SG:177:GLN:HG2	1.77	0.65
47:S2:557:U:O2'	47:S2:558:G:H5'	1.95	0.65
8:LD:40:ASP:HB2	8:LD:43:LYS:HG3	1.78	0.65
56:SI:110:ARG:O	56:SI:114:GLU:HG2	1.97	0.65
81:L5:4274:A:H2'	81:L5:4275:G:C8	2.31	0.65
8:LD:258:LYS:NZ	82:L7:119:U:O4	2.29	0.65
10:LF:182:TYR:HB3	10:LF:200:ARG:HG3	1.78	0.65
83:Lq:120:GLU:OE2	83:Lq:162:LYS:NZ	2.30	0.65
4:L8:62:A:OP1	37:Lh:51:ARG:NH2	2.30	0.65
14:LJ:171:ASP:O	63:SP:9:LYS:NZ	2.26	0.65
4:L8:85:U:OP1	4:L8:86:U:O2'	2.15	0.65
33:Ld:50:ARG:HG2	33:Ld:54:MET:HE3	1.78	0.65
7:LC:95:MET:HG3	81:L5:2351:OMC:HM22	1.79	0.64
12:LH:31:ARG:NH1	12:LH:149:ASN:OD1	2.29	0.64
13:LI:184:MET:HA	13:LI:187:LYS:HE2	1.79	0.64
20:LQ:87:THR:HG21	81:L5:1503:A:H62	1.61	0.64
55:SH:147:LYS:O	55:SH:149:ASP:N	2.29	0.64
81:L5:2839:PSU:N1	81:L5:3849:A:N1	2.38	0.64
47:S2:1399:C:O2	47:S2:1447:OMG:N2	2.15	0.64
21:LR:60:ARG:NH1	81:L5:2616:C:OP1	2.30	0.64
22:LS:15:ARG:HB3	22:LS:27:LEU:HD23	1.79	0.64
47:S2:420:G:OP1	70:SW:88:LYS:NZ	2.30	0.64
47:S2:1217:A:H2'	47:S2:1218:C:C6	2.32	0.64
81:L5:1179:U:H3'	81:L5:1180:C:H5''	1.78	0.64
81:L5:3689:G:O2'	81:L5:3818:UY1:OP2	2.12	0.64
4:L8:67:U:H5''	39:Lj:86:PRO:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SF:127:ARG:HD2	53:SF:136:ARG:HG3	1.79	0.64
76:Sc:22:GLY:O	76:Sc:26:GLN:NE2	2.31	0.64
6:LB:10:ARG:NH2	6:LB:265:SER:O	2.30	0.64
42:Lm:100:TYR:O	81:L5:4472:G:O2'	2.15	0.64
47:S2:448:A:H5''	56:SI:25:ARG:HA	1.79	0.64
47:S2:928:G:H2'	47:S2:929:G:C8	2.33	0.64
52:SE:211:LYS:HZ3	52:SE:215:GLY:HA2	1.63	0.64
26:LW:84:GLY:HA2	54:SG:161:PRO:HD3	1.80	0.64
48:SA:1:MET:HA	48:SA:59:LEU:HB2	1.79	0.64
56:SI:11:ARG:O	59:SL:136:LYS:NZ	2.31	0.64
5:LA:245[B]:ARG:NH2	81:L5:3698:G:OP2	2.31	0.64
6:LB:168:MET:HA	6:LB:171:LEU:HD12	1.79	0.64
12:LH:94:SER:HB2	12:LH:142:ASP:HB3	1.80	0.64
39:Lj:52:LYS:NZ	81:L5:375:G:OP2	2.27	0.64
63:SP:130:ARG:HG2	63:SP:130:ARG:HH11	1.63	0.64
81:L5:1175:A:H2	81:L5:1185:G:H22	1.46	0.64
81:L5:4239:A:H2'	81:L5:4240:G:C8	2.33	0.64
11:LG:108:GLN:N	11:LG:108:GLN:OE1	2.31	0.63
23:LT:43:LYS:O	23:LT:58:HIS:ND1	2.31	0.63
26:LW:99:GLU:HA	26:LW:102:LYS:HG2	1.78	0.63
74:Sa:45:VAL:O	74:Sa:46:GLU:HG3	1.97	0.63
11:LG:37:LYS:NZ	81:L5:4126:C:OP1	2.31	0.63
60:SM:81:ASP:HB3	60:SM:84:LYS:HB2	1.81	0.63
1:CB:42:LYS:NZ	1:CB:348:ASP:OD1	2.31	0.63
5:LA:245[A]:ARG:NH2	81:L5:3698:G:OP2	2.31	0.63
11:LG:73:ARG:HH12	81:L5:4162:C:H5	1.46	0.63
14:LJ:54:ARG:NH2	81:L5:4259:C:OP2	2.30	0.63
43:Ln:4:LYS:NZ	47:S2:1844:U:O4	2.19	0.63
34:Le:38:PRO:HB2	34:Le:46:ARG:HB2	1.81	0.63
56:SI:202:ILE:HG22	56:SI:206:LYS:HE3	1.80	0.63
17:LN:45:PRO:O	17:LN:49:ARG:HG3	1.98	0.63
81:L5:4077:A:N1	81:L5:4171:C:N4	2.46	0.63
78:Se:53:LYS:HA	78:Se:53:LYS:HE3	1.81	0.63
48:SA:205:ARG:NH2	48:SA:214:GLU:OE1	2.32	0.62
72:SY:12:PHE:HZ	72:SY:21:LYS:HD2	1.64	0.62
81:L5:4227:OMU:HM21	81:L5:4336:A:H1'	1.79	0.62
4:L8:17:A:N6	81:L5:417:G:H1'	2.13	0.62
10:LF:216:PRO:HD3	10:LF:247:MET:HE2	1.80	0.62
14:LJ:35:ARG:HB3	14:LJ:123:ILE:HG23	1.79	0.62
15:LL:47:ALA:HB3	15:LL:48:PRO:HD3	1.81	0.62
63:SP:30:TYR:O	63:SP:34:MET:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:141:ARG:NH1	9:LE:191:GLN:O	2.32	0.62
24:LU:18:VAL:HG11	24:LU:77:PRO:HA	1.81	0.62
28:LY:59:ARG:HB2	28:LY:103:LYS:HG3	1.81	0.62
52:SE:102:ILE:HG23	52:SE:182:MET:HE1	1.81	0.62
1:CB:138:GLN:HA	1:CB:141:THR:HG22	1.81	0.62
48:SA:137:ALA:HB1	48:SA:142:LEU:HB3	1.80	0.62
6:LB:83:PRO:O	6:LB:167:GLN:NE2	2.31	0.62
1:CB:451:ILE:HD11	1:CB:458:VAL:HG22	1.80	0.62
8:LD:50:ARG:NH2	8:LD:72:ASP:OD2	2.31	0.62
5:LA:37:ARG:NH2	81:L5:4088:C:OP1	2.33	0.62
22:LS:127:MET:HA	23:LT:153:PRO:HG2	1.81	0.62
47:S2:943:U:O2'	62:SO:135:ILE:O	2.18	0.62
81:L5:4227:OMU:H5'	81:L5:4227:OMU:H6	1.82	0.62
37:Lh:107:GLN:O	37:Lh:111:GLU:HG3	1.99	0.62
47:S2:1256:G:H8	68:SU:66:ARG:HB2	1.65	0.62
51:SD:172:VAL:HG22	51:SD:185:LYS:HG2	1.82	0.62
52:SE:100:ARG:HB2	52:SE:114:ILE:HD13	1.82	0.62
80:Sg:83:TRP:HA	80:Sg:107:ASP:HB2	1.82	0.62
60:SM:87:GLU:HG3	60:SM:92:CYS:HB3	1.82	0.62
47:S2:1445:PSU:HO2'	47:S2:1446:A:H8	1.48	0.61
81:L5:1339:U:H2'	81:L5:1340:OMC:C6	2.34	0.61
81:L5:3923:A:H2'	81:L5:3924:C:C6	2.35	0.61
7:LC:197:ARG:NH1	81:L5:351:C:OP2	2.31	0.61
23:LT:111:GLU:O	23:LT:115:LYS:HD2	2.00	0.61
47:S2:1612:G:OP1	63:SP:18:ARG:NH2	2.33	0.61
73:SZ:68:ILE:HB	73:SZ:109:TYR:HB2	1.81	0.61
80:Sg:212:LYS:HA	80:Sg:235:ILE:HG23	1.82	0.61
81:L5:3723:A:H2'	81:L5:3724:A2M:H8	1.81	0.61
24:LU:56:LEU:HD21	24:LU:63:ILE:HD12	1.82	0.61
81:L5:4219:A:C6	81:L5:4220:6MZ:H9	2.36	0.61
47:S2:126:G:OP1	54:SG:198:ARG:NH1	2.28	0.61
47:S2:993:G:N7	74:Sa:15:ARG:NH1	2.48	0.61
81:L5:4859:C:H3'	81:L5:4860:G:H8	1.66	0.61
7:LC:66:SER:HA	7:LC:77:PRO:HA	1.82	0.61
15:LL:80:GLU:HG3	15:LL:110:LEU:HD12	1.83	0.61
31:Lb:90:SER:OG	81:L5:1266:G:N7	2.34	0.61
47:S2:1679:A:H2'	53:SF:60:ARG:HD2	1.81	0.61
81:L5:4111:U:H2'	81:L5:4112:C:C6	2.34	0.61
83:Lq:159:GLN:HB3	83:Lq:162:LYS:NZ	2.14	0.61
47:S2:204:G:H2'	47:S2:205:G:C8	2.35	0.61
47:S2:1230:C:OP1	66:SS:130:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1332:A:O2'	51:SD:145:GLN:O	2.12	0.61
81:L5:1625:OMG:N1	81:L5:3918:G:OP1	2.30	0.61
27:LX:82:THR:HG21	37:Lh:37:THR:HG22	1.82	0.61
47:S2:367:U:H4'	47:S2:371:A:C8	2.36	0.61
10:LF:52:GLU:OE2	81:L5:1238:A:O2'	2.18	0.61
23:LT:68:THR:HG21	81:L5:4314:C:H4'	1.83	0.61
31:Lb:7:HIS:HB3	81:L5:4219:A:H4'	1.83	0.61
32:Lc:34:THR:HG23	32:Lc:95:ALA:HB2	1.83	0.61
81:L5:139:G:H2'	81:L5:140:G:C8	2.35	0.61
83:Lq:123:VAL:HB	83:Lq:158:VAL:HG13	1.83	0.61
26:LW:97:LYS:HD3	26:LW:98:PRO:HD2	1.82	0.61
8:LD:273:LEU:O	8:LD:277:LYS:HG3	2.01	0.60
47:S2:52:G:O2'	72:SY:105:LYS:NZ	2.34	0.60
47:S2:925:G:H1	47:S2:1017:U:H3	1.47	0.60
48:SA:59:LEU:HD22	48:SA:181:GLU:HG2	1.83	0.60
81:L5:4111:U:H2'	81:L5:4112:C:H6	1.65	0.60
26:LW:109:ILE:O	26:LW:113:LYS:HG2	2.01	0.60
47:S2:1857:G:OP1	62:SO:141:ARG:NH1	2.34	0.60
60:SM:93:LYS:NZ	60:SM:102:LYS:O	2.32	0.60
66:SS:39:ARG:HE	67:ST:38:LYS:HD2	1.65	0.60
17:LN:143:ARG:O	17:LN:149:GLN:NE2	2.26	0.60
37:Lh:73:TYR:HB3	37:Lh:79:LYS:HG2	1.83	0.60
47:S2:118:C:H1'	47:S2:445:A:C5	2.37	0.60
74:Sa:22:ARG:NH1	74:Sa:29:CYS:SG	2.73	0.60
81:L5:138:G:H2'	81:L5:139:G:C8	2.36	0.60
56:SI:57:ALA:HB2	56:SI:183:GLY:HA2	1.84	0.60
57:SJ:136:ARG:HD3	57:SJ:160:SER:HA	1.82	0.60
65:SR:34:VAL:O	65:SR:38:ILE:HG13	2.02	0.60
4:L8:70:G:H5''	28:LY:27:ARG:CZ	2.31	0.60
19:LP:115:GLU:HG2	19:LP:151:THR:HG23	1.82	0.60
47:S2:981:A:H2'	47:S2:982:G:C8	2.36	0.60
54:SG:159:ARG:HD2	54:SG:173:ALA:HB2	1.82	0.60
9:LE:190:HIS:HB3	9:LE:193:PHE:HD2	1.66	0.60
47:S2:28:U:H2'	47:S2:29:G:H8	1.65	0.60
47:S2:1560:U:HO2'	47:S2:1583:C:HO2'	1.50	0.60
7:LC:218:ILE:HG12	7:LC:229:LEU:HG	1.84	0.60
7:LC:335:MET:O	7:LC:339:THR:HG23	2.02	0.60
9:LE:243:THR:HG22	9:LE:245:GLN:H	1.67	0.60
14:LJ:19:LYS:NZ	81:L5:4261:C:OP1	2.23	0.60
16:LM:81:ASP:N	16:LM:81:ASP:OD1	2.34	0.60
22:LS:95:ARG:NH2	22:LS:112:ASP:OD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:847:A:OP1	52:SE:108:ARG:NH1	2.35	0.60
80:Sg:8:ARG:HG3	80:Sg:311:GLN:HG3	1.83	0.60
6:LB:107:ALA:HB2	6:LB:201:LEU:HD22	1.82	0.60
81:L5:267:G:H2'	81:L5:268:G:H8	1.64	0.60
8:LD:223:PHE:HB3	8:LD:226:TYR:HB2	1.82	0.60
29:LZ:36:ARG:NH2	81:L5:2580:U:OP1	2.35	0.60
35:Lf:14:TYR:OH	35:Lf:92:LEU:O	2.17	0.60
47:S2:168:C:OP1	54:SG:131:ARG:NE	2.31	0.60
48:SA:13:GLU:CD	48:SA:13:GLU:H	2.09	0.60
81:L5:661:C:H2'	81:L5:662:C:C6	2.37	0.60
81:L5:1998:A:C8	83:Lq:55:MET:HB2	2.37	0.60
81:L5:3599:A:H2'	81:L5:3600:G:C8	2.36	0.60
83:Lq:44:ARG:HE	83:Lq:53:VAL:HB	1.67	0.60
1:CB:727:ARG:NH2	1:CB:856:ASP:OD2	2.33	0.60
55:SH:18:GLU:O	55:SH:21:SER:OG	2.20	0.60
80:Sg:129:ILE:HB	80:Sg:142:VAL:HG22	1.83	0.59
80:Sg:278:SER:O	80:Sg:280:LYS:NZ	2.33	0.59
4:L8:23:C:H1'	28:LY:16:LYS:HG3	1.84	0.59
81:L5:1358:G:O2'	81:L5:1360:G:O6	2.20	0.59
18:LO:168:TYR:CE2	18:LO:172:LYS:HD2	2.37	0.59
27:LX:82:THR:HG22	27:LX:155:ILE:HG23	1.83	0.59
49:SB:107:ARG:NH1	62:SO:133:THR:O	2.17	0.59
59:SL:33:LEU:HD23	59:SL:33:LEU:H	1.68	0.59
62:SO:56:VAL:HG13	62:SO:60:MET:HE2	1.84	0.59
67:ST:13:GLU:OE1	67:ST:142:ASN:ND2	2.34	0.59
47:S2:186:C:H2'	47:S2:187:G:C8	2.37	0.59
47:S2:1203:G:H2'	47:S2:1204:A:C8	2.37	0.59
81:L5:4992:G:H2'	81:L5:4993:G:C8	2.36	0.59
1:CB:259:LYS:HG2	1:CB:264:ARG:NH1	2.16	0.59
83:Lq:26:LYS:NZ	83:Lq:93:GLU:O	2.36	0.59
81:L5:2008:U:H1'	81:L5:2011:C:H5	1.66	0.59
29:LZ:83:THR:HG22	29:LZ:85:TYR:HD1	1.66	0.59
39:Lj:46:LYS:NZ	81:L5:24:G:N7	2.51	0.59
74:Sa:88:SER:O	74:Sa:92:ARG:HB2	2.01	0.59
81:L5:1257:A:H3'	81:L5:1258:G:C8	2.37	0.59
29:LZ:17:ARG:NH2	29:LZ:18:TYR:OH	2.36	0.59
81:L5:711:A:H2'	81:L5:712:C:C6	2.38	0.59
17:LN:203:TYR:HB2	81:L5:1359:G:H4'	1.85	0.59
27:LX:104:ALA:O	27:LX:108:GLN:HB2	2.03	0.59
81:L5:683:C:H2'	81:L5:684:G:O4'	2.03	0.59
13:LI:73:ASN:HB2	13:LI:87:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1115:U:H4'	47:S2:1116:C:H5'	1.85	0.59
47:S2:1388:A:H61	51:SD:161:GLY:HA3	1.68	0.59
11:LG:165:GLU:OE1	17:LN:26:ARG:NH2	2.32	0.58
19:LP:94:MET:HE2	19:LP:148:MET:HE3	1.85	0.58
47:S2:528:A:H2'	47:S2:529:A:C8	2.38	0.58
81:L5:5027:C:O2'	81:L5:5028:G:H5''	2.03	0.58
4:L8:144:U:H2'	4:L8:145:C:C6	2.38	0.58
9:LE:161:ARG:NH1	9:LE:273:SER:OG	2.37	0.58
47:S2:640:A:H2'	47:S2:641:A:C8	2.37	0.58
6:LB:246:ARG:NH1	81:L5:4525:C:OP1	2.32	0.58
20:LQ:172:ARG:NH1	30:La:56:VAL:O	2.35	0.58
68:SU:18:HIS:NE2	68:SU:94:PRO:O	2.36	0.58
71:SX:66:ILE:HD13	78:Se:5:SER:HB3	1.84	0.58
81:L5:666:G:N7	81:L5:668:C:N4	2.51	0.58
81:L5:2520:C:H2'	81:L5:2521:G:C8	2.38	0.58
81:L5:4260:U:H2'	81:L5:4261:C:C6	2.37	0.58
8:LD:84:PRO:O	8:LD:89:LYS:NZ	2.36	0.58
13:LI:3:ARG:NH2	81:L5:4431:PSU:OP2	2.36	0.58
35:Lf:36:ARG:NH1	35:Lf:79:GLY:O	2.35	0.58
47:S2:1139:C:H2'	47:S2:1140:G:O4'	2.03	0.58
81:L5:267:G:H2'	81:L5:268:G:C8	2.37	0.58
30:La:27:LYS:NZ	81:L5:1518:A:OP1	2.36	0.58
47:S2:113:G:N2	47:S2:293:C:H5'	2.18	0.58
61:SN:25:TRP:CD2	75:Sb:82:LYS:HE2	2.39	0.58
80:Sg:217:MET:HG2	80:Sg:229:THR:HB	1.85	0.58
81:L5:162:A:H2'	81:L5:163:A:C8	2.38	0.58
81:L5:4740:G:H1'	81:L5:4742:G:H5''	1.86	0.58
1:CB:295:ASP:O	1:CB:299:LYS:HG2	2.04	0.58
24:LU:100:LEU:HD13	24:LU:112:LEU:HD23	1.85	0.58
55:SH:17:ASP:HB2	55:SH:20:GLU:HB2	1.84	0.58
55:SH:17:ASP:OD1	55:SH:17:ASP:N	2.36	0.58
81:L5:1095:A:H61	81:L5:1200:G:H1	1.50	0.58
81:L5:2529:A:O2'	81:L5:2531:C:OP2	2.21	0.58
1:CB:602:LEU:HD23	1:CB:604:MET:HE3	1.85	0.58
4:L8:83:C:H4'	4:L8:84:A:C5	2.39	0.58
10:LF:57:TYR:OH	10:LF:189:ASP:OD1	2.15	0.58
15:LL:119:GLU:HG2	15:LL:123:LYS:HD2	1.84	0.58
31:Lb:120:ARG:NH1	81:L5:1242:G:N3	2.52	0.58
56:SI:69:SER:OG	56:SI:191:GLU:OE2	2.19	0.58
81:L5:268:G:H2'	81:L5:269:G:H8	1.69	0.58
81:L5:909:A:H2'	81:L5:910:G:H8	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LB:30:LYS:NZ	81:L5:4717:A:OP2	2.26	0.58
17:LN:191:ALA:O	17:LN:195:ARG:HG2	2.03	0.58
47:S2:1588:A:H2'	47:S2:1589:A:C8	2.39	0.58
62:SO:90:ILE:HG22	62:SO:124:MET:HE1	1.85	0.58
81:L5:2474:G:N2	81:L5:2502:G:O2'	2.37	0.58
1:CB:697:MET:HE1	1:CB:702:PHE:HZ	1.69	0.58
47:S2:1256:G:C8	68:SU:66:ARG:HB2	2.39	0.58
30:La:59:LYS:NZ	81:L5:89:C:OP1	2.31	0.58
51:SD:40:ARG:HB3	51:SD:47:GLU:HG3	1.86	0.58
76:Sc:13:ARG:HH21	76:Sc:35:MET:HE1	1.69	0.58
81:L5:2474:G:H2'	81:L5:2502:G:N2	2.18	0.58
81:L5:4739:C:H2'	81:L5:4740:G:H5'	1.85	0.58
47:S2:942:G:H2'	47:S2:943:U:C6	2.39	0.57
81:L5:218:A:H3'	81:L5:219:G:H21	1.69	0.57
81:L5:1942:A:H2'	81:L5:1943:A:C8	2.38	0.57
44:Lo:39:ARG:NH1	81:L5:295:A:OP2	2.34	0.57
50:SC:167:ARG:HB3	50:SC:177:PRO:HB2	1.86	0.57
80:Sg:157:SER:OG	80:Sg:159:ASN:OD1	2.16	0.57
12:LH:14:GLU:H	12:LH:14:GLU:CD	2.13	0.57
15:LL:180:ALA:O	15:LL:184:MET:HG3	2.04	0.57
47:S2:1407:U:H2'	47:S2:1408:U:C6	2.40	0.57
55:SH:162:GLN:OE1	55:SH:165:ASN:ND2	2.38	0.57
56:SI:128:LYS:HD2	56:SI:129:LEU:H	1.69	0.57
81:L5:3654:G:O2'	81:L5:3693:U:OP1	2.20	0.57
40:Lk:51:GLU:OE1	40:Lk:51:GLU:N	2.34	0.57
42:Lm:80:PRO:O	42:Lm:84:GLN:HG3	2.04	0.57
47:S2:186:C:H2'	47:S2:187:G:H8	1.68	0.57
47:S2:1401:A:H4'	68:SU:52:GLY:HA3	1.85	0.57
47:S2:1447:OMG:OP1	68:SU:87:ARG:NH2	2.37	0.57
67:ST:116:ASP:OD1	67:ST:117:GLN:NE2	2.38	0.57
80:Sg:191:HIS:CG	80:Sg:195:LEU:HD21	2.40	0.57
81:L5:2318:G:N2	81:L5:2321:G:OP2	2.30	0.57
3:CD:288:LYS:O	3:CD:292:ASN:ND2	2.37	0.57
6:LB:74:GLU:OE1	6:LB:285:TYR:OH	2.16	0.57
27:LX:105:ASN:OD1	27:LX:106:LYS:N	2.38	0.57
47:S2:655:A:H4'	47:S2:656:G:H3'	1.87	0.57
47:S2:1277:C:H2'	47:S2:1278:A:H8	1.69	0.57
58:SK:42:ASN:O	58:SK:46:MET:HG3	2.05	0.57
80:Sg:17:TRP:HB2	80:Sg:36:ARG:HD2	1.87	0.57
81:L5:4537:C:H2'	81:L5:4538:G:C8	2.40	0.57
6:LB:56:ILE:HD13	6:LB:365:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Lf:43:LEU:O	35:Lf:109:ARG:NH1	2.37	0.57
81:L5:453:G:H2'	81:L5:453:G:N3	2.19	0.57
81:L5:2520:C:H2'	81:L5:2521:G:H8	1.70	0.57
12:LH:12:ILE:HG12	12:LH:18:ILE:HD12	1.86	0.57
47:S2:874:G:H2'	47:S2:875:A:C8	2.40	0.57
53:SF:71:ARG:NH2	53:SF:148:ASN:OD1	2.31	0.57
58:SK:80:ARG:HG3	58:SK:85:LEU:HB2	1.86	0.57
65:SR:57:LEU:O	65:SR:61:ILE:HG23	2.05	0.57
75:Sb:40:CYS:SG	75:Sb:42:LYS:NZ	2.67	0.57
81:L5:4913:G:H4'	81:L5:4914:C:O5'	2.04	0.57
1:CB:779:THR:HG22	1:CB:781:MET:H	1.69	0.57
1:CB:272:LYS:HE3	1:CB:273:PHE:H	1.70	0.57
9:LE:86:GLU:O	81:L5:2258:C:N4	2.38	0.57
18:LO:140:ARG:O	18:LO:144:GLU:HG2	2.04	0.57
55:SH:138:GLU:H	55:SH:159:ASP:HB2	1.70	0.57
5:LA:28:ARG:HB3	5:LA:123:ARG:HD3	1.86	0.56
39:Lj:49:TRP:O	81:L5:1646:A:O2'	2.22	0.56
81:L5:1633:G:H5'	81:L5:1634:A:OP1	2.04	0.56
26:LW:87:LEU:O	26:LW:91:MET:HG2	2.03	0.56
81:L5:176:G:H2'	81:L5:177:G:C8	2.40	0.56
16:LM:113:MET:HE2	16:LM:114:LYS:HD3	1.86	0.56
32:Lc:104:ILE:HD12	32:Lc:105:ILE:HG12	1.88	0.56
47:S2:928:G:H1	47:S2:1013:U:H3	1.54	0.56
68:SU:80:PHE:HB3	77:Sd:52:PHE:HB3	1.88	0.56
81:L5:717:U:H2'	81:L5:718:C:C6	2.41	0.56
81:L5:2362:U:H2'	81:L5:2363:A2M:H8	1.87	0.56
81:L5:3711:A:H2'	81:L5:3712:A:O4'	2.05	0.56
81:L5:4291:G:H5'	81:L5:4293:U:C6	2.40	0.56
81:L5:4922:C:H2'	81:L5:4923:C:C6	2.40	0.56
1:CB:665:ILE:HG12	1:CB:703:ASP:HB3	1.87	0.56
8:LD:62:CYS:HB3	8:LD:105:LEU:HD22	1.87	0.56
9:LE:154:THR:HG23	81:L5:4942:C:H4'	1.87	0.56
25:LV:13:LYS:HD2	25:LV:128:LEU:HD11	1.87	0.56
40:Lk:49:ASP:HB3	40:Lk:52:LYS:HB2	1.87	0.56
47:S2:54:A:OP1	72:SY:111:LYS:NZ	2.33	0.56
47:S2:145:G:H2'	47:S2:146:G:C8	2.40	0.56
47:S2:563:G:O2'	47:S2:564:A:OP1	2.23	0.56
51:SD:136:VAL:HG12	51:SD:186:VAL:HG22	1.88	0.56
62:SO:117:ARG:O	62:SO:121:ARG:HG2	2.05	0.56
81:L5:1577:G:O2'	81:L5:1612:G:H4'	2.05	0.56
1:CB:206:ASP:OD2	1:CB:208:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:132:PRO:HG2	9:LE:135:GLN:HG3	1.87	0.56
47:S2:601:OMG:N2	47:S2:621:C:O2	2.19	0.56
64:SQ:51:LEU:HD13	64:SQ:81:ILE:HG23	1.86	0.56
81:L5:1964:A:H2'	81:L5:1965:G:H8	1.69	0.56
4:L8:148:A:H2'	4:L8:149:G:C8	2.41	0.56
8:LD:119:TYR:OH	8:LD:139:PRO:O	2.23	0.56
28:LY:32:SER:OG	28:LY:101:PRO:O	2.18	0.56
47:S2:204:G:H2'	47:S2:205:G:H8	1.69	0.56
51:SD:211:VAL:O	65:SR:20:TYR:OH	2.22	0.56
47:S2:1382:A:H2'	47:S2:1383:A2M:H8	1.88	0.56
81:L5:176:G:H2'	81:L5:177:G:H8	1.70	0.56
10:LF:60:GLU:O	10:LF:64:MET:HG3	2.06	0.56
81:L5:153:G:H2'	81:L5:154:G:H8	1.70	0.56
83:Lq:159:GLN:HB3	83:Lq:162:LYS:HZ1	1.71	0.56
4:L8:141:C:H5''	17:LN:60:VAL:HG11	1.87	0.56
25:LV:32:THR:HG21	25:LV:105:ILE:HD12	1.86	0.56
67:ST:108:GLU:OE2	67:ST:121:ARG:NE	2.25	0.56
81:L5:3910:C:H2'	81:L5:3911:C:C6	2.40	0.56
8:LD:262:LYS:HD3	8:LD:262:LYS:H	1.71	0.56
9:LE:180:VAL:HG21	9:LE:258:LEU:HD11	1.87	0.56
11:LG:95:LEU:HD21	11:LG:156:VAL:HG21	1.88	0.56
47:S2:1413:G:H2'	47:S2:1414:A:H8	1.71	0.56
71:SX:68:LYS:HB3	71:SX:91:LEU:HD22	1.88	0.56
81:L5:452:A:H4'	81:L5:453:G:H5'	1.88	0.56
81:L5:665:C:H4'	81:L5:666:G:H5'	1.88	0.56
1:CB:451:ILE:HD12	1:CB:452:LEU:H	1.71	0.55
4:L8:69:PSU:H3'	4:L8:70:G:C8	2.41	0.55
47:S2:906:U:H2'	47:S2:907:G:C8	2.41	0.55
47:S2:1531:A:H4'	47:S2:1605:G:H4'	1.87	0.55
51:SD:75:LYS:HE2	58:SK:20:VAL:HG23	1.87	0.55
81:L5:662:C:H2'	81:L5:663:G:C8	2.41	0.55
81:L5:2745:A:H2'	81:L5:2746:A:C8	2.40	0.55
4:L8:141:C:H2'	4:L8:142:U:C6	2.41	0.55
32:Lc:31:TYR:OH	32:Lc:59:GLU:OE1	2.20	0.55
47:S2:806:U:H3	47:S2:857:U:H3	1.54	0.55
47:S2:1441:U:O2	47:S2:1443:C:N4	2.39	0.55
74:Sa:7:ASN:O	74:Sa:9:GLY:N	2.35	0.55
80:Sg:234:ASP:OD1	80:Sg:234:ASP:N	2.27	0.55
81:L5:909:A:H2'	81:L5:910:G:C8	2.41	0.55
44:Lo:33:LEU:HA	44:Lo:38:LYS:HG2	1.87	0.55
52:SE:18:TRP:HH2	52:SE:31:PRO:HD3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:4108:G:H2'	81:L5:4109:G:O4'	2.06	0.55
5:LA:183:GLY:CA	81:L5:1613:A:H5''	2.37	0.55
6:LB:153:MET:HB3	6:LB:194:LEU:HD11	1.88	0.55
67:ST:5:THR:HG22	67:ST:7:LYS:H	1.71	0.55
80:Sg:112:ALA:HB3	80:Sg:121:VAL:HG12	1.87	0.55
81:L5:1316:OMG:N1	81:L5:1327:C:N3	2.50	0.55
81:L5:3923:A:H2'	81:L5:3924:C:H6	1.72	0.55
16:LM:24:LEU:HB2	16:LM:43:THR:HG21	1.89	0.55
16:LM:123:ILE:HD11	18:LO:189:ILE:HD13	1.89	0.55
35:Lf:106:TYR:HB2	35:Lf:107:PRO:HD3	1.87	0.55
48:SA:110:ASN:HB3	48:SA:113:GLN:HG3	1.89	0.55
81:L5:99:A:H2'	81:L5:100:C:O2	2.07	0.55
1:CB:649:ILE:HG12	1:CB:663:THR:HG22	1.89	0.55
8:LD:200:MET:HA	8:LD:200:MET:HE3	1.87	0.55
45:Lp:51:ALA:HB3	45:Lp:54:ILE:HD12	1.89	0.55
47:S2:554:A:C8	47:S2:589:G:H5''	2.41	0.55
47:S2:587:A:H5'	47:S2:592:C:H42	1.71	0.55
47:S2:1354:G:N2	47:S2:1357:A:OP2	2.35	0.55
48:SA:80:ARG:NH2	48:SA:165:ASN:O	2.39	0.55
81:L5:179:G:N2	81:L5:258:G:H1'	2.22	0.55
81:L5:4967:A:H2'	81:L5:4968:A:C8	2.42	0.55
2:CC:28:U:H2'	2:CC:29:G:C8	2.42	0.55
13:LI:162:ARG:NH2	81:L5:2033:A:OP1	2.39	0.55
49:SB:88:THR:HG22	49:SB:98:THR:HG22	1.89	0.55
81:L5:460:C:H2'	81:L5:461:G:H8	1.70	0.55
2:CC:39:U:H2'	2:CC:40:C:H6	1.71	0.55
47:S2:1532:C:O2'	47:S2:1601:A:N1	2.40	0.55
68:SU:24:LEU:HD23	68:SU:112:VAL:HG22	1.89	0.55
76:Sc:36:ASP:OD2	76:Sc:37:ASP:N	2.39	0.55
1:CB:531:ASP:HB3	1:CB:534:VAL:HG12	1.88	0.55
6:LB:378:ARG:HG2	26:LW:32:LEU:HD21	1.87	0.55
18:LO:106:ASP:O	81:L5:4910:G:N2	2.39	0.55
24:LU:101:ARG:NH2	81:L5:2702:C:OP1	2.39	0.55
47:S2:874:G:H2'	47:S2:875:A:H8	1.72	0.55
56:SI:172:LEU:HD13	56:SI:190:LEU:HD12	1.88	0.55
57:SJ:31:LEU:HD13	57:SJ:102:ILE:HD11	1.89	0.55
80:Sg:153:CYS:HB3	80:Sg:198:VAL:HG12	1.87	0.55
81:L5:188:G:H4'	81:L5:189:G:H5''	1.89	0.55
4:L8:116:C:C2'	4:L8:117:C:H5'	2.37	0.55
41:Ll:41:ARG:NH2	81:L5:2431:A:OP1	2.40	0.55
54:SG:136:LYS:NZ	54:SG:175:LYS:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SV:32:ILE:HG12	69:SV:60:ARG:HD2	1.88	0.55
81:L5:737:C:C5	81:L5:739:G:H5''	2.42	0.55
1:CB:85:ASP:HA	1:CB:88:PHE:HD1	1.72	0.54
6:LB:252:ALA:HB3	81:L5:4457:PSU:H1'	1.89	0.54
47:S2:29:G:H2'	47:S2:30:C:C6	2.43	0.54
55:SH:164:ASN:OD1	55:SH:164:ASN:N	2.40	0.54
81:L5:268:G:H2'	81:L5:269:G:C8	2.42	0.54
81:L5:914:U:O2'	81:L5:915:A:OP2	2.20	0.54
81:L5:1094:G:H3'	81:L5:1095:A:H8	1.72	0.54
81:L5:2693:G:H2'	81:L5:2694:G:N2	2.21	0.54
1:CB:286:PRO:HB2	1:CB:291:GLN:HG2	1.88	0.54
25:LV:15:ARG:HB2	81:L5:4618:OMG:H5''	1.90	0.54
30:La:72:THR:HG22	30:La:110:LYS:HB3	1.89	0.54
48:SA:2:SER:OG	48:SA:56:GLU:OE2	2.22	0.54
55:SH:78:ARG:O	55:SH:82:GLU:HG2	2.07	0.54
81:L5:175:C:H2'	81:L5:176:G:H8	1.72	0.54
81:L5:1186:U:H2'	81:L5:1187:G:N3	2.22	0.54
81:L5:1327:C:H2'	81:L5:1328:G:C8	2.43	0.54
81:L5:1332:C:H2'	81:L5:1333:A:H8	1.72	0.54
81:L5:4966:A:H2'	81:L5:4967:A:O4'	2.07	0.54
9:LE:98:GLY:HA3	9:LE:101:ASN:HD21	1.72	0.54
47:S2:484:A2M:H8	47:S2:484:A2M:O5'	2.06	0.54
53:SF:102:LEU:HD11	73:SZ:100:VAL:HG21	1.89	0.54
65:SR:103:LYS:HG3	65:SR:119:VAL:HG22	1.89	0.54
81:L5:369:G:N2	81:L5:372:A:OP2	2.36	0.54
81:L5:3614:G:O2'	81:L5:3615:G:OP1	2.24	0.54
81:L5:3718:A2M:H2	81:L5:3934:G:O4'	2.07	0.54
13:LI:116:ARG:NH2	81:L5:4194:U:O2'	2.40	0.54
14:LJ:38:LYS:HD3	14:LJ:38:LYS:N	2.21	0.54
37:Lh:89:ARG:O	37:Lh:93:ARG:HG2	2.08	0.54
40:Lk:35:LYS:HE2	81:L5:2696:A:H62	1.72	0.54
47:S2:1232:PSU:H2'	47:S2:1233:G:C8	2.43	0.54
68:SU:62:ARG:HB3	68:SU:62:ARG:HH11	1.72	0.54
19:LP:74:LYS:NZ	81:L5:4982:A:OP1	2.32	0.54
22:LS:99:ASP:OD2	22:LS:108:GLN:NE2	2.41	0.54
46:Lr:65:LYS:O	46:Lr:102:TYR:OH	2.20	0.54
47:S2:28:U:H2'	47:S2:29:G:C8	2.41	0.54
47:S2:1084:A:OP1	47:S2:1858:G:O2'	2.23	0.54
47:S2:1279:C:H2'	47:S2:1280:G:C8	2.42	0.54
60:SM:23:LYS:O	60:SM:27:ILE:HG23	2.07	0.54
76:Sc:37:ASP:OD2	76:Sc:39:SER:OG	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:175:C:H2'	81:L5:176:G:C8	2.42	0.54
81:L5:1669:A:H4'	81:L5:1685:G:N2	2.22	0.54
1:CB:45:ILE:HG22	1:CB:46:ILE:HG13	1.89	0.54
64:SQ:97:GLN:HB3	64:SQ:105:LYS:HG3	1.88	0.54
81:L5:66:A:O2'	81:L5:326:C:O2	2.24	0.54
81:L5:3597:G:H4'	81:L5:3598:C:O5'	2.08	0.54
3:CD:304:LYS:HG3	3:CD:305:PRO:HD2	1.90	0.54
24:LU:47:ILE:HD12	24:LU:63:ILE:HD11	1.89	0.54
81:L5:181:C:C2	81:L5:182:G:N7	2.75	0.54
81:L5:2092:G:O2'	81:L5:2262:G:N2	2.41	0.54
81:L5:3861:A:H2'	81:L5:3862:A:C8	2.43	0.54
1:CB:616:ASP:OD2	1:CB:639:TYR:OH	2.20	0.54
10:LF:135:ILE:HD11	81:L5:1726:U:H5'	1.89	0.54
26:LW:93:LYS:O	26:LW:101:ARG:NH2	2.41	0.54
57:SJ:114:VAL:HG23	57:SJ:126:ALA:HB1	1.90	0.54
65:SR:116:ASN:N	65:SR:116:ASN:OD1	2.39	0.54
80:Sg:215:GLN:NE2	80:Sg:231:ASP:OD1	2.41	0.54
81:L5:1174:G:H1	81:L5:1186:U:H3	1.56	0.54
15:LL:55:ILE:HG23	15:LL:76:PHE:HE1	1.73	0.54
22:LS:19:THR:HG22	22:LS:21:LYS:H	1.73	0.54
81:L5:1317:U:H2'	81:L5:1318:C:C6	2.43	0.54
81:L5:1961:G:O2'	81:L5:2025:A:N6	2.41	0.54
81:L5:2414:G:H2'	81:L5:2415:OMU:H6	1.90	0.54
6:LB:36:ASP:HB3	6:LB:39:LYS:HE2	1.89	0.54
11:LG:231:ASP:OD1	11:LG:234:ARG:NH2	2.41	0.54
12:LH:72:THR:HG21	81:L5:4700:A:N1	2.22	0.54
47:S2:874:G:H21	55:SH:114:GLN:HE22	1.56	0.54
47:S2:1117:C:H2'	47:S2:1118:C:C6	2.43	0.54
47:S2:1714:U:H2'	47:S2:1715:A:C8	2.43	0.54
56:SI:113:TYR:OH	56:SI:156:ALA:O	2.25	0.54
5:LA:116:LEU:HD23	5:LA:164:ALA:HB2	1.89	0.53
42:Lm:93:LYS:HD2	42:Lm:102:ARG:HG2	1.90	0.53
63:SP:130:ARG:HG2	63:SP:130:ARG:NH1	2.21	0.53
1:CB:279:SER:HB3	1:CB:285:LEU:HD21	1.89	0.53
5:LA:208:GLU:HG2	81:L5:1629:G:H1	1.73	0.53
14:LJ:127:GLY:HA3	81:L5:4251:A:C2	2.43	0.53
47:S2:455:A:H2'	47:S2:456:C:C6	2.43	0.53
47:S2:1037:G:H4'	47:S2:1845:A:H4'	1.90	0.53
50:SC:183:LYS:HA	50:SC:195:LEU:O	2.08	0.53
51:SD:113:LEU:HD11	51:SD:117:ARG:HD2	1.90	0.53
6:LB:57:VAL:HG22	6:LB:73:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SB:224:GLU:HB2	49:SB:227:LYS:HG3	1.90	0.53
51:SD:135:GLU:HG3	51:SD:153:VAL:HG12	1.90	0.53
81:L5:163:A:H2'	81:L5:164:G:H8	1.73	0.53
81:L5:739:G:O2'	81:L5:740:G:O5'	2.26	0.53
83:Lq:108:PRO:O	83:Lq:181:SER:OG	2.26	0.53
4:L8:126:C:O2'	4:L8:127:U:H6	1.91	0.53
47:S2:1595:U:H2'	47:S2:1596:U:C6	2.43	0.53
54:SG:216:ARG:C	54:SG:218:LYS:H	2.17	0.53
83:Lq:172:ALA:O	83:Lq:176:ASN:ND2	2.32	0.53
15:LL:18:TRP:NE1	81:L5:1516:G:O2'	2.38	0.53
47:S2:1283:C:O2'	47:S2:1313:A:N1	2.38	0.53
63:SP:61:ARG:NH1	63:SP:88:GLU:OE2	2.41	0.53
80:Sg:236:ILE:HG12	80:Sg:252:THR:HG22	1.90	0.53
81:L5:1307:A:H2'	81:L5:1308:C:C6	2.43	0.53
83:Lq:107:VAL:HG22	83:Lq:108:PRO:HD2	1.89	0.53
1:CB:479:LEU:HD21	1:CB:483:GLY:HA3	1.91	0.53
3:CD:201:ARG:NH1	3:CD:201:ARG:HB2	2.24	0.53
33:Ld:26:THR:HG22	33:Ld:85:ARG:HH11	1.73	0.53
43:Ln:1:MET:HG3	47:S2:1706:G:H5'	1.90	0.53
47:S2:1461:G:H3'	47:S2:1463:U:H3	1.73	0.53
62:SO:34:PHE:HB3	62:SO:41:PHE:HB2	1.91	0.53
1:CB:545:ILE:HD12	1:CB:575:PRO:HB3	1.90	0.53
1:CB:845:LYS:NZ	1:CB:845:LYS:HB3	2.24	0.53
47:S2:17:C:H2'	47:S2:18:C:C6	2.43	0.53
47:S2:51:U:H2'	47:S2:52:G:C8	2.44	0.53
52:SE:43:PRO:HG2	52:SE:46:ILE:HG13	1.90	0.53
56:SI:160:SER:HA	56:SI:163:GLU:HG2	1.90	0.53
81:L5:1604:G:H2'	81:L5:1605:G:C8	2.44	0.53
81:L5:3713:U:H5''	81:L5:3714:G:OP1	2.09	0.53
81:L5:3717:A:H2'	81:L5:3718:A2M:C8	2.38	0.53
4:L8:125:C:H4'	4:L8:126:C:C5	2.44	0.53
11:LG:99:ALA:HB1	11:LG:136:LEU:HD11	1.89	0.53
13:LI:36:LEU:HD11	13:LI:69:ARG:HD2	1.89	0.53
40:Lk:12:LEU:O	40:Lk:16:ARG:HG3	2.08	0.53
47:S2:1252:C:OP1	68:SU:75:LYS:NZ	2.39	0.53
64:SQ:89:SER:HB3	64:SQ:112:LEU:HD13	1.89	0.53
81:L5:2765:A:H2'	81:L5:2766:A:C8	2.44	0.53
81:L5:2844:A:O2'	81:L5:4631:G:H4'	2.09	0.53
81:L5:4238:G:H2'	81:L5:4239:A:C8	2.44	0.53
81:L5:4536:OMC:HM22	81:L5:4537:C:O4'	2.09	0.53
10:LF:34:ARG:HG2	81:L5:1272:C:H5''	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LO:185:VAL:O	18:LO:189:ILE:HG12	2.09	0.53
46:Lr:19:LYS:HG2	46:Lr:24:THR:HG23	1.91	0.53
47:S2:78:C:H1'	54:SG:175:LYS:HB2	1.91	0.53
51:SD:10:LYS:NZ	68:SU:111:GLU:OE1	2.42	0.53
81:L5:1332:C:H2'	81:L5:1333:A:C8	2.43	0.53
81:L5:3641:U:OP2	81:L5:3646:A:N6	2.41	0.53
4:L8:93:C:O2'	4:L8:94:G:H8	1.92	0.53
79:Sf:123:SER:OG	79:Sf:124:ASP:N	2.42	0.53
80:Sg:174:VAL:HB	80:Sg:188:HIS:HB2	1.90	0.53
81:L5:4114:C:H2'	81:L5:4115:G:N3	2.24	0.53
81:L5:4860:G:H2'	81:L5:4861:G:H8	1.73	0.53
11:LG:107:LYS:HG3	11:LG:108:GLN:OE1	2.09	0.52
47:S2:1017:U:H5'	61:SN:55:ARG:HD3	1.91	0.52
77:Sd:13:LYS:HB2	77:Sd:13:LYS:NZ	2.25	0.52
81:L5:163:A:H2'	81:L5:164:G:C8	2.44	0.52
19:LP:85:LYS:O	19:LP:89:GLU:HG3	2.08	0.52
36:Lg:26:PRO:HD2	81:L5:2521:G:H4'	1.90	0.52
38:Li:73:ILE:O	38:Li:77:VAL:HG22	2.09	0.52
47:S2:508:A:H5'	47:S2:509:OMG:OP2	2.09	0.52
5:LA:183:GLY:HA2	81:L5:1613:A:H5''	1.92	0.52
6:LB:21:ARG:NH2	81:L5:4981:G:O6	2.42	0.52
7:LC:156:ASP:OD2	7:LC:255:SER:OG	2.28	0.52
18:LO:27:VAL:HG13	18:LO:98:ALA:HB1	1.91	0.52
24:LU:92:LYS:NZ	81:L5:2627:C:OP1	2.42	0.52
28:LY:103:LYS:HD3	81:L5:231:U:O2'	2.10	0.52
37:Lh:6:ALA:O	37:Lh:10:ARG:HG3	2.08	0.52
47:S2:1560:U:H2'	47:S2:1561:A:H8	1.73	0.52
52:SE:112:HIS:NE2	52:SE:237:SER:O	2.37	0.52
75:Sb:49:HIS:CE1	75:Sb:70:LYS:HG2	2.44	0.52
81:L5:1333:A:H2'	81:L5:1334:A:C8	2.45	0.52
81:L5:2847:G:N1	81:L5:3841:OMC:H5	2.04	0.52
4:L8:8:U:H2'	4:L8:9:A:C8	2.45	0.52
6:LB:128:LYS:O	6:LB:131:THR:OG1	2.22	0.52
6:LB:252:ALA:HB1	81:L5:4524:G:C2	2.45	0.52
47:S2:575:A:H2'	47:S2:576:A2M:O4'	2.08	0.52
54:SG:126:ASP:O	54:SG:127:THR:HG22	2.10	0.52
81:L5:433:A:C2	81:L5:3867:A2M:H4'	2.45	0.52
81:L5:691:C:H2'	81:L5:692:A:C8	2.43	0.52
81:L5:1617:G:H1'	81:L5:2513:A:N6	2.24	0.52
81:L5:1933:G:H2'	81:L5:1934:A:C8	2.45	0.52
81:L5:4927:G:H5'	81:L5:4928:C:H5	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:22:MET:HE1	1:CB:126:LEU:HB2	1.91	0.52
10:LF:232:ASP:OD1	10:LF:236:ARG:NH2	2.37	0.52
63:SP:34:MET:HB3	63:SP:42:ARG:HG3	1.90	0.52
65:SR:70:SER:O	65:SR:70:SER:OG	2.23	0.52
81:L5:178:C:H5	81:L5:258:G:H21	1.56	0.52
83:Lq:173:THR:O	83:Lq:177:MET:HG3	2.08	0.52
25:LV:43:LYS:HG3	25:LV:60:MET:HG2	1.92	0.52
47:S2:1741:U:H2'	47:S2:1742:C:O4'	2.10	0.52
62:SO:97:LEU:HD11	62:SO:112:ALA:HB1	1.92	0.52
81:L5:1964:A:H2'	81:L5:1965:G:C8	2.45	0.52
81:L5:4625:C:O2'	81:L5:4626:A:H5'	2.09	0.52
1:CB:697:MET:HE1	1:CB:702:PHE:CZ	2.45	0.52
8:LD:204:VAL:O	8:LD:208:MET:HG3	2.09	0.52
13:LI:87:MET:HG2	13:LI:138:ILE:HG23	1.90	0.52
17:LN:14:LYS:HE2	81:L5:280:G:H5''	1.90	0.52
47:S2:1597:C:OP2	73:SZ:85:ARG:NH2	2.38	0.52
76:Sc:11:LEU:HB3	76:Sc:35:MET:HG3	1.90	0.52
80:Sg:213:ASP:OD1	80:Sg:213:ASP:N	2.40	0.52
83:Lq:132:PRO:HB3	83:Lq:147:ILE:HD12	1.92	0.52
4:L8:122:G:H3'	4:L8:125:C:H42	1.75	0.52
17:LN:104:GLU:HA	17:LN:160:GLU:HG3	1.92	0.52
19:LP:14:SER:O	19:LP:105:LYS:NZ	2.37	0.52
34:Le:105:SER:HA	34:Le:108:ARG:HG2	1.92	0.52
54:SG:181:THR:HG22	54:SG:183:ARG:H	1.74	0.52
55:SH:65:PRO:HB2	55:SH:68:GLN:HG3	1.90	0.52
56:SI:91:VAL:HG21	56:SI:205:ARG:HH22	1.74	0.52
81:L5:2570:U:H2'	81:L5:2571:C:C6	2.45	0.52
81:L5:3641:U:H5	81:L5:3646:A:N7	2.07	0.52
1:CB:77:LEU:HD11	1:CB:102:LEU:HD12	1.92	0.52
38:Li:72:PHE:O	38:Li:76:ARG:HG2	2.09	0.52
40:Lk:10:ASP:O	40:Lk:14:THR:HG23	2.09	0.52
40:Lk:26:LYS:HB2	40:Lk:69:LEU:HD12	1.91	0.52
47:S2:399:C:H5	47:S2:680:G:H5''	1.75	0.52
47:S2:1751:C:H1'	47:S2:1784:G:N2	2.24	0.52
66:SS:35:GLY:O	66:SS:97:GLN:NE2	2.40	0.52
81:L5:2811:G:N1	81:L5:2814:C:OP2	2.38	0.52
81:L5:5030:U:H2'	81:L5:5031:G:H8	1.75	0.52
28:LY:37:GLU:H	28:LY:37:GLU:CD	2.18	0.52
28:LY:52:ASP:HB2	28:LY:110:LYS:HD3	1.93	0.52
47:S2:385:G:H3'	59:SL:136:LYS:HB2	1.92	0.52
50:SC:72:ASP:OD2	50:SC:272:HIS:NE2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:147:LEU:HD21	54:SG:156:TYR:CD2	2.45	0.52
81:L5:1940:G:H22	81:L5:4434:C:H5''	1.74	0.52
81:L5:3664:G:H2'	81:L5:3665:G:H8	1.74	0.52
81:L5:4924:C:O2'	81:L5:4926:C:O2	2.24	0.52
19:LP:33:ALA:HB1	19:LP:117:ILE:HG12	1.92	0.51
28:LY:15:ARG:NH1	81:L5:230:G:OP1	2.40	0.51
30:La:36:GLY:HA3	30:La:40:HIS:CE1	2.45	0.51
34:Le:19:LYS:NZ	81:L5:2318:G:O6	2.43	0.51
47:S2:441:C:H2'	47:S2:442:C:C6	2.45	0.51
49:SB:185:VAL:O	49:SB:189:ILE:HG12	2.09	0.51
68:SU:20:ILE:HD13	68:SU:97:ILE:HG21	1.92	0.51
81:L5:2520:C:O2	81:L5:2640:G:N2	2.42	0.51
81:L5:3873:G:H2'	81:L5:3874:G:C8	2.45	0.51
81:L5:4743:G:H2'	81:L5:4744:A:C8	2.45	0.51
4:L8:96:C:OP1	37:Lh:70:ARG:NH1	2.42	0.51
14:LJ:10:ASN:HB3	14:LJ:13:ARG:HG3	1.92	0.51
39:Lj:12:ARG:HH11	81:L5:2404:A:H1'	1.75	0.51
46:Lr:28:GLU:HG2	46:Lr:31:ASN:HB2	1.92	0.51
47:S2:948:C:H2'	47:S2:949:G:H8	1.75	0.51
49:SB:72:ALA:HB2	49:SB:80:ALA:HB2	1.92	0.51
81:L5:1971:C:H5	81:L5:2000:G:H2'	1.75	0.51
81:L5:4260:U:H2'	81:L5:4261:C:H6	1.74	0.51
4:L8:50:C:N4	4:L8:51:U:O4	2.43	0.51
17:LN:116:LEU:HD22	17:LN:135:ILE:HD11	1.92	0.51
21:LR:105:LEU:HD13	21:LR:135:LYS:HE2	1.91	0.51
26:LW:102:LYS:HA	26:LW:105:ARG:HD3	1.91	0.51
47:S2:1098:C:H2'	47:S2:1099:G:C8	2.46	0.51
47:S2:1410:C:H2'	47:S2:1411:G:H8	1.74	0.51
47:S2:1653:U:H2'	47:S2:1654:G:C8	2.45	0.51
56:SI:190:LEU:HD22	56:SI:194:GLU:HG2	1.93	0.51
70:SW:30:CYS:HB2	70:SW:61:ILE:HG13	1.92	0.51
73:SZ:65:TYR:HB2	73:SZ:68:ILE:HG12	1.92	0.51
81:L5:1437:C:N4	81:L5:1438:U:O4	2.43	0.51
81:L5:1693:U:H2'	81:L5:1694:C:O4'	2.09	0.51
81:L5:3787:G:H1'	81:L5:3789:C:N4	2.25	0.51
4:L8:75:OMG:OP2	28:LY:74:TYR:OH	2.27	0.51
22:LS:83:ARG:HG3	22:LS:125:GLN:HB2	1.91	0.51
33:Ld:64:ILE:HG23	33:Ld:68:LEU:HD23	1.93	0.51
36:Lg:15:THR:O	36:Lg:19:LYS:NZ	2.43	0.51
47:S2:1278:A:H2'	47:S2:1279:C:C6	2.45	0.51
52:SE:182:MET:HG3	52:SE:192:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:164:LYS:HB3	54:SG:167:LYS:HB2	1.92	0.51
62:SO:53:ILE:HG23	62:SO:88:LEU:HD12	1.92	0.51
81:L5:455:C:O2'	81:L5:456:C:H5'	2.11	0.51
81:L5:1857:C:H2'	81:L5:1858:A:H8	1.76	0.51
9:LE:141:ARG:NH2	35:Lf:110:ILE:O	2.43	0.51
45:Lp:23:ARG:NH2	81:L5:2875:C:OP1	2.43	0.51
46:Lr:98:ARG:HG3	46:Lr:107:ARG:HD3	1.93	0.51
47:S2:964:A:H2'	47:S2:965:U:H6	1.76	0.51
47:S2:1406:G:H2'	47:S2:1407:U:C6	2.45	0.51
47:S2:1538:C:H2'	47:S2:1539:U:C6	2.45	0.51
51:SD:225:GLU:HG2	80:Sg:187:ASN:HB3	1.92	0.51
56:SI:26:LYS:HD2	56:SI:29:LEU:HD23	1.93	0.51
66:SS:15:VAL:HG21	66:SS:20:ILE:HD12	1.92	0.51
76:Sc:42:ILE:HD11	76:Sc:44:ARG:HD3	1.92	0.51
81:L5:318:A:H2'	81:L5:319:A:C8	2.45	0.51
81:L5:2745:A:H2'	81:L5:2746:A:H8	1.76	0.51
12:LH:59:LYS:HE2	12:LH:66:GLU:HB3	1.93	0.51
15:LL:201:GLU:O	15:LL:205:GLN:HG2	2.11	0.51
47:S2:562:U:H2'	47:S2:563:G:C8	2.46	0.51
48:SA:94:THR:HG23	48:SA:186:ARG:HH22	1.75	0.51
81:L5:460:C:H2'	81:L5:461:G:C8	2.44	0.51
81:L5:4541:G:N2	81:L5:4544:A:OP2	2.32	0.51
1:CB:594:LYS:HG2	1:CB:601:ARG:HG2	1.93	0.51
4:L8:19:C:H2'	4:L8:20:A:C8	2.46	0.51
8:LD:120:GLU:O	8:LD:248:ARG:NH1	2.32	0.51
24:LU:24:ASP:OD1	24:LU:26:THR:HG23	2.11	0.51
48:SA:80:ARG:NH1	48:SA:126:ASP:OD2	2.44	0.51
56:SI:128:LYS:O	56:SI:130:THR:N	2.43	0.51
81:L5:91:G:H5'	81:L5:93:G:N7	2.26	0.51
1:CB:434:TYR:CE1	1:CB:442:LEU:HD23	2.46	0.51
21:LR:39:GLN:NE2	81:L5:2711:G:OP2	2.43	0.51
47:S2:106:C:H2'	47:S2:107:A:H8	1.76	0.51
47:S2:344:U:H2'	47:S2:345:U:C6	2.46	0.51
47:S2:1328:OMG:N1	47:S2:1501:C:N3	2.51	0.51
50:SC:105:GLU:HB3	50:SC:216:MET:HE1	1.93	0.51
57:SJ:58:ARG:O	57:SJ:62:THR:HG23	2.10	0.51
57:SJ:107:GLU:O	57:SJ:113:GLN:NE2	2.42	0.51
81:L5:1940:G:N2	81:L5:4434:C:OP1	2.44	0.51
16:LM:136:LEU:O	16:LM:137:LYS:HG3	2.11	0.51
47:S2:12:U:H2'	47:S2:13:C:C6	2.45	0.51
47:S2:1010:G:H2'	47:S2:1011:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1445:PSU:O2'	47:S2:1446:A:H8	1.94	0.51
47:S2:1564:C:P	67:ST:121:ARG:HH22	2.34	0.51
50:SC:185:THR:O	50:SC:246:LYS:HD2	2.11	0.51
52:SE:174:LYS:O	52:SE:179:ASN:ND2	2.44	0.51
58:SK:32:HIS:CE1	58:SK:34:GLU:HB2	2.46	0.51
81:L5:469:C:H2'	81:L5:470:A:C8	2.46	0.51
1:CB:423:THR:HG22	1:CB:450:THR:H	1.76	0.51
11:LG:53:ARG:NH2	81:L5:4165:C:OP1	2.44	0.51
18:LO:5:GLN:HG3	18:LO:6:VAL:N	2.26	0.51
24:LU:105:ASN:HD21	24:LU:111:GLU:HG2	1.76	0.51
38:Li:63:VAL:HG12	38:Li:65:LYS:HG3	1.93	0.51
47:S2:907:G:H2'	47:S2:908:A:C8	2.46	0.51
47:S2:1102:G:OP2	49:SB:151:ARG:NH2	2.44	0.51
52:SE:45:ILE:HA	52:SE:61:VAL:HG11	1.93	0.51
66:SS:14:ARG:NH2	66:SS:17:ASN:O	2.43	0.51
81:L5:907:C:H2'	81:L5:908:G:C8	2.44	0.51
81:L5:2497:C:H2'	81:L5:2498:C:H6	1.75	0.51
1:CB:756:VAL:HG11	1:CB:782:PHE:HB2	1.93	0.50
3:CD:200:ASP:OD1	3:CD:200:ASP:N	2.40	0.50
10:LF:95:ILE:HB	10:LF:220:MET:HE1	1.93	0.50
13:LI:180:GLU:O	13:LI:184:MET:HG3	2.11	0.50
20:LQ:2:GLY:N	81:L5:2072:C:OP1	2.44	0.50
47:S2:557:U:H2'	47:S2:558:G:C8	2.45	0.50
47:S2:1016:U:H5''	61:SN:14:SER:HB3	1.93	0.50
47:S2:1118:C:O2'	75:Sb:75:GLU:OE2	2.30	0.50
47:S2:1457:U:H2'	47:S2:1458:G:C8	2.46	0.50
74:Sa:60:ASP:OD1	74:Sa:60:ASP:N	2.44	0.50
80:Sg:304:ASP:O	80:Sg:306:LEU:N	2.43	0.50
81:L5:406:C:O2'	81:L5:407:A:OP1	2.27	0.50
81:L5:4370:OMG:C5	92:L5:5109:3HE:H20	2.46	0.50
3:CD:223:ASP:HB3	51:SD:117:ARG:HB2	1.92	0.50
22:LS:48:VAL:HG13	22:LS:54:MET:HB3	1.93	0.50
40:Lk:59:SER:O	40:Lk:59:SER:OG	2.24	0.50
47:S2:26:U:O2'	47:S2:27:A2M:H5'	2.12	0.50
47:S2:352:U:H2'	47:S2:353:C:C6	2.47	0.50
80:Sg:29:ASP:OD1	80:Sg:47:ARG:NH2	2.45	0.50
80:Sg:48:ASP:OD2	80:Sg:50:THR:OG1	2.21	0.50
81:L5:1444:G:H2'	81:L5:1445:U:O4'	2.12	0.50
81:L5:1734:G:N2	81:L5:1735:U:O4	2.29	0.50
81:L5:4460:U:H2'	81:L5:4461:C:C6	2.46	0.50
55:SH:10:LYS:HD2	55:SH:12:ASN:OD1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SM:43:ASP:OD1	79:Sf:106:TYR:OH	2.16	0.50
81:L5:1962:A:H2	81:L5:2024:G:H21	1.59	0.50
5:LA:50:HIS:CD2	81:L5:2741:U:H2'	2.47	0.50
10:LF:96:ARG:NH2	81:L5:1895:G:OP1	2.44	0.50
20:LQ:12:LYS:HD2	81:L5:2082:G:H5''	1.94	0.50
47:S2:215:G:H2'	47:S2:216:C:H6	1.77	0.50
47:S2:809:A:OP1	52:SE:187:ALA:N	2.44	0.50
47:S2:1736:G:H2'	47:S2:1737:G:C8	2.46	0.50
81:L5:1994:C:H2'	81:L5:1995:G:C8	2.47	0.50
81:L5:2744:A:H2'	81:L5:2745:A:C8	2.46	0.50
81:L5:5004:C:H2'	81:L5:5005:G:O4'	2.11	0.50
83:Lq:28:PHE:HB2	83:Lq:89:VAL:HB	1.93	0.50
1:CB:610:PRO:HG2	1:CB:639:TYR:HB3	1.93	0.50
6:LB:230:GLY:O	6:LB:234:ARG:HB2	2.12	0.50
29:LZ:28:ASN:HB2	29:LZ:77:TYR:OH	2.12	0.50
32:Lc:78:ASN:HB2	32:Lc:90:ARG:HB3	1.94	0.50
47:S2:1280:G:H2'	47:S2:1281:G:H8	1.77	0.50
47:S2:1410:C:H2'	47:S2:1411:G:C8	2.46	0.50
47:S2:1720:U:H5''	47:S2:1721:U:H5''	1.93	0.50
47:S2:1849:G:H3'	47:S2:1850:MA6:H8	1.93	0.50
81:L5:1202:C:H3'	81:L5:1203:G:C5'	2.41	0.50
81:L5:2448:G:H2'	81:L5:2449:A:C8	2.46	0.50
81:L5:4107:G:H2'	81:L5:4108:G:H8	1.75	0.50
53:SF:73:THR:HG22	53:SF:93:VAL:HG21	1.93	0.50
70:SW:3:ARG:HD3	70:SW:6:VAL:HG12	1.93	0.50
81:L5:1273:G:C2'	81:L5:1274:A:H5'	2.41	0.50
81:L5:1538:U:H2'	81:L5:1539:G:H8	1.76	0.50
3:CD:210:ARG:NH2	47:S2:624:C:O2'	2.45	0.50
24:LU:105:ASN:HD21	24:LU:111:GLU:CG	2.25	0.50
27:LX:87:MET:HE1	27:LX:155:ILE:HG22	1.92	0.50
31:Lb:6:ASN:HB2	81:L5:4219:A:O3'	2.12	0.50
47:S2:1182:A:C5	47:S2:1183:A:H1'	2.47	0.50
60:SM:117:GLU:HA	60:SM:121:LYS:HD3	1.93	0.50
76:Sc:20:ARG:NH2	76:Sc:25:GLY:O	2.38	0.50
15:LL:63:THR:CG2	30:La:66:ASN:HB3	2.39	0.50
16:LM:113:MET:HG3	81:L5:4881:U:C4	2.47	0.50
33:Ld:37:GLY:O	33:Ld:41:ARG:HG3	2.11	0.50
60:SM:60:MET:HA	60:SM:63:LYS:HG2	1.94	0.50
80:Sg:24:THR:HG23	80:Sg:27:PHE:H	1.77	0.50
81:L5:1820:C:O2'	81:L5:1821:G:N7	2.44	0.50
81:L5:2104:G:H2'	81:L5:2105:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:3772:U:H3'	81:L5:3773:U:H5''	1.93	0.50
17:LN:90:ASN:ND2	81:L5:3928:A:OP1	2.41	0.50
28:LY:83:GLU:OE2	28:LY:84:ARG:NH2	2.45	0.50
47:S2:38:A:OP1	57:SJ:5:ARG:HG2	2.12	0.50
53:SF:112:LEU:O	53:SF:116:ILE:HG12	2.12	0.50
53:SF:136:ARG:O	53:SF:203:ASN:HB3	2.12	0.50
54:SG:137:ARG:HB3	54:SG:140:ARG:HG3	1.93	0.50
57:SJ:53:ILE:HD13	57:SJ:81:LEU:HD21	1.93	0.50
66:SS:89:ASP:OD1	66:SS:90:VAL:N	2.45	0.50
1:CB:21:ASN:ND2	1:CB:415:ARG:HH11	2.05	0.49
49:SB:129:THR:OG1	49:SB:131:ASP:OD1	2.29	0.49
57:SJ:45:ARG:O	57:SJ:49:THR:HG23	2.11	0.49
71:SX:28:LYS:HE3	71:SX:32:LEU:HD22	1.93	0.49
81:L5:1076:C:H2'	81:L5:1077:C:C6	2.47	0.49
81:L5:1345:A:H2'	81:L5:1346:C:C6	2.46	0.49
81:L5:2016:C:H2'	81:L5:2017:A:H8	1.77	0.49
81:L5:3717:A:H2'	81:L5:3718:A2M:H8	1.94	0.49
83:Lq:28:PHE:CE1	83:Lq:192:VAL:HB	2.47	0.49
3:CD:226:THR:HG22	3:CD:227:GLU:HG3	1.93	0.49
6:LB:176:LYS:HG3	81:L5:4986:G:H5''	1.93	0.49
7:LC:254:GLU:O	7:LC:258:ARG:HG3	2.12	0.49
22:LS:53:LYS:NZ	82:L7:74:A:O2'	2.38	0.49
47:S2:1713:C:H2'	47:S2:1714:U:C6	2.48	0.49
56:SI:61:ASP:OD1	56:SI:61:ASP:N	2.37	0.49
66:SS:64:VAL:O	66:SS:68:ILE:HG12	2.12	0.49
81:L5:2803:U:H2'	81:L5:2804:OMC:H6	1.77	0.49
1:CB:829:SER:HB2	1:CB:831:PRO:HD2	1.94	0.49
15:LL:200:LYS:O	15:LL:204:GLU:HG2	2.12	0.49
32:Lc:38:ILE:HG21	32:Lc:63:TYR:HB3	1.92	0.49
39:Lj:65:ARG:O	39:Lj:69:ILE:HD12	2.12	0.49
47:S2:15:U:H2'	47:S2:16:G:O4'	2.11	0.49
47:S2:501:C:O2	47:S2:501:C:H2'	2.12	0.49
47:S2:799:U:H2'	47:S2:800:U:C6	2.46	0.49
47:S2:988:C:H5''	49:SB:116:LYS:HG2	1.93	0.49
51:SD:214:LYS:HA	51:SD:214:LYS:HE2	1.95	0.49
54:SG:22:ARG:HA	54:SG:25:ARG:HH21	1.75	0.49
81:L5:264:C:H2'	81:L5:265:C:C6	2.47	0.49
81:L5:1081:C:C2'	81:L5:1082:C:H5'	2.41	0.49
81:L5:4770:U:H2'	81:L5:4771:C:C5	2.46	0.49
83:Lq:26:LYS:HB3	83:Lq:95:LEU:HD21	1.93	0.49
7:LC:334:THR:HG21	10:LF:51:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:133:PHE:O	9:LE:138:ARG:NH2	2.43	0.49
31:Lb:32:LEU:HD12	81:L5:1464:C:H5''	1.94	0.49
31:Lb:56:LYS:HE2	81:L5:1812:C:H5''	1.94	0.49
52:SE:255:ARG:O	52:SE:259:LYS:HG2	2.13	0.49
80:Sg:124:SER:OG	80:Sg:125:ARG:N	2.44	0.49
2:CC:39:U:H2'	2:CC:40:C:C6	2.48	0.49
8:LD:41:LYS:HB2	23:LT:68:THR:O	2.11	0.49
20:LQ:87:THR:HG21	81:L5:1503:A:N6	2.28	0.49
47:S2:1457:U:H2'	47:S2:1458:G:H8	1.78	0.49
47:S2:1562:C:H2'	47:S2:1563:G:H8	1.77	0.49
47:S2:1678:A2M:O2'	47:S2:1679:A:H5'	2.13	0.49
52:SE:97:GLU:HB3	52:SE:99:PHE:CE2	2.47	0.49
81:L5:753:C:H41	81:L5:910:G:H1	1.59	0.49
81:L5:1700:G:O2'	81:L5:1701:A:O5'	2.29	0.49
81:L5:3720:G:H22	81:L5:3733:A:H2	1.59	0.49
81:L5:4859:C:H3'	81:L5:4860:G:C8	2.45	0.49
1:CB:143:LEU:O	1:CB:147:ILE:HG12	2.12	0.49
1:CB:327:ASP:HA	1:CB:330:LYS:HE2	1.92	0.49
6:LB:213:GLN:HG3	6:LB:214:ASP:OD2	2.13	0.49
6:LB:247:GLY:HA2	81:L5:2838:G:H5'	1.93	0.49
8:LD:181:PRO:HD2	8:LD:195:HIS:CD2	2.48	0.49
18:LO:72:HIS:O	18:LO:74:ARG:NH1	2.43	0.49
49:SB:124:HIS:HA	49:SB:137:LEU:O	2.12	0.49
50:SC:65:LYS:HE3	50:SC:273:LEU:HD13	1.93	0.49
63:SP:13:ARG:HA	63:SP:13:ARG:HE	1.77	0.49
79:Sf:126:CYS:HB3	79:Sf:143:LYS:HD3	1.94	0.49
81:L5:244:G:H2'	81:L5:246:G:H5''	1.95	0.49
81:L5:1503:A:H4'	81:L5:1504:G:H5'	1.94	0.49
81:L5:1786:A:H2'	81:L5:1789:C:C5	2.48	0.49
81:L5:3723:A:H2'	81:L5:3724:A2M:C8	2.42	0.49
81:L5:3911:C:H2'	81:L5:3912:U:H6	1.77	0.49
81:L5:4584:A:H2'	81:L5:4585:U:O4'	2.12	0.49
81:L5:4860:G:H2'	81:L5:4861:G:C8	2.47	0.49
12:LH:60:TRP:HB2	81:L5:4764:A:N1	2.28	0.49
47:S2:113:G:H21	47:S2:293:C:H5'	1.77	0.49
47:S2:1860:A:H3'	74:Sa:8:ASN:HB3	1.94	0.49
51:SD:192:TRP:NE1	51:SD:201:LYS:O	2.39	0.49
56:SI:192:GLY:O	56:SI:196:GLU:HG3	2.12	0.49
79:Sf:118:ARG:HG2	79:Sf:118:ARG:HH11	1.78	0.49
80:Sg:165:ILE:HD11	80:Sg:179:LEU:HD13	1.94	0.49
81:L5:162:A:H2'	81:L5:163:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:1366:G:O2'	81:L5:1367:C:O2	2.28	0.49
81:L5:1656:U:O2'	81:L5:3906:A:N1	2.39	0.49
81:L5:2409:U:H5	81:L5:2783:A:N1	2.11	0.49
81:L5:4738:C:H2'	81:L5:4739:C:H6	1.76	0.49
4:L8:26:C:O2'	7:LC:53:ALA:O	2.29	0.49
18:LO:31:ARG:O	18:LO:33:VAL:HG23	2.13	0.49
23:LT:27:LEU:HB3	23:LT:31:MET:HE3	1.95	0.49
26:LW:113:LYS:O	26:LW:116:LYS:HG3	2.13	0.49
34:Le:35:TRP:CH2	34:Le:55:MET:HG2	2.47	0.49
47:S2:554:A:N7	47:S2:589:G:H5''	2.28	0.49
48:SA:30:LEU:HD21	48:SA:35:GLU:HG2	1.95	0.49
55:SH:60:ILE:HB	55:SH:92:VAL:HG12	1.95	0.49
59:SL:76:VAL:HG12	59:SL:125:ILE:HG13	1.94	0.49
81:L5:158:A:H5''	81:L5:159:C:H2'	1.95	0.49
81:L5:325:U:H2'	81:L5:326:C:C6	2.47	0.49
81:L5:1443:A:H2'	81:L5:1444:G:C4	2.47	0.49
81:L5:4770:U:H2'	81:L5:4771:C:C6	2.48	0.49
81:L5:5023:C:H3'	81:L5:5024:C:H4'	1.93	0.49
16:LM:119:ARG:O	16:LM:123:ILE:HG12	2.13	0.49
47:S2:1013:U:OP1	47:S2:1129:G:O2'	2.31	0.49
47:S2:1270:G:O2'	47:S2:1301:A:N7	2.41	0.49
47:S2:1784:G:P	47:S2:1784:G:H8	2.36	0.49
48:SA:82:THR:O	48:SA:82:THR:OG1	2.28	0.49
55:SH:51:ILE:HG12	55:SH:61:ILE:HD11	1.94	0.49
56:SI:165:GLN:HB3	56:SI:171:LEU:HD23	1.95	0.49
60:SM:92:CYS:HA	60:SM:103:VAL:HG22	1.95	0.49
80:Sg:241:PHE:HE1	80:Sg:261:LEU:HD11	1.78	0.49
81:L5:753:C:H5	81:L5:910:G:H22	1.61	0.49
81:L5:2543:A:H2	81:L5:2773:G:H22	1.60	0.49
81:L5:4239:A:H2'	81:L5:4240:G:H8	1.76	0.49
81:L5:4537:C:H2'	81:L5:4538:G:H8	1.78	0.49
11:LG:131:LYS:HD2	11:LG:132:ARG:H	1.77	0.49
19:LP:40:HIS:CE1	19:LP:157:VAL:HB	2.48	0.49
24:LU:28:PRO:HB2	24:LU:34:MET:HB2	1.94	0.49
47:S2:953:C:H2'	47:S2:954:U:O4'	2.13	0.49
47:S2:1636:G:O2'	53:SF:164:ARG:NH1	2.45	0.49
47:S2:1705:C:H2'	47:S2:1706:G:C8	2.48	0.49
49:SB:180:ASP:OD1	49:SB:180:ASP:N	2.41	0.49
50:SC:236:PHE:O	50:SC:240:THR:HG22	2.12	0.49
52:SE:98:ASN:O	52:SE:114:ILE:HG12	2.13	0.49
1:CB:112:SER:O	1:CB:116:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CD:204:LEU:HD12	47:S2:1489:A:C8	2.48	0.48
32:Lc:57:LYS:HB2	32:Lc:57:LYS:HE2	1.68	0.48
47:S2:16:G:H2'	47:S2:17:C:C6	2.48	0.48
62:SO:142:ARG:HB3	74:Sa:22:ARG:HE	1.77	0.48
81:L5:1773:U:H2'	81:L5:1774:C:C6	2.48	0.48
81:L5:4136:G:H2'	81:L5:4137:C:C6	2.48	0.48
81:L5:4460:U:H2'	81:L5:4461:C:H6	1.78	0.48
8:LD:41:LYS:HD2	23:LT:93:ILE:HG13	1.94	0.48
8:LD:83:LEU:HB3	8:LD:88:VAL:HG13	1.96	0.48
32:Lc:38:ILE:HD11	32:Lc:46:VAL:HG21	1.94	0.48
47:S2:1016:U:O2	75:Sb:30:SER:OG	2.31	0.48
58:SK:74:GLU:CD	58:SK:74:GLU:H	2.21	0.48
81:L5:4095:G:H1	81:L5:4113:U:H3	1.59	0.48
81:L5:4274:A:H2'	81:L5:4275:G:H8	1.72	0.48
81:L5:4967:A:H2'	81:L5:4968:A:H8	1.78	0.48
6:LB:80:GLU:OE1	6:LB:323:TYR:OH	2.28	0.48
18:LO:87:MET:SD	81:L5:1912:G:N2	2.86	0.48
47:S2:156:G:OP1	54:SG:2:LYS:NZ	2.40	0.48
47:S2:394:G:H5'	59:SL:81:LYS:HD3	1.96	0.48
47:S2:445:A:N7	89:S2:1939:PUT:H12	2.28	0.48
64:SQ:81:ILE:O	64:SQ:85:ARG:HG3	2.13	0.48
81:L5:4169:G:H4'	81:L5:4171:C:C2	2.48	0.48
81:L5:4630:G:N2	95:L5:5418:HOH:O	2.46	0.48
1:CB:94:ASP:OD1	1:CB:94:ASP:N	2.45	0.48
2:CC:28:U:H2'	2:CC:29:G:H8	1.78	0.48
10:LF:76:ARG:HD2	81:L5:729:G:H5''	1.95	0.48
24:LU:19:LEU:HB2	24:LU:73:THR:HG23	1.95	0.48
47:S2:207:G:H3'	47:S2:208:G:H8	1.77	0.48
47:S2:1017:U:H2'	47:S2:1018:U:H6	1.79	0.48
47:S2:1147:C:OP1	74:Sa:6:ARG:NH1	2.46	0.48
51:SD:61:GLU:O	51:SD:61:GLU:HG2	2.13	0.48
51:SD:162:ASP:N	51:SD:163:PRO:HD2	2.29	0.48
54:SG:5:ILE:HD13	54:SG:111:LEU:HB2	1.94	0.48
57:SJ:78:LEU:HB3	57:SJ:92:MET:HE3	1.95	0.48
81:L5:1095:A:N6	81:L5:1200:G:H1	2.09	0.48
81:L5:4628:PSU:N1	95:L5:5403:HOH:O	2.34	0.48
27:LX:110:LYS:HG2	27:LX:114:LYS:HD2	1.95	0.48
52:SE:138:HIS:CD2	52:SE:148:ARG:HG3	2.49	0.48
54:SG:67:VAL:HG12	54:SG:69:THR:HG22	1.96	0.48
80:Sg:67:SER:HG	80:Sg:83:TRP:CD1	2.32	0.48
81:L5:1178:G:H2'	81:L5:1178:G:N3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:2469:C:H5'	81:L5:2470:C:OP2	2.14	0.48
81:L5:2497:C:H2'	81:L5:2498:C:C6	2.48	0.48
81:L5:2601:A:N6	81:L5:2744:A:OP2	2.42	0.48
81:L5:4738:C:H2'	81:L5:4739:C:C6	2.49	0.48
83:Lq:112:ARG:HG3	83:Lq:112:ARG:HH11	1.77	0.48
17:LN:85:VAL:HA	44:Lo:49:GLY:HA2	1.94	0.48
41:Ll:44:TRP:CZ3	41:Ll:45:ARG:HD3	2.48	0.48
47:S2:1405:A:H2'	47:S2:1406:G:O4'	2.14	0.48
57:SJ:136:ARG:NH1	57:SJ:159:PHE:O	2.46	0.48
66:SS:38:ARG:HB3	67:ST:45:LEU:HD21	1.95	0.48
81:L5:934:C:H5''	81:L5:935:A:OP1	2.14	0.48
81:L5:2640:G:H2'	81:L5:2641:A:C8	2.49	0.48
1:CB:381:ALA:HB1	1:CB:395:MET:SD	2.53	0.48
10:LF:24:ASN:HA	10:LF:27:GLU:OE2	2.13	0.48
15:LL:16:LYS:HG2	81:L5:46:U:H5''	1.96	0.48
19:LP:76:TRP:CD1	19:LP:76:TRP:H	2.32	0.48
21:LR:6:LEU:HD12	21:LR:9:ARG:HH21	1.78	0.48
21:LR:126:LYS:HG2	21:LR:131:VAL:HG21	1.96	0.48
52:SE:151:ASP:HB3	52:SE:154:ILE:HG13	1.95	0.48
66:SS:66:ARG:O	66:SS:70:ILE:HG13	2.13	0.48
67:ST:32:GLU:CD	67:ST:32:GLU:H	2.22	0.48
81:L5:153:G:H2'	81:L5:154:G:C8	2.47	0.48
81:L5:2465:C:H2'	81:L5:2466:G:O4'	2.14	0.48
81:L5:4611:A:H2'	81:L5:4612:C:H6	1.79	0.48
16:LM:94:LYS:HE3	81:L5:4871:C:OP1	2.13	0.48
17:LN:189:ARG:HE	17:LN:193:ARG:NH1	2.12	0.48
20:LQ:178:ARG:HA	20:LQ:184:ARG:O	2.14	0.48
29:LZ:46:ILE:HG23	29:LZ:68:ILE:HG23	1.95	0.48
30:La:29:PRO:HG3	81:L5:1654:G:H5'	1.96	0.48
30:La:119:LYS:HA	30:La:140:VAL:HG22	1.96	0.48
46:Lr:68:SER:HB2	81:L5:669:C:H5'	1.96	0.48
47:S2:1533:A:C2	47:S2:1536:G:N3	2.81	0.48
57:SJ:33:GLY:HA3	78:Se:38:TYR:CG	2.49	0.48
72:SY:7:ILE:HG23	72:SY:25:ILE:HG23	1.96	0.48
81:L5:494:U:H2'	81:L5:495:C:C6	2.48	0.48
81:L5:1247:U:H2'	81:L5:1248:C:C6	2.49	0.48
81:L5:1346:C:H2'	81:L5:1347:G:H8	1.78	0.48
81:L5:2496:G:H2'	81:L5:2497:C:C6	2.49	0.48
8:LD:208:MET:HB2	8:LD:233:PRO:HG3	1.96	0.48
9:LE:277:LEU:HD23	9:LE:277:LEU:HA	1.72	0.48
14:LJ:73:THR:HG22	82:L7:39:C:N3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LO:181:ALA:O	18:LO:185:VAL:HG22	2.13	0.48
34:Le:38:PRO:HB3	34:Le:43:ASN:OD1	2.14	0.48
42:Lm:109:ASN:ND2	42:Lm:117:HIS:O	2.39	0.48
47:S2:27:A2M:H5''	47:S2:484:A2M:H1'	1.96	0.48
47:S2:218:U:H2'	47:S2:219:U:C6	2.49	0.48
47:S2:1213:C:H2'	47:S2:1214:A:C8	2.48	0.48
47:S2:1455:A:H2'	47:S2:1456:G:H8	1.79	0.48
47:S2:1865:C:O2	74:Sa:92:ARG:HG2	2.14	0.48
58:SK:21:MET:HE2	58:SK:21:MET:HB2	1.78	0.48
61:SN:3:ARG:HG2	61:SN:3:ARG:HH11	1.79	0.48
81:L5:1733:G:N3	81:L5:4214:A:H2'	2.28	0.48
81:L5:2264:C:H2'	81:L5:2265:G:O4'	2.14	0.48
81:L5:3925:OMU:HM23	81:L5:3925:OMU:H1'	1.55	0.48
1:CB:584:SER:HB3	1:CB:739:ARG:HG3	1.95	0.48
5:LA:248:GLY:HA3	47:S2:1069:U:H5''	1.95	0.48
20:LQ:151:HIS:CE1	20:LQ:164:LYS:HG2	2.48	0.48
46:Lr:37:SER:HB2	81:L5:2267:U:OP1	2.14	0.48
47:S2:1227:G:C2	47:S2:1228:A:C8	3.02	0.48
47:S2:1365:G:H2'	47:S2:1366:G:C8	2.48	0.48
47:S2:1861:G:H5''	74:Sa:3:LYS:HA	1.95	0.48
54:SG:22:ARG:HA	54:SG:25:ARG:NE	2.26	0.48
81:L5:2706:G:N2	81:L5:2707:U:O2'	2.47	0.48
19:LP:54:GLN:HA	19:LP:83:TRP:CD1	2.48	0.47
47:S2:1687:C:H2'	47:S2:1688:C:H6	1.78	0.47
57:SJ:60:LEU:HD22	57:SJ:70:ARG:HA	1.96	0.47
74:Sa:90:GLU:H	74:Sa:90:GLU:CD	2.22	0.47
81:L5:2498:C:H2'	81:L5:2499:C:H6	1.79	0.47
81:L5:3732:A:H2'	81:L5:3733:A:C8	2.49	0.47
81:L5:4500:U:H2'	81:L5:4501:U:H6	1.79	0.47
11:LG:200:THR:HB	81:L5:150:U:OP2	2.14	0.47
29:LZ:85:TYR:OH	36:Lg:99:GLU:OE2	2.32	0.47
34:Le:82:VAL:HG13	34:Le:114:ARG:HG2	1.96	0.47
49:SB:144:LYS:HD3	49:SB:208:HIS:CG	2.48	0.47
68:SU:101:ILE:HD12	68:SU:102:THR:N	2.28	0.47
81:L5:106:A:H2'	81:L5:107:G:O4'	2.14	0.47
81:L5:2539:C:H2'	81:L5:2540:C:C6	2.49	0.47
1:CB:176:GLN:O	1:CB:180:ARG:HG2	2.15	0.47
4:L8:90:C:O2'	28:LY:24:HIS:ND1	2.42	0.47
9:LE:66:LYS:HD3	81:L5:979:C:OP2	2.13	0.47
10:LF:223:LYS:HB2	10:LF:223:LYS:HE2	1.78	0.47
11:LG:165:GLU:HA	11:LG:168:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LQ:11:ARG:HG3	81:L5:2081:C:H5''	1.96	0.47
47:S2:149:A:H3'	47:S2:150:A:H8	1.80	0.47
47:S2:532:C:H2'	47:S2:533:A:C8	2.50	0.47
51:SD:154:ASP:OD2	51:SD:155:GLY:N	2.48	0.47
60:SM:55:ASN:ND2	60:SM:81:ASP:HA	2.26	0.47
63:SP:65:LYS:C	63:SP:65:LYS:HD2	2.39	0.47
81:L5:1821:G:H2'	81:L5:1821:G:N3	2.29	0.47
81:L5:4258:C:H2'	81:L5:4259:C:H6	1.79	0.47
6:LB:238:LYS:HE2	6:LB:238:LYS:HB2	1.61	0.47
9:LE:67:ALA:HA	9:LE:69:TYR:CE1	2.49	0.47
17:LN:82:GLY:HA2	81:L5:4187:G:H4'	1.97	0.47
19:LP:117:ILE:HD12	19:LP:148:MET:HE2	1.97	0.47
47:S2:996:A:H2'	47:S2:997:A:C8	2.50	0.47
81:L5:23:C:H2'	81:L5:24:G:O4'	2.15	0.47
81:L5:3656:A:H2'	81:L5:3657:U:H6	1.78	0.47
4:L8:80:A:H8	4:L8:84:A:OP1	1.98	0.47
15:LL:94:ILE:HG13	15:LL:124:LEU:HD21	1.96	0.47
22:LS:93:MET:HG2	81:L5:1952:G:H4'	1.96	0.47
47:S2:433:A:H5''	56:SI:22:HIS:HB3	1.97	0.47
47:S2:573:U:O2	47:S2:576:A2M:H8	2.15	0.47
51:SD:116:ARG:HD2	51:SD:150:MET:HE1	1.96	0.47
52:SE:160:ILE:HD12	52:SE:169:ILE:HG12	1.97	0.47
57:SJ:103:GLU:OE1	57:SJ:103:GLU:N	2.48	0.47
66:SS:15:VAL:HG13	66:SS:68:ILE:CD1	2.43	0.47
74:Sa:51:ARG:O	74:Sa:55:GLU:HG3	2.15	0.47
82:L7:4:U:H2'	82:L7:5:A:H8	1.79	0.47
12:LH:40:HIS:CD2	12:LH:40:HIS:H	2.31	0.47
12:LH:120:GLU:HG2	81:L5:4611:A:H2	1.79	0.47
32:Lc:78:ASN:OD1	32:Lc:78:ASN:N	2.42	0.47
40:Lk:33:LYS:HG2	40:Lk:46:VAL:HG22	1.96	0.47
47:S2:102:A:H4'	47:S2:104:A:C8	2.48	0.47
47:S2:323:C:H3'	47:S2:327:G:H1	1.79	0.47
47:S2:384:U:O4	56:SI:5:ARG:NH2	2.28	0.47
47:S2:1563:G:OP1	67:ST:121:ARG:NH1	2.48	0.47
81:L5:318:A:H2'	81:L5:319:A:H8	1.78	0.47
81:L5:1548:G:O2'	81:L5:2812:A:N3	2.41	0.47
81:L5:4238:G:H2'	81:L5:4239:A:H8	1.79	0.47
1:CB:9:ILE:O	1:CB:13:MET:HG3	2.15	0.47
1:CB:27:HIS:ND1	1:CB:138:GLN:HB2	2.30	0.47
4:L8:16:G:N2	81:L5:417:G:O2'	2.47	0.47
4:L8:128:C:H2'	4:L8:129:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LA:178:PRO:HB2	5:LA:180:LEU:HD13	1.96	0.47
21:LR:128:LYS:HD2	81:L5:2666:U:O4	2.15	0.47
22:LS:70:LYS:HA	22:LS:70:LYS:HD3	1.72	0.47
23:LT:111:GLU:HB3	23:LT:115:LYS:HZ1	1.79	0.47
29:LZ:109:LYS:HE3	29:LZ:109:LYS:HB3	1.61	0.47
42:Lm:94:MET:HE3	42:Lm:94:MET:HB3	1.87	0.47
64:SQ:42:ILE:HG22	64:SQ:44:PRO:HD2	1.95	0.47
77:Sd:22:ARG:HD2	77:Sd:38:MET:HE2	1.95	0.47
80:Sg:185:LYS:HG2	80:Sg:186:THR:OG1	2.14	0.47
81:L5:1866:U:H2'	81:L5:1867:A:O4'	2.15	0.47
81:L5:1971:C:C5	81:L5:2000:G:H2'	2.49	0.47
81:L5:2554:U:H1'	81:L5:2574:G:N2	2.29	0.47
81:L5:2758:G:O2'	81:L5:2765:A:N3	2.47	0.47
81:L5:4088:C:H2'	81:L5:4089:G:C8	2.50	0.47
81:L5:4578:G:H2'	81:L5:4579:PSU:C6	2.50	0.47
81:L5:4954:G:H2'	81:L5:4955:A:C8	2.50	0.47
10:LF:148:LYS:HD3	10:LF:245:ARG:NH2	2.30	0.47
20:LQ:14:ARG:NH2	81:L5:2083:C:OP2	2.44	0.47
20:LQ:69:LYS:HD2	81:L5:1458:C:H5''	1.97	0.47
40:Lk:54:GLU:O	40:Lk:58:GLN:HG2	2.15	0.47
44:Lo:61:LYS:HG2	81:L5:4372:U:OP2	2.15	0.47
45:Lp:75:SER:O	45:Lp:79:VAL:HG13	2.15	0.47
47:S2:641:A:O2'	47:S2:645:C:OP1	2.31	0.47
47:S2:944:A:H5''	62:SO:134:PRO:HB3	1.97	0.47
47:S2:1258:A:C2	47:S2:1663:A:H2'	2.50	0.47
47:S2:1621:U:O2'	47:S2:1622:U:H2'	2.15	0.47
47:S2:1797:U:H2'	47:S2:1798:C:C6	2.50	0.47
59:SL:91:ASP:HB3	59:SL:104:LYS:HE2	1.95	0.47
72:SY:63:HIS:CE1	72:SY:68:LYS:HG2	2.50	0.47
81:L5:700:G:H4'	81:L5:969:C:C2	2.50	0.47
81:L5:980:U:H2'	81:L5:981:C:C6	2.50	0.47
81:L5:3861:A:H2'	81:L5:3862:A:H8	1.80	0.47
81:L5:4591:U:H2'	81:L5:4592:C:C6	2.50	0.47
6:LB:241:PRO:HD3	81:L5:4456:OMC:HM21	1.97	0.47
9:LE:219:LYS:NZ	81:L5:4940:C:OP2	2.31	0.47
34:Le:85:LEU:HD21	34:Le:115:ALA:HB2	1.95	0.47
40:Lk:24:LYS:HD2	40:Lk:69:LEU:HD21	1.96	0.47
48:SA:127:PRO:HA	48:SA:134:LEU:HD11	1.96	0.47
66:SS:121:ARG:HG2	66:SS:131:VAL:HB	1.97	0.47
74:Sa:50:VAL:O	74:Sa:54:SER:OG	2.25	0.47
81:L5:116:G:H2'	81:L5:117:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:1857:C:H2'	81:L5:1858:A:C8	2.50	0.47
81:L5:4392:OMG:HM21	81:L5:4394:A:H2'	1.96	0.47
81:L5:4399:U:H2'	81:L5:4400:G:O4'	2.15	0.47
5:LA:130:SER:HA	5:LA:169:VAL:HG22	1.96	0.47
8:LD:93:THR:O	8:LD:158:LYS:NZ	2.39	0.47
46:Lr:28:GLU:OE1	46:Lr:31:ASN:ND2	2.45	0.47
55:SH:86:LYS:HE3	55:SH:86:LYS:HB2	1.53	0.47
55:SH:162:GLN:O	55:SH:166:VAL:HG22	2.13	0.47
80:Sg:164:ILE:HG22	80:Sg:178:ASN:HA	1.97	0.47
81:L5:180:C:H2'	81:L5:181:C:C1'	2.45	0.47
81:L5:388:A:H1'	81:L5:403:G:N2	2.30	0.47
81:L5:1858:A:H2'	81:L5:1859:C:H6	1.80	0.47
81:L5:2475:G:H5''	81:L5:2476:G:C8	2.50	0.47
81:L5:4068:U:H2'	81:L5:4069:U:C6	2.50	0.47
4:L8:144:U:H2'	4:L8:145:C:H6	1.81	0.46
6:LB:224:LYS:NZ	81:L5:4626:A:OP2	2.42	0.46
6:LB:258:HIS:HB2	81:L5:4518:A:OP2	2.15	0.46
12:LH:89:ARG:HG3	12:LH:145:ILE:HG23	1.97	0.46
34:Le:35:TRP:CZ2	34:Le:56:PRO:HD2	2.50	0.46
47:S2:555:A:H2'	47:S2:557:U:H6	1.80	0.46
47:S2:1277:C:H2'	47:S2:1278:A:C8	2.50	0.46
47:S2:1511:U:H2'	47:S2:1512:C:C6	2.49	0.46
47:S2:1533:A:H2	47:S2:1536:G:N3	2.14	0.46
47:S2:1644:C:H4'	64:SQ:140:ARG:HB2	1.95	0.46
53:SF:85:LYS:O	53:SF:89:THR:HG23	2.15	0.46
55:SH:130:LEU:HD21	55:SH:156:VAL:HG21	1.97	0.46
72:SY:105:LYS:O	72:SY:109:GLU:HG3	2.15	0.46
76:Sc:29:GLN:NE2	76:Sc:45:ASN:OD1	2.32	0.46
81:L5:469:C:H2'	81:L5:470:A:H8	1.79	0.46
81:L5:3877:A:N3	81:L5:4401:G:O2'	2.38	0.46
3:CD:185:PHE:HA	3:CD:191:ARG:HA	1.96	0.46
12:LH:6:SER:HB3	12:LH:67:LEU:HD22	1.98	0.46
34:Le:107:ASN:O	34:Le:111:ILE:HG13	2.15	0.46
44:Lo:44:LYS:HE3	44:Lo:52:THR:HB	1.97	0.46
47:S2:10:G:H21	50:SC:114:LYS:HA	1.80	0.46
47:S2:184:G:H2'	47:S2:185:G:C8	2.50	0.46
47:S2:1425:G:H2'	47:S2:1426:U:C6	2.50	0.46
65:SR:71:ILE:O	65:SR:75:GLU:HG2	2.15	0.46
70:SW:28:ARG:HB3	70:SW:29:PRO:HD3	1.97	0.46
76:Sc:16:LYS:HD3	76:Sc:18:LEU:HD23	1.97	0.46
80:Sg:11:LEU:HB2	80:Sg:307:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:462:G:H2'	81:L5:463:A:C8	2.50	0.46
81:L5:1678:C:O2	89:L5:5382:PUT:N2	2.48	0.46
81:L5:1739:G:H2'	81:L5:1740:C:C6	2.51	0.46
81:L5:1994:C:H2'	81:L5:1995:G:H8	1.81	0.46
81:L5:2415:OMU:H2'	81:L5:2416:G:C8	2.50	0.46
81:L5:2602:G:H2'	81:L5:2603:C:C6	2.50	0.46
81:L5:3944:G:H1	81:L5:4069:U:H3	1.63	0.46
1:CB:835:VAL:O	1:CB:839:ARG:HG3	2.15	0.46
6:LB:168:MET:HG3	6:LB:178:ALA:HA	1.97	0.46
7:LC:84:THR:OG1	7:LC:85:HIS:N	2.48	0.46
7:LC:339:THR:HG22	7:LC:342:ARG:HH22	1.80	0.46
8:LD:193:GLU:O	8:LD:197:LYS:HG2	2.15	0.46
12:LH:106:GLN:HE21	12:LH:113:GLU:CD	2.22	0.46
28:LY:50:ARG:HD3	28:LY:115:ARG:HD2	1.98	0.46
33:Ld:92:ARG:HA	33:Ld:102:LEU:HD23	1.96	0.46
46:Lr:32:LEU:O	46:Lr:33:LYS:HB2	2.15	0.46
47:S2:568:C:H2'	47:S2:569:A:C8	2.50	0.46
47:S2:747:U:H2'	47:S2:748:C:O4'	2.14	0.46
47:S2:1272:C:O2'	47:S2:1273:C:H5'	2.15	0.46
72:SY:102:THR:HG23	72:SY:107:ARG:HE	1.80	0.46
81:L5:46:U:OP2	81:L5:47:A:O2'	2.23	0.46
81:L5:3786:U:OP1	81:L5:4550:G:O2'	2.23	0.46
81:L5:4523:A2M:H5''	81:L5:4524:G:H5'	1.98	0.46
81:L5:4741:C:H4'	81:L5:4742:G:H5'	1.97	0.46
82:L7:4:U:H2'	82:L7:5:A:C8	2.50	0.46
82:L7:16:A:H2'	82:L7:17:C:C6	2.51	0.46
1:CB:144:ARG:HG2	1:CB:144:ARG:HH11	1.80	0.46
4:L8:92:U:H2'	4:L8:93:C:O4'	2.15	0.46
6:LB:252:ALA:HB1	81:L5:4524:G:N3	2.30	0.46
7:LC:150:LEU:HD12	7:LC:150:LEU:HA	1.67	0.46
10:LF:46:ARG:HH21	31:Lb:102:PRO:HG3	1.80	0.46
15:LL:79:GLU:HG2	15:LL:110:LEU:CD1	2.44	0.46
34:Le:43:ASN:HD21	34:Le:45:VAL:HG13	1.80	0.46
34:Le:113:GLU:O	34:Le:117:GLN:HG3	2.15	0.46
47:S2:443:U:H2'	47:S2:444:G:O4'	2.15	0.46
59:SL:111:VAL:HG12	59:SL:140:PHE:HB2	1.97	0.46
64:SQ:53:GLU:HG2	64:SQ:54:PRO:HD3	1.97	0.46
81:L5:406:C:H2'	81:L5:407:A:C8	2.50	0.46
81:L5:753:C:H5	81:L5:910:G:H1	1.62	0.46
81:L5:1551:C:H2'	81:L5:1552:G:O4'	2.16	0.46
81:L5:1588:U:H2'	81:L5:1589:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:1941:A:C2	81:L5:4434:C:H5'	2.51	0.46
81:L5:1961:G:OP2	83:Lq:59:THR:OG1	2.34	0.46
81:L5:4254:G:H2'	81:L5:4254:G:N3	2.31	0.46
81:L5:4750:G:H2'	81:L5:4751:G:C8	2.51	0.46
3:CD:287:TRP:O	3:CD:291:GLN:HG2	2.16	0.46
4:L8:17:A:H1'	81:L5:418:A:C2	2.51	0.46
12:LH:57:VAL:HG23	12:LH:70:VAL:HG13	1.97	0.46
24:LU:105:ASN:HD22	24:LU:113:ARG:HH21	1.62	0.46
46:Lr:47:LYS:O	46:Lr:103:ARG:HD2	2.16	0.46
47:S2:453:C:O2'	54:SG:92:ARG:O	2.25	0.46
47:S2:1403:C:C4	47:S2:1433:C:H2'	2.51	0.46
48:SA:50:ASN:O	48:SA:54:THR:HG23	2.16	0.46
50:SC:187:ARG:HB3	50:SC:187:ARG:HH11	1.81	0.46
53:SF:77:MET:HE2	53:SF:86:LYS:HD3	1.96	0.46
54:SG:22:ARG:CA	54:SG:25:ARG:HH21	2.28	0.46
81:L5:2611:A:H2'	81:L5:2612:G:C8	2.49	0.46
81:L5:3753:G:C8	81:L5:3776:G:C8	3.04	0.46
1:CB:846:GLU:OE2	1:CB:846:GLU:N	2.25	0.46
5:LA:31:ALA:HB2	5:LA:123:ARG:HH21	1.81	0.46
6:LB:305:THR:C	6:LB:307:TYR:H	2.23	0.46
7:LC:1:MET:SD	7:LC:3:CYS:N	2.86	0.46
27:LX:148:ASP:OD1	27:LX:149:VAL:N	2.49	0.46
53:SF:35:LEU:HD22	53:SF:147:VAL:HG23	1.97	0.46
62:SO:98:ARG:NH1	62:SO:99:ALA:O	2.48	0.46
81:L5:1273:G:O2'	81:L5:1274:A:H5'	2.16	0.46
81:L5:2411:C:H2'	81:L5:2412:A:H8	1.80	0.46
5:LA:194:ASN:ND2	95:LA:401:HOH:O	2.44	0.46
7:LC:11:TYR:CZ	7:LC:148:PRO:HB2	2.51	0.46
8:LD:278:ASP:O	8:LD:282:GLN:HG3	2.16	0.46
11:LG:164:ILE:HG13	11:LG:168:VAL:HG13	1.96	0.46
14:LJ:140:SER:O	14:LJ:144:LYS:HG3	2.16	0.46
47:S2:43:U:OP2	47:S2:485:A:N6	2.48	0.46
47:S2:606:G:H1'	78:Se:58:ASN:OD1	2.16	0.46
47:S2:948:C:H2'	47:S2:949:G:C8	2.51	0.46
47:S2:1328:OMG:HM23	47:S2:1328:OMG:H1'	1.79	0.46
51:SD:158:ILE:HG12	51:SD:189:MET:HE3	1.97	0.46
81:L5:128:C:H2'	81:L5:129:C:C6	2.51	0.46
81:L5:270:U:H2'	81:L5:271:C:C6	2.50	0.46
81:L5:1326:A2M:H2'	81:L5:1327:C:C6	2.50	0.46
81:L5:4507:A:H2'	81:L5:4508:C:C6	2.51	0.46
8:LD:184:ASP:OD2	8:LD:187:SER:OG	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:176:THR:HG23	9:LE:177:GLY:N	2.30	0.46
11:LG:176:LYS:HD2	38:Li:43:MET:CE	2.45	0.46
12:LH:90:TYR:CE2	12:LH:184:LYS:HD3	2.51	0.46
28:LY:8:THR:OG1	81:L5:347:A:OP2	2.28	0.46
44:Lo:2:VAL:N	44:Lo:90[B]:HIS:O	2.49	0.46
44:Lo:2:VAL:N	44:Lo:90[A]:HIS:O	2.49	0.46
47:S2:1279:C:H2'	47:S2:1280:G:H8	1.81	0.46
47:S2:1374:C:H2'	47:S2:1375:G:O4'	2.15	0.46
47:S2:1703:OMC:H5	47:S2:1871:6MZ:N6	2.09	0.46
47:S2:1740:C:H2'	47:S2:1741:U:C6	2.51	0.46
48:SA:34:MET:HE2	48:SA:149:ASN:O	2.16	0.46
54:SG:143:LYS:HB2	54:SG:143:LYS:HE3	1.67	0.46
54:SG:165:GLU:CD	54:SG:165:GLU:H	2.24	0.46
55:SH:106:ARG:HG3	55:SH:109:ARG:NH1	2.31	0.46
56:SI:22:HIS:C	56:SI:22:HIS:ND1	2.73	0.46
62:SO:120:ALA:HB2	74:Sa:53:ILE:HD13	1.98	0.46
79:Sf:120:GLU:OE2	79:Sf:129:GLY:N	2.49	0.46
81:L5:182:G:H2'	81:L5:183:C:C6	2.51	0.46
81:L5:2588:C:OP1	81:L5:2768:C:O2'	2.23	0.46
7:LC:116:ASN:HB2	7:LC:119:GLN:HG3	1.98	0.46
7:LC:221:PHE:O	7:LC:222:ARG:HB3	2.16	0.46
11:LG:108:GLN:O	11:LG:112:GLN:HG2	2.16	0.46
18:LO:44:SER:OG	81:L5:2054:U:OP2	2.26	0.46
31:Lb:51:LYS:HB3	31:Lb:51:LYS:HE3	1.84	0.46
37:Lh:4:ILE:HG22	37:Lh:56:ARG:HD2	1.98	0.46
47:S2:85:A:H2'	47:S2:86:C:H6	1.80	0.46
47:S2:1189:A:OP1	71:SX:28:LYS:HE2	2.16	0.46
61:SN:87:ASP:OD1	61:SN:87:ASP:N	2.47	0.46
74:Sa:18:VAL:HG21	74:Sa:33:ASP:OD2	2.16	0.46
80:Sg:3:GLU:OE1	80:Sg:245:ARG:NE	2.43	0.46
80:Sg:35:SER:OG	80:Sg:36:ARG:N	2.49	0.46
81:L5:1308:C:H2'	81:L5:1309:C:C6	2.50	0.46
81:L5:1735:U:H5'	89:L5:5387:PUT:H21	1.97	0.46
81:L5:1846:G:H2'	81:L5:1847:C:C6	2.51	0.46
81:L5:1977:C:O2'	81:L5:1978:C:OP1	2.32	0.46
81:L5:2306:G:H1'	81:L5:2332:A:N6	2.31	0.46
81:L5:4699:U:H1'	81:L5:4700:A:H5''	1.97	0.46
81:L5:5030:U:H2'	81:L5:5031:G:C8	2.50	0.46
11:LG:212:LYS:HB2	11:LG:212:LYS:HE2	1.63	0.46
18:LO:142:ALA:HA	18:LO:145:VAL:HG22	1.98	0.46
47:S2:1238:PSU:O4	47:S2:1242:U:H5	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1472:C:H2'	47:S2:1473:G:O4'	2.16	0.46
53:SF:69:VAL:O	53:SF:73:THR:HG23	2.16	0.46
81:L5:3697:U:H5''	81:L5:3698:G:H5'	1.98	0.46
81:L5:4894:A:H5''	81:L5:4896:G:H5'	1.98	0.46
1:CB:830:ARG:O	1:CB:834:VAL:HG22	2.16	0.45
5:LA:204:MET:HG2	81:L5:1631:A:C2	2.51	0.45
18:LO:176:ARG:HD3	81:L5:4769:G:H5''	1.97	0.45
21:LR:172:ARG:O	21:LR:175:GLU:HG3	2.16	0.45
47:S2:158:A:H3'	47:S2:159:A2M:H8	1.98	0.45
56:SI:131:PRO:C	56:SI:133:GLU:H	2.23	0.45
65:SR:32:LYS:HG3	65:SR:47:ARG:NE	2.31	0.45
67:ST:27:LYS:HB2	67:ST:27:LYS:HE3	1.71	0.45
81:L5:908:G:H2'	81:L5:909:A:H8	1.81	0.45
81:L5:1079:C:C2	81:L5:1080:C:C5	3.03	0.45
81:L5:1194:G:H2'	81:L5:1195:G:C8	2.51	0.45
81:L5:2693:G:H2'	81:L5:2694:G:C2	2.51	0.45
81:L5:4734:A:H1'	81:L5:4735:G:C8	2.51	0.45
5:LA:54:ARG:HG2	5:LA:56:ALA:H	1.82	0.45
11:LG:243:GLY:O	11:LG:247:VAL:HG13	2.17	0.45
15:LL:79:GLU:HG2	15:LL:110:LEU:HD13	1.99	0.45
17:LN:184:ILE:HD12	81:L5:99:A:H5''	1.98	0.45
21:LR:99:MET:HE2	21:LR:99:MET:HA	1.98	0.45
23:LT:107:LYS:NZ	23:LT:111:GLU:OE1	2.48	0.45
41:LI:33:ASN:O	41:LI:34:LYS:HG2	2.16	0.45
47:S2:44:U:O2	47:S2:482:G:H1'	2.16	0.45
47:S2:1010:G:H2'	47:S2:1011:A:H8	1.82	0.45
47:S2:1203:G:H4'	50:SC:116:THR:HA	1.97	0.45
47:S2:1378:A:OP2	48:SA:102:ARG:NH1	2.47	0.45
47:S2:1444:U:O2'	47:S2:1445:PSU:H5''	2.16	0.45
51:SD:16:ILE:HG21	77:Sd:22:ARG:NH1	2.31	0.45
55:SH:139:ILE:HG23	55:SH:156:VAL:HG13	1.98	0.45
56:SI:129:LEU:HG	56:SI:131:PRO:HD3	1.98	0.45
60:SM:35:ILE:HG13	79:Sf:102:VAL:HG21	1.97	0.45
60:SM:49:LEU:HD11	60:SM:77:ILE:HG13	1.99	0.45
81:L5:461:G:H2'	81:L5:462:G:C8	2.52	0.45
81:L5:1172:C:N4	81:L5:1188:C:N3	2.63	0.45
81:L5:2411:C:H2'	81:L5:2412:A:C8	2.51	0.45
81:L5:4991:U:H2'	81:L5:4992:G:C8	2.51	0.45
3:CD:220:THR:OG1	3:CD:221:VAL:N	2.47	0.45
4:L8:55:U:H2'	4:L8:56:G:C8	2.52	0.45
5:LA:199:VAL:HG21	81:L5:1631:A:N7	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LD:289:ARG:O	8:LD:293:ARG:HG2	2.17	0.45
10:LF:104:LYS:HE2	10:LF:104:LYS:HB2	1.72	0.45
10:LF:241:ASN:O	10:LF:245:ARG:HG2	2.16	0.45
47:S2:159:A2M:HM'3	47:S2:159:A2M:H1'	1.58	0.45
47:S2:806:U:H2'	47:S2:807:G:C8	2.51	0.45
47:S2:1259:A:H1'	47:S2:1264:C:N4	2.30	0.45
52:SE:126:VAL:HG22	52:SE:156:VAL:HA	1.98	0.45
67:ST:44:GLU:O	67:ST:45:LEU:HB2	2.16	0.45
74:Sa:41:ILE:HG12	74:Sa:68:TYR:CD2	2.52	0.45
81:L5:1244:G:H2'	81:L5:1245:C:H6	1.82	0.45
81:L5:1893:C:H1'	81:L5:1937:C:O2	2.16	0.45
5:LA:107:MET:O	5:LA:139:HIS:NE2	2.47	0.45
12:LH:103:VAL:HG11	12:LH:144:LEU:HD21	1.99	0.45
13:LI:52:MET:HB2	13:LI:152:LEU:HD22	1.99	0.45
14:LJ:64:ARG:HB3	44:Lo:104:ILE:HG12	1.99	0.45
29:LZ:29:ILE:HG22	29:LZ:32:GLY:H	1.80	0.45
33:Ld:44:ARG:O	33:Ld:48:GLU:HG2	2.15	0.45
47:S2:690:G:N2	47:S2:690:G:OP2	2.50	0.45
47:S2:690:G:H2'	47:S2:691:G:C4	2.51	0.45
47:S2:1325:G:H1'	47:S2:1510:G:H5''	1.99	0.45
47:S2:1337:4AC:H4'	68:SU:67:LYS:O	2.16	0.45
47:S2:1407:U:H2'	47:S2:1408:U:H6	1.78	0.45
48:SA:51:LEU:HA	48:SA:54:THR:HG23	1.99	0.45
50:SC:252:THR:HG22	50:SC:254:ASP:OD1	2.16	0.45
51:SD:35:SER:O	51:SD:35:SER:OG	2.30	0.45
59:SL:126:VAL:HG12	59:SL:145:VAL:HG22	1.98	0.45
62:SO:26:ASN:OD1	62:SO:26:ASN:N	2.48	0.45
80:Sg:48:ASP:OD1	80:Sg:49:GLU:N	2.50	0.45
81:L5:1199:G:H2'	81:L5:1200:G:C8	2.51	0.45
1:CB:13:MET:HB3	1:CB:468:ASN:ND2	2.31	0.45
4:L8:3:A:O2'	19:LP:61:ARG:HD3	2.15	0.45
16:LM:33:GLN:NE2	81:L5:1925:G:OP1	2.50	0.45
34:Le:5:ARG:NH2	81:L5:703:G:O2'	2.50	0.45
43:Ln:2:ARG:HH22	47:S2:1842:4AC:CM7	2.30	0.45
47:S2:1019:C:H2'	47:S2:1020:A:O4'	2.17	0.45
47:S2:1308:U:H2'	47:S2:1309:C:C6	2.51	0.45
56:SI:91:VAL:HG21	56:SI:205:ARG:NH2	2.31	0.45
81:L5:679:C:H2'	81:L5:680:G:H8	1.82	0.45
81:L5:3648:A:H1'	81:L5:3785:A2M:N6	2.31	0.45
81:L5:4070:U:H2'	81:L5:4071:U:C6	2.52	0.45
81:L5:4370:OMG:C4	92:L5:5109:3HE:H20	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LB:90:VAL:HG13	6:LB:161:ARG:HB2	1.98	0.45
11:LG:51:LEU:O	11:LG:55:VAL:HG23	2.17	0.45
17:LN:195:ARG:HD3	81:L5:98:A:OP1	2.16	0.45
34:Le:98:GLU:OE2	34:Le:123:THR:OG1	2.29	0.45
47:S2:1291:A:OP2	47:S2:1302:G:O2'	2.26	0.45
48:SA:94:THR:O	48:SA:186:ARG:NH2	2.49	0.45
49:SB:94:LYS:HA	49:SB:94:LYS:HD2	1.66	0.45
61:SN:31:ASP:OD1	61:SN:31:ASP:N	2.50	0.45
62:SO:117:ARG:HD2	74:Sa:49:ALA:HB2	1.98	0.45
63:SP:123:TYR:OH	66:SS:124:ARG:NH1	2.50	0.45
68:SU:65:THR:HG22	68:SU:67:LYS:H	1.80	0.45
68:SU:106:ILE:HG21	68:SU:112:VAL:HG21	1.99	0.45
81:L5:653:U:H2'	81:L5:654:C:C6	2.51	0.45
81:L5:4096:C:N4	81:L5:4097:G:O6	2.49	0.45
1:CB:404:THR:HG22	1:CB:411:TYR:CE2	2.52	0.45
4:L8:106:G:H5''	4:L8:137:A:H5''	1.98	0.45
8:LD:92:LEU:O	8:LD:93:THR:HG22	2.17	0.45
33:Ld:19:GLU:HG3	33:Ld:102:LEU:HD11	1.98	0.45
33:Ld:75:LYS:HB2	33:Ld:79:ASN:O	2.16	0.45
34:Le:38:PRO:HG2	34:Le:45:VAL:HG22	1.97	0.45
47:S2:1845:A:H2'	47:S2:1846:G:C8	2.52	0.45
48:SA:200:ASP:N	48:SA:200:ASP:OD1	2.49	0.45
67:ST:31:PRO:HG2	67:ST:34:VAL:HG13	1.99	0.45
72:SY:108:LYS:O	72:SY:112:ASN:ND2	2.50	0.45
81:L5:180:C:H2'	81:L5:181:C:N1	2.31	0.45
81:L5:300:A:H2'	81:L5:301:G:H8	1.80	0.45
81:L5:452:A:H62	81:L5:1293:G:H3'	1.82	0.45
81:L5:2350:U:O5'	81:L5:2351:OMC:H5'	2.17	0.45
81:L5:2815:A2M:H2'	81:L5:2816:G:C8	2.51	0.45
81:L5:3664:G:H2'	81:L5:3665:G:C8	2.51	0.45
81:L5:4459:U:H2'	81:L5:4460:U:C6	2.51	0.45
5:LA:24:LYS:HA	5:LA:24:LYS:HD3	1.76	0.45
6:LB:257:TRP:CD1	6:LB:257:TRP:C	2.95	0.45
6:LB:382:MET:HE3	6:LB:382:MET:HB3	1.83	0.45
9:LE:170:SER:OG	9:LE:214:ASP:OD2	2.30	0.45
10:LF:221:LYS:HB2	10:LF:222:LYS:H	1.61	0.45
12:LH:15:ASN:OD1	12:LH:15:ASN:N	2.43	0.45
17:LN:144:ARG:NH2	81:L5:125:C:OP2	2.50	0.45
29:LZ:123:LYS:O	29:LZ:124:THR:OG1	2.30	0.45
37:Lh:4:ILE:HG23	37:Lh:9:LEU:HD11	1.99	0.45
47:S2:17:C:H2'	47:S2:18:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:508:A:H3'	47:S2:509:OMG:H8	1.82	0.45
47:S2:569:A:H2'	47:S2:570:C:O4'	2.17	0.45
47:S2:875:A:H1'	55:SH:114:GLN:NE2	2.32	0.45
47:S2:1154:U:H2'	50:SC:192:LEU:HD11	1.98	0.45
47:S2:1409:A:H2'	47:S2:1410:C:C6	2.52	0.45
47:S2:1687:C:H2'	47:S2:1688:C:C6	2.51	0.45
47:S2:1798:C:H2'	47:S2:1799:G:O4'	2.17	0.45
52:SE:95:THR:OG1	52:SE:97:GLU:HG2	2.16	0.45
59:SL:94:HIS:HB2	59:SL:105:ARG:HD2	1.98	0.45
60:SM:23:LYS:HB3	60:SM:23:LYS:HE3	1.73	0.45
62:SO:150:ARG:H	62:SO:150:ARG:HG2	1.64	0.45
66:SS:36:VAL:HG23	66:SS:99:LEU:HD22	1.99	0.45
81:L5:1445:U:H2'	81:L5:1446:C:C5	2.51	0.45
81:L5:1774:C:H2'	81:L5:1775:A:O4'	2.17	0.45
81:L5:4859:C:H5''	81:L5:4860:G:N7	2.32	0.45
81:L5:4894:A:H3'	81:L5:4895:C:C5'	2.39	0.45
1:CB:395:MET:HB3	1:CB:395:MET:HE2	1.83	0.45
4:L8:8:U:H2'	4:L8:9:A:H8	1.81	0.45
4:L8:31:G:OP1	15:LL:34:ARG:HD3	2.17	0.45
4:L8:58:G:N7	39:Lj:63:ARG:NH2	2.49	0.45
6:LB:224:LYS:HD2	6:LB:340:THR:HG22	1.99	0.45
8:LD:117:LYS:HD3	8:LD:117:LYS:HA	1.64	0.45
8:LD:256:LYS:HD2	82:L7:117:G:H5'	1.99	0.45
11:LG:215:LEU:O	11:LG:219:VAL:HG13	2.17	0.45
14:LJ:114:ASP:OD1	14:LJ:114:ASP:N	2.50	0.45
47:S2:689:U:H2'	47:S2:690:G:C4	2.52	0.45
47:S2:1280:G:H2'	47:S2:1281:G:C8	2.51	0.45
47:S2:1546:G:H5'	64:SQ:18:THR:HG21	1.99	0.45
47:S2:1678:A2M:HM'3	47:S2:1678:A2M:H1'	1.60	0.45
49:SB:165:ARG:HG2	49:SB:169:MET:HE2	1.99	0.45
50:SC:113:GLN:OE1	50:SC:122:THR:OG1	2.33	0.45
57:SJ:131:ARG:HA	57:SJ:131:ARG:HD2	1.78	0.45
62:SO:34:PHE:CD1	62:SO:98:ARG:HD3	2.52	0.45
81:L5:1346:C:H2'	81:L5:1347:G:C8	2.51	0.45
81:L5:3607:U:H2'	81:L5:3608:A:C8	2.52	0.45
81:L5:4340:U:O2	91:L5:5101:SPD:N10	2.50	0.45
83:Lq:124:PRO:HA	83:Lq:157:ASP:OD2	2.17	0.45
12:LH:57:VAL:CG2	12:LH:70:VAL:HG13	2.47	0.45
13:LI:48:LEU:O	13:LI:139:ARG:HA	2.17	0.45
13:LI:51:HIS:ND1	13:LI:137:SER:OG	2.46	0.45
16:LM:117:LYS:NZ	81:L5:4882:U:OP1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LS:95:ARG:NH1	81:L5:1951:G:O2'	2.48	0.45
23:LT:116:LYS:HB3	23:LT:116:LYS:HE2	1.81	0.45
31:Lb:107:ARG:NH2	81:L5:1270:A:OP2	2.49	0.45
34:Le:43:ASN:ND2	34:Le:45:VAL:HG13	2.32	0.45
49:SB:175:GLU:O	49:SB:179:ASN:ND2	2.49	0.45
67:ST:117:GLN:CD	67:ST:117:GLN:H	2.25	0.45
68:SU:51:LYS:HG2	68:SU:92:HIS:HE2	1.80	0.45
74:Sa:13:LYS:HD3	74:Sa:13:LYS:HA	1.80	0.45
80:Sg:172:LYS:HG2	80:Sg:193:GLY:C	2.42	0.45
81:L5:679:C:H2'	81:L5:680:G:C8	2.52	0.45
81:L5:919:C:H2'	81:L5:920:C:C6	2.52	0.45
81:L5:4518:A:OP2	81:L5:4518:A:H8	1.99	0.45
81:L5:4637:OMG:HM23	81:L5:4637:OMG:H1'	1.78	0.45
81:L5:4730:C:H2'	81:L5:4731:G:C8	2.52	0.45
1:CB:426:LYS:HA	1:CB:446:PRO:HA	1.99	0.44
1:CB:444:LEU:C	1:CB:445:LYS:HD2	2.42	0.44
1:CB:610:PRO:HD2	1:CB:613:LEU:HD12	1.99	0.44
6:LB:17:LEU:HD12	6:LB:17:LEU:HA	1.75	0.44
6:LB:165:HIS:HB3	6:LB:180:LEU:HD23	1.98	0.44
12:LH:50:LYS:O	12:LH:51:LYS:HB3	2.17	0.44
24:LU:23:LEU:HD21	24:LU:83:LEU:HB3	1.99	0.44
32:Lc:77:ASN:OD1	32:Lc:80:GLU:HG3	2.16	0.44
33:Ld:33:ILE:HG22	33:Ld:44:ARG:HG3	1.98	0.44
47:S2:440:G:H5''	47:S2:1798:C:O2'	2.17	0.44
47:S2:527:C:H2'	47:S2:528:A:C8	2.52	0.44
47:S2:1093:A:H2'	47:S2:1094:C:C6	2.52	0.44
47:S2:1231:C:O2'	47:S2:1253:A:N6	2.49	0.44
47:S2:1554:C:N4	77:Sd:37:ASN:OD1	2.51	0.44
68:SU:66:ARG:HG3	68:SU:68:THR:HG22	1.99	0.44
75:Sb:30:SER:HB3	75:Sb:49:HIS:CD2	2.45	0.44
80:Sg:263:GLY:O	80:Sg:265:ILE:HG12	2.16	0.44
81:L5:470:A:H2'	81:L5:471:A:O4'	2.16	0.44
81:L5:1320:U:O2'	81:L5:1891:A:N1	2.37	0.44
81:L5:1705:G:H2'	81:L5:1706:A:O4'	2.17	0.44
81:L5:2351:OMC:HM23	81:L5:2351:OMC:H1'	1.69	0.44
81:L5:4563:U:H2'	81:L5:4564:A:H8	1.83	0.44
81:L5:4680:G:H2'	81:L5:4681:A:C8	2.52	0.44
81:L5:5047:C:O2'	81:L5:5050:C:OP2	2.31	0.44
21:LR:98:ARG:NH1	21:LR:132:PHE:O	2.49	0.44
21:LR:181:LYS:HA	21:LR:181:LYS:HD3	1.63	0.44
34:Le:31:ILE:HD11	81:L5:2347:A:C4	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:860:G:H21	70:SW:107:SER:HG	1.59	0.44
59:SL:79:LYS:HB2	59:SL:87:VAL:HG13	1.99	0.44
65:SR:33:ARG:HG3	80:Sg:125:ARG:NH1	2.31	0.44
81:L5:62:A:N3	81:L5:77:U:O2'	2.41	0.44
81:L5:1087:A:H2'	81:L5:1088:C:C6	2.52	0.44
81:L5:1677:U:H4'	81:L5:1680:G:C2	2.51	0.44
81:L5:2747:U:H2'	81:L5:2748:C:C6	2.52	0.44
81:L5:3619:G:H22	81:L5:3624:A:H1'	1.82	0.44
81:L5:3928:A:H2'	81:L5:3929:G:O4'	2.17	0.44
81:L5:4771:C:H2'	81:L5:4772:C:C6	2.52	0.44
4:L8:36:G:O2'	4:L8:103:A:N1	2.38	0.44
15:LL:59:VAL:HG22	81:L5:74:G:H5'	1.99	0.44
15:LL:128:PRO:HB3	15:LL:134:PRO:HA	2.00	0.44
17:LN:93:LYS:HD3	81:L5:300:A:H2	1.82	0.44
18:LO:165:LYS:O	18:LO:169:ARG:HG3	2.16	0.44
22:LS:133:ALA:HB3	22:LS:136:LYS:HG2	1.98	0.44
25:LV:43:LYS:HE2	81:L5:4508:C:H5''	1.98	0.44
33:Ld:24:GLU:OE2	33:Ld:87:ARG:NH2	2.41	0.44
47:S2:291:G:HO2'	47:S2:292:A:P	2.40	0.44
47:S2:1749:G:H2'	47:S2:1750:C:C6	2.52	0.44
48:SA:38:ILE:HD11	48:SA:150:THR:HG22	1.99	0.44
52:SE:9:LEU:HB2	52:SE:30:ARG:HD3	1.99	0.44
81:L5:223:G:H4'	81:L5:225:G:N7	2.32	0.44
81:L5:492:U:H2'	81:L5:493:G:C8	2.53	0.44
81:L5:1244:G:H2'	81:L5:1245:C:C6	2.53	0.44
81:L5:1662:C:H2'	81:L5:1663:C:C6	2.52	0.44
81:L5:4095:G:C2	81:L5:4114:C:C2	3.05	0.44
81:L5:4110:C:H2'	81:L5:4111:U:C6	2.52	0.44
81:L5:4935:C:H2'	81:L5:4936:G:C8	2.53	0.44
1:CB:747:VAL:HA	1:CB:811:GLN:O	2.17	0.44
6:LB:308:ASP:OD1	6:LB:309:LEU:N	2.50	0.44
7:LC:80:ARG:NH1	81:L5:1645:C:OP1	2.47	0.44
7:LC:336:ARG:HE	7:LC:336:ARG:HB2	1.62	0.44
31:Lb:63:LYS:HE3	31:Lb:63:LYS:HB3	1.76	0.44
33:Ld:29:ILE:O	33:Ld:33:ILE:HG12	2.17	0.44
47:S2:685:A:H5''	70:SW:31:SER:HB3	1.99	0.44
47:S2:1378:A:H4'	47:S2:1379:A:O5'	2.17	0.44
47:S2:1512:C:H5''	77:Sd:8:TRP:CZ3	2.52	0.44
47:S2:1564:C:OP1	67:ST:121:ARG:NH2	2.50	0.44
52:SE:143:ASP:OD1	52:SE:143:ASP:N	2.44	0.44
55:SH:159:ASP:O	55:SH:160:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SN:60:VAL:HG13	61:SN:66:VAL:HG21	1.97	0.44
64:SQ:48:GLN:HE21	64:SQ:52:LEU:HD21	1.82	0.44
81:L5:4406:U:C2	81:L5:4407:G:C8	3.05	0.44
1:CB:146:ALA:HB1	1:CB:151:ILE:HB	1.99	0.44
4:L8:59:A:H4'	4:L8:60:G:H3'	1.99	0.44
20:LQ:71:LYS:HE2	20:LQ:71:LYS:HB3	1.64	0.44
21:LR:98:ARG:NH2	21:LR:130:ASN:OD1	2.39	0.44
47:S2:563:G:HO2'	47:S2:564:A:P	2.40	0.44
47:S2:1309:C:H41	79:Sf:96:LYS:NZ	2.15	0.44
47:S2:1389:C:H4'	51:SD:205:PRO:HB3	2.00	0.44
48:SA:22:GLY:C	48:SA:24:HIS:H	2.24	0.44
81:L5:4991:U:H2'	81:L5:4992:G:H8	1.83	0.44
81:L5:5024:C:N4	81:L5:5029:C:O4'	2.51	0.44
1:CB:27:HIS:HB2	1:CB:139:THR:HG23	2.00	0.44
11:LG:44:ASP:OD1	11:LG:44:ASP:N	2.49	0.44
17:LN:170:LYS:O	81:L5:299:C:H5''	2.18	0.44
25:LV:43:LYS:HE3	25:LV:62:MET:HE3	1.99	0.44
28:LY:72:GLN:HB3	28:LY:81:TYR:HB2	1.99	0.44
47:S2:555:A:H2'	47:S2:557:U:C6	2.53	0.44
47:S2:1286:G:O6	60:SM:36:ARG:HB3	2.18	0.44
47:S2:1801:A:H2'	47:S2:1802:C:C6	2.53	0.44
50:SC:169:TYR:CD2	50:SC:173:LYS:HB3	2.52	0.44
57:SJ:47:LYS:HB3	57:SJ:47:LYS:HE3	1.59	0.44
80:Sg:57:ARG:HD3	80:Sg:95:GLY:HA3	1.99	0.44
80:Sg:272:GLN:OE1	80:Sg:284:PRO:HG2	2.18	0.44
81:L5:482:G:H2'	81:L5:485:C:C6	2.53	0.44
81:L5:488:G:H8	81:L5:488:G:O5'	2.00	0.44
81:L5:1183:C:H2'	81:L5:1184:A:C8	2.53	0.44
81:L5:1637:A:OP1	81:L5:1640:C:N4	2.44	0.44
81:L5:2335:C:H2'	81:L5:2336:G:H8	1.83	0.44
81:L5:4159:C:H2'	81:L5:4160:C:C6	2.52	0.44
81:L5:4742:G:H2'	81:L5:4743:G:C8	2.53	0.44
83:Lq:20:LEU:HD12	83:Lq:54:LEU:HD22	1.99	0.44
1:CB:10:ARG:NE	1:CB:463:ASP:OD1	2.50	0.44
6:LB:36:ASP:O	6:LB:187:GLY:HA2	2.18	0.44
9:LE:181:LEU:O	81:L5:4883:C:N4	2.47	0.44
11:LG:111:LYS:NZ	11:LG:111:LYS:HB2	2.33	0.44
27:LX:156:ILE:O	84:CA:290:ARG:NH2	2.49	0.44
47:S2:64:A:N6	47:S2:83:A:OP2	2.51	0.44
47:S2:804:U:H2'	47:S2:805:U:C6	2.52	0.44
47:S2:945:U:H2'	47:S2:946:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SZ:73:VAL:HG12	73:SZ:79:ILE:HD11	2.00	0.44
81:L5:966:A:N1	81:L5:2093:A:H2	2.16	0.44
81:L5:1932:A:H2'	81:L5:1933:G:C8	2.53	0.44
81:L5:4742:G:H2'	81:L5:4743:G:H8	1.83	0.44
81:L5:4919:G:H2'	81:L5:4920:C:C6	2.53	0.44
83:Lq:26:LYS:HB2	83:Lq:26:LYS:HE3	1.63	0.44
2:CC:31:A:O3'	47:S2:1641:A:O2'	2.36	0.44
14:LJ:22:LEU:HA	14:LJ:129:ASP:O	2.18	0.44
15:LL:46:ILE:HB	15:LL:49:ARG:HB2	2.00	0.44
17:LN:9:GLU:HB2	38:Li:44:ILE:HG13	2.00	0.44
20:LQ:155:ALA:O	20:LQ:158:THR:OG1	2.29	0.44
24:LU:52:LYS:HE2	24:LU:52:LYS:HB2	1.69	0.44
24:LU:80:LYS:HE2	24:LU:110:TYR:CZ	2.52	0.44
33:Ld:53:ALA:HA	33:Ld:88:LEU:HD21	1.99	0.44
47:S2:428:OMU:H6	47:S2:428:OMU:H2'	1.80	0.44
47:S2:1025:U:H2'	47:S2:1026:C:O4'	2.18	0.44
47:S2:1397:U:O4'	47:S2:1442:OMU:H5''	2.18	0.44
47:S2:1736:G:H2'	47:S2:1737:G:H8	1.83	0.44
50:SC:194:ARG:HD3	50:SC:196:ILE:HD11	2.00	0.44
60:SM:74:ILE:HD13	60:SM:74:ILE:HA	1.84	0.44
71:SX:54:LYS:HE3	71:SX:91:LEU:HG	2.00	0.44
81:L5:82:U:H2'	81:L5:83:C:O4'	2.17	0.44
81:L5:1577:G:H5'	81:L5:1578:U:H5''	2.00	0.44
81:L5:4957:C:H2'	81:L5:4958:C:C6	2.53	0.44
3:CD:201:ARG:HB2	3:CD:201:ARG:HH11	1.83	0.44
6:LB:92:TYR:HB3	6:LB:99:LEU:HG	2.00	0.44
7:LC:242:PRO:O	81:L5:2296:G:O2'	2.32	0.44
16:LM:3:PHE:H	22:LS:175:PHE:HZ	1.65	0.44
18:LO:81:TRP:HB2	18:LO:104:VAL:HG21	2.00	0.44
22:LS:163:HIS:O	22:LS:164:LYS:HD3	2.18	0.44
28:LY:113:LYS:HG3	28:LY:114:ASP:N	2.32	0.44
34:Le:35:TRP:HH2	34:Le:55:MET:HG2	1.83	0.44
37:Lh:31:LEU:HB3	37:Lh:47:ILE:HG12	1.99	0.44
42:Lm:97:ARG:HG2	42:Lm:122:ARG:HG2	1.99	0.44
47:S2:115:U:H2'	47:S2:116:OMU:C6	2.48	0.44
47:S2:689:U:H2'	47:S2:690:G:C2	2.53	0.44
47:S2:940:U:H2'	47:S2:941:C:C6	2.53	0.44
47:S2:1733:U:H2'	47:S2:1734:G:O4'	2.18	0.44
47:S2:1823:A:H3'	47:S2:1824:A:N3	2.33	0.44
50:SC:61:MET:HA	50:SC:61:MET:HE3	2.00	0.44
56:SI:162:LEU:HD11	56:SI:191:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:Sa:10:ARG:HB2	74:Sa:33:ASP:OD1	2.18	0.44
81:L5:1:C:H1'	81:L5:2:G:C8	2.52	0.44
81:L5:86:U:H2'	81:L5:87:A:C8	2.53	0.44
81:L5:93:G:H2'	81:L5:94:A:C8	2.53	0.44
81:L5:965:G:O2'	81:L5:2092:G:N2	2.51	0.44
81:L5:1251:C:H2'	81:L5:1252:C:C6	2.53	0.44
81:L5:1420:A:C5	81:L5:1500:A:H4'	2.53	0.44
81:L5:4486:C:H2'	81:L5:4487:A:O4'	2.18	0.44
83:Lq:94:ASP:HB3	83:Lq:97:GLU:HB3	2.00	0.44
5:LA:101:VAL:HG22	5:LA:165:VAL:HG22	1.99	0.43
6:LB:288:GLY:HA3	6:LB:330:PHE:CE1	2.53	0.43
7:LC:322:LEU:O	7:LC:326:LEU:HG	2.17	0.43
10:LF:127:LYS:HB2	23:LT:133:ALA:HB3	2.00	0.43
18:LO:61:ARG:HA	18:LO:70:PRO:HD2	1.99	0.43
26:LW:107:GLN:O	26:LW:110:ARG:HG3	2.18	0.43
38:Li:103:LYS:HE2	38:Li:103:LYS:HB3	1.76	0.43
47:S2:461:U:H2'	47:S2:462:C:C6	2.53	0.43
47:S2:1189:A:H2'	47:S2:1190:A:C8	2.53	0.43
55:SH:34:SER:O	55:SH:36:LEU:N	2.49	0.43
55:SH:157:HIS:HB3	55:SH:190:PRO:HG3	1.99	0.43
63:SP:18:ARG:HD3	66:SS:88:LYS:HG2	2.00	0.43
65:SR:59:LYS:HB3	65:SR:59:LYS:HE2	1.79	0.43
80:Sg:302:TYR:CE2	80:Sg:308:ARG:HD2	2.53	0.43
81:L5:1689:G:OP2	89:L5:5385:PUT:N1	2.49	0.43
81:L5:1963:C:C2	81:L5:1964:A:C8	3.06	0.43
81:L5:2000:G:H4'	81:L5:2017:A:C2	2.52	0.43
1:CB:42:LYS:HE2	1:CB:79:TYR:HE1	1.83	0.43
1:CB:722:ILE:HB	1:CB:723:PRO:HD3	2.00	0.43
3:CD:284:LEU:HD13	58:SK:85:LEU:HD11	2.01	0.43
4:L8:97:A:H2'	4:L8:98:C:O4'	2.18	0.43
5:LA:30:ARG:O	5:LA:163:ARG:NH1	2.44	0.43
5:LA:183:GLY:HA3	81:L5:1613:A:H5''	2.00	0.43
8:LD:211:LEU:HD23	8:LD:211:LEU:HA	1.84	0.43
9:LE:219:LYS:HE2	81:L5:4941:G:OP1	2.17	0.43
11:LG:120:LYS:HE3	11:LG:120:LYS:HB3	1.81	0.43
26:LW:119:LYS:HD3	26:LW:119:LYS:HA	1.53	0.43
47:S2:84:A:N3	47:S2:150:A:O2'	2.45	0.43
47:S2:161:U:H5'	72:SY:116:LYS:HG3	2.00	0.43
47:S2:932:G:O2'	47:S2:934:G:OP2	2.32	0.43
47:S2:1070:A:H2'	47:S2:1071:G:O4'	2.18	0.43
47:S2:1246:A:N6	47:S2:1247:C:H41	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Sb:32:PHE:O	75:Sb:82:LYS:HG2	2.17	0.43
81:L5:1672:U:H2'	81:L5:1673:U:C6	2.54	0.43
81:L5:1683:PSU:H2'	81:L5:1684:A:C8	2.53	0.43
81:L5:2415:OMU:HM23	81:L5:2415:OMU:H1'	1.50	0.43
83:Lq:50:LYS:H	83:Lq:50:LYS:HD3	1.83	0.43
83:Lq:138:PHE:HE2	83:Lq:154:ILE:HD11	1.83	0.43
1:CB:383:MET:HE3	1:CB:383:MET:HB3	1.75	0.43
3:CD:210:ARG:O	3:CD:213:SER:OG	2.35	0.43
3:CD:289:ALA:HA	3:CD:292:ASN:HD21	1.82	0.43
5:LA:192:LYS:HE2	5:LA:192:LYS:HB3	1.75	0.43
6:LB:182:GLU:OE2	81:L5:4580:U:O2'	2.23	0.43
18:LO:61:ARG:HH21	18:LO:66:PRO:HG2	1.84	0.43
19:LP:122:ALA:HB3	19:LP:143:PRO:HB2	1.99	0.43
21:LR:96:MET:HG3	81:L5:2667:C:O4'	2.17	0.43
31:Lb:10:HIS:NE2	81:L5:1877:G:O6	2.48	0.43
47:S2:158:A:H2'	47:S2:159:A2M:O4'	2.18	0.43
47:S2:502:C:O4'	52:SE:66:MET:HG3	2.18	0.43
47:S2:1550:G:H3'	47:S2:1579:A:H61	1.81	0.43
76:Sc:21:THR:HB	76:Sc:68:LEU:HD21	2.00	0.43
81:L5:2417:A:C4	81:L5:2418:A:C8	3.06	0.43
81:L5:2862:G:H4'	81:L5:3625:G:N7	2.33	0.43
81:L5:3880:G:H2'	81:L5:3881:G:C8	2.53	0.43
81:L5:4069:U:H2'	81:L5:4070:U:C6	2.54	0.43
81:L5:4504:C:H2'	81:L5:4505:C:C6	2.53	0.43
1:CB:539:GLU:HG2	1:CB:545:ILE:HG13	2.01	0.43
5:LA:241:ARG:HG3	81:L5:3659:G:OP1	2.18	0.43
7:LC:163:LYS:HB2	7:LC:166:GLU:HG3	1.99	0.43
8:LD:228:LYS:C	8:LD:230:SER:H	2.26	0.43
11:LG:103:ARG:NH2	11:LG:192:ARG:O	2.51	0.43
11:LG:117:ARG:NH1	11:LG:117:ARG:O	2.51	0.43
17:LN:148:THR:O	17:LN:151:ILE:HG22	2.19	0.43
19:LP:83:TRP:O	81:L5:3856:A:H5''	2.18	0.43
30:La:44:ASN:ND2	81:L5:1683:PSU:OP1	2.46	0.43
47:S2:13:C:H4'	47:S2:1355:C:O2	2.18	0.43
47:S2:17:C:O2'	47:S2:1194:A:N1	2.41	0.43
47:S2:647:U:H2'	47:S2:648:A:C8	2.53	0.43
47:S2:1124:C:H5''	49:SB:150:ILE:HG12	2.01	0.43
47:S2:1500:G:H2'	47:S2:1501:C:C6	2.53	0.43
47:S2:1528:G:O2'	47:S2:1666:C:OP1	2.32	0.43
55:SH:50:GLU:OE1	55:SH:60:ILE:HG12	2.19	0.43
81:L5:457:G:H2'	81:L5:458:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:1186:U:H3'	81:L5:1187:G:H21	1.84	0.43
81:L5:1328:G:O2'	81:L5:2349:A:OP1	2.37	0.43
81:L5:1450:C:H2'	81:L5:1451:G:O4'	2.18	0.43
81:L5:2579:G:N2	81:L5:2582:A:OP2	2.40	0.43
81:L5:2656:U:H2'	81:L5:2657:G:O4'	2.19	0.43
81:L5:4685:U:H2'	81:L5:4686:G:C8	2.53	0.43
83:Lq:55:MET:HE3	83:Lq:55:MET:HB3	1.89	0.43
83:Lq:72:ASN:OD1	83:Lq:75:LEU:HG	2.18	0.43
4:L8:125:C:H4'	4:L8:126:C:H5	1.82	0.43
9:LE:165:LEU:HD11	9:LE:176:THR:HB	2.00	0.43
13:LI:38:ARG:HD3	13:LI:83:ASP:HB3	2.00	0.43
17:LN:83:LYS:HB3	17:LN:85:VAL:HG12	2.00	0.43
20:LQ:154:LYS:HE2	20:LQ:161:SER:HB3	2.00	0.43
23:LT:78:LYS:HE3	23:LT:87:LYS:HD3	2.00	0.43
35:Lf:27:LEU:HB3	35:Lf:83:MET:HE1	2.00	0.43
41:Ll:33:ASN:ND2	41:Ll:35:ILE:O	2.47	0.43
47:S2:512:A2M:H4'	47:S2:576:A2M:H2	2.00	0.43
47:S2:554:A:O4'	78:Se:25:LYS:NZ	2.51	0.43
47:S2:1164:G:O2'	47:S2:1165:G:H5'	2.18	0.43
47:S2:1631:U:H5''	66:SS:34:LYS:HG2	2.00	0.43
47:S2:1704:C:H6	47:S2:1831:A:H61	1.67	0.43
55:SH:145:ARG:NH1	70:SW:51:GLU:OE1	2.40	0.43
58:SK:47:LYS:HA	58:SK:47:LYS:HD3	1.82	0.43
60:SM:41:ALA:HB3	60:SM:110:VAL:HG21	2.01	0.43
66:SS:98:VAL:HG23	66:SS:103:LEU:HD13	2.01	0.43
81:L5:923:C:H2'	81:L5:925:C:C5	2.53	0.43
81:L5:1431:C:H2'	81:L5:1432:G:O4'	2.19	0.43
81:L5:3669:G:H21	81:L5:3672:G:N2	2.17	0.43
81:L5:5025:C:H5''	81:L5:5026:U:C5	2.54	0.43
1:CB:81:LEU:HD23	1:CB:81:LEU:HA	1.86	0.43
6:LB:175:GLN:NE2	6:LB:177:LYS:O	2.42	0.43
7:LC:169:LEU:O	7:LC:173:LYS:HG2	2.18	0.43
8:LD:236:MET:HA	8:LD:239:MET:HG2	1.99	0.43
9:LE:155:GLY:HA2	81:L5:4942:C:H5''	2.00	0.43
9:LE:190:HIS:ND1	9:LE:192:LYS:HB2	2.33	0.43
18:LO:89:PRO:HD3	81:L5:1914:C:H4'	1.99	0.43
19:LP:6:LEU:HD21	81:L5:425:U:H4'	2.00	0.43
23:LT:124:THR:OG1	23:LT:125:TRP:N	2.52	0.43
47:S2:434:G:OP1	56:SI:23:LYS:HG3	2.19	0.43
47:S2:815:U:C2	47:S2:816:A:C8	3.06	0.43
48:SA:183:LEU:HB3	48:SA:189:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SE:102:ILE:HG21	52:SE:239:PRO:HD3	2.00	0.43
52:SE:141:THR:OG1	52:SE:143:ASP:OD1	2.26	0.43
80:Sg:147:HIS:CD2	80:Sg:169:GLY:HA3	2.54	0.43
81:L5:667:A:H5''	81:L5:668:C:H5''	2.01	0.43
81:L5:2632:PSU:H2'	81:L5:2633:U:C6	2.54	0.43
81:L5:3818:UY1:O3'	81:L5:3819:G:OP2	2.36	0.43
81:L5:3911:C:H2'	81:L5:3912:U:C6	2.52	0.43
81:L5:4188:U:H2'	81:L5:4189:U:C6	2.53	0.43
81:L5:4684:A:H2'	81:L5:4685:U:O4'	2.19	0.43
82:L7:58:A:H2'	82:L7:59:G:C8	2.53	0.43
83:Lq:112:ARG:HG3	83:Lq:112:ARG:NH1	2.33	0.43
83:Lq:160:LEU:HD12	83:Lq:160:LEU:HA	1.78	0.43
1:CB:22:MET:HE2	1:CB:22:MET:HB2	1.84	0.43
1:CB:533:MET:HE3	1:CB:533:MET:HB3	1.79	0.43
4:L8:94:G:H21	39:Lj:82:THR:HB	1.83	0.43
13:LI:62:SER:HB3	13:LI:93:PRO:HG3	2.01	0.43
14:LJ:44:THR:O	14:LJ:78:LYS:HD3	2.18	0.43
22:LS:115:ALA:HB2	81:L5:2060:G:N2	2.34	0.43
23:LT:102:ARG:HH21	23:LT:105:PHE:HE2	1.67	0.43
29:LZ:54:THR:H	29:LZ:57:MET:HG3	1.83	0.43
45:Lp:59:SER:O	81:L5:2652:G:N2	2.51	0.43
47:S2:1134:G:H2'	47:S2:1135:C:C6	2.53	0.43
47:S2:1471:C:H2'	47:S2:1472:C:C6	2.53	0.43
47:S2:1745:A:H1'	54:SG:66:GLY:HA2	2.01	0.43
65:SR:114:LEU:HD12	65:SR:117:LEU:HD11	1.99	0.43
67:ST:104:LEU:O	67:ST:108:GLU:HG3	2.19	0.43
80:Sg:68:ASP:HB3	80:Sg:111:VAL:HG22	2.00	0.43
81:L5:183:C:H2'	81:L5:185:C:C6	2.54	0.43
81:L5:256:G:H2'	81:L5:257:C:C6	2.54	0.43
81:L5:1082:C:HO2'	81:L5:1083:U:P	2.39	0.43
81:L5:1461:C:H2'	81:L5:1462:A:C8	2.54	0.43
6:LB:247:GLY:CA	81:L5:2838:G:H5'	2.48	0.43
9:LE:220:LYS:HB3	9:LE:220:LYS:HE3	1.74	0.43
10:LF:92:VAL:O	10:LF:120:GLY:HA2	2.19	0.43
17:LN:96:ARG:NH1	17:LN:100:SER:OG	2.52	0.43
20:LQ:55:ARG:NH1	81:L5:1351:G:O6	2.50	0.43
22:LS:158:VAL:HG11	81:L5:2055:G:C8	2.54	0.43
23:LT:111:GLU:HB3	23:LT:115:LYS:NZ	2.34	0.43
30:La:35:ALA:HB1	81:L5:39:A:H5''	2.00	0.43
32:Lc:18:LEU:O	32:Lc:22:MET:HG2	2.19	0.43
47:S2:5:U:H2'	47:S2:6:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:92:A:H4'	47:S2:93:PSU:OP2	2.18	0.43
47:S2:101:U:H3'	47:S2:408:A:H61	1.82	0.43
47:S2:159:A2M:H2	47:S2:468:A2M:H4'	2.00	0.43
47:S2:1455:A:OP1	65:SR:5:ARG:NH2	2.46	0.43
47:S2:1549:U:H2'	47:S2:1550:G:C8	2.54	0.43
54:SG:98:ARG:NH2	54:SG:103:ASP:OD1	2.50	0.43
60:SM:61:TYR:O	60:SM:65:VAL:HG12	2.19	0.43
67:ST:56:ARG:HG3	67:ST:103:VAL:HG21	2.00	0.43
80:Sg:101:PHE:CD2	80:Sg:136:GLY:HA2	2.54	0.43
81:L5:662:C:H2'	81:L5:663:G:H8	1.83	0.43
81:L5:1996:C:H2'	81:L5:1997:U:O4'	2.19	0.43
81:L5:4208:U:OP1	81:L5:4334:U:O2'	2.30	0.43
1:CB:294:LEU:HD23	1:CB:294:LEU:HA	1.86	0.43
4:L8:6:C:H2'	4:L8:7:U:C6	2.54	0.43
4:L8:155:C:OP2	11:LG:89:ARG:HD3	2.19	0.43
5:LA:171:GLY:O	45:Lp:68:ALA:HB2	2.19	0.43
6:LB:301:ASN:OD1	6:LB:301:ASN:N	2.52	0.43
8:LD:5:LYS:HG2	81:L5:1778:C:H5''	2.01	0.43
16:LM:38:VAL:HG11	16:LM:50:MET:HE3	2.00	0.43
18:LO:110:PRO:N	18:LO:111:PRO:HD2	2.34	0.43
27:LX:38:LYS:HA	27:LX:38:LYS:HD3	1.67	0.43
29:LZ:79:HIS:CE1	81:L5:2580:U:HO2'	2.30	0.43
31:Lb:115:GLY:HA2	81:L5:1241:C:O2	2.18	0.43
33:Ld:84:ILE:HG23	33:Ld:86:VAL:HG13	2.00	0.43
47:S2:218:U:O2	56:SI:184:ARG:NH2	2.52	0.43
47:S2:1497:G:N7	58:SK:25:LYS:NZ	2.64	0.43
47:S2:1545:A:H2'	47:S2:1546:G:C8	2.53	0.43
52:SE:254:LYS:HB2	52:SE:254:LYS:HE2	1.78	0.43
55:SH:63:PHE:HA	55:SH:95:ILE:O	2.19	0.43
72:SY:5:VAL:HG23	72:SY:32:LYS:HE2	2.01	0.43
74:Sa:32:LYS:O	74:Sa:37:LYS:NZ	2.49	0.43
81:L5:666:G:H2'	81:L5:668:C:OP1	2.19	0.43
81:L5:750:U:H1'	81:L5:917:A:C8	2.53	0.43
81:L5:1294:A:H1'	81:L5:1296:G:N1	2.34	0.43
81:L5:1567:U:H2'	81:L5:1568:C:C6	2.54	0.43
81:L5:2683:C:H2'	81:L5:2684:C:C6	2.54	0.43
81:L5:3783:A:OP2	81:L5:3808:OMC:N4	2.51	0.43
81:L5:4500:U:H2'	81:L5:4501:U:C6	2.54	0.43
82:L7:27:G:H21	82:L7:55:A:N6	2.17	0.43
1:CB:692:LEU:HD22	1:CB:848:ILE:HD13	2.01	0.43
6:LB:29:VAL:HG21	6:LB:32:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:62:MET:HE3	9:LE:62:MET:HB3	1.88	0.43
13:LI:66:GLU:HG3	13:LI:69:ARG:HH21	1.84	0.43
15:LL:200:LYS:HE3	15:LL:200:LYS:HB2	1.87	0.43
26:LW:61:LYS:HE2	81:L5:5041:G:OP2	2.19	0.43
37:Lh:14:LYS:HE3	37:Lh:61:ILE:HG23	2.01	0.43
40:Lk:51:GLU:O	40:Lk:55:LYS:HG2	2.18	0.43
47:S2:1017:U:H2'	47:S2:1018:U:C6	2.54	0.43
47:S2:1450:G:H5'	47:S2:1451:G:OP2	2.19	0.43
47:S2:1531:A:H2'	47:S2:1532:C:C6	2.54	0.43
50:SC:110:MET:O	50:SC:110:MET:HG3	2.19	0.43
53:SF:30:ILE:HD13	53:SF:39:ILE:HB	2.00	0.43
60:SM:86:GLY:HA2	60:SM:89:VAL:HG22	2.00	0.43
71:SX:98:ASP:OD2	71:SX:140:ARG:NH1	2.48	0.43
81:L5:1607:C:N4	91:L5:5102:SPD:H71	2.34	0.43
81:L5:1787:A:H4'	89:L5:5387:PUT:H11	2.00	0.43
81:L5:3621:A:C8	81:L5:4642:U:H1'	2.54	0.43
81:L5:3656:A:H2'	81:L5:3657:U:C6	2.53	0.43
81:L5:3721:U:H2'	81:L5:3722:G:C8	2.54	0.43
81:L5:4633:G:O2'	81:L5:4635:A:OP2	2.31	0.43
81:L5:4744:A:H2'	81:L5:4745:G:O4'	2.19	0.43
81:L5:4973:U:H1'	81:L5:4986:G:C2	2.54	0.43
1:CB:235:LYS:C	1:CB:235:LYS:HZ2	2.27	0.42
1:CB:502:SER:O	1:CB:504:VAL:HG22	2.18	0.42
4:L8:141:C:H2'	4:L8:142:U:H6	1.83	0.42
6:LB:332:MET:HE1	6:LB:368:ILE:HD13	2.00	0.42
7:LC:101:MET:HE2	7:LC:104:PRO:HA	2.00	0.42
13:LI:19:LYS:HE2	13:LI:26:VAL:HB	2.01	0.42
15:LL:36:ARG:NH1	81:L5:1364:U:OP2	2.41	0.42
17:LN:84:PRO:HA	17:LN:87:HIS:CG	2.54	0.42
36:Lg:83:CYS:O	36:Lg:87:VAL:HG23	2.19	0.42
47:S2:881:G:H2'	47:S2:882:U:H5'	2.01	0.42
47:S2:941:C:H2'	47:S2:942:G:C8	2.53	0.42
50:SC:270:THR:O	50:SC:274:VAL:HG23	2.18	0.42
61:SN:45:LEU:HB3	61:SN:49:GLN:HG3	2.01	0.42
79:Sf:118:ARG:HB2	79:Sf:131:PHE:CD1	2.54	0.42
81:L5:3736:A:H2'	81:L5:3737:A:C8	2.53	0.42
81:L5:3910:C:N3	81:L5:4392:OMG:N1	2.62	0.42
81:L5:4113:U:O2'	81:L5:4114:C:H5'	2.18	0.42
81:L5:4619:U:H2'	81:L5:4620:OMU:C6	2.49	0.42
4:L8:145:C:H2'	4:L8:146:U:C6	2.53	0.42
9:LE:87:LYS:HD2	9:LE:87:LYS:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LF:27:GLU:OE1	10:LF:27:GLU:N	2.41	0.42
26:LW:52:THR:O	26:LW:56:ARG:HG3	2.18	0.42
26:LW:72:THR:O	26:LW:74:ARG:NH2	2.51	0.42
39:Lj:50:SER:HB3	39:Lj:53:ALA:HB3	2.02	0.42
47:S2:464:A:H5''	47:S2:465:A:N7	2.33	0.42
47:S2:1201:U:H2'	47:S2:1202:U:C6	2.53	0.42
54:SG:85:ARG:O	54:SG:87:ARG:NH1	2.50	0.42
63:SP:133:ILE:HD12	63:SP:133:ILE:HA	1.80	0.42
66:SS:106:LYS:HD3	66:SS:106:LYS:HA	1.74	0.42
79:Sf:107:LYS:O	79:Sf:115:SER:OG	2.33	0.42
81:L5:37:U:H2'	81:L5:38:A:O4'	2.18	0.42
81:L5:129:C:H2'	81:L5:130:C:C6	2.54	0.42
81:L5:1847:C:H2'	81:L5:1848:C:C6	2.54	0.42
81:L5:1974:U:O4'	81:L5:1976:G:H5'	2.19	0.42
81:L5:2020:U:H2'	81:L5:2021:G:H8	1.84	0.42
81:L5:3910:C:H2'	81:L5:3911:C:H6	1.82	0.42
81:L5:4301:U:OP2	81:L5:4303:C:N4	2.52	0.42
81:L5:5016:A:N6	81:L5:5033:G:O2'	2.52	0.42
1:CB:309:LYS:HB3	1:CB:309:LYS:HE2	1.80	0.42
4:L8:86:U:H4'	4:L8:87:G:OP2	2.20	0.42
10:LF:199:LYS:HB2	10:LF:199:LYS:HE2	1.90	0.42
12:LH:63:ASN:O	12:LH:67:LEU:HG	2.18	0.42
13:LI:36:LEU:HD13	13:LI:87:MET:HE3	2.00	0.42
15:LL:184:MET:HE2	15:LL:184:MET:HB3	1.81	0.42
40:Lk:29:LYS:NZ	40:Lk:29:LYS:HB2	2.34	0.42
47:S2:216:C:C2	47:S2:217:A:C8	3.07	0.42
47:S2:529:A:C2	47:S2:555:A:H2	2.36	0.42
47:S2:1559:C:H2'	47:S2:1560:U:O4'	2.19	0.42
51:SD:212:GLU:OE1	65:SR:19:LYS:HE3	2.19	0.42
52:SE:101:LEU:HD23	52:SE:101:LEU:HA	1.89	0.42
56:SI:139:LYS:HE3	56:SI:139:LYS:HB3	1.88	0.42
61:SN:43:LYS:HE3	61:SN:43:LYS:HB2	1.91	0.42
66:SS:89:ASP:OD1	66:SS:91:LYS:N	2.46	0.42
72:SY:101:LYS:HA	72:SY:101:LYS:HD3	1.76	0.42
79:Sf:100:LEU:HB3	79:Sf:103:LEU:HG	2.00	0.42
81:L5:1270:A:O2'	81:L5:1439:C:O2	2.36	0.42
81:L5:2034:G:H2'	81:L5:2035:C:C6	2.54	0.42
81:L5:2413:U:H2'	81:L5:2414:G:C8	2.54	0.42
81:L5:3893:C:O2'	81:L5:4979:A:N1	2.49	0.42
81:L5:4481:U:H2'	81:L5:4482:U:C6	2.54	0.42
81:L5:4563:U:H2'	81:L5:4564:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:4772:C:H2'	81:L5:4773:C:C6	2.54	0.42
83:Lq:65:ILE:HG23	83:Lq:75:LEU:HB3	2.01	0.42
6:LB:13:SER:HB2	81:L5:4622:A:H4'	2.01	0.42
7:LC:109:ARG:O	7:LC:109:ARG:HG2	2.20	0.42
18:LO:76:PRO:HB3	18:LO:138:LEU:HG	2.00	0.42
18:LO:189:ILE:O	18:LO:193:THR:HG23	2.20	0.42
21:LR:46:LYS:HB3	21:LR:46:LYS:HE3	1.89	0.42
47:S2:1831:A:H3'	47:S2:1871:6MZ:O1P	2.19	0.42
55:SH:181:THR:OG1	55:SH:183:LYS:HG2	2.20	0.42
69:SV:51:LYS:HG3	69:SV:78:ILE:HD11	2.02	0.42
76:Sc:29:GLN:NE2	76:Sc:66:ARG:O	2.52	0.42
76:Sc:47:LYS:HB2	76:Sc:47:LYS:HE3	1.78	0.42
81:L5:1562:G:H5'	81:L5:1563:A:OP2	2.20	0.42
81:L5:3718:A2M:HM'3	81:L5:3718:A2M:H1'	1.86	0.42
1:CB:16:LYS:HB2	1:CB:16:LYS:HE3	1.54	0.42
1:CB:226:LYS:HZ2	1:CB:226:LYS:HG2	1.80	0.42
1:CB:452:LEU:HD12	1:CB:452:LEU:HA	1.77	0.42
6:LB:304:SER:OG	6:LB:310:SER:O	2.37	0.42
7:LC:237:ILE:HD12	7:LC:237:ILE:HA	1.90	0.42
9:LE:72:LYS:HB2	31:Lb:119:CYS:HB2	2.01	0.42
12:LH:118:LEU:HD11	12:LH:167:VAL:HG22	2.01	0.42
18:LO:34:VAL:HG22	18:LO:103:LYS:HB2	2.01	0.42
30:La:35:ALA:HB2	81:L5:38:A:H5''	2.02	0.42
30:La:94:LYS:HD3	30:La:94:LYS:HA	1.90	0.42
38:Li:85:ARG:NH2	81:L5:310:G:H5''	2.35	0.42
47:S2:27:A2M:H8	47:S2:27:A2M:H2'	1.90	0.42
47:S2:67:C:C2	54:SG:167:LYS:HD2	2.53	0.42
47:S2:941:C:H2'	47:S2:942:G:H8	1.85	0.42
49:SB:168:MET:HG2	49:SB:197:ILE:HG21	2.01	0.42
52:SE:11:ARG:HA	52:SE:28:ALA:HB2	2.01	0.42
52:SE:52:LEU:HD13	52:SE:54:TYR:HE2	1.84	0.42
53:SF:135:ARG:HD2	53:SF:135:ARG:HA	1.80	0.42
58:SK:95:ARG:HA	58:SK:95:ARG:HD2	1.84	0.42
63:SP:109:PRO:O	63:SP:112:ILE:HB	2.20	0.42
72:SY:82:ALA:O	72:SY:86:GLU:HB3	2.19	0.42
81:L5:490:C:H2'	81:L5:491:G:C8	2.54	0.42
81:L5:965:G:H2'	81:L5:2256:C:O2	2.19	0.42
81:L5:1342:A:O2'	81:L5:1343:A:H5'	2.20	0.42
81:L5:3721:U:H2'	81:L5:3722:G:H8	1.83	0.42
81:L5:3845:A:H2'	81:L5:3846:C:C6	2.55	0.42
81:L5:4344:U:H2'	81:L5:4345:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:4488:A:H4'	81:L5:4489:G:C8	2.54	0.42
1:CB:84:ASN:OD1	1:CB:84:ASN:N	2.51	0.42
1:CB:127:VAL:HG21	1:CB:143:LEU:HD13	2.02	0.42
5:LA:180:LEU:HD22	45:Lp:26:VAL:HG21	2.01	0.42
7:LC:207:PRO:HG2	7:LC:227:ILE:HD13	2.00	0.42
14:LJ:74:VAL:CG1	14:LJ:78:LYS:HD2	2.50	0.42
15:LL:145:LYS:HE2	15:LL:145:LYS:HB2	1.78	0.42
21:LR:38:ARG:O	21:LR:39:GLN:HB2	2.19	0.42
28:LY:103:LYS:HD2	28:LY:103:LYS:N	2.34	0.42
29:LZ:29:ILE:HD11	29:LZ:98:LYS:HD2	2.00	0.42
36:Lg:69:LYS:HG3	36:Lg:73:HIS:CE1	2.54	0.42
37:Lh:40:ALA:O	37:Lh:44:LEU:HG	2.19	0.42
47:S2:380:G:OP1	56:SI:31:ARG:HD2	2.19	0.42
47:S2:382:C:H2'	47:S2:383:G:C8	2.55	0.42
47:S2:384:U:H5'	59:SL:133:PRO:O	2.20	0.42
47:S2:1115:U:H1'	47:S2:1117:C:OP2	2.18	0.42
47:S2:1177:PSU:H2'	47:S2:1178:U:C6	2.55	0.42
47:S2:1794:C:H2'	47:S2:1795:G:C8	2.55	0.42
47:S2:1806:A:H2'	47:S2:1807:C:C6	2.55	0.42
49:SB:28:LYS:HB3	49:SB:28:LYS:HE2	1.67	0.42
53:SF:127:ARG:HB3	53:SF:135:ARG:HH21	1.84	0.42
56:SI:168:GLN:HA	81:L5:5026:U:H1'	2.02	0.42
61:SN:33:VAL:HG21	61:SN:66:VAL:HG11	2.01	0.42
81:L5:1895:G:H2'	81:L5:1896:A:O4'	2.20	0.42
81:L5:2671:C:H2'	81:L5:2672:C:C6	2.55	0.42
81:L5:2730:U:H2'	81:L5:2731:C:C6	2.54	0.42
3:CD:285:ASP:OD1	3:CD:286:GLU:N	2.52	0.42
4:L8:14:OMU:H2'	4:L8:15:G:O4'	2.19	0.42
5:LA:114:CYS:N	5:LA:165:VAL:O	2.49	0.42
6:LB:3:HIS:CD2	6:LB:5:LYS:H	2.37	0.42
12:LH:60:TRP:O	12:LH:61:TRP:HB2	2.18	0.42
12:LH:105:ILE:HG23	12:LH:109:GLY:HA2	2.00	0.42
14:LJ:95:ARG:C	14:LJ:97:ASN:H	2.28	0.42
21:LR:39:GLN:HG2	21:LR:42:ARG:HH11	1.85	0.42
26:LW:34:ALA:HA	26:LW:37:GLU:HB2	2.02	0.42
47:S2:94:G:O2'	47:S2:508:A:O2'	2.31	0.42
47:S2:880:G:H3'	47:S2:881:G:H8	1.84	0.42
47:S2:1348:G:C8	47:S2:1349:G:C8	3.07	0.42
47:S2:1395:C:H1'	47:S2:1474:A:C5	2.55	0.42
47:S2:1748:G:H2'	47:S2:1749:G:C8	2.54	0.42
51:SD:118:ALA:O	51:SD:122:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:25:ARG:CZ	54:SG:25:ARG:HB2	2.49	0.42
80:Sg:302:TYR:HE2	80:Sg:308:ARG:HB2	1.83	0.42
81:L5:461:G:H2'	81:L5:462:G:H8	1.83	0.42
81:L5:1326:A2M:HM'2	81:L5:1327:C:O4'	2.20	0.42
81:L5:1375:C:O2'	81:L5:1376:C:H5'	2.20	0.42
81:L5:1433:A:H2'	81:L5:1434:G:O4'	2.20	0.42
81:L5:4265:U:H5'	81:L5:4267:G:O6	2.19	0.42
5:LA:145:LYS:HA	5:LA:145:LYS:HD3	1.92	0.42
8:LD:150:LEU:HD23	14:LJ:146:ARG:HG3	2.01	0.42
14:LJ:28:GLU:OE1	14:LJ:32:ARG:NE	2.40	0.42
22:LS:93:MET:HE1	22:LS:117:HIS:CE1	2.55	0.42
26:LW:9:SER:H	26:LW:9:SER:HG	1.61	0.42
29:LZ:83:THR:HG23	36:Lg:95:PHE:CZ	2.54	0.42
37:Lh:81:LEU:HD23	37:Lh:84:ARG:HD2	2.01	0.42
47:S2:5:U:H2'	47:S2:6:G:H8	1.85	0.42
47:S2:54:A:H5'	72:SY:108:LYS:NZ	2.35	0.42
47:S2:306:C:H1'	47:S2:308:G:C5	2.54	0.42
47:S2:595:U:H2'	47:S2:596:U:C6	2.55	0.42
47:S2:1397:U:O4	64:SQ:12:VAL:HA	2.18	0.42
51:SD:32:ASP:OD2	51:SD:65:ARG:NH1	2.53	0.42
60:SM:24:THR:O	60:SM:27:ILE:HG12	2.20	0.42
64:SQ:51:LEU:HA	64:SQ:51:LEU:HD12	1.78	0.42
81:L5:1179:U:O2'	81:L5:1180:C:OP1	2.31	0.42
81:L5:2377:C:H2'	81:L5:2378:G:O4'	2.19	0.42
81:L5:2669:C:H2'	81:L5:2670:C:O4'	2.20	0.42
81:L5:4096:C:H42	81:L5:4112:C:H42	1.68	0.42
81:L5:4112:C:H2'	81:L5:4113:U:C6	2.55	0.42
81:L5:4236:G:H4'	81:L5:4328:G:O2'	2.19	0.42
81:L5:4927:G:H5'	81:L5:4928:C:C5	2.54	0.42
83:Lq:32:ALA:O	83:Lq:85:ASN:ND2	2.52	0.42
4:L8:40:A:H2'	4:L8:41:A:C8	2.55	0.42
4:L8:116:C:O2'	4:L8:117:C:H5'	2.20	0.42
14:LJ:159:LYS:O	14:LJ:163:MET:HG3	2.20	0.42
16:LM:8:GLU:HB3	22:LS:151:LYS:HG3	2.01	0.42
22:LS:116:ARG:NH1	81:L5:1950:U:O2'	2.53	0.42
37:Lh:99:GLU:HA	37:Lh:102:LEU:HG	2.00	0.42
37:Lh:112:ARG:NH2	81:L5:264:C:O2	2.53	0.42
47:S2:203:G:OP1	56:SI:147:LYS:NZ	2.51	0.42
47:S2:352:U:H2'	47:S2:353:C:H6	1.85	0.42
47:S2:952:G:H2'	47:S2:953:C:C6	2.55	0.42
47:S2:1088:U:H4'	47:S2:1089:G:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1144:A:H5'	47:S2:1355:C:C5	2.54	0.42
48:SA:164:ASN:O	48:SA:170:SER:OG	2.28	0.42
59:SL:60:CYS:SG	59:SL:114:SER:OG	2.72	0.42
61:SN:3:ARG:HG2	61:SN:3:ARG:NH1	2.35	0.42
70:SW:42:MET:HB3	70:SW:42:MET:HE2	1.71	0.42
81:L5:65:A:N6	81:L5:75:G:H1'	2.35	0.42
81:L5:2045:G:O6	81:L5:3870:C:O2'	2.37	0.42
81:L5:2376:A:H2'	81:L5:2377:C:C6	2.55	0.42
81:L5:2809:G:N7	91:L5:5105:SPD:H92	2.35	0.42
81:L5:5001:PSU:H2'	81:L5:5002:U:O4'	2.19	0.42
9:LE:153:LEU:HD11	9:LE:195:ILE:HG13	2.02	0.42
12:LH:50:LYS:C	12:LH:52:LYS:H	2.27	0.42
15:LL:2:ALA:HA	15:LL:3:PRO:HD3	1.88	0.42
22:LS:71:SER:O	22:LS:76:LYS:NZ	2.52	0.42
26:LW:44:ARG:HD3	81:L5:3615:G:H21	1.85	0.42
28:LY:11:ARG:HG3	81:L5:229:G:H5''	2.02	0.42
29:LZ:25:ILE:HA	29:LZ:43:VAL:HG12	2.01	0.42
33:Ld:46:LEU:HD22	33:Ld:72:VAL:HG11	2.01	0.42
47:S2:67:C:O2'	54:SG:164:LYS:HD3	2.19	0.42
47:S2:689:U:H2'	47:S2:690:G:N3	2.35	0.42
47:S2:799:U:H5''	55:SH:109:ARG:HB3	2.02	0.42
47:S2:943:U:C2	47:S2:944:A:C8	3.08	0.42
47:S2:1144:A:H2'	47:S2:1145:A:C8	2.54	0.42
47:S2:1365:G:H2'	47:S2:1366:G:H8	1.84	0.42
47:S2:1432:U:P	47:S2:1433:C:H5'	2.59	0.42
48:SA:145:ILE:HG12	48:SA:159:ILE:HB	2.01	0.42
51:SD:28:GLU:HG2	51:SD:69:LEU:HD21	2.01	0.42
52:SE:232:ASN:OD1	52:SE:232:ASN:N	2.52	0.42
69:SV:81:LYS:HB2	69:SV:81:LYS:HE2	1.74	0.42
73:SZ:91:LEU:HD22	73:SZ:96:LEU:HD12	2.01	0.42
75:Sb:38:PRO:O	75:Sb:40:CYS:N	2.52	0.42
81:L5:1669:A:H4'	81:L5:1685:G:H22	1.85	0.42
81:L5:1739:G:H5''	82:L7:102:U:H1'	2.01	0.42
83:Lq:27:CYS:SG	83:Lq:193:PHE:HB3	2.60	0.42
83:Lq:32:ALA:HB3	83:Lq:55:MET:HE1	2.00	0.42
1:CB:354:ILE:HG23	1:CB:358:LEU:HD12	2.02	0.41
4:L8:28:C:O2'	81:L5:1371:A:N1	2.49	0.41
15:LL:10:LEU:HD11	81:L5:1344:C:H1'	2.02	0.41
26:LW:102:LYS:N	26:LW:102:LYS:HD2	2.34	0.41
34:Le:28:TYR:CD2	34:Le:30:LYS:HE2	2.55	0.41
43:Ln:2:ARG:HH22	47:S2:1842:4AC:HM72	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:746:C:H2'	47:S2:747:U:O4'	2.20	0.41
47:S2:1518:C:OP1	47:S2:1519:U:O2'	2.36	0.41
48:SA:198:MET:HG2	48:SA:200:ASP:H	1.83	0.41
50:SC:132:ASP:OD1	50:SC:136:HIS:HB2	2.20	0.41
55:SH:10:LYS:HE2	55:SH:46:THR:C	2.45	0.41
58:SK:59:LYS:HE2	58:SK:59:LYS:HB2	1.59	0.41
60:SM:89:VAL:HG23	60:SM:91:LEU:HG	2.01	0.41
60:SM:124:ILE:HD13	60:SM:124:ILE:HA	1.90	0.41
62:SO:62:VAL:HG11	62:SO:67:ASP:HB2	2.01	0.41
71:SX:95:GLU:O	71:SX:98:ASP:HB2	2.20	0.41
80:Sg:93:THR:O	80:Sg:94:THR:OG1	2.30	0.41
81:L5:1077:C:C2	81:L5:1078:A:C8	3.08	0.41
81:L5:1480:C:O2'	81:L5:1482:G:OP2	2.38	0.41
81:L5:1875:C:H2'	81:L5:1876:U:C6	2.54	0.41
81:L5:4589:A:N1	81:L5:4621:C:O2'	2.47	0.41
81:L5:4861:G:H2'	81:L5:4862:G:H8	1.85	0.41
1:CB:308:LYS:O	1:CB:312:THR:HG23	2.21	0.41
1:CB:619:LYS:HE3	1:CB:619:LYS:HB2	1.74	0.41
3:CD:298:VAL:HG13	3:CD:300:PHE:CD2	2.56	0.41
5:LA:46:LYS:HD2	5:LA:46:LYS:HA	1.76	0.41
9:LE:45:SER:C	9:LE:47:ASN:H	2.28	0.41
10:LF:52:GLU:HG3	31:Lb:96:LEU:CD1	2.50	0.41
13:LI:47:PRO:HB3	13:LI:171:TRP:CZ2	2.55	0.41
19:LP:13:LYS:HD3	19:LP:152:GLU:OE1	2.20	0.41
22:LS:74:ARG:O	22:LS:76:LYS:NZ	2.49	0.41
22:LS:103:ALA:O	22:LS:107:THR:OG1	2.38	0.41
47:S2:1203:G:N3	47:S2:1699:A:H2	2.18	0.41
47:S2:1670:C:H2'	47:S2:1671:G:C8	2.55	0.41
56:SI:203:LYS:HB3	56:SI:203:LYS:HE2	1.73	0.41
59:SL:78:THR:HG21	59:SL:89:ARG:HB2	2.01	0.41
59:SL:90:ARG:HD3	59:SL:109:MET:HE2	2.02	0.41
60:SM:25:ALA:O	60:SM:30:GLY:N	2.53	0.41
61:SN:49:GLN:H	61:SN:49:GLN:HG2	1.60	0.41
64:SQ:97:GLN:CB	64:SQ:105:LYS:HG3	2.50	0.41
74:Sa:2:THR:HG23	74:Sa:3:LYS:N	2.29	0.41
81:L5:965:G:H21	81:L5:2092:G:H1'	1.85	0.41
81:L5:1279:A:O2'	81:L5:1281:G:N7	2.50	0.41
81:L5:2022:C:H2'	81:L5:2023:C:O4'	2.19	0.41
81:L5:2079:G:H2'	81:L5:2080:U:C6	2.55	0.41
81:L5:4232:U:H4'	81:L5:4233:A:O4'	2.20	0.41
1:CB:252:LYS:HE2	1:CB:252:LYS:HB2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LC:143:ARG:HA	7:LC:143:ARG:HD2	1.98	0.41
9:LE:178:PRO:HG2	9:LE:181:LEU:HD12	2.02	0.41
11:LG:43:GLN:HE22	81:L5:4117:U:H5'	1.84	0.41
22:LS:154:LEU:HB3	22:LS:157:ARG:HD3	2.03	0.41
23:LT:28:ALA:O	23:LT:32:ARG:HG2	2.20	0.41
33:Ld:39:LYS:HA	33:Ld:39:LYS:HD3	1.90	0.41
44:Lo:11:PHE:O	44:Lo:81:ARG:NH1	2.35	0.41
47:S2:153:G:N3	54:SG:13:GLN:NE2	2.67	0.41
47:S2:1534:C:H5''	47:S2:1536:G:O4'	2.20	0.41
50:SC:176:LYS:HB2	50:SC:176:LYS:HE2	1.74	0.41
53:SF:143:PRO:HA	53:SF:146:ARG:HG2	2.02	0.41
54:SG:218:LYS:HG2	54:SG:222:GLU:OE2	2.20	0.41
57:SJ:111:GLN:NE2	57:SJ:127:ARG:HB2	2.35	0.41
61:SN:29:THR:OG1	61:SN:31:ASP:OD1	2.32	0.41
75:Sb:41:TYR:CD1	75:Sb:42:LYS:HD3	2.55	0.41
80:Sg:254:PRO:O	80:Sg:272:GLN:NE2	2.49	0.41
80:Sg:260:ASP:HB2	80:Sg:267:VAL:HG11	2.02	0.41
81:L5:751:G:H2'	81:L5:752:G:O4'	2.21	0.41
81:L5:3599:A:H2'	81:L5:3600:G:H8	1.84	0.41
81:L5:4478:G:O2'	81:L5:4602:A:N1	2.47	0.41
81:L5:4518:A:O5'	81:L5:4520:G:H4'	2.20	0.41
81:L5:4578:G:H2'	81:L5:4579:PSU:H6	1.85	0.41
81:L5:4638:U:OP1	81:L5:5044:A:O2'	2.37	0.41
81:L5:5003:U:H2'	81:L5:5004:C:C6	2.55	0.41
81:L5:5007:A:N7	81:L5:5042:A:O2'	2.46	0.41
1:CB:130:ASP:OD1	1:CB:132:VAL:HG22	2.21	0.41
1:CB:462:GLU:H	1:CB:462:GLU:CD	2.28	0.41
5:LA:48:ILE:HG22	45:Lp:54:ILE:HG12	2.01	0.41
9:LE:178:PRO:C	9:LE:180:VAL:H	2.28	0.41
11:LG:162:ASP:CB	11:LG:163:PRO:HD3	2.49	0.41
14:LJ:35:ARG:O	14:LJ:39:VAL:HG13	2.21	0.41
20:LQ:178:ARG:HB3	30:La:53:PHE:O	2.20	0.41
23:LT:107:LYS:HG2	23:LT:111:GLU:OE1	2.20	0.41
24:LU:60:VAL:HG12	24:LU:61:VAL:HG23	2.02	0.41
27:LX:91:GLU:HG3	84:CA:291:MET:HE3	2.02	0.41
29:LZ:27:LYS:HE3	29:LZ:27:LYS:HB2	1.96	0.41
45:Lp:2:ALA:HA	81:L5:1569:U:C5	2.56	0.41
47:S2:106:C:H2'	47:S2:107:A:C8	2.53	0.41
47:S2:293:C:O2	47:S2:293:C:H2'	2.19	0.41
47:S2:554:A:C8	47:S2:589:G:H4'	2.55	0.41
47:S2:1174:U:H2'	47:S2:1175:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SS:24:ARG:HG3	66:SS:29:ALA:HB2	2.02	0.41
71:SX:52:LEU:N	71:SX:71:ARG:O	2.45	0.41
81:L5:699:C:O2'	81:L5:968:C:N3	2.53	0.41
81:L5:1188:C:H2'	81:L5:1189:G:H8	1.86	0.41
81:L5:1696:C:H2'	81:L5:1697:G:O4'	2.20	0.41
3:CD:222:LYS:H	3:CD:222:LYS:HE2	1.85	0.41
3:CD:282:MET:HB3	58:SK:89:ILE:HD13	2.01	0.41
8:LD:291:GLN:HE22	13:LI:214:SER:HG	1.63	0.41
9:LE:179:LEU:HD22	9:LE:250:GLN:HG2	2.02	0.41
10:LF:36:LYS:HE2	10:LF:36:LYS:HB3	1.71	0.41
12:LH:53:LYS:O	12:LH:54:ARG:HB2	2.20	0.41
16:LM:55:MET:HB2	16:LM:55:MET:HE2	1.85	0.41
31:Lb:36:ASP:OD1	81:L5:4314:C:O2'	2.35	0.41
47:S2:85:A:H2'	47:S2:86:C:C6	2.56	0.41
47:S2:109:PSU:H2'	47:S2:110:U:O4'	2.20	0.41
47:S2:308:G:H8	47:S2:308:G:OP2	2.03	0.41
47:S2:1303:C:H2'	47:S2:1304:U:C6	2.55	0.41
48:SA:22:GLY:O	48:SA:24:HIS:ND1	2.44	0.41
51:SD:157:MET:HE2	51:SD:157:MET:HB2	1.95	0.41
53:SF:120:GLY:HA2	53:SF:121:PRO:HD3	1.96	0.41
54:SG:2:LYS:HG2	54:SG:17:GLU:HG2	2.03	0.41
54:SG:3:LEU:HB2	54:SG:16:ILE:HG12	2.01	0.41
73:SZ:92:LEU:HD22	73:SZ:109:TYR:HE1	1.84	0.41
81:L5:317:A:C2	81:L5:4361:PSU:H1'	2.56	0.41
81:L5:733:A:H2'	81:L5:734:G:O4'	2.20	0.41
81:L5:741:C:C4	81:L5:742:G:C8	3.08	0.41
81:L5:1538:U:H2'	81:L5:1539:G:C8	2.54	0.41
81:L5:1908:A:H2'	81:L5:1909:G:O4'	2.20	0.41
81:L5:2542:G:H2'	81:L5:2543:A:C8	2.55	0.41
81:L5:3726:A:H2'	81:L5:3727:A:C8	2.55	0.41
81:L5:4458:C:H2'	81:L5:4459:U:C6	2.55	0.41
81:L5:4551:U:H2'	81:L5:4552:PSU:C6	2.56	0.41
83:Lq:77:LYS:H	83:Lq:77:LYS:HG3	1.66	0.41
1:CB:539:GLU:CG	1:CB:545:ILE:HG13	2.51	0.41
4:L8:5:U:H2'	4:L8:6:C:H6	1.86	0.41
7:LC:76:ILE:HG21	81:L5:2352:U:H5'	2.01	0.41
7:LC:209:ILE:HD13	7:LC:251:ILE:HB	2.01	0.41
8:LD:286:SER:HB3	81:L5:1178:G:C2'	2.46	0.41
11:LG:154:LEU:HB3	11:LG:204:PHE:HB2	2.03	0.41
16:LM:85:LYS:O	16:LM:89:THR:HG23	2.20	0.41
24:LU:19:LEU:HD12	24:LU:73:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Lg:84:ALA:O	36:Lg:88:ARG:HG3	2.21	0.41
46:Lr:64:ILE:HG23	46:Lr:102:TYR:CZ	2.56	0.41
47:S2:433:A:H2'	47:S2:434:G:C8	2.56	0.41
47:S2:1824:A:H3'	47:S2:1825:A:H8	1.85	0.41
55:SH:113:LYS:HD2	55:SH:113:LYS:H	1.86	0.41
64:SQ:113:ILE:HG12	64:SQ:120:LEU:HD12	2.02	0.41
72:SY:117:VAL:O	72:SY:122:LYS:NZ	2.39	0.41
81:L5:10:A:H2'	81:L5:11:G:C8	2.55	0.41
81:L5:728:U:H2'	81:L5:730:G:H5'	2.02	0.41
81:L5:3727:A:H8	81:L5:3727:A:OP2	2.04	0.41
81:L5:4347:G:H2'	81:L5:4348:A:C8	2.56	0.41
81:L5:4862:G:H2'	81:L5:4863:G:C8	2.56	0.41
81:L5:5010:PSU:H2'	81:L5:5011:A:C8	2.56	0.41
1:CB:283:LYS:HB3	1:CB:283:LYS:HE3	1.77	0.41
1:CB:302:ASP:OD2	1:CB:306:ASN:ND2	2.53	0.41
4:L8:37:A:OP2	37:Lh:89:ARG:HD2	2.21	0.41
6:LB:258:HIS:C	6:LB:260:ALA:N	2.77	0.41
6:LB:331:VAL:HG12	6:LB:333:LEU:HG	2.03	0.41
7:LC:63:SER:O	7:LC:80:ARG:HD2	2.20	0.41
8:LD:262:LYS:H	8:LD:262:LYS:CD	2.33	0.41
13:LI:204:GLY:O	82:L7:63:C:H3'	2.20	0.41
15:LL:170:THR:OG1	15:LL:173:GLU:HG3	2.21	0.41
17:LN:179:LYS:HE2	81:L5:313:U:H5''	2.03	0.41
36:Lg:19:LYS:HD3	36:Lg:19:LYS:HA	1.92	0.41
40:Lk:9:LYS:HE3	40:Lk:9:LYS:HB2	1.93	0.41
40:Lk:35:LYS:HE3	81:L5:2693:G:OP1	2.21	0.41
47:S2:1333:U:H5'	51:SD:147:ALA:HB2	2.03	0.41
47:S2:1631:U:H2'	47:S2:1632:G:O4'	2.20	0.41
48:SA:159:ILE:HD11	69:SV:34:MET:HE1	2.02	0.41
50:SC:178:HIS:ND1	50:SC:221:ASP:OD2	2.44	0.41
51:SD:137:VAL:HG22	51:SD:151:LYS:HG3	2.02	0.41
74:Sa:11:ALA:HB3	74:Sa:33:ASP:HB2	2.02	0.41
79:Sf:92:LYS:HA	79:Sf:92:LYS:HD2	1.76	0.41
81:L5:2479:G:H2'	81:L5:2480:G:C8	2.56	0.41
81:L5:2811:G:H1'	81:L5:2815:A2M:N6	2.35	0.41
81:L5:4174:U:H2'	81:L5:4175:G:C8	2.55	0.41
1:CB:45:ILE:HG21	1:CB:454:MET:HE1	2.03	0.41
1:CB:745:TYR:HB2	1:CB:788:LEU:O	2.20	0.41
3:CD:186:ASP:OD2	3:CD:186:ASP:C	2.64	0.41
7:LC:230:LEU:HD12	7:LC:230:LEU:HA	1.91	0.41
9:LE:101:ASN:HB3	81:L5:684:G:O2'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:161:ARG:O	9:LE:182:ASN:ND2	2.54	0.41
9:LE:183:ARG:HD2	9:LE:183:ARG:HA	1.84	0.41
17:LN:12:ARG:NH1	81:L5:308:G:O6	2.53	0.41
47:S2:853:C:C2	47:S2:854:A:C8	3.09	0.41
47:S2:1562:C:H2'	47:S2:1563:G:C8	2.55	0.41
47:S2:1673:U:O2'	53:SF:84:GLY:O	2.33	0.41
50:SC:204:ILE:O	50:SC:211:LYS:NZ	2.54	0.41
51:SD:148:LYS:HE2	51:SD:150:MET:HG3	2.02	0.41
53:SF:100:ILE:O	53:SF:104:THR:OG1	2.38	0.41
57:SJ:28:GLU:OE2	57:SJ:44:TRP:NE1	2.50	0.41
67:ST:50:GLU:H	67:ST:50:GLU:CD	2.28	0.41
80:Sg:157:SER:HB2	80:Sg:164:ILE:CD1	2.50	0.41
81:L5:737:C:C4	81:L5:739:G:H5''	2.56	0.41
81:L5:1720:C:H2'	81:L5:1721:G:O4'	2.20	0.41
81:L5:4389:C:H2'	81:L5:4390:A:C8	2.56	0.41
81:L5:4538:G:H2'	81:L5:4539:U:C6	2.56	0.41
81:L5:4710:C:H2'	81:L5:4711:C:C6	2.55	0.41
81:L5:4723:A:H2'	81:L5:4724:A:C8	2.56	0.41
1:CB:585:GLU:HG2	1:CB:737:GLN:HB2	2.03	0.41
1:CB:651:CYS:SG	1:CB:680:VAL:HG22	2.61	0.41
5:LA:118:GLU:HG3	5:LA:126:LEU:HD21	2.02	0.41
6:LB:66:LYS:HG3	25:LV:11:GLY:HA2	2.02	0.41
6:LB:156:TYR:OH	81:L5:4912:G:N2	2.54	0.41
6:LB:228:TYR:O	81:L5:2835:A:O2'	2.34	0.41
6:LB:359:ALA:O	6:LB:360:LEU:HG	2.20	0.41
7:LC:66:SER:O	7:LC:67:TRP:HB2	2.21	0.41
7:LC:209:ILE:HB	7:LC:229:LEU:HD13	2.03	0.41
7:LC:318:PRO:C	7:LC:320:LYS:H	2.29	0.41
8:LD:129:GLU:HB3	8:LD:177:THR:CG2	2.51	0.41
11:LG:48:LYS:HD2	27:LX:42:THR:HB	2.02	0.41
12:LH:72:THR:HG22	81:L5:4691:A:H1'	2.03	0.41
13:LI:91:LEU:HD23	13:LI:91:LEU:HA	1.95	0.41
13:LI:115:MET:HB2	81:L5:4442:PSU:OP1	2.20	0.41
15:LL:80:GLU:OE1	15:LL:102:ARG:NH2	2.54	0.41
15:LL:165:LYS:HB3	15:LL:165:LYS:HE2	1.58	0.41
21:LR:62:ARG:NH2	81:L5:4648:A:OP1	2.54	0.41
21:LR:172:ARG:HH21	47:S2:909:G:P	2.44	0.41
24:LU:25:CYS:HB3	24:LU:112:LEU:HD22	2.03	0.41
29:LZ:14:LEU:O	36:Lg:88:ARG:HG2	2.21	0.41
30:La:59:LYS:HD2	30:La:61:TYR:HE1	1.85	0.41
31:Lb:18:ARG:HD2	81:L5:1686:C:O3'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Lb:106:LYS:HE2	31:Lb:106:LYS:HB2	1.79	0.41
33:Ld:26:THR:HG22	33:Ld:85:ARG:NH1	2.35	0.41
34:Le:43:ASN:HD22	34:Le:44:ARG:N	2.19	0.41
38:Li:43:MET:HE2	38:Li:43:MET:HA	2.03	0.41
42:Lm:95:ILE:HD12	81:L5:4473:A:H5''	2.02	0.41
47:S2:51:U:H2'	47:S2:52:G:H8	1.84	0.41
47:S2:96:C:H2'	47:S2:97:U:C6	2.55	0.41
47:S2:107:A:H2'	47:S2:108:G:H8	1.84	0.41
47:S2:215:G:H2'	47:S2:216:C:C6	2.54	0.41
47:S2:943:U:H2'	47:S2:944:A:C8	2.54	0.41
47:S2:964:A:H2'	47:S2:965:U:C6	2.56	0.41
47:S2:1025:U:OP1	47:S2:1090:C:O2'	2.39	0.41
47:S2:1351:G:O2'	47:S2:1378:A:N1	2.47	0.41
47:S2:1553:C:H2'	47:S2:1554:C:O4'	2.21	0.41
47:S2:1589:A:H2'	47:S2:1590:C:O4'	2.20	0.41
47:S2:1616:U:H2'	47:S2:1617:G:O4'	2.21	0.41
47:S2:1628:C:H2'	47:S2:1629:C:C6	2.55	0.41
47:S2:1667:U:H2'	47:S2:1668:U:C6	2.56	0.41
47:S2:1686:G:H2'	47:S2:1687:C:C6	2.56	0.41
47:S2:1730:U:H2'	47:S2:1731:A:C8	2.55	0.41
48:SA:107:THR:HG23	48:SA:115:ALA:O	2.21	0.41
49:SB:77:ASP:OD1	49:SB:77:ASP:N	2.50	0.41
52:SE:233:LYS:HE3	52:SE:233:LYS:HB3	1.87	0.41
53:SF:24:SER:OG	53:SF:27:ASP:OD1	2.37	0.41
53:SF:167:LYS:HG2	53:SF:171:GLU:OE1	2.21	0.41
54:SG:215:LYS:HE3	54:SG:216:ARG:NH1	2.35	0.41
66:SS:116:LYS:HB3	66:SS:116:LYS:HE3	1.68	0.41
72:SY:57:VAL:HB	72:SY:60:PHE:HE2	1.86	0.41
80:Sg:260:ASP:O	80:Sg:264:LYS:HA	2.21	0.41
81:L5:25:A:H2'	81:L5:26:C:H6	1.86	0.41
81:L5:126:C:H2'	81:L5:127:G:H8	1.85	0.41
81:L5:286:U:H2'	81:L5:287:U:C6	2.55	0.41
81:L5:382:G:O2'	81:L5:407:A:N6	2.48	0.41
81:L5:385:A:N3	81:L5:387:G:H5''	2.36	0.41
81:L5:650:C:H2'	81:L5:651:C:C6	2.56	0.41
81:L5:1175:A:H2	81:L5:1185:G:H1	1.68	0.41
81:L5:1253:G:O2'	81:L5:1257:A:N6	2.50	0.41
81:L5:1905:U:H2'	81:L5:1906:U:O4'	2.21	0.41
81:L5:2021:G:H5''	83:Lq:58:ASN:OD1	2.20	0.41
81:L5:2276:A:H2'	81:L5:2277:C:O4'	2.21	0.41
81:L5:2634:C:H2'	81:L5:2635:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:L5:4413:C:H2'	81:L5:4414:A:O4'	2.21	0.41
81:L5:4611:A:H2'	81:L5:4612:C:C6	2.56	0.41
1:CB:664:ASP:C	1:CB:665:ILE:HD13	2.45	0.41
4:L8:20:A:H2'	4:L8:21:C:O4'	2.20	0.41
8:LD:208:MET:HE2	8:LD:208:MET:HB3	1.87	0.41
9:LE:205:ASN:C	9:LE:205:ASN:OD1	2.63	0.41
21:LR:80:LYS:HE3	21:LR:80:LYS:HB3	1.92	0.41
24:LU:19:LEU:HD23	24:LU:19:LEU:H	1.86	0.41
31:Lb:114:LYS:HB2	31:Lb:114:LYS:HE2	1.80	0.41
31:Lb:120:ARG:CZ	81:L5:1241:C:H5	2.34	0.41
47:S2:1473:G:N1	47:S2:1476:A:OP2	2.52	0.41
49:SB:138:PHE:O	49:SB:213:ARG:N	2.54	0.41
62:SO:71:PRO:HB3	62:SO:114:SER:OG	2.20	0.41
64:SQ:113:ILE:HD13	64:SQ:113:ILE:HA	1.95	0.41
67:ST:11:GLN:OE1	67:ST:62:ARG:HD2	2.21	0.41
81:L5:271:C:H2'	81:L5:272:U:C6	2.56	0.41
81:L5:689:U:H2'	81:L5:690:C:C6	2.56	0.41
81:L5:1475:G:N2	81:L5:1490:G:C4	2.89	0.41
81:L5:1779:PSU:H2'	81:L5:1780:A:C8	2.56	0.41
81:L5:3772:U:H3'	81:L5:3773:U:C5'	2.50	0.41
81:L5:4115:G:H4'	81:L5:4116:C:H5'	2.03	0.41
83:Lq:39:GLN:CG	83:Lq:107:VAL:HG21	2.51	0.41
1:CB:10:ARG:NE	1:CB:465:PRO:HD3	2.36	0.40
1:CB:325:SER:HA	1:CB:328:LYS:NZ	2.36	0.40
1:CB:750:GLN:O	1:CB:808:ALA:HA	2.21	0.40
6:LB:28:LYS:O	6:LB:220:ILE:HG21	2.21	0.40
7:LC:293:LEU:O	7:LC:299:GLN:NE2	2.37	0.40
9:LE:73:TYR:HB2	81:L5:1273:G:C6	2.56	0.40
11:LG:102:TYR:OH	11:LG:208:ASN:HB2	2.21	0.40
13:LI:208:LYS:O	13:LI:211:VAL:HG22	2.21	0.40
15:LL:46:ILE:O	15:LL:149:GLN:NE2	2.53	0.40
25:LV:60:MET:HE3	25:LV:60:MET:HB2	1.87	0.40
26:LW:71:ARG:HB2	26:LW:73:ARG:HH22	1.86	0.40
28:LY:47:MET:HE3	28:LY:47:MET:HB3	1.97	0.40
30:La:43:ILE:HG23	81:L5:4304:A:C2	2.55	0.40
36:Lg:109:ALA:O	36:Lg:112:GLN:HG3	2.21	0.40
40:Lk:36:VAL:HG13	40:Lk:43:TYR:HB2	2.02	0.40
47:S2:193:C:H2'	47:S2:194:C:C6	2.56	0.40
47:S2:555:A:OP1	47:S2:555:A:H8	2.04	0.40
47:S2:959:G:O2'	47:S2:1065:G:H4'	2.20	0.40
47:S2:1047:C:H2'	47:S2:1048:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1809:A:H2'	47:S2:1810:U:O4'	2.20	0.40
74:Sa:59:PHE:HB2	74:Sa:62:TYR:HB2	2.03	0.40
79:Sf:133:ALA:N	79:Sf:140:TYR:O	2.47	0.40
81:L5:734:G:C2	81:L5:735:G:C8	3.09	0.40
81:L5:965:G:N2	81:L5:2092:G:H1'	2.36	0.40
81:L5:1284:G:O2'	81:L5:1285:U:H5''	2.21	0.40
81:L5:1662:C:H2'	81:L5:1663:C:H6	1.87	0.40
81:L5:1942:A:H2'	81:L5:1943:A:H8	1.85	0.40
81:L5:1962:A:N6	81:L5:2026:A:O2'	2.54	0.40
81:L5:2463:G:C2'	81:L5:2464:C:H5'	2.51	0.40
81:L5:2898:G:H2'	81:L5:2899:C:C6	2.56	0.40
81:L5:4088:C:H2'	81:L5:4089:G:H8	1.85	0.40
81:L5:4691:A:H2'	81:L5:4692:A:O4'	2.20	0.40
81:L5:4749:C:H2'	81:L5:4750:G:O4'	2.21	0.40
1:CB:505:VAL:HG22	1:CB:797:THR:HG21	2.04	0.40
13:LI:22:PHE:CZ	81:L5:1788:A:H2'	2.57	0.40
15:LL:3:PRO:O	81:L5:1682:A:H5''	2.21	0.40
29:LZ:10:VAL:HG11	29:LZ:129:TRP:HZ3	1.86	0.40
38:Li:25[A]:ARG:NH1	81:L5:159:C:H5'	2.36	0.40
38:Li:25[B]:ARG:NH1	81:L5:159:C:H5'	2.36	0.40
47:S2:162:C:H2'	47:S2:163:U:O4'	2.21	0.40
47:S2:344:U:H2'	47:S2:345:U:H6	1.85	0.40
47:S2:929:G:H2'	47:S2:930:C:O4'	2.20	0.40
47:S2:1253:A:N6	47:S2:1665:G:O2'	2.54	0.40
47:S2:1398:G:H22	47:S2:1448:A:H2	1.70	0.40
52:SE:124:CYS:HB3	52:SE:141:THR:HB	2.03	0.40
53:SF:119:SER:HB2	53:SF:189:ALA:HB1	2.04	0.40
53:SF:127:ARG:O	53:SF:127:ARG:NE	2.54	0.40
54:SG:93:LYS:HE3	54:SG:93:LYS:HB3	1.77	0.40
81:L5:182:G:H2'	81:L5:183:C:H6	1.86	0.40
81:L5:259:C:H2'	81:L5:260:C:C6	2.57	0.40
81:L5:1078:A:C5	81:L5:1079:C:C5	3.09	0.40
81:L5:2293:U:H2'	81:L5:2294:G:C8	2.56	0.40
81:L5:2805:C:C2'	81:L5:2806:A:H5'	2.51	0.40
81:L5:4219:A:H3'	81:L5:4220:6MZ:P	2.60	0.40
81:L5:4895:C:H3'	81:L5:4895:C:OP2	2.21	0.40
83:Lq:107:VAL:HG12	83:Lq:185:PHE:O	2.21	0.40
1:CB:454:MET:HE3	1:CB:454:MET:HB3	1.85	0.40
6:LB:306:ASP:O	6:LB:306:ASP:OD1	2.39	0.40
10:LF:222:LYS:HE3	10:LF:222:LYS:HB3	1.86	0.40
13:LI:47:PRO:HG2	13:LI:142:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LL:18:TRP:CD1	15:LL:18:TRP:H	2.38	0.40
15:LL:128:PRO:HA	15:LL:138:ASP:CG	2.46	0.40
22:LS:95:ARG:HE	22:LS:95:ARG:HB3	1.73	0.40
47:S2:564:A:H2'	47:S2:565:G:O4'	2.21	0.40
47:S2:1439:A:H2'	47:S2:1440:C:O4'	2.21	0.40
57:SJ:179:LYS:HB2	57:SJ:179:LYS:HE2	1.97	0.40
80:Sg:5:MET:HB2	80:Sg:270:LEU:HD21	2.04	0.40
81:L5:1247:U:H2'	81:L5:1248:C:H6	1.85	0.40
81:L5:1689:G:N7	89:L5:5385:PUT:H41	2.37	0.40
81:L5:1751:A:H2'	81:L5:1752:G:C8	2.56	0.40
81:L5:2809:G:O2'	81:L5:4644:G:OP1	2.30	0.40
81:L5:3785:A2M:H8	81:L5:3785:A2M:H2'	1.96	0.40
81:L5:3934:G:H2'	81:L5:3935:C:C6	2.57	0.40
81:L5:4322:G:N2	81:L5:4325:A:OP2	2.47	0.40
1:CB:599:HIS:NE2	3:CD:183:ASP:HB2	2.36	0.40
10:LF:88:LYS:HE3	10:LF:88:LYS:HB2	1.81	0.40
13:LI:207:ASP:O	13:LI:211:VAL:HG13	2.22	0.40
43:Ln:15:ARG:HG3	43:Ln:18:ARG:NH2	2.36	0.40
44:Lo:77:CYS:SG	44:Lo:79:SER:HB2	2.62	0.40
47:S2:601:OMG:HM23	47:S2:601:OMG:H1'	1.92	0.40
47:S2:1005:G:H2'	47:S2:1006:C:H6	1.86	0.40
47:S2:1390:U:H2'	47:S2:1391:OMC:C6	2.56	0.40
47:S2:1473:G:H5'	47:S2:1474:A:OP2	2.22	0.40
51:SD:110:LEU:HG	51:SD:175:VAL:HG13	2.04	0.40
53:SF:88:MET:O	53:SF:91:ARG:HG2	2.21	0.40
55:SH:66:VAL:HG22	55:SH:96:ALA:HB1	2.03	0.40
60:SM:85:LEU:HD21	60:SM:109:VAL:HG12	2.04	0.40
66:SS:51:ASP:O	66:SS:54:LYS:HG2	2.22	0.40
67:ST:6:VAL:O	67:ST:11:GLN:NE2	2.44	0.40
80:Sg:153:CYS:O	80:Sg:167:SER:HA	2.22	0.40
81:L5:5024:C:H3'	81:L5:5025:C:O4'	2.21	0.40
1:CB:505:VAL:O	1:CB:547:ALA:HA	2.22	0.40
4:L8:102:G:OP2	4:L8:104:A:O2'	2.33	0.40
6:LB:56:ILE:HG22	6:LB:368:ILE:HG12	2.03	0.40
6:LB:206:PRO:HG2	6:LB:209:GLN:HG3	2.04	0.40
21:LR:3:MET:HG2	81:L5:2385:U:H4'	2.03	0.40
21:LR:171:LYS:O	21:LR:174:GLU:HG3	2.20	0.40
25:LV:69:LYS:HD3	25:LV:71:GLU:OE2	2.22	0.40
47:S2:116:OMU:H1'	47:S2:116:OMU:HM23	1.71	0.40
47:S2:553:U:H2'	47:S2:555:A:C5	2.56	0.40
47:S2:674:C:H2'	47:S2:675:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:S2:1395:C:H1'	47:S2:1474:A:C4	2.57	0.40
48:SA:21:ALA:O	48:SA:23:THR:OG1	2.38	0.40
51:SD:206:ASP:OD1	51:SD:206:ASP:N	2.53	0.40
67:ST:38:LYS:HE2	67:ST:43:LYS:O	2.21	0.40
68:SU:56:MET:HG3	68:SU:86:LYS:HD2	2.03	0.40
74:Sa:64:LEU:HA	74:Sa:65:PRO:HD3	1.94	0.40
75:Sb:21:LYS:C	75:Sb:23:ARG:H	2.29	0.40
76:Sc:26:GLN:H	76:Sc:26:GLN:HG2	1.57	0.40
81:L5:113:A:H2'	81:L5:114:G:O4'	2.21	0.40
81:L5:137:G:C2	81:L5:138:G:C5	3.09	0.40
81:L5:750:U:C2	81:L5:751:G:C8	3.09	0.40
81:L5:2029:A:H2'	81:L5:2030:A:C8	2.57	0.40
81:L5:2538:U:H2'	81:L5:2539:C:C6	2.56	0.40
81:L5:2675:G:H1'	81:L5:2676:A:OP2	2.21	0.40
81:L5:3606:U:H2'	81:L5:3607:U:C6	2.57	0.40
81:L5:3713:U:H4'	81:L5:3714:G:O5'	2.21	0.40
81:L5:3932:U:H2'	81:L5:3933:G:C8	2.56	0.40
81:L5:4344:U:H2'	81:L5:4345:C:H6	1.87	0.40
81:L5:4397:A:N1	93:L5:5388:ANM:H13	2.36	0.40
81:L5:4734:A:O2'	81:L5:4735:G:OP2	2.29	0.40
83:Lq:77:LYS:HB2	83:Lq:198:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CB	813/858 (95%)	794 (98%)	19 (2%)	0	100	100
3	CD	68/402 (17%)	63 (93%)	5 (7%)	0	100	100
5	LA	246/257 (96%)	237 (96%)	9 (4%)	0	100	100
6	LB	397/403 (98%)	382 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	LC	362/427 (85%)	344 (95%)	18 (5%)	0	100	100
8	LD	290/297 (98%)	278 (96%)	12 (4%)	0	100	100
9	LE	219/288 (76%)	204 (93%)	15 (7%)	0	100	100
10	LF	224/248 (90%)	217 (97%)	7 (3%)	0	100	100
11	LG	223/266 (84%)	216 (97%)	7 (3%)	0	100	100
12	LH	188/192 (98%)	175 (93%)	12 (6%)	1 (0%)	24	42
13	LI	199/214 (93%)	195 (98%)	4 (2%)	0	100	100
14	LJ	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
15	LL	204/211 (97%)	195 (96%)	8 (4%)	1 (0%)	24	42
16	LM	135/215 (63%)	129 (96%)	6 (4%)	0	100	100
17	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
18	LO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
19	LP	156/184 (85%)	148 (95%)	8 (5%)	0	100	100
20	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
21	LR	179/196 (91%)	174 (97%)	5 (3%)	0	100	100
22	LS	173/176 (98%)	165 (95%)	8 (5%)	0	100	100
23	LT	156/160 (98%)	151 (97%)	4 (3%)	1 (1%)	21	38
24	LU	98/128 (77%)	94 (96%)	3 (3%)	1 (1%)	12	25
25	LV	128/140 (91%)	123 (96%)	5 (4%)	0	100	100
26	LW	109/157 (69%)	107 (98%)	2 (2%)	0	100	100
27	LX	119/156 (76%)	117 (98%)	2 (2%)	0	100	100
28	LY	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
29	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
30	La	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
31	Lb	101/159 (64%)	97 (96%)	4 (4%)	0	100	100
32	Lc	92/115 (80%)	90 (98%)	2 (2%)	0	100	100
33	Ld	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
34	Le	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
35	Lf	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
36	Lg	111/117 (95%)	111 (100%)	0	0	100	100
37	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	Li	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
39	Lj	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
40	Lk	66/70 (94%)	66 (100%)	0	0	100	100
41	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
42	Lm	50/128 (39%)	50 (100%)	0	0	100	100
43	Ln	22/25 (88%)	22 (100%)	0	0	100	100
44	Lo	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
45	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
46	Lr	124/137 (90%)	119 (96%)	5 (4%)	0	100	100
48	SA	213/295 (72%)	205 (96%)	8 (4%)	0	100	100
49	SB	211/264 (80%)	205 (97%)	6 (3%)	0	100	100
50	SC	218/293 (74%)	209 (96%)	9 (4%)	0	100	100
51	SD	224/243 (92%)	221 (99%)	2 (1%)	1 (0%)	30	48
52	SE	258/263 (98%)	249 (96%)	9 (4%)	0	100	100
53	SF	180/204 (88%)	170 (94%)	10 (6%)	0	100	100
54	SG	233/249 (94%)	228 (98%)	4 (2%)	1 (0%)	30	48
55	SH	181/194 (93%)	172 (95%)	8 (4%)	1 (1%)	21	38
56	SI	203/208 (98%)	193 (95%)	10 (5%)	0	100	100
57	SJ	178/194 (92%)	173 (97%)	5 (3%)	0	100	100
58	SK	95/165 (58%)	89 (94%)	6 (6%)	0	100	100
59	SL	141/158 (89%)	137 (97%)	4 (3%)	0	100	100
60	SM	109/132 (83%)	102 (94%)	7 (6%)	0	100	100
61	SN	148/151 (98%)	148 (100%)	0	0	100	100
62	SO	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
63	SP	126/145 (87%)	120 (95%)	6 (5%)	0	100	100
64	SQ	140/146 (96%)	134 (96%)	6 (4%)	0	100	100
65	SR	130/135 (96%)	123 (95%)	7 (5%)	0	100	100
66	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
67	ST	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
68	SU	98/119 (82%)	93 (95%)	5 (5%)	0	100	100
69	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
71	SX	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
72	SY	121/133 (91%)	120 (99%)	1 (1%)	0	100	100
73	SZ	70/125 (56%)	64 (91%)	5 (7%)	1 (1%)	9	19
74	Sa	100/115 (87%)	96 (96%)	4 (4%)	0	100	100
75	Sb	76/84 (90%)	70 (92%)	6 (8%)	0	100	100
76	Sc	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
77	Sd	53/56 (95%)	53 (100%)	0	0	100	100
78	Se	48/133 (36%)	46 (96%)	2 (4%)	0	100	100
79	Sf	63/156 (40%)	60 (95%)	3 (5%)	0	100	100
80	Sg	311/317 (98%)	288 (93%)	23 (7%)	0	100	100
83	Lq	197/317 (62%)	184 (93%)	12 (6%)	1 (0%)	24	42
84	CA	13/394 (3%)	13 (100%)	0	0	100	100
All	All	12260/14733 (83%)	11805 (96%)	446 (4%)	9 (0%)	49	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
55	SH	148	LEU
54	SG	127	THR
73	SZ	103	HIS
24	LU	67	LYS
23	LT	80	VAL
12	LH	54	ARG
15	LL	135	LYS
83	Lq	154	ILE
51	SD	217	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CB	697/730 (96%)	669 (96%)	28 (4%)	28	53
3	CD	62/322 (19%)	60 (97%)	2 (3%)	34	59
5	LA	189/199 (95%)	180 (95%)	9 (5%)	23	46
6	LB	347/349 (99%)	337 (97%)	10 (3%)	37	61
7	LC	302/348 (87%)	295 (98%)	7 (2%)	44	68
8	LD	246/250 (98%)	233 (95%)	13 (5%)	20	42
9	LE	197/252 (78%)	189 (96%)	8 (4%)	27	52
10	LF	195/215 (91%)	191 (98%)	4 (2%)	47	70
11	LG	196/223 (88%)	191 (97%)	5 (3%)	40	65
12	LH	169/171 (99%)	167 (99%)	2 (1%)	63	80
13	LI	174/182 (96%)	166 (95%)	8 (5%)	24	48
14	LJ	144/149 (97%)	135 (94%)	9 (6%)	16	34
15	LL	172/177 (97%)	169 (98%)	3 (2%)	53	75
16	LM	116/161 (72%)	111 (96%)	5 (4%)	26	50
17	LN	171/172 (99%)	165 (96%)	6 (4%)	32	57
18	LO	173/174 (99%)	166 (96%)	7 (4%)	28	53
19	LP	139/163 (85%)	132 (95%)	7 (5%)	22	44
20	LQ	164/165 (99%)	161 (98%)	3 (2%)	51	73
21	LR	160/175 (91%)	153 (96%)	7 (4%)	25	49
22	LS	156/157 (99%)	143 (92%)	13 (8%)	10	22
23	LT	139/140 (99%)	129 (93%)	10 (7%)	13	28
24	LU	90/115 (78%)	87 (97%)	3 (3%)	33	58
25	LV	100/107 (94%)	94 (94%)	6 (6%)	17	36
26	LW	94/126 (75%)	93 (99%)	1 (1%)	65	81
27	LX	109/133 (82%)	106 (97%)	3 (3%)	38	62
28	LY	124/135 (92%)	118 (95%)	6 (5%)	23	46
29	LZ	117/118 (99%)	114 (97%)	3 (3%)	40	65
30	La	120/121 (99%)	113 (94%)	7 (6%)	18	38
31	Lb	86/126 (68%)	82 (95%)	4 (5%)	23	47
32	Lc	79/97 (81%)	74 (94%)	5 (6%)	16	34
33	Ld	98/110 (89%)	93 (95%)	5 (5%)	21	43
34	Le	114/121 (94%)	110 (96%)	4 (4%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Lf	88/89 (99%)	86 (98%)	2 (2%)	44	68
36	Lg	97/100 (97%)	95 (98%)	2 (2%)	47	70
37	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	84
38	Li	87/89 (98%)	84 (97%)	3 (3%)	32	58
39	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	78
40	Lk	63/65 (97%)	60 (95%)	3 (5%)	23	46
41	Ll	47/48 (98%)	47 (100%)	0	100	100
42	Lm	47/116 (40%)	47 (100%)	0	100	100
43	Ln	23/24 (96%)	23 (100%)	0	100	100
44	Lo	93/94 (99%)	92 (99%)	1 (1%)	65	81
45	Lp	73/75 (97%)	70 (96%)	3 (4%)	27	52
46	Lr	109/121 (90%)	107 (98%)	2 (2%)	51	73
48	SA	180/243 (74%)	177 (98%)	3 (2%)	53	75
49	SB	194/231 (84%)	189 (97%)	5 (3%)	40	65
50	SC	186/225 (83%)	177 (95%)	9 (5%)	23	46
51	SD	189/202 (94%)	184 (97%)	5 (3%)	40	65
52	SE	223/225 (99%)	220 (99%)	3 (1%)	61	79
53	SF	157/170 (92%)	152 (97%)	5 (3%)	34	59
54	SG	205/218 (94%)	197 (96%)	8 (4%)	28	54
55	SH	157/174 (90%)	152 (97%)	5 (3%)	34	59
56	SI	177/180 (98%)	171 (97%)	6 (3%)	32	58
57	SJ	160/168 (95%)	156 (98%)	4 (2%)	42	66
58	SK	88/136 (65%)	86 (98%)	2 (2%)	44	68
59	SL	131/142 (92%)	129 (98%)	2 (2%)	57	77
60	SM	93/108 (86%)	90 (97%)	3 (3%)	34	59
61	SN	130/131 (99%)	126 (97%)	4 (3%)	35	60
62	SO	104/119 (87%)	100 (96%)	4 (4%)	29	54
63	SP	114/130 (88%)	111 (97%)	3 (3%)	40	65
64	SQ	115/121 (95%)	112 (97%)	3 (3%)	40	65
65	SR	119/122 (98%)	116 (98%)	3 (2%)	42	66
66	SS	125/132 (95%)	122 (98%)	3 (2%)	43	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	ST	112/115 (97%)	109 (97%)	3 (3%)	39	63
68	SU	92/107 (86%)	89 (97%)	3 (3%)	33	58
69	SV	67/67 (100%)	66 (98%)	1 (2%)	57	77
70	SW	111/113 (98%)	107 (96%)	4 (4%)	31	56
71	SX	112/115 (97%)	111 (99%)	1 (1%)	70	84
72	SY	107/115 (93%)	106 (99%)	1 (1%)	70	84
73	SZ	64/103 (62%)	61 (95%)	3 (5%)	23	47
74	Sa	87/98 (89%)	86 (99%)	1 (1%)	65	81
75	Sb	73/76 (96%)	71 (97%)	2 (3%)	39	63
76	Sc	56/62 (90%)	51 (91%)	5 (9%)	9	20
77	Sd	45/49 (92%)	44 (98%)	1 (2%)	45	69
78	Se	42/104 (40%)	41 (98%)	1 (2%)	43	67
79	Sf	57/140 (41%)	54 (95%)	3 (5%)	20	42
80	Sg	270/275 (98%)	260 (96%)	10 (4%)	30	55
83	Lq	167/258 (65%)	163 (98%)	4 (2%)	43	67
84	CA	12/336 (4%)	12 (100%)	0	100	100
All	All	10669/12504 (85%)	10315 (97%)	354 (3%)	34	58

All (354) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CB	4	PHE
1	CB	14	ASP
1	CB	16	LYS
1	CB	22	MET
1	CB	110	ASP
1	CB	128	VAL
1	CB	154	VAL
1	CB	209	LEU
1	CB	233	VAL
1	CB	274	SER
1	CB	278	THR
1	CB	328	LYS
1	CB	398	ILE
1	CB	421	VAL
1	CB	458	VAL

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Mol	Chain	Res	Type
1	CB	473	VAL
1	CB	480	VAL
1	CB	484	THR
1	CB	487	THR
1	CB	504	VAL
1	CB	533	MET
1	CB	613	LEU
1	CB	755	VAL
1	CB	762	VAL
1	CB	779	THR
1	CB	790	VAL
1	CB	791	ASN
1	CB	855	LEU
3	CD	225	LEU
3	CD	297	LYS
5	LA	15	VAL
5	LA	32	VAL
5	LA	77	ILE
5	LA	102	LEU
5	LA	116	LEU
5	LA	169	VAL
5	LA	192	LYS
5	LA	207	VAL
5	LA	228	ASP
6	LB	60	VAL
6	LB	67	VAL
6	LB	159	VAL
6	LB	162	VAL
6	LB	174	ARG
6	LB	258	HIS
6	LB	317	LEU
6	LB	337	VAL
6	LB	338	VAL
6	LB	350	SER
7	LC	1	MET
7	LC	45	ARG
7	LC	56	GLU
7	LC	154	VAL
7	LC	209	ILE
7	LC	334	THR
7	LC	353	LYS
8	LD	37	VAL

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Mol	Chain	Res	Type
8	LD	88	VAL
8	LD	115	MET
8	LD	118	ILE
8	LD	132	VAL
8	LD	150	LEU
8	LD	154	THR
8	LD	163	LEU
8	LD	167	VAL
8	LD	176	SER
8	LD	213	GLU
8	LD	272	SER
8	LD	291	GLN
9	LE	49	VAL
9	LE	51	VAL
9	LE	54	ILE
9	LE	71	ARG
9	LE	104	THR
9	LE	109	LEU
9	LE	120	ASP
9	LE	251	LYS
10	LF	55	LYS
10	LF	130	ILE
10	LF	223	LYS
10	LF	229	GLU
11	LG	140	VAL
11	LG	198	THR
11	LG	200	THR
11	LG	207	VAL
11	LG	247	VAL
12	LH	10	VAL
12	LH	72	THR
13	LI	33	ILE
13	LI	43	VAL
13	LI	56	GLU
13	LI	61	SER
13	LI	123	GLN
13	LI	125	THR
13	LI	133	GLN
13	LI	183	ASP
14	LJ	14	GLU
14	LJ	26	VAL
14	LJ	39	VAL

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Mol	Chain	Res	Type
14	LJ	40	LEU
14	LJ	49	VAL
14	LJ	57	VAL
14	LJ	96	LYS
14	LJ	133	VAL
14	LJ	148	THR
15	LL	59	VAL
15	LL	70	VAL
15	LL	138	ASP
16	LM	2	VAL
16	LM	25	VAL
16	LM	38	VAL
16	LM	70	GLN
16	LM	112	VAL
17	LN	18	VAL
17	LN	60	VAL
17	LN	80	THR
17	LN	101	VAL
17	LN	182	HIS
17	LN	184	ILE
18	LO	27	VAL
18	LO	64	THR
18	LO	108	ILE
18	LO	119	VAL
18	LO	141	LEU
18	LO	175	MET
18	LO	203	VAL
19	LP	6	LEU
19	LP	9	GLU
19	LP	53	LEU
19	LP	57	CYS
19	LP	80	GLN
19	LP	104	LEU
19	LP	141	SER
20	LQ	3	VAL
20	LQ	17	GLU
20	LQ	137	VAL
21	LR	6	LEU
21	LR	8	LYS
21	LR	29	THR
21	LR	63	CYS
21	LR	110	ARG

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Mol	Chain	Res	Type
21	LR	112	SER
21	LR	177	LEU
22	LS	19	THR
22	LS	42	SER
22	LS	48	VAL
22	LS	62	VAL
22	LS	82	LEU
22	LS	88	SER
22	LS	90	THR
22	LS	107	THR
22	LS	131	GLU
22	LS	135	SER
22	LS	138	ARG
22	LS	158	VAL
22	LS	169	THR
23	LT	4	THR
23	LT	27	LEU
23	LT	29	THR
23	LT	68	THR
23	LT	72	VAL
23	LT	79	GLN
23	LT	87	LYS
23	LT	93	ILE
23	LT	116	LYS
23	LT	147	GLU
24	LU	25	CYS
24	LU	60	VAL
24	LU	103	VAL
25	LV	22	VAL
25	LV	32	THR
25	LV	65	VAL
25	LV	91	LYS
25	LV	101	ASN
25	LV	138	SER
26	LW	119	LYS
27	LX	50	LYS
27	LX	97	VAL
27	LX	102	VAL
28	LY	9	SER
28	LY	28	LYS
28	LY	44	VAL
28	LY	46	SER

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Mol	Chain	Res	Type
28	LY	55	VAL
28	LY	112	ASP
29	LZ	11	VAL
29	LZ	35	ASP
29	LZ	100	VAL
30	La	15	VAL
30	La	56	VAL
30	La	103	VAL
30	La	120	GLN
30	La	130	SER
30	La	140	VAL
30	La	147	VAL
31	Lb	4	SER
31	Lb	9	THR
31	Lb	13	SER
31	Lb	65	MET
32	Lc	28	VAL
32	Lc	78	ASN
32	Lc	91	VAL
32	Lc	92	CYS
32	Lc	94	LEU
33	Ld	26	THR
33	Ld	46	LEU
33	Ld	62	VAL
33	Ld	118	GLN
33	Ld	122	VAL
34	Le	45	VAL
34	Le	87	VAL
34	Le	91	CYS
34	Le	94	SER
35	Lf	33	VAL
35	Lf	81	SER
36	Lg	48	VAL
36	Lg	104	VAL
37	Lh	88	THR
38	Li	12	ASN
38	Li	18	THR
38	Li	88	GLU
39	Lj	22	CYS
40	Lk	9	LYS
40	Lk	59	SER
40	Lk	68	GLU

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Mol	Chain	Res	Type
44	Lo	79	SER
45	Lp	77	VAL
45	Lp	83	ILE
45	Lp	89	LEU
46	Lr	63	VAL
46	Lr	101	LYS
48	SA	54	THR
48	SA	75	SER
48	SA	82	THR
49	SB	29	ASP
49	SB	50	THR
49	SB	77	ASP
49	SB	108	ASP
49	SB	154	SER
50	SC	73	MET
50	SC	76	LYS
50	SC	147	VAL
50	SC	149	THR
50	SC	173	LYS
50	SC	240	THR
50	SC	259	THR
50	SC	270	THR
50	SC	271	ASP
51	SD	35	SER
51	SD	41	VAL
51	SD	42	THR
51	SD	44	THR
51	SD	115	VAL
52	SE	67	GLN
52	SE	105	THR
52	SE	126	VAL
53	SF	82	ASN
53	SF	83	ASN
53	SF	119	SER
53	SF	140	ASP
53	SF	202	SER
54	SG	13	GLN
54	SG	16	ILE
54	SG	26	THR
54	SG	75	LEU
54	SG	102	VAL
54	SG	139	SER

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Mol	Chain	Res	Type
54	SG	146	ASN
54	SG	163	ASN
55	SH	11	PRO
55	SH	137	SER
55	SH	148	LEU
55	SH	164	ASN
55	SH	165	ASN
56	SI	22	HIS
56	SI	107	THR
56	SI	128	LYS
56	SI	151	GLU
56	SI	172	LEU
56	SI	199	LEU
57	SJ	3	VAL
57	SJ	47	LYS
57	SJ	63	LEU
57	SJ	163	SER
58	SK	3	MET
58	SK	40	VAL
59	SL	39	ASN
59	SL	87	VAL
60	SM	58	GLU
60	SM	77	ILE
60	SM	78	LYS
61	SN	49	GLN
61	SN	53	ILE
61	SN	63	VAL
61	SN	120	SER
62	SO	26	ASN
62	SO	62	VAL
62	SO	103	ASN
62	SO	116	LEU
63	SP	12	PHE
63	SP	112	ILE
63	SP	133	ILE
64	SQ	18	THR
64	SQ	118	THR
64	SQ	144	SER
65	SR	70	SER
65	SR	116	ASN
65	SR	124	VAL
66	SS	73	ASN

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Mol	Chain	Res	Type
66	SS	90	VAL
66	SS	145	THR
67	ST	6	VAL
67	ST	98	SER
67	ST	124	THR
68	SU	29	VAL
68	SU	39	LEU
68	SU	78	ASP
69	SV	82	ASN
70	SW	30	CYS
70	SW	80	ASP
70	SW	90	GLN
70	SW	107	SER
71	SX	72	VAL
72	SY	35	VAL
73	SZ	49	LEU
73	SZ	82	SER
73	SZ	113	THR
74	Sa	42	ARG
75	Sb	41	TYR
75	Sb	44	THR
76	Sc	28	THR
76	Sc	38	THR
76	Sc	46	VAL
76	Sc	57	THR
76	Sc	61	SER
77	Sd	30	LEU
78	Se	29	THR
79	Sf	87	THR
79	Sf	100	LEU
79	Sf	102	VAL
80	Sg	15	ASN
80	Sg	113	PHE
80	Sg	141	THR
80	Sg	178	ASN
80	Sg	181	ASN
80	Sg	229	THR
80	Sg	234	ASP
80	Sg	240	CYS
80	Sg	267	VAL
80	Sg	303	THR
83	Lq	23	ASP

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Mol	Chain	Res	Type
83	Lq	92	LYS
83	Lq	184	SER
83	Lq	192	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	CB	145	GLN
1	CB	168	GLN
1	CB	291	GLN
1	CB	357	HIS
1	CB	565	HIS
1	CB	705	HIS
3	CD	196	HIS
3	CD	292	ASN
5	LA	83	HIS
5	LA	95	GLN
5	LA	205	ASN
5	LA	216	HIS
6	LB	203	GLN
6	LB	289	GLN
6	LB	354	GLN
7	LC	310	HIS
7	LC	317	ASN
7	LC	329	ASN
8	LD	45	ASN
8	LD	111	ASN
8	LD	229	ASN
8	LD	282	GLN
9	LE	101	ASN
9	LE	182	ASN
9	LE	245	GLN
10	LF	24	ASN
11	LG	66	GLN
11	LG	141	ASN
12	LH	102	ASN
12	LH	138	GLN
12	LH	189	GLN
13	LI	92	HIS
13	LI	123	GLN
14	LJ	46	GLN
15	LL	67	HIS

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Mol	Chain	Res	Type
15	LL	111	GLN
15	LL	115	GLN
15	LL	149	GLN
16	LM	34	ASN
16	LM	69	HIS
17	LN	15	GLN
17	LN	29	GLN
18	LO	63	ASN
18	LO	180	GLN
19	LP	137	ASN
20	LQ	21	GLN
20	LQ	151	HIS
20	LQ	160	HIS
21	LR	40	GLN
21	LR	134	ASN
23	LT	66	ASN
23	LT	90	ASN
24	LU	105	ASN
25	LV	27	ASN
26	LW	17	HIS
26	LW	96	GLN
28	LY	72	GLN
30	La	19	HIS
30	La	60	HIS
30	La	67	GLN
33	Ld	116	ASN
33	Ld	121	ASN
34	Le	43	ASN
34	Le	52	GLN
37	Lh	98	HIS
38	Li	15	HIS
38	Li	36	HIS
41	Ll	33	ASN
45	Lp	33	GLN
46	Lr	4	HIS
46	Lr	30	ASN
46	Lr	41	ASN
48	SA	33	GLN
48	SA	111	GLN
48	SA	132	GLN
49	SB	95	ASN
49	SB	99	ASN

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Mol	Chain	Res	Type
51	SD	165	ASN
51	SD	179	GLN
51	SD	226	GLN
52	SE	36	HIS
52	SE	98	ASN
52	SE	188	ASN
53	SF	83	ASN
53	SF	118	ASN
53	SF	203	ASN
54	SG	81	HIS
55	SH	44	ASN
55	SH	68	GLN
55	SH	97	GLN
55	SH	114	GLN
56	SI	116	HIS
58	SK	7	ASN
59	SL	19	ASN
59	SL	94	HIS
60	SM	48	HIS
60	SM	55	ASN
61	SN	49	GLN
61	SN	58	HIS
63	SP	41	GLN
64	SQ	48	GLN
64	SQ	77	HIS
64	SQ	114	GLN
66	SS	10	GLN
67	ST	63	HIS
67	ST	85	ASN
67	ST	117	GLN
72	SY	63	HIS
75	Sb	49	HIS
75	Sb	65	GLN
77	Sd	5	GLN
78	Se	3	HIS
80	Sg	51	ASN
80	Sg	181	ASN
80	Sg	237	ASN
80	Sg	285	GLN
80	Sg	305	ASN
80	Sg	311	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	CC	21/85 (24%)	4 (19%)	0
4	L8	153/156 (98%)	52 (33%)	3 (1%)
47	S2	1579/1871 (84%)	403 (25%)	4 (0%)
81	L5	3447/5069 (68%)	752 (21%)	17 (0%)
82	L7	118/120 (98%)	14 (11%)	0
All	All	5318/7301 (72%)	1225 (23%)	24 (0%)

All (1225) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	CC	25	C
2	CC	26	G
2	CC	31	A
2	CC	41	C
4	L8	3	A
4	L8	17	A
4	L8	23	C
4	L8	24	G
4	L8	25	G
4	L8	34	U
4	L8	35	C
4	L8	38	U
4	L8	39	G
4	L8	43	A
4	L8	45	C
4	L8	48	A
4	L8	51	U
4	L8	52	A
4	L8	58	G
4	L8	59	A
4	L8	60	G
4	L8	61	A
4	L8	62	A
4	L8	63	U
4	L8	64	U
4	L8	67	U
4	L8	69	PSU
4	L8	70	G
4	L8	73	U
4	L8	75	OMG
4	L8	79	G

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Mol	Chain	Res	Type
4	L8	80	A
4	L8	81	C
4	L8	82	A
4	L8	83	C
4	L8	85	U
4	L8	86	U
4	L8	87	G
4	L8	91	A
4	L8	100	U
4	L8	101	C
4	L8	103	A
4	L8	105	C
4	L8	110	U
4	L8	112	G
4	L8	114	G
4	L8	115	G
4	L8	116	C
4	L8	117	C
4	L8	118	C
4	L8	125	C
4	L8	126	C
4	L8	127	U
4	L8	128	C
4	L8	137	A
4	L8	148	A
47	S2	2	A
47	S2	4	C
47	S2	17	C
47	S2	19	A
47	S2	23	G
47	S2	25	A
47	S2	27	A2M
47	S2	28	U
47	S2	33	G
47	S2	41	G
47	S2	45	A
47	S2	46	A
47	S2	54	A
47	S2	56	G
47	S2	57	U
47	S2	59	U
47	S2	64	A

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Mol	Chain	Res	Type
47	S2	65	C
47	S2	67	C
47	S2	68	A
47	S2	70	G
47	S2	72	C
47	S2	99	A2M
47	S2	103	A
47	S2	110	U
47	S2	113	G
47	S2	115	U
47	S2	116	OMU
47	S2	126	G
47	S2	128	U
47	S2	129	C
47	S2	130	G
47	S2	142	C
47	S2	143	U
47	S2	144	U
47	S2	149	A
47	S2	153	G
47	S2	160	U
47	S2	161	U
47	S2	162	C
47	S2	179	C
47	S2	184	G
47	S2	189	U
47	S2	190	G
47	S2	193	C
47	S2	204	G
47	S2	206	G
47	S2	207	G
47	S2	208	G
47	S2	211	G
47	S2	212	C
47	S2	213	G
47	S2	214	U
47	S2	289	G
47	S2	290	U
47	S2	291	G
47	S2	292	A
47	S2	293	C
47	S2	295	C

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Mol	Chain	Res	Type
47	S2	302	A
47	S2	306	C
47	S2	307	G
47	S2	308	G
47	S2	309	G
47	S2	311	C
47	S2	312	G
47	S2	314	U
47	S2	317	C
47	S2	319	C
47	S2	321	C
47	S2	323	C
47	S2	329	G
47	S2	332	G
47	S2	333	G
47	S2	339	A
47	S2	340	C
47	S2	351	G
47	S2	360	A
47	S2	361	U
47	S2	362	C
47	S2	363	A
47	S2	364	A
47	S2	367	U
47	S2	368	U
47	S2	370	G
47	S2	377	G
47	S2	381	C
47	S2	385	G
47	S2	386	C
47	S2	399	C
47	S2	407	G
47	S2	408	A
47	S2	409	C
47	S2	424	C
47	S2	428	OMU
47	S2	429	C
47	S2	438	G
47	S2	448	A
47	S2	449	A
47	S2	450	C
47	S2	452	G

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Mol	Chain	Res	Type
47	S2	464	A
47	S2	465	A
47	S2	471	G
47	S2	472	C
47	S2	473	A
47	S2	474	G
47	S2	475	C
47	S2	482	G
47	S2	487	U
47	S2	488	U
47	S2	492	C
47	S2	500	A
47	S2	501	C
47	S2	502	C
47	S2	503	C
47	S2	516	A
47	S2	517	OMC
47	S2	525	A
47	S2	533	A
47	S2	552	G
47	S2	554	A
47	S2	555	A
47	S2	558	G
47	S2	559	G
47	S2	560	A
47	S2	563	G
47	S2	564	A
47	S2	566	U
47	S2	570	C
47	S2	576	A2M
47	S2	583	A
47	S2	587	A
47	S2	589	G
47	S2	591	U
47	S2	592	C
47	S2	594	A
47	S2	596	U
47	S2	597	G
47	S2	606	G
47	S2	608	C
47	S2	617	G
47	S2	622	C

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Mol	Chain	Res	Type
47	S2	623	G
47	S2	627	U
47	S2	628	A
47	S2	629	A
47	S2	631	U
47	S2	632	C
47	S2	635	G
47	S2	638	C
47	S2	643	A
47	S2	644	OMG
47	S2	655	A
47	S2	656	G
47	S2	660	C
47	S2	663	C
47	S2	664	A
47	S2	668	A
47	S2	669	A
47	S2	671	A
47	S2	672	A
47	S2	683	OMG
47	S2	684	G
47	S2	687	C
47	S2	688	U
47	S2	689	U
47	S2	691	G
47	S2	808	A
47	S2	810	A
47	S2	811	A
47	S2	821	G
47	S2	822	U
47	S2	823	U
47	S2	824	C
47	S2	830	A
47	S2	833	C
47	S2	842	C
47	S2	844	U
47	S2	845	G
47	S2	847	A
47	S2	850	C
47	S2	853	C
47	S2	869	A
47	S2	870	A

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Mol	Chain	Res	Type
47	S2	871	U
47	S2	872	A
47	S2	873	G
47	S2	878	G
47	S2	879	C
47	S2	880	G
47	S2	881	G
47	S2	882	U
47	S2	884	C
47	S2	907	G
47	S2	909	G
47	S2	913	A
47	S2	918	U
47	S2	920	A
47	S2	930	C
47	S2	933	G
47	S2	934	G
47	S2	943	U
47	S2	947	G
47	S2	949	G
47	S2	955	A
47	S2	963	A
47	S2	967	C
47	S2	968	U
47	S2	970	G
47	S2	971	G
47	S2	972	A
47	S2	986	G
47	S2	990	A
47	S2	992	A
47	S2	999	G
47	S2	1001	A
47	S2	1008	A
47	S2	1017	U
47	S2	1023	A
47	S2	1039	C
47	S2	1044	G
47	S2	1045	U
47	S2	1047	C
47	S2	1060	A
47	S2	1061	U
47	S2	1062	A

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Mol	Chain	Res	Type
47	S2	1067	C
47	S2	1080	A
47	S2	1083	A
47	S2	1085	C
47	S2	1088	U
47	S2	1109	C
47	S2	1116	C
47	S2	1117	C
47	S2	1121	G
47	S2	1123	C
47	S2	1133	A
47	S2	1138	C
47	S2	1148	A
47	S2	1153	C
47	S2	1154	U
47	S2	1195	A
47	S2	1208	A
47	S2	1215	C
47	S2	1216	C
47	S2	1217	A
47	S2	1224	G
47	S2	1227	G
47	S2	1242	U
47	S2	1243	U
47	S2	1251	A
47	S2	1253	A
47	S2	1256	G
47	S2	1257	G
47	S2	1259	A
47	S2	1260	A
47	S2	1263	U
47	S2	1264	C
47	S2	1273	C
47	S2	1274	G
47	S2	1275	G
47	S2	1280	G
47	S2	1290	G
47	S2	1292	C
47	S2	1293	A
47	S2	1294	G
47	S2	1295	A
47	S2	1302	G

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Mol	Chain	Res	Type
47	S2	1303	C
47	S2	1304	U
47	S2	1305	C
47	S2	1308	U
47	S2	1312	G
47	S2	1314	U
47	S2	1320	G
47	S2	1322	G
47	S2	1326	U
47	S2	1327	G
47	S2	1330	G
47	S2	1341	C
47	S2	1342	U
47	S2	1348	G
47	S2	1363	C
47	S2	1364	U
47	S2	1371	U
47	S2	1372	U
47	S2	1373	C
47	S2	1376	A
47	S2	1378	A
47	S2	1396	A
47	S2	1397	U
47	S2	1401	A
47	S2	1402	A
47	S2	1404	U
47	S2	1407	U
47	S2	1408	U
47	S2	1413	G
47	S2	1415	C
47	S2	1426	U
47	S2	1431	G
47	S2	1433	C
47	S2	1442	OMU
47	S2	1446	A
47	S2	1447	OMG
47	S2	1450	G
47	S2	1454	A
47	S2	1455	A
47	S2	1462	U
47	S2	1463	U
47	S2	1478	U

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Mol	Chain	Res	Type
47	S2	1480	A
47	S2	1486	A
47	S2	1488	C
47	S2	1489	A
47	S2	1490	OMG
47	S2	1494	U
47	S2	1495	G
47	S2	1497	G
47	S2	1498	A
47	S2	1508	A
47	S2	1510	G
47	S2	1520	G
47	S2	1521	C
47	S2	1523	C
47	S2	1529	C
47	S2	1533	A
47	S2	1535	U
47	S2	1536	G
47	S2	1539	U
47	S2	1544	C
47	S2	1552	G
47	S2	1555	U
47	S2	1556	A
47	S2	1557	C
47	S2	1558	C
47	S2	1570	G
47	S2	1573	G
47	S2	1578	U
47	S2	1579	A
47	S2	1580	A
47	S2	1582	C
47	S2	1585	U
47	S2	1586	U
47	S2	1587	G
47	S2	1588	A
47	S2	1594	A
47	S2	1598	G
47	S2	1601	A
47	S2	1602	U
47	S2	1603	G
47	S2	1621	U
47	S2	1623	A

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Mol	Chain	Res	Type
47	S2	1631	U
47	S2	1633	A
47	S2	1639	G
47	S2	1640	A
47	S2	1641	A
47	S2	1648	G
47	S2	1654	G
47	S2	1663	A
47	S2	1665	G
47	S2	1671	G
47	S2	1680	G
47	S2	1693	G
47	S2	1694	U
47	S2	1695	A
47	S2	1696	C
47	S2	1698	C
47	S2	1700	C
47	S2	1715	A
47	S2	1721	U
47	S2	1722	G
47	S2	1726	G
47	S2	1732	G
47	S2	1742	C
47	S2	1743	G
47	S2	1744	G
47	S2	1745	A
47	S2	1748	G
47	S2	1785	C
47	S2	1787	G
47	S2	1797	U
47	S2	1798	C
47	S2	1805	G
47	S2	1809	A
47	S2	1810	U
47	S2	1822	A
47	S2	1823	A
47	S2	1824	A
47	S2	1826	G
47	S2	1829	G
47	S2	1835	A
47	S2	1838	U
47	S2	1849	G

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Mol	Chain	Res	Type
47	S2	1851	MA6
47	S2	1852	C
47	S2	1861	G
47	S2	1862	G
47	S2	1863	A
47	S2	1864	U
47	S2	1865	C
47	S2	1867	U
81	L5	4	G
81	L5	15	A
81	L5	25	A
81	L5	26	C
81	L5	27	C
81	L5	30	C
81	L5	39	A
81	L5	42	A
81	L5	48	G
81	L5	56	A
81	L5	58	G
81	L5	59	A
81	L5	64	A
81	L5	65	A
81	L5	66	A
81	L5	67	C
81	L5	69	A
81	L5	72	C
81	L5	73	A
81	L5	91	G
81	L5	98	A
81	L5	104	G
81	L5	108	A
81	L5	109	G
81	L5	110	C
81	L5	119	G
81	L5	120	A
81	L5	141	C
81	L5	145	G
81	L5	152	U
81	L5	159	C
81	L5	165	A
81	L5	166	C
81	L5	170	C

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Mol	Chain	Res	Type
81	L5	178	C
81	L5	179	G
81	L5	180	C
81	L5	181	C
81	L5	185	C
81	L5	186	G
81	L5	194	C
81	L5	200	U
81	L5	201	C
81	L5	209	U
81	L5	210	C
81	L5	218	A
81	L5	219	G
81	L5	220	C
81	L5	233	U
81	L5	246	G
81	L5	250	C
81	L5	253	G
81	L5	258	G
81	L5	265	C
81	L5	266	C
81	L5	267	G
81	L5	278	G
81	L5	280	G
81	L5	297	U
81	L5	306	A
81	L5	315	G
81	L5	316	U
81	L5	340	C
81	L5	350	C
81	L5	373	G
81	L5	381	U
81	L5	387	G
81	L5	388	A
81	L5	406	C
81	L5	407	A
81	L5	408	A
81	L5	410	A
81	L5	411	G
81	L5	412	G
81	L5	413	G
81	L5	417	G

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Mol	Chain	Res	Type
81	L5	418	A
81	L5	431	G
81	L5	432	U
81	L5	433	A
81	L5	449	C
81	L5	450	G
81	L5	452	A
81	L5	453	G
81	L5	454	U
81	L5	456	C
81	L5	457	G
81	L5	466	A
81	L5	467	U
81	L5	468	U
81	L5	472	C
81	L5	473	C
81	L5	479	G
81	L5	484	U
81	L5	485	C
81	L5	486	C
81	L5	489	C
81	L5	493	G
81	L5	494	U
81	L5	509	A
81	L5	510	U
81	L5	512	U
81	L5	654	C
81	L5	655	C
81	L5	657	C
81	L5	658	C
81	L5	659	G
81	L5	666	G
81	L5	667	A
81	L5	668	C
81	L5	669	C
81	L5	672	C
81	L5	673	C
81	L5	685	C
81	L5	686	A
81	L5	687	U
81	L5	696	C
81	L5	704	C

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Mol	Chain	Res	Type
81	L5	706	C
81	L5	708	G
81	L5	730	G
81	L5	731	G
81	L5	738	C
81	L5	739	G
81	L5	740	G
81	L5	742	G
81	L5	746	A
81	L5	747	A
81	L5	753	C
81	L5	754	U
81	L5	755	C
81	L5	758	G
81	L5	759	G
81	L5	907	C
81	L5	911	U
81	L5	913	U
81	L5	914	U
81	L5	915	A
81	L5	917	A
81	L5	918	G
81	L5	923	C
81	L5	924	C
81	L5	926	G
81	L5	932	A
81	L5	933	G
81	L5	935	A
81	L5	936	C
81	L5	937	U
81	L5	941	C
81	L5	943	A
81	L5	945	U
81	L5	956	A
81	L5	959	G
81	L5	960	A
81	L5	961	G
81	L5	962	C
81	L5	965	G
81	L5	966	A
81	L5	968	C
81	L5	969	C

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Mol	Chain	Res	Type
81	L5	970	G
81	L5	977	C
81	L5	982	U
81	L5	985	C
81	L5	986	C
81	L5	1070	G
81	L5	1072	C
81	L5	1075	G
81	L5	1076	C
81	L5	1082	C
81	L5	1083	U
81	L5	1084	C
81	L5	1095	A
81	L5	1171	G
81	L5	1172	C
81	L5	1174	G
81	L5	1179	U
81	L5	1180	C
81	L5	1187	G
81	L5	1193	C
81	L5	1202	C
81	L5	1203	G
81	L5	1204	C
81	L5	1210	C
81	L5	1211	G
81	L5	1214	C
81	L5	1215	C
81	L5	1216	C
81	L5	1218	G
81	L5	1219	G
81	L5	1235	G
81	L5	1241	C
81	L5	1243	C
81	L5	1246	G
81	L5	1247	U
81	L5	1253	G
81	L5	1258	G
81	L5	1260	G
81	L5	1262	G
81	L5	1266	G
81	L5	1267	C
81	L5	1272	C

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Mol	Chain	Res	Type
81	L5	1273	G
81	L5	1274	A
81	L5	1275	G
81	L5	1278	C
81	L5	1280	C
81	L5	1284	G
81	L5	1285	U
81	L5	1287	G
81	L5	1293	G
81	L5	1294	A
81	L5	1295	C
81	L5	1301	C
81	L5	1312	A
81	L5	1313	C
81	L5	1314	C
81	L5	1324	A
81	L5	1326	A2M
81	L5	1354	A
81	L5	1358	G
81	L5	1359	G
81	L5	1360	G
81	L5	1365	C
81	L5	1366	G
81	L5	1367	C
81	L5	1387	A
81	L5	1394	G
81	L5	1397	A
81	L5	1420	A
81	L5	1435	G
81	L5	1437	C
81	L5	1439	C
81	L5	1441	C
81	L5	1442	C
81	L5	1443	A
81	L5	1444	G
81	L5	1445	U
81	L5	1446	C
81	L5	1452	A
81	L5	1457	G
81	L5	1482	G
81	L5	1483	C
81	L5	1493	G

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Mol	Chain	Res	Type
81	L5	1497	A
81	L5	1498	G
81	L5	1502	G
81	L5	1514	U
81	L5	1515	A
81	L5	1517	G
81	L5	1518	A
81	L5	1534	A2M
81	L5	1535	C
81	L5	1547	A
81	L5	1562	G
81	L5	1566	C
81	L5	1574	G
81	L5	1578	U
81	L5	1582	U
81	L5	1586	G
81	L5	1591	U
81	L5	1596	U
81	L5	1624	G
81	L5	1625	OMG
81	L5	1631	A
81	L5	1632	A
81	L5	1633	G
81	L5	1634	A
81	L5	1638	A
81	L5	1640	C
81	L5	1642	A
81	L5	1643	A
81	L5	1654	G
81	L5	1661	C
81	L5	1663	C
81	L5	1670	G
81	L5	1676	C
81	L5	1677	U
81	L5	1678	C
81	L5	1680	G
81	L5	1681	G
81	L5	1685	G
81	L5	1694	C
81	L5	1701	A
81	L5	1704	C
81	L5	1705	G

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Mol	Chain	Res	Type
81	L5	1724	G
81	L5	1726	U
81	L5	1730	U
81	L5	1734	G
81	L5	1741	G
81	L5	1742	A
81	L5	1750	G
81	L5	1775	A
81	L5	1785	C
81	L5	1787	A
81	L5	1797	G
81	L5	1803	G
81	L5	1804	A
81	L5	1810	G
81	L5	1815	G
81	L5	1820	C
81	L5	1821	G
81	L5	1822	U
81	L5	1831	G
81	L5	1834	U
81	L5	1836	G
81	L5	1837	A
81	L5	1842	G
81	L5	1843	A
81	L5	1855	G
81	L5	1869	G
81	L5	1871	A2M
81	L5	1872	G
81	L5	1873	A
81	L5	1882	U
81	L5	1892	A
81	L5	1893	C
81	L5	1897	A
81	L5	1917	A
81	L5	1918	U
81	L5	1919	G
81	L5	1920	C
81	L5	1921	C
81	L5	1922	G
81	L5	1925	G
81	L5	1930	U
81	L5	1931	C

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Mol	Chain	Res	Type
81	L5	1932	A
81	L5	1936	C
81	L5	1940	G
81	L5	1948	G
81	L5	1949	U
81	L5	1951	G
81	L5	1959	U
81	L5	1960	A
81	L5	1961	G
81	L5	1962	A
81	L5	1964	A
81	L5	1965	G
81	L5	1975	G
81	L5	1978	C
81	L5	1984	A
81	L5	1985	G
81	L5	1991	A
81	L5	1997	U
81	L5	2002	A
81	L5	2004	U
81	L5	2005	G
81	L5	2011	C
81	L5	2014	C
81	L5	2017	A
81	L5	2026	A
81	L5	2033	A
81	L5	2034	G
81	L5	2044	U
81	L5	2046	G
81	L5	2048	U
81	L5	2055	G
81	L5	2056	G
81	L5	2069	A
81	L5	2070	U
81	L5	2084	C
81	L5	2085	G
81	L5	2090	U
81	L5	2091	C
81	L5	2092	G
81	L5	2093	A
81	L5	2096	G
81	L5	2098	G

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Mol	Chain	Res	Type
81	L5	2101	C
81	L5	2102	G
81	L5	2103	G
81	L5	2106	G
81	L5	2107	C
81	L5	2258	C
81	L5	2261	G
81	L5	2262	G
81	L5	2263	A
81	L5	2289	C
81	L5	2300	A
81	L5	2301	G
81	L5	2313	A
81	L5	2316	G
81	L5	2333	G
81	L5	2345	G
81	L5	2348	G
81	L5	2350	U
81	L5	2351	OMC
81	L5	2352	U
81	L5	2357	G
81	L5	2360	A
81	L5	2364	OMG
81	L5	2366	A
81	L5	2367	A
81	L5	2369	U
81	L5	2382	A
81	L5	2383	C
81	L5	2395	A
81	L5	2396	A
81	L5	2397	G
81	L5	2408	U
81	L5	2412	A
81	L5	2417	A
81	L5	2421	G
81	L5	2424	OMG
81	L5	2425	U
81	L5	2441	C
81	L5	2450	G
81	L5	2464	C
81	L5	2465	C
81	L5	2469	C

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Mol	Chain	Res	Type
81	L5	2471	G
81	L5	2474	G
81	L5	2475	G
81	L5	2478	C
81	L5	2479	G
81	L5	2503	G
81	L5	2504	C
81	L5	2505	C
81	L5	2506	G
81	L5	2507	A
81	L5	2513	A
81	L5	2514	G
81	L5	2519	U
81	L5	2529	A
81	L5	2537	A
81	L5	2554	U
81	L5	2556	G
81	L5	2573	A
81	L5	2583	C
81	L5	2586	G
81	L5	2587	A
81	L5	2589	C
81	L5	2601	A
81	L5	2611	A
81	L5	2618	G
81	L5	2627	C
81	L5	2638	G
81	L5	2652	G
81	L5	2653	C
81	L5	2659	A
81	L5	2662	G
81	L5	2669	C
81	L5	2676	A
81	L5	2686	G
81	L5	2687	U
81	L5	2694	G
81	L5	2695	A
81	L5	2696	A
81	L5	2708	U
81	L5	2710	C
81	L5	2711	G
81	L5	2721	G

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Mol	Chain	Res	Type
81	L5	2724	G
81	L5	2726	G
81	L5	2732	G
81	L5	2738	C
81	L5	2739	C
81	L5	2742	G
81	L5	2743	A
81	L5	2746	A
81	L5	2756	G
81	L5	2761	U
81	L5	2769	U
81	L5	2770	C
81	L5	2787	A2M
81	L5	2788	U
81	L5	2790	U
81	L5	2806	A
81	L5	2814	C
81	L5	2815	A2M
81	L5	2826	U
81	L5	2827	G
81	L5	2829	U
81	L5	2834	C
81	L5	2838	G
81	L5	2839	PSU
81	L5	2842	G
81	L5	2846	G
81	L5	2848	G
81	L5	2855	G
81	L5	2867	C
81	L5	2892	C
81	L5	2900	U
81	L5	3597	G
81	L5	3598	C
81	L5	3599	A
81	L5	3604	A
81	L5	3605	C
81	L5	3615	G
81	L5	3618	C
81	L5	3626	G
81	L5	3630	A
81	L5	3635	A
81	L5	3644	U

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Mol	Chain	Res	Type
81	L5	3646	A
81	L5	3648	A
81	L5	3662	A
81	L5	3664	G
81	L5	3670	C
81	L5	3672	G
81	L5	3673	C
81	L5	3674	G
81	L5	3685	C
81	L5	3696	C
81	L5	3701	OMC
81	L5	3702	A
81	L5	3709	U
81	L5	3710	G
81	L5	3711	A
81	L5	3714	G
81	L5	3717	A
81	L5	3719	A
81	L5	3726	A
81	L5	3727	A
81	L5	3753	G
81	L5	3756	A
81	L5	3759	A
81	L5	3760	A
81	L5	3773	U
81	L5	3774	A
81	L5	3777	G
81	L5	3784	A
81	L5	3785	A2M
81	L5	3786	U
81	L5	3788	C
81	L5	3802	U
81	L5	3810	C
81	L5	3811	G
81	L5	3812	C
81	L5	3814	U
81	L5	3817	A
81	L5	3818	UY1
81	L5	3819	G
81	L5	3823	G
81	L5	3838	U
81	L5	3839	G

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Mol	Chain	Res	Type
81	L5	3840	U
81	L5	3867	A2M
81	L5	3877	A
81	L5	3878	C
81	L5	3879	G
81	L5	3885	G
81	L5	3887	OMC
81	L5	3892	U
81	L5	3897	G
81	L5	3901	A
81	L5	3906	A
81	L5	3907	G
81	L5	3908	A
81	L5	3915	U
81	L5	3924	C
81	L5	3930	U
81	L5	3938	G
81	L5	3939	G
81	L5	3942	A
81	L5	3943	A
81	L5	3944	G
81	L5	4073	A
81	L5	4076	G
81	L5	4084	G
81	L5	4095	G
81	L5	4097	G
81	L5	4098	A
81	L5	4099	G
81	L5	4111	U
81	L5	4115	G
81	L5	4119	C
81	L5	4127	A
81	L5	4135	G
81	L5	4150	G
81	L5	4160	C
81	L5	4162	C
81	L5	4163	U
81	L5	4168	G
81	L5	4170	A
81	L5	4177	C
81	L5	4183	G
81	L5	4184	G

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Mol	Chain	Res	Type
81	L5	4191	G
81	L5	4196	G
81	L5	4197	G
81	L5	4202	U
81	L5	4219	A
81	L5	4221	C
81	L5	4222	G
81	L5	4225	G
81	L5	4227	OMU
81	L5	4228	OMG
81	L5	4229	U
81	L5	4233	A
81	L5	4237	C
81	L5	4251	A
81	L5	4254	G
81	L5	4257	A
81	L5	4265	U
81	L5	4268	A
81	L5	4273	A
81	L5	4281	A
81	L5	4304	A
81	L5	4305	G
81	L5	4306	OMU
81	L5	4314	C
81	L5	4329	G
81	L5	4330	G
81	L5	4332	C
81	L5	4338	G
81	L5	4339	A
81	L5	4349	C
81	L5	4350	C
81	L5	4364	G
81	L5	4371	G
81	L5	4372	U
81	L5	4373	G
81	L5	4376	A
81	L5	4377	G
81	L5	4378	A
81	L5	4379	A
81	L5	4387	C
81	L5	4391	G
81	L5	4394	A

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Mol	Chain	Res	Type
81	L5	4405	G
81	L5	4421	C
81	L5	4422	A
81	L5	4426	C
81	L5	4448	G
81	L5	4449	A
81	L5	4464	A
81	L5	4466	C
81	L5	4471	PSU
81	L5	4475	G
81	L5	4488	A
81	L5	4500	U
81	L5	4512	U
81	L5	4513	A
81	L5	4515	G
81	L5	4518	A
81	L5	4519	C
81	L5	4524	G
81	L5	4531	U
81	L5	4532	PSU
81	L5	4545	G
81	L5	4548	A
81	L5	4549	G
81	L5	4557	U
81	L5	4560	C
81	L5	4567	G
81	L5	4569	PSU
81	L5	4570	G
81	L5	4575	G
81	L5	4589	A
81	L5	4590	A2M
81	L5	4617	G
81	L5	4618	OMG
81	L5	4627	U
81	L5	4632	U
81	L5	4636	U
81	L5	4637	OMG
81	L5	4638	U
81	L5	4639	G
81	L5	4647	G
81	L5	4649	G
81	L5	4656	A

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Mol	Chain	Res	Type
81	L5	4657	U
81	L5	4670	C
81	L5	4672	A
81	L5	4687	A
81	L5	4700	A
81	L5	4707	A
81	L5	4708	A
81	L5	4709	U
81	L5	4719	G
81	L5	4733	C
81	L5	4734	A
81	L5	4740	G
81	L5	4741	C
81	L5	4742	G
81	L5	4745	G
81	L5	4747	C
81	L5	4751	G
81	L5	4754	G
81	L5	4757	C
81	L5	4759	C
81	L5	4761	G
81	L5	4765	G
81	L5	4771	C
81	L5	4772	C
81	L5	4773	C
81	L5	4775	C
81	L5	4860	G
81	L5	4867	G
81	L5	4870	G
81	L5	4871	C
81	L5	4875	G
81	L5	4882	U
81	L5	4883	C
81	L5	4889	G
81	L5	4894	A
81	L5	4895	C
81	L5	4896	G
81	L5	4900	C
81	L5	4901	G
81	L5	4910	G
81	L5	4912	G
81	L5	4914	C

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Mol	Chain	Res	Type
81	L5	4922	C
81	L5	4925	U
81	L5	4926	C
81	L5	4927	G
81	L5	4934	A
81	L5	4937	C
81	L5	4940	C
81	L5	4941	G
81	L5	4943	A
81	L5	4944	C
81	L5	4951	G
81	L5	4960	G
81	L5	4963	G
81	L5	4966	A
81	L5	4967	A
81	L5	4973	U
81	L5	4975	G
81	L5	4976	U
81	L5	4982	A
81	L5	4985	U
81	L5	4988	U
81	L5	4995	U
81	L5	5008	C
81	L5	5009	G
81	L5	5013	C
81	L5	5014	A
81	L5	5017	G
81	L5	5022	U
81	L5	5023	C
81	L5	5024	C
81	L5	5025	C
81	L5	5026	U
81	L5	5027	C
81	L5	5028	G
81	L5	5029	C
81	L5	5030	U
81	L5	5032	C
81	L5	5034	A
81	L5	5041	G
81	L5	5047	C
81	L5	5050	C
81	L5	5054	C

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Mol	Chain	Res	Type
81	L5	5055	G
81	L5	5058	A
81	L5	5061	A
81	L5	5069	U
82	L7	7	G
82	L7	25	G
82	L7	33	U
82	L7	38	U
82	L7	49	A
82	L7	53	U
82	L7	54	A
82	L7	64	G
82	L7	66	G
82	L7	76	U
82	L7	97	G
82	L7	100	A
82	L7	110	G
82	L7	111	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L8	69	PSU
4	L8	86	U
4	L8	125	C
47	S2	291	G
47	S2	563	G
47	S2	688	U
47	S2	970	G
81	L5	406	C
81	L5	914	U
81	L5	1633	G
81	L5	1977	C
81	L5	2033	A
81	L5	2084	C
81	L5	2416	G
81	L5	2675	G
81	L5	2760	G
81	L5	3597	G
81	L5	3614	G
81	L5	3673	C
81	L5	3701	OMC

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Mol	Chain	Res	Type
81	L5	3713	U
81	L5	3923	A
81	L5	4699	U
81	L5	4913	G

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

154 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$
81	OMG	L5	4370	81	23,26,27	2.34	9 (39%)	32,38,41	2.35	11 (34%)
47	PSU	S2	406	47	18,21,22	4.53	7 (38%)	21,30,33	2.00	5 (23%)
81	PSU	L5	4628	81	18,21,22	4.45	7 (38%)	21,30,33	1.95	6 (28%)
47	OMU	S2	172	47	19,22,23	3.06	8 (42%)	25,31,34	1.83	4 (16%)
47	6MZ	S2	1871	86	26,26,26	2.30	4 (15%)	36,39,39	2.01	11 (30%)
47	A2M	S2	590	47	22,25,26	3.49	9 (40%)	30,36,39	2.56	12 (40%)
81	PSU	L5	1781	81	18,21,22	4.60	7 (38%)	21,30,33	1.89	4 (19%)
81	UR3	L5	4530	81	19,22,23	2.81	6 (31%)	26,32,35	1.86	5 (19%)
81	UY1	L5	3818	86	19,22,23	4.02	7 (36%)	21,31,34	1.89	6 (28%)
81	PSU	L5	4552	81	18,21,22	4.53	7 (38%)	21,30,33	1.96	5 (23%)
47	B8N	S2	1870	-	25,29,30	3.33	9 (36%)	28,42,45	2.10	7 (25%)
81	PSU	L5	3639	81	18,21,22	4.51	7 (38%)	21,30,33	2.03	5 (23%)
47	A2M	S2	576	47	22,25,26	3.54	9 (40%)	30,36,39	2.30	11 (36%)
47	PSU	S2	1177	47	18,21,22	4.46	7 (38%)	21,30,33	2.07	5 (23%)
81	PSU	L5	1862	81	18,21,22	4.55	7 (38%)	21,30,33	2.05	5 (23%)
4	OMG	L8	75	4	23,26,27	2.35	8 (34%)	32,38,41	2.41	10 (31%)
81	OMG	L5	3792	81	23,26,27	2.34	8 (34%)	32,38,41	2.41	8 (25%)
4	PSU	L8	69	4	18,21,22	4.59	8 (44%)	21,30,33	2.17	5 (23%)
81	OMG	L5	1316	81	23,26,27	2.31	8 (34%)	32,38,41	2.36	12 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	OMU	L5	4498	81	19,22,23	2.98	8 (42%)	25,31,34	1.80	4 (16%)
47	A2M	S2	99	47,86	22,25,26	3.58	9 (40%)	30,36,39	2.30	11 (36%)
47	A2M	S2	27	47,86	22,25,26	3.40	9 (40%)	30,36,39	2.80	14 (46%)
81	A2M	L5	400	81	22,25,26	3.57	9 (40%)	30,36,39	2.31	10 (33%)
47	PSU	S2	1238	47	18,21,22	4.59	7 (38%)	21,30,33	2.05	5 (23%)
81	A2M	L5	3718	81	22,25,26	3.53	9 (40%)	30,36,39	2.29	12 (40%)
4	OMU	L8	14	81,4	19,22,23	2.98	8 (42%)	25,31,34	1.83	4 (16%)
47	4AC	S2	1842	47	21,24,25	3.10	10 (47%)	28,34,37	1.72	5 (17%)
81	A2M	L5	2787	81	22,25,26	3.52	9 (40%)	30,36,39	2.28	10 (33%)
47	OMG	S2	436	47	23,26,27	2.33	9 (39%)	32,38,41	2.31	11 (34%)
81	PSU	L5	4312	81	18,21,22	4.54	7 (38%)	21,30,33	1.99	5 (23%)
81	PSU	L5	4576	81	18,21,22	4.57	7 (38%)	21,30,33	1.96	5 (23%)
81	PSU	L5	5001	81	18,21,22	4.54	7 (38%)	21,30,33	1.96	5 (23%)
81	PSU	L5	4403	81	18,21,22	4.45	7 (38%)	21,30,33	2.10	6 (28%)
81	PSU	L5	4579	81	18,21,22	4.52	7 (38%)	21,30,33	1.95	5 (23%)
47	PSU	S2	1232	47	18,21,22	4.58	7 (38%)	21,30,33	1.94	5 (23%)
81	OMG	L5	4623	81	23,26,27	2.30	8 (34%)	32,38,41	2.32	10 (31%)
81	OMG	L5	4499	81	23,26,27	2.37	8 (34%)	32,38,41	2.46	9 (28%)
81	OMC	L5	1340	81	19,22,23	2.91	8 (42%)	25,31,34	0.83	0
47	PSU	S2	109	47	18,21,22	4.55	7 (38%)	21,30,33	2.04	6 (28%)
47	OMC	S2	517	47	19,22,23	2.98	8 (42%)	25,31,34	0.76	1 (4%)
47	MA6	S2	1851	47	23,26,27	1.45	4 (17%)	33,38,41	2.99	12 (36%)
81	A2M	L5	1871	81	22,25,26	3.61	9 (40%)	30,36,39	2.46	12 (40%)
47	A2M	S2	468	47	22,25,26	3.57	9 (40%)	30,36,39	2.36	11 (36%)
81	OMG	L5	1625	81	23,26,27	2.35	8 (34%)	32,38,41	2.51	9 (28%)
47	OMC	S2	1391	47	19,22,23	2.93	8 (42%)	25,31,34	0.80	1 (4%)
47	PSU	S2	93	47	18,21,22	4.59	7 (38%)	21,30,33	1.89	4 (19%)
47	A2M	S2	166	47	22,25,26	3.54	9 (40%)	30,36,39	2.33	10 (33%)
81	A2M	L5	2401	81	22,25,26	3.54	9 (40%)	30,36,39	2.36	11 (36%)
81	OMG	L5	4637	81	23,26,27	2.34	8 (34%)	32,38,41	2.49	10 (31%)
47	OMU	S2	354	47	19,22,23	3.01	8 (42%)	25,31,34	1.78	4 (16%)
47	A2M	S2	1678	47	22,25,26	3.62	9 (40%)	30,36,39	2.36	11 (36%)
81	OMG	L5	2876	81	23,26,27	2.30	8 (34%)	32,38,41	2.53	10 (31%)
81	5MC	L5	3782	81,86	19,22,23	3.68	8 (42%)	26,32,35	1.24	3 (11%)
81	A2M	L5	1534	81,86	22,25,26	3.49	9 (40%)	30,36,39	2.38	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PSU	S2	1643	47,86	18,21,22	4.55	7 (38%)	21,30,33	1.94	5 (23%)
81	OMG	L5	2424	81	23,26,27	2.39	8 (34%)	32,38,41	2.59	9 (28%)
47	4AC	S2	1337	47	21,24,25	2.92	9 (42%)	28,34,37	1.62	6 (21%)
81	PSU	L5	4471	81	18,21,22	4.56	7 (38%)	21,30,33	2.02	5 (23%)
47	OMU	S2	121	47	19,22,23	3.01	8 (42%)	25,31,34	1.76	4 (16%)
81	OMC	L5	2351	81	19,22,23	2.88	8 (42%)	25,31,34	0.82	1 (4%)
81	OMU	L5	4620	81	19,22,23	2.99	8 (42%)	25,31,34	1.75	4 (16%)
81	A2M	L5	3724	81	22,25,26	3.54	9 (40%)	30,36,39	2.30	12 (40%)
81	A2M	L5	3825	81	22,25,26	3.56	9 (40%)	30,36,39	2.35	10 (33%)
81	OMC	L5	2804	81	19,22,23	2.89	8 (42%)	25,31,34	0.85	1 (4%)
47	OMG	S2	644	47	23,26,27	2.35	8 (34%)	32,38,41	2.45	10 (31%)
81	PSU	L5	5010	81	18,21,22	4.60	7 (38%)	21,30,33	1.94	5 (23%)
81	OMC	L5	3887	81	19,22,23	2.96	8 (42%)	25,31,34	0.88	0
47	OMC	S2	174	47	19,22,23	3.01	8 (42%)	25,31,34	0.83	0
81	OMU	L5	2415	81	19,22,23	3.05	8 (42%)	25,31,34	1.82	5 (20%)
81	OMG	L5	2364	81	23,26,27	2.31	9 (39%)	32,38,41	2.31	11 (34%)
81	A2M	L5	4590	81	22,25,26	3.56	9 (40%)	30,36,39	2.32	10 (33%)
81	PSU	L5	2839	81	18,21,22	4.47	7 (38%)	21,30,33	1.86	5 (23%)
81	PSU	L5	3884	81	18,21,22	4.49	7 (38%)	21,30,33	1.87	4 (19%)
47	OMG	S2	1328	87,47	23,26,27	2.30	8 (34%)	32,38,41	2.34	9 (28%)
47	PSU	S2	681	47	18,21,22	4.56	7 (38%)	21,30,33	1.93	5 (23%)
47	PSU	S2	34	47	18,21,22	4.59	7 (38%)	21,30,33	2.00	5 (23%)
81	PSU	L5	4569	81	18,21,22	4.51	7 (38%)	21,30,33	1.95	5 (23%)
81	A2M	L5	4523	81,86	22,25,26	3.53	9 (40%)	30,36,39	2.35	11 (36%)
47	OMG	S2	1490	47,86	23,26,27	2.33	8 (34%)	32,38,41	2.13	7 (21%)
47	A2M	S2	512	47	22,25,26	3.55	9 (40%)	30,36,39	2.31	10 (33%)
47	PSU	S2	1056	47	18,21,22	4.63	7 (38%)	21,30,33	1.97	5 (23%)
81	OMC	L5	2365	81,86	19,22,23	2.92	8 (42%)	25,31,34	0.83	0
81	PSU	L5	4457	81	18,21,22	4.48	7 (38%)	21,30,33	1.98	6 (28%)
81	PSU	L5	4972	81	18,21,22	4.56	7 (38%)	21,30,33	1.98	5 (23%)
47	MA6	S2	1850	47	23,26,27	1.48	5 (21%)	33,38,41	2.87	12 (36%)
47	PSU	S2	651	47	18,21,22	4.57	7 (38%)	21,30,33	2.00	5 (23%)
81	PSU	L5	4532	81	18,21,22	4.51	7 (38%)	21,30,33	1.87	4 (19%)
47	OMU	S2	116	47	19,22,23	3.06	8 (42%)	25,31,34	1.77	4 (16%)
81	PSU	L5	3770	81	18,21,22	4.50	7 (38%)	21,30,33	2.06	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	OMC	S2	1703	47	19,22,23	3.03	8 (42%)	25,31,34	1.25	2 (8%)
81	PSU	L5	3637	81	18,21,22	4.47	7 (38%)	21,30,33	1.82	4 (19%)
81	PSU	L5	4353	81	18,21,22	4.53	7 (38%)	21,30,33	2.00	5 (23%)
47	PSU	S2	649	47	18,21,22	4.56	7 (38%)	21,30,33	1.98	5 (23%)
81	OMG	L5	4618	81	23,26,27	2.32	9 (39%)	32,38,41	2.31	11 (34%)
81	OMC	L5	1881	81,87	19,22,23	2.91	8 (42%)	25,31,34	0.82	0
47	OMG	S2	601	47	23,26,27	2.34	9 (39%)	32,38,41	2.44	10 (31%)
81	OMU	L5	2837	81	19,22,23	3.02	8 (42%)	25,31,34	1.81	4 (16%)
81	A2M	L5	3785	81	22,25,26	3.44	9 (40%)	30,36,39	2.48	13 (43%)
47	A2M	S2	1031	47	22,25,26	3.56	9 (40%)	30,36,39	2.33	10 (33%)
47	PSU	S2	1692	47	18,21,22	4.53	7 (38%)	21,30,33	2.03	5 (23%)
81	PSU	L5	4442	81	18,21,22	4.49	8 (44%)	21,30,33	2.13	6 (28%)
81	OMG	L5	4228	81	23,26,27	2.32	9 (39%)	32,38,41	2.25	8 (25%)
47	A2M	S2	1383	47	22,25,26	3.53	9 (40%)	30,36,39	2.35	12 (40%)
81	PSU	L5	3695	81	18,21,22	4.44	7 (38%)	21,30,33	2.10	5 (23%)
47	OMG	S2	683	47	23,26,27	2.35	9 (39%)	32,38,41	2.36	11 (34%)
81	OMG	L5	1522	81	23,26,27	2.32	8 (34%)	32,38,41	2.36	11 (34%)
81	A2M	L5	1524	81	22,25,26	3.52	9 (40%)	30,36,39	2.47	13 (43%)
81	A2M	L5	3830	81	22,25,26	3.50	9 (40%)	30,36,39	2.34	10 (33%)
81	OMU	L5	4306	81	19,22,23	3.01	8 (42%)	25,31,34	1.76	4 (16%)
47	A2M	S2	484	47	22,25,26	3.51	9 (40%)	30,36,39	2.31	10 (33%)
47	PSU	S2	686	47	18,21,22	4.53	7 (38%)	21,30,33	1.96	5 (23%)
81	PSU	L5	4361	81	18,21,22	4.53	7 (38%)	21,30,33	1.97	5 (23%)
47	OMG	S2	1447	47	23,26,27	2.36	9 (39%)	32,38,41	2.42	9 (28%)
81	PSU	L5	2632	81	18,21,22	4.57	7 (38%)	21,30,33	1.93	5 (23%)
81	OMC	L5	3808	81	19,22,23	2.90	8 (42%)	25,31,34	0.78	1 (4%)
81	A2M	L5	2363	81,86	22,25,26	3.58	9 (40%)	30,36,39	2.33	10 (33%)
81	OMG	L5	3744	81	23,26,27	0.31	0	32,38,41	0.43	0
47	OMU	S2	1442	47,86	19,22,23	3.09	8 (42%)	25,31,34	1.93	7 (28%)
81	OMC	L5	3869	81	19,22,23	2.95	8 (42%)	25,31,34	0.80	0
81	OMU	L5	3925	81	19,22,23	3.01	8 (42%)	25,31,34	1.83	4 (16%)
81	OMC	L5	2824	81	19,22,23	2.94	8 (42%)	25,31,34	0.84	1 (4%)
81	PSU	L5	4431	81	18,21,22	4.55	7 (38%)	21,30,33	1.95	4 (19%)
81	A2M	L5	4571	81	22,25,26	3.62	9 (40%)	30,36,39	2.30	11 (36%)
81	PSU	L5	3851	81	18,21,22	4.50	7 (38%)	21,30,33	2.01	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PSU	S2	1244	47	18,21,22	4.53	7 (38%)	21,30,33	1.98	5 (23%)
47	OMU	S2	1288	47	19,22,23	3.05	8 (42%)	25,31,34	1.73	4 (16%)
47	PSU	S2	1445	47	18,21,22	4.58	7 (38%)	21,30,33	1.97	4 (19%)
81	6MZ	L5	4220	-	26,26,26	2.26	5 (19%)	36,39,39	2.04	11 (30%)
81	OMU	L5	4227	81	19,22,23	3.03	8 (42%)	25,31,34	1.76	4 (16%)
81	A2M	L5	3867	81	22,25,26	3.55	9 (40%)	30,36,39	2.33	11 (36%)
81	OMC	L5	2861	81	19,22,23	2.97	8 (42%)	25,31,34	0.78	1 (4%)
81	PSU	L5	1683	81	18,21,22	4.53	7 (38%)	21,30,33	1.92	5 (23%)
81	OMC	L5	4456	81	19,22,23	2.92	8 (42%)	25,31,34	0.84	1 (4%)
81	PSU	L5	4689	81	18,21,22	4.54	7 (38%)	21,30,33	1.97	5 (23%)
81	OMC	L5	3701	81,87,86	19,22,23	0.38	0	25,31,34	0.60	0
81	OMG	L5	4494	81	23,26,27	2.33	9 (39%)	32,38,41	2.36	9 (28%)
81	OMG	L5	4392	81	23,26,27	2.31	8 (34%)	32,38,41	2.33	9 (28%)
81	PSU	L5	3758	81	18,21,22	4.48	7 (38%)	21,30,33	2.01	5 (23%)
81	A2M	L5	398	81	22,25,26	3.55	9 (40%)	30,36,39	2.32	10 (33%)
47	A2M	S2	159	47	22,25,26	3.53	9 (40%)	30,36,39	2.36	12 (40%)
47	PSU	S2	36	47	18,21,22	4.56	7 (38%)	21,30,33	1.99	5 (23%)
81	OMC	L5	2422	81,86	19,22,23	2.91	8 (42%)	25,31,34	0.84	1 (4%)
81	PSU	L5	1782	81	18,21,22	4.54	7 (38%)	21,30,33	1.96	5 (23%)
81	PSU	L5	3920	81,86	18,21,22	4.47	7 (38%)	21,30,33	1.96	5 (23%)
81	PSU	L5	4423	81	18,21,22	4.59	7 (38%)	21,30,33	2.01	5 (23%)
81	A2M	L5	2815	81	22,25,26	3.52	9 (40%)	30,36,39	2.34	11 (36%)
81	PSU	L5	1779	81	18,21,22	4.55	7 (38%)	21,30,33	1.94	5 (23%)
81	A2M	L5	1326	81	22,25,26	3.54	9 (40%)	30,36,39	2.33	9 (30%)
81	PSU	L5	4299	81	18,21,22	4.54	7 (38%)	21,30,33	1.99	5 (23%)
81	OMC	L5	4536	81	19,22,23	2.91	8 (42%)	25,31,34	0.82	1 (4%)
81	OMC	L5	3841	81	19,22,23	2.95	8 (42%)	25,31,34	1.43	3 (12%)
47	OMU	S2	428	47	19,22,23	3.03	8 (42%)	25,31,34	1.81	4 (16%)
47	OMG	S2	509	47	23,26,27	2.32	8 (34%)	32,38,41	2.39	9 (28%)
81	OMG	L5	3627	81	23,26,27	2.27	8 (34%)	32,38,41	2.26	10 (31%)

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
81	OMG	L5	4370	81	-	0/9/27/28	0/3/3/3
47	PSU	S2	406	47	-	0/7/25/26	0/2/2/2
81	PSU	L5	4628	81	-	0/7/25/26	0/2/2/2
47	OMU	S2	172	47	-	0/9/27/28	0/2/2/2
47	6MZ	S2	1871	86	-	2/12/28/28	0/3/3/3
47	A2M	S2	590	47	-	1/9/27/28	0/3/3/3
81	PSU	L5	1781	81	-	1/7/25/26	0/2/2/2
81	UR3	L5	4530	81	-	2/7/25/26	0/2/2/2
81	UY1	L5	3818	86	-	5/9/27/28	0/2/2/2
81	PSU	L5	4552	81	-	0/7/25/26	0/2/2/2
47	B8N	S2	1870	-	-	8/16/34/35	0/2/2/2
81	PSU	L5	3639	81	-	0/7/25/26	0/2/2/2
47	A2M	S2	576	47	-	3/9/27/28	0/3/3/3
47	PSU	S2	1177	47	-	0/7/25/26	0/2/2/2
81	PSU	L5	1862	81	-	0/7/25/26	0/2/2/2
4	OMG	L8	75	4	-	2/9/27/28	0/3/3/3
81	OMG	L5	3792	81	-	0/9/27/28	0/3/3/3
4	PSU	L8	69	4	-	2/7/25/26	0/2/2/2
81	OMG	L5	1316	81	-	0/9/27/28	0/3/3/3
81	OMU	L5	4498	81	-	0/9/27/28	0/2/2/2
47	A2M	S2	99	47,86	-	2/9/27/28	0/3/3/3
47	A2M	S2	27	47,86	-	3/9/27/28	0/3/3/3
81	A2M	L5	400	81	-	0/9/27/28	0/3/3/3
47	PSU	S2	1238	47	-	0/7/25/26	0/2/2/2
81	A2M	L5	3718	81	-	0/9/27/28	0/3/3/3
4	OMU	L8	14	81,4	-	1/9/27/28	0/2/2/2
47	4AC	S2	1842	47	-	2/11/29/30	0/2/2/2
81	A2M	L5	2787	81	-	5/9/27/28	0/3/3/3
47	OMG	S2	436	47	-	0/9/27/28	0/3/3/3
81	PSU	L5	4312	81	-	0/7/25/26	0/2/2/2
81	PSU	L5	4576	81	-	0/7/25/26	0/2/2/2
81	PSU	L5	5001	81	-	0/7/25/26	0/2/2/2
81	PSU	L5	4403	81	-	0/7/25/26	0/2/2/2
81	PSU	L5	4579	81	-	0/7/25/26	0/2/2/2
47	PSU	S2	1232	47	-	0/7/25/26	0/2/2/2
81	OMG	L5	4623	81	-	0/9/27/28	0/3/3/3
81	OMG	L5	4499	81	-	0/9/27/28	0/3/3/3
81	OMC	L5	1340	81	-	0/9/27/28	0/2/2/2
47	PSU	S2	109	47	-	0/7/25/26	0/2/2/2
47	OMC	S2	517	47	-	0/9/27/28	0/2/2/2
47	MA6	S2	1851	47	-	1/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	A2M	L5	1871	81	-	2/9/27/28	0/3/3/3
47	A2M	S2	468	47	-	0/9/27/28	0/3/3/3
81	OMG	L5	1625	81	-	0/9/27/28	0/3/3/3
47	OMC	S2	1391	47	-	0/9/27/28	0/2/2/2
47	PSU	S2	93	47	-	0/7/25/26	0/2/2/2
47	A2M	S2	166	47	-	0/9/27/28	0/3/3/3
81	A2M	L5	2401	81	-	0/9/27/28	0/3/3/3
81	OMG	L5	4637	81	-	1/9/27/28	0/3/3/3
47	OMU	S2	354	47	-	0/9/27/28	0/2/2/2
47	A2M	S2	1678	47	-	1/9/27/28	0/3/3/3
81	OMG	L5	2876	81	-	2/9/27/28	0/3/3/3
81	5MC	L5	3782	81,86	-	1/7/25/26	0/2/2/2
81	A2M	L5	1534	81,86	-	2/9/27/28	0/3/3/3
47	PSU	S2	1643	47,86	-	0/7/25/26	0/2/2/2
81	OMG	L5	2424	81	-	2/9/27/28	0/3/3/3
47	4AC	S2	1337	47	-	2/11/29/30	0/2/2/2
81	PSU	L5	4471	81	-	2/7/25/26	0/2/2/2
47	OMU	S2	121	47	-	1/9/27/28	0/2/2/2
81	OMC	L5	2351	81	-	4/9/27/28	0/2/2/2
81	OMU	L5	4620	81	-	0/9/27/28	0/2/2/2
81	A2M	L5	3724	81	-	0/9/27/28	0/3/3/3
81	A2M	L5	3825	81	-	0/9/27/28	0/3/3/3
81	OMC	L5	2804	81	-	0/9/27/28	0/2/2/2
47	OMG	S2	644	47	-	3/9/27/28	0/3/3/3
81	PSU	L5	5010	81	-	0/7/25/26	0/2/2/2
81	OMC	L5	3887	81	-	2/9/27/28	0/2/2/2
47	OMC	S2	174	47	-	0/9/27/28	0/2/2/2
81	OMU	L5	2415	81	-	1/9/27/28	0/2/2/2
81	OMG	L5	2364	81	-	2/9/27/28	0/3/3/3
81	A2M	L5	4590	81	-	1/9/27/28	0/3/3/3
81	PSU	L5	2839	81	-	4/7/25/26	0/2/2/2
81	PSU	L5	3884	81	-	0/7/25/26	0/2/2/2
47	OMG	S2	1328	87,47	-	0/9/27/28	0/3/3/3
47	PSU	S2	681	47	-	0/7/25/26	0/2/2/2
47	PSU	S2	34	47	-	0/7/25/26	0/2/2/2
81	PSU	L5	4569	81	-	2/7/25/26	0/2/2/2
81	A2M	L5	4523	81,86	-	1/9/27/28	0/3/3/3
47	OMG	S2	1490	47,86	-	1/9/27/28	0/3/3/3
47	A2M	S2	512	47	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PSU	S2	1056	47	-	0/7/25/26	0/2/2/2
81	OMC	L5	2365	81,86	-	0/9/27/28	0/2/2/2
81	PSU	L5	4457	81	-	0/7/25/26	0/2/2/2
81	PSU	L5	4972	81	-	0/7/25/26	0/2/2/2
47	MA6	S2	1850	47	-	0/11/29/30	0/3/3/3
47	PSU	S2	651	47	-	0/7/25/26	0/2/2/2
81	PSU	L5	4532	81	-	2/7/25/26	0/2/2/2
47	OMU	S2	116	47	-	3/9/27/28	0/2/2/2
81	PSU	L5	3770	81	-	0/7/25/26	0/2/2/2
47	OMC	S2	1703	47	-	4/9/27/28	0/2/2/2
81	PSU	L5	3637	81	-	3/7/25/26	0/2/2/2
81	PSU	L5	4353	81	-	0/7/25/26	0/2/2/2
47	PSU	S2	649	47	-	0/7/25/26	0/2/2/2
81	OMG	L5	4618	81	-	2/9/27/28	0/3/3/3
81	OMC	L5	1881	81,87	-	0/9/27/28	0/2/2/2
47	OMG	S2	601	47	-	0/9/27/28	0/3/3/3
81	OMU	L5	2837	81	-	0/9/27/28	0/2/2/2
81	A2M	L5	3785	81	-	3/9/27/28	0/3/3/3
47	A2M	S2	1031	47	-	0/9/27/28	0/3/3/3
47	PSU	S2	1692	47	-	0/7/25/26	0/2/2/2
81	PSU	L5	4442	81	-	0/7/25/26	0/2/2/2
81	OMG	L5	4228	81	-	2/9/27/28	0/3/3/3
47	A2M	S2	1383	47	-	0/9/27/28	0/3/3/3
81	PSU	L5	3695	81	-	0/7/25/26	0/2/2/2
47	OMG	S2	683	47	-	2/9/27/28	0/3/3/3
81	OMG	L5	1522	81	-	0/9/27/28	0/3/3/3
81	A2M	L5	1524	81	-	0/9/27/28	0/3/3/3
81	A2M	L5	3830	81	-	0/9/27/28	0/3/3/3
81	OMU	L5	4306	81	-	2/9/27/28	0/2/2/2
47	A2M	S2	484	47	-	0/9/27/28	0/3/3/3
47	PSU	S2	686	47	-	0/7/25/26	0/2/2/2
81	PSU	L5	4361	81	-	0/7/25/26	0/2/2/2
47	OMG	S2	1447	47	-	3/9/27/28	0/3/3/3
81	PSU	L5	2632	81	-	0/7/25/26	0/2/2/2
81	OMC	L5	3808	81	-	0/9/27/28	0/2/2/2
81	A2M	L5	2363	81,86	-	0/9/27/28	0/3/3/3
81	OMG	L5	3744	81	-	0/9/27/28	0/3/3/3
47	OMU	S2	1442	47,86	-	4/9/27/28	0/2/2/2
81	OMC	L5	3869	81	-	0/9/27/28	0/2/2/2
81	OMU	L5	3925	81	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	OMC	L5	2824	81	-	0/9/27/28	0/2/2/2
81	PSU	L5	4431	81	-	0/7/25/26	0/2/2/2
81	A2M	L5	4571	81	-	0/9/27/28	0/3/3/3
81	PSU	L5	3851	81	-	2/7/25/26	0/2/2/2
47	PSU	S2	1244	47	-	0/7/25/26	0/2/2/2
47	OMU	S2	1288	47	-	0/9/27/28	0/2/2/2
47	PSU	S2	1445	47	-	1/7/25/26	0/2/2/2
81	6MZ	L5	4220	-	-	5/12/28/28	0/3/3/3
81	OMU	L5	4227	81	-	2/9/27/28	0/2/2/2
81	A2M	L5	3867	81	-	3/9/27/28	0/3/3/3
81	OMC	L5	2861	81	-	0/9/27/28	0/2/2/2
81	PSU	L5	1683	81	-	0/7/25/26	0/2/2/2
81	OMC	L5	4456	81	-	0/9/27/28	0/2/2/2
81	PSU	L5	4689	81	-	0/7/25/26	0/2/2/2
81	OMC	L5	3701	81,87,86	-	5/9/27/28	0/2/2/2
81	OMG	L5	4494	81	-	0/9/27/28	0/3/3/3
81	OMG	L5	4392	81	-	0/9/27/28	0/3/3/3
81	PSU	L5	3758	81	-	0/7/25/26	0/2/2/2
81	A2M	L5	398	81	-	1/9/27/28	0/3/3/3
47	A2M	S2	159	47	-	2/9/27/28	0/3/3/3
47	PSU	S2	36	47	-	0/7/25/26	0/2/2/2
81	OMC	L5	2422	81,86	-	2/9/27/28	0/2/2/2
81	PSU	L5	1782	81	-	0/7/25/26	0/2/2/2
81	PSU	L5	3920	81,86	-	0/7/25/26	0/2/2/2
81	PSU	L5	4423	81	-	0/7/25/26	0/2/2/2
81	A2M	L5	2815	81	-	2/9/27/28	0/3/3/3
81	PSU	L5	1779	81	-	0/7/25/26	0/2/2/2
81	A2M	L5	1326	81	-	3/9/27/28	0/3/3/3
81	PSU	L5	4299	81	-	0/7/25/26	0/2/2/2
81	OMC	L5	4536	81	-	0/9/27/28	0/2/2/2
81	OMC	L5	3841	81	-	2/9/27/28	0/2/2/2
47	OMU	S2	428	47	-	6/9/27/28	0/2/2/2
47	OMG	S2	509	47	-	0/9/27/28	0/3/3/3
81	OMG	L5	3627	81	-	1/9/27/28	0/3/3/3

All (1192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	1781	PSU	C6-C5	12.27	1.48	1.35
81	L5	5010	PSU	C6-C5	12.23	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	93	PSU	C6-C5	12.18	1.48	1.35
47	S2	1445	PSU	C6-C5	12.13	1.48	1.35
81	L5	4552	PSU	C6-C5	12.12	1.48	1.35
81	L5	4312	PSU	C6-C5	12.10	1.48	1.35
47	S2	651	PSU	C6-C5	12.08	1.48	1.35
81	L5	4471	PSU	C6-C5	12.07	1.48	1.35
47	S2	34	PSU	C6-C5	12.07	1.48	1.35
47	S2	1056	PSU	C6-C5	12.06	1.48	1.35
81	L5	4423	PSU	C6-C5	12.06	1.48	1.35
47	S2	649	PSU	C6-C5	12.06	1.48	1.35
81	L5	4576	PSU	C6-C5	12.04	1.48	1.35
47	S2	1232	PSU	C6-C5	12.04	1.48	1.35
47	S2	681	PSU	C6-C5	12.02	1.48	1.35
4	L8	69	PSU	C6-C5	12.02	1.48	1.35
81	L5	2632	PSU	C6-C5	12.02	1.48	1.35
81	L5	4361	PSU	C6-C5	11.99	1.48	1.35
81	L5	1683	PSU	C6-C5	11.99	1.48	1.35
47	S2	36	PSU	C6-C5	11.99	1.48	1.35
81	L5	4299	PSU	C6-C5	11.98	1.48	1.35
47	S2	1238	PSU	C6-C5	11.97	1.48	1.35
81	L5	1779	PSU	C6-C5	11.96	1.48	1.35
81	L5	4353	PSU	C6-C5	11.95	1.48	1.35
47	S2	1692	PSU	C6-C5	11.94	1.48	1.35
47	S2	406	PSU	C6-C5	11.94	1.48	1.35
81	L5	4431	PSU	C6-C5	11.94	1.48	1.35
81	L5	3884	PSU	C6-C5	11.93	1.48	1.35
81	L5	4689	PSU	C6-C5	11.92	1.48	1.35
81	L5	5001	PSU	C6-C5	11.92	1.48	1.35
81	L5	4972	PSU	C6-C5	11.91	1.48	1.35
81	L5	4532	PSU	C6-C5	11.91	1.48	1.35
81	L5	4579	PSU	C6-C5	11.91	1.48	1.35
47	S2	109	PSU	C6-C5	11.90	1.48	1.35
47	S2	1244	PSU	C6-C5	11.89	1.48	1.35
81	L5	1862	PSU	C6-C5	11.89	1.48	1.35
47	S2	1643	PSU	C6-C5	11.89	1.48	1.35
81	L5	1782	PSU	C6-C5	11.89	1.48	1.35
81	L5	3851	PSU	C6-C5	11.88	1.48	1.35
47	S2	686	PSU	C6-C5	11.88	1.48	1.35
81	L5	4569	PSU	C6-C5	11.86	1.48	1.35
81	L5	3770	PSU	C6-C5	11.81	1.48	1.35
81	L5	3639	PSU	C6-C5	11.79	1.48	1.35
81	L5	2839	PSU	C6-C5	11.79	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	4457	PSU	C6-C5	11.77	1.48	1.35
81	L5	3637	PSU	C6-C5	11.74	1.48	1.35
81	L5	3920	PSU	C6-C5	11.74	1.48	1.35
81	L5	4442	PSU	C6-C5	11.65	1.48	1.35
81	L5	4628	PSU	C6-C5	11.64	1.48	1.35
47	S2	1177	PSU	C6-C5	11.63	1.48	1.35
81	L5	3758	PSU	C6-C5	11.63	1.48	1.35
81	L5	3695	PSU	C6-C5	11.61	1.48	1.35
81	L5	4403	PSU	C6-C5	11.59	1.48	1.35
81	L5	3818	UY1	C6-C5	10.76	1.47	1.35
47	S2	1871	6MZ	C6-N6	10.17	1.45	1.34
47	S2	1056	PSU	C2-N1	10.04	1.49	1.36
47	S2	1238	PSU	C2-N1	9.92	1.49	1.36
81	L5	4423	PSU	C2-N1	9.91	1.49	1.36
4	L8	69	PSU	C2-N1	9.89	1.49	1.36
81	L5	4972	PSU	C2-N1	9.89	1.49	1.36
47	S2	1232	PSU	C2-N1	9.88	1.49	1.36
47	S2	1445	PSU	C2-N1	9.84	1.49	1.36
47	S2	34	PSU	C2-N1	9.84	1.49	1.36
81	L5	1782	PSU	C2-N1	9.82	1.49	1.36
81	L5	2839	PSU	C2-N1	9.82	1.49	1.36
81	L5	5010	PSU	C2-N1	9.82	1.49	1.36
47	S2	649	PSU	C2-N1	9.80	1.49	1.36
81	L5	4471	PSU	C2-N1	9.80	1.49	1.36
81	L5	3758	PSU	C2-N1	9.80	1.49	1.36
81	L5	4431	PSU	C2-N1	9.80	1.49	1.36
81	L5	1862	PSU	C2-N1	9.79	1.49	1.36
81	L5	1781	PSU	C2-N1	9.79	1.49	1.36
81	L5	2632	PSU	C2-N1	9.79	1.49	1.36
81	L5	5001	PSU	C2-N1	9.79	1.49	1.36
81	L5	4220	6MZ	C6-N6	9.78	1.45	1.34
47	S2	1643	PSU	C2-N1	9.78	1.49	1.36
81	L5	1779	PSU	C2-N1	9.78	1.49	1.36
47	S2	36	PSU	C2-N1	9.77	1.49	1.36
81	L5	4569	PSU	C2-N1	9.77	1.49	1.36
47	S2	651	PSU	C2-N1	9.76	1.49	1.36
47	S2	109	PSU	C2-N1	9.76	1.49	1.36
47	S2	681	PSU	C2-N1	9.76	1.49	1.36
81	L5	4576	PSU	C2-N1	9.75	1.49	1.36
47	S2	686	PSU	C2-N1	9.74	1.49	1.36
47	S2	1244	PSU	C2-N1	9.73	1.49	1.36
81	L5	4457	PSU	C2-N1	9.72	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	4689	PSU	C2-N1	9.71	1.49	1.36
47	S2	93	PSU	C2-N1	9.70	1.49	1.36
81	L5	1683	PSU	C2-N1	9.70	1.49	1.36
47	S2	406	PSU	C2-N1	9.69	1.49	1.36
81	L5	4299	PSU	C2-N1	9.69	1.49	1.36
81	L5	4361	PSU	C2-N1	9.69	1.49	1.36
81	L5	4353	PSU	C2-N1	9.68	1.49	1.36
81	L5	4579	PSU	C2-N1	9.67	1.49	1.36
81	L5	4442	PSU	C2-N1	9.67	1.49	1.36
81	L5	3639	PSU	C2-N1	9.66	1.49	1.36
81	L5	3637	PSU	C2-N1	9.65	1.49	1.36
81	L5	3770	PSU	C2-N1	9.65	1.49	1.36
47	S2	1692	PSU	C2-N1	9.64	1.49	1.36
81	L5	4312	PSU	C2-N1	9.63	1.49	1.36
47	S2	1177	PSU	C2-N1	9.61	1.49	1.36
81	L5	4403	PSU	C2-N1	9.60	1.49	1.36
81	L5	3920	PSU	C2-N1	9.59	1.49	1.36
81	L5	4532	PSU	C2-N1	9.59	1.49	1.36
81	L5	3695	PSU	C2-N1	9.56	1.49	1.36
81	L5	3851	PSU	C2-N1	9.56	1.49	1.36
81	L5	4552	PSU	C2-N1	9.56	1.49	1.36
81	L5	4571	A2M	C2'-C1'	-9.52	1.29	1.53
81	L5	4628	PSU	C2-N1	9.50	1.49	1.36
47	S2	1678	A2M	C2'-C1'	-9.49	1.29	1.53
81	L5	3884	PSU	C2-N1	9.43	1.49	1.36
81	L5	2363	A2M	C2'-C1'	-9.42	1.29	1.53
81	L5	1326	A2M	C2'-C1'	-9.39	1.30	1.53
47	S2	468	A2M	C2'-C1'	-9.34	1.30	1.53
47	S2	99	A2M	C2'-C1'	-9.30	1.30	1.53
47	S2	512	A2M	C2'-C1'	-9.29	1.30	1.53
81	L5	3818	UY1	C2-N1	9.28	1.48	1.36
81	L5	4590	A2M	C2'-C1'	-9.27	1.30	1.53
47	S2	1031	A2M	C2'-C1'	-9.27	1.30	1.53
81	L5	1871	A2M	C2'-C1'	-9.26	1.30	1.53
81	L5	3825	A2M	C2'-C1'	-9.25	1.30	1.53
81	L5	3867	A2M	C2'-C1'	-9.23	1.30	1.53
81	L5	2401	A2M	C2'-C1'	-9.20	1.30	1.53
81	L5	3724	A2M	C2'-C1'	-9.20	1.30	1.53
47	S2	166	A2M	C2'-C1'	-9.19	1.30	1.53
81	L5	398	A2M	C2'-C1'	-9.19	1.30	1.53
81	L5	400	A2M	C2'-C1'	-9.18	1.30	1.53
47	S2	576	A2M	C2'-C1'	-9.18	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	159	A2M	C2'-C1'	-9.11	1.30	1.53
81	L5	3830	A2M	C2'-C1'	-9.10	1.30	1.53
47	S2	1383	A2M	C2'-C1'	-9.09	1.30	1.53
81	L5	4523	A2M	C2'-C1'	-9.09	1.30	1.53
81	L5	398	A2M	O4'-C1'	9.09	1.63	1.42
81	L5	2787	A2M	C2'-C1'	-9.06	1.30	1.53
47	S2	484	A2M	C2'-C1'	-9.05	1.30	1.53
81	L5	2815	A2M	C2'-C1'	-9.03	1.30	1.53
81	L5	3785	A2M	C2'-C1'	-9.01	1.30	1.53
81	L5	3718	A2M	C2'-C1'	-9.00	1.30	1.53
81	L5	1524	A2M	C2'-C1'	-8.98	1.31	1.53
81	L5	3724	A2M	O4'-C1'	8.96	1.62	1.42
81	L5	1871	A2M	O4'-C1'	8.95	1.62	1.42
47	S2	590	A2M	O4'-C1'	8.95	1.62	1.42
81	L5	3718	A2M	O4'-C1'	8.95	1.62	1.42
47	S2	1678	A2M	O4'-C1'	8.94	1.62	1.42
47	S2	99	A2M	O4'-C1'	8.93	1.62	1.42
81	L5	1534	A2M	O4'-C1'	8.93	1.62	1.42
47	S2	166	A2M	O4'-C1'	8.92	1.62	1.42
81	L5	1534	A2M	C2'-C1'	-8.91	1.31	1.53
81	L5	4590	A2M	O4'-C1'	8.91	1.62	1.42
81	L5	2401	A2M	O4'-C1'	8.88	1.62	1.42
81	L5	400	A2M	O4'-C1'	8.87	1.62	1.42
47	S2	590	A2M	C2'-C1'	-8.86	1.31	1.53
47	S2	27	A2M	C2'-C1'	-8.86	1.31	1.53
81	L5	2815	A2M	O4'-C1'	8.85	1.62	1.42
47	S2	1383	A2M	O4'-C1'	8.85	1.62	1.42
47	S2	512	A2M	O4'-C1'	8.84	1.62	1.42
81	L5	4523	A2M	O4'-C1'	8.84	1.62	1.42
81	L5	4571	A2M	O4'-C1'	8.83	1.62	1.42
81	L5	3825	A2M	O4'-C1'	8.82	1.62	1.42
47	S2	468	A2M	O4'-C1'	8.79	1.62	1.42
81	L5	2787	A2M	O4'-C1'	8.78	1.62	1.42
81	L5	3782	5MC	C6-C5	8.78	1.48	1.34
81	L5	3830	A2M	O4'-C1'	8.78	1.62	1.42
47	S2	484	A2M	O4'-C1'	8.77	1.62	1.42
81	L5	2363	A2M	O4'-C1'	8.76	1.62	1.42
47	S2	159	A2M	O4'-C1'	8.74	1.62	1.42
47	S2	576	A2M	O4'-C1'	8.72	1.62	1.42
47	S2	1031	A2M	O4'-C1'	8.72	1.62	1.42
47	S2	27	A2M	O4'-C1'	8.69	1.62	1.42
81	L5	1524	A2M	O4'-C1'	8.67	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	1326	A2M	O4'-C1'	8.66	1.62	1.42
81	L5	3867	A2M	O4'-C1'	8.63	1.61	1.42
47	S2	1870	B8N	C6-N1	8.31	1.56	1.36
81	L5	3785	A2M	O4'-C1'	8.29	1.61	1.42
47	S2	1056	PSU	C2-N3	7.75	1.50	1.37
47	S2	651	PSU	C2-N3	7.72	1.50	1.37
47	S2	34	PSU	C2-N3	7.69	1.50	1.37
47	S2	1445	PSU	C2-N3	7.69	1.50	1.37
4	L8	69	PSU	C2-N3	7.68	1.50	1.37
81	L5	2632	PSU	C2-N3	7.67	1.50	1.37
47	S2	109	PSU	C2-N3	7.67	1.50	1.37
47	S2	1442	OMU	C2-N1	7.67	1.50	1.38
47	S2	1692	PSU	C2-N3	7.66	1.50	1.37
81	L5	4423	PSU	C2-N3	7.65	1.50	1.37
81	L5	5010	PSU	C2-N3	7.65	1.50	1.37
47	S2	1643	PSU	C2-N3	7.64	1.50	1.37
47	S2	93	PSU	C2-N3	7.64	1.50	1.37
81	L5	1779	PSU	C2-N3	7.64	1.50	1.37
47	S2	1232	PSU	C2-N3	7.64	1.50	1.37
81	L5	4576	PSU	C2-N3	7.64	1.50	1.37
47	S2	1870	B8N	C4-N3	-7.62	1.26	1.40
47	S2	406	PSU	C2-N3	7.62	1.50	1.37
47	S2	36	PSU	C2-N3	7.62	1.50	1.37
47	S2	686	PSU	C2-N3	7.61	1.50	1.37
81	L5	4689	PSU	C2-N3	7.61	1.50	1.37
81	L5	3639	PSU	C2-N3	7.60	1.50	1.37
47	S2	649	PSU	C2-N3	7.59	1.50	1.37
81	L5	3770	PSU	C2-N3	7.58	1.50	1.37
47	S2	1238	PSU	C2-N3	7.58	1.50	1.37
47	S2	1244	PSU	C2-N3	7.57	1.49	1.37
47	S2	681	PSU	C2-N3	7.57	1.49	1.37
81	L5	4431	PSU	C2-N3	7.56	1.49	1.37
81	L5	4972	PSU	C2-N3	7.56	1.49	1.37
81	L5	5001	PSU	C2-N3	7.56	1.49	1.37
81	L5	4353	PSU	C2-N3	7.56	1.49	1.37
81	L5	4299	PSU	C2-N3	7.56	1.49	1.37
81	L5	3884	PSU	C2-N3	7.56	1.49	1.37
81	L5	1683	PSU	C2-N3	7.54	1.49	1.37
81	L5	4579	PSU	C2-N3	7.54	1.49	1.37
81	L5	1862	PSU	C2-N3	7.54	1.49	1.37
81	L5	4530	UR3	C2-N1	7.54	1.48	1.38
81	L5	1782	PSU	C2-N3	7.53	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	1781	PSU	C2-N3	7.53	1.49	1.37
81	L5	4442	PSU	C2-N3	7.53	1.49	1.37
81	L5	4312	PSU	C2-N3	7.53	1.49	1.37
81	L5	4628	PSU	C2-N3	7.52	1.49	1.37
81	L5	4471	PSU	C2-N3	7.51	1.49	1.37
81	L5	4552	PSU	C2-N3	7.51	1.49	1.37
81	L5	4532	PSU	C2-N3	7.49	1.49	1.37
81	L5	3851	PSU	C2-N3	7.48	1.49	1.37
81	L5	4403	PSU	C2-N3	7.47	1.49	1.37
81	L5	3637	PSU	C2-N3	7.45	1.49	1.37
81	L5	3920	PSU	C2-N3	7.44	1.49	1.37
81	L5	4457	PSU	C2-N3	7.44	1.49	1.37
81	L5	4569	PSU	C2-N3	7.43	1.49	1.37
81	L5	3758	PSU	C2-N3	7.42	1.49	1.37
47	S2	1177	PSU	C2-N3	7.40	1.49	1.37
81	L5	4361	PSU	C2-N3	7.39	1.49	1.37
81	L5	3695	PSU	C2-N3	7.35	1.49	1.37
81	L5	3818	UY1	C2-N3	7.34	1.49	1.37
47	S2	172	OMU	C2-N1	7.27	1.49	1.38
47	S2	428	OMU	C2-N1	7.22	1.49	1.38
47	S2	116	OMU	C2-N1	7.19	1.49	1.38
81	L5	2839	PSU	C2-N3	7.19	1.49	1.37
81	L5	2415	OMU	C2-N1	7.18	1.49	1.38
47	S2	1870	B8N	C4-C5	7.16	1.63	1.47
81	L5	4227	OMU	C2-N1	7.13	1.49	1.38
47	S2	1288	OMU	C2-N1	7.11	1.49	1.38
81	L5	3925	OMU	C2-N1	7.10	1.49	1.38
81	L5	4620	OMU	C2-N1	7.08	1.49	1.38
47	S2	354	OMU	C2-N1	7.04	1.49	1.38
81	L5	2837	OMU	C2-N1	6.99	1.49	1.38
47	S2	121	OMU	C2-N1	6.97	1.49	1.38
81	L5	4306	OMU	C2-N1	6.95	1.49	1.38
81	L5	4498	OMU	C2-N1	6.94	1.49	1.38
47	S2	172	OMU	C2-N3	6.93	1.50	1.38
4	L8	14	OMU	C2-N1	6.92	1.49	1.38
47	S2	1288	OMU	C2-N3	6.85	1.49	1.38
47	S2	428	OMU	C2-N3	6.82	1.49	1.38
47	S2	116	OMU	C2-N3	6.76	1.49	1.38
81	L5	1524	A2M	O4'-C4'	-6.75	1.30	1.45
81	L5	2837	OMU	C2-N3	6.74	1.49	1.38
81	L5	2415	OMU	C2-N3	6.71	1.49	1.38
81	L5	4571	A2M	O4'-C4'	-6.71	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	4306	OMU	C2-N3	6.71	1.49	1.38
81	L5	4227	OMU	C2-N3	6.68	1.49	1.38
47	S2	1442	OMU	C2-N3	6.67	1.49	1.38
81	L5	1871	A2M	O4'-C4'	-6.66	1.30	1.45
81	L5	400	A2M	O4'-C4'	-6.64	1.30	1.45
47	S2	1337	4AC	C2-N3	6.64	1.49	1.36
47	S2	1678	A2M	O4'-C4'	-6.61	1.30	1.45
81	L5	2363	A2M	O4'-C4'	-6.61	1.30	1.45
81	L5	4620	OMU	C2-N3	6.61	1.49	1.38
47	S2	354	OMU	C2-N3	6.60	1.49	1.38
81	L5	3925	OMU	C2-N3	6.58	1.49	1.38
47	S2	1031	A2M	O4'-C4'	-6.58	1.30	1.45
81	L5	3867	A2M	O4'-C4'	-6.58	1.30	1.45
47	S2	121	OMU	C2-N3	6.56	1.49	1.38
47	S2	159	A2M	O4'-C4'	-6.53	1.30	1.45
47	S2	576	A2M	O4'-C4'	-6.50	1.30	1.45
81	L5	4498	OMU	C2-N3	6.50	1.49	1.38
81	L5	2815	A2M	O4'-C4'	-6.49	1.30	1.45
4	L8	14	OMU	C2-N3	6.49	1.49	1.38
81	L5	4590	A2M	O4'-C4'	-6.48	1.30	1.45
81	L5	4523	A2M	O4'-C4'	-6.47	1.30	1.45
81	L5	1326	A2M	O4'-C4'	-6.47	1.30	1.45
47	S2	468	A2M	O4'-C4'	-6.47	1.30	1.45
47	S2	590	A2M	O4'-C4'	-6.46	1.30	1.45
81	L5	2424	OMG	C4-N3	6.44	1.49	1.34
47	S2	484	A2M	O4'-C4'	-6.42	1.30	1.45
81	L5	3825	A2M	O4'-C4'	-6.41	1.30	1.45
81	L5	2787	A2M	O4'-C4'	-6.41	1.30	1.45
47	S2	1703	OMC	C2-N3	6.38	1.49	1.36
47	S2	174	OMC	C2-N3	6.37	1.49	1.36
81	L5	4499	OMG	C4-N3	6.36	1.48	1.34
4	L8	75	OMG	C4-N3	6.35	1.48	1.34
81	L5	4637	OMG	C4-N3	6.35	1.48	1.34
47	S2	166	A2M	O4'-C4'	-6.34	1.30	1.45
47	S2	99	A2M	O4'-C4'	-6.34	1.30	1.45
81	L5	3785	A2M	O4'-C4'	-6.33	1.30	1.45
47	S2	512	A2M	O4'-C4'	-6.33	1.30	1.45
47	S2	1383	A2M	O4'-C4'	-6.33	1.30	1.45
81	L5	3792	OMG	C4-N3	6.32	1.48	1.34
47	S2	644	OMG	C4-N3	6.32	1.48	1.34
81	L5	1625	OMG	C4-N3	6.32	1.48	1.34
47	S2	1842	4AC	C6-C5	6.30	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	3718	A2M	O4'-C4'	-6.30	1.31	1.45
81	L5	3782	5MC	C4-N3	6.29	1.44	1.34
81	L5	398	A2M	O4'-C4'	-6.28	1.31	1.45
81	L5	3724	A2M	O4'-C4'	-6.28	1.31	1.45
81	L5	1534	A2M	O4'-C4'	-6.26	1.31	1.45
81	L5	2401	A2M	O4'-C4'	-6.26	1.31	1.45
81	L5	1881	OMC	C2-N3	6.25	1.48	1.36
81	L5	3782	5MC	C5-C4	6.25	1.48	1.44
81	L5	4494	OMG	C4-N3	6.24	1.48	1.34
47	S2	601	OMG	C4-N3	6.23	1.48	1.34
47	S2	1447	OMG	C4-N3	6.23	1.48	1.34
47	S2	509	OMG	C4-N3	6.22	1.48	1.34
47	S2	517	OMC	C2-N3	6.22	1.48	1.36
81	L5	2861	OMC	C2-N3	6.22	1.48	1.36
81	L5	3887	OMC	C2-N3	6.21	1.48	1.36
81	L5	2824	OMC	C2-N3	6.20	1.48	1.36
81	L5	3869	OMC	C2-N3	6.20	1.48	1.36
81	L5	2876	OMG	C4-N3	6.20	1.48	1.34
81	L5	3830	A2M	O4'-C4'	-6.20	1.31	1.45
81	L5	1340	OMC	C2-N3	6.18	1.48	1.36
81	L5	1522	OMG	C4-N3	6.17	1.48	1.34
81	L5	4456	OMC	C2-N3	6.16	1.48	1.36
81	L5	4370	OMG	C4-N3	6.15	1.48	1.34
81	L5	2365	OMC	C2-N3	6.15	1.48	1.36
81	L5	2804	OMC	C2-N3	6.14	1.48	1.36
81	L5	2364	OMG	C4-N3	6.14	1.48	1.34
81	L5	4530	UR3	C6-C5	6.13	1.49	1.35
47	S2	1391	OMC	C2-N3	6.12	1.48	1.36
81	L5	3782	5MC	C2-N3	6.12	1.48	1.36
47	S2	683	OMG	C4-N3	6.12	1.48	1.34
81	L5	1316	OMG	C4-N3	6.11	1.48	1.34
81	L5	4618	OMG	C4-N3	6.10	1.48	1.34
47	S2	1490	OMG	C4-N3	6.10	1.48	1.34
81	L5	3841	OMC	C2-N3	6.09	1.48	1.36
81	L5	4623	OMG	C4-N3	6.09	1.48	1.34
81	L5	4392	OMG	C4-N3	6.07	1.48	1.34
47	S2	436	OMG	C4-N3	6.06	1.48	1.34
81	L5	2422	OMC	C2-N3	6.04	1.48	1.36
47	S2	1337	4AC	C4-N3	6.04	1.43	1.32
81	L5	4536	OMC	C2-N3	6.03	1.48	1.36
47	S2	174	OMC	C6-C5	6.03	1.49	1.35
81	L5	2351	OMC	C2-N3	6.02	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	1328	OMG	C4-N3	6.02	1.48	1.34
47	S2	1842	4AC	C2-N3	5.99	1.48	1.36
47	S2	1337	4AC	C6-C5	5.99	1.49	1.35
81	L5	3808	OMC	C2-N3	5.98	1.48	1.36
81	L5	4228	OMG	C4-N3	5.97	1.47	1.34
47	S2	517	OMC	C6-C5	5.96	1.48	1.35
47	S2	1391	OMC	C6-C5	5.95	1.48	1.35
81	L5	3887	OMC	C6-C5	5.94	1.48	1.35
81	L5	4536	OMC	C6-C5	5.91	1.48	1.35
81	L5	2861	OMC	C6-C5	5.91	1.48	1.35
81	L5	3627	OMG	C4-N3	5.91	1.47	1.34
81	L5	3869	OMC	C6-C5	5.91	1.48	1.35
47	S2	1842	4AC	C4-N3	5.89	1.42	1.32
81	L5	4456	OMC	C6-C5	5.87	1.48	1.35
81	L5	2365	OMC	C6-C5	5.87	1.48	1.35
81	L5	2824	OMC	C6-C5	5.87	1.48	1.35
47	S2	1703	OMC	C6-C5	5.86	1.48	1.35
81	L5	3808	OMC	C6-C5	5.83	1.48	1.35
81	L5	2804	OMC	C6-C5	5.83	1.48	1.35
81	L5	2422	OMC	C6-C5	5.81	1.48	1.35
81	L5	1881	OMC	C6-C5	5.79	1.48	1.35
47	S2	121	OMU	C6-C5	5.78	1.48	1.35
81	L5	1340	OMC	C6-C5	5.76	1.48	1.35
81	L5	2837	OMU	C6-C5	5.75	1.48	1.35
81	L5	3841	OMC	C6-C5	5.74	1.48	1.35
47	S2	116	OMU	C6-C5	5.74	1.48	1.35
47	S2	354	OMU	C6-C5	5.73	1.48	1.35
81	L5	2351	OMC	C6-C5	5.73	1.48	1.35
81	L5	4306	OMU	C6-C5	5.73	1.48	1.35
47	S2	1442	OMU	C6-C5	5.70	1.48	1.35
81	L5	2415	OMU	C6-C5	5.69	1.48	1.35
47	S2	1288	OMU	C6-C5	5.69	1.48	1.35
47	S2	172	OMU	C6-C5	5.65	1.48	1.35
81	L5	4227	OMU	C6-C5	5.62	1.48	1.35
81	L5	3925	OMU	C6-C5	5.62	1.48	1.35
4	L8	14	OMU	C6-C5	5.57	1.48	1.35
47	S2	27	A2M	O4'-C4'	-5.57	1.32	1.45
81	L5	4620	OMU	C6-C5	5.56	1.48	1.35
81	L5	4498	OMU	C6-C5	5.55	1.47	1.35
47	S2	1870	B8N	C2-N1	5.54	1.55	1.39
47	S2	428	OMU	C6-C5	5.53	1.47	1.35
47	S2	1056	PSU	C6-N1	5.33	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	1781	PSU	C6-N1	5.32	1.45	1.36
81	L5	4576	PSU	C6-N1	5.27	1.44	1.36
47	S2	681	PSU	C6-N1	5.27	1.44	1.36
47	S2	93	PSU	C6-N1	5.27	1.44	1.36
47	S2	1238	PSU	C6-N1	5.26	1.44	1.36
81	L5	5010	PSU	C6-N1	5.26	1.44	1.36
81	L5	2424	OMG	C2-N3	5.23	1.45	1.33
81	L5	4532	PSU	C6-N1	5.20	1.44	1.36
47	S2	36	PSU	C6-N1	5.20	1.44	1.36
81	L5	1782	PSU	C6-N1	5.19	1.44	1.36
81	L5	4471	PSU	C6-N1	5.19	1.44	1.36
47	S2	517	OMC	C4-N3	5.19	1.44	1.34
81	L5	4972	PSU	C6-N1	5.18	1.44	1.36
81	L5	4689	PSU	C6-N1	5.18	1.44	1.36
47	S2	34	PSU	C6-N1	5.18	1.44	1.36
81	L5	4423	PSU	C6-N1	5.18	1.44	1.36
81	L5	2632	PSU	C6-N1	5.18	1.44	1.36
47	S2	1232	PSU	C6-N1	5.17	1.44	1.36
81	L5	1862	PSU	C6-N1	5.16	1.44	1.36
47	S2	649	PSU	C6-N1	5.16	1.44	1.36
47	S2	1643	PSU	C6-N1	5.16	1.44	1.36
47	S2	406	PSU	C6-N1	5.16	1.44	1.36
47	S2	109	PSU	C6-N1	5.16	1.44	1.36
81	L5	4431	PSU	C6-N1	5.13	1.44	1.36
81	L5	4579	PSU	C6-N1	5.13	1.44	1.36
47	S2	686	PSU	C6-N1	5.13	1.44	1.36
47	S2	174	OMC	C4-N3	5.13	1.44	1.34
81	L5	5001	PSU	C6-N1	5.13	1.44	1.36
81	L5	1779	PSU	C6-N1	5.12	1.44	1.36
81	L5	4361	PSU	C6-N1	5.11	1.44	1.36
81	L5	4569	PSU	C6-N1	5.11	1.44	1.36
47	S2	1445	PSU	C6-N1	5.11	1.44	1.36
81	L5	4312	PSU	C6-N1	5.09	1.44	1.36
81	L5	2861	OMC	C4-N3	5.09	1.44	1.34
47	S2	1244	PSU	C6-N1	5.09	1.44	1.36
81	L5	3869	OMC	C4-N3	5.08	1.44	1.34
81	L5	1340	OMC	C4-N3	5.08	1.44	1.34
81	L5	3758	PSU	C6-N1	5.08	1.44	1.36
47	S2	651	PSU	C6-N1	5.07	1.44	1.36
81	L5	4499	OMG	C2-N3	5.07	1.45	1.33
81	L5	3770	PSU	C6-N1	5.05	1.44	1.36
81	L5	4299	PSU	C6-N1	5.05	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	1447	OMG	C2-N3	5.05	1.45	1.33
81	L5	4353	PSU	C6-N1	5.05	1.44	1.36
81	L5	1625	OMG	C2-N3	5.05	1.45	1.33
4	L8	69	PSU	C6-N1	5.03	1.44	1.36
47	S2	1703	OMC	C4-N3	5.02	1.44	1.34
81	L5	4552	PSU	C6-N1	5.02	1.44	1.36
81	L5	1683	PSU	C6-N1	5.01	1.44	1.36
81	L5	3887	OMC	C4-N3	5.01	1.44	1.34
81	L5	3841	OMC	C2-N1	5.00	1.50	1.40
81	L5	3851	PSU	C6-N1	5.00	1.44	1.36
47	S2	1177	PSU	C6-N1	5.00	1.44	1.36
81	L5	3884	PSU	C6-N1	5.00	1.44	1.36
47	S2	1703	OMC	C2-N1	4.99	1.50	1.40
81	L5	2824	OMC	C4-N3	4.98	1.44	1.34
47	S2	1692	PSU	C6-N1	4.98	1.44	1.36
81	L5	3639	PSU	C6-N1	4.97	1.44	1.36
4	L8	75	OMG	C2-N3	4.96	1.45	1.33
81	L5	2422	OMC	C4-N3	4.96	1.44	1.34
81	L5	4457	PSU	C6-N1	4.96	1.44	1.36
81	L5	2839	PSU	C6-N1	4.96	1.44	1.36
81	L5	2365	OMC	C4-N3	4.95	1.44	1.34
47	S2	644	OMG	C2-N3	4.95	1.45	1.33
81	L5	4628	PSU	C6-N1	4.95	1.44	1.36
47	S2	1391	OMC	C4-N3	4.94	1.44	1.34
81	L5	4530	UR3	C2-N3	4.91	1.48	1.39
81	L5	3695	PSU	C6-N1	4.91	1.44	1.36
81	L5	4536	OMC	C4-N3	4.91	1.44	1.34
81	L5	3920	PSU	C6-N1	4.90	1.44	1.36
81	L5	3637	PSU	C6-N1	4.89	1.44	1.36
81	L5	4442	PSU	C6-N1	4.89	1.44	1.36
81	L5	1881	OMC	C4-N3	4.89	1.44	1.34
47	S2	683	OMG	C2-N3	4.88	1.45	1.33
47	S2	509	OMG	C2-N3	4.88	1.45	1.33
81	L5	2351	OMC	C4-N3	4.87	1.44	1.34
81	L5	2804	OMC	C4-N3	4.87	1.44	1.34
81	L5	4637	OMG	C2-N3	4.87	1.45	1.33
47	S2	601	OMG	C2-N3	4.86	1.45	1.33
81	L5	3792	OMG	C2-N3	4.84	1.44	1.33
81	L5	4403	PSU	C6-N1	4.84	1.44	1.36
47	S2	1842	4AC	C2-N1	4.83	1.50	1.40
81	L5	3695	PSU	C1'-C5	-4.83	1.39	1.50
81	L5	4456	OMC	C4-N3	4.82	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	4370	OMG	C2-N3	4.80	1.44	1.33
81	L5	4494	OMG	C2-N3	4.79	1.44	1.33
47	S2	1177	PSU	C1'-C5	-4.78	1.39	1.50
81	L5	1862	PSU	C1'-C5	-4.78	1.39	1.50
47	S2	1870	B8N	C6-C5	4.78	1.41	1.35
81	L5	3808	OMC	C4-N3	4.76	1.44	1.34
47	S2	1238	PSU	C1'-C5	-4.75	1.39	1.50
81	L5	4618	OMG	C2-N3	4.75	1.44	1.33
47	S2	174	OMC	C4-N4	4.73	1.45	1.33
81	L5	1522	OMG	C2-N3	4.73	1.44	1.33
81	L5	4442	PSU	C1'-C5	-4.72	1.39	1.50
47	S2	1692	PSU	C1'-C5	-4.72	1.39	1.50
47	S2	436	OMG	C2-N3	4.71	1.44	1.33
47	S2	1703	OMC	C4-N4	4.70	1.45	1.33
81	L5	4361	PSU	C1'-C5	-4.70	1.39	1.50
81	L5	4392	OMG	C2-N3	4.70	1.44	1.33
47	S2	1244	PSU	C1'-C5	-4.70	1.39	1.50
81	L5	4403	PSU	C1'-C5	-4.69	1.39	1.50
81	L5	2876	OMG	C2-N3	4.69	1.44	1.33
81	L5	2861	OMC	C4-N4	4.68	1.45	1.33
81	L5	4299	PSU	C1'-C5	-4.68	1.39	1.50
81	L5	3818	UY1	C6-N1	4.68	1.44	1.36
81	L5	4353	PSU	C1'-C5	-4.68	1.39	1.50
81	L5	3851	PSU	C1'-C5	-4.67	1.39	1.50
81	L5	2364	OMG	C2-N3	4.67	1.44	1.33
81	L5	3758	PSU	C1'-C5	-4.66	1.39	1.50
47	S2	651	PSU	C1'-C5	-4.64	1.39	1.50
81	L5	3887	OMC	C4-N4	4.64	1.45	1.33
81	L5	3639	PSU	C1'-C5	-4.64	1.39	1.50
47	S2	109	PSU	C1'-C5	-4.64	1.39	1.50
81	L5	4228	OMG	C2-N3	4.64	1.44	1.33
47	S2	36	PSU	C1'-C5	-4.63	1.39	1.50
81	L5	4623	OMG	C2-N3	4.63	1.44	1.33
81	L5	1316	OMG	C2-N3	4.62	1.44	1.33
81	L5	1779	PSU	C1'-C5	-4.61	1.39	1.50
47	S2	1232	PSU	C1'-C5	-4.61	1.39	1.50
81	L5	3841	OMC	C4-N4	4.61	1.45	1.33
47	S2	1643	PSU	C1'-C5	-4.61	1.39	1.50
81	L5	2824	OMC	C4-N4	4.60	1.45	1.33
81	L5	4628	PSU	C1'-C5	-4.60	1.39	1.50
81	L5	3841	OMC	C4-N3	4.60	1.43	1.34
47	S2	1328	OMG	C2-N3	4.60	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	4579	PSU	C1'-C5	-4.60	1.39	1.50
47	S2	1056	PSU	C1'-C5	-4.59	1.39	1.50
81	L5	3770	PSU	C1'-C5	-4.59	1.39	1.50
81	L5	4576	PSU	C1'-C5	-4.59	1.39	1.50
47	S2	34	PSU	C1'-C5	-4.58	1.39	1.50
81	L5	5010	PSU	C1'-C5	-4.58	1.39	1.50
47	S2	686	PSU	C1'-C5	-4.58	1.39	1.50
81	L5	4972	PSU	C1'-C5	-4.57	1.39	1.50
81	L5	3808	OMC	C4-N4	4.57	1.45	1.33
47	S2	517	OMC	C4-N4	4.57	1.45	1.33
81	L5	3869	OMC	C4-N4	4.57	1.45	1.33
81	L5	2422	OMC	C4-N4	4.56	1.45	1.33
81	L5	1683	PSU	C1'-C5	-4.56	1.40	1.50
81	L5	3920	PSU	C1'-C5	-4.56	1.40	1.50
47	S2	1391	OMC	C4-N4	4.56	1.44	1.33
47	S2	681	PSU	C1'-C5	-4.56	1.40	1.50
47	S2	406	PSU	C1'-C5	-4.56	1.40	1.50
81	L5	1781	PSU	C1'-C5	-4.56	1.40	1.50
81	L5	2365	OMC	C4-N4	4.56	1.44	1.33
81	L5	1340	OMC	C4-N4	4.55	1.44	1.33
47	S2	649	PSU	C1'-C5	-4.55	1.40	1.50
81	L5	4456	OMC	C4-N4	4.55	1.44	1.33
81	L5	4536	OMC	C4-N4	4.55	1.44	1.33
81	L5	4431	PSU	C1'-C5	-4.54	1.40	1.50
81	L5	4689	PSU	C1'-C5	-4.54	1.40	1.50
81	L5	1782	PSU	C1'-C5	-4.54	1.40	1.50
81	L5	4552	PSU	C1'-C5	-4.54	1.40	1.50
81	L5	4471	PSU	C1'-C5	-4.54	1.40	1.50
81	L5	2804	OMC	C4-N4	4.53	1.44	1.33
81	L5	4569	PSU	C1'-C5	-4.53	1.40	1.50
81	L5	4423	PSU	C1'-C5	-4.53	1.40	1.50
81	L5	2424	OMG	C2-N2	4.53	1.44	1.34
81	L5	2632	PSU	C1'-C5	-4.52	1.40	1.50
81	L5	4499	OMG	C2-N2	4.51	1.44	1.34
47	S2	1490	OMG	C2-N3	4.51	1.44	1.33
81	L5	4532	PSU	C1'-C5	-4.50	1.40	1.50
81	L5	4312	PSU	C1'-C5	-4.50	1.40	1.50
81	L5	5001	PSU	C1'-C5	-4.49	1.40	1.50
47	S2	1391	OMC	C2-N1	4.49	1.49	1.40
47	S2	1490	OMG	C2-N2	4.48	1.44	1.34
47	S2	174	OMC	C2-N1	4.48	1.49	1.40
47	S2	1447	OMG	C2-N2	4.48	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	1870	B8N	C1'-C5	-4.47	1.40	1.50
81	L5	3884	PSU	C1'-C5	-4.46	1.40	1.50
47	S2	683	OMG	C2-N2	4.46	1.44	1.34
47	S2	93	PSU	C1'-C5	-4.46	1.40	1.50
47	S2	517	OMC	C2-N1	4.46	1.49	1.40
4	L8	75	OMG	C2-N2	4.45	1.44	1.34
81	L5	3792	OMG	C2-N2	4.45	1.44	1.34
81	L5	4370	OMG	C2-N2	4.45	1.44	1.34
81	L5	1881	OMC	C4-N4	4.44	1.44	1.33
47	S2	436	OMG	C2-N2	4.44	1.44	1.34
81	L5	2824	OMC	C2-N1	4.43	1.49	1.40
81	L5	3782	5MC	C2-N1	4.43	1.49	1.40
81	L5	1625	OMG	C2-N2	4.43	1.44	1.34
47	S2	644	OMG	C2-N2	4.43	1.44	1.34
47	S2	512	A2M	C6-N6	4.43	1.45	1.34
81	L5	2861	OMC	C2-N1	4.42	1.49	1.40
81	L5	4494	OMG	C2-N2	4.42	1.44	1.34
47	S2	601	OMG	C2-N2	4.42	1.44	1.34
81	L5	4228	OMG	C2-N2	4.42	1.44	1.34
81	L5	4618	OMG	C2-N2	4.41	1.44	1.34
81	L5	4457	PSU	C1'-C5	-4.41	1.40	1.50
81	L5	4456	OMC	C2-N1	4.41	1.49	1.40
81	L5	3808	OMC	C2-N1	4.41	1.49	1.40
81	L5	2351	OMC	C4-N4	4.39	1.44	1.33
47	S2	576	A2M	C6-N6	4.39	1.45	1.34
47	S2	1678	A2M	C6-N6	4.39	1.45	1.34
81	L5	2815	A2M	C6-N6	4.39	1.45	1.34
47	S2	509	OMG	C2-N2	4.38	1.44	1.34
81	L5	3637	PSU	C1'-C5	-4.38	1.40	1.50
81	L5	2351	OMC	C2-N1	4.38	1.49	1.40
47	S2	166	A2M	C6-N6	4.38	1.45	1.34
47	S2	159	A2M	C6-N6	4.38	1.45	1.34
47	S2	590	A2M	C6-N6	4.37	1.45	1.34
81	L5	2422	OMC	C2-N1	4.37	1.49	1.40
81	L5	3724	A2M	C6-N6	4.37	1.45	1.34
47	S2	484	A2M	C6-N6	4.36	1.45	1.34
81	L5	398	A2M	C6-N6	4.36	1.45	1.34
81	L5	1534	A2M	C6-N6	4.36	1.45	1.34
4	L8	69	PSU	C1'-C5	-4.36	1.40	1.50
81	L5	4571	A2M	C6-N6	4.35	1.45	1.34
81	L5	400	A2M	C6-N6	4.35	1.45	1.34
81	L5	3887	OMC	C2-N1	4.34	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	468	A2M	C6-N6	4.34	1.45	1.34
81	L5	2876	OMG	C2-N2	4.33	1.44	1.34
81	L5	4637	OMG	C2-N2	4.33	1.44	1.34
81	L5	3869	OMC	C2-N1	4.32	1.49	1.40
81	L5	1881	OMC	C2-N1	4.32	1.49	1.40
47	S2	1383	A2M	C6-N6	4.32	1.45	1.34
81	L5	4623	OMG	C2-N2	4.32	1.44	1.34
81	L5	1316	OMG	C2-N2	4.32	1.44	1.34
81	L5	2364	OMG	C2-N2	4.32	1.44	1.34
47	S2	1445	PSU	C1'-C5	-4.31	1.40	1.50
81	L5	1524	A2M	C6-N6	4.31	1.45	1.34
81	L5	4392	OMG	C2-N2	4.31	1.44	1.34
81	L5	4590	A2M	C6-N6	4.30	1.45	1.34
47	S2	1288	OMU	C4-N3	4.30	1.46	1.38
81	L5	3627	OMG	C2-N3	4.30	1.43	1.33
47	S2	1328	OMG	C2-N2	4.30	1.44	1.34
47	S2	99	A2M	C6-N6	4.30	1.45	1.34
47	S2	1842	4AC	C7-N4	4.30	1.45	1.37
81	L5	3718	A2M	C6-N6	4.29	1.45	1.34
81	L5	3867	A2M	C6-N6	4.29	1.45	1.34
81	L5	1522	OMG	C2-N2	4.29	1.44	1.34
81	L5	4523	A2M	C6-N6	4.28	1.45	1.34
47	S2	1031	A2M	C6-N6	4.28	1.45	1.34
47	S2	27	A2M	C6-N6	4.27	1.45	1.34
81	L5	2804	OMC	C2-N1	4.27	1.49	1.40
81	L5	2401	A2M	C6-N6	4.27	1.45	1.34
81	L5	3782	5MC	C4-N4	4.26	1.45	1.34
81	L5	4536	OMC	C2-N1	4.25	1.49	1.40
81	L5	3830	A2M	C6-N6	4.25	1.45	1.34
81	L5	4227	OMU	C4-N3	4.25	1.45	1.38
81	L5	1871	A2M	C6-N6	4.24	1.45	1.34
81	L5	3825	A2M	C6-N6	4.23	1.45	1.34
47	S2	116	OMU	C4-N3	4.23	1.45	1.38
81	L5	2787	A2M	C6-N6	4.23	1.45	1.34
81	L5	2365	OMC	C2-N1	4.23	1.48	1.40
81	L5	1340	OMC	C2-N1	4.23	1.48	1.40
81	L5	2415	OMU	C4-N3	4.21	1.45	1.38
81	L5	2363	A2M	C6-N6	4.21	1.45	1.34
81	L5	3627	OMG	C2-N2	4.21	1.44	1.34
81	L5	3782	5MC	C6-N1	4.19	1.45	1.38
81	L5	1326	A2M	C6-N6	4.15	1.44	1.34
47	S2	428	OMU	C4-N3	4.15	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	121	OMU	C4-N3	4.14	1.45	1.38
47	S2	1337	4AC	C2-N1	4.14	1.48	1.40
47	S2	172	OMU	C4-N3	4.13	1.45	1.38
81	L5	4306	OMU	C4-N3	4.12	1.45	1.38
81	L5	3785	A2M	C6-N6	4.10	1.44	1.34
4	L8	14	OMU	C4-N3	4.09	1.45	1.38
47	S2	354	OMU	C4-N3	4.09	1.45	1.38
81	L5	2839	PSU	C1'-C5	-4.08	1.41	1.50
81	L5	2837	OMU	C4-N3	4.05	1.45	1.38
81	L5	4498	OMU	C4-N3	4.05	1.45	1.38
81	L5	3925	OMU	C4-N3	4.02	1.45	1.38
81	L5	4620	OMU	C4-N3	3.97	1.45	1.38
47	S2	1442	OMU	C4-N3	3.88	1.45	1.38
47	S2	1445	PSU	C4-N3	3.80	1.46	1.38
47	S2	1842	4AC	O2-C2	-3.73	1.16	1.23
47	S2	1851	MA6	C6-N6	3.69	1.47	1.36
47	S2	1337	4AC	C7-N4	3.64	1.44	1.37
47	S2	1850	MA6	C6-N6	3.64	1.46	1.36
47	S2	93	PSU	C4-N3	3.62	1.45	1.38
47	S2	1643	PSU	C4-N3	3.56	1.45	1.38
47	S2	651	PSU	C4-N3	3.56	1.45	1.38
47	S2	1842	4AC	C5-C4	3.56	1.48	1.41
81	L5	4423	PSU	C4-N3	3.55	1.45	1.38
47	S2	34	PSU	C4-N3	3.55	1.45	1.38
47	S2	1056	PSU	C4-N3	3.54	1.45	1.38
47	S2	109	PSU	C4-N3	3.54	1.45	1.38
47	S2	681	PSU	C4-N3	3.54	1.45	1.38
47	S2	1232	PSU	C4-N3	3.54	1.45	1.38
81	L5	2632	PSU	C4-N3	3.52	1.45	1.38
81	L5	5010	PSU	C4-N3	3.52	1.45	1.38
47	S2	36	PSU	C4-N3	3.51	1.45	1.38
81	L5	4312	PSU	C4-N3	3.51	1.45	1.38
81	L5	3884	PSU	C4-N3	3.51	1.45	1.38
81	L5	4689	PSU	C4-N3	3.50	1.45	1.38
81	L5	4972	PSU	C4-N3	3.50	1.45	1.38
81	L5	3637	PSU	C4-N3	3.49	1.45	1.38
47	S2	649	PSU	C4-N3	3.49	1.45	1.38
47	S2	686	PSU	C4-N3	3.49	1.45	1.38
81	L5	1779	PSU	C4-N3	3.48	1.45	1.38
81	L5	4532	PSU	C4-N3	3.48	1.45	1.38
47	S2	1244	PSU	C4-N3	3.48	1.45	1.38
47	S2	1692	PSU	C4-N3	3.48	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	4431	PSU	C4-N3	3.47	1.45	1.38
81	L5	5001	PSU	C4-N3	3.47	1.45	1.38
81	L5	1782	PSU	C4-N3	3.46	1.45	1.38
81	L5	3841	OMC	O2-C2	-3.46	1.17	1.23
81	L5	4353	PSU	C4-N3	3.45	1.45	1.38
81	L5	3920	PSU	C4-N3	3.45	1.45	1.38
81	L5	1683	PSU	C4-N3	3.44	1.45	1.38
47	S2	406	PSU	C4-N3	3.44	1.45	1.38
81	L5	4576	PSU	C4-N3	3.43	1.45	1.38
81	L5	4579	PSU	C4-N3	3.42	1.45	1.38
81	L5	2351	OMC	C6-N1	3.42	1.46	1.38
47	S2	1238	PSU	C4-N3	3.42	1.45	1.38
81	L5	3770	PSU	C4-N3	3.42	1.45	1.38
81	L5	1871	A2M	O3'-C3'	-3.41	1.34	1.43
81	L5	1862	PSU	C4-N3	3.40	1.45	1.38
81	L5	4361	PSU	C4-N3	3.40	1.45	1.38
81	L5	1781	PSU	C4-N3	3.40	1.45	1.38
81	L5	4628	PSU	C4-N3	3.39	1.45	1.38
81	L5	4299	PSU	C4-N3	3.39	1.45	1.38
81	L5	2424	OMG	C5-N7	-3.38	1.32	1.39
81	L5	3639	PSU	C4-N3	3.38	1.45	1.38
81	L5	4403	PSU	C4-N3	3.37	1.45	1.38
81	L5	4552	PSU	C4-N3	3.37	1.45	1.38
81	L5	4442	PSU	C4-N3	3.37	1.45	1.38
81	L5	3825	A2M	C5-C4	-3.35	1.33	1.39
81	L5	3887	OMC	C6-N1	3.35	1.46	1.38
81	L5	3869	OMC	C6-N1	3.34	1.46	1.38
81	L5	4457	PSU	C4-N3	3.34	1.45	1.38
4	L8	69	PSU	C4-N3	3.33	1.45	1.38
81	L5	4569	PSU	C4-N3	3.33	1.45	1.38
81	L5	1625	OMG	C5-N7	-3.32	1.32	1.39
81	L5	3851	PSU	C4-N3	3.31	1.45	1.38
47	S2	1490	OMG	C5-N7	-3.31	1.32	1.39
81	L5	4471	PSU	C4-N3	3.31	1.45	1.38
81	L5	2839	PSU	C4-N3	3.29	1.45	1.38
81	L5	3758	PSU	C4-N3	3.29	1.45	1.38
47	S2	1703	OMC	C6-N1	3.28	1.45	1.38
81	L5	3867	A2M	O3'-C3'	-3.28	1.34	1.43
47	S2	517	OMC	C6-N1	3.27	1.45	1.38
47	S2	1177	PSU	C4-N3	3.26	1.45	1.38
81	L5	4523	A2M	C5-C4	-3.26	1.33	1.39
81	L5	4590	A2M	O3'-C3'	-3.26	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	174	OMC	C6-N1	3.26	1.45	1.38
81	L5	4571	A2M	O3'-C3'	-3.25	1.34	1.43
81	L5	2839	PSU	O4-C4	-3.25	1.17	1.23
47	S2	468	A2M	O3'-C3'	-3.25	1.34	1.43
81	L5	3818	UY1	C4-N3	3.24	1.44	1.38
81	L5	4536	OMC	C6-N1	3.24	1.45	1.38
47	S2	1842	4AC	C6-N1	3.23	1.45	1.38
81	L5	3718	A2M	O3'-C3'	-3.23	1.35	1.43
81	L5	2861	OMC	C6-N1	3.22	1.45	1.38
47	S2	1391	OMC	C6-N1	3.22	1.45	1.38
81	L5	1871	A2M	C5-C4	-3.21	1.33	1.39
81	L5	2401	A2M	C5-C4	-3.21	1.33	1.39
47	S2	468	A2M	C5-C4	-3.21	1.33	1.39
81	L5	398	A2M	O3'-C3'	-3.21	1.35	1.43
47	S2	99	A2M	O3'-C3'	-3.20	1.35	1.43
81	L5	400	A2M	O3'-C3'	-3.19	1.35	1.43
81	L5	1340	OMC	C6-N1	3.19	1.45	1.38
81	L5	2365	OMC	C6-N1	3.19	1.45	1.38
81	L5	2804	OMC	C6-N1	3.18	1.45	1.38
47	S2	159	A2M	O2'-C2'	3.18	1.50	1.42
47	S2	1031	A2M	C5-C4	-3.18	1.33	1.39
81	L5	2824	OMC	C6-N1	3.18	1.45	1.38
81	L5	3808	OMC	O2-C2	-3.18	1.17	1.23
81	L5	3695	PSU	C4-N3	3.18	1.44	1.38
81	L5	1326	A2M	O3'-C3'	-3.17	1.35	1.43
81	L5	1524	A2M	C5-C4	-3.17	1.33	1.39
81	L5	1881	OMC	C6-N1	3.16	1.45	1.38
47	S2	1328	OMG	C5-N7	-3.16	1.32	1.39
47	S2	1703	OMC	O2-C2	-3.16	1.17	1.23
81	L5	3830	A2M	C5-C4	-3.16	1.33	1.39
81	L5	2422	OMC	C6-N1	3.15	1.45	1.38
81	L5	2787	A2M	C5-C4	-3.15	1.33	1.39
47	S2	512	A2M	O3'-C3'	-3.15	1.35	1.43
47	S2	1490	OMG	C4-N9	-3.14	1.30	1.38
81	L5	4456	OMC	C6-N1	3.14	1.45	1.38
47	S2	1678	A2M	C5-C4	-3.14	1.33	1.39
81	L5	2363	A2M	O3'-C3'	-3.14	1.35	1.43
81	L5	1881	OMC	O2-C2	-3.14	1.17	1.23
81	L5	3808	OMC	C6-N1	3.13	1.45	1.38
81	L5	4494	OMG	C5-N7	-3.12	1.32	1.39
81	L5	2876	OMG	C5-N7	-3.12	1.32	1.39
81	L5	3825	A2M	O3'-C3'	-3.11	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	3925	OMU	O4-C4	-3.11	1.18	1.24
47	S2	1383	A2M	C5-C4	-3.11	1.33	1.39
81	L5	3792	OMG	C5-N7	-3.11	1.32	1.39
47	S2	1678	A2M	O3'-C3'	-3.11	1.35	1.43
81	L5	4499	OMG	C5-N7	-3.11	1.32	1.39
47	S2	1031	A2M	O3'-C3'	-3.10	1.35	1.43
47	S2	576	A2M	O3'-C3'	-3.10	1.35	1.43
4	L8	75	OMG	C5-N7	-3.10	1.32	1.39
81	L5	3785	A2M	O2'-C2'	3.09	1.50	1.42
47	S2	644	OMG	C5-N7	-3.09	1.32	1.39
81	L5	1522	OMG	C5-N7	-3.09	1.32	1.39
81	L5	3887	OMC	O2-C2	-3.09	1.18	1.23
47	S2	601	OMG	C5-N7	-3.09	1.32	1.39
47	S2	436	OMG	C5-N7	-3.09	1.32	1.39
81	L5	2422	OMC	O2-C2	-3.08	1.18	1.23
81	L5	4220	6MZ	C5-C4	-3.08	1.33	1.39
81	L5	4571	A2M	C5-C4	-3.08	1.33	1.39
81	L5	2861	OMC	O2-C2	-3.08	1.18	1.23
81	L5	3637	PSU	O4-C4	-3.08	1.17	1.23
47	S2	1383	A2M	O3'-C3'	-3.08	1.35	1.43
81	L5	4370	OMG	C5-N7	-3.07	1.32	1.39
81	L5	3724	A2M	O3'-C3'	-3.07	1.35	1.43
81	L5	1316	OMG	C5-N7	-3.07	1.32	1.39
81	L5	3785	A2M	C5-C4	-3.07	1.33	1.39
81	L5	1326	A2M	C5-C4	-3.06	1.33	1.39
81	L5	4530	UR3	C6-N1	3.06	1.45	1.38
47	S2	683	OMG	C5-N7	-3.06	1.32	1.39
47	S2	484	A2M	C5-C4	-3.06	1.33	1.39
81	L5	2363	A2M	C5-C4	-3.06	1.33	1.39
81	L5	4456	OMC	O2-C2	-3.06	1.18	1.23
81	L5	3841	OMC	C6-N1	3.06	1.45	1.38
47	S2	166	A2M	O3'-C3'	-3.06	1.35	1.43
81	L5	4637	OMG	C5-N7	-3.06	1.32	1.39
47	S2	1850	MA6	C5-C4	-3.05	1.33	1.39
81	L5	2365	OMC	O2-C2	-3.05	1.18	1.23
47	S2	27	A2M	O2'-C2'	3.05	1.50	1.42
81	L5	3724	A2M	C5-C4	-3.05	1.33	1.39
81	L5	4392	OMG	C5-N7	-3.05	1.33	1.39
81	L5	2824	OMC	O2-C2	-3.05	1.18	1.23
47	S2	159	A2M	O3'-C3'	-3.04	1.35	1.43
81	L5	3830	A2M	O3'-C3'	-3.04	1.35	1.43
81	L5	2815	A2M	O3'-C3'	-3.04	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	3867	A2M	C5-C4	-3.03	1.33	1.39
47	S2	428	OMU	O4-C4	-3.03	1.18	1.24
81	L5	4536	OMC	O2-C2	-3.03	1.18	1.23
47	S2	590	A2M	O3'-C3'	-3.03	1.35	1.43
47	S2	166	A2M	C5-C4	-3.03	1.33	1.39
47	S2	99	A2M	C5-C4	-3.02	1.33	1.39
47	S2	512	A2M	C5-C4	-3.02	1.33	1.39
81	L5	1340	OMC	O2-C2	-3.02	1.18	1.23
81	L5	4457	PSU	O4-C4	-3.01	1.17	1.23
81	L5	400	A2M	C5-C4	-3.01	1.33	1.39
81	L5	2351	OMC	O2-C2	-3.01	1.18	1.23
81	L5	3627	OMG	C4-N9	-3.01	1.30	1.38
81	L5	4498	OMU	O4-C4	-3.01	1.18	1.24
81	L5	2364	OMG	C5-N7	-3.00	1.33	1.39
81	L5	3718	A2M	C5-C4	-3.00	1.33	1.39
47	S2	517	OMC	O2-C2	-2.99	1.18	1.23
81	L5	4620	OMU	O4-C4	-2.99	1.18	1.24
47	S2	509	OMG	C5-N7	-2.99	1.33	1.39
47	S2	1851	MA6	C5-C4	-2.98	1.33	1.39
47	S2	174	OMC	O2-C2	-2.98	1.18	1.23
81	L5	2401	A2M	O3'-C3'	-2.98	1.35	1.43
81	L5	2804	OMC	O2-C2	-2.98	1.18	1.23
4	L8	14	OMU	O4-C4	-2.98	1.18	1.24
47	S2	1678	A2M	O2'-C2'	2.98	1.50	1.42
81	L5	4623	OMG	C5-N7	-2.98	1.33	1.39
81	L5	3869	OMC	O2-C2	-2.97	1.18	1.23
81	L5	4306	OMU	O4-C4	-2.97	1.18	1.24
81	L5	4228	OMG	C4-N9	-2.97	1.30	1.38
47	S2	1238	PSU	O4-C4	-2.97	1.17	1.23
47	S2	1447	OMG	C5-N7	-2.96	1.33	1.39
47	S2	27	A2M	O3'-C3'	-2.95	1.35	1.43
81	L5	2787	A2M	C5-N7	-2.94	1.33	1.39
47	S2	576	A2M	C5-C4	-2.94	1.33	1.39
81	L5	2815	A2M	O2'-C2'	2.94	1.49	1.42
81	L5	2415	OMU	O4-C4	-2.94	1.18	1.24
47	S2	1442	OMU	O4-C4	-2.93	1.18	1.24
81	L5	4590	A2M	C5-C4	-2.93	1.33	1.39
81	L5	1534	A2M	C5-C4	-2.92	1.33	1.39
47	S2	1337	4AC	O7-C7	-2.92	1.16	1.23
81	L5	4227	OMU	O4-C4	-2.92	1.18	1.24
47	S2	99	A2M	O2'-C2'	2.92	1.49	1.42
81	L5	4523	A2M	O3'-C3'	-2.92	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	484	A2M	O2'-C2'	2.91	1.49	1.42
47	S2	590	A2M	C5-C4	-2.91	1.33	1.39
81	L5	3724	A2M	O2'-C2'	2.91	1.49	1.42
81	L5	4618	OMG	C5-N7	-2.90	1.33	1.39
81	L5	2787	A2M	O2'-C2'	2.90	1.49	1.42
81	L5	3867	A2M	O2'-C2'	2.90	1.49	1.42
47	S2	27	A2M	C5-C4	-2.90	1.33	1.39
47	S2	1177	PSU	O4-C4	-2.89	1.18	1.23
47	S2	121	OMU	O4-C4	-2.89	1.18	1.24
81	L5	3627	OMG	C5-N7	-2.89	1.33	1.39
47	S2	116	OMU	O4-C4	-2.89	1.18	1.24
47	S2	590	A2M	O2'-C2'	2.89	1.49	1.42
81	L5	400	A2M	O2'-C2'	2.89	1.49	1.42
81	L5	1683	PSU	O4-C4	-2.88	1.18	1.23
47	S2	1031	A2M	O2'-C2'	2.88	1.49	1.42
81	L5	3718	A2M	C5-N7	-2.88	1.33	1.39
81	L5	1524	A2M	O3'-C3'	-2.88	1.35	1.43
81	L5	398	A2M	C5-C4	-2.88	1.34	1.39
81	L5	3695	PSU	O4-C4	-2.87	1.18	1.23
47	S2	1391	OMC	O2-C2	-2.87	1.18	1.23
81	L5	3718	A2M	O2'-C2'	2.87	1.49	1.42
81	L5	3825	A2M	O2'-C2'	2.87	1.49	1.42
81	L5	4972	PSU	O4-C4	-2.87	1.18	1.23
81	L5	4228	OMG	C5-N7	-2.86	1.33	1.39
81	L5	1782	PSU	O4-C4	-2.86	1.18	1.23
47	S2	172	OMU	O4-C4	-2.86	1.18	1.24
47	S2	99	A2M	C5-N7	-2.86	1.33	1.39
47	S2	354	OMU	O4-C4	-2.86	1.18	1.24
81	L5	1862	PSU	O4-C4	-2.86	1.18	1.23
81	L5	3851	PSU	O4-C4	-2.86	1.18	1.23
47	S2	1383	A2M	O2'-C2'	2.85	1.49	1.42
81	L5	4590	A2M	O2'-C2'	2.85	1.49	1.42
81	L5	4431	PSU	O4-C4	-2.85	1.18	1.23
81	L5	4569	PSU	O4-C4	-2.85	1.18	1.23
81	L5	1534	A2M	O2'-C2'	2.85	1.49	1.42
81	L5	4299	PSU	O4-C4	-2.85	1.18	1.23
81	L5	2815	A2M	C5-C4	-2.85	1.34	1.39
47	S2	1442	OMU	C6-N1	2.84	1.44	1.38
81	L5	1524	A2M	O2'-C2'	2.84	1.49	1.42
81	L5	4571	A2M	O2'-C2'	2.83	1.49	1.42
81	L5	4361	PSU	O4-C4	-2.83	1.18	1.23
81	L5	4552	PSU	O4-C4	-2.83	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	2837	OMU	O4-C4	-2.83	1.19	1.24
47	S2	484	A2M	O3'-C3'	-2.83	1.35	1.43
81	L5	2363	A2M	C5-N7	-2.83	1.33	1.39
47	S2	512	A2M	O2'-C2'	2.83	1.49	1.42
81	L5	3758	PSU	O4-C4	-2.82	1.18	1.23
47	S2	121	OMU	C6-N1	2.82	1.44	1.38
81	L5	3867	A2M	C5-N7	-2.82	1.33	1.39
81	L5	2415	OMU	C6-N1	2.82	1.44	1.38
81	L5	4523	A2M	O2'-C2'	2.82	1.49	1.42
81	L5	2815	A2M	C5-N7	-2.82	1.33	1.39
47	S2	428	OMU	C6-N1	2.82	1.44	1.38
81	L5	1316	OMG	O6-C6	-2.82	1.18	1.23
47	S2	159	A2M	C5-C4	-2.81	1.34	1.39
81	L5	3627	OMG	O6-C6	-2.81	1.18	1.23
81	L5	3920	PSU	O4-C4	-2.81	1.18	1.23
47	S2	576	A2M	O2'-C2'	2.81	1.49	1.42
81	L5	2363	A2M	O2'-C2'	2.81	1.49	1.42
4	L8	69	PSU	O4-C4	-2.81	1.18	1.23
47	S2	1871	6MZ	C5-C4	-2.81	1.34	1.39
81	L5	398	A2M	O2'-C2'	2.81	1.49	1.42
81	L5	1781	PSU	O4-C4	-2.80	1.18	1.23
81	L5	4579	PSU	O4-C4	-2.80	1.18	1.23
81	L5	4392	OMG	O6-C6	-2.80	1.18	1.23
47	S2	166	A2M	O2'-C2'	2.80	1.49	1.42
81	L5	1326	A2M	C5-N7	-2.80	1.34	1.39
81	L5	4576	PSU	O4-C4	-2.79	1.18	1.23
47	S2	116	OMU	C6-N1	2.79	1.44	1.38
81	L5	5001	PSU	O4-C4	-2.79	1.18	1.23
47	S2	1031	A2M	C5-N7	-2.79	1.34	1.39
81	L5	4523	A2M	C5-N7	-2.79	1.34	1.39
47	S2	354	OMU	C6-N1	2.79	1.44	1.38
47	S2	1328	OMG	C4-N9	-2.79	1.31	1.38
47	S2	1288	OMU	O4-C4	-2.78	1.19	1.24
81	L5	2787	A2M	O3'-C3'	-2.78	1.36	1.43
81	L5	1534	A2M	C5-N7	-2.78	1.34	1.39
81	L5	2401	A2M	O2'-C2'	2.78	1.49	1.42
47	S2	1328	OMG	O6-C6	-2.78	1.18	1.23
81	L5	4392	OMG	C4-N9	-2.77	1.31	1.38
81	L5	4442	PSU	O4-C4	-2.77	1.18	1.23
47	S2	1288	OMU	C6-N1	2.77	1.44	1.38
47	S2	436	OMG	C4-N9	-2.77	1.31	1.38
81	L5	2632	PSU	O4-C4	-2.77	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	1056	PSU	O4-C4	-2.77	1.18	1.23
47	S2	93	PSU	O4-C4	-2.76	1.18	1.23
81	L5	3830	A2M	O2'-C2'	2.76	1.49	1.42
47	S2	1692	PSU	O4-C4	-2.76	1.18	1.23
81	L5	4306	OMU	C6-N1	2.76	1.44	1.38
47	S2	601	OMG	C2-N1	2.76	1.44	1.37
4	L8	14	OMU	C6-N1	2.76	1.44	1.38
81	L5	1779	PSU	O4-C4	-2.76	1.18	1.23
47	S2	1447	OMG	C2-N1	2.76	1.44	1.37
81	L5	4689	PSU	O4-C4	-2.76	1.18	1.23
81	L5	3639	PSU	O4-C4	-2.75	1.18	1.23
81	L5	4403	PSU	O4-C4	-2.75	1.18	1.23
47	S2	683	OMG	C2-N1	2.75	1.44	1.37
81	L5	4471	PSU	O4-C4	-2.75	1.18	1.23
81	L5	4532	PSU	O4-C4	-2.75	1.18	1.23
47	S2	1337	4AC	C6-N1	2.75	1.44	1.38
81	L5	3925	OMU	C6-N1	2.74	1.44	1.38
47	S2	406	PSU	O4-C4	-2.74	1.18	1.23
47	S2	172	OMU	C6-N1	2.74	1.44	1.38
47	S2	34	PSU	O4-C4	-2.74	1.18	1.23
47	S2	1244	PSU	O4-C4	-2.74	1.18	1.23
81	L5	5010	PSU	O4-C4	-2.74	1.18	1.23
81	L5	1871	A2M	O2'-C2'	2.73	1.49	1.42
47	S2	681	PSU	O4-C4	-2.73	1.18	1.23
47	S2	686	PSU	O4-C4	-2.73	1.18	1.23
81	L5	1534	A2M	O3'-C3'	-2.73	1.36	1.43
47	S2	649	PSU	O4-C4	-2.73	1.18	1.23
81	L5	4370	OMG	C2-N1	2.72	1.44	1.37
81	L5	3830	A2M	C5-N7	-2.72	1.34	1.39
47	S2	484	A2M	C5-N7	-2.72	1.34	1.39
81	L5	4628	PSU	O4-C4	-2.72	1.18	1.23
81	L5	3770	PSU	O4-C4	-2.72	1.18	1.23
81	L5	4498	OMU	O2-C2	-2.72	1.18	1.23
47	S2	109	PSU	O4-C4	-2.72	1.18	1.23
81	L5	1522	OMG	O6-C6	-2.72	1.18	1.23
47	S2	436	OMG	C2-N1	2.72	1.44	1.37
81	L5	4423	PSU	O4-C4	-2.71	1.18	1.23
81	L5	2876	OMG	O6-C6	-2.71	1.18	1.23
81	L5	3818	UY1	O4-C4	-2.71	1.18	1.23
47	S2	1643	PSU	O4-C4	-2.71	1.18	1.23
81	L5	3884	PSU	O4-C4	-2.70	1.18	1.23
81	L5	1871	A2M	C5-N7	-2.70	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	4353	PSU	O4-C4	-2.70	1.18	1.23
81	L5	2837	OMU	C6-N1	2.70	1.44	1.38
81	L5	2401	A2M	C5-N7	-2.70	1.34	1.39
81	L5	4571	A2M	C5-N7	-2.70	1.34	1.39
47	S2	36	PSU	O4-C4	-2.70	1.18	1.23
81	L5	4623	OMG	O6-C6	-2.70	1.18	1.23
47	S2	468	A2M	O2'-C2'	2.70	1.49	1.42
81	L5	2364	OMG	C4-N9	-2.70	1.31	1.38
47	S2	576	A2M	C5-N7	-2.70	1.34	1.39
81	L5	4228	OMG	C2-N1	2.70	1.44	1.37
81	L5	4618	OMG	C2-N1	2.70	1.44	1.37
47	S2	1232	PSU	O4-C4	-2.69	1.18	1.23
81	L5	4312	PSU	O4-C4	-2.69	1.18	1.23
47	S2	683	OMG	C4-N9	-2.69	1.31	1.38
47	S2	1490	OMG	O6-C6	-2.69	1.18	1.23
47	S2	1850	MA6	C5-N7	-2.69	1.34	1.39
47	S2	651	PSU	O4-C4	-2.69	1.18	1.23
81	L5	4620	OMU	C6-N1	2.69	1.44	1.38
81	L5	1522	OMG	C2-N1	2.68	1.44	1.37
81	L5	4498	OMU	C6-N1	2.68	1.44	1.38
47	S2	1383	A2M	C5-N7	-2.68	1.34	1.39
81	L5	1316	OMG	C4-N9	-2.68	1.31	1.38
81	L5	4637	OMG	O6-C6	-2.68	1.18	1.23
47	S2	1678	A2M	C5-N7	-2.67	1.34	1.39
4	L8	75	OMG	C2-N1	2.67	1.44	1.37
81	L5	4618	OMG	C4-N9	-2.67	1.31	1.38
47	S2	512	A2M	C5-N7	-2.66	1.34	1.39
81	L5	4623	OMG	C2-N1	2.66	1.44	1.37
81	L5	3825	A2M	C5-N7	-2.66	1.34	1.39
81	L5	2364	OMG	O6-C6	-2.66	1.18	1.23
81	L5	4227	OMU	C6-N1	2.66	1.44	1.38
81	L5	1524	A2M	C5-N7	-2.66	1.34	1.39
81	L5	4494	OMG	C2-N1	2.66	1.44	1.37
47	S2	159	A2M	C5-N7	-2.66	1.34	1.39
81	L5	4228	OMG	O6-C6	-2.66	1.18	1.23
81	L5	4623	OMG	C4-N9	-2.66	1.31	1.38
47	S2	1442	OMU	O2-C2	-2.66	1.18	1.23
47	S2	644	OMG	C2-N1	2.66	1.44	1.37
81	L5	1326	A2M	O2'-C2'	2.65	1.49	1.42
81	L5	4370	OMG	C4-N9	-2.65	1.31	1.38
47	S2	1031	A2M	C8-N9	-2.65	1.33	1.37
81	L5	3792	OMG	C4-N9	-2.65	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	1871	A2M	C8-N9	-2.63	1.33	1.37
47	S2	436	OMG	O6-C6	-2.63	1.18	1.23
81	L5	1534	A2M	C8-N9	-2.63	1.33	1.37
4	L8	69	PSU	O4'-C1'	-2.63	1.40	1.43
81	L5	400	A2M	C5-N7	-2.63	1.34	1.39
81	L5	4618	OMG	O6-C6	-2.63	1.18	1.23
81	L5	3785	A2M	C5-N7	-2.62	1.34	1.39
81	L5	4637	OMG	C2-N1	2.62	1.44	1.37
81	L5	4499	OMG	C2-N1	2.62	1.44	1.37
81	L5	1522	OMG	C4-N9	-2.62	1.31	1.38
47	S2	166	A2M	C5-N7	-2.62	1.34	1.39
81	L5	398	A2M	C5-N7	-2.62	1.34	1.39
81	L5	2401	A2M	C8-N9	-2.61	1.33	1.37
47	S2	1337	4AC	C5-C4	2.61	1.46	1.41
81	L5	3718	A2M	C8-N9	-2.61	1.33	1.37
47	S2	1445	PSU	O4-C4	-2.61	1.18	1.23
81	L5	3724	A2M	C5-N7	-2.61	1.34	1.39
81	L5	3825	A2M	C8-N9	-2.61	1.33	1.37
47	S2	27	A2M	C5-N7	-2.61	1.34	1.39
81	L5	4590	A2M	C5-N7	-2.61	1.34	1.39
47	S2	509	OMG	O6-C6	-2.61	1.18	1.23
81	L5	2363	A2M	C8-N9	-2.60	1.33	1.37
81	L5	3792	OMG	O6-C6	-2.60	1.18	1.23
47	S2	468	A2M	C5-N7	-2.60	1.34	1.39
81	L5	2424	OMG	O6-C6	-2.59	1.18	1.23
81	L5	4499	OMG	O6-C6	-2.59	1.18	1.23
4	L8	75	OMG	O6-C6	-2.59	1.18	1.23
47	S2	590	A2M	C5-N7	-2.59	1.34	1.39
81	L5	2424	OMG	C2-N1	2.59	1.43	1.37
81	L5	3782	5MC	O2-C2	-2.59	1.18	1.23
47	S2	1678	A2M	C8-N9	-2.59	1.33	1.37
47	S2	644	OMG	O6-C6	-2.59	1.18	1.23
81	L5	1316	OMG	C2-N1	2.58	1.43	1.37
81	L5	1326	A2M	C8-N9	-2.58	1.33	1.37
47	S2	509	OMG	C2-N1	2.58	1.43	1.37
47	S2	99	A2M	C8-N9	-2.58	1.33	1.37
47	S2	601	OMG	O6-C6	-2.58	1.18	1.23
4	L8	14	OMU	O2-C2	-2.58	1.18	1.23
81	L5	3627	OMG	C2-N1	2.58	1.43	1.37
81	L5	3785	A2M	O3'-C3'	-2.58	1.36	1.43
47	S2	1337	4AC	O2-C2	-2.57	1.18	1.23
47	S2	1871	6MZ	C5-N7	-2.57	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	2364	OMG	C2-N1	2.57	1.43	1.37
47	S2	1383	A2M	C8-N9	-2.57	1.33	1.37
47	S2	1871	6MZ	C8-N9	-2.56	1.33	1.37
47	S2	121	OMU	O2-C2	-2.56	1.18	1.23
47	S2	159	A2M	C8-N9	-2.56	1.33	1.37
81	L5	4494	OMG	O6-C6	-2.56	1.18	1.23
81	L5	3867	A2M	C8-N9	-2.55	1.33	1.37
81	L5	3792	OMG	C2-N1	2.55	1.43	1.37
81	L5	2876	OMG	C4-N9	-2.55	1.31	1.38
81	L5	4370	OMG	O6-C6	-2.55	1.18	1.23
47	S2	576	A2M	C8-N9	-2.54	1.33	1.37
81	L5	400	A2M	C8-N9	-2.54	1.33	1.37
81	L5	2837	OMU	O2-C2	-2.54	1.18	1.23
81	L5	4571	A2M	C8-N9	-2.53	1.33	1.37
47	S2	1328	OMG	C2-N1	2.52	1.43	1.37
47	S2	1851	MA6	C5-N7	-2.51	1.34	1.39
81	L5	1625	OMG	O6-C6	-2.51	1.18	1.23
81	L5	3925	OMU	O2-C2	-2.51	1.18	1.23
81	L5	3724	A2M	C8-N9	-2.51	1.33	1.37
81	L5	4392	OMG	C2-N1	2.50	1.43	1.37
81	L5	4220	6MZ	C5-N7	-2.50	1.34	1.39
81	L5	1625	OMG	C2-N1	2.50	1.43	1.37
81	L5	2787	A2M	C8-N9	-2.49	1.33	1.37
81	L5	4494	OMG	C4-N9	-2.49	1.31	1.38
81	L5	1524	A2M	C8-N9	-2.48	1.33	1.37
81	L5	2415	OMU	O2-C2	-2.48	1.18	1.23
81	L5	4227	OMU	C5-C4	2.48	1.49	1.43
81	L5	3785	A2M	C8-N9	-2.48	1.33	1.37
47	S2	116	OMU	O2-C2	-2.48	1.18	1.23
81	L5	4620	OMU	O2-C2	-2.48	1.18	1.23
47	S2	683	OMG	O6-C6	-2.47	1.18	1.23
81	L5	2876	OMG	C2-N1	2.46	1.43	1.37
47	S2	512	A2M	C8-N9	-2.46	1.33	1.37
47	S2	484	A2M	C8-N9	-2.45	1.33	1.37
47	S2	1288	OMU	C5-C4	2.45	1.49	1.43
81	L5	4306	OMU	O2-C2	-2.45	1.18	1.23
47	S2	354	OMU	O2-C2	-2.44	1.18	1.23
47	S2	601	OMG	C4-N9	-2.43	1.31	1.38
47	S2	1447	OMG	O6-C6	-2.43	1.19	1.23
47	S2	468	A2M	C8-N9	-2.43	1.33	1.37
81	L5	2837	OMU	C5-C4	2.43	1.49	1.43
47	S2	1490	OMG	C2-N1	2.42	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	2815	A2M	C8-N9	-2.42	1.33	1.37
47	S2	1447	OMG	C4-N9	-2.42	1.31	1.38
4	L8	14	OMU	C5-C4	2.42	1.48	1.43
81	L5	4220	6MZ	C8-N9	-2.42	1.33	1.37
47	S2	174	OMC	C5-C4	2.42	1.48	1.42
81	L5	3808	OMC	C5-C4	2.41	1.48	1.42
47	S2	1842	4AC	C4-N4	2.41	1.43	1.39
47	S2	1447	OMG	C5-C6	2.40	1.53	1.44
81	L5	3830	A2M	C8-N9	-2.40	1.33	1.37
81	L5	4227	OMU	O2-C2	-2.39	1.18	1.23
81	L5	4523	A2M	C8-N9	-2.39	1.33	1.37
47	S2	116	OMU	C5-C4	2.39	1.48	1.43
47	S2	172	OMU	O2-C2	-2.39	1.18	1.23
81	L5	398	A2M	C8-N9	-2.38	1.33	1.37
47	S2	1870	B8N	O4'-C1'	-2.38	1.40	1.43
47	S2	509	OMG	C4-N9	-2.38	1.32	1.38
81	L5	2861	OMC	C5-C4	2.38	1.48	1.42
81	L5	2415	OMU	C5-C4	2.38	1.48	1.43
47	S2	1288	OMU	O2-C2	-2.38	1.18	1.23
81	L5	4590	A2M	C8-N9	-2.37	1.33	1.37
47	S2	683	OMG	C5-C6	2.37	1.53	1.44
81	L5	4228	OMG	C5-C6	2.37	1.53	1.44
4	L8	75	OMG	C4-N9	-2.37	1.32	1.38
47	S2	166	A2M	C8-N9	-2.37	1.33	1.37
47	S2	121	OMU	C5-C4	2.37	1.48	1.43
81	L5	1625	OMG	C5-C6	2.36	1.53	1.44
81	L5	4637	OMG	C4-N9	-2.36	1.32	1.38
47	S2	354	OMU	C5-C4	2.36	1.48	1.43
81	L5	4530	UR3	O2-C2	-2.36	1.18	1.22
47	S2	517	OMC	C5-C4	2.36	1.48	1.42
47	S2	1851	MA6	C4-N9	-2.35	1.32	1.37
47	S2	590	A2M	C8-N9	-2.35	1.33	1.37
47	S2	509	OMG	C5-C6	2.35	1.53	1.44
81	L5	4370	OMG	C5-C6	2.34	1.53	1.44
81	L5	4499	OMG	C4-N9	-2.34	1.32	1.38
81	L5	4498	OMU	C5-C4	2.34	1.48	1.43
47	S2	428	OMU	O2-C2	-2.33	1.18	1.23
81	L5	4530	UR3	O4-C4	-2.33	1.18	1.23
81	L5	4499	OMG	C5-C6	2.33	1.53	1.44
47	S2	27	A2M	C8-N9	-2.33	1.33	1.37
81	L5	4618	OMG	C5-C6	2.32	1.53	1.44
81	L5	3887	OMC	C5-C4	2.32	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S2	644	OMG	C4-N9	-2.32	1.32	1.38
47	S2	1442	OMU	C5-C4	2.32	1.48	1.43
81	L5	4306	OMU	C5-C4	2.32	1.48	1.43
81	L5	3925	OMU	C5-C4	2.32	1.48	1.43
47	S2	644	OMG	C5-C6	2.30	1.53	1.44
47	S2	1870	B8N	O4-C4	-2.29	1.18	1.23
81	L5	2365	OMC	C5-C4	2.29	1.48	1.42
81	L5	4637	OMG	C5-C6	2.29	1.53	1.44
47	S2	601	OMG	C5-C6	2.28	1.52	1.44
81	L5	4620	OMU	C5-C4	2.28	1.48	1.43
47	S2	1842	4AC	O7-C7	-2.28	1.18	1.23
4	L8	75	OMG	C5-C6	2.28	1.52	1.44
81	L5	4623	OMG	C5-C6	2.27	1.52	1.44
81	L5	4456	OMC	C5-C4	2.27	1.48	1.42
81	L5	2824	OMC	C5-C4	2.27	1.48	1.42
81	L5	4494	OMG	C5-C6	2.27	1.52	1.44
81	L5	4536	OMC	C5-C4	2.27	1.48	1.42
81	L5	1625	OMG	C4-N9	-2.27	1.32	1.38
81	L5	3792	OMG	C5-C6	2.26	1.52	1.44
81	L5	2364	OMG	C5-C6	2.26	1.52	1.44
47	S2	172	OMU	C5-C4	2.26	1.48	1.43
47	S2	1391	OMC	C5-C4	2.24	1.48	1.42
47	S2	436	OMG	C5-C6	2.24	1.52	1.44
47	S2	1870	B8N	O2-C2	-2.22	1.18	1.22
47	S2	1703	OMC	C5-C4	2.22	1.48	1.42
81	L5	2422	OMC	C5-C4	2.22	1.48	1.42
81	L5	3869	OMC	C5-C4	2.22	1.48	1.42
81	L5	4392	OMG	C5-C6	2.21	1.52	1.44
47	S2	428	OMU	C5-C4	2.21	1.48	1.43
81	L5	2876	OMG	C5-C6	2.21	1.52	1.44
81	L5	3627	OMG	C5-C6	2.19	1.52	1.44
81	L5	1522	OMG	C5-C6	2.19	1.52	1.44
81	L5	1316	OMG	C5-C6	2.19	1.52	1.44
81	L5	3841	OMC	C5-C4	2.17	1.48	1.42
81	L5	4228	OMG	C6-N1	2.17	1.42	1.38
81	L5	4220	6MZ	C4-N9	-2.17	1.33	1.37
81	L5	2424	OMG	C5-C6	2.17	1.52	1.44
47	S2	1850	MA6	C4-N9	-2.17	1.33	1.37
47	S2	683	OMG	C6-N1	2.16	1.42	1.38
81	L5	3818	UY1	O4'-C1'	-2.14	1.40	1.43
81	L5	1881	OMC	C5-C4	2.13	1.47	1.42
47	S2	1328	OMG	C5-C6	2.12	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	L5	2804	OMC	C5-C4	2.12	1.47	1.42
47	S2	1447	OMG	C6-N1	2.09	1.42	1.38
81	L5	2424	OMG	C4-N9	-2.08	1.32	1.38
81	L5	1340	OMC	C5-C4	2.07	1.47	1.42
47	S2	1850	MA6	C8-N9	-2.06	1.34	1.37
81	L5	4442	PSU	O4'-C1'	-2.06	1.41	1.43
81	L5	4618	OMG	C6-N1	2.06	1.42	1.38
47	S2	601	OMG	C6-N1	2.06	1.42	1.38
47	S2	1490	OMG	C5-C6	2.05	1.52	1.44
81	L5	4370	OMG	C6-N1	2.05	1.42	1.38
81	L5	2351	OMC	C5-C4	2.04	1.47	1.42
47	S2	436	OMG	C6-N1	2.04	1.42	1.38
81	L5	2364	OMG	C6-N1	2.02	1.42	1.38
81	L5	4494	OMG	C6-N1	2.01	1.42	1.38

All (1004) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1851	MA6	N1-C6-N6	-10.68	103.84	116.86
47	S2	1850	MA6	N1-C6-N6	-9.85	104.86	116.86
81	L5	2876	OMG	C1'-N9-C8	-8.29	103.17	126.73
81	L5	2424	OMG	C1'-N9-C8	-8.23	103.35	126.73
81	L5	3792	OMG	C1'-N9-C8	-7.83	104.47	126.73
81	L5	4637	OMG	C1'-N9-C8	-7.83	104.50	126.73
81	L5	1625	OMG	C1'-N9-C8	-7.80	104.58	126.73
47	S2	601	OMG	C1'-N9-C8	-7.77	104.65	126.73
81	L5	4499	OMG	C1'-N9-C8	-7.67	104.95	126.73
4	L8	75	OMG	C1'-N9-C8	-7.62	105.09	126.73
81	L5	2424	OMG	C1'-N9-C4	7.50	148.65	126.49
47	S2	644	OMG	C1'-N9-C8	-7.47	105.51	126.73
47	S2	1328	OMG	C1'-N9-C8	-7.40	105.72	126.73
81	L5	4494	OMG	C1'-N9-C8	-7.28	106.06	126.73
81	L5	1522	OMG	C1'-N9-C8	-7.23	106.19	126.73
47	S2	1447	OMG	C1'-N9-C8	-7.18	106.33	126.73
81	L5	2876	OMG	C1'-N9-C4	7.18	147.69	126.49
47	S2	683	OMG	C1'-N9-C8	-7.16	106.38	126.73
81	L5	1625	OMG	C1'-N9-C4	7.12	147.52	126.49
81	L5	4392	OMG	C1'-N9-C8	-7.10	106.56	126.73
47	S2	509	OMG	C1'-N9-C8	-7.08	106.62	126.73
81	L5	4370	OMG	C1'-N9-C8	-7.03	106.77	126.73
81	L5	1316	OMG	C1'-N9-C8	-6.91	107.09	126.73
81	L5	2364	OMG	C1'-N9-C8	-6.89	107.16	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4623	OMG	C1'-N9-C8	-6.87	107.21	126.73
47	S2	1851	MA6	C5-C6-N6	6.86	136.19	125.33
47	S2	436	OMG	C1'-N9-C8	-6.86	107.25	126.73
81	L5	4637	OMG	C1'-N9-C4	6.79	146.53	126.49
47	S2	601	OMG	C1'-N9-C4	6.77	146.50	126.49
81	L5	4499	OMG	C1'-N9-C4	6.72	146.34	126.49
81	L5	3792	OMG	C1'-N9-C4	6.69	146.25	126.49
81	L5	4618	OMG	C1'-N9-C8	-6.61	107.96	126.73
47	S2	1490	OMG	C1'-N9-C8	-6.59	108.00	126.73
4	L8	75	OMG	C1'-N9-C4	6.58	145.92	126.49
81	L5	4228	OMG	C1'-N9-C8	-6.52	108.20	126.73
47	S2	644	OMG	C1'-N9-C4	6.41	145.42	126.49
81	L5	4494	OMG	C1'-N9-C4	6.39	145.35	126.49
47	S2	1328	OMG	C1'-N9-C4	6.30	145.09	126.49
81	L5	3627	OMG	C1'-N9-C8	-6.29	108.87	126.73
47	S2	1850	MA6	C5-C6-N6	6.23	135.19	125.33
47	S2	1447	OMG	C1'-N9-C4	6.20	144.80	126.49
47	S2	509	OMG	C1'-N9-C4	6.18	144.74	126.49
81	L5	4220	6MZ	N1-C2-N3	-6.12	119.31	128.58
81	L5	4392	OMG	C1'-N9-C4	6.12	144.56	126.49
47	S2	683	OMG	C1'-N9-C4	6.11	144.54	126.49
81	L5	1522	OMG	C1'-N9-C4	6.04	144.34	126.49
81	L5	4370	OMG	C1'-N9-C4	6.04	144.32	126.49
47	S2	27	A2M	N3-C2-N1	-5.96	119.56	128.58
81	L5	1316	OMG	C1'-N9-C4	5.82	143.68	126.49
81	L5	4623	OMG	C1'-N9-C4	5.80	143.63	126.49
47	S2	1851	MA6	N1-C2-N3	-5.80	119.80	128.58
4	L8	14	OMU	C4-N3-C2	-5.79	119.42	126.61
81	L5	2364	OMG	C1'-N9-C4	5.79	143.59	126.49
47	S2	1871	6MZ	N1-C2-N3	-5.76	119.86	128.58
81	L5	3785	A2M	N3-C2-N1	-5.72	119.92	128.58
47	S2	436	OMG	C1'-N9-C4	5.70	143.31	126.49
81	L5	1871	A2M	N3-C2-N1	-5.67	120.00	128.58
47	S2	590	A2M	N3-C2-N1	-5.64	120.04	128.58
47	S2	1850	MA6	N1-C2-N3	-5.62	120.08	128.58
81	L5	3925	OMU	C4-N3-C2	-5.60	119.66	126.61
81	L5	2787	A2M	N3-C2-N1	-5.59	120.12	128.58
47	S2	1870	B8N	C1'-C5-C4	5.59	126.09	117.61
81	L5	4590	A2M	N3-C2-N1	-5.59	120.13	128.58
81	L5	1524	A2M	N3-C2-N1	-5.57	120.15	128.58
47	S2	1842	4AC	CM7-C7-N4	5.55	124.23	115.27
81	L5	1326	A2M	N3-C2-N1	-5.52	120.22	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4618	OMG	C1'-N9-C4	5.50	142.75	126.49
47	S2	172	OMU	C4-N3-C2	-5.50	119.78	126.61
47	S2	428	OMU	C4-N3-C2	-5.48	119.80	126.61
47	S2	590	A2M	C5-C4-N3	-5.48	119.17	126.72
47	S2	1031	A2M	N3-C2-N1	-5.46	120.31	128.58
81	L5	4228	OMG	C1'-N9-C4	5.46	142.61	126.49
81	L5	4227	OMU	C4-N3-C2	-5.45	119.84	126.61
47	S2	512	A2M	N3-C2-N1	-5.45	120.33	128.58
81	L5	4498	OMU	C4-N3-C2	-5.45	119.84	126.61
81	L5	2415	OMU	C4-N3-C2	-5.45	119.85	126.61
47	S2	1490	OMG	C1'-N9-C4	5.45	142.58	126.49
47	S2	166	A2M	N3-C2-N1	-5.42	120.38	128.58
47	S2	354	OMU	C4-N3-C2	-5.41	119.90	126.61
81	L5	398	A2M	N3-C2-N1	-5.40	120.41	128.58
81	L5	2837	OMU	C4-N3-C2	-5.39	119.92	126.61
47	S2	468	A2M	N3-C2-N1	-5.38	120.44	128.58
81	L5	4306	OMU	C4-N3-C2	-5.37	119.94	126.61
47	S2	590	A2M	N6-C6-N1	-5.37	106.42	118.38
81	L5	400	A2M	N3-C2-N1	-5.36	120.47	128.58
81	L5	2401	A2M	N3-C2-N1	-5.35	120.48	128.58
47	S2	1288	OMU	C4-N3-C2	-5.34	119.98	126.61
47	S2	1383	A2M	N3-C2-N1	-5.32	120.53	128.58
81	L5	3825	A2M	N3-C2-N1	-5.31	120.54	128.58
47	S2	1870	B8N	C5-C4-N3	5.31	125.80	116.15
81	L5	1534	A2M	N6-C6-N1	-5.30	106.58	118.38
81	L5	2363	A2M	N3-C2-N1	-5.28	120.59	128.58
81	L5	4590	A2M	N6-C6-N1	-5.25	106.68	118.38
47	S2	116	OMU	C4-N3-C2	-5.25	120.09	126.61
47	S2	1442	OMU	C4-N3-C2	-5.23	120.12	126.61
47	S2	121	OMU	C4-N3-C2	-5.23	120.12	126.61
47	S2	484	A2M	N3-C2-N1	-5.23	120.67	128.58
81	L5	2363	A2M	N6-C6-N1	-5.23	106.73	118.38
81	L5	1534	A2M	N3-C2-N1	-5.22	120.67	128.58
81	L5	4571	A2M	N3-C2-N1	-5.22	120.69	128.58
81	L5	3830	A2M	N3-C2-N1	-5.21	120.69	128.58
81	L5	2839	PSU	C4-N3-C2	-5.20	119.21	126.37
81	L5	4523	A2M	N3-C2-N1	-5.20	120.72	128.58
81	L5	2815	A2M	N3-C2-N1	-5.19	120.72	128.58
81	L5	1534	A2M	C5-C4-N3	-5.19	119.57	126.72
81	L5	3724	A2M	N3-C2-N1	-5.18	120.74	128.58
81	L5	3718	A2M	C5-C4-N3	-5.16	119.61	126.72
47	S2	576	A2M	N3-C2-N1	-5.16	120.77	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4620	OMU	C4-N3-C2	-5.15	120.22	126.61
47	S2	27	A2M	N6-C6-N1	-5.15	106.91	118.38
47	S2	1678	A2M	N3-C2-N1	-5.15	120.79	128.58
47	S2	159	A2M	N6-C6-N1	-5.13	106.95	118.38
81	L5	3825	A2M	N6-C6-N1	-5.12	106.97	118.38
47	S2	484	A2M	N6-C6-N1	-5.12	106.97	118.38
81	L5	2815	A2M	N6-C6-N1	-5.11	107.00	118.38
81	L5	3830	A2M	N6-C6-N1	-5.10	107.02	118.38
81	L5	2424	OMG	C5-C4-N3	-5.10	120.27	128.39
81	L5	3785	A2M	N6-C6-N1	-5.10	107.02	118.38
81	L5	2815	A2M	C5-C4-N3	-5.09	119.71	126.72
81	L5	1524	A2M	N6-C6-N1	-5.09	107.05	118.38
47	S2	99	A2M	N3-C2-N1	-5.08	120.89	128.58
81	L5	3627	OMG	C1'-N9-C4	5.08	141.49	126.49
81	L5	2787	A2M	C5-C4-N3	-5.08	119.72	126.72
47	S2	1445	PSU	C4-N3-C2	-5.06	119.40	126.37
81	L5	1326	A2M	C5-C4-N3	-5.06	119.76	126.72
47	S2	159	A2M	C5-C4-N3	-5.04	119.77	126.72
47	S2	468	A2M	N6-C6-N1	-5.04	107.15	118.38
47	S2	166	A2M	N6-C6-N1	-5.04	107.15	118.38
4	L8	69	PSU	N1-C2-N3	5.03	120.48	115.17
47	S2	1238	PSU	C4-N3-C2	-5.03	119.44	126.37
47	S2	1031	A2M	N6-C6-N1	-5.03	107.18	118.38
47	S2	1678	A2M	N6-C6-N1	-5.02	107.20	118.38
81	L5	3867	A2M	N6-C6-N1	-5.00	107.24	118.38
81	L5	1326	A2M	N6-C6-N1	-5.00	107.25	118.38
81	L5	4571	A2M	N6-C6-N1	-4.97	107.30	118.38
47	S2	99	A2M	C5-C4-N3	-4.97	119.87	126.72
81	L5	3718	A2M	N6-C6-N1	-4.97	107.31	118.38
81	L5	3724	A2M	N6-C6-N1	-4.96	107.33	118.38
81	L5	4523	A2M	C5-C4-N3	-4.95	119.89	126.72
47	S2	1383	A2M	N6-C6-N1	-4.95	107.35	118.38
47	S2	484	A2M	C5-C4-N3	-4.95	119.90	126.72
81	L5	3867	A2M	C5-C4-N3	-4.95	119.91	126.72
47	S2	512	A2M	N6-C6-N1	-4.94	107.38	118.38
81	L5	398	A2M	N6-C6-N1	-4.94	107.38	118.38
81	L5	2401	A2M	N6-C6-N1	-4.94	107.38	118.38
47	S2	99	A2M	N6-C6-N1	-4.93	107.39	118.38
81	L5	3695	PSU	C4-N3-C2	-4.93	119.58	126.37
81	L5	4403	PSU	C4-N3-C2	-4.93	119.58	126.37
81	L5	2363	A2M	C5-C4-N3	-4.92	119.94	126.72
81	L5	3867	A2M	N3-C2-N1	-4.92	121.13	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	3825	A2M	C5-C4-N3	-4.92	119.94	126.72
47	S2	1177	PSU	C4-N3-C2	-4.92	119.60	126.37
81	L5	398	A2M	C5-C4-N3	-4.92	119.95	126.72
81	L5	4523	A2M	N6-C6-N1	-4.91	107.44	118.38
81	L5	400	A2M	N6-C6-N1	-4.91	107.44	118.38
81	L5	4457	PSU	C4-N3-C2	-4.90	119.62	126.37
81	L5	1871	A2M	N6-C6-N1	-4.90	107.47	118.38
4	L8	69	PSU	C4-N3-C2	-4.90	119.63	126.37
47	S2	576	A2M	N6-C6-N1	-4.89	107.48	118.38
81	L5	3724	A2M	C5-C4-N3	-4.88	120.00	126.72
81	L5	3758	PSU	C4-N3-C2	-4.88	119.66	126.37
47	S2	1678	A2M	C5-C4-N3	-4.87	120.01	126.72
81	L5	4442	PSU	C4-N3-C2	-4.86	119.67	126.37
81	L5	4442	PSU	N1-C2-N3	4.86	120.29	115.17
81	L5	3770	PSU	C4-N3-C2	-4.85	119.69	126.37
81	L5	3785	A2M	C5-C4-N3	-4.85	120.03	126.72
81	L5	2401	A2M	C5-C4-N3	-4.84	120.05	126.72
81	L5	3718	A2M	N3-C2-N1	-4.83	121.27	128.58
81	L5	1625	OMG	C5-C4-N3	-4.83	120.70	128.39
81	L5	4972	PSU	C4-N3-C2	-4.82	119.73	126.37
81	L5	4403	PSU	N1-C2-N3	4.82	120.25	115.17
47	S2	1383	A2M	C5-C4-N3	-4.82	120.08	126.72
47	S2	1031	A2M	C5-C4-N3	-4.81	120.10	126.72
81	L5	1782	PSU	C4-N3-C2	-4.81	119.75	126.37
81	L5	1862	PSU	C4-N3-C2	-4.81	119.75	126.37
81	L5	3695	PSU	N1-C2-N3	4.81	120.24	115.17
47	S2	1871	6MZ	C5-C4-N3	-4.80	120.11	126.72
47	S2	1056	PSU	C4-N3-C2	-4.79	119.77	126.37
81	L5	4471	PSU	N1-C2-N3	4.78	120.21	115.17
81	L5	4571	A2M	C5-C4-N3	-4.77	120.15	126.72
47	S2	109	PSU	C4-N3-C2	-4.76	119.81	126.37
47	S2	159	A2M	N3-C2-N1	-4.76	121.38	128.58
81	L5	400	A2M	C5-C4-N3	-4.75	120.17	126.72
81	L5	2787	A2M	N6-C6-N1	-4.75	107.80	118.38
81	L5	3830	A2M	C5-C4-N3	-4.75	120.18	126.72
81	L5	4423	PSU	C4-N3-C2	-4.74	119.84	126.37
47	S2	1445	PSU	N1-C2-N3	4.73	120.16	115.17
81	L5	1524	A2M	C5-C4-N3	-4.73	120.20	126.72
81	L5	3770	PSU	N1-C2-N3	4.71	120.14	115.17
47	S2	1692	PSU	C4-N3-C2	-4.71	119.89	126.37
47	S2	1177	PSU	N1-C2-N3	4.70	120.13	115.17
81	L5	4471	PSU	C4-N3-C2	-4.70	119.89	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	5001	PSU	C4-N3-C2	-4.69	119.91	126.37
81	L5	1862	PSU	N1-C2-N3	4.69	120.12	115.17
47	S2	27	A2M	O4'-C1'-N9	4.69	117.10	108.09
47	S2	34	PSU	C4-N3-C2	-4.69	119.91	126.37
81	L5	3851	PSU	C4-N3-C2	-4.68	119.92	126.37
81	L5	3851	PSU	N1-C2-N3	4.68	120.11	115.17
81	L5	1871	A2M	C5-C4-N3	-4.68	120.27	126.72
47	S2	686	PSU	C4-N3-C2	-4.68	119.93	126.37
81	L5	4353	PSU	C4-N3-C2	-4.68	119.93	126.37
47	S2	166	A2M	C5-C4-N3	-4.68	120.28	126.72
81	L5	4423	PSU	N1-C2-N3	4.67	120.09	115.17
81	L5	4569	PSU	C4-N3-C2	-4.67	119.94	126.37
47	S2	406	PSU	C4-N3-C2	-4.66	119.95	126.37
47	S2	36	PSU	C4-N3-C2	-4.66	119.95	126.37
47	S2	93	PSU	C4-N3-C2	-4.66	119.95	126.37
47	S2	1232	PSU	C4-N3-C2	-4.66	119.95	126.37
47	S2	651	PSU	C4-N3-C2	-4.66	119.95	126.37
81	L5	4361	PSU	C4-N3-C2	-4.65	119.96	126.37
47	S2	649	PSU	C4-N3-C2	-4.65	119.96	126.37
47	S2	576	A2M	C5-C4-N3	-4.65	120.32	126.72
47	S2	512	A2M	C5-C4-N3	-4.64	120.33	126.72
47	S2	1692	PSU	N1-C2-N3	4.64	120.06	115.17
81	L5	3920	PSU	C4-N3-C2	-4.64	119.98	126.37
47	S2	27	A2M	C5-C4-N3	-4.63	120.33	126.72
47	S2	1244	PSU	C4-N3-C2	-4.63	119.99	126.37
47	S2	1238	PSU	N1-C2-N3	4.62	120.05	115.17
81	L5	1779	PSU	C4-N3-C2	-4.62	120.00	126.37
81	L5	4431	PSU	C4-N3-C2	-4.60	120.03	126.37
81	L5	4530	UR3	C4-N3-C2	-4.60	120.88	124.58
81	L5	4576	PSU	C4-N3-C2	-4.60	120.03	126.37
81	L5	5010	PSU	C4-N3-C2	-4.60	120.04	126.37
81	L5	1683	PSU	C4-N3-C2	-4.60	120.04	126.37
47	S2	34	PSU	N1-C2-N3	4.59	120.01	115.17
47	S2	1643	PSU	C4-N3-C2	-4.59	120.04	126.37
81	L5	4312	PSU	C4-N3-C2	-4.59	120.04	126.37
47	S2	109	PSU	N1-C2-N3	4.59	120.01	115.17
81	L5	3639	PSU	C4-N3-C2	-4.59	120.05	126.37
81	L5	4299	PSU	N1-C2-N3	4.58	120.00	115.17
81	L5	3639	PSU	N1-C2-N3	4.57	119.99	115.17
81	L5	4353	PSU	N1-C2-N3	4.57	119.99	115.17
81	L5	4590	A2M	C5-C4-N3	-4.57	120.42	126.72
81	L5	4499	OMG	C5-C4-N3	-4.57	121.12	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4689	PSU	C4-N3-C2	-4.57	120.08	126.37
47	S2	681	PSU	C4-N3-C2	-4.56	120.09	126.37
81	L5	4312	PSU	N1-C2-N3	4.56	119.97	115.17
81	L5	4457	PSU	N1-C2-N3	4.54	119.96	115.17
81	L5	4972	PSU	N1-C2-N3	4.54	119.96	115.17
81	L5	4299	PSU	C4-N3-C2	-4.54	120.12	126.37
81	L5	4579	PSU	C4-N3-C2	-4.54	120.12	126.37
81	L5	3818	UY1	C4-N3-C2	-4.53	120.13	126.37
47	S2	406	PSU	N1-C2-N3	4.53	119.95	115.17
81	L5	4628	PSU	C4-N3-C2	-4.53	120.13	126.37
81	L5	4532	PSU	C4-N3-C2	-4.52	120.15	126.37
81	L5	4361	PSU	N1-C2-N3	4.51	119.93	115.17
81	L5	4628	PSU	N1-C2-N3	4.51	119.93	115.17
47	S2	649	PSU	N1-C2-N3	4.51	119.92	115.17
47	S2	651	PSU	N1-C2-N3	4.51	119.92	115.17
81	L5	4552	PSU	C4-N3-C2	-4.50	120.17	126.37
81	L5	4689	PSU	N1-C2-N3	4.50	119.91	115.17
47	S2	1870	B8N	C4-N3-C2	-4.50	120.08	125.62
81	L5	2632	PSU	N1-C2-N3	4.49	119.90	115.17
81	L5	3758	PSU	N1-C2-N3	4.48	119.90	115.17
47	S2	36	PSU	N1-C2-N3	4.48	119.89	115.17
47	S2	468	A2M	C5-C4-N3	-4.48	120.55	126.72
81	L5	1782	PSU	N1-C2-N3	4.48	119.89	115.17
81	L5	4552	PSU	N1-C2-N3	4.47	119.89	115.17
47	S2	1447	OMG	C5-C4-N3	-4.47	121.27	128.39
81	L5	2632	PSU	C4-N3-C2	-4.47	120.22	126.37
81	L5	3637	PSU	C4-N3-C2	-4.46	120.23	126.37
47	S2	1056	PSU	N1-C2-N3	4.45	119.87	115.17
81	L5	5001	PSU	N1-C2-N3	4.45	119.87	115.17
47	S2	1244	PSU	N1-C2-N3	4.45	119.86	115.17
81	L5	3920	PSU	N1-C2-N3	4.45	119.86	115.17
81	L5	4569	PSU	N1-C2-N3	4.45	119.86	115.17
81	L5	4576	PSU	N1-C2-N3	4.45	119.86	115.17
81	L5	4579	PSU	N1-C2-N3	4.45	119.86	115.17
81	L5	1781	PSU	C4-N3-C2	-4.44	120.26	126.37
81	L5	4431	PSU	N1-C2-N3	4.42	119.83	115.17
47	S2	1337	4AC	C6-C5-C4	4.42	122.32	117.00
47	S2	644	OMG	C5-C4-N3	-4.42	121.36	128.39
47	S2	1850	MA6	C5-C4-N3	-4.41	120.64	126.72
47	S2	681	PSU	N1-C2-N3	4.40	119.81	115.17
47	S2	686	PSU	N1-C2-N3	4.40	119.81	115.17
47	S2	509	OMG	C5-C4-N3	-4.39	121.40	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	5010	PSU	N1-C2-N3	4.39	119.80	115.17
47	S2	27	A2M	C2'-C1'-N9	-4.38	106.54	113.75
47	S2	93	PSU	N1-C2-N3	4.38	119.79	115.17
81	L5	4220	6MZ	N9-C8-N7	-4.38	107.72	113.94
81	L5	3884	PSU	C4-N3-C2	-4.38	120.34	126.37
81	L5	4637	OMG	C5-C4-N3	-4.37	121.43	128.39
81	L5	2401	A2M	N9-C8-N7	-4.36	107.74	113.94
81	L5	1781	PSU	N1-C2-N3	4.35	119.76	115.17
47	S2	1232	PSU	N1-C2-N3	4.35	119.75	115.17
47	S2	468	A2M	N9-C8-N7	-4.35	107.77	113.94
47	S2	1678	A2M	N9-C8-N7	-4.34	107.78	113.94
4	L8	75	OMG	C5-C4-N3	-4.34	121.49	128.39
81	L5	1683	PSU	N1-C2-N3	4.33	119.74	115.17
47	S2	1643	PSU	N1-C2-N3	4.33	119.73	115.17
47	S2	1851	MA6	N9-C8-N7	-4.33	107.80	113.94
81	L5	1871	A2M	N9-C8-N7	-4.31	107.82	113.94
81	L5	4530	UR3	C6-N1-C2	-4.30	118.28	121.80
81	L5	1779	PSU	N1-C2-N3	4.30	119.71	115.17
81	L5	3884	PSU	N1-C2-N3	4.30	119.70	115.17
81	L5	4532	PSU	N1-C2-N3	4.27	119.67	115.17
81	L5	3825	A2M	N9-C8-N7	-4.26	107.89	113.94
47	S2	1442	OMU	N3-C2-N1	4.24	120.41	114.89
81	L5	2876	OMG	C5-C4-N3	-4.22	121.68	128.39
81	L5	4530	UR3	C1'-N1-C2	4.19	123.90	117.04
81	L5	3830	A2M	N9-C8-N7	-4.19	107.99	113.94
47	S2	601	OMG	C5-C4-N3	-4.18	121.73	128.39
47	S2	1850	MA6	N9-C8-N7	-4.17	108.02	113.94
81	L5	3841	OMC	O2-C2-N3	-4.16	115.77	122.33
47	S2	1383	A2M	N9-C8-N7	-4.16	108.03	113.94
81	L5	4494	OMG	C5-C4-N3	-4.16	121.78	128.39
47	S2	166	A2M	N9-C8-N7	-4.14	108.07	113.94
47	S2	512	A2M	N9-C8-N7	-4.13	108.08	113.94
47	S2	172	OMU	N3-C2-N1	4.13	120.26	114.89
81	L5	4523	A2M	N9-C8-N7	-4.12	108.09	113.94
47	S2	1031	A2M	N9-C8-N7	-4.11	108.10	113.94
47	S2	576	A2M	N9-C8-N7	-4.11	108.10	113.94
81	L5	3637	PSU	N1-C2-N3	4.10	119.49	115.17
47	S2	683	OMG	C5-C4-N3	-4.09	121.87	128.39
81	L5	3792	OMG	C5-C4-N3	-4.09	121.88	128.39
81	L5	2839	PSU	N1-C2-N3	4.08	119.47	115.17
81	L5	4370	OMG	C5-C4-N3	-4.08	121.89	128.39
47	S2	1851	MA6	C5-C4-N3	-4.08	121.09	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	2837	OMU	N3-C2-N1	4.06	120.18	114.89
81	L5	1534	A2M	C5-C6-N6	4.06	133.35	123.29
81	L5	400	A2M	N9-C8-N7	-4.06	108.17	113.94
47	S2	159	A2M	C5-C6-N6	4.06	133.34	123.29
81	L5	4590	A2M	C5-C6-N6	4.06	133.34	123.29
81	L5	3867	A2M	N9-C8-N7	-4.05	108.19	113.94
81	L5	1524	A2M	N9-C8-N7	-4.04	108.20	113.94
81	L5	2815	A2M	C5-C6-N6	4.04	133.28	123.29
81	L5	4571	A2M	N9-C8-N7	-4.03	108.22	113.94
4	L8	14	OMU	C5-C4-N3	4.03	120.44	114.80
4	L8	69	PSU	C6-N1-C2	-4.01	118.97	122.69
47	S2	99	A2M	N9-C8-N7	-4.00	108.27	113.94
47	S2	590	A2M	C5-C6-N6	3.99	133.18	123.29
81	L5	3724	A2M	N9-C8-N7	-3.99	108.27	113.94
81	L5	4498	OMU	N3-C2-N1	3.99	120.08	114.89
81	L5	4590	A2M	N9-C8-N7	-3.98	108.28	113.94
47	S2	159	A2M	N9-C8-N7	-3.98	108.30	113.94
81	L5	1625	OMG	C2-N3-C4	3.97	119.14	112.30
47	S2	1871	6MZ	N9-C8-N7	-3.97	108.30	113.94
81	L5	1316	OMG	C5-C4-N3	-3.96	122.08	128.39
81	L5	2363	A2M	N9-C8-N7	-3.96	108.32	113.94
81	L5	2363	A2M	C5-C6-N6	3.95	133.07	123.29
47	S2	354	OMU	N3-C2-N1	3.93	120.01	114.89
81	L5	4392	OMG	C5-C4-N3	-3.93	122.13	128.39
47	S2	27	A2M	C5-C6-N6	3.92	132.99	123.29
47	S2	121	OMU	N3-C2-N1	3.92	119.99	114.89
47	S2	116	OMU	N3-C2-N1	3.91	119.98	114.89
81	L5	3830	A2M	C5-C6-N6	3.91	132.96	123.29
47	S2	590	A2M	N9-C8-N7	-3.90	108.40	113.94
81	L5	1522	OMG	C5-C4-N3	-3.90	122.19	128.39
81	L5	2364	OMG	C5-C4-N3	-3.90	122.19	128.39
47	S2	166	A2M	C5-C6-N6	3.86	132.85	123.29
47	S2	576	A2M	C5-C6-N6	3.85	132.83	123.29
47	S2	468	A2M	C5-C6-N6	3.85	132.82	123.29
47	S2	484	A2M	C5-C6-N6	3.85	132.82	123.29
81	L5	1326	A2M	N9-C8-N7	-3.85	108.48	113.94
81	L5	398	A2M	N9-C8-N7	-3.84	108.48	113.94
47	S2	1678	A2M	C5-C6-N6	3.84	132.80	123.29
81	L5	4689	PSU	C6-N1-C2	-3.84	119.12	122.69
47	S2	27	A2M	O2'-C2'-C1'	3.84	116.28	108.99
81	L5	4623	OMG	C5-C4-N3	-3.84	122.28	128.39
81	L5	2632	PSU	C6-N1-C2	-3.83	119.13	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	1534	A2M	N9-C8-N7	-3.83	108.50	113.94
81	L5	2415	OMU	N3-C2-N1	3.83	119.88	114.89
81	L5	3639	PSU	C6-N1-C2	-3.82	119.14	122.69
47	S2	512	A2M	C5-C6-N6	3.82	132.75	123.29
81	L5	3785	A2M	N9-C8-N7	-3.82	108.52	113.94
81	L5	4220	6MZ	C5-C4-N3	-3.82	121.46	126.72
81	L5	4618	OMG	C5-C4-N3	-3.81	122.33	128.39
81	L5	4571	A2M	C5-C6-N6	3.81	132.72	123.29
81	L5	4471	PSU	C6-N1-C2	-3.81	119.16	122.69
81	L5	2424	OMG	C2-N3-C4	3.81	118.86	112.30
81	L5	4306	OMU	N3-C2-N1	3.80	119.84	114.89
47	S2	484	A2M	N9-C8-N7	-3.80	108.54	113.94
81	L5	3925	OMU	N3-C2-N1	3.80	119.84	114.89
47	S2	1383	A2M	C5-C6-N6	3.80	132.69	123.29
81	L5	398	A2M	C5-C6-N6	3.79	132.68	123.29
81	L5	3724	A2M	C5-C6-N6	3.79	132.68	123.29
47	S2	1447	OMG	C2-N3-C4	3.79	118.83	112.30
81	L5	1524	A2M	C5-C6-N6	3.79	132.67	123.29
81	L5	3867	A2M	C5-C6-N6	3.79	132.66	123.29
81	L5	4423	PSU	C6-N1-C2	-3.78	119.18	122.69
81	L5	4499	OMG	C2-N3-C4	3.78	118.81	112.30
4	L8	14	OMU	N3-C2-N1	3.78	119.81	114.89
81	L5	3627	OMG	N9-C8-N7	-3.77	106.40	113.40
81	L5	3825	A2M	C5-C6-N6	3.77	132.63	123.29
81	L5	3925	OMU	C5-C4-N3	3.77	120.08	114.80
81	L5	3718	A2M	C5-C6-N6	3.77	132.62	123.29
81	L5	4579	PSU	C6-N1-C2	-3.77	119.19	122.69
81	L5	4552	PSU	C6-N1-C2	-3.76	119.20	122.69
81	L5	1326	A2M	C5-C6-N6	3.76	132.59	123.29
47	S2	27	A2M	N9-C8-N7	-3.75	108.61	113.94
81	L5	3818	UY1	N1-C2-N3	3.75	119.12	115.17
81	L5	400	A2M	C5-C6-N6	3.75	132.56	123.29
47	S2	428	OMU	C5-C4-N3	3.74	120.05	114.80
47	S2	1031	A2M	C5-C6-N6	3.74	132.56	123.29
47	S2	1328	OMG	C5-C4-N3	-3.74	122.43	128.39
47	S2	644	OMG	C2-N3-C4	3.74	118.75	112.30
81	L5	4523	A2M	C5-C6-N6	3.74	132.54	123.29
81	L5	3851	PSU	C6-N1-C2	-3.73	119.22	122.69
47	S2	509	OMG	C2-N3-C4	3.73	118.72	112.30
81	L5	2787	A2M	N9-C8-N7	-3.72	108.65	113.94
81	L5	4299	PSU	C6-N1-C2	-3.72	119.24	122.69
81	L5	1781	PSU	C6-N1-C2	-3.72	119.24	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	99	A2M	C5-C6-N6	3.71	132.48	123.29
81	L5	2401	A2M	C5-C6-N6	3.71	132.48	123.29
81	L5	3695	PSU	C6-N1-C2	-3.71	119.25	122.69
81	L5	4227	OMU	N3-C2-N1	3.71	119.72	114.89
47	S2	1445	PSU	C6-N1-C2	-3.71	119.25	122.69
47	S2	436	OMG	C5-C4-N3	-3.71	122.49	128.39
81	L5	1871	A2M	C5-C6-N6	3.71	132.46	123.29
81	L5	3884	PSU	C6-N1-C2	-3.71	119.25	122.69
81	L5	4637	OMG	C2-N3-C4	3.71	118.68	112.30
81	L5	4370	OMG	C2-N3-C4	3.70	118.67	112.30
81	L5	2815	A2M	N9-C8-N7	-3.70	108.69	113.94
47	S2	406	PSU	C6-N1-C2	-3.70	119.26	122.69
47	S2	1692	PSU	C6-N1-C2	-3.70	119.26	122.69
81	L5	4628	PSU	C6-N1-C2	-3.68	119.27	122.69
81	L5	4312	PSU	C6-N1-C2	-3.68	119.27	122.69
81	L5	1862	PSU	C6-N1-C2	-3.68	119.28	122.69
47	S2	1871	6MZ	C4-C5-C6	3.68	119.83	116.78
47	S2	590	A2M	C2-N3-C4	3.67	120.79	111.83
47	S2	428	OMU	N3-C2-N1	3.67	119.67	114.89
81	L5	2415	OMU	C5-C4-N3	3.67	119.94	114.80
47	S2	34	PSU	C6-N1-C2	-3.67	119.29	122.69
81	L5	4227	OMU	C5-C4-N3	3.66	119.93	114.80
81	L5	3818	UY1	C6-C5-C4	3.66	120.64	118.17
47	S2	109	PSU	C6-N1-C2	-3.65	119.30	122.69
81	L5	4431	PSU	C6-N1-C2	-3.65	119.30	122.69
81	L5	4618	OMG	N9-C8-N7	-3.65	106.64	113.40
47	S2	436	OMG	N9-C8-N7	-3.64	106.64	113.40
81	L5	2364	OMG	C2-N3-C4	3.64	118.57	112.30
81	L5	4392	OMG	C2-N3-C4	3.64	118.57	112.30
81	L5	1316	OMG	C2-N3-C4	3.64	118.56	112.30
81	L5	4620	OMU	N3-C2-N1	3.64	119.63	114.89
81	L5	4403	PSU	C6-N1-C2	-3.63	119.32	122.69
81	L5	4618	OMG	C2-N3-C4	3.63	118.55	112.30
47	S2	36	PSU	C6-N1-C2	-3.63	119.32	122.69
47	S2	649	PSU	C6-N1-C2	-3.63	119.33	122.69
47	S2	681	PSU	C6-N1-C2	-3.62	119.33	122.69
81	L5	3718	A2M	N9-C8-N7	-3.62	108.80	113.94
47	S2	1288	OMU	N3-C2-N1	3.62	119.61	114.89
81	L5	4442	PSU	C6-N1-C2	-3.62	119.33	122.69
81	L5	4306	OMU	C5-C4-N3	3.62	119.86	114.80
81	L5	3785	A2M	C5-C6-N6	3.62	132.24	123.29
47	S2	651	PSU	C6-N1-C2	-3.61	119.34	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4494	OMG	C2-N3-C4	3.61	118.51	112.30
81	L5	2876	OMG	C2-N3-C4	3.58	118.47	112.30
47	S2	1851	MA6	C2-N1-C6	3.57	120.56	111.83
81	L5	4228	OMG	C2-N3-C4	3.57	118.45	112.30
47	S2	1177	PSU	C6-N1-C2	-3.57	119.38	122.69
81	L5	4576	PSU	C6-N1-C2	-3.57	119.38	122.69
47	S2	1288	OMU	C5-C4-N3	3.56	119.79	114.80
81	L5	4498	OMU	C5-C4-N3	3.56	119.78	114.80
47	S2	601	OMG	C2-N3-C4	3.56	118.42	112.30
81	L5	4620	OMU	C5-C4-N3	3.55	119.78	114.80
47	S2	683	OMG	C2-N3-C4	3.55	118.42	112.30
81	L5	4353	PSU	C6-N1-C2	-3.55	119.40	122.69
47	S2	1842	4AC	C6-C5-C4	3.54	121.27	117.00
81	L5	3770	PSU	C6-N1-C2	-3.53	119.41	122.69
81	L5	3792	OMG	C2-N3-C4	3.53	118.38	112.30
81	L5	4442	PSU	C6-C5-C4	3.52	120.55	118.17
47	S2	1238	PSU	C6-N1-C2	-3.51	119.43	122.69
81	L5	1316	OMG	N9-C8-N7	-3.51	106.89	113.40
47	S2	1850	MA6	C4-C5-C6	3.51	119.54	115.91
81	L5	4361	PSU	C6-N1-C2	-3.51	119.44	122.69
81	L5	1522	OMG	N9-C8-N7	-3.51	106.89	113.40
81	L5	3920	PSU	C6-N1-C2	-3.51	119.44	122.69
4	L8	75	OMG	C2-N3-C4	3.51	118.34	112.30
47	S2	1870	B8N	N3-C2-N1	3.50	120.99	116.72
81	L5	2787	A2M	C5-C6-N6	3.50	131.95	123.29
81	L5	2364	OMG	N9-C8-N7	-3.50	106.91	113.40
81	L5	3785	A2M	C2-N3-C4	3.49	120.36	111.83
47	S2	436	OMG	C2-N3-C4	3.49	118.30	112.30
81	L5	4530	UR3	C5-C4-N3	3.48	119.63	115.04
81	L5	3627	OMG	C2-N3-C4	3.48	118.30	112.30
81	L5	4623	OMG	N9-C8-N7	-3.48	106.94	113.40
47	S2	116	OMU	C5-C4-N3	3.48	119.67	114.80
47	S2	1232	PSU	C6-N1-C2	-3.48	119.46	122.69
47	S2	1643	PSU	C6-N1-C2	-3.47	119.47	122.69
47	S2	1842	4AC	O7-C7-CM7	-3.47	115.87	122.05
81	L5	5010	PSU	C6-N1-C2	-3.47	119.47	122.69
81	L5	1683	PSU	C6-N1-C2	-3.47	119.47	122.69
81	L5	3782	5MC	C5-C6-N1	-3.47	119.55	123.31
81	L5	4623	OMG	C2-N3-C4	3.46	118.25	112.30
81	L5	4457	PSU	C6-N1-C2	-3.45	119.49	122.69
47	S2	354	OMU	C5-C4-N3	3.45	119.63	114.80
47	S2	93	PSU	C6-N1-C2	-3.45	119.49	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	5001	PSU	C6-N1-C2	-3.45	119.49	122.69
47	S2	1244	PSU	C6-N1-C2	-3.45	119.49	122.69
47	S2	121	OMU	C5-C4-N3	3.44	119.62	114.80
81	L5	1782	PSU	C6-N1-C2	-3.44	119.50	122.69
81	L5	1522	OMG	C2-N3-C4	3.44	118.22	112.30
47	S2	1328	OMG	C2-N3-C4	3.44	118.22	112.30
81	L5	4228	OMG	C5-C4-N3	-3.44	122.92	128.39
81	L5	2787	A2M	C2-N3-C4	3.43	120.22	111.83
47	S2	1703	OMC	O2-C2-N3	-3.43	116.92	122.33
47	S2	1850	MA6	C2-N1-C6	3.43	120.21	111.83
47	S2	27	A2M	C2-N3-C4	3.43	120.20	111.83
47	S2	1490	OMG	N9-C8-N7	-3.43	107.05	113.40
47	S2	644	OMG	N9-C8-N7	-3.41	107.08	113.40
47	S2	172	OMU	C5-C4-N3	3.41	119.57	114.80
47	S2	683	OMG	N9-C8-N7	-3.40	107.09	113.40
81	L5	4532	PSU	C6-N1-C2	-3.40	119.53	122.69
47	S2	1871	6MZ	C2-N3-C4	3.40	120.14	111.83
81	L5	4569	PSU	C6-N1-C2	-3.39	119.54	122.69
47	S2	1056	PSU	C6-N1-C2	-3.39	119.55	122.69
81	L5	4228	OMG	N9-C8-N7	-3.39	107.12	113.40
81	L5	3637	PSU	C6-N1-C2	-3.39	119.55	122.69
47	S2	1442	OMU	C1'-N1-C2	3.38	123.67	117.59
47	S2	686	PSU	C6-N1-C2	-3.38	119.55	122.69
81	L5	1524	A2M	C2-N3-C4	3.38	120.08	111.83
81	L5	1326	A2M	C2-N3-C4	3.38	120.08	111.83
47	S2	1328	OMG	N9-C8-N7	-3.37	107.16	113.40
47	S2	1337	4AC	C5-C4-N3	-3.37	117.33	122.60
47	S2	1447	OMG	N9-C8-N7	-3.37	107.16	113.40
81	L5	1779	PSU	C6-N1-C2	-3.36	119.57	122.69
81	L5	3627	OMG	C5-C4-N3	-3.35	123.05	128.39
81	L5	4972	PSU	C6-N1-C2	-3.35	119.58	122.69
81	L5	3785	A2M	C4'-O4'-C1'	-3.34	102.09	109.47
81	L5	1534	A2M	C2-N3-C4	3.34	119.98	111.83
47	S2	590	A2M	N3-C4-N9	3.34	132.84	127.17
81	L5	3758	PSU	C6-N1-C2	-3.32	119.61	122.69
81	L5	4370	OMG	N9-C8-N7	-3.32	107.25	113.40
81	L5	2876	OMG	N9-C8-N7	-3.30	107.28	113.40
81	L5	3792	OMG	N9-C8-N7	-3.30	107.28	113.40
47	S2	1442	OMU	C5-C4-N3	3.30	119.42	114.80
81	L5	3825	A2M	C2-N3-C4	3.29	119.88	111.83
47	S2	1031	A2M	C2-N3-C4	3.29	119.86	111.83
47	S2	1490	OMG	C2-N3-C4	3.29	117.96	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4392	OMG	N9-C8-N7	-3.28	107.33	113.40
47	S2	484	A2M	C2-N3-C4	3.27	119.82	111.83
81	L5	2424	OMG	N9-C4-N3	3.27	132.49	125.95
81	L5	1871	A2M	C2-N3-C4	3.26	119.80	111.83
81	L5	2415	OMU	O4-C4-C5	-3.26	119.55	125.16
81	L5	398	A2M	C2-N3-C4	3.25	119.78	111.83
81	L5	2815	A2M	C2-N3-C4	3.25	119.78	111.83
47	S2	428	OMU	O4-C4-C5	-3.25	119.56	125.16
81	L5	4637	OMG	N9-C8-N7	-3.24	107.39	113.40
81	L5	2837	OMU	C5-C4-N3	3.24	119.34	114.80
81	L5	4220	6MZ	C2-N3-C4	3.24	119.74	111.83
47	S2	509	OMG	N9-C8-N7	-3.22	107.42	113.40
47	S2	1851	MA6	C2-N3-C4	3.22	119.70	111.83
47	S2	601	OMG	N9-C8-N7	-3.22	107.43	113.40
81	L5	2363	A2M	C2-N3-C4	3.22	119.69	111.83
81	L5	2401	A2M	C2-N3-C4	3.21	119.68	111.83
81	L5	4523	A2M	C2-N3-C4	3.19	119.63	111.83
4	L8	75	OMG	N9-C8-N7	-3.19	107.48	113.40
81	L5	400	A2M	C2-N3-C4	3.19	119.63	111.83
81	L5	3724	A2M	C2-N3-C4	3.19	119.63	111.83
4	L8	69	PSU	O2-C2-N1	-3.19	119.50	122.79
47	S2	166	A2M	C2-N3-C4	3.18	119.60	111.83
81	L5	4590	A2M	C2-N3-C4	3.18	119.59	111.83
47	S2	1383	A2M	C2-N3-C4	3.18	119.59	111.83
47	S2	1850	MA6	C2-N3-C4	3.17	119.58	111.83
47	S2	1678	A2M	C2-N3-C4	3.17	119.58	111.83
47	S2	512	A2M	C2-N3-C4	3.17	119.58	111.83
81	L5	3925	OMU	O4-C4-C5	-3.17	119.70	125.16
47	S2	27	A2M	O4'-C1'-C2'	-3.15	101.16	106.59
81	L5	4571	A2M	C2-N3-C4	3.14	119.51	111.83
47	S2	1871	6MZ	C5-N7-C8	3.14	108.39	103.45
81	L5	3639	PSU	O2-C2-N1	-3.14	119.55	122.79
4	L8	14	OMU	O4-C4-C5	-3.14	119.75	125.16
47	S2	99	A2M	C2-N3-C4	3.14	119.49	111.83
81	L5	3830	A2M	C2-N3-C4	3.12	119.46	111.83
81	L5	4499	OMG	N9-C8-N7	-3.12	107.61	113.40
81	L5	3718	A2M	C2-N3-C4	3.12	119.45	111.83
81	L5	3867	A2M	C2-N3-C4	3.12	119.45	111.83
81	L5	4494	OMG	N9-C8-N7	-3.12	107.62	113.40
47	S2	1692	PSU	O2-C2-N1	-3.11	119.58	122.79
47	S2	468	A2M	C2-N3-C4	3.11	119.43	111.83
47	S2	576	A2M	C2-N3-C4	3.09	119.39	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4220	6MZ	C5-N7-C8	3.09	108.31	103.45
47	S2	1678	A2M	C5-N7-C8	3.08	108.30	103.45
81	L5	2401	A2M	N3-C4-N9	3.08	132.41	127.17
81	L5	4220	6MZ	C4-N9-C1'	-3.08	119.44	126.63
81	L5	3770	PSU	O2-C2-N1	-3.07	119.63	122.79
81	L5	1524	A2M	C2'-C1'-N9	-3.06	108.72	113.75
81	L5	1326	A2M	N3-C4-N9	3.05	132.35	127.17
81	L5	1871	A2M	N3-C4-N9	3.03	132.32	127.17
47	S2	159	A2M	C2-N3-C4	3.02	119.22	111.83
47	S2	116	OMU	O4-C4-C5	-3.02	119.95	125.16
81	L5	3825	A2M	C5-N7-C8	3.02	108.20	103.45
81	L5	1534	A2M	N3-C4-N9	3.01	132.29	127.17
47	S2	159	A2M	C5-N7-C8	3.01	108.18	103.45
81	L5	4498	OMU	O4-C4-C5	-3.01	119.97	125.16
81	L5	4552	PSU	O2-C2-N1	-3.00	119.69	122.79
81	L5	3830	A2M	C5-N7-C8	3.00	108.16	103.45
47	S2	99	A2M	N3-C4-N9	2.99	132.26	127.17
81	L5	2401	A2M	C5-N7-C8	2.99	108.15	103.45
81	L5	3867	A2M	N3-C4-N9	2.99	132.25	127.17
81	L5	4403	PSU	C6-C5-C4	2.99	120.19	118.17
47	S2	1031	A2M	N3-C4-N9	2.99	132.24	127.17
81	L5	3718	A2M	N3-C4-N9	2.98	132.24	127.17
81	L5	4312	PSU	O2-C2-N1	-2.98	119.71	122.79
47	S2	1490	OMG	C5-C4-N3	-2.98	123.65	128.39
81	L5	2363	A2M	N3-C4-N9	2.98	132.23	127.17
81	L5	4299	PSU	O2-C2-N1	-2.98	119.72	122.79
47	S2	1383	A2M	N3-C4-N9	2.97	132.23	127.17
81	L5	1862	PSU	O2-C2-N1	-2.97	119.72	122.79
81	L5	4620	OMU	O4-C4-C5	-2.97	120.05	125.16
47	S2	468	A2M	C5-N7-C8	2.96	108.11	103.45
47	S2	34	PSU	O2-C2-N1	-2.96	119.74	122.79
81	L5	2815	A2M	C5-N7-C8	2.96	108.10	103.45
81	L5	3782	5MC	CM5-C5-C6	-2.96	118.85	122.85
47	S2	121	OMU	O4-C4-C5	-2.96	120.06	125.16
81	L5	4423	PSU	O2-C2-N1	-2.95	119.75	122.79
47	S2	354	OMU	O4-C4-C5	-2.94	120.09	125.16
47	S2	590	A2M	C5-N7-C8	2.94	108.07	103.45
81	L5	4227	OMU	O4-C4-C5	-2.94	120.09	125.16
47	S2	1445	PSU	O2-C2-N1	-2.94	119.76	122.79
47	S2	651	PSU	O2-C2-N1	-2.93	119.76	122.79
81	L5	3695	PSU	C6-C5-C4	2.93	120.15	118.17
47	S2	1383	A2M	C5-N7-C8	2.92	108.05	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1031	A2M	C5-N7-C8	2.92	108.05	103.45
47	S2	1678	A2M	N3-C4-N9	2.92	132.13	127.17
81	L5	4523	A2M	N3-C4-N9	2.92	132.13	127.17
81	L5	4523	A2M	C5-N7-C8	2.92	108.04	103.45
81	L5	4220	6MZ	C4-C5-N7	-2.92	107.25	110.58
81	L5	3825	A2M	N3-C4-N9	2.91	132.12	127.17
81	L5	3695	PSU	O2-C2-N1	-2.91	119.78	122.79
47	S2	686	PSU	O2-C2-N1	-2.91	119.78	122.79
47	S2	1244	PSU	O2-C2-N1	-2.91	119.79	122.79
47	S2	99	A2M	C5-N7-C8	2.91	108.02	103.45
81	L5	4403	PSU	O2-C2-N1	-2.91	119.79	122.79
47	S2	159	A2M	N3-C4-N9	2.90	132.10	127.17
47	S2	1288	OMU	O4-C4-C5	-2.90	120.16	125.16
81	L5	3851	PSU	O2-C2-N1	-2.90	119.80	122.79
81	L5	1534	A2M	C5-N7-C8	2.90	108.00	103.45
81	L5	1683	PSU	O2-C2-N1	-2.90	119.80	122.79
81	L5	4306	OMU	O4-C4-C5	-2.89	120.17	125.16
47	S2	1870	B8N	O4-C4-N3	-2.89	115.29	119.99
47	S2	406	PSU	O2-C2-N1	-2.89	119.80	122.79
81	L5	2363	A2M	C5-N7-C8	2.89	108.00	103.45
81	L5	3724	A2M	C5-N7-C8	2.89	108.00	103.45
81	L5	4353	PSU	O2-C2-N1	-2.89	119.81	122.79
47	S2	1177	PSU	C6-C5-C4	2.89	120.12	118.17
47	S2	576	A2M	C5-N7-C8	2.89	107.99	103.45
81	L5	2787	A2M	N3-C4-N9	2.89	132.08	127.17
47	S2	109	PSU	O2-C2-N1	-2.88	119.81	122.79
81	L5	3867	A2M	C5-N7-C8	2.88	107.97	103.45
81	L5	4689	PSU	O2-C2-N1	-2.87	119.82	122.79
47	S2	1842	4AC	C5-C4-N4	2.87	127.78	122.94
47	S2	109	PSU	C6-C5-C4	2.87	120.11	118.17
47	S2	1851	MA6	C4-C5-C6	2.86	118.87	115.91
81	L5	4571	A2M	N3-C4-N9	2.86	132.04	127.17
47	S2	1871	6MZ	C4-C5-N7	-2.86	107.31	110.58
81	L5	3770	PSU	C6-C5-C4	2.86	120.10	118.17
47	S2	512	A2M	N3-C4-N9	2.86	132.03	127.17
81	L5	3785	A2M	N3-C4-N9	2.85	132.02	127.17
47	S2	649	PSU	O2-C2-N1	-2.85	119.84	122.79
81	L5	3841	OMC	C1'-N1-C2	2.85	124.74	118.44
81	L5	1871	A2M	C5-N7-C8	2.85	107.93	103.45
81	L5	4431	PSU	O2-C2-N1	-2.85	119.85	122.79
47	S2	512	A2M	C5-N7-C8	2.84	107.92	103.45
81	L5	1326	A2M	C5-N7-C8	2.84	107.91	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	166	A2M	C5-N7-C8	2.84	107.91	103.45
81	L5	4442	PSU	O2-C2-N1	-2.83	119.87	122.79
81	L5	5001	PSU	O2-C2-N1	-2.83	119.87	122.79
81	L5	400	A2M	N3-C4-N9	2.83	131.97	127.17
81	L5	398	A2M	N3-C4-N9	2.82	131.97	127.17
81	L5	2632	PSU	O2-C2-N1	-2.82	119.88	122.79
81	L5	4628	PSU	O2-C2-N1	-2.82	119.88	122.79
81	L5	2815	A2M	N3-C4-N9	2.81	131.95	127.17
47	S2	1337	4AC	N4-C4-N3	2.81	118.44	113.87
81	L5	398	A2M	C5-N7-C8	2.81	107.87	103.45
81	L5	2424	OMG	C2-N1-C6	-2.81	120.01	125.11
81	L5	3724	A2M	N3-C4-N9	2.81	131.95	127.17
81	L5	400	A2M	C5-N7-C8	2.81	107.86	103.45
47	S2	172	OMU	O4-C4-C5	-2.81	120.32	125.16
81	L5	4571	A2M	C5-N7-C8	2.80	107.86	103.45
47	S2	1703	OMC	C1'-N1-C2	2.80	124.63	118.44
81	L5	1871	A2M	C4-N9-C8	2.80	108.68	105.74
81	L5	2837	OMU	O4-C4-C5	-2.80	120.33	125.16
81	L5	1871	A2M	C2'-C1'-N9	-2.80	109.14	113.75
47	S2	166	A2M	N3-C4-N9	2.79	131.92	127.17
81	L5	3920	PSU	O2-C2-N1	-2.78	119.92	122.79
47	S2	1177	PSU	O2-C2-N1	-2.78	119.92	122.79
47	S2	509	OMG	C2-N1-C6	-2.78	120.07	125.11
81	L5	4353	PSU	C6-C5-C4	2.78	120.05	118.17
81	L5	1779	PSU	O2-C2-N1	-2.77	119.93	122.79
47	S2	1851	MA6	C5-N7-C8	2.77	107.81	103.45
47	S2	651	PSU	C6-C5-C4	2.77	120.04	118.17
81	L5	3830	A2M	N3-C4-N9	2.77	131.87	127.17
47	S2	484	A2M	C5-N7-C8	2.76	107.79	103.45
47	S2	1850	MA6	C5-N7-C8	2.76	107.79	103.45
81	L5	3639	PSU	C6-C5-C4	2.76	120.04	118.17
47	S2	1692	PSU	C6-C5-C4	2.76	120.04	118.17
81	L5	4532	PSU	O2-C2-N1	-2.76	119.94	122.79
81	L5	1625	OMG	C2-N1-C6	-2.76	120.11	125.11
81	L5	4590	A2M	C5-N7-C8	2.75	107.78	103.45
47	S2	1232	PSU	O2-C2-N1	-2.75	119.95	122.79
47	S2	36	PSU	C6-C5-C4	2.75	120.03	118.17
81	L5	3758	PSU	O2-C2-N1	-2.75	119.95	122.79
47	S2	1244	PSU	C6-C5-C4	2.74	120.03	118.17
81	L5	3785	A2M	O4'-C1'-N9	2.74	113.35	108.09
81	L5	4392	OMG	C2-N1-C6	-2.74	120.15	125.11
81	L5	1625	OMG	N9-C4-N3	2.73	131.42	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1447	OMG	C2-N1-C6	-2.73	120.16	125.11
47	S2	1643	PSU	C6-C5-C4	2.73	120.02	118.17
81	L5	1524	A2M	C5-N7-C8	2.73	107.74	103.45
81	L5	5010	PSU	O2-C2-N1	-2.73	119.97	122.79
81	L5	3718	A2M	C5-N7-C8	2.73	107.73	103.45
81	L5	4576	PSU	O2-C2-N1	-2.72	119.98	122.79
81	L5	4530	UR3	O2-C2-N3	-2.72	117.57	121.33
47	S2	484	A2M	N3-C4-N9	2.72	131.79	127.17
47	S2	93	PSU	O2-C2-N1	-2.72	119.99	122.79
81	L5	1625	OMG	N9-C8-N7	-2.71	108.37	113.40
81	L5	2401	A2M	C4-N9-C8	2.71	108.58	105.74
81	L5	2876	OMG	C2-N1-C6	-2.71	120.20	125.11
81	L5	4471	PSU	O2-C2-N1	-2.70	120.00	122.79
47	S2	1442	OMU	O2-C2-N3	-2.70	116.51	121.49
47	S2	1871	6MZ	N3-C4-N9	2.70	131.75	127.17
47	S2	1337	4AC	O7-C7-CM7	-2.69	117.26	122.05
47	S2	1056	PSU	C6-C5-C4	2.69	119.99	118.17
81	L5	4579	PSU	O2-C2-N1	-2.69	120.02	122.79
81	L5	2787	A2M	C5-N7-C8	2.69	107.67	103.45
81	L5	4590	A2M	N3-C4-N9	2.69	131.74	127.17
47	S2	683	OMG	C2-N1-C6	-2.69	120.24	125.11
47	S2	36	PSU	O2-C2-N1	-2.68	120.02	122.79
81	L5	4637	OMG	C2-N1-C6	-2.68	120.25	125.11
81	L5	3758	PSU	C6-C5-C4	2.68	119.98	118.17
4	L8	69	PSU	C6-C5-C4	2.68	119.98	118.17
81	L5	4972	PSU	O2-C2-N1	-2.68	120.03	122.79
81	L5	1862	PSU	C6-C5-C4	2.67	119.98	118.17
47	S2	1337	4AC	C4-N3-C2	2.67	123.64	120.11
47	S2	1842	4AC	C5-C4-N3	-2.67	118.42	122.60
47	S2	27	A2M	C5-N7-C8	2.66	107.64	103.45
47	S2	159	A2M	C4-C5-N7	-2.66	107.54	110.58
81	L5	4361	PSU	O2-C2-N1	-2.66	120.04	122.79
81	L5	1522	OMG	C2-N1-C6	-2.66	120.28	125.11
81	L5	1316	OMG	C2-N1-C6	-2.66	120.29	125.11
81	L5	4499	OMG	N9-C4-N3	2.66	131.27	125.95
47	S2	1850	MA6	N3-C4-N9	2.66	131.69	127.17
81	L5	4499	OMG	C2-N1-C6	-2.66	120.30	125.11
81	L5	1524	A2M	N3-C4-N9	2.65	131.68	127.17
47	S2	644	OMG	C2-N1-C6	-2.65	120.30	125.11
81	L5	4457	PSU	O2-C2-N1	-2.65	120.05	122.79
47	S2	576	A2M	N3-C4-N9	2.65	131.68	127.17
81	L5	1782	PSU	O2-C2-N1	-2.65	120.05	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	3627	OMG	C2'-C1'-N9	-2.65	109.21	114.24
47	S2	601	OMG	C2-N1-C6	-2.65	120.31	125.11
81	L5	4370	OMG	C2-N1-C6	-2.64	120.32	125.11
4	L8	75	OMG	N9-C4-N3	2.63	131.22	125.95
81	L5	4972	PSU	C6-C5-C4	2.63	119.95	118.17
47	S2	1328	OMG	C2-N1-C6	-2.63	120.34	125.11
81	L5	4361	PSU	C6-C5-C4	2.63	119.95	118.17
81	L5	4471	PSU	C6-C5-C4	2.62	119.94	118.17
81	L5	3818	UY1	O2-C2-N1	-2.62	120.09	122.79
81	L5	2815	A2M	C4-C5-N7	-2.62	107.59	110.58
47	S2	1238	PSU	C6-C5-C4	2.61	119.94	118.17
81	L5	4618	OMG	C2-N1-C6	-2.61	120.38	125.11
81	L5	1779	PSU	C6-C5-C4	2.61	119.94	118.17
81	L5	2364	OMG	C2-N1-C6	-2.60	120.39	125.11
47	S2	468	A2M	N3-C4-N9	2.60	131.59	127.17
81	L5	3785	A2M	C5-N7-C8	2.59	107.53	103.45
47	S2	590	A2M	O4'-C1'-N9	2.59	113.07	108.09
81	L5	4569	PSU	O2-C2-N1	-2.59	120.12	122.79
4	L8	75	OMG	C2-N1-C6	-2.59	120.42	125.11
47	S2	34	PSU	C6-C5-C4	2.58	119.91	118.17
47	S2	1643	PSU	O2-C2-N1	-2.58	120.13	122.79
81	L5	3818	UY1	C6-N1-C2	-2.57	120.30	122.69
81	L5	3851	PSU	C6-C5-C4	2.57	119.91	118.17
47	S2	686	PSU	C6-C5-C4	2.57	119.91	118.17
47	S2	681	PSU	O2-C2-N1	-2.57	120.14	122.79
81	L5	4623	OMG	C2-N1-C6	-2.57	120.46	125.11
47	S2	1442	OMU	O4-C4-C5	-2.55	120.76	125.16
47	S2	406	PSU	C6-C5-C4	2.55	119.90	118.17
81	L5	4637	OMG	N9-C4-N3	2.54	131.04	125.95
47	S2	1851	MA6	C4-N9-C8	2.54	108.41	105.74
81	L5	3884	PSU	O2-C2-N1	-2.54	120.17	122.79
47	S2	1238	PSU	O2-C2-N1	-2.53	120.17	122.79
47	S2	27	A2M	N3-C4-N9	2.53	131.48	127.17
81	L5	4576	PSU	C6-C5-C4	2.53	119.88	118.17
81	L5	1534	A2M	C4-C5-N7	-2.53	107.69	110.58
81	L5	2424	OMG	N9-C8-N7	-2.53	108.71	113.40
81	L5	4299	PSU	C6-C5-C4	2.53	119.88	118.17
47	S2	468	A2M	C4-N9-C8	2.52	108.39	105.74
81	L5	3920	PSU	C6-C5-C4	2.52	119.88	118.17
81	L5	3627	OMG	C2-N1-C6	-2.52	120.54	125.11
81	L5	4569	PSU	C6-C5-C4	2.52	119.87	118.17
81	L5	4494	OMG	C2-N1-C6	-2.52	120.55	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	644	OMG	N9-C4-N3	2.52	130.99	125.95
47	S2	1678	A2M	C4-C5-N7	-2.51	107.71	110.58
81	L5	4228	OMG	C2-N1-C6	-2.51	120.56	125.11
47	S2	1678	A2M	C4-N9-C8	2.50	108.36	105.74
47	S2	1056	PSU	O2-C2-N1	-2.50	120.21	122.79
81	L5	1781	PSU	O2-C2-N1	-2.49	120.22	122.79
47	S2	436	OMG	C2-N1-C6	-2.49	120.60	125.11
81	L5	3724	A2M	C4-C5-N7	-2.48	107.74	110.58
81	L5	3627	OMG	N2-C2-N1	2.48	122.00	116.76
47	S2	576	A2M	C4-C5-N7	-2.48	107.75	110.58
47	S2	590	A2M	C4'-O4'-C1'	-2.47	104.02	109.47
81	L5	4628	PSU	C6-C5-C4	2.47	119.84	118.17
81	L5	3782	5MC	O2-C2-N3	-2.46	118.45	122.33
81	L5	3825	A2M	C4-C5-N7	-2.46	107.77	110.58
81	L5	3792	OMG	N9-C4-N3	2.45	130.84	125.95
47	S2	512	A2M	C4-N9-C8	2.44	108.30	105.74
81	L5	2876	OMG	N9-C4-N3	2.44	130.83	125.95
47	S2	1870	B8N	C31-N3-C4	2.44	120.63	117.18
47	S2	1850	MA6	C4-N9-C8	2.43	108.29	105.74
81	L5	4228	OMG	N2-C2-N1	2.43	121.90	116.76
81	L5	4220	6MZ	C4-N9-C8	2.43	108.29	105.74
47	S2	484	A2M	C4-C5-N7	-2.43	107.80	110.58
81	L5	5010	PSU	C6-C5-C4	2.43	119.81	118.17
81	L5	4392	OMG	C5-C6-N1	2.41	119.40	113.25
47	S2	590	A2M	C4-C5-N7	-2.41	107.83	110.58
81	L5	4220	6MZ	C5-C4-N9	2.41	108.44	105.81
81	L5	3830	A2M	C4-C5-N7	-2.41	107.83	110.58
81	L5	3718	A2M	C6-C5-C4	2.40	120.46	117.18
81	L5	4312	PSU	C6-C5-C4	2.40	119.79	118.17
47	S2	649	PSU	C6-C5-C4	2.40	119.79	118.17
47	S2	1383	A2M	C4-N9-C8	2.40	108.25	105.74
81	L5	398	A2M	C4-C5-N7	-2.39	107.85	110.58
81	L5	4579	PSU	C6-C5-C4	2.38	119.78	118.17
47	S2	159	A2M	C6-C5-C4	2.38	120.43	117.18
81	L5	3718	A2M	C4-C5-N7	-2.37	107.87	110.58
81	L5	5001	PSU	C6-C5-C4	2.37	119.78	118.17
47	S2	468	A2M	C4-C5-N7	-2.37	107.87	110.58
47	S2	1447	OMG	N9-C4-N3	2.36	130.68	125.95
81	L5	3637	PSU	O2-C2-N1	-2.36	120.36	122.79
47	S2	99	A2M	C4-C5-N7	-2.35	107.89	110.58
81	L5	3825	A2M	C4-N9-C8	2.35	108.20	105.74
47	S2	1031	A2M	C4-N9-C8	2.34	108.20	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	S2	1232	PSU	C6-C5-C4	2.34	119.75	118.17
81	L5	2424	OMG	O6-C6-C5	-2.34	120.35	126.53
47	S2	166	A2M	C4-N9-C8	2.34	108.19	105.74
47	S2	436	OMG	C2'-C1'-N9	-2.34	109.80	114.24
81	L5	4220	6MZ	C1'-N9-C8	2.33	132.27	127.09
81	L5	1524	A2M	C4-C5-N7	-2.33	107.92	110.58
81	L5	3841	OMC	C6-C5-C4	2.33	121.35	117.53
81	L5	400	A2M	C4-N9-C8	2.33	108.18	105.74
81	L5	2363	A2M	C4-C5-N7	-2.33	107.92	110.58
81	L5	400	A2M	C4-C5-N7	-2.32	107.92	110.58
47	S2	27	A2M	C4-C5-N7	-2.32	107.93	110.58
81	L5	4423	PSU	C6-C5-C4	2.32	119.74	118.17
81	L5	2422	OMC	O2-C2-N3	-2.32	118.67	122.33
81	L5	1326	A2M	C4-C5-N7	-2.32	107.93	110.58
81	L5	1625	OMG	C5-C6-N1	2.31	119.14	113.25
81	L5	2876	OMG	C5-C6-N1	2.31	119.14	113.25
81	L5	2815	A2M	C5-C4-N9	2.31	108.33	105.81
81	L5	1316	OMG	C5-C6-N1	2.31	119.13	113.25
81	L5	3867	A2M	C4-C5-N7	-2.31	107.94	110.58
81	L5	4523	A2M	C4-C5-N7	-2.31	107.94	110.58
47	S2	509	OMG	C5-C6-N1	2.30	119.12	113.25
47	S2	601	OMG	N9-C4-N3	2.30	130.56	125.95
47	S2	576	A2M	C4-N9-C8	2.30	108.15	105.74
47	S2	681	PSU	C6-C5-C4	2.30	119.72	118.17
81	L5	2364	OMG	C5-C6-N1	2.29	119.09	113.25
47	S2	509	OMG	N9-C4-N3	2.29	130.54	125.95
47	S2	484	A2M	C5-C4-N9	2.29	108.31	105.81
47	S2	1328	OMG	C5-C6-N1	2.29	119.08	113.25
81	L5	4618	OMG	C5-C6-N1	2.29	119.07	113.25
47	S2	1383	A2M	C4-C5-N7	-2.29	107.97	110.58
81	L5	4571	A2M	C4-N9-C8	2.28	108.13	105.74
81	L5	4637	OMG	C5-C6-N1	2.27	119.04	113.25
81	L5	2401	A2M	C4-C5-N7	-2.27	107.98	110.58
81	L5	4571	A2M	C4-C5-N7	-2.27	107.98	110.58
81	L5	4456	OMC	O2-C2-N3	-2.27	118.75	122.33
47	S2	1031	A2M	C4-C5-N7	-2.27	107.99	110.58
81	L5	4228	OMG	C5-C6-N1	2.26	119.02	113.25
81	L5	4618	OMG	C8-N7-C5	2.26	108.29	104.26
47	S2	644	OMG	C8-N7-C5	2.26	108.28	104.26
81	L5	4499	OMG	C5-C6-N1	2.26	119.00	113.25
81	L5	2424	OMG	C5-C6-N1	2.26	118.99	113.25
47	S2	644	OMG	C5-C6-N1	2.25	118.99	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4523	A2M	C6-C5-C4	2.25	120.25	117.18
81	L5	1522	OMG	C5-C6-N1	2.25	118.99	113.25
81	L5	3627	OMG	C5-C6-N1	2.25	118.97	113.25
81	L5	4370	OMG	C5-C6-N1	2.25	118.97	113.25
47	S2	1851	MA6	N3-C4-N9	2.24	130.98	127.17
81	L5	4590	A2M	C4-C5-N7	-2.24	108.02	110.58
81	L5	1316	OMG	O6-C6-C5	-2.24	120.63	126.53
47	S2	166	A2M	C4-C5-N7	-2.23	108.03	110.58
81	L5	3808	OMC	O2-C2-N3	-2.23	118.82	122.33
81	L5	1782	PSU	C6-C5-C4	2.23	119.68	118.17
47	S2	1447	OMG	C5-C6-N1	2.22	118.92	113.25
81	L5	1524	A2M	C4'-O4'-C1'	-2.22	104.56	109.47
81	L5	2787	A2M	C4-C5-N7	-2.22	108.04	110.58
81	L5	4623	OMG	N2-C2-N1	2.22	121.45	116.76
81	L5	4442	PSU	O4'-C1'-C2'	2.22	108.22	105.15
81	L5	4590	A2M	C4-N9-C8	2.22	108.07	105.74
81	L5	2815	A2M	C6-C5-C4	2.22	120.21	117.18
81	L5	1871	A2M	C5'-C4'-C3'	-2.21	107.25	115.21
81	L5	3867	A2M	C4-N9-C8	2.21	108.06	105.74
81	L5	4220	6MZ	C4-C5-C6	2.21	118.62	116.78
81	L5	1316	OMG	N2-C2-N1	2.21	121.42	116.76
81	L5	3830	A2M	C4-N9-C8	2.21	108.06	105.74
47	S2	512	A2M	C4-C5-N7	-2.21	108.06	110.58
81	L5	2415	OMU	C1'-N1-C2	2.21	121.55	117.59
47	S2	1447	OMG	C8-N7-C5	2.20	108.19	104.26
47	S2	1851	MA6	C4-C5-N7	-2.20	108.06	110.58
81	L5	1522	OMG	N9-C4-N3	2.20	130.35	125.95
47	S2	1490	OMG	N1-C2-N3	-2.20	119.30	123.32
47	S2	468	A2M	C2'-C1'-N9	-2.19	110.15	113.75
81	L5	2787	A2M	C5-C4-N9	2.19	108.20	105.81
47	S2	99	A2M	C6-C5-C4	2.19	120.17	117.18
47	S2	436	OMG	C8-N7-C5	2.19	108.16	104.26
4	L8	75	OMG	C5-C6-N1	2.18	118.81	113.25
81	L5	3792	OMG	C2-N1-C6	-2.18	121.16	125.11
47	S2	27	A2M	C5-C4-N9	2.18	108.19	105.81
47	S2	1871	6MZ	C9-N6-C6	2.18	124.87	122.85
81	L5	4494	OMG	N9-C4-N3	2.18	130.31	125.95
81	L5	1524	A2M	C4-N9-C8	2.18	108.02	105.74
81	L5	2364	OMG	N2-C2-N1	2.18	121.36	116.76
81	L5	4623	OMG	C5-C6-N1	2.17	118.79	113.25
47	S2	1337	4AC	C5-C6-N1	-2.17	118.31	121.84
47	S2	601	OMG	C5-C6-N1	2.17	118.78	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4403	PSU	O4'-C1'-C2'	2.17	108.15	105.15
81	L5	2876	OMG	O6-C6-C5	-2.17	120.81	126.53
81	L5	1316	OMG	C8-N7-C5	2.17	108.12	104.26
81	L5	4370	OMG	N2-C2-N1	2.16	121.33	116.76
81	L5	4689	PSU	C6-C5-C4	2.16	119.63	118.17
81	L5	4494	OMG	C5-C6-N1	2.16	118.75	113.25
47	S2	436	OMG	C5-C6-N1	2.16	118.74	113.25
81	L5	2839	PSU	C5-C4-N3	2.16	121.30	116.55
81	L5	2824	OMC	O2-C2-N3	-2.15	118.94	122.33
47	S2	1383	A2M	C2'-C1'-N9	-2.15	110.21	113.75
81	L5	3718	A2M	C5-C4-N9	2.15	108.15	105.81
47	S2	590	A2M	O4'-C4'-C3'	-2.15	100.89	105.15
47	S2	1328	OMG	O6-C6-C5	-2.14	120.88	126.53
47	S2	601	OMG	O6-C6-C5	-2.14	120.89	126.53
81	L5	2632	PSU	C6-C5-C4	2.14	119.62	118.17
81	L5	1534	A2M	C5-C4-N9	2.14	108.14	105.81
81	L5	4623	OMG	C8-N7-C5	2.13	108.06	104.26
81	L5	4618	OMG	N2-C2-N1	2.13	121.26	116.76
47	S2	683	OMG	N9-C4-N3	2.13	130.22	125.95
81	L5	4618	OMG	C2'-C1'-N9	-2.13	110.19	114.24
47	S2	1678	A2M	C6-C5-C4	2.13	120.09	117.18
81	L5	2804	OMC	O2-C2-N3	-2.13	118.97	122.33
47	S2	1871	6MZ	C5-C4-N9	2.13	108.13	105.81
47	S2	683	OMG	C5-C6-N1	2.13	118.67	113.25
4	L8	75	OMG	O6-C6-C5	-2.12	120.93	126.53
81	L5	3627	OMG	C8-N7-C5	2.12	108.04	104.26
81	L5	4392	OMG	O6-C6-C5	-2.12	120.93	126.53
47	S2	1870	B8N	O4-C4-C5	-2.12	118.91	122.58
47	S2	159	A2M	C5-C4-N9	2.12	108.12	105.81
81	L5	3785	A2M	C4-C5-N7	-2.12	108.16	110.58
81	L5	1534	A2M	C6-C5-C4	2.12	120.07	117.18
81	L5	1524	A2M	C5-C4-N9	2.11	108.12	105.81
81	L5	1871	A2M	C4-C5-N7	-2.11	108.16	110.58
47	S2	1391	OMC	O2-C2-N3	-2.11	119.00	122.33
81	L5	4523	A2M	C4-N9-C8	2.11	107.95	105.74
81	L5	4637	OMG	O6-C6-C5	-2.11	120.97	126.53
81	L5	4552	PSU	C6-C5-C4	2.11	119.59	118.17
47	S2	509	OMG	C8-N7-C5	2.10	108.01	104.26
47	S2	99	A2M	C4-N9-C8	2.10	107.95	105.74
81	L5	1522	OMG	C8-N7-C5	2.10	108.01	104.26
81	L5	4392	OMG	N2-C2-N1	2.10	121.20	116.76
47	S2	1442	OMU	C6-N1-C2	-2.10	118.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	1316	OMG	C2'-C1'-N9	-2.10	110.25	114.24
81	L5	3818	UY1	O4'-C1'-C2'	2.10	108.24	104.56
81	L5	4623	OMG	O6-C6-C5	-2.10	120.99	126.53
47	S2	1328	OMG	N2-C2-N1	2.10	121.19	116.76
81	L5	1522	OMG	O6-C6-C5	-2.10	120.99	126.53
81	L5	4499	OMG	O6-C6-C5	-2.10	120.99	126.53
81	L5	2364	OMG	O6-C6-C5	-2.10	121.00	126.53
81	L5	2351	OMC	O2-C2-N3	-2.09	119.03	122.33
81	L5	3867	A2M	C6-C5-C4	2.09	120.03	117.18
81	L5	2363	A2M	C4-N9-C8	2.09	107.93	105.74
81	L5	3724	A2M	C4-N9-C8	2.09	107.93	105.74
81	L5	2401	A2M	C2'-C1'-N9	-2.09	110.32	113.75
81	L5	398	A2M	C5-C4-N9	2.08	108.08	105.81
81	L5	3785	A2M	O4'-C1'-C2'	-2.08	103.00	106.59
81	L5	1625	OMG	O6-C6-C5	-2.08	121.05	126.53
81	L5	4370	OMG	N9-C4-N3	2.08	130.10	125.95
47	S2	644	OMG	O6-C6-C5	-2.07	121.06	126.53
81	L5	4637	OMG	C8-N7-C5	2.07	107.95	104.26
81	L5	4571	A2M	C6-C5-C4	2.07	120.01	117.18
81	L5	2839	PSU	C6-N1-C2	-2.07	120.77	122.69
47	S2	683	OMG	C8-N7-C5	2.07	107.94	104.26
81	L5	2364	OMG	C8-N7-C5	2.07	107.94	104.26
81	L5	2839	PSU	O2-C2-N1	-2.07	120.66	122.79
47	S2	683	OMG	N2-C2-N1	2.07	121.12	116.76
47	S2	1850	MA6	C4-C5-N7	-2.06	108.22	110.58
81	L5	1316	OMG	N9-C4-N3	2.06	130.08	125.95
81	L5	3724	A2M	C6-C5-C4	2.06	119.99	117.18
81	L5	3724	A2M	C5-C4-N9	2.06	108.06	105.81
81	L5	1522	OMG	C2'-C1'-N9	-2.06	110.33	114.24
81	L5	2876	OMG	C8-N7-C5	2.06	107.93	104.26
47	S2	517	OMC	O2-C2-N3	-2.06	119.09	122.33
81	L5	4618	OMG	O6-C6-C5	-2.06	121.11	126.53
81	L5	1683	PSU	C6-C5-C4	2.06	119.56	118.17
47	S2	1383	A2M	C6-C5-C4	2.06	119.98	117.18
81	L5	4370	OMG	O6-C6-C5	-2.05	121.12	126.53
81	L5	3792	OMG	C5-C6-N1	2.05	118.47	113.25
47	S2	436	OMG	N2-C2-N1	2.05	121.09	116.76
81	L5	3718	A2M	C5'-C4'-C3'	-2.05	107.83	115.21
81	L5	4494	OMG	O6-C6-C5	-2.05	121.12	126.53
47	S2	683	OMG	O6-C6-C5	-2.05	121.13	126.53
81	L5	4370	OMG	C8-N7-C5	2.04	107.90	104.26
81	L5	2364	OMG	N9-C4-N3	2.04	130.04	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	L5	4536	OMC	O2-C2-N3	-2.03	119.12	122.33
47	S2	601	OMG	C8-N7-C5	2.03	107.88	104.26
81	L5	2861	OMC	O2-C2-N3	-2.03	119.13	122.33
81	L5	4457	PSU	C6-C5-C4	2.03	119.54	118.17
47	S2	1490	OMG	N2-C2-N1	2.03	121.05	116.76
81	L5	4457	PSU	O4'-C1'-C2'	2.02	107.95	105.15
81	L5	4628	PSU	O4'-C1'-C2'	2.02	107.95	105.15
47	S2	1871	6MZ	C4-N9-C8	2.02	107.86	105.74
47	S2	159	A2M	C4-N9-C8	2.02	107.86	105.74
4	L8	75	OMG	C8-N7-C5	2.02	107.85	104.26
47	S2	109	PSU	O4'-C1'-C2'	2.02	107.94	105.15
47	S2	576	A2M	C5-C4-N9	2.01	108.01	105.81
81	L5	3785	A2M	C4-N9-C8	2.01	107.85	105.74
47	S2	436	OMG	O6-C6-C5	-2.01	121.23	126.53

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L8	14	OMU	C1'-C2'-O2'-CM2
4	L8	75	OMG	O4'-C4'-C5'-O5'
47	S2	116	OMU	C1'-C2'-O2'-CM2
47	S2	116	OMU	O4'-C4'-C5'-O5'
47	S2	159	A2M	C1'-C2'-O2'-CM'
47	S2	428	OMU	C2'-C1'-N1-C6
47	S2	428	OMU	O4'-C4'-C5'-O5'
47	S2	644	OMG	O4'-C4'-C5'-O5'
47	S2	683	OMG	O4'-C4'-C5'-O5'
47	S2	1442	OMU	O4'-C1'-N1-C2
47	S2	1442	OMU	O4'-C1'-N1-C6
47	S2	1447	OMG	O4'-C4'-C5'-O5'
47	S2	1447	OMG	C3'-C4'-C5'-O5'
47	S2	1678	A2M	C1'-C2'-O2'-CM'
47	S2	1703	OMC	O4'-C1'-N1-C2
47	S2	1703	OMC	O4'-C1'-N1-C6
47	S2	1870	B8N	O4'-C1'-C5-C6
47	S2	1870	B8N	O4'-C1'-C5-C4
47	S2	1870	B8N	N3-C31-C32-C33
47	S2	1870	B8N	C31-C32-C33-C34
47	S2	1870	B8N	C31-C32-C33-N34
81	L5	1326	A2M	O4'-C4'-C5'-O5'
81	L5	1871	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
81	L5	1871	A2M	C3'-C4'-C5'-O5'
81	L5	2351	OMC	C1'-C2'-O2'-CM2
81	L5	2415	OMU	C1'-C2'-O2'-CM2
81	L5	2424	OMG	O4'-C4'-C5'-O5'
81	L5	2815	A2M	O4'-C4'-C5'-O5'
81	L5	2839	PSU	O4'-C1'-C5-C4
81	L5	2839	PSU	O4'-C1'-C5-C6
81	L5	3637	PSU	C2'-C1'-C5-C4
81	L5	3637	PSU	O4'-C1'-C5-C4
81	L5	3637	PSU	O4'-C1'-C5-C6
81	L5	3701	OMC	C2'-C1'-N1-C2
81	L5	3701	OMC	C2'-C1'-N1-C6
81	L5	3818	UY1	C4'-C5'-O5'-P
81	L5	3841	OMC	O4'-C1'-N1-C2
81	L5	3841	OMC	O4'-C1'-N1-C6
81	L5	3887	OMC	O4'-C4'-C5'-O5'
81	L5	3925	OMU	C1'-C2'-O2'-CM2
81	L5	4220	6MZ	C5-C6-N6-C9
81	L5	4220	6MZ	N1-C6-N6-C9
81	L5	4220	6MZ	O4'-C4'-C5'-O5'
81	L5	4227	OMU	C3'-C4'-C5'-O5'
81	L5	4306	OMU	C3'-C4'-C5'-O5'
81	L5	4523	A2M	C1'-C2'-O2'-CM'
81	L5	4530	UR3	O4'-C1'-N1-C6
81	L5	4530	UR3	O4'-C1'-N1-C2
81	L5	4532	PSU	O4'-C4'-C5'-O5'
81	L5	4569	PSU	O4'-C4'-C5'-O5'
81	L5	4590	A2M	C4'-C5'-O5'-P
81	L5	4637	OMG	C1'-C2'-O2'-CM2
4	L8	69	PSU	C3'-C4'-C5'-O5'
4	L8	75	OMG	C3'-C4'-C5'-O5'
47	S2	116	OMU	C3'-C4'-C5'-O5'
47	S2	428	OMU	C3'-C4'-C5'-O5'
47	S2	512	A2M	O4'-C4'-C5'-O5'
47	S2	576	A2M	O4'-C4'-C5'-O5'
47	S2	576	A2M	C3'-C4'-C5'-O5'
47	S2	644	OMG	C3'-C4'-C5'-O5'
47	S2	1870	B8N	O4'-C4'-C5'-O5'
47	S2	1871	6MZ	O4'-C4'-C5'-O5'
81	L5	2364	OMG	O4'-C4'-C5'-O5'
81	L5	2424	OMG	C3'-C4'-C5'-O5'
81	L5	2876	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
81	L5	2876	OMG	C3'-C4'-C5'-O5'
81	L5	3851	PSU	C3'-C4'-C5'-O5'
81	L5	3867	A2M	O4'-C4'-C5'-O5'
81	L5	3867	A2M	C3'-C4'-C5'-O5'
81	L5	3887	OMC	C3'-C4'-C5'-O5'
81	L5	4228	OMG	C3'-C4'-C5'-O5'
81	L5	4532	PSU	C3'-C4'-C5'-O5'
81	L5	4569	PSU	C3'-C4'-C5'-O5'
81	L5	4618	OMG	O4'-C4'-C5'-O5'
47	S2	27	A2M	O4'-C4'-C5'-O5'
47	S2	27	A2M	C3'-C4'-C5'-O5'
47	S2	99	A2M	O4'-C4'-C5'-O5'
47	S2	1442	OMU	O4'-C4'-C5'-O5'
47	S2	1703	OMC	C3'-C4'-C5'-O5'
81	L5	1326	A2M	C3'-C4'-C5'-O5'
81	L5	2351	OMC	C3'-C4'-C5'-O5'
81	L5	2351	OMC	O4'-C4'-C5'-O5'
81	L5	2787	A2M	O4'-C4'-C5'-O5'
81	L5	2839	PSU	C3'-C4'-C5'-O5'
81	L5	3818	UY1	O4'-C4'-C5'-O5'
81	L5	4227	OMU	O4'-C4'-C5'-O5'
81	L5	4228	OMG	O4'-C4'-C5'-O5'
81	L5	4306	OMU	O4'-C4'-C5'-O5'
81	L5	4471	PSU	C3'-C4'-C5'-O5'
47	S2	428	OMU	C2'-C1'-N1-C2
47	S2	683	OMG	C3'-C4'-C5'-O5'
47	S2	1703	OMC	O4'-C4'-C5'-O5'
81	L5	2815	A2M	C3'-C4'-C5'-O5'
81	L5	3818	UY1	C3'-C4'-C5'-O5'
4	L8	69	PSU	O4'-C4'-C5'-O5'
81	L5	4220	6MZ	C3'-C4'-C5'-O5'
81	L5	4618	OMG	C3'-C4'-C5'-O5'
47	S2	1870	B8N	C3'-C4'-C5'-O5'
47	S2	1871	6MZ	C3'-C4'-C5'-O5'
81	L5	2364	OMG	C3'-C4'-C5'-O5'
81	L5	2839	PSU	O4'-C4'-C5'-O5'
81	L5	4471	PSU	O4'-C4'-C5'-O5'
81	L5	2787	A2M	C2'-C1'-N9-C8
47	S2	1337	4AC	O4'-C4'-C5'-O5'
81	L5	3785	A2M	O4'-C4'-C5'-O5'
81	L5	3851	PSU	O4'-C4'-C5'-O5'
47	S2	512	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
47	S2	1442	OMU	C3'-C4'-C5'-O5'
81	L5	2787	A2M	C2'-C1'-N9-C4
81	L5	3785	A2M	C3'-C4'-C5'-O5'
47	S2	1842	4AC	O7-C7-N4-C4
47	S2	1842	4AC	CM7-C7-N4-C4
81	L5	2422	OMC	C3'-C4'-C5'-O5'
81	L5	1781	PSU	C3'-C4'-C5'-O5'
81	L5	1326	A2M	C4'-C5'-O5'-P
81	L5	2422	OMC	O4'-C4'-C5'-O5'
47	S2	428	OMU	O4'-C1'-N1-C2
47	S2	428	OMU	O4'-C1'-N1-C6
81	L5	3818	UY1	C1'-C2'-O2'-CM2
81	L5	3818	UY1	C3'-C2'-O2'-CM2
47	S2	644	OMG	C4'-C5'-O5'-P
81	L5	1534	A2M	C4'-C5'-O5'-P
47	S2	1851	MA6	C4'-C5'-O5'-P
81	L5	3701	OMC	O4'-C1'-N1-C6
47	S2	1447	OMG	C4'-C5'-O5'-P
81	L5	3701	OMC	O4'-C1'-N1-C2
47	S2	576	A2M	C4'-C5'-O5'-P
81	L5	398	A2M	C3'-C4'-C5'-O5'
81	L5	3782	5MC	O4'-C4'-C5'-O5'
47	S2	1870	B8N	C4'-C5'-O5'-P
81	L5	3867	A2M	C4'-C5'-O5'-P
47	S2	121	OMU	C3'-C4'-C5'-O5'
81	L5	4220	6MZ	C5'-O5'-P-O1P
47	S2	159	A2M	O4'-C4'-C5'-O5'
81	L5	3785	A2M	C2'-C1'-N9-C8
47	S2	1445	PSU	C2'-C1'-C5-C6
81	L5	2787	A2M	O4'-C1'-N9-C8
47	S2	99	A2M	C3'-C4'-C5'-O5'
81	L5	2351	OMC	C2'-C1'-N1-C2
81	L5	1534	A2M	O4'-C4'-C5'-O5'
81	L5	2787	A2M	C3'-C4'-C5'-O5'
81	L5	3627	OMG	O4'-C4'-C5'-O5'
47	S2	1490	OMG	C4'-C5'-O5'-P
81	L5	3701	OMC	C4'-C5'-O5'-P
47	S2	590	A2M	O4'-C1'-N9-C8
47	S2	27	A2M	C2'-C1'-N9-C8
47	S2	1337	4AC	C3'-C4'-C5'-O5'

There are no ring outliers.

76 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	L5	4370	OMG	3	0
81	L5	4628	PSU	1	0
47	S2	1871	6MZ	3	0
81	L5	3818	UY1	2	0
81	L5	4552	PSU	1	0
47	S2	576	A2M	3	0
47	S2	1177	PSU	1	0
4	L8	75	OMG	1	0
4	L8	69	PSU	1	0
81	L5	1316	OMG	2	0
47	S2	27	A2M	3	0
47	S2	1238	PSU	1	0
81	L5	3718	A2M	4	0
4	L8	14	OMU	1	0
47	S2	1842	4AC	2	0
81	L5	5001	PSU	1	0
81	L5	4579	PSU	2	0
47	S2	1232	PSU	1	0
81	L5	4623	OMG	1	0
81	L5	1340	OMC	1	0
47	S2	109	PSU	1	0
47	S2	468	A2M	1	0
81	L5	1625	OMG	1	0
47	S2	1391	OMC	1	0
47	S2	93	PSU	1	0
81	L5	4637	OMG	1	0
47	S2	1678	A2M	2	0
47	S2	1337	4AC	1	0
81	L5	2351	OMC	3	0
81	L5	4620	OMU	1	0
81	L5	3724	A2M	2	0
81	L5	2804	OMC	1	0
81	L5	5010	PSU	1	0
81	L5	2415	OMU	3	0
81	L5	2364	OMG	1	0
81	L5	2839	PSU	1	0
47	S2	1328	OMG	3	0
81	L5	4523	A2M	1	0
47	S2	512	A2M	1	0
81	L5	4457	PSU	1	0
47	S2	1850	MA6	1	0
47	S2	116	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	S2	1703	OMC	2	0
81	L5	4618	OMG	2	0
47	S2	601	OMG	2	0
81	L5	3785	A2M	2	0
81	L5	4442	PSU	1	0
81	L5	4228	OMG	1	0
47	S2	1383	A2M	1	0
47	S2	683	OMG	1	0
81	L5	1522	OMG	1	0
47	S2	484	A2M	2	0
81	L5	4361	PSU	1	0
47	S2	1447	OMG	2	0
81	L5	2632	PSU	1	0
81	L5	3808	OMC	1	0
81	L5	2363	A2M	1	0
47	S2	1442	OMU	1	0
81	L5	3925	OMU	1	0
81	L5	4431	PSU	1	0
47	S2	1445	PSU	3	0
81	L5	4220	6MZ	2	0
81	L5	4227	OMU	2	0
81	L5	3867	A2M	1	0
81	L5	1683	PSU	2	0
81	L5	4456	OMC	1	0
81	L5	4392	OMG	3	0
47	S2	159	A2M	4	0
81	L5	2815	A2M	2	0
81	L5	1779	PSU	1	0
81	L5	1326	A2M	2	0
81	L5	4536	OMC	1	0
81	L5	3841	OMC	2	0
47	S2	428	OMU	1	0
47	S2	509	OMG	2	0
81	L5	3627	OMG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 403 ligands modelled in this entry, 384 are monoatomic - leaving 19 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
91	SPD	L5	5108	-	9,9,9	0.30	0	8,8,8	0.76	0
89	PUT	L5	5386	-	5,5,5	0.10	0	4,4,4	0.11	0
85	GDP	CB	901	-	29,30,30	0.45	0	45,47,47	0.47	0
90	HYG	S2	1979	-	36,39,39	0.77	1 (2%)	44,60,60	1.35	6 (13%)
91	SPD	L5	5104	-	9,9,9	0.32	0	8,8,8	0.76	0
92	3HE	L5	5109	-	21,21,21	0.10	0	23,30,30	0.23	0
89	PUT	L5	5382	-	5,5,5	0.09	0	4,4,4	0.12	0
89	PUT	L5	5384	-	5,5,5	0.11	0	4,4,4	0.12	0
91	SPD	L5	5106	-	9,9,9	0.33	0	8,8,8	0.84	0
91	SPD	L5	5107	-	9,9,9	0.32	0	8,8,8	0.88	0
91	SPD	L5	5102	-	9,9,9	0.31	0	8,8,8	0.80	0
89	PUT	L5	5387	-	5,5,5	0.07	0	4,4,4	0.14	0
91	SPD	L5	5103	-	9,9,9	0.32	0	8,8,8	0.90	0
89	PUT	L5	5383	-	5,5,5	0.09	0	4,4,4	0.14	0
89	PUT	S2	1939	-	5,5,5	0.08	0	4,4,4	0.14	0
91	SPD	L5	5101	-	9,9,9	0.31	0	8,8,8	0.78	0
89	PUT	L5	5385	-	5,5,5	0.09	0	4,4,4	0.15	0
93	ANM	L5	5388	-	20,20,20	0.58	0	24,27,27	0.44	0
91	SPD	L5	5105	-	9,9,9	0.31	0	8,8,8	0.88	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
91	SPD	L5	5108	-	-	1/7/7/7	-
89	PUT	L5	5386	-	-	1/3/3/3	-
85	GDP	CB	901	-	-	6/16/32/32	0/3/3/3
90	HYG	S2	1979	-	-	2/12/87/87	0/4/4/4
91	SPD	L5	5104	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	3HE	L5	5109	-	-	0/8/36/36	0/2/2/2
89	PUT	L5	5382	-	-	0/3/3/3	-
89	PUT	L5	5384	-	-	0/3/3/3	-
91	SPD	L5	5106	-	-	1/7/7/7	-
91	SPD	L5	5107	-	-	5/7/7/7	-
91	SPD	L5	5102	-	-	1/7/7/7	-
89	PUT	L5	5387	-	-	1/3/3/3	-
91	SPD	L5	5103	-	-	4/7/7/7	-
89	PUT	L5	5383	-	-	0/3/3/3	-
89	PUT	S2	1939	-	-	0/3/3/3	-
91	SPD	L5	5101	-	-	0/7/7/7	-
89	PUT	L5	5385	-	-	0/3/3/3	-
93	ANM	L5	5388	-	-	0/10/23/23	0/2/2/2
91	SPD	L5	5105	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	S2	1979	HYG	C4-N9	2.62	1.50	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	S2	1979	HYG	O22-C17-C16	4.19	121.21	111.22
90	S2	1979	HYG	C16-C17-C12	-4.13	103.64	113.50
90	S2	1979	HYG	O14-C13-C12	-3.18	103.30	109.49
90	S2	1979	HYG	O11-C5-C4	-3.02	103.13	109.40
90	S2	1979	HYG	O29-C12-C13	2.28	116.70	110.89
90	S2	1979	HYG	O35-C34-C33	-2.22	106.73	111.55

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	CB	901	GDP	C5'-O5'-PA-O3A
85	CB	901	GDP	O4'-C4'-C5'-O5'
85	CB	901	GDP	C3'-C4'-C5'-O5'
90	S2	1979	HYG	O14-C13-O18-C6
91	L5	5107	SPD	C3-C4-C5-N6
91	L5	5104	SPD	C2-C3-C4-C5
91	L5	5103	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
91	L5	5106	SPD	C3-C4-C5-N6
90	S2	1979	HYG	C3-C4-N9-C10
91	L5	5108	SPD	C4-C5-N6-C7
91	L5	5105	SPD	C2-C3-C4-C5
91	L5	5104	SPD	C3-C4-C5-N6
91	L5	5107	SPD	C7-C8-C9-N10
91	L5	5107	SPD	C8-C7-N6-C5
91	L5	5103	SPD	C2-C3-C4-C5
85	CB	901	GDP	C5'-O5'-PA-O1A
91	L5	5103	SPD	C7-C8-C9-N10
85	CB	901	GDP	PB-O3A-PA-O2A
89	L5	5386	PUT	C1-C2-C3-C4
91	L5	5103	SPD	N1-C2-C3-C4
89	L5	5387	PUT	C1-C2-C3-C4
91	L5	5107	SPD	C4-C5-N6-C7
85	CB	901	GDP	PB-O3A-PA-O1A
91	L5	5107	SPD	N6-C7-C8-C9
91	L5	5102	SPD	C7-C8-C9-N10

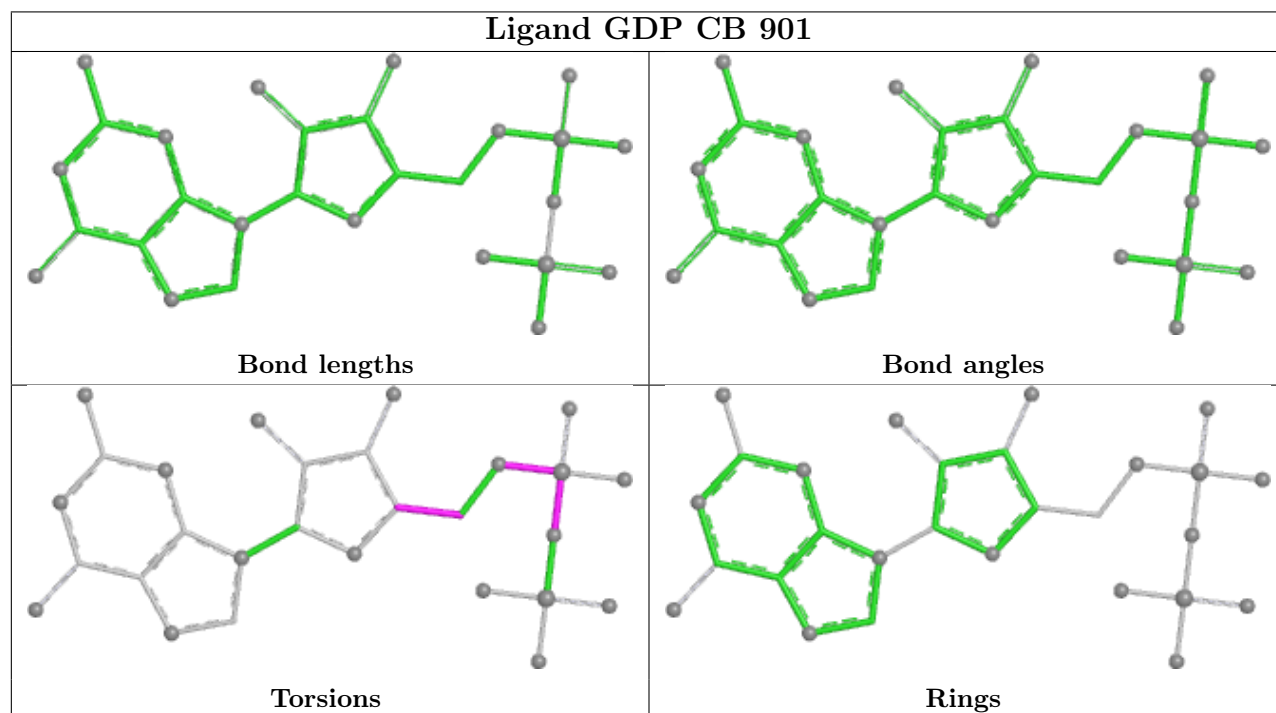
There are no ring outliers.

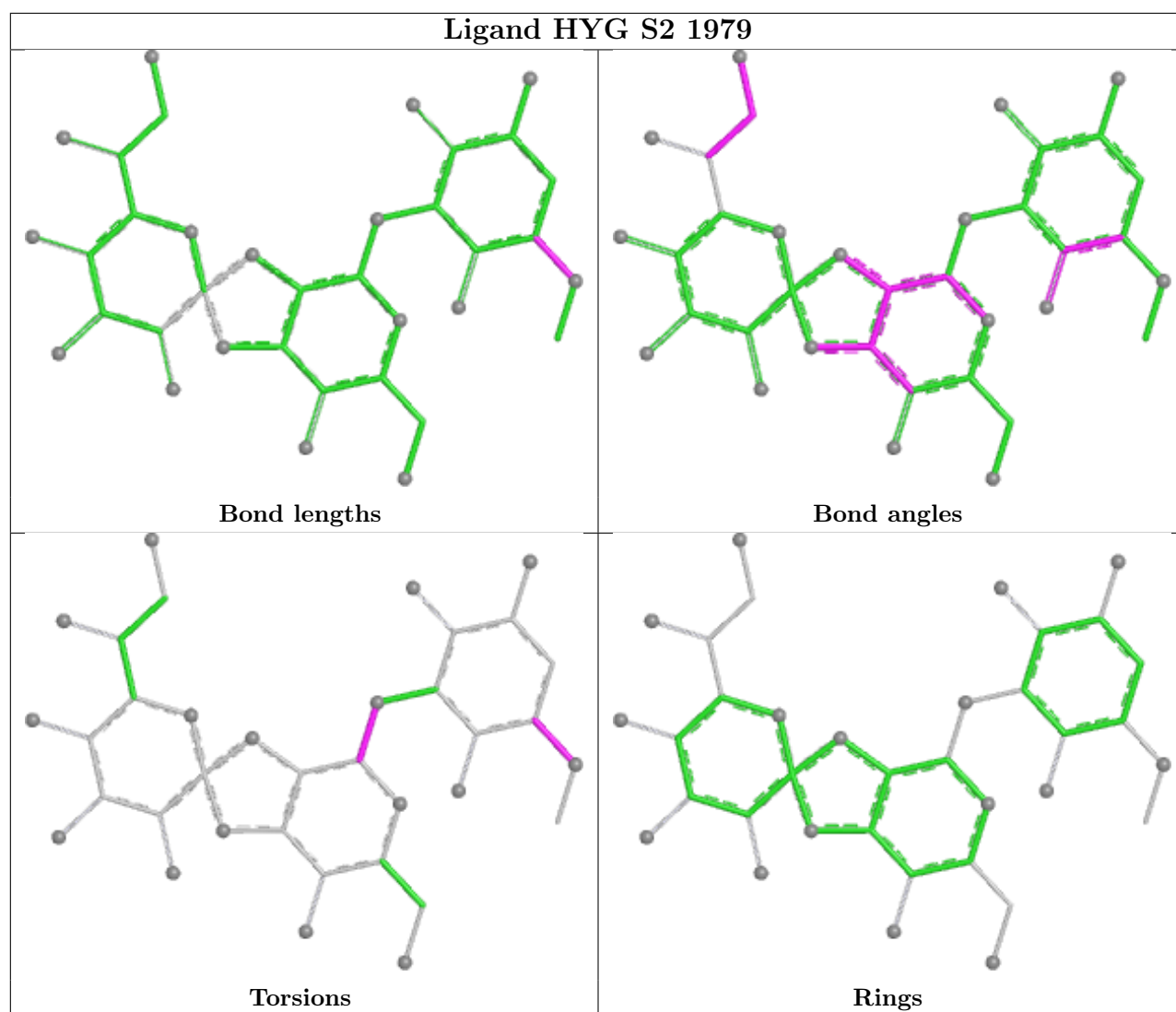
10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	L5	5109	3HE	2	0
89	L5	5382	PUT	1	0
91	L5	5107	SPD	1	0
91	L5	5102	SPD	1	0
89	L5	5387	PUT	2	0
89	S2	1939	PUT	1	0
91	L5	5101	SPD	1	0
89	L5	5385	PUT	2	0
93	L5	5388	ANM	1	0
91	L5	5105	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
81	L5	4
47	S2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1869:A	O3'	1870:B8N	P	61.81
1	S2	1870:B8N	O3'	1871:6MZ	P	34.71
1	L5	4219:A	O3'	4220:6MZ	P	4.27
1	L5	3817:A	O3'	3818:UY1	P	2.93
1	L5	3818:UY1	O3'	3819:G	P	2.92
1	L5	4220:6MZ	O3'	4221:C	P	2.88

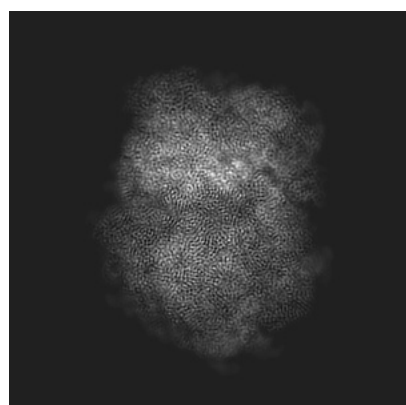
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50673. These allow visual inspection of the internal detail of the map and identification of artifacts.

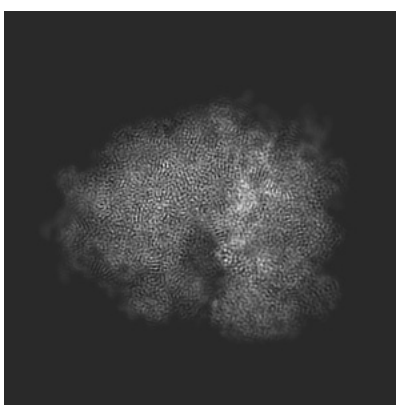
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

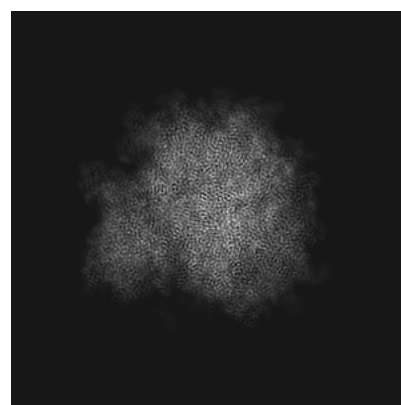
6.1.1 Primary map



X



Y

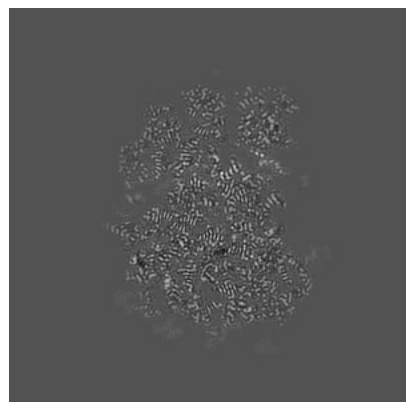


Z

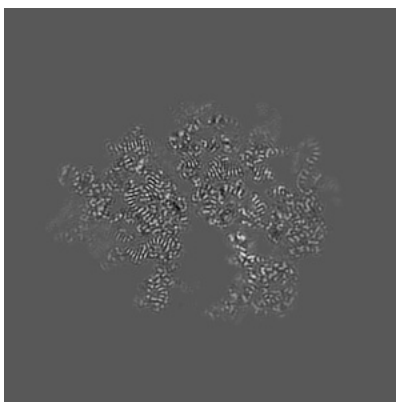
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

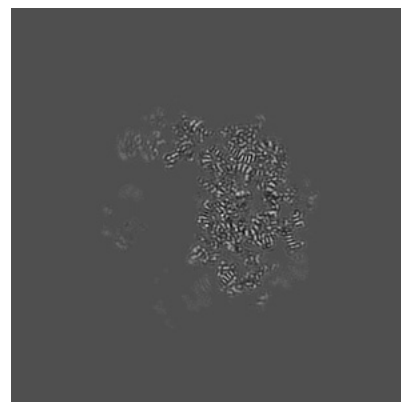
6.2.1 Primary map



X Index: 240



Y Index: 240

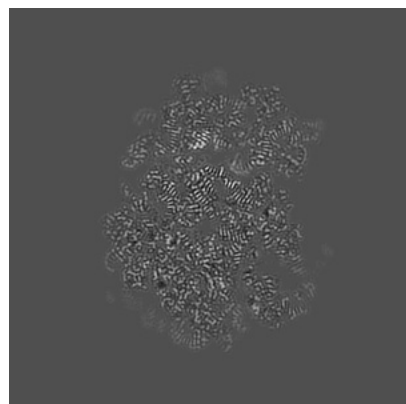


Z Index: 240

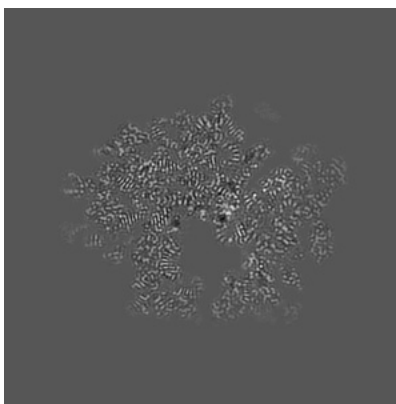
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

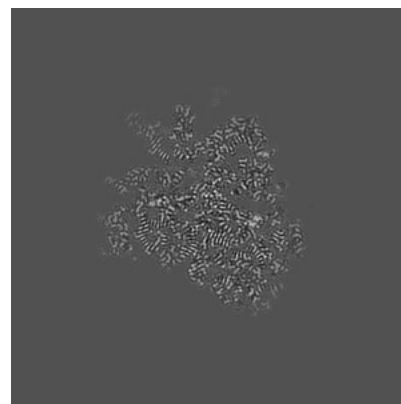
6.3.1 Primary map



X Index: 261



Y Index: 223

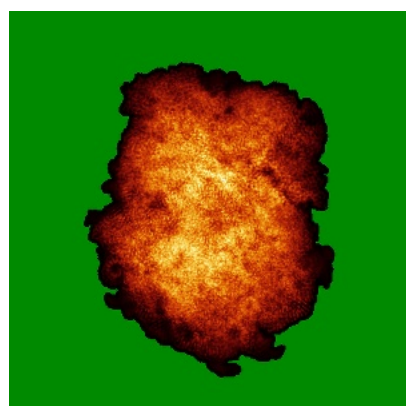


Z Index: 196

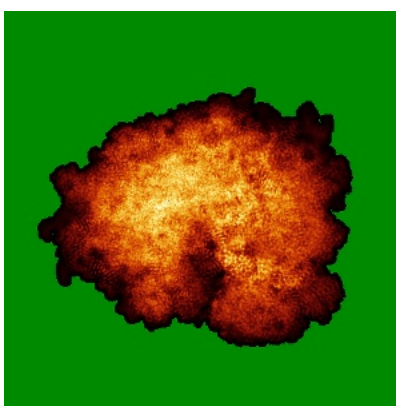
The images above show the largest variance slices of the map in three orthogonal directions.

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

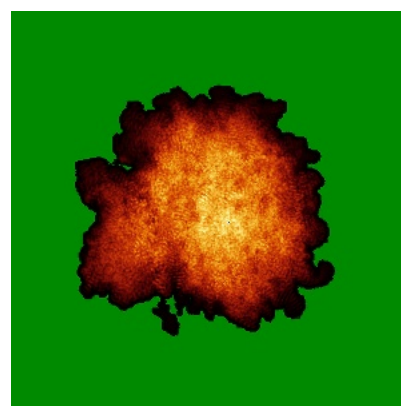
6.4.1 Primary map



X



Y

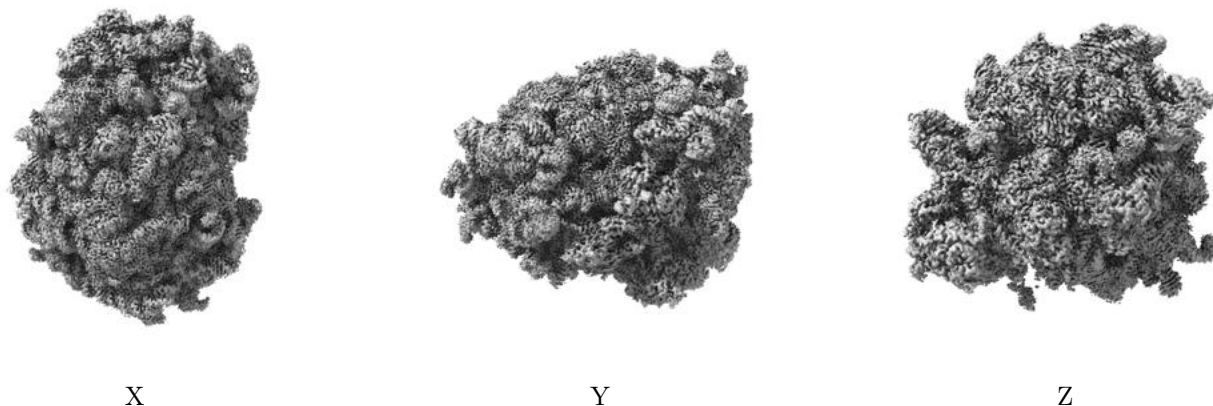


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

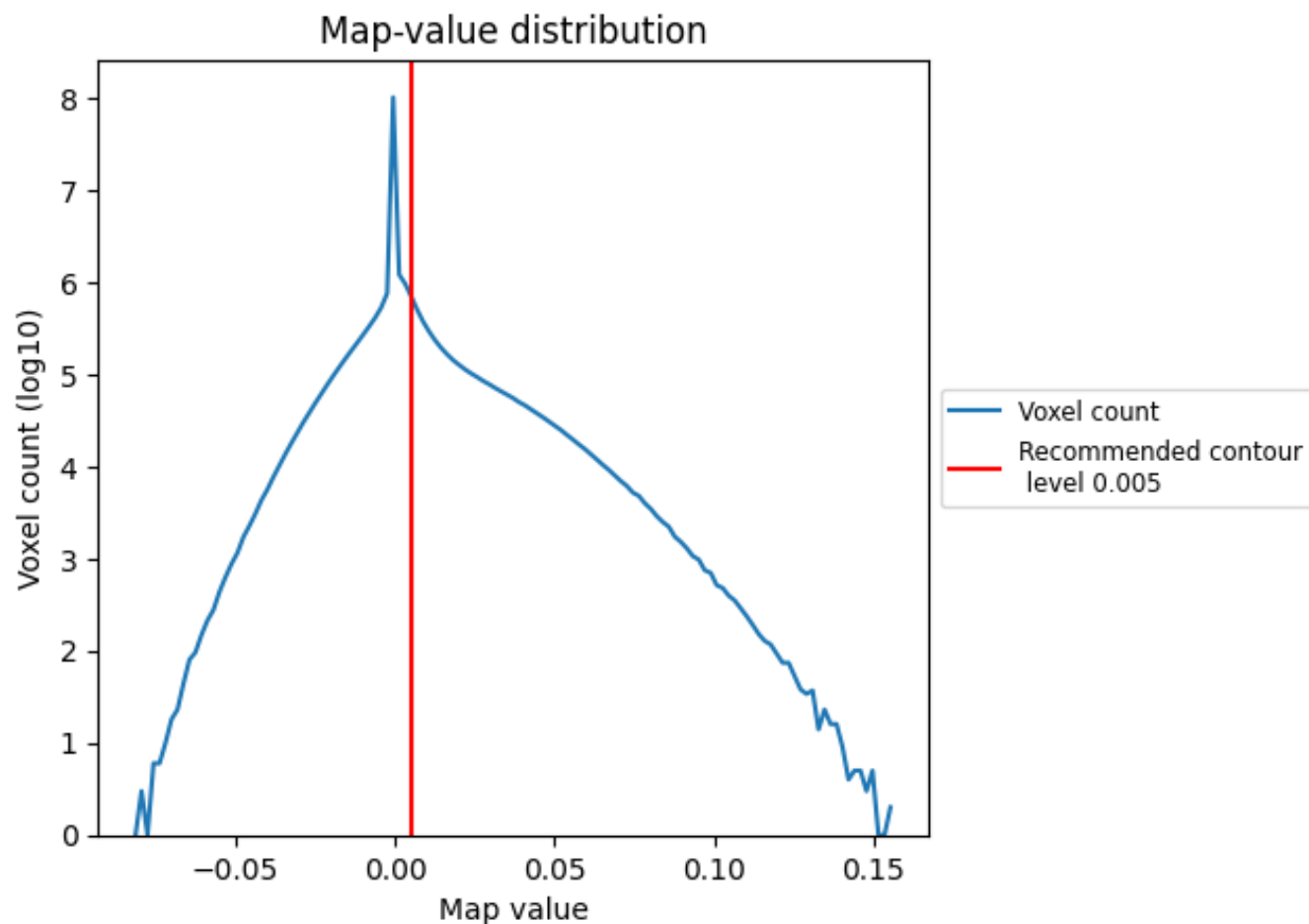
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

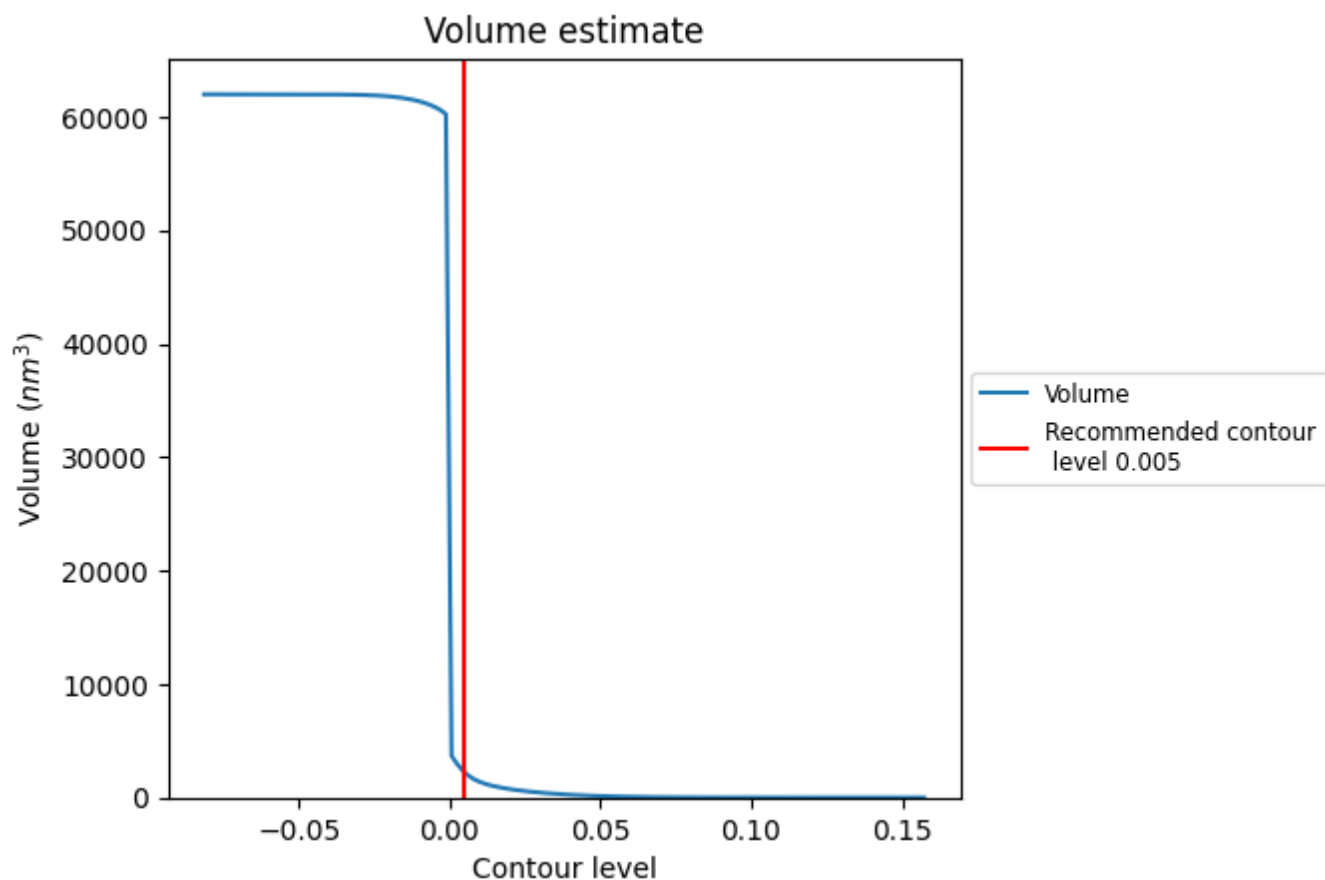
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

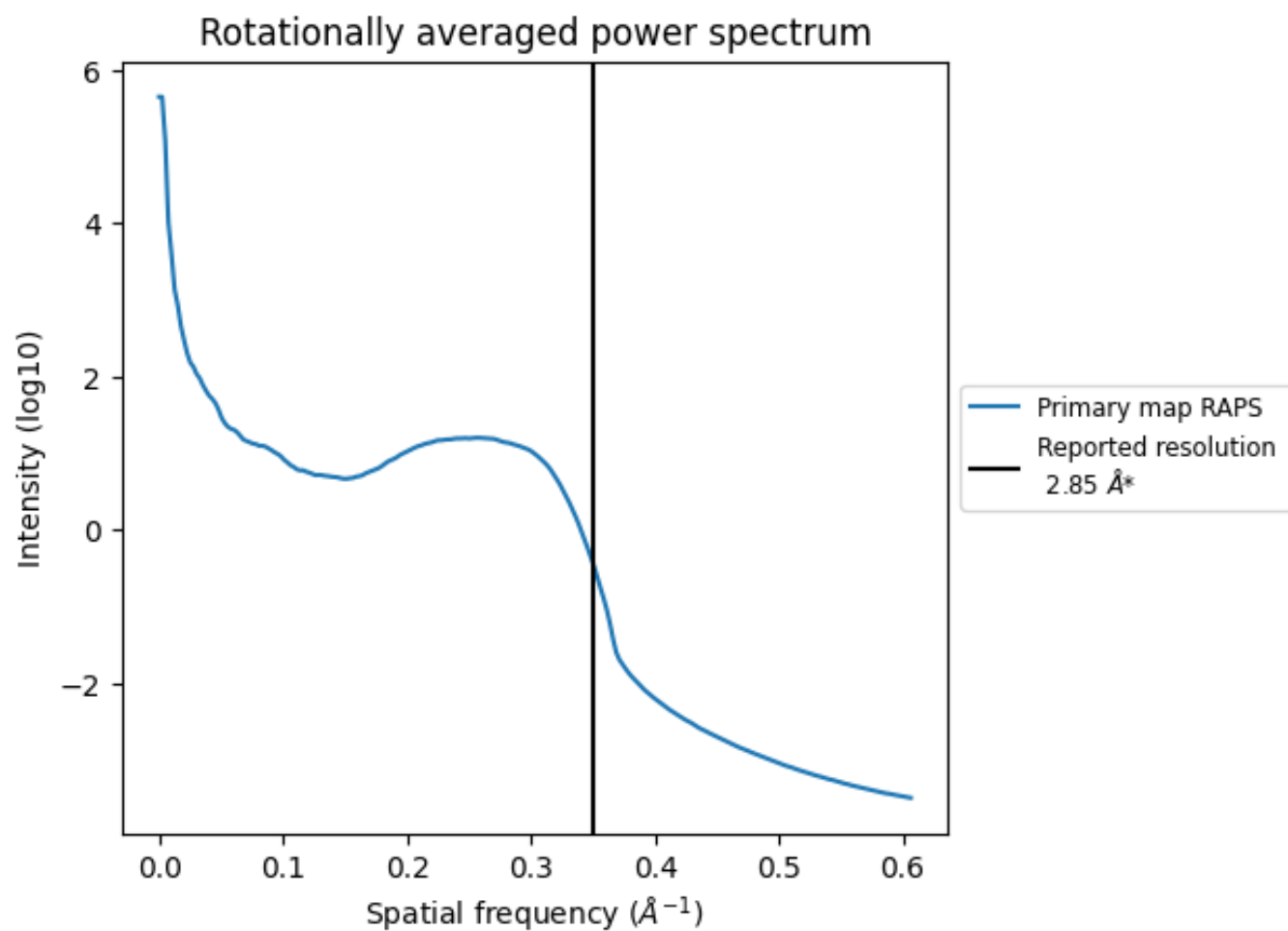
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2225 nm³; this corresponds to an approximate mass of 2010 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 ⓘ

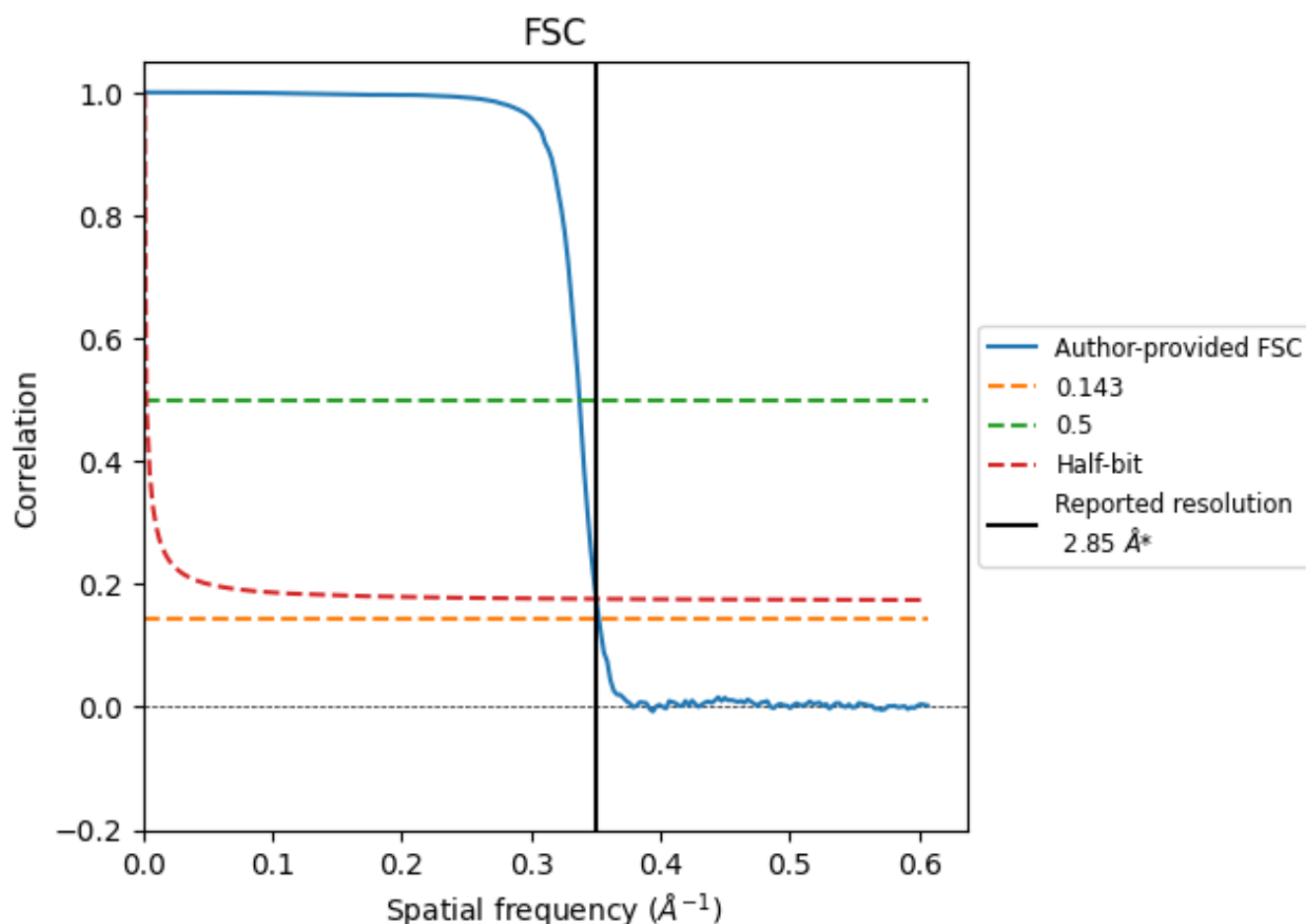


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 Å⁻¹

8.2 Resolution estimates [i](#)

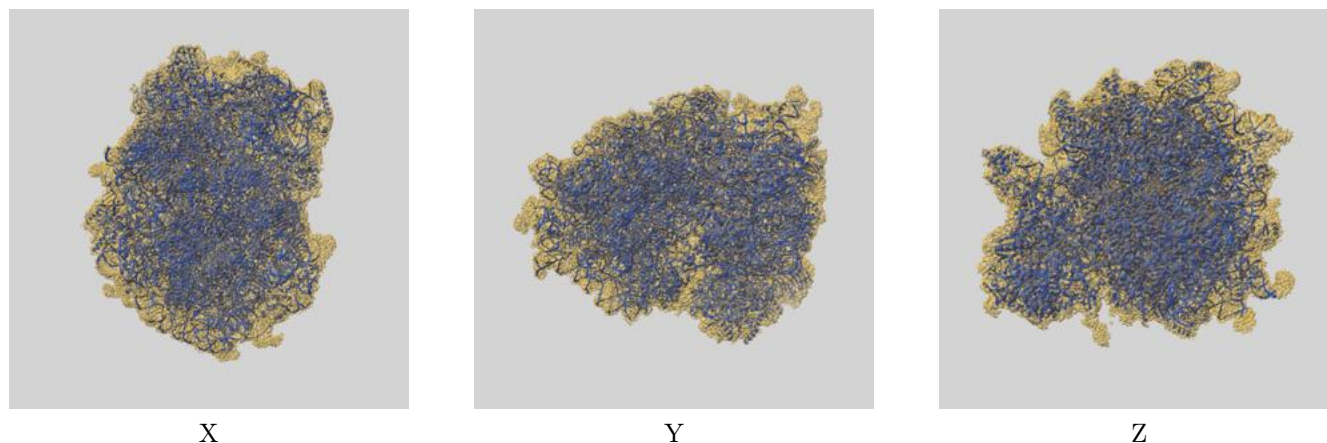
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.84	2.96	2.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

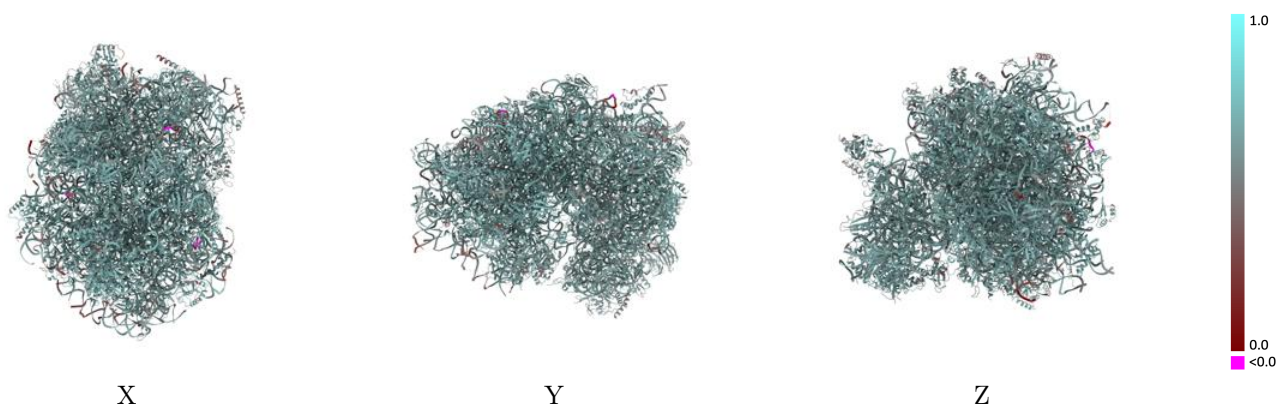
This section contains information regarding the fit between EMDB map EMD-50673 and PDB model 9FQZ. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



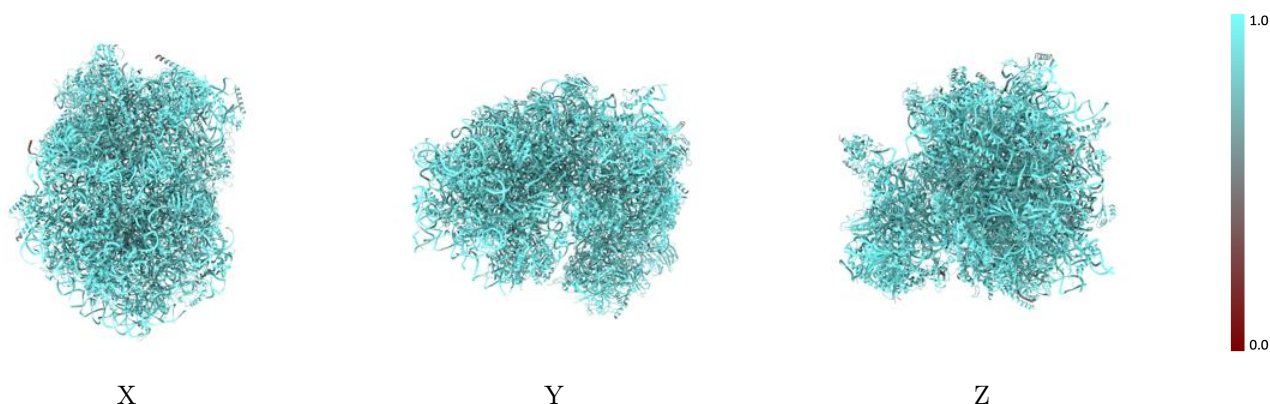
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



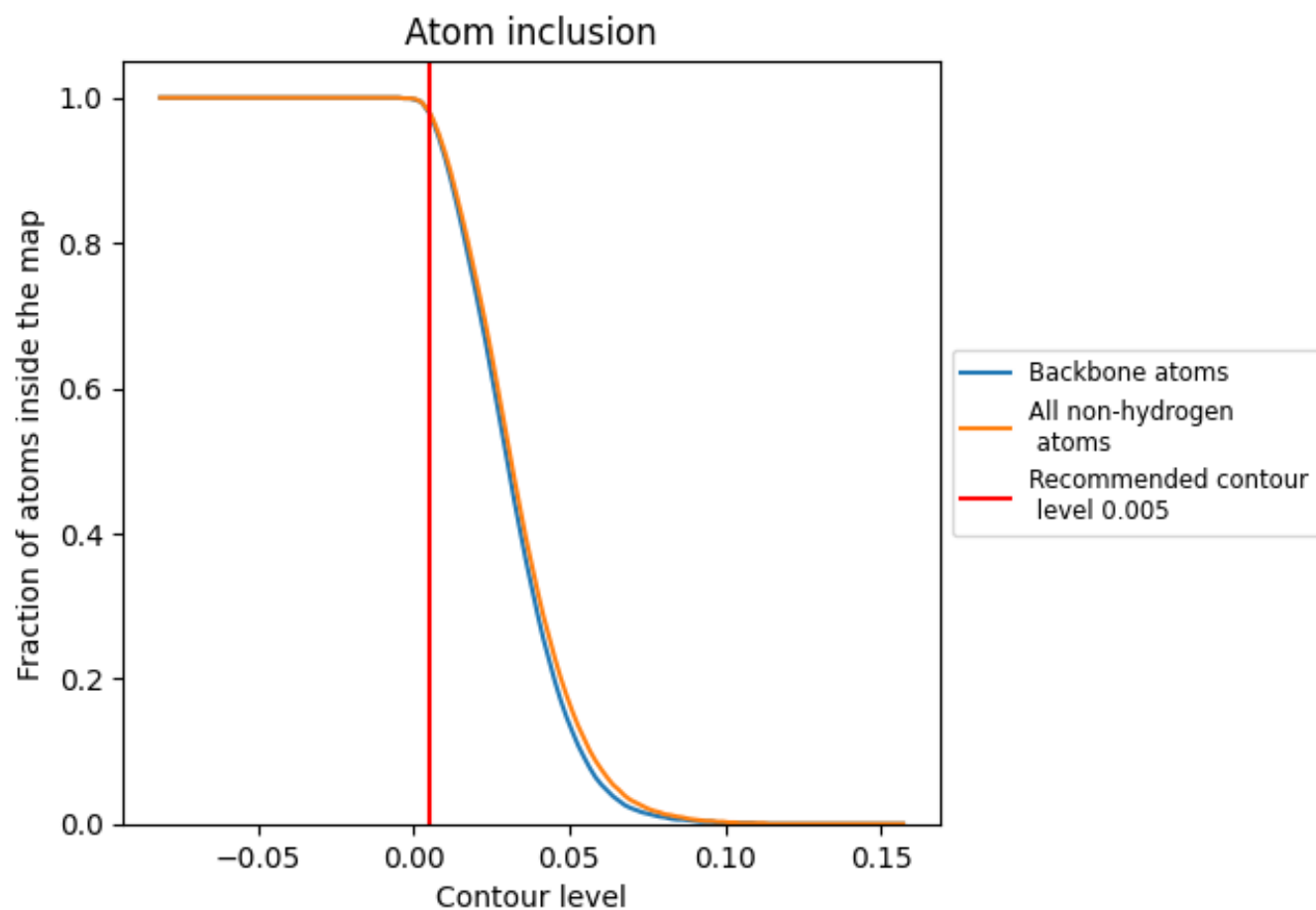
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.5 Map-model fit summary ⓘ





















































































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

Chain	Atom inclusion	Q-score
All	 0.9810	 0.6200
CA	 0.7170	 0.5430
CB	 0.9720	 0.5870
CC	 0.7510	 0.4660
CD	 0.8800	 0.5550
L5	 0.9860	 0.6180
L7	 1.0000	 0.6470
L8	 0.9800	 0.6060
LA	 0.9930	 0.6530
LB	 0.9850	 0.6490
LC	 0.9850	 0.6450
LD	 0.9760	 0.6350
LE	 0.9790	 0.6270
LF	 0.9920	 0.6490
LG	 0.9770	 0.6250
LH	 0.9820	 0.6380
LI	 0.9860	 0.6450
LJ	 0.9670	 0.6160
LL	 0.9750	 0.6290
LM	 0.9890	 0.6420
LN	 0.9960	 0.6600
LO	 0.9920	 0.6490
LP	 0.9870	 0.6490
LQ	 0.9970	 0.6580
LR	 0.9630	 0.6160
LS	 0.9930	 0.6560
LT	 0.9840	 0.6370
LU	 0.9590	 0.5960
LV	 0.9970	 0.6530
LW	 0.8900	 0.5530
LX	 0.9840	 0.6400
LY	 0.9790	 0.6450
LZ	 0.9890	 0.6410
La	 0.9940	 0.6600
Lb	 0.9700	 0.6170



















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Chain	Atom inclusion	Q-score
Lc	 0.9920	 0.6330
Ld	 0.9670	 0.6250
Le	 0.9920	 0.6540
Lf	 0.9910	 0.6590
Lg	 0.9760	 0.6380
Lh	 0.9870	 0.6420
Li	 0.9880	 0.6320
Lj	 0.9880	 0.6470
Lk	 0.9650	 0.6290
Ll	 0.9950	 0.6470
Lm	 0.9980	 0.6480
Ln	 0.9950	 0.6460
Lo	 0.9830	 0.6410
Lp	 1.0000	 0.6480
Lq	 0.9100	 0.5580
Lr	 0.9910	 0.6500
S2	 0.9910	 0.6160
SA	 0.9620	 0.6200
SB	 0.9870	 0.6260
SC	 0.9880	 0.6350
SD	 0.9690	 0.6040
SE	 0.9840	 0.6360
SF	 0.9780	 0.6090
SG	 0.9540	 0.5930
SH	 0.9190	 0.5740
SI	 0.9670	 0.6080
SJ	 0.9830	 0.6260
SK	 0.9670	 0.6100
SL	 0.9660	 0.6280
SM	 0.8990	 0.5550
SN	 0.9900	 0.6270
SO	 0.9740	 0.6250
SP	 0.9740	 0.6050
SQ	 0.9790	 0.6220
SR	 0.9360	 0.5990
SS	 0.9710	 0.6130
ST	 0.9750	 0.6170
SU	 0.9480	 0.5910
SV	 0.9820	 0.6330
SW	 0.9840	 0.6350
SX	 0.9930	 0.6370
SY	 0.9830	 0.6290

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Chain	Atom inclusion	Q-score
SZ	 0.9660	 0.6130
Sa	 0.9730	 0.6190
Sb	 0.9530	 0.6050
Sc	 0.9620	 0.5780
Sd	 0.9840	 0.6280
Se	 0.9750	 0.6140
Sf	 0.9360	 0.5660
Sg	 0.9520	 0.5980