



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 09:06 am BST

PDB ID : 7ZJW / pdb_00007zjw
EMDB ID : EMD-14751
Title : Rabbit 80S ribosome as it decodes the Sec-UGA codon
Authors : Hilal, T.; Simonovic, M.; Spahn, C.M.T.
Deposited on : 2022-04-12
Resolution : 2.80 Å(reported)
Based on initial model : 7O7Y

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

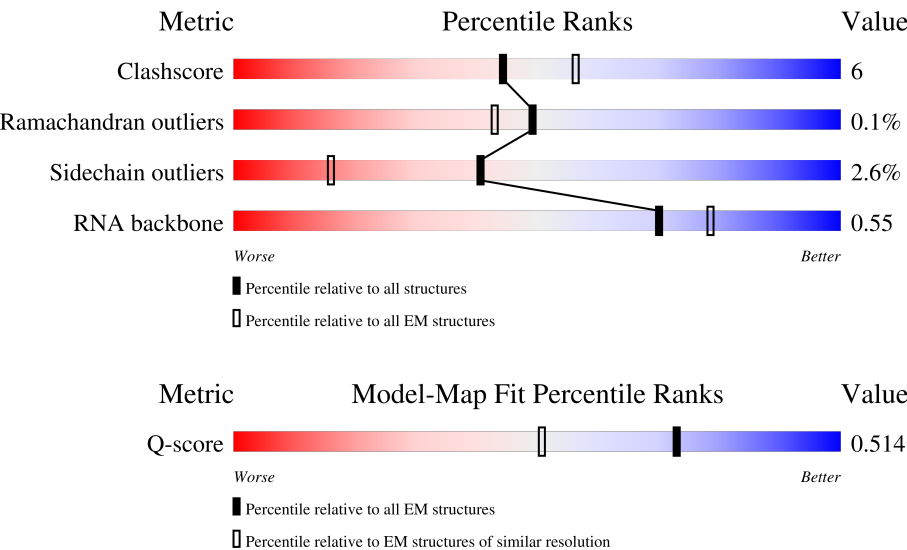
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.80 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.



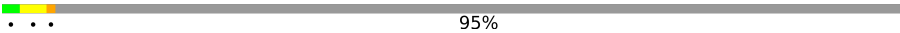
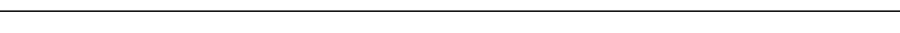
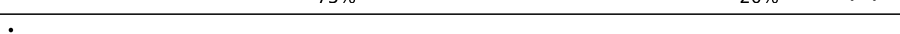
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	E	616	
2	F	90	
3	I	1072	

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Mol	Chain	Length	Quality of chain
4	S	855	 95%
5	B	854	 19% 5% 76%
6	L5	4808	 53% 21% 22%
7	L7	119	 82% 17%
8	L8	158	 78% 20%
9	LD	257	 81% 18%
10	LE	403	 79% 18%
11	LF	413	 75% 12% 12%
12	LG	297	 81% 17%
13	LH	291	 65% 14% 20%
14	LI	247	 74% 17% 9%
15	LJ	266	 77% 10% 12%
16	LK	192	 82% 16%
17	LL	214	 5% 80% 17%
18	LM	178	 75% 20%
19	LO	211	 85% 13%
20	LP	218	 55% 9% 37%
21	LQ	204	 80% 19%
22	LR	203	 87% 11%
23	LS	184	 67% 19% 14%
24	LT	188	 86% 13%
25	LU	196	 73% 15% 8%
26	LV	176	 83% 17%
27	LW	160	 84% 14%
28	LX	128	 62% 15% 23%

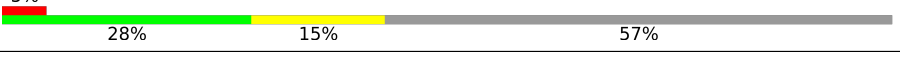
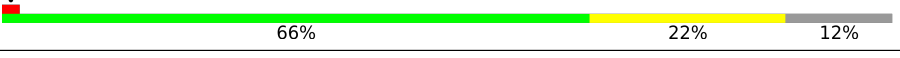
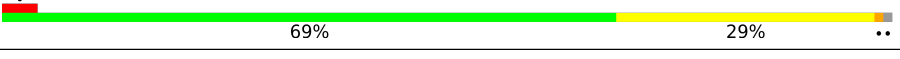
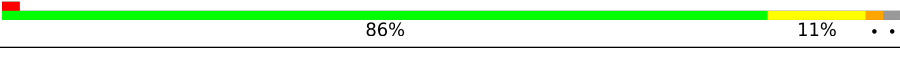
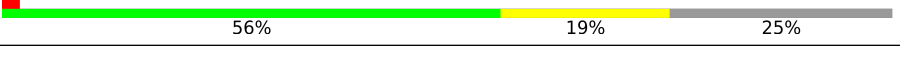
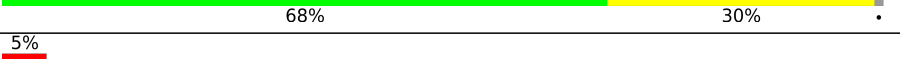
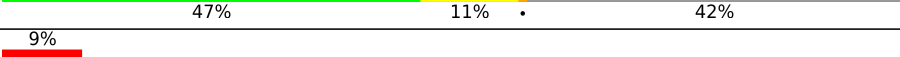
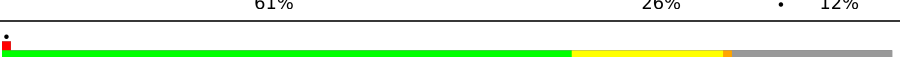
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Mol	Chain	Length	Quality of chain
29	LY	140	
30	LZ	157	
31	La	156	
32	Lb	145	
33	Lc	136	
34	Ld	148	
35	Le	245	
36	Lf	115	
37	Lg	125	
38	Lh	135	
39	Li	110	
40	Lj	117	
41	Lk	123	
42	Ll	105	
43	Lm	97	
44	Ln	70	
45	Lo	51	
46	Lp	128	
47	Lq	106	
48	Lr	92	
49	Ls	137	
50	Lt	318	
51	Lx	217	
52	S2	1870	
53	SB	84	

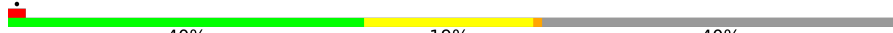
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Mol	Chain	Length	Quality of chain
54	SC	69	
55	SD	156	
56	SE	133	
57	SF	115	
58	SG	317	
59	SH	56	
60	SL	295	
61	SM	264	
62	SN	293	
63	SO	281	
64	SP	263	
65	SQ	204	
66	SR	249	
67	SS	432	
68	ST	208	
69	SU	194	
70	SV	165	
71	SW	158	
72	SX	132	
73	SY	151	
74	SZ	151	
75	Sa	145	
76	Sb	172	
77	Sc	135	
78	Sd	152	

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Mol	Chain	Length	Quality of chain
79	Se	145	
80	Sf	119	
81	Sg	83	
82	Sh	130	
83	Si	143	
84	Sj	130	
85	Sk	124	
86	Sl	25	

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 230266 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 eEFSec.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	519	Total	C	N	O	S	0	0
			3335	2110	616	599	10		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP P57772
E	-18	GLY	-	expression tag	UNP P57772
E	-17	SER	-	expression tag	UNP P57772
E	-16	SER	-	expression tag	UNP P57772
E	-15	HIS	-	expression tag	UNP P57772
E	-14	HIS	-	expression tag	UNP P57772
E	-13	HIS	-	expression tag	UNP P57772
E	-12	HIS	-	expression tag	UNP P57772
E	-11	HIS	-	expression tag	UNP P57772
E	-10	HIS	-	expression tag	UNP P57772
E	-9	SER	-	expression tag	UNP P57772
E	-8	SER	-	expression tag	UNP P57772
E	-7	GLY	-	expression tag	UNP P57772
E	-6	LEU	-	expression tag	UNP P57772
E	-5	VAL	-	expression tag	UNP P57772
E	-4	PRO	-	expression tag	UNP P57772
E	-3	ARG	-	expression tag	UNP P57772
E	-2	GLY	-	expression tag	UNP P57772
E	-1	SER	-	expression tag	UNP P57772
E	0	HIS	-	expression tag	UNP P57772
E	409	GLU	GLN	conflict	UNP P57772

- Molecule 2 is a RNA chain called human Ser-tRNA-Sec.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	90	Total	C	N	O	P	0	0
			1914	853	334	637	90		

- Molecule 3 is a RNA chain called CrPV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	183	Total	C	N	O	P	0	0
			3882	1739	675	1285	183		

- Molecule 4 is a RNA chain called GPX4 SECIS element.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	46	Total	C	N	O	P	0	0
			983	438	179	320	46		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1118	U	C	conflict	GB 25123295
S	1126	A	C	conflict	GB 25123295
S	1132	A	U	conflict	GB 25123295
S	1133	G	-	insertion	GB 25123295
S	1134	C	-	insertion	GB 25123295
S	1135	C	-	insertion	GB 25123295
S	1136	C	-	insertion	GB 25123295
S	1150	U	A	conflict	GB 25123295

- Molecule 5 is a protein called SECIS Binding Protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	204	Total	C	N	O	S	0	0
			1379	881	257	238	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	687	ARG	LYS	conflict	UNP Q96T21
B	692	ILE	VAL	conflict	UNP Q96T21

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	3764	Total	C	N	O	P	0	0
			80771	36002	14762	26243	3764		

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- Molecule 8 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 9 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LD	253	Total	C	N	O	S	0	0
			1939	1214	396	323	6		

- Molecule 10 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LF	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 12 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LG	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 13 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LH	232	Total	C	N	O	S	0	0
			1859	1197	354	305	3		

- Molecule 14 is a protein called 60S ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	182	ASN	GLY	conflict	UNP A0A7J8C453
LI	199	HIS	ARG	conflict	UNP A0A7J8C453

- Molecule 15 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LJ	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LJ	184	LEU	ILE	conflict	UNP P62424

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LK	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 17 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LL	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 18 is a protein called 60S ribosomal protein L11.

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

- Molecule 19 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LO	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LO	74	ARG	HIS	conflict	UNP G1TKB3
LO	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 20 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LP	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 21 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LQ	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 22 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LR	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LR	174	LEU	ILE	conflict	UNP A0A0N8ETI8
LR	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 23 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LS	159	Total	C	N	O	S	0	0
			1288	808	249	222	9		

- Molecule 24 is a protein called 60S ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LT	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LT	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 25 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LU	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 26 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LV	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LV	36	ASN	ILE	conflict	UNP A0A1Z5LHJ5

- Molecule 27 is a protein called 60S ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 28 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LX	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LX	60	ALA	VAL	conflict	UNP Q4R5I3

- Molecule 29 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LY	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 30 is a protein called 60S ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LZ	93	Total	C	N	O	S	0	0
			766	480	153	129	4		

- Molecule 31 is a protein called 60S ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	La	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 32 is a protein called 60S ribosomal protein L26.

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

- Molecule 33 is a protein called 60S ribosomal protein L27.

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

- Molecule 34 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 35 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 36 is a protein called 60S ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 37 is a protein called 60S ribosomal protein eL31.

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

- Molecule 38 is a protein called 60S ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lh	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 39 is a protein called 60S ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Li	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 40 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lj	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 41 is a protein called 60S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lk	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 42 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ll	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 43 is a protein called 60S ribosomal protein L37.

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

- Molecule 44 is a protein called 60S ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ln	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 45 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lo	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 46 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lp	52	Total	C	N	O	S	0	0
			431	269	90	66	6		

- Molecule 47 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lq	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 48 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lr	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 49 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ls	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

- Molecule 50 is a protein called 60S ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lt	115	Total	C	N	O		0	0
			567	337	115	115			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lt	106	LEU	LYS	conflict	UNP G1SPK4

- Molecule 51 is a protein called 60S ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lx	196	Total	C	N	O		0	0
			972	580	196	196			

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S2	1770	Total	C	N	O	P	0	0
			37825	16906	6780	12369	1770		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	251	C	U	conflict	GB 37956930
S2	583	U	C	conflict	GB 37956930
S2	584	A	C	conflict	GB 37956930
S2	585	A	G	conflict	GB 37956930
S2	1338	4AC	C	conflict	GB 37956930
S2	1843	4AC	C	conflict	GB 37956930

- Molecule 53 is a protein called 40S ribosomal protein S27.

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

- Molecule 54 is a protein called 40S ribosomal protein S28.

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

- Molecule 55 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SD	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 56 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SE	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 57 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SF	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 58 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SG	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 59 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SH	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SL	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 61 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SM	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 62 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SN	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SN	33	ILE	VAL	conflict	UNP O18789
SN	101	ALA	SER	conflict	UNP O18789

- Molecule 63 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 64 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 65 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 66 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SR	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 67 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SS	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 68 is a protein called 40S ribosomal protein S8.

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

- Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SU	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 70 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SV	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 71 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SW	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 72 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SX	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 73 is a protein called 40S ribosomal protein uS15.

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

- Molecule 74 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SZ	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 75 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sa	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 76 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sb	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 77 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sc	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 78 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sd	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 79 is a protein called 40S Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Se	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 80 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sf	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 81 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sg	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 82 is a protein called 40S ribosomal protein S15a.

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

- Molecule 83 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Si	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 84 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Sj	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

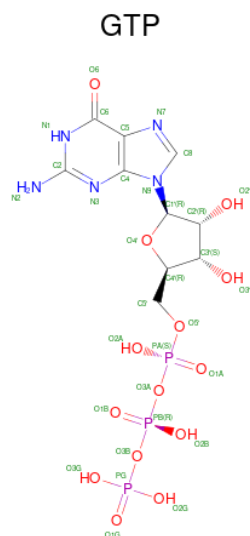
- Molecule 85 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Sk	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 86 is a protein called 60S ribosomal protein L41.

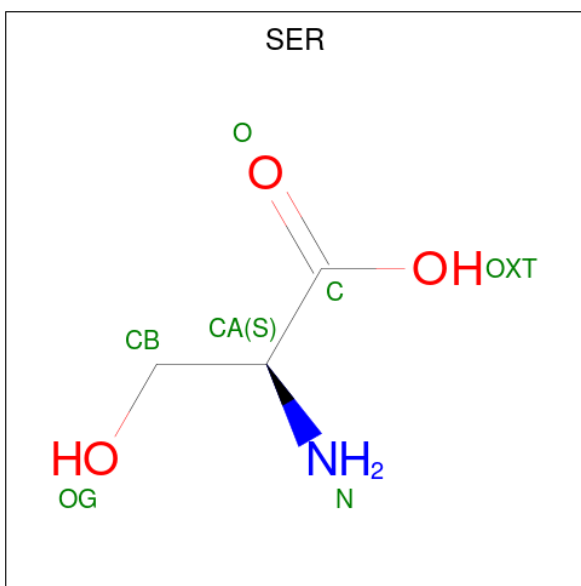
Mol	Chain	Residues	Atoms					AltConf	Trace
86	Sl	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 87 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
87	E	1	Total 32	C 10	N 5	O 14	P 3	0
87	L7	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 88 is SERINE (CCD ID: SER) (formula: $\text{C}_3\text{H}_7\text{NO}_3$).



Mol	Chain	Residues	Atoms				AltConf
88	F	1	Total	C	N	O	0
			6	3	1	2	

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	I	2	Total 2	Mg 2	0
89	L5	162	Total 162	Mg 162	0
89	L7	2	Total 2	Mg 2	0
89	L8	1	Total 1	Mg 1	0
89	LD	1	Total 1	Mg 1	0
89	LS	1	Total 1	Mg 1	0
89	LY	1	Total 1	Mg 1	0
89	S2	55	Total 55	Mg 55	0

- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
90	L5	17	Total 17	K 17	0
90	S2	1	Total 1	K 1	0

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	Lj	1	Total 1	Zn 1	0
91	Lm	1	Total 1	Zn 1	0
91	Lp	1	Total 1	Zn 1	0
91	Lq	1	Total 1	Zn 1	0
91	Lr	1	Total 1	Zn 1	0
91	SD	1	Total 1	Zn 1	0
91	SF	2	Total 2	Zn 2	0
91	SH	1	Total 1	Zn 1	0

- Molecule 92 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
92	SZ	1	Total 1	Na 1	0

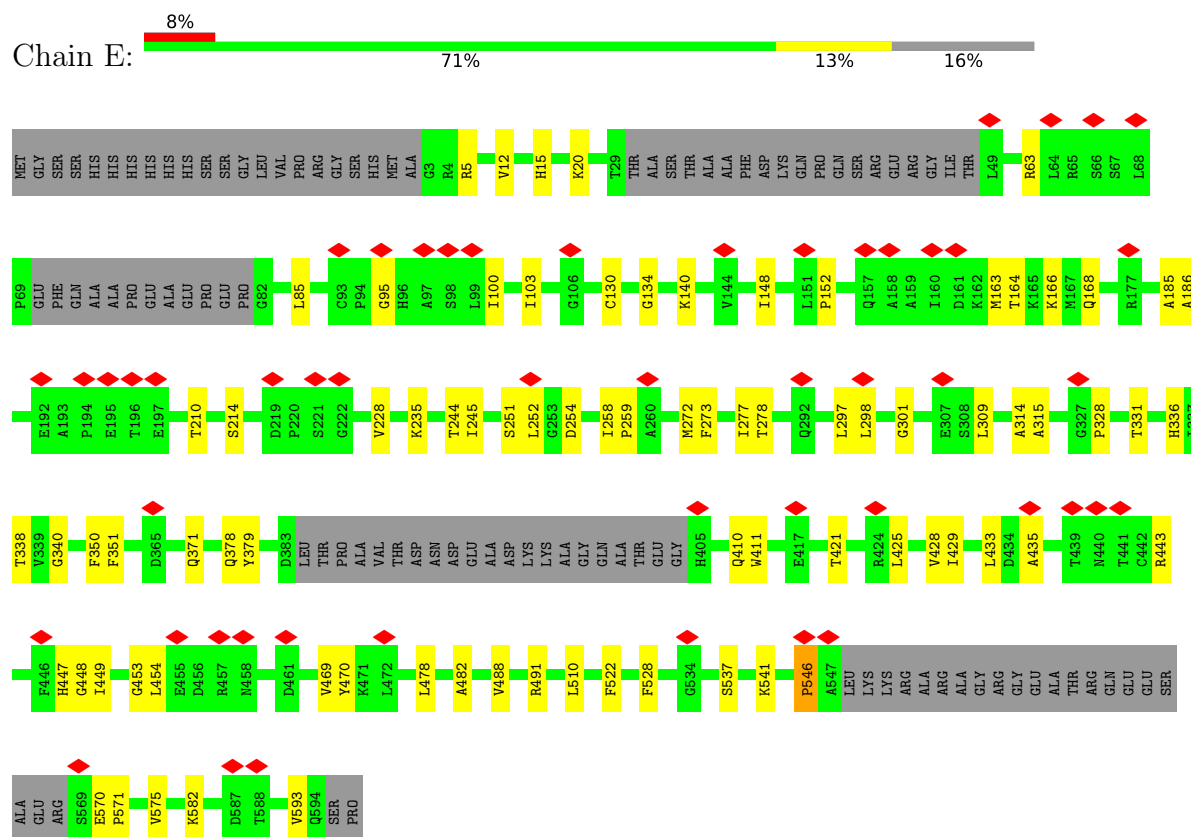
- Molecule 93 is water.

Mol	Chain	Residues	Atoms		AltConf
93	L5	56	Total 56	O 56	0
93	L7	1	Total 1	O 1	0
93	L8	1	Total 1	O 1	0
93	LD	1	Total 1	O 1	0
93	LE	1	Total 1	O 1	0
93	LH	1	Total 1	O 1	0
93	LK	1	Total 1	O 1	0
93	LL	1	Total 1	O 1	0
93	LQ	1	Total 1	O 1	0
93	LV	1	Total 1	O 1	0
93	Ld	1	Total 1	O 1	0
93	S2	34	Total 34	O 34	0
93	SF	1	Total 1	O 1	0
93	SH	1	Total 1	O 1	0
93	SW	1	Total 1	O 1	0
93	Sd	1	Total 1	O 1	0
93	Se	1	Total 1	O 1	0
93	Si	2	Total 2	O 2	0

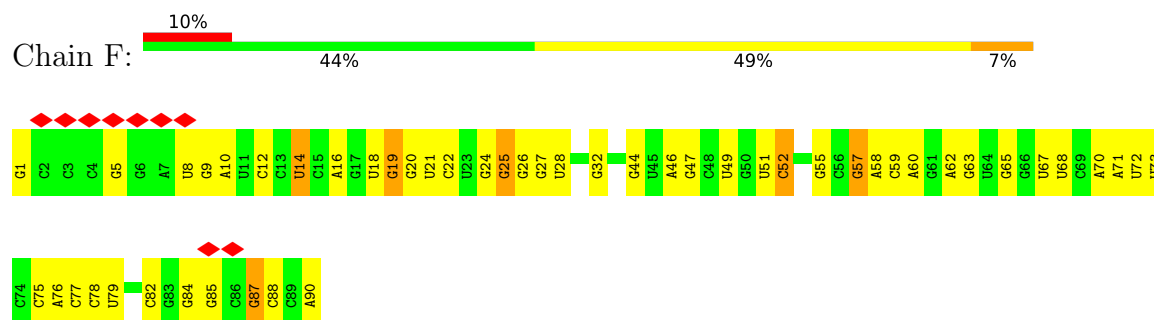
3 Residue-property plots [i](#)

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

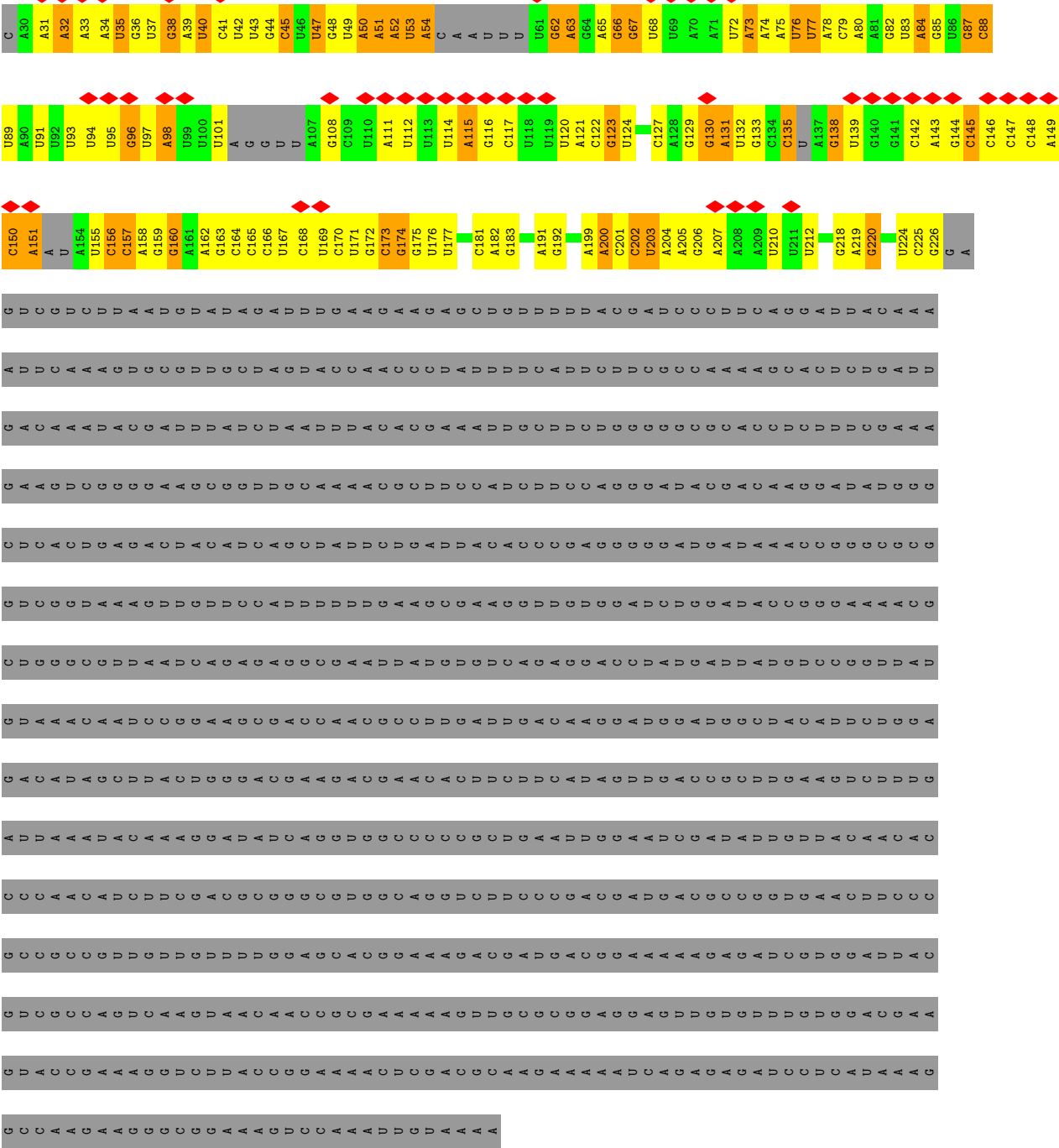
- Molecule 1: eEFSec



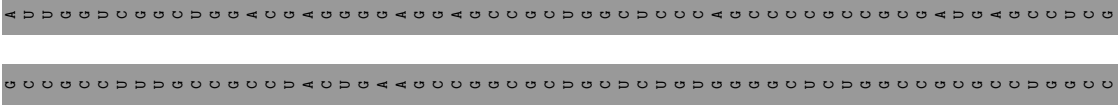
- Molecule 2: human Ser-tRNA-Sec

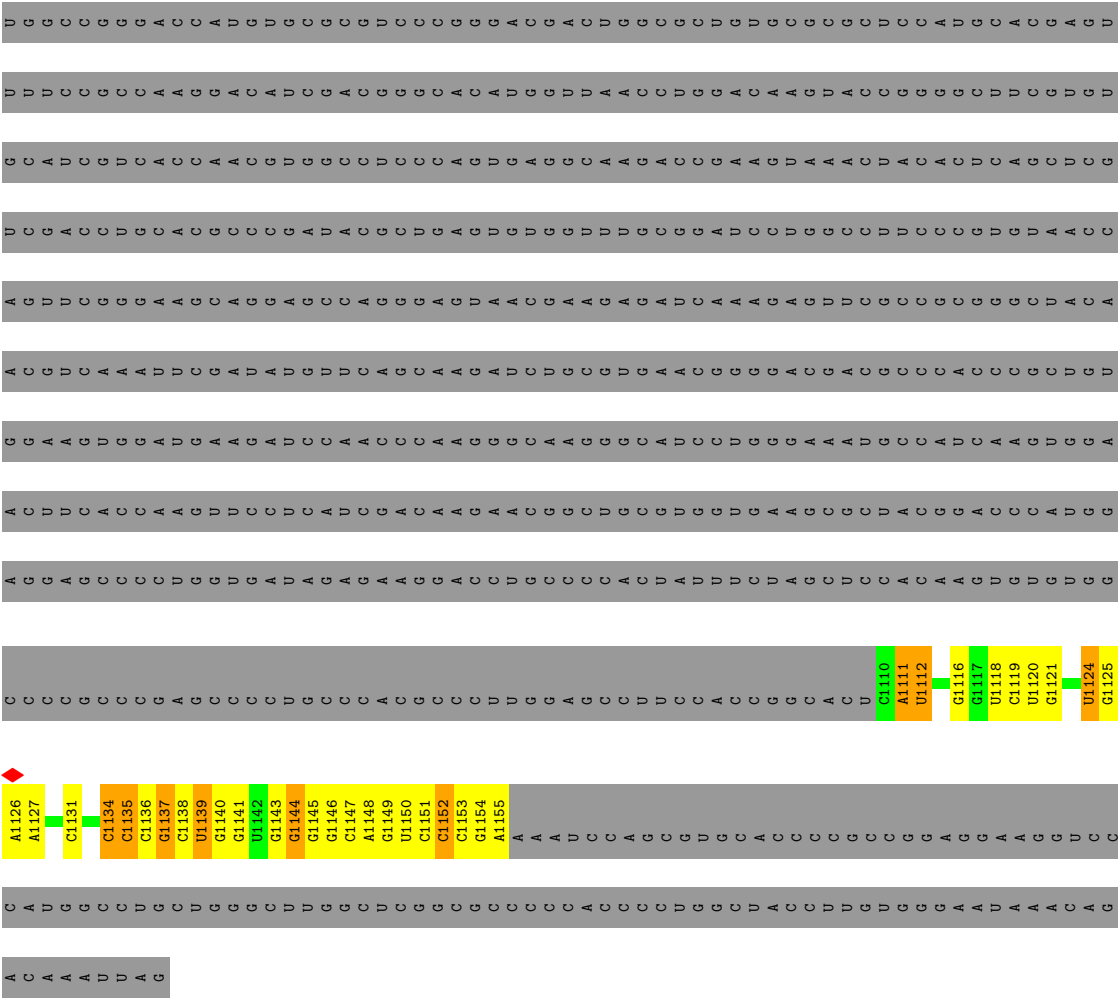


- Molecule 3: CrPV IRES

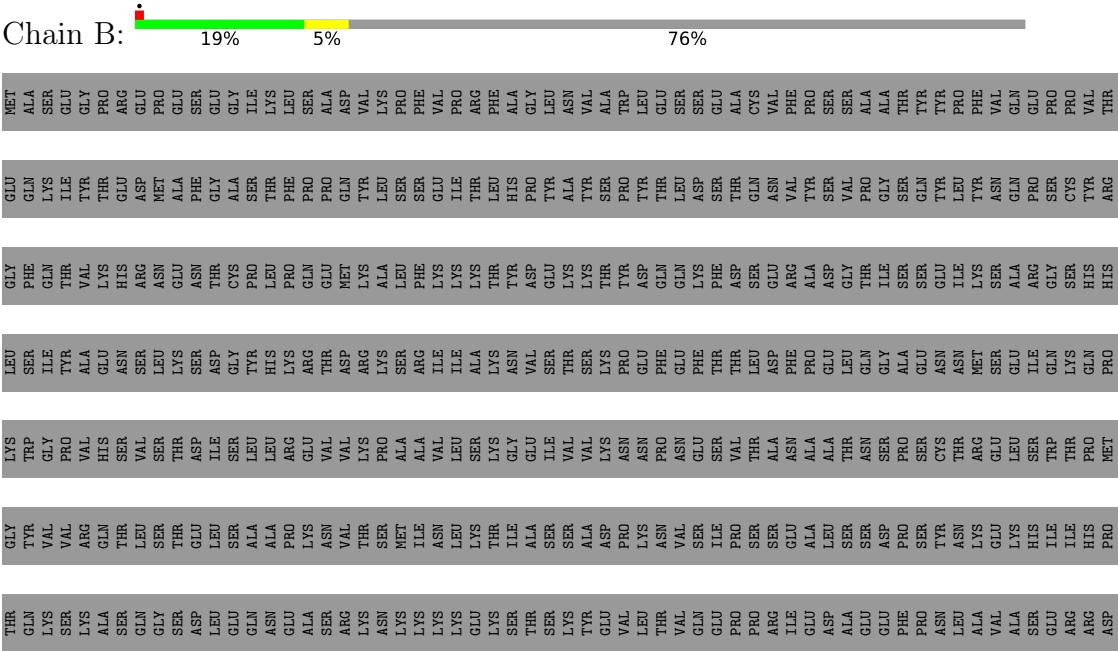


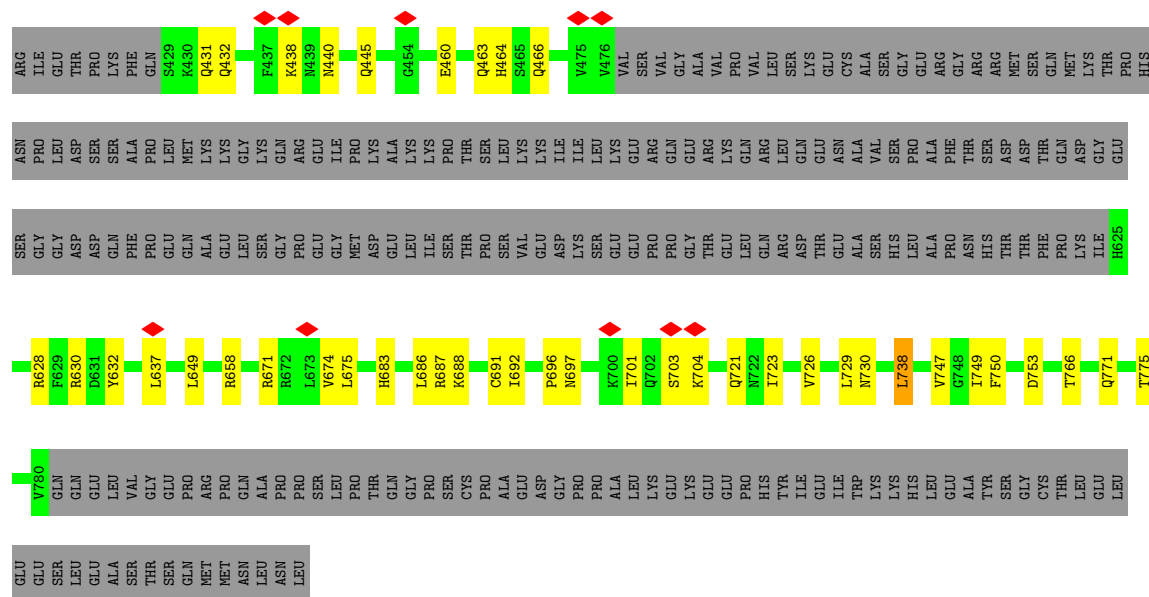
● Molecule 4: GPX4 SECIS element





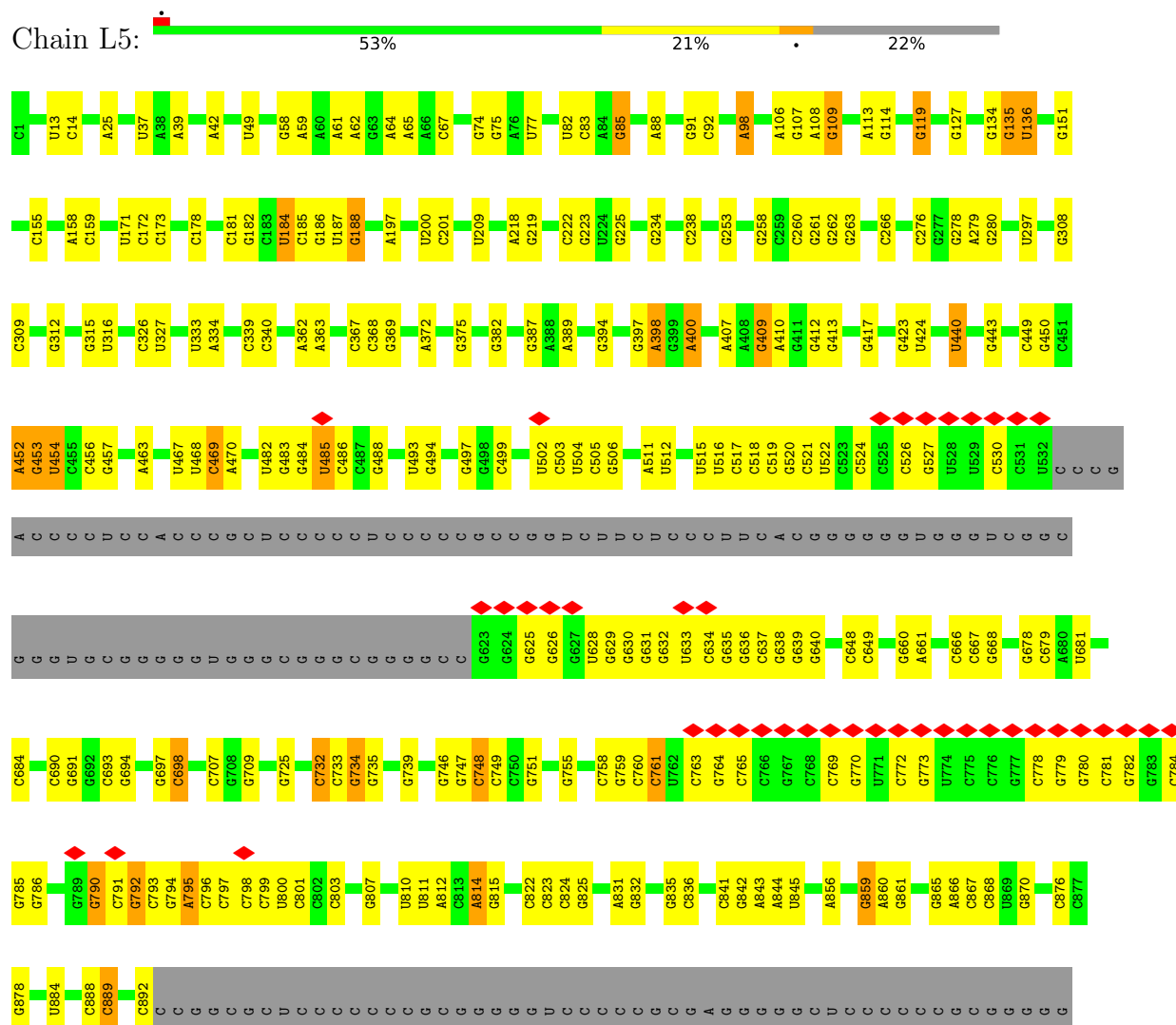
● Molecule 5: SECIS Binding Protein 2

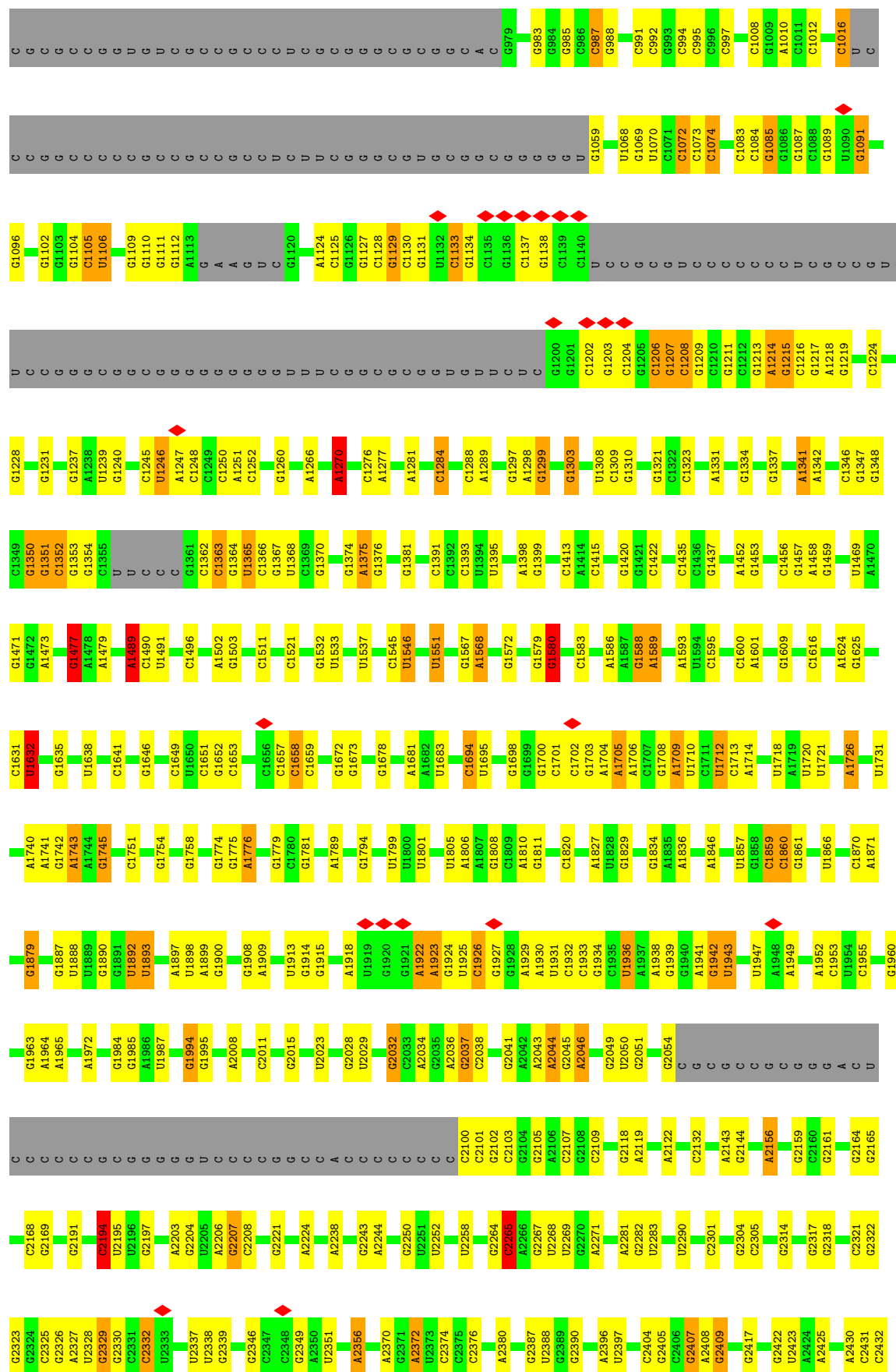




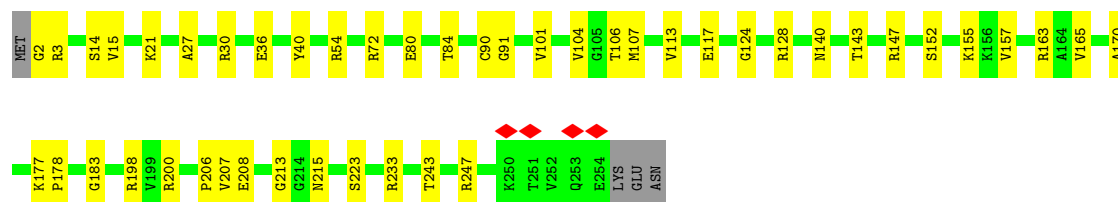
• Molecule 6: 28S rRNA

Chain L5:



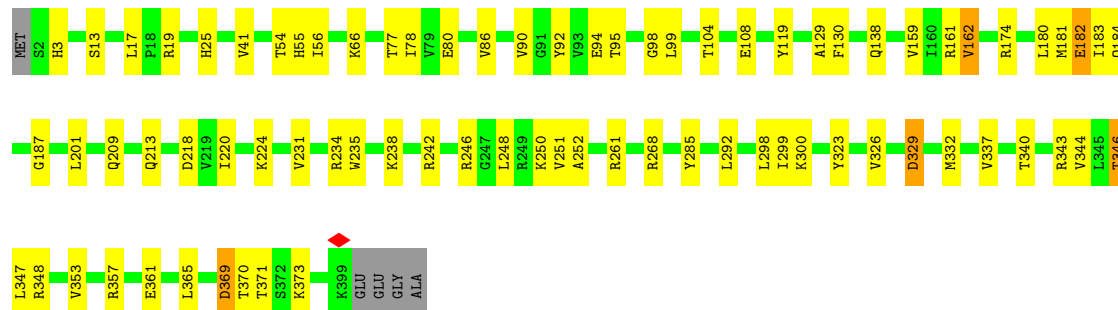






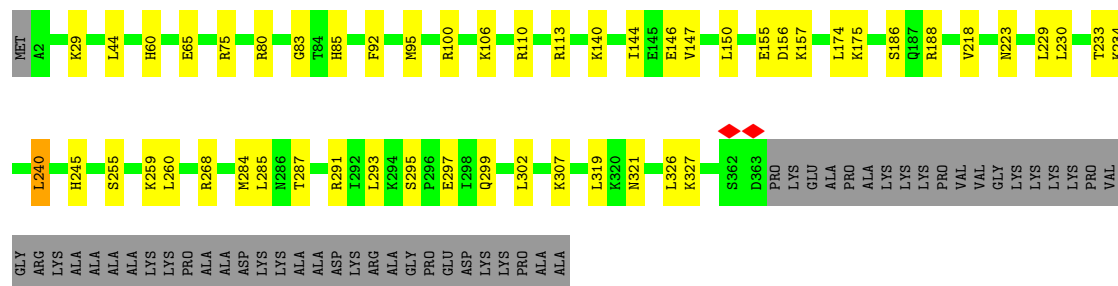
• Molecule 10: 60S ribosomal protein L3

Chain LE: 79% 18% ..



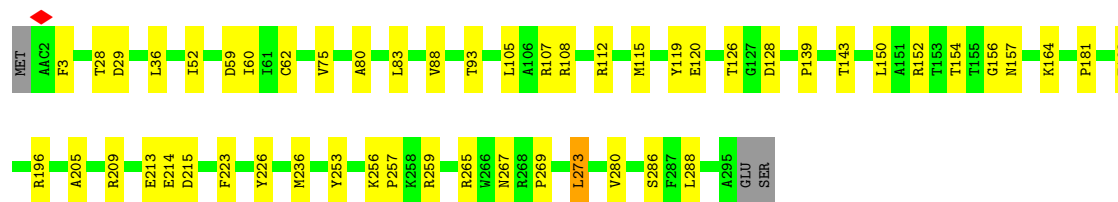
• Molecule 11: 60S ribosomal protein L4

Chain LF: 75% 12% 12%



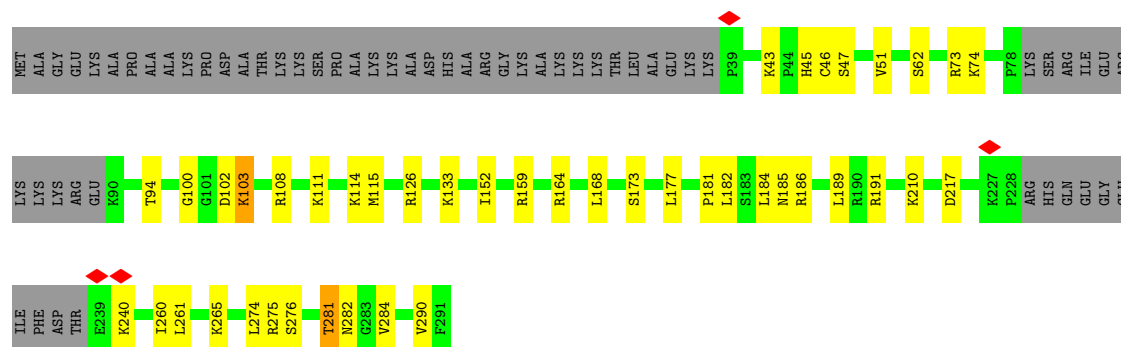
• Molecule 12: Ribosomal_L18_c domain-containing protein

Chain LG: 81% 17%



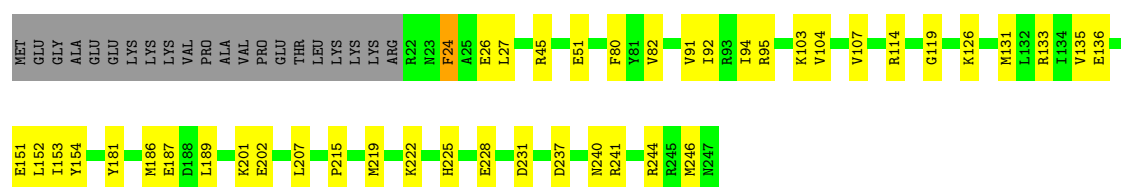
• Molecule 13: 60S ribosomal protein L6

Chain LH: 65% 14% 20%



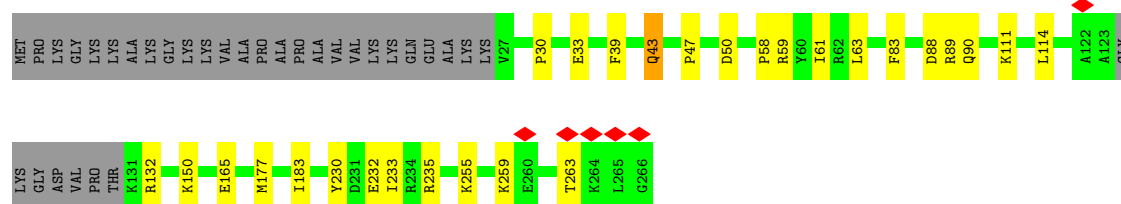
• Molecule 14: 60S ribosomal Protein uL30

Chain LI: 74% 17% 9%



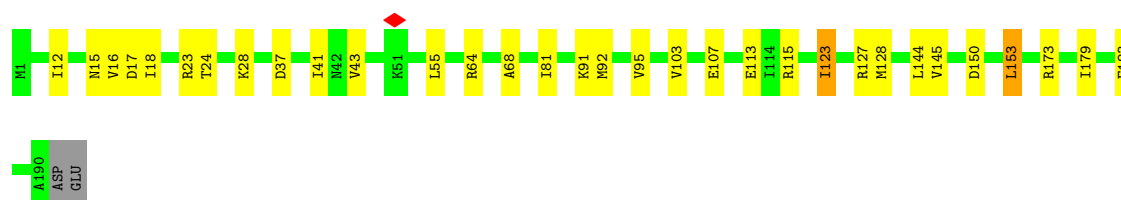
• Molecule 15: 60S ribosomal protein eL8

Chain LJ: 77% 10% 12%



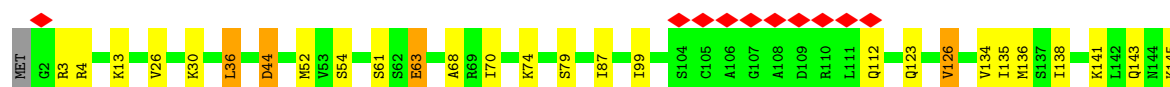
• Molecule 16: 60S ribosomal protein L9

Chain LK: 82% 16% ..



• Molecule 17: 60S ribosomal protein L10

Chain LL: 5% 80% 17% .





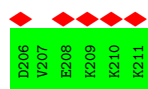
- Molecule 18: 60S ribosomal protein L11

Chain LM: 75% 20% . .



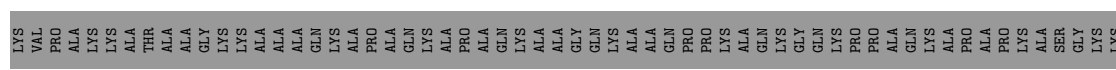
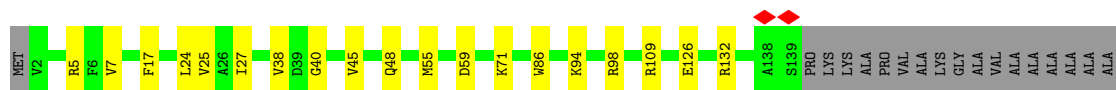
- Molecule 19: 60S ribosomal protein eL13

Chain LO: 85% 13% .



- Molecule 20: 60S ribosomal protein L14

Chain LP: 55% 9% 37%



- Molecule 21: 60S ribosomal protein L15

Chain LQ: 80% 19%

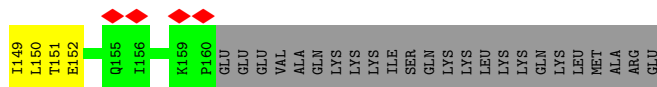


- Molecule 22: 60S ribosomal protein uL13

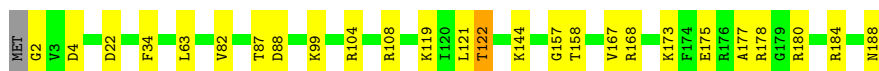
Chain LR: 87% 11% .



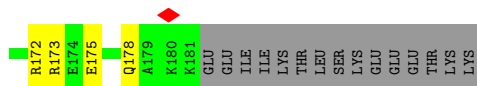
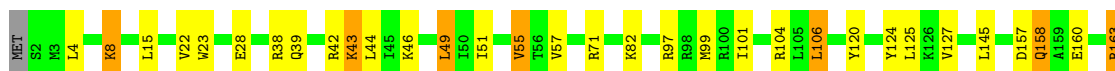
- Molecule 23: 60S ribosomal protein uL22



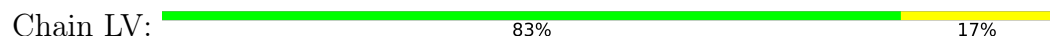
- Molecule 24: 60S ribosomal Protein eL18



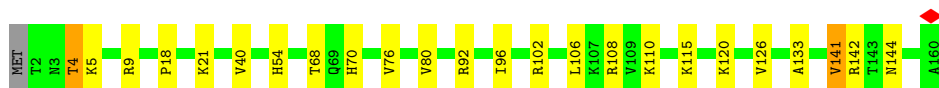
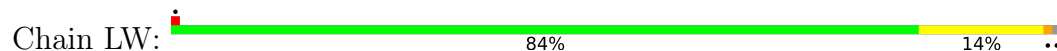
- Molecule 25: 60S ribosomal protein L19



- Molecule 26: 60S ribosomal protein eL20

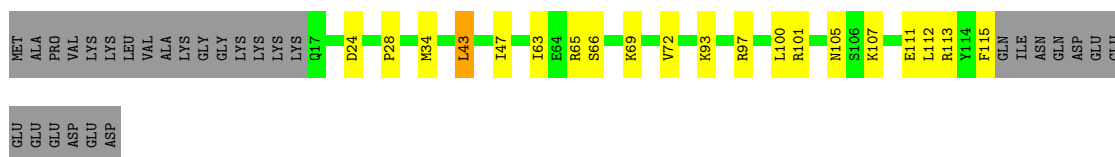


- Molecule 27: 60S ribosomal protein eL21



- Molecule 28: 60S ribosomal protein eL22

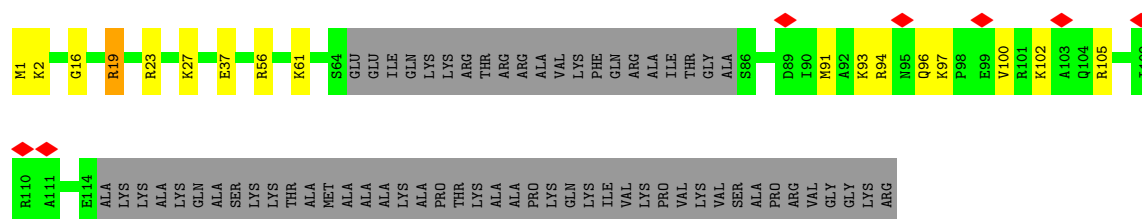




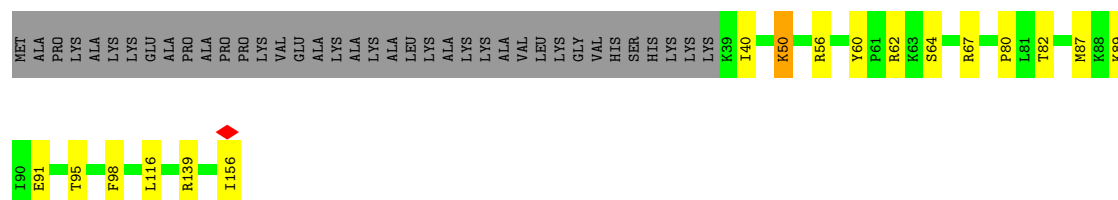
- Molecule 29: 60S ribosomal protein L23



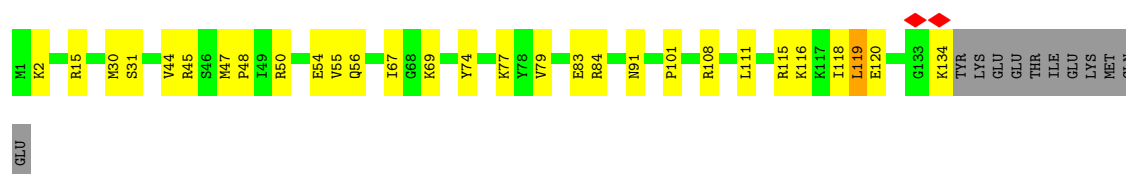
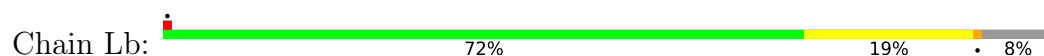
- Molecule 30: 60S ribosomal protein eL24



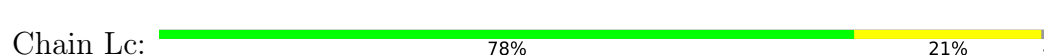
- Molecule 31: 60S ribosomal protein uL23



- Molecule 32: 60S ribosomal protein L26

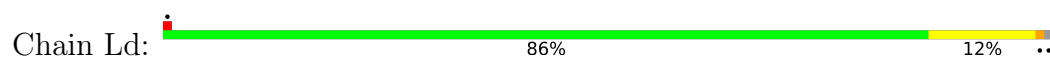


- Molecule 33: 60S ribosomal protein L27

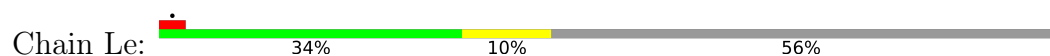




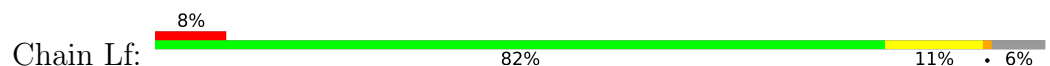
- Molecule 34: 60S ribosomal protein L27a



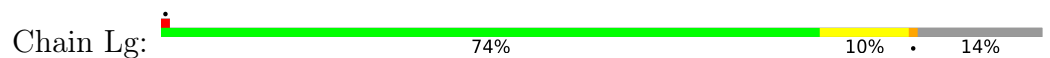
- Molecule 35: 60S ribosomal protein L29



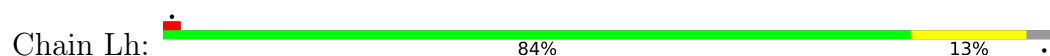
- Molecule 36: 60S ribosomal protein eL30



- Molecule 37: 60S ribosomal protein eL31



- Molecule 38: 60S ribosomal protein eL32



- Molecule 39: 60S ribosomal protein eL33

Chain Li:  87% 12%



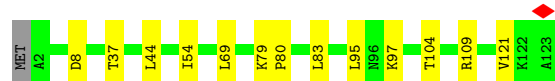
- Molecule 40: 60S ribosomal protein L34

Chain Lj:  86% 10%



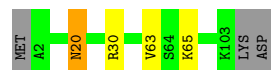
- Molecule 41: 60S ribosomal protein uL29

Chain Lk:  89% 11%



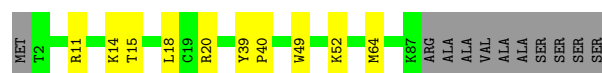
- Molecule 42: 60S ribosomal protein L36

Chain Ll:  93%



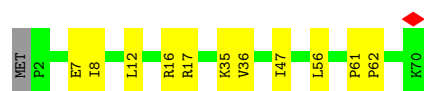
- Molecule 43: 60S ribosomal protein L37

Chain Lm:  78% 10% 11%



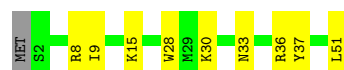
- Molecule 44: 60S ribosomal protein eL38

Chain Ln:  83% 16%

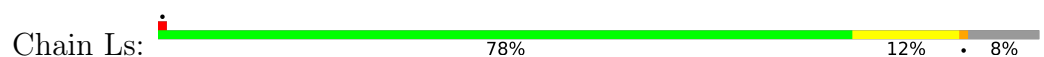
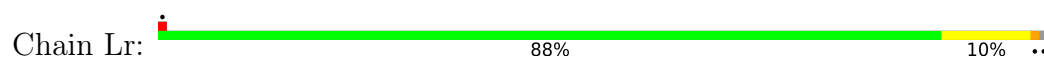
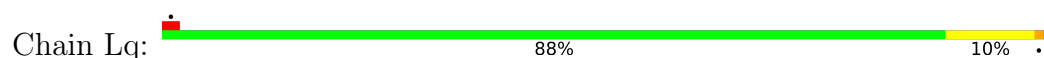


- Molecule 45: 60S ribosomal protein eL39

Chain Lo:  80% 18%

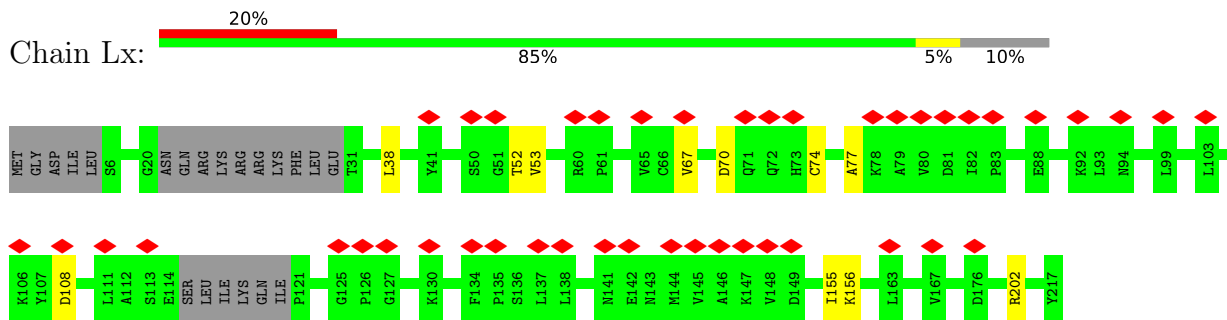


- Chain Lp:

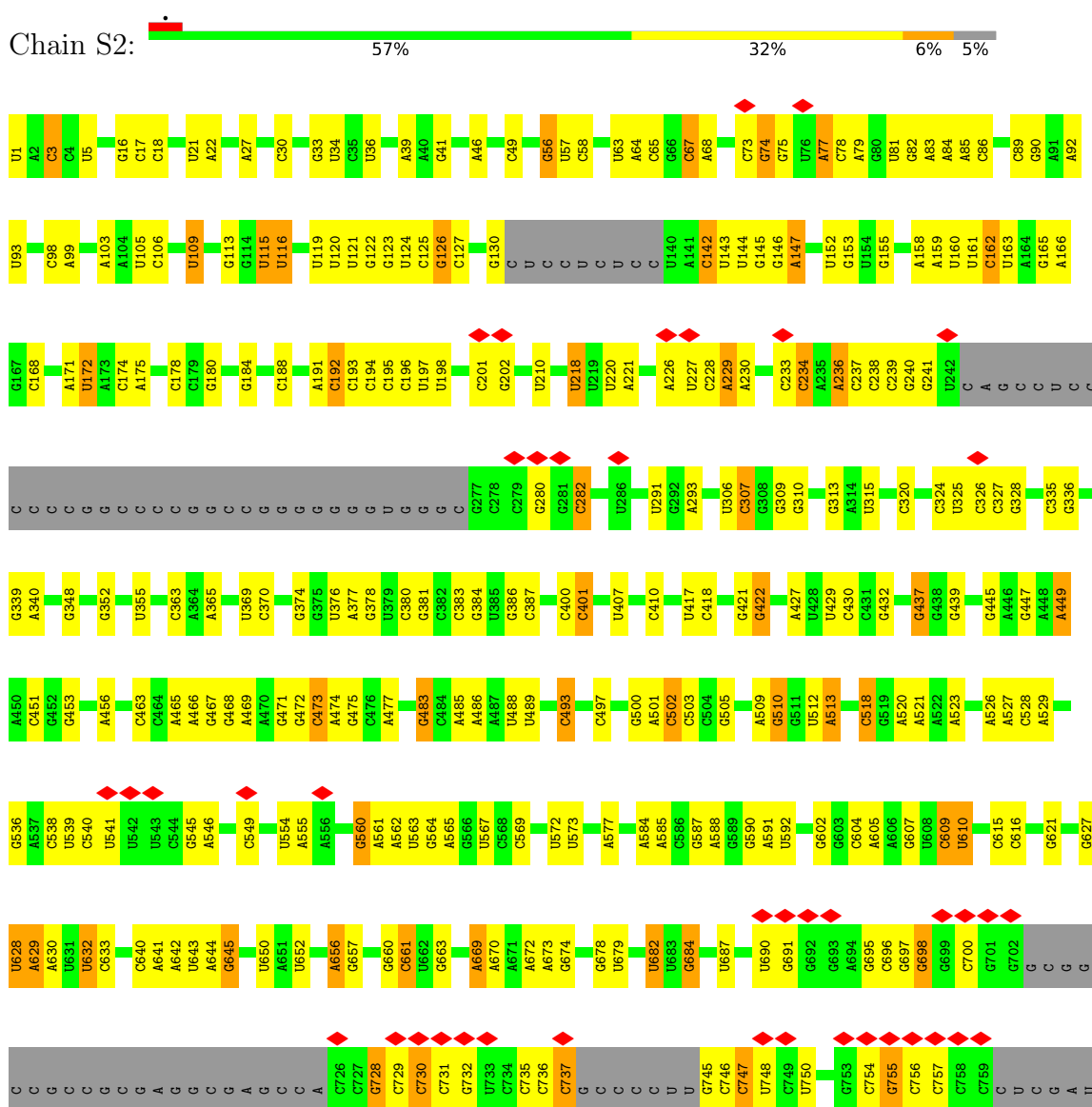


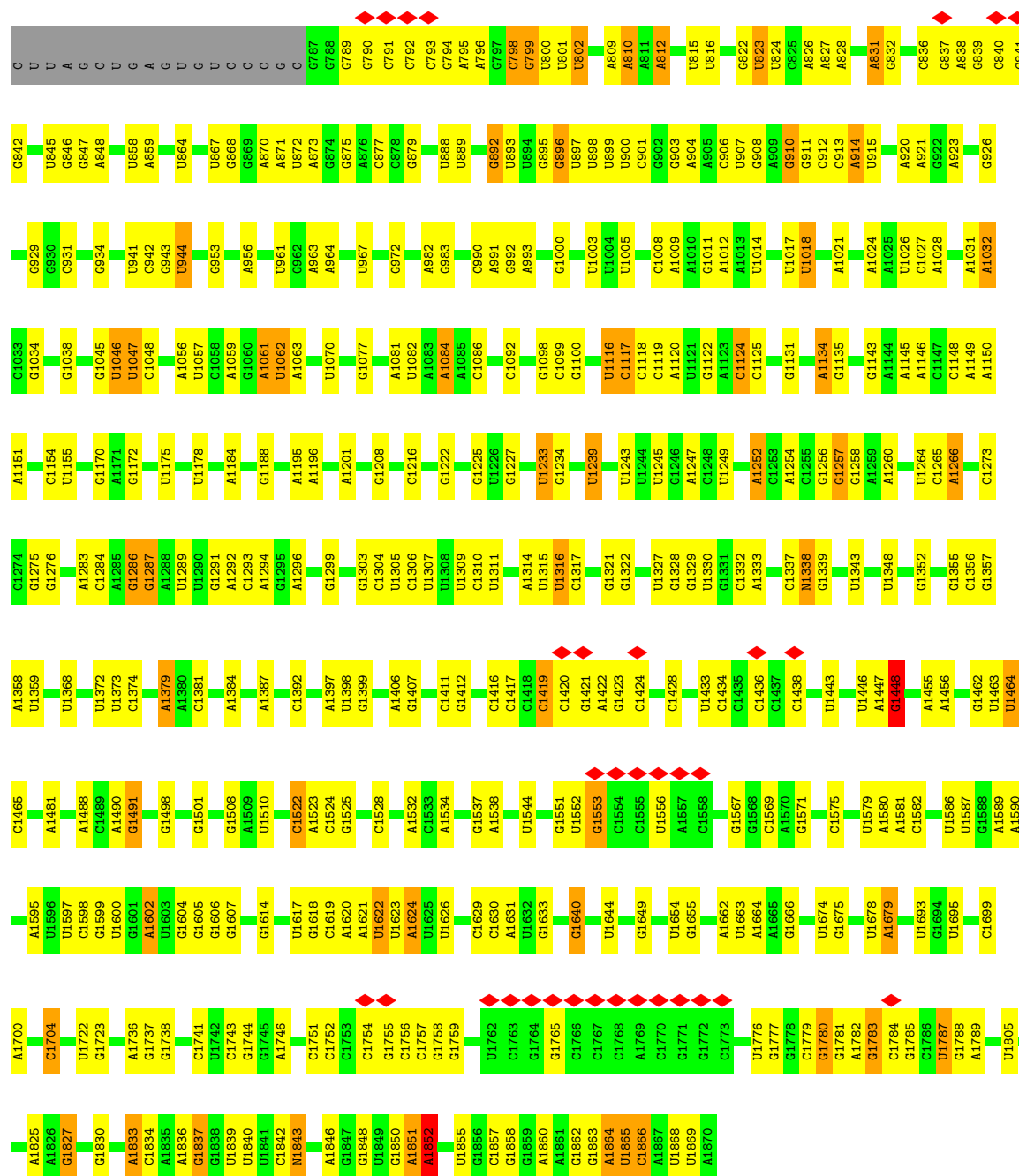
ALA
ALA
ALA
ASP
ALA
ALA
LEU
PRO
ALA
LYS
VAL
GLU
GLU
LYS
LYS
GLU
SER
GLU
GLU
SER
ASP
GLU
MET
ASP
GLY
PHE
GLY
LEU
PHE
ASP

• Molecule 51: 60S ribosomal protein uL1

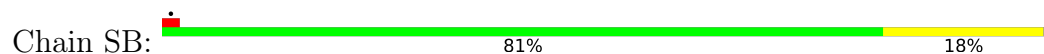


• Molecule 52: 18S rRNA





- Molecule 53: 40S ribosomal protein S27

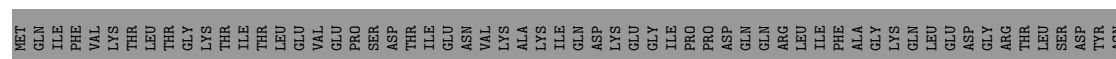
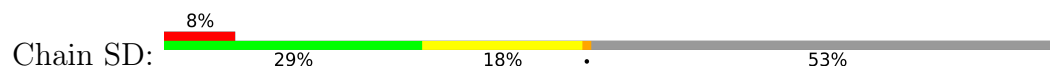


- Molecule 54: 40S ribosomal protein S28

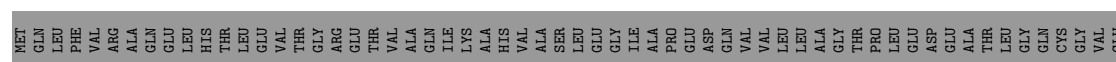




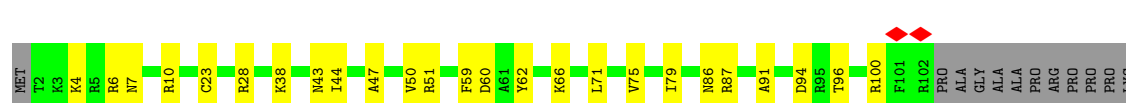
- Molecule 55: 40S ribosomal protein S27a



- Molecule 56: 40S ribosomal protein S30



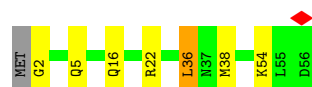
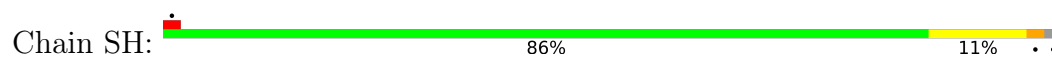
- Molecule 57: Ribosomal protein eS26



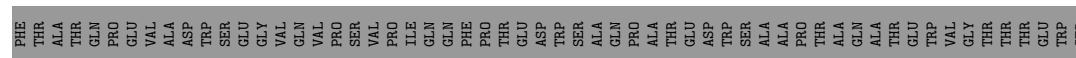
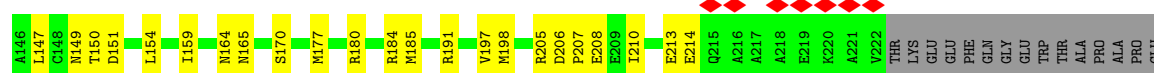
- Molecule 58: RACK1



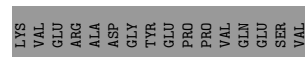
- Molecule 59: 40S ribosomal protein uS14



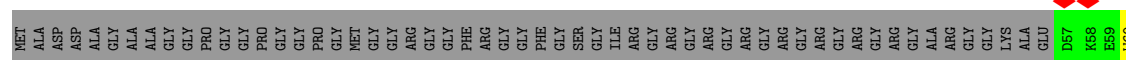
- Molecule 60: 40S ribosomal protein SA

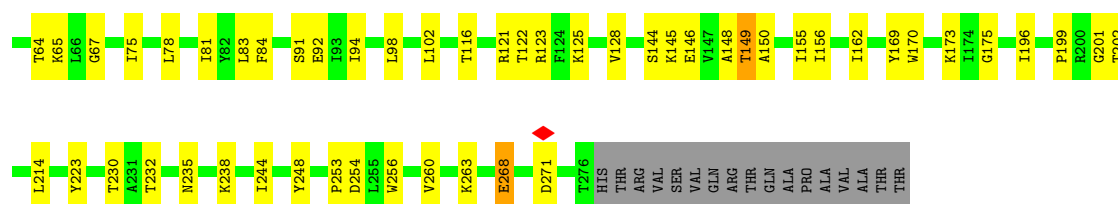


- Molecule 61: 40S ribosomal protein S3a

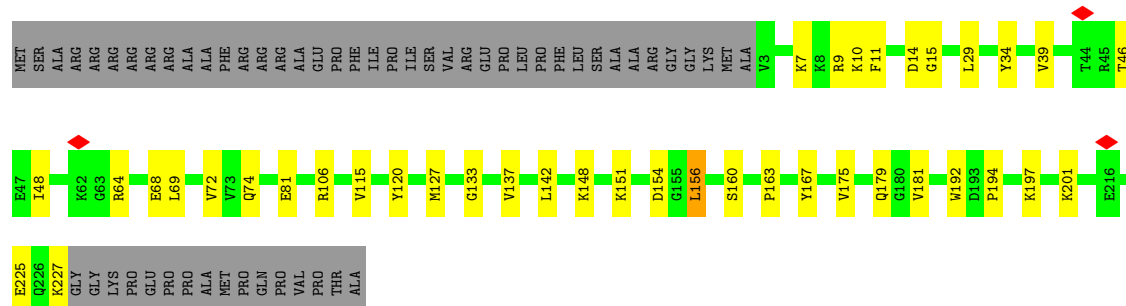


- Molecule 62: 40S ribosomal protein uS5

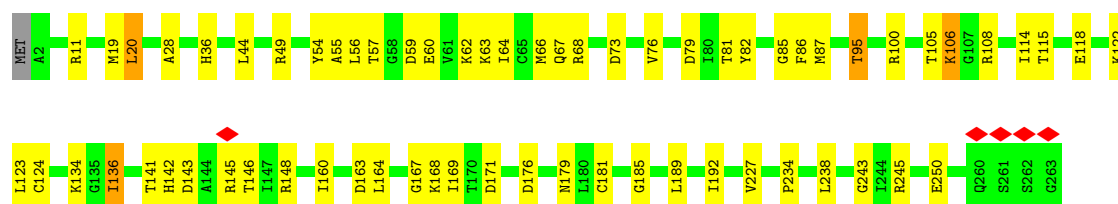




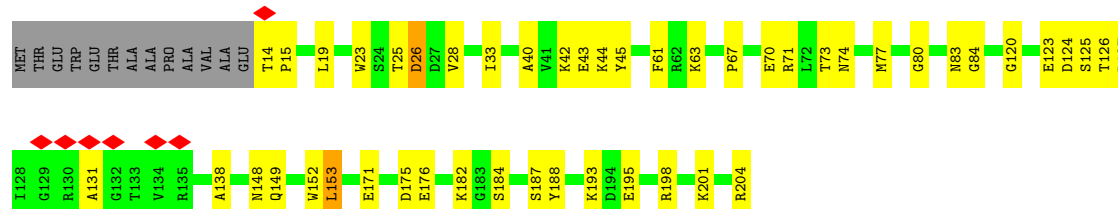
• Molecule 63: 40S ribosomal protein S3



• Molecule 64: 40S ribosomal protein eS4



• Molecule 65: Ribosomal protein S5



• Molecule 66: 40S ribosomal protein S6

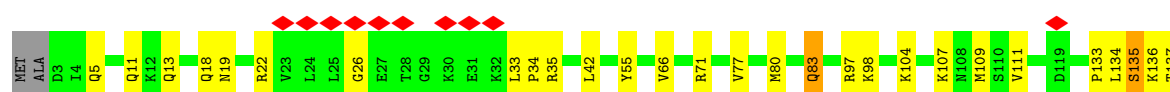
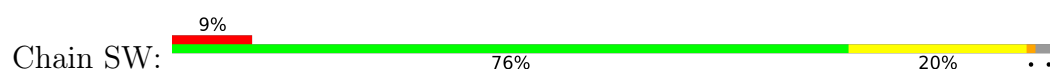




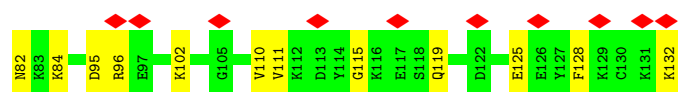
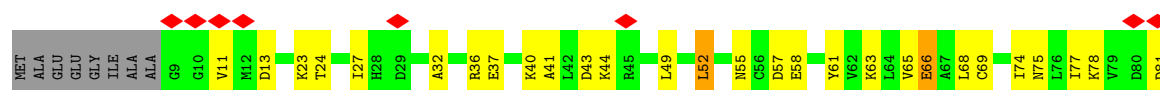
- Molecule 70: 40S ribosomal protein eS10



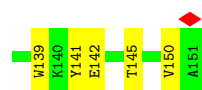
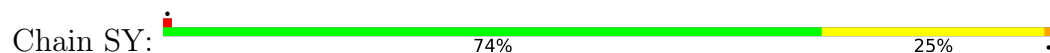
- Molecule 71: 40S ribosomal protein S11



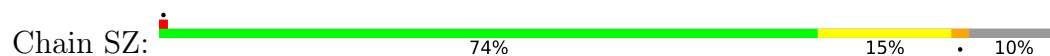
- Molecule 72: 40S ribosomal protein S12



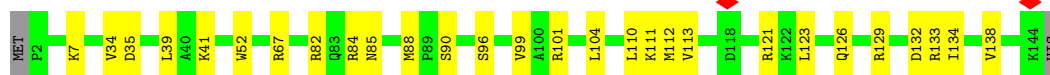
- Molecule 73: 40S ribosomal protein uS15



- Molecule 74: 40S ribosomal protein uS11

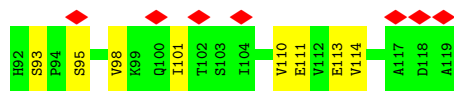
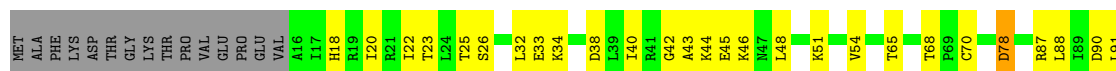


Chain Se:  79% 19%



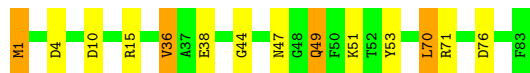
- Molecule 80: 40S ribosomal protein uS10

Chain Sf:  6% 58% 29% 13%



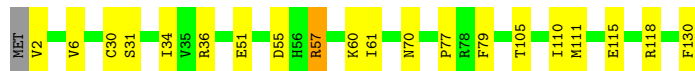
- Molecule 81: 40S ribosomal protein eS21

Chain Sg:  83% 12% 5%



- Molecule 82: 40S ribosomal protein S15a

Chain Sh:  84% 15% ..



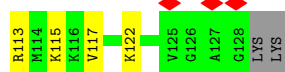
- Molecule 83: 40S ribosomal protein S23

Chain Si:  80% 17% ...

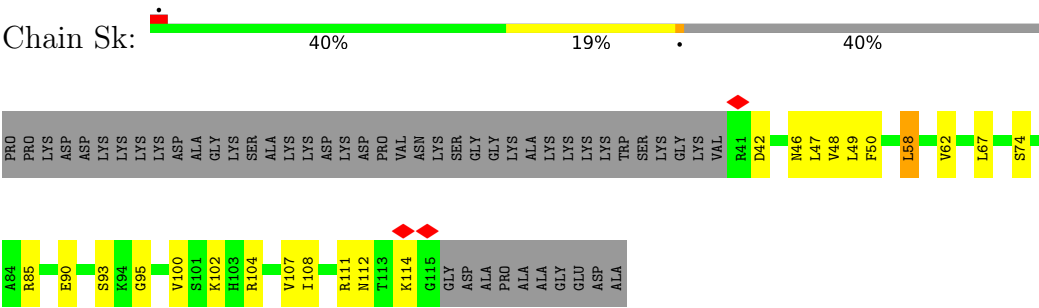


- Molecule 84: 40S ribosomal protein S24

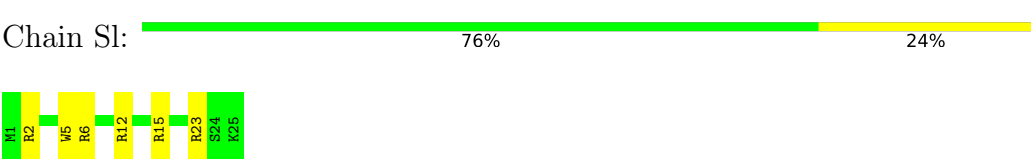
Chain Sj:  68% 28%



● Molecule 85: 40S ribosomal protein S25



● Molecule 86: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77142	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.629	Depositor
Minimum map value	0.000	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	520.704, 520.704, 520.704	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.017, 1.017, 1.017	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, OMG, 7MG, OMC, PSU, NA, AME, SAC, GTP, MLZ, ZN, AAC, HIC, AYA, UR3, MA6, 1MA, NMM, 6MZ, OMU, HY3, A2M, 4AC, MG, K, M3L

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	E	0.10	0/3403	0.37	2/4656 (0.0%)
2	F	0.15	1/2136 (0.0%)	0.18	0/3325
3	I	0.10	0/4335	0.21	0/6738
4	S	0.09	0/1098	0.22	0/1710
5	B	0.15	0/1398	0.34	1/1905 (0.1%)
6	L5	0.18	1/87426 (0.0%)	0.19	0/136397
7	L7	0.16	0/2835	0.17	0/4418
8	L8	0.16	0/3635	0.17	0/5661
9	LD	0.16	0/1977	0.26	0/2651
10	LE	0.16	0/3261	0.26	0/4364
11	LF	0.16	0/2932	0.24	0/3939
12	LG	0.15	0/2437	0.23	0/3264
13	LH	0.13	0/1896	0.24	0/2541
14	LI	0.16	0/1922	0.24	0/2563
15	LJ	0.14	0/1908	0.23	0/2566
16	LK	0.14	0/1535	0.22	0/2063
17	LL	0.15	0/1756	0.25	0/2346
18	LM	0.13	0/1385	0.27	0/1852
19	LO	0.15	0/1733	0.24	0/2316
20	LP	0.15	0/1158	0.24	0/1547
21	LQ	0.18	0/1746	0.24	0/2338
22	LR	0.17	0/1662	0.24	0/2222
23	LS	0.16	0/1315	0.24	0/1763
24	LT	0.17	0/1539	0.27	0/2054
25	LU	0.13	0/1524	0.21	0/2013
26	LV	0.16	0/1497	0.23	0/2008
27	LW	0.15	0/1326	0.23	0/1770
28	LX	0.12	0/820	0.27	0/1100
29	LY	0.15	0/1048	0.25	0/1402
30	LZ	0.13	0/779	0.23	0/1034
31	La	0.14	0/984	0.24	0/1323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.14	0/1132	0.22	0/1504
33	Lc	0.13	0/1130	0.20	0/1507
34	Ld	0.17	0/1191	0.26	0/1590
35	Le	0.13	0/884	0.28	0/1169
36	Lf	0.13	0/847	0.20	0/1134
37	Lg	0.15	0/903	0.23	0/1216
38	Lh	0.17	0/1088	0.24	0/1451
39	Li	0.17	0/903	0.28	0/1208
40	Lj	0.15	0/916	0.25	0/1220
41	Lk	0.13	0/1021	0.19	0/1348
42	Ll	0.12	0/841	0.21	0/1112
43	Lm	0.17	0/720	0.27	0/952
44	Ln	0.13	0/575	0.22	0/761
45	Lo	0.15	0/459	0.22	0/608
46	Lp	0.15	0/425	0.26	0/562
47	Lq	0.14	0/866	0.22	0/1141
48	Lr	0.14	0/718	0.24	0/953
49	Ls	0.16	0/1020	0.25	0/1366
50	Lt	0.09	0/565	0.26	0/783
51	Lx	0.09	0/969	0.26	0/1347
52	S2	0.16	0/40365	0.17	0/62915
53	SB	0.10	0/665	0.23	0/891
54	SC	0.10	0/497	0.22	0/666
55	SD	0.09	0/622	0.25	0/822
56	SE	0.08	0/462	0.24	0/607
57	SF	0.12	0/828	0.23	0/1109
58	SG	0.09	0/2493	0.25	0/3394
59	SH	0.12	0/470	0.23	0/623
60	SL	0.11	0/1771	0.23	0/2406
61	SM	0.11	0/1841	0.23	0/2459
62	SN	0.12	0/1742	0.24	0/2354
63	SO	0.11	0/1779	0.23	0/2395
64	SP	0.09	0/2118	0.24	0/2849
65	SQ	0.10	0/1531	0.25	0/2059
66	SR	0.09	0/1946	0.24	0/2590
67	SS	0.10	0/1552	0.24	0/2079
68	ST	0.10	0/1715	0.24	0/2287
69	SU	0.10	0/1550	0.25	0/2069
70	SV	0.11	0/834	0.25	0/1125
71	SW	0.11	0/1284	0.24	0/1717
72	SX	0.09	0/968	0.25	0/1296
73	SY	0.11	0/1232	0.22	0/1656
74	SZ	0.12	0/1029	0.27	0/1380

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sa	0.10	0/1069	0.23	0/1429
76	Sb	0.11	0/1142	0.29	0/1528
77	Sc	0.10	0/1094	0.24	0/1469
78	Sd	0.11	0/1226	0.26	0/1643
79	Se	0.09	0/1119	0.21	0/1498
80	Sf	0.11	0/831	0.24	0/1115
81	Sg	0.10	0/636	0.22	0/852
82	Sh	0.12	0/1051	0.23	0/1406
83	Si	0.12	0/1107	0.27	0/1475
84	Sj	0.09	0/1032	0.23	0/1371
85	Sk	0.09	0/604	0.25	0/810
86	Sl	0.14	0/240	0.16	0/305
All	All	0.16	2/242024 (0.0%)	0.21	3/355430 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
83	Si	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	52	C	C4-N4	-5.20	1.23	1.33
6	L5	3517	A2M	O3'-P	5.04	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	571	PRO	N-CA-CB	11.87	110.78	102.35
1	E	546	PRO	N-CA-CB	7.34	110.95	103.25
5	B	704	LYS	CB-CA-C	-5.31	110.43	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	Si	62	HY3	Mainchain

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	E	3335	0	2684	42	0
2	F	1914	0	966	22	0
3	I	3882	0	1960	55	0
4	S	983	0	500	12	0
5	B	1379	0	1208	30	0
6	L5	80771	0	40889	609	0
7	L7	2538	0	1284	13	0
8	L8	3319	0	1684	12	0
9	LD	1939	0	2036	32	0
10	LE	3206	0	3353	51	0
11	LF	2886	0	3057	38	0
12	LG	2398	0	2430	35	0
13	LH	1859	0	2033	35	0
14	LI	1886	0	2008	29	0
15	LJ	1877	0	2023	18	0
16	LK	1516	0	1595	19	0
17	LL	1717	0	1762	27	0
18	LM	1362	0	1399	26	0
19	LO	1702	0	1820	22	0
20	LP	1137	0	1211	12	0
21	LQ	1701	0	1749	30	0
22	LR	1630	0	1776	18	0
23	LS	1288	0	1326	23	0
24	LT	1515	0	1634	22	0
25	LU	1508	0	1664	25	0
26	LV	1457	0	1492	17	0
27	LW	1298	0	1366	15	0
28	LX	806	0	827	14	0
29	LY	1034	0	1095	7	0
30	LZ	766	0	794	14	0
31	La	967	0	1040	13	0
32	Lb	1115	0	1205	21	0
33	Lc	1107	0	1182	22	0
34	Ld	1162	0	1205	15	0
35	Le	881	0	957	20	0
36	Lf	836	0	888	8	0
37	Lg	888	0	930	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lh	1070	0	1164	13	0
39	Li	884	0	924	8	0
40	Lj	906	0	998	10	0
41	Lk	1013	0	1147	9	0
42	Ll	830	0	916	3	0
43	Lm	705	0	737	7	0
44	Ln	569	0	637	9	0
45	Lo	447	0	480	7	0
46	Lp	431	0	471	7	0
47	Lq	863	0	929	8	0
48	Lr	708	0	756	8	0
49	Ls	1014	0	1083	11	0
50	Lt	567	0	251	5	0
51	Lx	972	0	429	5	0
52	S2	37825	0	19179	386	0
53	SB	651	0	672	10	0
54	SC	495	0	523	9	0
55	SD	610	0	634	29	0
56	SE	457	0	502	20	0
57	SF	814	0	862	21	0
58	SG	2436	0	2393	57	0
59	SH	459	0	448	7	0
60	SL	1743	0	1748	39	0
61	SM	1815	0	1908	29	0
62	SN	1706	0	1796	38	0
63	SO	1751	0	1846	26	0
64	SP	2076	0	2177	44	0
65	SQ	1509	0	1563	31	0
66	SR	1923	0	2089	54	0
67	SS	1529	0	1625	35	0
68	ST	1686	0	1772	49	0
69	SU	1525	0	1640	51	0
70	SV	810	0	836	13	0
71	SW	1262	0	1332	27	0
72	SX	958	0	993	31	0
73	SY	1208	0	1294	25	0
74	SZ	1016	0	1039	16	0
75	Sa	1048	0	1093	28	0
76	Sb	1124	0	1193	24	0
77	Sc	1080	0	1135	29	0
78	Sd	1217	0	1279	38	0
79	Se	1113	0	1145	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Sf	821	0	883	22	0
81	Sg	640	0	633	14	0
82	Sh	1034	0	1078	16	0
83	Si	1099	0	1162	17	0
84	Sj	1015	0	1085	28	0
85	Sk	598	0	656	16	0
86	Sl	239	0	286	5	0
87	E	32	0	10	1	0
87	L7	32	0	11	3	0
88	F	6	0	4	0	0
89	I	2	0	0	0	0
89	L5	162	0	0	0	0
89	L7	2	0	0	0	0
89	L8	1	0	0	0	0
89	LD	1	0	0	0	0
89	LS	1	0	0	0	0
89	LY	1	0	0	0	0
89	S2	55	0	0	0	0
90	L5	17	0	0	0	0
90	S2	1	0	0	0	0
91	Lj	1	0	0	0	0
91	Lm	1	0	0	0	0
91	Lp	1	0	0	0	0
91	Lq	1	0	0	0	0
91	Lr	1	0	0	0	0
91	SD	1	0	0	0	0
91	SF	2	0	0	0	0
91	SH	1	0	0	0	0
92	SZ	1	0	0	0	0
93	L5	56	0	0	2	0
93	L7	1	0	0	0	0
93	L8	1	0	0	0	0
93	LD	1	0	0	0	0
93	LE	1	0	0	0	0
93	LH	1	0	0	0	0
93	LK	1	0	0	0	0
93	LL	1	0	0	0	0
93	LQ	1	0	0	0	0
93	LV	1	0	0	0	0
93	Ld	1	0	0	0	0
93	S2	34	0	0	0	0
93	SF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	SH	1	0	0	0	0
93	SW	1	0	0	0	0
93	Sd	1	0	0	1	0
93	Se	1	0	0	0	0
93	Si	2	0	0	0	0
All	All	230266	0	168478	2304	0

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

All (2304) 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)
6:L5:278:G:H5''	21:LQ:8:GLN:HE22	1.45	0.80
76:Sb:102:GLU:HA	76:Sb:105:LYS:HB3	1.62	0.80
18:LM:164:ARG:HG2	18:LM:168:GLN:HE22	1.47	0.79
6:L5:1924:G:H1'	6:L5:1942:G:H5''	1.65	0.79
77:Sc:31:ASN:HD22	77:Sc:55:THR:HG22	1.47	0.78
6:L5:3669:C:H1'	21:LQ:125:SER:HB3	1.64	0.78
84:Sj:109:GLU:OE1	84:Sj:113:ARG:NH1	2.17	0.78
6:L5:3702:G:H1	6:L5:3779:C:H42	1.29	0.78
10:LE:329:ASP:OD1	10:LE:329:ASP:N	2.17	0.77
6:L5:3443:A:N6	6:L5:3468:A:OP1	2.18	0.77
52:S2:1092:C:HO2'	82:Sh:2:VAL:N	1.82	0.76
58:SG:87:LEU:HB2	58:SG:101:PHE:HB2	1.67	0.76
9:LD:104:VAL:HA	9:LD:107:MET:HE2	1.67	0.76
6:L5:3678:G:H1	6:L5:3794:U:H3	1.33	0.75
6:L5:3868:C:N4	6:L5:3889:G:O6	2.19	0.75
6:L5:1008:C:H1'	6:L5:1096:G:H22	1.52	0.75
64:SP:57:THR:HG22	64:SP:59:ASP:H	1.51	0.75
6:L5:1134:G:H22	6:L5:1206:C:H2'	1.50	0.75
52:S2:926:G:H1	52:S2:1018:U:H3	1.35	0.75
74:SZ:34:PHE:HB3	74:SZ:41:PHE:HB2	1.67	0.75
52:S2:307:C:H5'	52:S2:309:G:H5'	1.68	0.74
63:SO:106:ARG:HG3	63:SO:175:VAL:HG12	1.68	0.74
6:L5:3829:C:H1'	6:L5:3837:G:H22	1.53	0.74
71:SW:104:LYS:HE2	83:Si:8:ARG:HH22	1.51	0.74
6:L5:1012:C:O2	6:L5:1089:G:N2	2.19	0.73
13:LH:191:ARG:NH1	13:LH:217:ASP:OD1	2.20	0.73
50:Lt:192:VAL:H	50:Lt:200:ASN:HA	1.53	0.73
52:S2:153:G:N3	66:SR:13:GLN:NE2	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1866:C:H1'	57:SF:7:ASN:HD21	1.53	0.72
56:SE:102:ARG:NH1	56:SE:103:THR:O	2.22	0.72
6:L5:3555:G:N2	6:L5:3555:G:OP2	2.23	0.72
8:L8:133:G:OP1	31:La:67:ARG:NH1	2.23	0.72
6:L5:3395:A:N6	6:L5:3914:G:O2'	2.23	0.72
52:S2:929:G:H1	52:S2:1014:U:H3	1.36	0.71
52:S2:1866:C:O2	57:SF:7:ASN:ND2	2.22	0.71
25:LU:172:ARG:NH1	52:S2:910:G:OP1	2.24	0.71
6:L5:3831:C:N4	6:L5:3832:G:N3	2.38	0.71
6:L5:3831:C:H42	6:L5:3834:G:H1	1.39	0.71
55:SD:100:LEU:HB3	55:SD:103:LEU:HD23	1.72	0.71
68:ST:13:LYS:HD3	71:SW:137:THR:HG21	1.72	0.71
6:L5:684:C:OP2	13:LH:114:LYS:NZ	2.23	0.71
7:L7:51:G:H21	18:LM:12:MET:HE3	1.55	0.71
6:L5:3421:G:O2'	6:L5:3550:U:OP2	2.08	0.70
52:S2:642:A:OP1	69:SU:40:LYS:NZ	2.24	0.70
66:SR:2:LYS:HB3	66:SR:15:LEU:HD11	1.74	0.70
6:L5:3704:A:N6	6:L5:3768:C:O2'	2.25	0.70
51:Lx:38:LEU:HA	51:Lx:202:ARG:H	1.57	0.70
2:F:67:U:O2'	6:L5:4165:U:O2'	2.09	0.70
6:L5:518:C:H42	6:L5:639:G:H1	1.40	0.69
33:Lc:15:ALA:HB2	40:Lj:88:ARG:HH12	1.58	0.69
78:Sd:139:THR:O	78:Sd:144:ARG:NH2	2.26	0.69
1:E:435:ALA:HB3	2:F:77:C:H4'	1.75	0.69
6:L5:3373:U:OP2	6:L5:3378:A:N6	2.23	0.69
60:SL:57:LYS:HZ1	81:Sg:70:LEU:HD21	1.56	0.69
56:SE:102:ARG:HE	56:SE:106:ALA:HB3	1.57	0.69
6:L5:1308:U:OP2	19:LO:36:ARG:NH2	2.25	0.68
52:S2:682:PSU:H4'	83:Si:9:THR:HG22	1.74	0.68
75:Sa:18:ARG:NH1	78:Sd:88:LYS:O	2.26	0.68
3:I:53:U:O2'	3:I:157:C:O2	2.12	0.68
60:SL:205:ARG:NH2	77:Sc:81:ARG:O	2.27	0.68
68:ST:110:ARG:HH21	68:ST:123:ARG:HE	1.39	0.68
6:L5:178:C:O2	6:L5:258:G:N2	2.25	0.68
6:L5:2444:A:N6	6:L5:2587:A:OP2	2.24	0.68
6:L5:2496:C:OP1	40:Lj:54:ARG:NH2	2.27	0.68
84:Sj:117:VAL:HG23	84:Sj:122:LYS:HG2	1.74	0.68
13:LH:74:LYS:HE2	35:Le:119:SER:HB3	1.76	0.68
6:L5:1789:A:OP2	19:LO:5:ARG:NH2	2.27	0.68
54:SC:29:GLN:HE22	54:SC:67:ARG:HA	1.58	0.68
6:L5:1909:A:N6	6:L5:1955:C:OP2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4666:G:N2	6:L5:4666:G:OP2	2.27	0.67
14:LI:104:VAL:HG13	14:LI:135:VAL:HG12	1.74	0.67
6:L5:1415:C:H5''	24:LT:144:LYS:HG2	1.76	0.67
6:L5:1437:G:N7	19:LO:188:ASN:ND2	2.41	0.67
52:S2:1598:C:OP2	85:Sk:85:ARG:NH2	2.28	0.67
65:SQ:127:ARG:NH2	65:SQ:131:ALA:O	2.27	0.67
6:L5:4724:U:O2	10:LE:174:ARG:NH1	2.26	0.67
40:Lj:46:CYS:HB3	40:Lj:86:CYS:SG	2.33	0.67
52:S2:1131:G:OP2	52:S2:1131:G:N2	2.27	0.67
52:S2:1397:A:O2'	52:S2:1399:G:N7	2.26	0.67
6:L5:1299:G:OP1	24:LT:108:ARG:NH2	2.28	0.67
6:L5:3819:G:N2	6:L5:3905:C:O2	2.28	0.67
52:S2:1293:C:H1'	55:SD:147:THR:HG21	1.75	0.67
68:ST:37:LYS:NZ	68:ST:93:THR:O	2.25	0.67
52:S2:497:C:OP1	64:SP:49:ARG:NH2	2.26	0.67
6:L5:1297:G:N7	24:LT:104:ARG:NH2	2.43	0.67
6:L5:2422:G:N2	6:L5:2425:A:OP2	2.27	0.67
6:L5:2471:U:OP1	28:LX:93:LYS:NZ	2.27	0.67
66:SR:85:ARG:HG3	66:SR:87:ARG:HH12	1.59	0.67
1:E:63:ARG:NH1	1:E:210:THR:O	2.27	0.67
6:L5:3449:A:OP2	6:L5:3467:G:N2	2.28	0.67
52:S2:691:G:N2	67:SS:181:THR:O	2.28	0.67
58:SG:107:ASP:N	58:SG:107:ASP:OD1	2.26	0.67
62:SN:202:THR:OG1	69:SU:58:ARG:NH2	2.28	0.67
74:SZ:99:ALA:H	74:SZ:133:THR:HB	1.60	0.66
6:L5:4679:C:OP1	13:LH:159:ARG:NH1	2.28	0.66
9:LD:207:VAL:HG13	9:LD:208:GLU:HG3	1.77	0.66
71:SW:83:GLN:O	71:SW:83:GLN:NE2	2.28	0.66
22:LR:46:ASN:O	22:LR:50:ASN:ND2	2.28	0.66
52:S2:380:C:OP2	68:ST:178:ARG:NH2	2.29	0.66
64:SP:87:MET:HE2	64:SP:123:LEU:HB2	1.77	0.66
6:L5:454:U:O2'	38:Lh:5:ARG:NH1	2.28	0.66
52:S2:78:C:O2	66:SR:175:LYS:NZ	2.26	0.66
52:S2:1754:C:O2	52:S2:1781:G:N2	2.28	0.66
3:I:39:A:OP2	3:I:88:C:N4	2.29	0.66
19:LO:169:ILE:HD11	34:Ld:123:ILE:HG12	1.77	0.66
52:S2:1416:C:O2'	79:Se:132:ASP:OD2	2.13	0.66
6:L5:1214:A:N6	6:L5:2054:G:O2'	2.27	0.66
6:L5:1641:C:O2'	35:Le:18:ARG:NH1	2.28	0.66
45:Lo:30:LYS:HB2	45:Lo:33:ASN:HB2	1.78	0.66
52:S2:520:A:O2'	69:SU:9:CYS:SG	2.50	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:ST:37:LYS:NZ	68:ST:93:THR:OG1	2.29	0.66
6:L5:184:U:H3	6:L5:253:G:H1	1.41	0.66
6:L5:4636:G:O2'	6:L5:4666:G:N7	2.28	0.66
18:LM:113:ILE:HG21	18:LM:119:TYR:HD1	1.61	0.66
11:LF:65:GLU:OE1	11:LF:80:ARG:NH1	2.29	0.65
65:SQ:19:LEU:HB3	65:SQ:23:TRP:HB2	1.77	0.65
3:I:220:G:H22	52:S2:1332:C:H41	1.45	0.65
6:L5:4366:OMU:OP2	6:L5:4416:C:N4	2.28	0.65
6:L5:4627:C:O2	6:L5:4670:G:N2	2.28	0.65
7:L7:105:C:OP2	17:LL:203:ARG:NH1	2.22	0.65
84:Sj:21:LYS:HB2	84:Sj:75:ILE:HB	1.77	0.65
13:LH:115:MET:O	49:Ls:87:ARG:NH1	2.28	0.65
66:SR:20:ASP:OD1	66:SR:22:ARG:NH2	2.29	0.65
52:S2:953:G:H21	74:SZ:52:THR:HG21	1.60	0.65
60:SL:2:SAC:OAC	60:SL:63:ARG:NH1	2.29	0.65
6:L5:4756:G:H5'	68:ST:92:ARG:HE	1.61	0.65
14:LI:80:PHE:HB2	27:LW:141:VAL:HG22	1.79	0.65
16:LK:107:GLU:OE1	16:LK:127:ARG:NH1	2.28	0.65
52:S2:1120:A:O2'	53:SB:72:ARG:NH2	2.29	0.65
52:S2:1675:G:N7	76:Sb:17:LYS:NZ	2.44	0.65
65:SQ:43:GLU:HG2	65:SQ:44:LYS:HD3	1.79	0.65
72:SX:81:ASP:HB3	72:SX:84:LYS:HB2	1.77	0.65
6:L5:2538:A:OP1	44:Ln:35:LYS:NZ	2.26	0.65
31:La:64:SER:HB2	41:Lk:69:LEU:HD13	1.79	0.65
6:L5:4218:G:O2'	46:Lp:100:TYR:O	2.15	0.65
52:S2:30:C:O3'	83:Si:137:LYS:NZ	2.28	0.65
58:SG:247:TRP:HB3	58:SG:258:ILE:HD11	1.79	0.65
6:L5:2469:U:O4	28:LX:97:ARG:NH1	2.30	0.65
64:SP:19:MET:SD	64:SP:108:ARG:NH1	2.70	0.65
21:LQ:165:THR:HG23	21:LQ:168:GLY:H	1.61	0.64
52:S2:65:C:O2	66:SR:160:LYS:NZ	2.30	0.64
52:S2:1034:G:N1	52:S2:1081:A:O2'	2.26	0.64
63:SO:64:ARG:NH2	70:SV:71:LEU:O	2.30	0.64
52:S2:1299:G:OP2	75:Sa:77:LYS:NZ	2.30	0.64
6:L5:1213:G:OP1	35:Le:120:ARG:NH2	2.29	0.64
3:I:117:C:N4	3:I:151:A:OP1	2.31	0.64
6:L5:1698:G:H1	6:L5:1712:U:H3	1.43	0.64
6:L5:4175:C:N3	17:LL:158:LYS:NZ	2.45	0.64
11:LF:146:GLU:HG2	11:LF:175:LYS:HB3	1.79	0.64
52:S2:1787:U:H2'	52:S2:1788:G:H8	1.63	0.64
6:L5:4018:G:OP2	6:L5:4018:G:N2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1618:G:N1	52:S2:1621:A:OP2	2.30	0.64
58:SG:120:ILE:HB	58:SG:132:TRP:HB2	1.79	0.64
64:SP:95:THR:OG1	84:Sj:16:ARG:NH2	2.30	0.64
6:L5:1216:C:OP1	35:Le:117:ARG:NE	2.23	0.64
10:LE:54:THR:OG1	10:LE:369:ASP:OD1	2.16	0.64
50:Lt:30:VAL:HA	50:Lt:189:ILE:HA	1.79	0.64
52:S2:165:G:OP2	52:S2:165:G:N2	2.31	0.64
30:LZ:91:MET:HA	30:LZ:94:ARG:HG2	1.80	0.64
52:S2:920:A:OP2	73:SY:64:ARG:NH1	2.30	0.64
72:SX:95:ASP:OD1	72:SX:96:ARG:N	2.31	0.64
6:L5:1224:C:O2'	11:LF:321:ASN:OD1	2.15	0.64
6:L5:2688:A:H61	6:L5:3575:C:H42	1.45	0.64
68:ST:87:ASN:HB3	68:ST:90:LEU:HD23	1.79	0.64
1:E:478:LEU:HD11	1:E:491:ARG:HE	1.62	0.63
6:L5:3337:C:OP2	25:LU:71:ARG:NH1	2.31	0.63
9:LD:36:GLU:OE2	9:LD:163:ARG:NH1	2.28	0.63
6:L5:1694:C:O2	12:LG:3:PHE:N	2.31	0.63
23:LS:39:MET:HE3	23:LS:44:ALA:HA	1.79	0.63
52:S2:1148:C:OP1	57:SF:6:ARG:NH1	2.31	0.63
6:L5:524:C:O2	6:L5:631:G:N2	2.28	0.63
6:L5:1551:U:O2'	23:LS:135:ARG:NH2	2.31	0.63
6:L5:2603:G:O6	33:Lc:64:LYS:NZ	2.31	0.63
32:Lb:54:GLU:OE2	32:Lb:69:LYS:NZ	2.31	0.63
6:L5:4480:A:H61	6:L5:4704:U:H3	1.45	0.63
52:S2:564:G:N7	69:SU:172:ARG:NH2	2.47	0.63
1:E:100:ILE:HD12	1:E:103:ILE:HD11	1.80	0.63
2:F:67:U:HO2'	6:L5:4165:U:HO2'	1.37	0.63
6:L5:4492:G:H22	6:L5:4694:A:H2	1.45	0.63
24:LT:157:GLY:O	24:LT:188:ASN:ND2	2.32	0.63
62:SN:199:PRO:HG2	69:SU:58:ARG:HH21	1.62	0.63
6:L5:4416:C:O2'	6:L5:4418:A:OP2	2.16	0.63
23:LS:23:ARG:NH1	23:LS:125:MET:SD	2.72	0.63
17:LL:3:ARG:NH2	17:LL:63:GLU:OE2	2.32	0.63
17:LL:145:LYS:HE3	17:LL:167:ILE:HG13	1.80	0.63
55:SD:122:PRO:HG2	55:SD:148:TYR:HE2	1.63	0.63
82:Sh:115:GLU:O	82:Sh:118:ARG:NH1	2.32	0.63
19:LO:58:ILE:HG12	19:LO:157:ILE:HD12	1.80	0.63
52:S2:233:C:N3	52:S2:234:C:N4	2.47	0.63
67:SS:44:ASN:O	67:SS:68:GLN:NE2	2.32	0.63
6:L5:1375:A:H5''	6:L5:1456:C:H5	1.64	0.63
6:L5:2036:A:H3'	6:L5:2037:G:H5'	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4634:U:O2	20:LP:132:ARG:NH2	2.32	0.63
16:LK:91:LYS:HG2	16:LK:145:VAL:HG22	1.79	0.63
25:LU:28:GLU:HB2	25:LU:49:LEU:HD21	1.81	0.62
40:Lj:5:LEU:HD21	40:Lj:30:ILE:HG22	1.81	0.62
2:F:51:U:H3	2:F:58:A:H61	1.47	0.62
4:S:1120:U:N3	4:S:1121:G:O6	2.32	0.62
6:L5:2327:A:H61	6:L5:2337:U:H3	1.45	0.62
33:Lc:89:ILE:HD11	33:Lc:117:LYS:HB3	1.81	0.62
80:Sf:45:GLU:OE2	80:Sf:46:LYS:NZ	2.31	0.62
52:S2:483:G:N1	52:S2:486:A:OP2	2.30	0.62
6:L5:1532:G:OP1	48:Lr:17:ARG:NH1	2.32	0.62
6:L5:4287:G:N2	6:L5:4290:A:OP2	2.28	0.62
58:SG:111:VAL:HG23	58:SG:122:SER:HB3	1.80	0.62
82:Sh:111:MET:HE3	82:Sh:115:GLU:HG2	1.81	0.62
2:F:68:U:O2'	2:F:70:A:N7	2.24	0.62
52:S2:1273:C:H4'	59:SH:2:GLY:HA3	1.82	0.62
52:S2:1522:C:OP2	78:Sd:136:THR:OG1	2.14	0.62
67:SS:145:ARG:HE	82:Sh:51:GLU:HG2	1.64	0.62
6:L5:327:U:O2'	42:Ll:30:ARG:NH1	2.33	0.62
6:L5:522:U:OP1	19:LO:118:LYS:NZ	2.33	0.62
6:L5:3618:G:OP1	22:LR:85:ARG:NH2	2.32	0.62
52:S2:152:U:O4'	66:SR:132:ARG:NH1	2.32	0.62
25:LU:173:ARG:NH2	52:S2:911:G:OP2	2.32	0.62
52:S2:1337:C:N4	52:S2:1338:4AC:O7	2.32	0.62
52:S2:1567:G:N7	79:Se:101:ARG:NH2	2.48	0.62
6:L5:1347:G:N2	6:L5:1370:G:N3	2.47	0.62
3:I:63:A:N7	3:I:65:A:N6	2.47	0.62
9:LD:117:GLU:HG2	9:LD:124:GLY:H	1.64	0.62
13:LH:74:LYS:HB3	35:Le:119:SER:HB3	1.81	0.62
37:Lg:64:ILE:HG23	37:Lg:68:LEU:HD23	1.82	0.62
52:S2:126:G:H8	66:SR:199:THR:HG21	1.65	0.62
52:S2:1619:C:O3'	75:Sa:50:ARG:NH2	2.33	0.62
61:SM:47:THR:OG1	61:SM:65:ARG:NH1	2.33	0.62
6:L5:308:G:OP2	6:L5:308:G:N2	2.31	0.61
6:L5:1354:G:N2	6:L5:1364:G:OP2	2.31	0.61
6:L5:1829:G:OP2	6:L5:1829:G:N2	2.31	0.61
13:LH:281:THR:OG1	13:LH:282:ASN:N	2.33	0.61
37:Lg:123:ASP:N	37:Lg:123:ASP:OD1	2.32	0.61
69:SU:120:ALA:O	69:SU:125:HIS:ND1	2.31	0.61
6:L5:4068:G:N2	6:L5:4071:A:OP2	2.33	0.61
7:L7:107:G:H5''	12:LG:273:LEU:HD11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LJ:150:LYS:HE3	15:LJ:177:MET:HE3	1.81	0.61
69:SU:170:PRO:HB3	69:SU:174:LYS:HE3	1.82	0.61
6:L5:3812:G:O6	9:LD:72:ARG:NH2	2.33	0.61
18:LM:144:LYS:O	18:LM:148:THR:OG1	2.16	0.61
66:SR:147:LEU:HD13	66:SR:151:ASP:HB3	1.81	0.61
3:I:47:U:O4'	3:I:82:G:N2	2.33	0.61
6:L5:1805:U:OP1	17:LL:4:ARG:NH1	2.31	0.61
52:S2:700:C:N4	52:S2:730:C:O4'	2.34	0.61
14:LI:151:GLU:OE2	14:LI:244:ARG:NH1	2.34	0.61
56:SE:86:VAL:HA	56:SE:89:GLN:HE21	1.65	0.61
67:SS:82:GLU:HA	67:SS:85:LYS:HE2	1.83	0.61
72:SX:66:GLU:OE2	72:SX:78:LYS:NZ	2.34	0.61
6:L5:4335:A:N1	6:L5:4367:C:O2'	2.33	0.61
26:LV:112:ASP:OD1	26:LV:116:ARG:NH1	2.31	0.61
52:S2:755:G:N2	52:S2:791:C:O2	2.32	0.61
52:S2:1021:A:N7	73:SY:70:LYS:NZ	2.49	0.61
52:S2:127:C:O2	64:SP:134:LYS:NZ	2.33	0.60
6:L5:1972:A:OP1	17:LL:162:ARG:NH2	2.34	0.60
6:L5:3909:U:H5'	6:L5:3910:C:H5''	1.81	0.60
28:LX:100:LEU:HD13	28:LX:112:LEU:HD23	1.83	0.60
73:SY:136:PRO:HG2	73:SY:139:TRP:HB2	1.83	0.60
3:I:76:U:C5	3:I:156:C:H5''	2.36	0.60
6:L5:369:G:N2	6:L5:372:A:OP2	2.27	0.60
6:L5:3996:G:O2'	18:LM:129:ASP:OD1	2.16	0.60
8:L8:85:U:O4	32:Lb:50:ARG:NH2	2.34	0.60
12:LG:256:LYS:HD2	12:LG:257:PRO:HD2	1.82	0.60
27:LW:142:ARG:NH1	27:LW:144:ASN:OD1	2.35	0.60
62:SN:83:LEU:O	81:Sg:15:ARG:NH1	2.34	0.60
28:LX:111:GLU:OE2	28:LX:113:ARG:NE	2.33	0.60
1:E:522:PHE:H	1:E:528:PHE:HA	1.65	0.60
6:L5:3973:OMU:HM21	6:L5:4082:A:H1'	1.83	0.60
6:L5:4508:G:OP2	22:LR:37:ARG:NH1	2.32	0.60
14:LI:237:ASP:O	14:LI:240:ASN:ND2	2.35	0.60
6:L5:1399:G:OP2	6:L5:1399:G:N2	2.31	0.60
6:L5:3541:G:OP2	6:L5:3541:G:N2	2.28	0.60
26:LV:147:ASP:HB3	26:LV:150:ILE:HB	1.82	0.60
54:SC:39:SER:HB2	57:SF:51:ARG:HH22	1.67	0.60
55:SD:102:VAL:H	72:SX:36:ARG:HH22	1.49	0.60
61:SM:57:ILE:HG22	61:SM:59:SER:H	1.67	0.60
81:Sg:38:GLU:OE2	81:Sg:49:GLN:NE2	2.34	0.60
6:L5:186:G:N2	6:L5:186:G:OP2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1355:G:N2	52:S2:1358:A:OP2	2.31	0.60
64:SP:136:ILE:HD11	64:SP:148:ARG:HB3	1.83	0.60
70:SV:21:MET:HG2	70:SV:49:MET:HE3	1.83	0.60
76:Sb:101:ASP:OD1	76:Sb:102:GLU:N	2.35	0.60
26:LV:95:ARG:NH2	26:LV:112:ASP:OD2	2.35	0.60
66:SR:57:ASP:OD1	66:SR:61:PHE:N	2.34	0.60
6:L5:732:C:O2'	6:L5:735:G:OP1	2.17	0.59
6:L5:1936:U:N3	6:L5:1939:G:OP2	2.30	0.59
6:L5:2050:U:N3	6:L5:2051:G:N7	2.50	0.59
6:L5:4369:OMG:OP1	10:LE:19:ARG:NH2	2.34	0.59
6:L5:4610:C:N4	26:LV:171:ARG:O	2.35	0.59
18:LM:164:ARG:O	18:LM:168:GLN:NE2	2.35	0.59
37:Lg:59:THR:HG1	37:Lg:104:THR:HG1	1.39	0.59
42:Ll:63:VAL:HG23	42:Ll:65:LYS:HG3	1.84	0.59
6:L5:151:G:H3'	21:LQ:49:ARG:HH22	1.66	0.59
6:L5:3412:U:OP1	9:LD:54:ARG:NH2	2.30	0.59
61:SM:59:SER:OG	61:SM:63:LYS:NZ	2.33	0.59
64:SP:64:ILE:HD12	84:Sj:17:LEU:HB3	1.84	0.59
69:SU:97:ILE:HA	69:SU:100:LEU:HD23	1.84	0.59
6:L5:1458:A:H4'	6:L5:1459:G:H5'	1.85	0.59
20:LP:40:GLY:HA3	20:LP:45:VAL:HB	1.83	0.59
52:S2:1315:U:O2'	70:SV:8:ARG:NH2	2.35	0.59
76:Sb:31:LEU:HD11	76:Sb:33:LYS:HE3	1.84	0.59
6:L5:4792:U:OP1	6:L5:4793:C:N4	2.36	0.59
13:LH:181:PRO:HD2	13:LH:184:LEU:HD12	1.84	0.59
18:LM:35:ARG:HB3	18:LM:123:ILE:HG23	1.85	0.59
58:SG:60:ARG:NH2	76:Sb:97:GLN:OE1	2.35	0.59
67:SS:34:SER:HA	67:SS:37:LYS:HE3	1.83	0.59
6:L5:136:U:O4	41:Lk:79:LYS:NZ	2.29	0.59
13:LH:290:VAL:O	20:LP:109:ARG:NH2	2.34	0.59
52:S2:1788:G:H2'	52:S2:1789:A:H8	1.67	0.59
66:SR:10:THR:HG23	66:SR:12:CYS:H	1.67	0.59
75:Sa:81:ARG:NH1	75:Sa:120:SER:OG	2.34	0.59
6:L5:822:C:H5''	6:L5:823:C:H5''	1.85	0.59
52:S2:282:C:H42	52:S2:892:G:H4'	1.67	0.59
52:S2:1544:U:H5''	76:Sb:37:ARG:HH12	1.67	0.59
2:F:75:C:H2'	2:F:76:A:C8	2.37	0.59
5:B:726:VAL:HG22	5:B:766:THR:HG21	1.84	0.59
6:L5:1125:C:H5	13:LH:62:SER:HB2	1.68	0.59
6:L5:2597:G:OP2	33:Lc:133:LYS:NZ	2.35	0.59
6:L5:1458:A:H62	24:LT:87:THR:HG21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:2376:C:OP1	31:La:139:ARG:NH1	2.35	0.59
23:LS:132:ALA:O	23:LS:135:ARG:NH1	2.36	0.59
25:LU:39:GLN:OE1	25:LU:42:ARG:NH1	2.35	0.59
40:Lj:50:PRO:HG3	48:Lr:61:MET:HE3	1.85	0.59
52:S2:75:G:O2'	52:S2:77:A:OP1	2.21	0.59
52:S2:745:G:O2'	67:SS:109:ARG:NH1	2.36	0.59
53:SB:28:PRO:HG3	73:SY:17:PRO:HG3	1.85	0.59
57:SF:43:ASN:OD1	57:SF:66:LYS:NZ	2.35	0.59
80:Sf:68:THR:OG1	80:Sf:70:CYS:O	2.17	0.59
85:Sk:95:GLY:O	85:Sk:112:ASN:ND2	2.31	0.59
6:L5:1834:G:OP1	14:LI:95:ARG:NH2	2.36	0.59
6:L5:2011:C:OP1	24:LT:2:GLY:N	2.36	0.59
21:LQ:115:VAL:HG11	21:LQ:160:GLU:HB3	1.85	0.59
43:Lm:20:ARG:NH2	43:Lm:39:TYR:OH	2.35	0.59
52:S2:123:G:O5'	64:SP:145:ARG:NH2	2.35	0.59
52:S2:872:U:OP2	71:SW:156:GLN:NE2	2.36	0.59
6:L5:454:U:O2	38:Lh:5:ARG:NH2	2.35	0.59
6:L5:878:G:H4'	11:LF:326:LEU:HD23	1.85	0.59
6:L5:3820:G:N1	6:L5:3904:C:O2	2.35	0.59
6:L5:4219:A:OP1	46:Lp:124:LYS:NZ	2.35	0.59
6:L5:4639:C:O2'	6:L5:4641:C:OP2	2.20	0.59
53:SB:26:GLN:OE1	82:Sh:57:ARG:NH2	2.35	0.59
52:S2:870:A:OP2	71:SW:153:LYS:NZ	2.36	0.58
64:SP:176:ASP:OD1	64:SP:179:ASN:ND2	2.34	0.58
72:SX:32:ALA:HB3	72:SX:110:VAL:HB	1.84	0.58
5:B:691:CYS:HB3	5:B:749:ILE:HD11	1.84	0.58
6:L5:678:G:H5''	13:LH:103:LYS:HD3	1.85	0.58
6:L5:2221:G:N2	6:L5:2224:A:OP2	2.36	0.58
52:S2:64:A:H2	52:S2:83:A:H62	1.51	0.58
63:SO:29:LEU:HB2	63:SO:34:TYR:HB2	1.85	0.58
66:SR:142:ARG:HA	66:SR:147:LEU:HB2	1.85	0.58
1:E:148:ILE:HG12	1:E:185:ALA:HB2	1.84	0.58
3:I:33:A:H3'	3:I:34:A:H8	1.68	0.58
6:L5:3773:G:N2	6:L5:3776:A:OP2	2.29	0.58
23:LS:36:ILE:HA	23:LS:39:MET:HE2	1.86	0.58
6:L5:2197:G:OP1	11:LF:85:HIS:NE2	2.36	0.58
8:L8:75:OMG:OP2	32:Lb:74:TYR:OH	2.20	0.58
6:L5:2552:C:OP2	25:LU:43:LYS:NZ	2.31	0.58
6:L5:3707:C:O2'	6:L5:3764:G:N2	2.37	0.58
52:S2:1851:MA6:N6	52:S2:1852:MA6:H103	2.18	0.58
6:L5:4622:C:H5	13:LH:275:ARG:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LL:152:LEU:HB3	17:LL:165:ILE:HD12	1.85	0.58
17:LL:187:GLU:HG3	17:LL:189:ARG:HG3	1.86	0.58
6:L5:3631:OMG:N7	93:L5:5104:HOH:O	2.32	0.58
6:L5:1435:C:O2'	6:L5:1437:G:OP2	2.22	0.58
87:L7:203:GTP:O1G	87:L7:203:GTP:H5'	2.04	0.58
6:L5:1897:A:O2'	6:L5:1964:A:N1	2.35	0.58
52:S2:629:A:N6	52:S2:1501:G:O2'	2.37	0.58
60:SL:147:LEU:O	60:SL:165:ASN:ND2	2.37	0.58
30:LZ:96:GLN:OE1	66:SR:156:TYR:OH	2.22	0.58
56:SE:126:LYS:NZ	56:SE:127:LYS:O	2.37	0.58
58:SG:73:SER:HG	58:SG:117:ASN:HD21	1.50	0.58
68:ST:157:LYS:NZ	68:ST:158:ILE:O	2.32	0.58
3:I:76:U:H5	3:I:156:C:H5''	1.68	0.57
12:LG:75:VAL:O	12:LG:112:ARG:NH1	2.36	0.57
13:LH:168:LEU:HD21	13:LH:260:ILE:HD11	1.86	0.57
39:Li:36:ARG:NH1	39:Li:79:GLY:O	2.35	0.57
55:SD:133:ALA:N	55:SD:140:TYR:O	2.31	0.57
58:SG:154:VAL:O	58:SG:155:ARG:NH1	2.34	0.57
63:SO:192:TRP:NE1	63:SO:201:LYS:O	2.37	0.57
6:L5:2122:A:O2'	38:Lh:48:ARG:NH2	2.37	0.57
6:L5:4270:G:OP1	6:L5:4305:A:N6	2.33	0.57
55:SD:137:ASP:N	55:SD:137:ASP:OD1	2.36	0.57
77:Sc:103:LYS:HG3	77:Sc:119:VAL:HG12	1.86	0.57
85:Sk:47:LEU:HB2	85:Sk:79:ILE:HG22	1.86	0.57
3:I:173:C:H5'	3:I:174:G:C8	2.38	0.57
5:B:460:GLU:HG3	5:B:464:HIS:HE1	1.69	0.57
6:L5:37:U:H4'	34:Ld:32:ARG:HD2	1.86	0.57
12:LG:62:CYS:HB3	12:LG:105:LEU:HD22	1.85	0.57
32:Lb:54:GLU:HB2	32:Lb:108:ARG:HB2	1.84	0.57
51:Lx:67:VAL:H	51:Lx:77:ALA:HB2	1.67	0.57
63:SO:142:LEU:O	63:SO:148:LYS:NZ	2.37	0.57
3:I:131:A:N6	3:I:135:C:O4'	2.37	0.57
6:L5:3622:A:N6	6:L5:4316:G:O2'	2.36	0.57
11:LF:92:PHE:O	11:LF:100:ARG:NH1	2.37	0.57
52:S2:1864:A:OP2	57:SF:4:LYS:NZ	2.34	0.57
6:L5:1477:OMG:H4'	11:LF:75:ARG:HB3	1.86	0.57
72:SX:69:CYS:HA	72:SX:74:ILE:HD12	1.86	0.57
6:L5:1932:C:N4	6:L5:1941:A:O4'	2.38	0.57
6:L5:3480:A:O2'	9:LD:223:SER:OG	2.22	0.57
56:SE:108:ARG:HH21	69:SU:40:LYS:HG2	1.70	0.57
52:S2:1293:C:N3	55:SD:138:ARG:NH2	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SS:178:LYS:HG3	67:SS:179:LYS:HE2	1.87	0.57
1:E:328:PRO:O	1:E:378:GLN:NE2	2.38	0.57
6:L5:661:A:O2'	11:LF:29:LYS:NZ	2.38	0.57
6:L5:1931:U:O2'	6:L5:1941:A:OP1	2.15	0.57
6:L5:4622:C:O2'	39:Li:1:MET:SD	2.62	0.57
52:S2:521:A:O2'	52:S2:826:A:N3	2.34	0.57
52:S2:1569:C:OP1	79:Se:96:SER:OG	2.22	0.57
58:SG:214:GLY:HA2	58:SG:236:ILE:HG13	1.87	0.57
63:SO:64:ARG:NH1	70:SV:73:ASN:OD1	2.37	0.57
63:SO:225:GLU:OE2	63:SO:227:LYS:NZ	2.35	0.57
6:L5:1938:A:H61	50:Lt:37:SER:HA	1.69	0.57
6:L5:3706:G:H4'	6:L5:3779:C:H1'	1.87	0.57
6:L5:3850:G:O3'	40:Lj:90:ARG:NH2	2.37	0.57
52:S2:493:C:OP2	84:Sj:107:ARG:NH2	2.38	0.57
62:SN:64:THR:HG23	62:SN:67:GLY:H	1.69	0.57
65:SQ:28:VAL:O	65:SQ:42:LYS:NZ	2.38	0.57
80:Sf:22:ILE:HG12	80:Sf:114:VAL:HG12	1.86	0.57
11:LF:140:LYS:HE3	11:LF:245:HIS:HB2	1.85	0.56
23:LS:138:PRO:HB3	23:LS:140:MET:HE2	1.86	0.56
24:LT:88:ASP:OD2	24:LT:108:ARG:NH1	2.38	0.56
52:S2:831:A:OP2	52:S2:847:G:N2	2.38	0.56
60:SL:210:ILE:O	77:Sc:81:ARG:NH2	2.36	0.56
68:ST:194:GLU:OE2	71:SW:18:GLN:NE2	2.37	0.56
70:SV:85:LEU:HD12	70:SV:89:ILE:HG21	1.86	0.56
6:L5:2559:C:O3'	28:LX:107:LYS:NZ	2.35	0.56
9:LD:101:VAL:HG22	9:LD:165:VAL:HG22	1.86	0.56
50:Lt:29:ILE:N	50:Lt:191:GLN:O	2.38	0.56
52:S2:1614:G:OP1	78:Sd:88:LYS:NZ	2.30	0.56
52:S2:1758:G:H2'	52:S2:1759:G:C8	2.40	0.56
60:SL:145:ILE:HG13	60:SL:159:ILE:HB	1.85	0.56
71:SW:77:VAL:HG11	71:SW:80:MET:HE3	1.88	0.56
75:Sa:65:LYS:NZ	75:Sa:66:GLU:OE2	2.37	0.56
3:I:174:G:H1'	3:I:175:G:C8	2.40	0.56
6:L5:3491:A:HO2'	52:S2:1827:G:HO2'	1.53	0.56
11:LF:144:ILE:HD12	11:LF:150:LEU:HD11	1.87	0.56
12:LG:265:ARG:HE	12:LG:269:PRO:HG3	1.71	0.56
13:LH:281:THR:HG23	13:LH:284:VAL:HG21	1.86	0.56
22:LR:128:ARG:NH1	26:LV:162:GLN:OE1	2.38	0.56
51:Lx:52:THR:HA	51:Lx:156:LYS:HA	1.87	0.56
6:L5:423:G:OP1	23:LS:62:ARG:NH1	2.36	0.56
6:L5:1104:G:H5''	6:L5:1105:C:H5''	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LO:8:MET:HE3	24:LT:168:ARG:HB3	1.87	0.56
52:S2:171:A:H5''	66:SR:177:GLN:HG2	1.88	0.56
73:SY:54:LEU:HB3	73:SY:60:VAL:HB	1.88	0.56
6:L5:1879:G:N2	6:L5:4180:C:OP1	2.38	0.56
17:LL:179:ASP:OD1	17:LL:179:ASP:N	2.37	0.56
81:Sg:47:ASN:ND2	81:Sg:49:GLN:OE1	2.34	0.56
1:E:15:HIS:O	1:E:20:LYS:NZ	2.32	0.56
6:L5:3709:C:O2	6:L5:3762:G:N2	2.35	0.56
52:S2:1184:A:OP1	86:Sl:15:ARG:NH1	2.39	0.56
52:S2:1456:A:OP1	77:Sc:5:ARG:NH2	2.38	0.56
61:SM:179:ASN:OD1	61:SM:187:LYS:NZ	2.31	0.56
73:SY:99:ARG:NH2	73:SY:119:GLU:OE2	2.37	0.56
78:Sd:26:ILE:HG13	78:Sd:45:LEU:HD21	1.87	0.56
3:I:173:C:N4	3:I:203:U:OP1	2.37	0.56
31:La:60:TYR:O	31:La:62:ARG:NH1	2.39	0.56
52:S2:679:U:OP2	52:S2:1027:C:N4	2.29	0.56
55:SD:114:ILE:HD13	72:SX:68:LEU:HD22	1.87	0.56
68:ST:80:ASP:OD1	68:ST:94:LYS:NZ	2.38	0.56
3:I:33:A:H3'	3:I:34:A:C8	2.40	0.56
13:LH:46:CYS:SG	13:LH:47:SER:N	2.79	0.56
18:LM:151:ILE:HD11	18:LM:156:ARG:HG2	1.87	0.56
52:S2:67:C:H5'	66:SR:162:LEU:HD11	1.88	0.56
52:S2:1417:C:OP1	79:Se:133:ARG:NH1	2.31	0.56
69:SU:113:GLN:HG3	69:SU:149:VAL:HG21	1.88	0.56
75:Sa:18:ARG:HD2	78:Sd:88:LYS:HG2	1.88	0.56
6:L5:1351:G:H1	6:L5:1366:C:N4	2.04	0.56
6:L5:1740:A:O3'	27:LW:102:ARG:NH1	2.39	0.56
6:L5:4050:A:OP2	6:L5:4051:G:N2	2.38	0.56
9:LD:107:MET:HE1	9:LD:113:VAL:HG11	1.88	0.56
14:LI:215:PRO:HG3	14:LI:219:MET:HE3	1.87	0.56
52:S2:1124:C:O2'	61:SM:146:ARG:NH2	2.38	0.56
66:SR:85:ARG:O	66:SR:87:ARG:NH1	2.38	0.56
68:ST:57:ALA:HB2	68:ST:183:GLY:HA2	1.87	0.56
78:Sd:80:PRO:HG2	78:Sd:83:PHE:HB2	1.87	0.56
6:L5:648:C:O3'	11:LF:268:ARG:NH1	2.39	0.56
6:L5:4361:C:H5''	10:LE:357:ARG:HD2	1.88	0.56
7:L7:27:G:OP1	18:LM:146:ARG:NH2	2.39	0.56
17:LL:87:ILE:HG12	17:LL:138:ILE:HG12	1.88	0.56
52:S2:447:G:OP2	68:ST:47:ARG:NH2	2.31	0.56
66:SR:205:GLU:HA	66:SR:208:GLU:HG2	1.88	0.56
1:E:433:LEU:O	1:E:443:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:176:U:H3	3:I:200:A:H61	1.54	0.55
6:L5:632:G:H5''	6:L5:633:U:H5'	1.87	0.55
51:Lx:53:VAL:N	51:Lx:155:ILE:O	2.39	0.55
58:SG:20:GLN:HG2	58:SG:69:VAL:H	1.71	0.55
6:L5:484:G:H3'	6:L5:485:U:H2'	1.89	0.55
6:L5:1237:G:OP2	6:L5:1237:G:N2	2.25	0.55
33:Lc:57:MET:HB2	33:Lc:61:LYS:HD3	1.88	0.55
84:Sj:12:PHE:HD1	84:Sj:23:MET:HB3	1.71	0.55
5:B:637:LEU:HD21	5:B:696:PRO:HG3	1.88	0.55
6:L5:1110:G:H2'	6:L5:1111:G:C8	2.41	0.55
6:L5:1381:G:N1	6:L5:1413:C:OP2	2.32	0.55
6:L5:4123:G:O6	34:Ld:42:ARG:NH2	2.39	0.55
18:LM:35:ARG:NH1	18:LM:122:SER:O	2.40	0.55
48:Lr:38:THR:HA	48:Lr:45:THR:HA	1.88	0.55
54:SC:20:ARG:NH1	54:SC:28:THR:OG1	2.40	0.55
62:SN:146:GLU:HG3	62:SN:148:ALA:H	1.71	0.55
3:I:192:G:H4'	52:S2:1059:A:H5'	1.87	0.55
5:B:432:GLN:HG2	52:S2:1291:G:H1'	1.88	0.55
6:L5:151:G:OP2	21:LQ:4:TYR:OH	2.20	0.55
6:L5:859:G:C8	13:LH:126:ARG:HG2	2.41	0.55
52:S2:56:G:OP1	84:Sj:111:LYS:NZ	2.33	0.55
52:S2:503:C:N4	64:SP:67:GLN:OE1	2.38	0.55
52:S2:512:U:H2'	52:S2:513:A2M:H8	1.88	0.55
58:SG:256:ILE:HB	58:SG:270:LEU:HB3	1.87	0.55
84:Sj:27:VAL:HG11	84:Sj:35:VAL:HG21	1.89	0.55
6:L5:1580:OMG:HM23	21:LQ:81:TYR:HE1	1.71	0.55
6:L5:3497:G:O2'	6:L5:3499:C:N4	2.39	0.55
10:LE:56:ILE:HD12	10:LE:365:LEU:HD22	1.88	0.55
52:S2:122:G:O2'	64:SP:145:ARG:NH2	2.40	0.55
52:S2:877:C:OP1	67:SS:113:LYS:NZ	2.37	0.55
52:S2:1552:U:OP1	63:SO:9:ARG:NH1	2.39	0.55
68:ST:141:ARG:HB3	68:ST:146:GLN:HG2	1.87	0.55
78:Sd:27:ALA:HB2	78:Sd:52:LEU:HD12	1.89	0.55
6:L5:3420:U:OP2	9:LD:198:ARG:NH2	2.38	0.55
19:LO:78:LEU:HD11	19:LO:88:LYS:HD3	1.88	0.55
52:S2:896:G:H2'	52:S2:897:U:C6	2.41	0.55
52:S2:1869:U:H1'	57:SF:100:ARG:HH21	1.72	0.55
6:L5:1924:G:C8	6:L5:1942:G:H2'	2.42	0.55
6:L5:4766:C:O2	68:ST:77:ARG:NH1	2.40	0.55
38:Lh:108:ARG:HH22	38:Lh:127:ALA:HB3	1.72	0.55
69:SU:114:VAL:HG22	69:SU:120:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:37:U:C2	3:I:40:U:H5''	2.42	0.55
4:S:1152:C:N3	4:S:1153:C:N4	2.55	0.55
14:LI:94:ILE:HD11	14:LI:219:MET:HE1	1.88	0.55
20:LP:5:ARG:NE	20:LP:59:ASP:OD1	2.39	0.55
35:Le:113:ALA:O	35:Le:117:ARG:N	2.38	0.55
6:L5:67:C:OP2	6:L5:312:G:N2	2.38	0.55
6:L5:4268:G:O2'	6:L5:4271:C:OP2	2.20	0.55
52:S2:467:G:HO2'	66:SR:72:ARG:HH22	1.53	0.55
54:SC:51:ARG:HH21	65:SQ:61:PHE:HB3	1.72	0.55
58:SG:220:ASP:OD1	58:SG:225:LYS:N	2.28	0.55
60:SL:7:VAL:O	60:SL:11:LYS:NZ	2.40	0.55
1:E:315:ALA:HA	1:E:453:GLY:HA2	1.89	0.55
6:L5:3805:A:N1	6:L5:3917:C:N4	2.54	0.55
52:S2:1462:G:H3'	52:S2:1464:U:H3	1.72	0.55
61:SM:146:ARG:CZ	61:SM:146:ARG:HB2	2.37	0.55
76:Sb:19:ALA:HB2	76:Sb:75:GLY:HA3	1.89	0.55
14:LI:153:ILE:HG22	14:LI:186:MET:HE2	1.90	0.54
52:S2:563:U:H2'	52:S2:564:G:C8	2.43	0.54
52:S2:1600:U:OP2	85:Sk:46:ASN:ND2	2.40	0.54
55:SD:128:ALA:HB1	72:SX:43:ASP:HB3	1.89	0.54
60:SL:191:ARG:NH2	81:Sg:44:GLY:O	2.39	0.54
72:SX:11:VAL:HG13	72:SX:13:ASP:H	1.71	0.54
72:SX:49:LEU:HB3	72:SX:111:VAL:HB	1.89	0.54
75:Sa:86:LEU:H	75:Sa:89:MET:HE3	1.72	0.54
3:I:47:U:OP2	3:I:82:G:N2	2.40	0.54
5:B:463:GLN:HA	5:B:701:ILE:HG12	1.88	0.54
6:L5:394:G:N2	6:L5:397:G:OP2	2.33	0.54
11:LF:233:THR:HG23	11:LF:234:LYS:HG3	1.88	0.54
19:LO:81:LEU:HD12	19:LO:86:ILE:HB	1.90	0.54
30:LZ:1:MET:SD	30:LZ:1:MET:N	2.80	0.54
35:Le:56:LYS:O	35:Le:60:ASN:ND2	2.35	0.54
52:S2:1599:G:OP1	85:Sk:80:ARG:NH1	2.40	0.54
2:F:5:G:H1	2:F:82:C:H42	1.54	0.54
6:L5:2109:C:O2'	49:Ls:39:ARG:NH1	2.39	0.54
6:L5:4083:C:N3	47:Lq:61:LYS:NZ	2.54	0.54
11:LF:295:SER:OG	11:LF:297:GLU:OE1	2.24	0.54
15:LJ:30:PRO:HB2	33:Lc:125:GLY:HA3	1.88	0.54
52:S2:430:C:O2'	52:S2:812:A:N1	2.41	0.54
52:S2:1330:U:O2'	52:S2:1333:A:OP2	2.20	0.54
58:SG:103:GLY:O	58:SG:130:LYS:NZ	2.40	0.54
59:SH:36:LEU:HD12	59:SH:38:MET:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Sk:42:ASP:N	85:Sk:42:ASP:OD1	2.40	0.54
6:L5:1270:A2M:OP2	6:L5:4191:U:O2'	2.24	0.54
6:L5:1354:G:H2'	6:L5:1363:C:N3	2.22	0.54
6:L5:4745:U:H4'	6:L5:4746:A:H5'	1.89	0.54
57:SF:59:PHE:HB2	57:SF:62:TYR:HB2	1.89	0.54
72:SX:37:GLU:O	72:SX:41:ALA:N	2.40	0.54
76:Sb:132:PHE:O	76:Sb:140:ARG:NH2	2.38	0.54
80:Sf:23:THR:HB	80:Sf:113:GLU:HB3	1.89	0.54
83:Si:93:PHE:O	83:Si:140:ARG:NH1	2.40	0.54
3:I:67:G:O5'	3:I:165:C:N4	2.41	0.54
6:L5:2207:OMG:N1	6:L5:3590:C:N3	2.50	0.54
6:L5:4035:U:O2'	6:L5:4066:G:O2'	2.20	0.54
9:LD:27:ALA:O	9:LD:128:ARG:NH1	2.40	0.54
31:La:87:MET:HE1	31:La:156:ILE:HG12	1.90	0.54
56:SE:113:ASN:HA	56:SE:117:VAL:HB	1.90	0.54
68:ST:105:ASP:OD2	68:ST:107:THR:OG1	2.17	0.54
76:Sb:34:VAL:HG22	76:Sb:70:VAL:HB	1.89	0.54
6:L5:49:U:OP2	21:LQ:189:ARG:NH1	2.41	0.54
6:L5:1350:G:H2'	6:L5:1351:G:C8	2.43	0.54
10:LE:246:ARG:O	10:LE:250:LYS:NZ	2.37	0.54
67:SS:29:GLU:HA	67:SS:32:MET:HE2	1.90	0.54
84:Sj:88:LYS:HD3	84:Sj:91:LEU:HD12	1.90	0.54
7:L7:2:U:H5'	12:LG:267:ASN:ND2	2.22	0.54
52:S2:162:C:OP1	66:SR:85:ARG:NH2	2.35	0.54
52:S2:172:OMU:H6	52:S2:315:U:H1'	1.90	0.54
56:SE:105:ARG:HD3	69:SU:127:ARG:HD3	1.88	0.54
58:SG:260:ASP:O	58:SG:264:LYS:N	2.40	0.54
64:SP:11:ARG:HA	64:SP:28:ALA:HB2	1.90	0.54
69:SU:110:LEU:HB2	69:SU:147:PHE:HB3	1.90	0.54
6:L5:62:A:N3	6:L5:77:U:O2'	2.35	0.54
6:L5:2549:G:O6	25:LU:46:LYS:NZ	2.41	0.54
9:LD:30:ARG:NH1	9:LD:36:GLU:OE1	2.41	0.54
9:LD:177:LYS:HB2	48:Lr:29:ILE:HG21	1.89	0.54
46:Lp:94:MET:HG2	46:Lp:105:PRO:HA	1.90	0.54
63:SO:137:VAL:HG22	63:SO:151:LYS:HG3	1.90	0.54
68:ST:34:ALA:HB2	68:ST:56:ARG:HD2	1.88	0.54
6:L5:526:C:H2'	6:L5:527:G:C8	2.43	0.54
6:L5:2699:C:O2	10:LE:242:ARG:NH2	2.41	0.54
6:L5:4610:C:OP2	20:LP:98:ARG:NH2	2.41	0.54
25:LU:15:LEU:HD12	25:LU:22:VAL:HG12	1.90	0.54
26:LV:15:ARG:NH2	26:LV:60:GLU:OE2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LZ:94:ARG:NH1	66:SR:146:ASN:OD1	2.40	0.54
34:Ld:72:THR:HG22	34:Ld:110:LYS:HB3	1.90	0.54
52:S2:1528:C:OP1	76:Sb:142:GLN:NE2	2.40	0.54
69:SU:63:LEU:HB2	69:SU:70:ARG:HD2	1.90	0.54
78:Sd:98:VAL:HG21	78:Sd:106:LYS:HE2	1.88	0.54
10:LE:213:GLN:NE2	10:LE:285:TYR:O	2.38	0.54
52:S2:191:A:OP2	68:ST:141:ARG:NH1	2.41	0.54
52:S2:698:G:O5'	52:S2:732:G:N2	2.38	0.54
61:SM:92:GLN:HG2	61:SM:97:LEU:HD21	1.89	0.54
62:SN:91:SER:HB2	62:SN:156:ILE:HG23	1.89	0.54
78:Sd:33:ILE:HD13	78:Sd:71:MET:HE1	1.90	0.54
6:L5:679:C:OP2	13:LH:103:LYS:NZ	2.33	0.53
6:L5:995:C:H42	6:L5:1110:G:H1	1.55	0.53
6:L5:1933:C:H2'	6:L5:1934:G:H8	1.73	0.53
12:LG:223:PHE:HB3	12:LG:226:TYR:HB2	1.88	0.53
29:LY:13:LYS:HB3	29:LY:128:LEU:HD21	1.90	0.53
45:Lo:36:ARG:HG3	45:Lo:37:TYR:HD1	1.73	0.53
71:SW:136:LYS:O	71:SW:139:ARG:NH2	2.40	0.53
73:SY:87:ASP:OD1	73:SY:87:ASP:N	2.41	0.53
6:L5:2317:G:H22	6:L5:2346:G:H5''	1.73	0.53
17:LL:54:SER:HB2	17:LL:135:ILE:HD11	1.89	0.53
22:LR:10:ASP:HB2	22:LR:117:ARG:HB3	1.90	0.53
35:Le:117:ARG:HD3	35:Le:118:LEU:HG	1.88	0.53
52:S2:240:G:N2	52:S2:280:G:N7	2.52	0.53
61:SM:189:ILE:HB	61:SM:190:PRO:HD3	1.89	0.53
64:SP:181:CYS:HA	64:SP:227:VAL:HA	1.90	0.53
65:SQ:124:ASP:OD1	65:SQ:125:SER:N	2.42	0.53
65:SQ:195:GLU:OE2	65:SQ:198:ARG:NH2	2.40	0.53
78:Sd:92:ASP:OD1	78:Sd:92:ASP:N	2.40	0.53
17:LL:79:SER:OG	17:LL:147:HIS:ND1	2.40	0.53
27:LW:4:THR:OG1	27:LW:5:LYS:N	2.42	0.53
32:Lb:77:LYS:HG3	32:Lb:79:VAL:HG22	1.91	0.53
11:LF:284:MET:HE3	11:LF:287:THR:HG22	1.90	0.53
25:LU:8:LYS:HD2	25:LU:22:VAL:HG23	1.91	0.53
47:Lq:71:GLU:OE2	47:Lq:78:ARG:NH2	2.42	0.53
52:S2:827:A:O2'	69:SU:9:CYS:SG	2.62	0.53
56:SE:102:ARG:NE	56:SE:106:ALA:HB3	2.22	0.53
58:SG:73:SER:OG	58:SG:117:ASN:ND2	2.29	0.53
62:SN:170:TRP:HH2	69:SU:62:THR:HG22	1.74	0.53
2:F:75:C:H2'	2:F:76:A:H8	1.74	0.53
6:L5:119:G:OP1	15:LJ:132:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:1341:A:O2'	6:L5:1422:C:O2'	2.25	0.53
6:L5:1583:C:H42	9:LD:3:ARG:HH11	1.56	0.53
6:L5:2032:G:O2'	6:L5:2100:C:N4	2.40	0.53
17:LL:52:MET:HE2	17:LL:136:MET:HG2	1.91	0.53
52:S2:1256:G:OP1	52:S2:1257:G:O2'	2.18	0.53
55:SD:105:TYR:HD1	55:SD:118:ARG:HG3	1.74	0.53
57:SF:38:LYS:HB2	57:SF:71:LEU:HB2	1.90	0.53
66:SR:230:LYS:O	66:SR:234:LEU:N	2.40	0.53
67:SS:101:LEU:O	67:SS:116:ARG:NH1	2.42	0.53
68:ST:101:ILE:HD12	68:ST:190:LEU:HD11	1.90	0.53
1:E:425:LEU:HG	1:E:449:ILE:HD11	1.91	0.53
6:L5:842:G:OP1	14:LI:244:ARG:NH2	2.37	0.53
6:L5:1016:C:N4	6:L5:1085:G:O6	2.42	0.53
6:L5:3863:G:H1	6:L5:3895:C:H42	1.57	0.53
52:S2:383:C:H2'	52:S2:384:G:H8	1.74	0.53
52:S2:1264:U:O2	59:SH:16:GLN:NE2	2.41	0.53
1:E:252:LEU:HB2	1:E:278:THR:HA	1.91	0.53
1:E:429:ILE:HA	1:E:447:HIS:HA	1.91	0.53
6:L5:1834:G:O2'	6:L5:1846:A:N3	2.39	0.53
6:L5:3819:G:C2	6:L5:3820:G:C5	2.97	0.53
33:Lc:12:LEU:HB2	33:Lc:81:MET:HB3	1.89	0.53
64:SP:115:THR:HG23	64:SP:118:GLU:H	1.72	0.53
73:SY:100:LYS:HG2	73:SY:104:ARG:HH12	1.74	0.53
5:B:432:GLN:H	52:S2:1291:G:H4'	1.74	0.53
6:L5:2103:C:O2	49:Ls:99:LYS:NZ	2.32	0.53
10:LE:95:THR:OG1	10:LE:98:GLY:O	2.27	0.53
18:LM:111:GLU:HG3	18:LM:113:ILE:HG12	1.91	0.53
44:Ln:8:ILE:HG23	44:Ln:56:LEU:HD12	1.91	0.53
54:SC:47:LYS:HE3	65:SQ:126:THR:HG22	1.91	0.53
60:SL:184:ARG:HD3	60:SL:191:ARG:HG3	1.91	0.53
72:SX:32:ALA:HB1	72:SX:37:GLU:OE1	2.08	0.53
5:B:445:GLN:OE1	55:SD:147:THR:OG1	2.18	0.53
6:L5:155:C:OP1	41:Lk:109:ARG:NH1	2.35	0.53
6:L5:3679:A:H2	6:L5:3793:G:H22	1.56	0.53
52:S2:1143:G:N2	52:S2:1146:A:OP2	2.40	0.53
61:SM:136:ARG:HB2	61:SM:218:LEU:HD11	1.90	0.53
5:B:460:GLU:O	5:B:464:HIS:ND1	2.41	0.53
6:L5:1354:G:H1'	6:L5:1364:G:C5	2.44	0.53
6:L5:2539:A:H62	44:Ln:35:LYS:HZ2	1.57	0.53
10:LE:80:GLU:OE1	10:LE:323:TYR:OH	2.19	0.53
13:LH:164:ARG:NH1	13:LH:276:SER:OG	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:526:A:H2'	52:S2:527:A:H8	1.73	0.53
83:Si:54:LYS:HD2	83:Si:91:LEU:HD11	1.90	0.53
6:L5:1827:A:N6	6:L5:3605:G:O2'	2.43	0.52
6:L5:2548:G:O6	25:LU:46:LYS:NZ	2.31	0.52
26:LV:96:GLU:HG3	26:LV:139:ARG:HG2	1.89	0.52
64:SP:64:ILE:HD11	84:Sj:18:LEU:HG	1.92	0.52
2:F:26:G:H2'	2:F:27:G:C8	2.44	0.52
6:L5:85:G:N2	6:L5:98:A:OP2	2.40	0.52
6:L5:2330:G:OP2	6:L5:2332:C:N4	2.41	0.52
6:L5:4124:A:O2'	6:L5:4125:A:H2'	2.09	0.52
52:S2:1551:G:H3'	52:S2:1580:A:H61	1.74	0.52
58:SG:11:LEU:HB2	58:SG:307:VAL:HB	1.91	0.52
58:SG:197:THR:HG21	58:SG:239:LEU:H	1.73	0.52
80:Sf:54:VAL:HG22	80:Sf:88:LEU:HB2	1.91	0.52
6:L5:3852:G:N2	15:LJ:43:GLN:O	2.42	0.52
44:Ln:7:GLU:OE1	44:Ln:7:GLU:N	2.42	0.52
52:S2:1047:PSU:H1'	74:SZ:140:THR:HB	1.91	0.52
60:SL:213:GLU:OE1	77:Sc:81:ARG:NH2	2.42	0.52
6:L5:3432:C:O2'	6:L5:3506:A:N3	2.40	0.52
6:L5:4292:A:N7	9:LD:215:ASN:ND2	2.57	0.52
7:L7:6:C:H4'	12:LG:52:ILE:HD13	1.91	0.52
15:LJ:88:ASP:OD2	15:LJ:90:GLN:NE2	2.43	0.52
21:LQ:96:ARG:NH2	21:LQ:100:SER:OG	2.40	0.52
60:SL:42:LYS:HD2	60:SL:48:ILE:HD11	1.91	0.52
65:SQ:26:ASP:N	65:SQ:26:ASP:OD1	2.43	0.52
3:I:63:A:H1'	3:I:170:C:H42	1.75	0.52
6:L5:778:C:H2'	6:L5:779:G:C8	2.45	0.52
6:L5:3778:A:OP1	6:L5:3780:C:N4	2.42	0.52
6:L5:4437:A:O2'	16:LK:68:ALA:O	2.27	0.52
10:LE:119:TYR:OH	10:LE:129:ALA:N	2.42	0.52
38:Lh:35:TRP:CZ2	38:Lh:56:PRO:HD2	2.45	0.52
49:Ls:117:ILE:O	49:Ls:120:SER:OG	2.22	0.52
52:S2:234:C:H42	52:S2:897:U:H3	1.58	0.52
52:S2:1170:G:OP1	86:Sl:6:ARG:NH2	2.43	0.52
58:SG:283:PRO:O	58:SG:285:GLN:NE2	2.42	0.52
60:SL:214:GLU:HG2	77:Sc:81:ARG:HH12	1.73	0.52
84:Sj:112:ASN:HA	84:Sj:115:LYS:HE2	1.91	0.52
1:E:259:PRO:HB3	1:E:421:THR:HG21	1.91	0.52
52:S2:698:G:N3	52:S2:731:C:N4	2.58	0.52
52:S2:1227:G:N1	52:S2:1640:7MG:OP2	2.33	0.52
60:SL:207:PRO:HA	60:SL:210:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Sa:25:LEU:HD23	75:Sa:87:PRO:HB3	1.91	0.52
3:I:96:G:H8	3:I:98:A:H5''	1.75	0.52
6:L5:1133:C:N3	6:L5:1207:G:N1	2.58	0.52
6:L5:1741:A:O2'	6:L5:1776:A:OP1	2.26	0.52
38:Lh:80:HIS:N	38:Lh:84:GLU:OE2	2.43	0.52
39:Li:15:LYS:HB3	39:Li:25:THR:HG23	1.92	0.52
3:I:173:C:H5'	3:I:174:G:H8	1.73	0.52
6:L5:876:C:O2	11:LF:327:LYS:NZ	2.43	0.52
14:LI:181:TYR:CZ	14:LI:202:GLU:HG2	2.45	0.52
36:Lf:20:LEU:HB3	36:Lf:102:SER:HB2	1.92	0.52
52:S2:77:A:H61	66:SR:183:ARG:NH1	2.07	0.52
61:SM:137:LEU:HG	61:SM:215:VAL:HG22	1.92	0.52
76:Sb:82:TYR:O	76:Sb:86:GLN:HG2	2.10	0.52
6:L5:2601:G:O2'	6:L5:2608:A:N3	2.39	0.52
6:L5:3386:G:O2'	6:L5:3425:U:OP1	2.21	0.52
15:LJ:259:LYS:O	15:LJ:263:THR:OG1	2.25	0.52
18:LM:56:THR:HG23	18:LM:63:ARG:HA	1.92	0.52
23:LS:118:GLN:OE1	23:LS:120:ASN:ND2	2.42	0.52
24:LT:180:ARG:HE	34:Ld:50:PRO:HG2	1.75	0.52
52:S2:146:G:O2'	52:S2:147:A:O5'	2.26	0.52
64:SP:44:LEU:HD23	64:SP:82:TYR:HB3	1.91	0.52
3:I:87:G:H5''	3:I:88:C:OP2	2.09	0.52
5:B:658:ARG:NH1	52:S2:1575:C:OP2	2.30	0.52
6:L5:856:A:H1'	6:L5:2015:G:H5''	1.92	0.52
31:La:89:LYS:HB3	31:La:95:THR:HG23	1.91	0.52
32:Lb:44:VAL:HG11	32:Lb:119:LEU:HD12	1.91	0.52
60:SL:113:GLN:HB2	60:SL:116:PHE:HB2	1.91	0.52
69:SU:32:ILE:HD11	69:SU:40:LYS:HD3	1.92	0.52
78:Sd:139:THR:O	93:Sd:201:HOH:O	2.19	0.52
1:E:371:GLN:OE1	1:E:371:GLN:N	2.43	0.51
6:L5:469:C:OP2	6:L5:678:G:N1	2.35	0.51
6:L5:1846:A:H4'	14:LI:222:LYS:HE3	1.92	0.51
12:LG:152:ARG:HG3	12:LG:154:THR:HG23	1.91	0.51
25:LU:160:GLU:HA	25:LU:163:ARG:HE	1.75	0.51
26:LV:99:ASP:OD1	26:LV:100:LEU:N	2.41	0.51
52:S2:944:U:O2'	74:SZ:135:ILE:O	2.25	0.51
52:S2:1553:G:O2'	52:S2:1556:U:O2'	2.28	0.51
58:SG:201:SER:OG	58:SG:203:ASP:OD1	2.24	0.51
84:Sj:29:HIS:ND1	84:Sj:29:HIS:O	2.42	0.51
6:L5:13:U:H1'	31:La:56:ARG:HD2	1.93	0.51
32:Lb:47:MET:HG2	32:Lb:115:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1084:A:N7	52:S2:1842:C:O2'	2.42	0.51
75:Sa:13:ARG:HH12	75:Sa:14:LYS:HG2	1.74	0.51
80:Sf:26:SER:HB2	80:Sf:110:VAL:HA	1.90	0.51
16:LK:24:THR:HA	16:LK:37:ASP:HA	1.91	0.51
36:Lf:5:LYS:HB3	36:Lf:9:LYS:HE3	1.91	0.51
52:S2:380:C:O2	68:ST:5:ARG:NE	2.43	0.51
52:S2:1149:A:OP1	57:SF:6:ARG:NH2	2.36	0.51
53:SB:4:ALA:HB2	81:Sg:71:ARG:HH11	1.73	0.51
6:L5:238:C:OP2	32:Lb:45:ARG:NH2	2.44	0.51
35:Le:71:ALA:O	35:Le:75:LEU:N	2.36	0.51
59:SH:22:ARG:HG2	59:SH:38:MET:HG2	1.91	0.51
62:SN:201:GLY:O	69:SU:54:ARG:NH2	2.33	0.51
66:SR:168:LYS:HD2	66:SR:169:PRO:HD2	1.91	0.51
72:SX:55:ASN:HD21	72:SX:82:ASN:H	1.57	0.51
77:Sc:44:LYS:HG3	77:Sc:47:ARG:HH21	1.74	0.51
1:E:470:TYR:HB3	1:E:582:LYS:HD2	1.91	0.51
6:L5:1334:G:N2	6:L5:1337:G:OP2	2.39	0.51
6:L5:2037:G:H22	6:L5:2046:A:H5''	1.75	0.51
12:LG:107:ARG:HH12	12:LG:120:GLU:HA	1.76	0.51
52:S2:374:G:OP1	71:SW:135:SER:OG	2.29	0.51
52:S2:1338:4AC:H2'	52:S2:1339:G:H8	1.75	0.51
83:Si:46:HIS:HB3	83:Si:101:LEU:HD11	1.92	0.51
83:Si:124:LYS:HG2	83:Si:129:SER:HA	1.93	0.51
6:L5:1859:C:H3'	6:L5:1860:C:H5''	1.93	0.51
6:L5:3766:C:O2'	6:L5:3778:A:O2'	2.18	0.51
6:L5:4139:G:O4'	6:L5:4193:5MC:HM52	2.10	0.51
18:LM:91:GLU:HG2	18:LM:93:GLU:OE1	2.10	0.51
23:LS:94:MET:HE2	23:LS:148:MET:HE3	1.92	0.51
52:S2:57:U:O2	52:S2:500:G:O2'	2.28	0.51
68:ST:10:LYS:O	68:ST:18:ARG:NH1	2.43	0.51
6:L5:2102:G:O3'	13:LH:111:LYS:NZ	2.43	0.51
6:L5:4379:G:N2	6:L5:4410:A:N7	2.59	0.51
9:LD:117:GLU:OE2	9:LD:163:ARG:NH2	2.39	0.51
52:S2:1508:G:N2	55:SD:87:THR:O	2.35	0.51
58:SG:268:ASP:OD1	58:SG:268:ASP:N	2.42	0.51
61:SM:30:TRP:CE2	74:SZ:19:PRO:HD3	2.46	0.51
72:SX:75:ASN:OD1	72:SX:132:LYS:NZ	2.34	0.51
75:Sa:81:ARG:NH2	75:Sa:117:GLY:O	2.44	0.51
2:F:19:G:N2	2:F:71:A:O5'	2.40	0.51
3:I:201:C:N4	3:I:202:C:O2	2.44	0.51
6:L5:1942:G:N2	6:L5:1943:U:O4	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Lc:35:ASP:N	33:Lc:35:ASP:OD1	2.44	0.51
41:Lk:80:PRO:HD2	41:Lk:83:LEU:HD12	1.91	0.51
52:S2:65:C:H4'	66:SR:172:LYS:HD3	1.93	0.51
56:SE:96:GLN:HG3	56:SE:98:LYS:HE2	1.93	0.51
59:SH:54:LYS:NZ	80:Sf:78:ASP:OD1	2.36	0.51
78:Sd:36:VAL:HG21	78:Sd:71:MET:HE3	1.93	0.51
3:I:32:A:H2'	3:I:33:A:C8	2.46	0.51
6:L5:1860:C:O2'	26:LV:160:ARG:NH2	2.35	0.51
14:LI:154:TYR:OH	14:LI:187:GLU:OE2	2.28	0.51
17:LL:141:LYS:HD2	17:LL:143:GLN:HE22	1.75	0.51
27:LW:115:LYS:HG2	27:LW:126:VAL:HG11	1.91	0.51
30:LZ:94:ARG:HH12	66:SR:145:PHE:C	2.19	0.51
52:S2:554:U:O4	52:S2:555:A:N6	2.43	0.51
52:S2:941:U:H3	52:S2:1003:U:H3	1.58	0.51
65:SQ:63:LYS:HD2	65:SQ:71:ARG:HH12	1.76	0.51
66:SR:135:PRO:HB3	66:SR:140:ARG:HB3	1.93	0.51
71:SW:111:VAL:HG12	71:SW:140:PHE:HB2	1.93	0.51
74:SZ:53:ILE:HG23	74:SZ:88:LEU:HD12	1.93	0.51
81:Sg:36:VAL:HG13	81:Sg:51:LYS:HB2	1.93	0.51
3:I:62:G:O6	3:I:170:C:O2'	2.29	0.51
6:L5:1546:U:N3	6:L5:4301:U:OP1	2.39	0.51
6:L5:1918:A:N6	6:L5:1923:A:OP1	2.44	0.51
10:LE:220:ILE:HB	10:LE:346:THR:HG23	1.92	0.51
52:S2:1617:U:OP2	75:Sa:43:ARG:NH2	2.44	0.51
61:SM:36:PRO:HB2	61:SM:38:MET:SD	2.50	0.51
61:SM:87:ILE:HG22	61:SM:101:HIS:HB2	1.93	0.51
52:S2:731:C:O5'	82:Sh:118:ARG:NH2	2.44	0.50
60:SL:121:LEU:HD21	60:SL:145:ILE:HD13	1.93	0.50
63:SO:68:GLU:HG3	70:SV:93:THR:HG21	1.92	0.50
5:B:721:GLN:HB3	5:B:723:ILE:HG12	1.93	0.50
6:L5:734:G:H2'	6:L5:735:G:C8	2.46	0.50
6:L5:734:G:H2'	6:L5:735:G:H8	1.77	0.50
10:LE:261:ARG:HB2	22:LR:64:THR:HG21	1.91	0.50
52:S2:643:U:H5	56:SE:108:ARG:HH12	1.58	0.50
52:S2:943:G:N2	74:SZ:137:SER:OG	2.42	0.50
82:Sh:6:VAL:HG12	82:Sh:34:ILE:HD11	1.93	0.50
3:I:96:G:C8	3:I:98:A:H5''	2.46	0.50
6:L5:25:A:N3	6:L5:339:C:O2'	2.42	0.50
6:L5:4643:G:H1	6:L5:4656:C:H42	1.60	0.50
87:L7:203:GTP:H5''	12:LG:265:ARG:NH1	2.26	0.50
10:LE:292:LEU:HB2	10:LE:299:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LL:183:ASP:OD1	17:LL:183:ASP:N	2.42	0.50
19:LO:80:GLU:OE2	19:LO:102:ARG:NH2	2.35	0.50
47:Lq:11:PHE:O	47:Lq:81:ARG:NH2	2.44	0.50
52:S2:74:G:H1	66:SR:171:THR:HG22	1.75	0.50
52:S2:963:A:N1	52:S2:1056:A:O2'	2.44	0.50
52:S2:1338:4AC:H2'	52:S2:1339:G:C8	2.46	0.50
52:S2:1751:C:N4	52:S2:1783:G:O6	2.45	0.50
58:SG:196:ASN:HD22	58:SG:211:GLY:HA2	1.76	0.50
63:SO:127:MET:HE1	63:SO:133:GLY:HA2	1.92	0.50
79:Se:85:ASN:HB2	79:Se:88:MET:HB2	1.92	0.50
6:L5:2546:G:OP1	28:LX:113:ARG:NH1	2.43	0.50
6:L5:3518:U:OP1	6:L5:4296:G:O2'	2.17	0.50
6:L5:3930:G:H5'	9:LD:233:ARG:HB2	1.94	0.50
52:S2:77:A:H61	66:SR:183:ARG:HH12	1.59	0.50
71:SW:134:LEU:HD13	71:SW:138:VAL:HG12	1.93	0.50
3:I:35:U:H2'	3:I:36:G:C5	2.47	0.50
6:L5:470:A:N3	13:LH:108:ARG:NH1	2.60	0.50
6:L5:785:G:H2'	6:L5:786:G:C8	2.45	0.50
6:L5:1496:C:H5''	9:LD:21:LYS:HG2	1.93	0.50
8:L8:23:C:OP1	32:Lb:15:ARG:NH1	2.44	0.50
14:LI:126:LYS:HB2	27:LW:133:ALA:HB3	1.93	0.50
57:SF:60:ASP:N	57:SF:60:ASP:OD1	2.42	0.50
62:SN:78:LEU:HD23	62:SN:78:LEU:H	1.77	0.50
62:SN:128:VAL:HG11	62:SN:155:ILE:HG12	1.93	0.50
64:SP:141:THR:OG1	64:SP:143:ASP:OD1	2.25	0.50
66:SR:114:VAL:HG12	66:SR:115:LYS:HD3	1.93	0.50
6:L5:456:C:H2'	6:L5:457:G:C8	2.47	0.50
6:L5:3996:G:OP1	18:LM:98:ASN:ND2	2.45	0.50
6:L5:4271:C:OP1	10:LE:246:ARG:NH1	2.41	0.50
12:LG:59:ASP:OD1	12:LG:60:ILE:N	2.45	0.50
52:S2:1116:U:H1'	52:S2:1117:C:H2'	1.94	0.50
62:SN:214:LEU:HD12	62:SN:244:ILE:HD11	1.93	0.50
64:SP:55:ALA:HB1	64:SP:60:GLU:HG3	1.93	0.50
6:L5:1110:G:H2'	6:L5:1111:G:H8	1.77	0.50
6:L5:1511:C:O2'	6:L5:2512:C:OP1	2.24	0.50
12:LG:215:ASP:OD1	12:LG:215:ASP:N	2.45	0.50
26:LV:113:MET:HG3	26:LV:119:ALA:HB3	1.93	0.50
52:S2:1865:U:H5'	57:SF:79:ILE:HD11	1.93	0.50
67:SS:39:GLN:HG3	67:SS:75:ILE:HG21	1.93	0.50
68:ST:48:VAL:HG21	68:ST:54:LYS:HG3	1.92	0.50
69:SU:19:PRO:O	69:SU:24:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SU:38:ARG:NH1	69:SU:42:GLU:OE2	2.45	0.50
5:B:671:ARG:NH2	5:B:753:ASP:O	2.35	0.50
6:L5:88:A:N7	24:LT:173:LYS:NZ	2.59	0.50
6:L5:223:G:N3	11:LF:223:ASN:ND2	2.59	0.50
6:L5:761:C:H42	6:L5:792:G:H22	1.59	0.50
6:L5:1252:C:OP1	22:LR:93:LYS:NZ	2.45	0.50
6:L5:1811:G:O2'	6:L5:3965:A:N3	2.39	0.50
8:L8:110:U:OP2	45:Lo:8:ARG:NH2	2.45	0.50
52:S2:193:C:H2'	52:S2:194:C:C6	2.47	0.50
69:SU:55:LYS:HA	69:SU:58:ARG:HG3	1.92	0.50
3:I:165:C:OP2	3:I:166:C:N4	2.45	0.50
6:L5:781:C:H2'	6:L5:782:G:C8	2.47	0.50
6:L5:3850:G:O2'	33:Lc:136:PHE:OXT	2.29	0.50
7:L7:24:C:H2'	7:L7:25:G:O4'	2.12	0.50
21:LQ:155:VAL:O	21:LQ:162:ARG:NH2	2.38	0.50
31:La:80:PRO:HA	31:La:98:PHE:HA	1.94	0.50
52:S2:1419:C:O2'	52:S2:1421:G:OP2	2.21	0.50
61:SM:34:LYS:O	61:SM:98:THR:OG1	2.27	0.50
6:L5:1741:A:H5''	6:L5:1742:G:H5'	1.93	0.49
6:L5:3382:C:OP1	9:LD:200:ARG:NH2	2.43	0.49
6:L5:4485:C:O2	6:L5:4699:G:N2	2.35	0.49
12:LG:128:ASP:O	12:LG:164:LYS:NZ	2.45	0.49
14:LI:92:ILE:HD13	14:LI:246:MET:HE2	1.94	0.49
18:LM:164:ARG:HG2	18:LM:168:GLN:NE2	2.23	0.49
52:S2:477:A:N3	52:S2:489:U:O2'	2.36	0.49
78:Sd:46:ARG:HG2	79:Se:35:ASP:HB3	1.94	0.49
6:L5:2161:G:N2	6:L5:2164:G:OP2	2.34	0.49
32:Lb:30:MET:HB3	32:Lb:101:PRO:HG2	1.94	0.49
53:SB:84:HIS:OXT	73:SY:19:ARG:NH2	2.45	0.49
56:SE:103:THR:OG1	56:SE:104:GLY:N	2.44	0.49
64:SP:106:LYS:HZ2	64:SP:108:ARG:HE	1.59	0.49
68:ST:76:THR:OG1	68:ST:77:ARG:N	2.45	0.49
75:Sa:94:VAL:HG12	75:Sa:107:ILE:HD11	1.94	0.49
80:Sf:98:VAL:HG12	80:Sf:101:ILE:HD12	1.94	0.49
3:I:38:G:H3'	3:I:88:C:H42	1.76	0.49
3:I:54:A:H5'	3:I:159:G:H21	1.76	0.49
6:L5:2301:C:H5''	21:LQ:67:ARG:HD2	1.94	0.49
6:L5:3954:U:OP1	6:L5:4080:U:O2'	2.29	0.49
6:L5:4374:PSU:O2'	30:LZ:16:GLY:O	2.27	0.49
6:L5:4445:U:H1'	6:L5:4446:A:H5''	1.94	0.49
13:LH:102:ASP:N	13:LH:102:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LK:92:MET:HE2	16:LK:179:ILE:HG22	1.93	0.49
52:S2:142:C:OP2	66:SR:188:LYS:NZ	2.40	0.49
58:SG:236:ILE:HG12	58:SG:252:THR:HG22	1.94	0.49
80:Sf:33:GLU:OE2	80:Sf:87:ARG:NH2	2.38	0.49
6:L5:1347:G:N1	6:L5:1348:G:N7	2.61	0.49
27:LW:40:VAL:HG21	27:LW:96:ILE:HD12	1.94	0.49
52:S2:1045:G:HO2'	52:S2:1046:PSU:HN1	1.60	0.49
55:SD:128:ALA:HB3	72:SX:44:LYS:HD2	1.93	0.49
58:SG:147:HIS:HA	58:SG:175:LYS:HZ3	1.77	0.49
62:SN:196:ILE:HB	62:SN:223:TYR:HB2	1.93	0.49
44:Ln:12:LEU:HB3	44:Ln:16:ARG:HH12	1.77	0.49
61:SM:38:MET:HE1	61:SM:231:LEU:HD11	1.93	0.49
84:Sj:55:ILE:HD12	84:Sj:75:ILE:HD12	1.94	0.49
1:E:163:MET:HG3	1:E:166:LYS:HD2	1.95	0.49
2:F:8:U:H2'	2:F:9:G:C8	2.47	0.49
6:L5:1010:A:N6	6:L5:1091:G:O6	2.45	0.49
6:L5:1211:G:O6	35:Le:111:ARG:NH2	2.45	0.49
6:L5:1477:OMG:H8	6:L5:1477:OMG:OP2	1.95	0.49
6:L5:1888:U:OP1	16:LK:64:ARG:NH1	2.45	0.49
6:L5:1892:U:O2'	6:L5:1893:U:OP1	2.30	0.49
6:L5:4026:A:N6	12:LG:28:THR:O	2.38	0.49
6:L5:4624:U:O4	13:LH:275:ARG:NH2	2.46	0.49
12:LG:126:THR:OG1	12:LG:128:ASP:OD1	2.27	0.49
19:LO:174:LYS:O	34:Ld:138:LYS:NZ	2.40	0.49
1:E:235:LYS:NZ	52:S2:49:C:O2'	2.46	0.49
6:L5:2194:OMC:HM22	6:L5:2195:U:H5'	1.94	0.49
58:SG:245:ARG:NH2	58:SG:295:GLY:O	2.46	0.49
62:SN:232:THR:HG22	62:SN:235:ASN:H	1.78	0.49
65:SQ:149:GLN:HG3	65:SQ:153:LEU:HD23	1.95	0.49
75:Sa:123:TYR:OH	78:Sd:124:ARG:NH1	2.45	0.49
77:Sc:66:VAL:HG23	77:Sc:69:ILE:HB	1.95	0.49
1:E:537:SER:O	1:E:541:LYS:N	2.43	0.49
6:L5:400:A2M:OP1	23:LS:4:TYR:OH	2.24	0.49
6:L5:1276:C:H2'	6:L5:1277:A:C8	2.48	0.49
6:L5:1350:G:H2'	6:L5:1351:G:H8	1.77	0.49
6:L5:1473:A:OP1	34:Ld:27:LYS:NZ	2.30	0.49
6:L5:4381:A:OP1	6:L5:4382:PSU:O2'	2.31	0.49
51:Lx:70:ASP:O	51:Lx:74:CYS:N	2.40	0.49
52:S2:1837:G:OP1	52:S2:1840:U:H4'	2.13	0.49
60:SL:198:MET:HE2	77:Sc:89:SER:HB2	1.95	0.49
76:Sb:52:LEU:HB3	76:Sb:56:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:G:H2'	2:F:26:G:C8	2.47	0.49
3:I:73:A:N6	3:I:160:G:OP2	2.46	0.49
6:L5:1879:G:H22	6:L5:4180:C:H5''	1.77	0.49
6:L5:3413:G:OP2	9:LD:128:ARG:NH2	2.46	0.49
6:L5:3491:A:O2'	52:S2:1827:G:O2'	2.26	0.49
6:L5:4304:U:OP2	10:LE:246:ARG:NH2	2.45	0.49
6:L5:4516:G:OP1	22:LR:176:ARG:NH1	2.44	0.49
52:S2:1532:A:H4'	52:S2:1606:G:H4'	1.94	0.49
6:L5:769:C:H2'	6:L5:770:G:C8	2.48	0.49
6:L5:3609:A:N3	6:L5:4147:G:O2'	2.40	0.49
6:L5:4138:OMG:H2'	6:L5:4193:5MC:HM51	1.95	0.49
6:L5:4635:G:H2'	6:L5:4636:G:H8	1.78	0.49
10:LE:90:VAL:HG22	10:LE:104:THR:HG23	1.95	0.49
21:LQ:158:HIS:HB3	21:LQ:161:MET:HG3	1.94	0.49
35:Le:57:MET:O	35:Le:61:ASN:ND2	2.45	0.49
52:S2:630:A:O2'	52:S2:632:U:OP1	2.30	0.49
52:S2:678:G:N1	52:S2:1028:A:OP2	2.41	0.49
52:S2:745:G:N3	67:SS:109:ARG:NH2	2.61	0.49
65:SQ:176:GLU:OE2	65:SQ:188:TYR:N	2.44	0.49
67:SS:51:ILE:HD13	67:SS:61:ILE:HD11	1.94	0.49
67:SS:149:ASP:OD1	67:SS:149:ASP:N	2.45	0.49
6:L5:181:C:H2'	6:L5:182:G:C8	2.47	0.48
6:L5:2028:G:H1	6:L5:2038:C:H41	1.60	0.48
6:L5:4326:U:O2'	10:LE:182:GLU:OE1	2.19	0.48
6:L5:4637:G:O6	6:L5:4660:C:N4	2.45	0.48
11:LF:285:LEU:HD23	24:LT:122:THR:HG21	1.94	0.48
52:S2:1031:A:H2'	52:S2:1032:A2M:H8	1.95	0.48
65:SQ:125:SER:HA	65:SQ:138:ALA:HA	1.95	0.48
69:SU:111:GLN:HB2	69:SU:145:PRO:HB3	1.95	0.48
3:I:174:G:O6	3:I:203:U:O2'	2.26	0.48
6:L5:417:G:H1'	8:L8:16:G:N2	2.28	0.48
6:L5:784:C:H2'	6:L5:785:G:H8	1.78	0.48
10:LE:224:LYS:HG2	10:LE:340:THR:HG22	1.95	0.48
11:LF:110:ARG:O	11:LF:113:ARG:NH1	2.35	0.48
12:LG:29:ASP:HB2	12:LG:150:LEU:HD21	1.95	0.48
30:LZ:56:ARG:HH21	30:LZ:61:LYS:HG2	1.78	0.48
52:S2:1233:PSU:H2'	52:S2:1234:G:C8	2.48	0.48
62:SN:84:PHE:HA	81:Sg:15:ARG:NH1	2.28	0.48
69:SU:18:ARG:HB3	69:SU:21:GLU:OE1	2.13	0.48
2:F:78:C:H2'	2:F:79:U:H6	1.78	0.48
10:LE:19:ARG:HB2	10:LE:234:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LE:41:VAL:HA	10:LE:187:GLY:HA3	1.96	0.48
52:S2:501:A:O2'	52:S2:502:C:O4'	2.28	0.48
71:SW:5:GLN:NE2	71:SW:11:GLN:O	2.39	0.48
71:SW:135:SER:OG	71:SW:136:LYS:N	2.43	0.48
4:S:1118:U:H2'	4:S:1119:C:C6	2.49	0.48
6:L5:158:A:N1	6:L5:276:C:O2'	2.42	0.48
6:L5:3393:G:N7	9:LD:152:SER:OG	2.41	0.48
6:L5:3679:A:H2	6:L5:3793:G:H1	1.60	0.48
6:L5:3692:A:N3	6:L5:3772:U:O2'	2.35	0.48
6:L5:3830:C:H2'	6:L5:3831:C:H6	1.79	0.48
6:L5:4089:U:O2'	47:Lq:31:ASP:OD1	2.31	0.48
12:LG:193:GLU:OE2	12:LG:196:ARG:NH2	2.44	0.48
14:LI:114:ARG:NH1	24:LT:4:ASP:O	2.45	0.48
33:Lc:50:PRO:HD3	33:Lc:68:ILE:HG12	1.94	0.48
52:S2:1011:G:H2'	52:S2:1012:A:C8	2.48	0.48
3:I:84:A:H2'	3:I:85:G:O4'	2.13	0.48
12:LG:108:ARG:CZ	12:LG:253:TYR:HB2	2.43	0.48
30:LZ:102:LYS:HA	30:LZ:105:ARG:HB3	1.95	0.48
33:Lc:54:THR:HG22	33:Lc:56:ALA:H	1.78	0.48
35:Le:5:MLZ:NZ	35:Le:8:THR:OG1	2.47	0.48
38:Lh:9:LYS:NZ	38:Lh:71:PRO:O	2.40	0.48
52:S2:1620:A:OP1	75:Sa:47:ARG:NE	2.45	0.48
78:Sd:109:GLU:HA	78:Sd:112:GLU:HB3	1.94	0.48
1:E:140:LYS:HD2	1:E:214:SER:HB2	1.95	0.48
6:L5:511:A:C6	34:Ld:105:ARG:HD3	2.48	0.48
6:L5:1215:G:H5'	35:Le:110:ALA:HB1	1.95	0.48
6:L5:3514:5MC:OP1	86:Sl:23:ARG:NH2	2.46	0.48
9:LD:140:ASN:OD1	9:LD:143:THR:OG1	2.22	0.48
24:LT:177:ALA:O	24:LT:184:ARG:HB2	2.13	0.48
52:S2:238:C:H3'	52:S2:892:G:N2	2.29	0.48
52:S2:1299:G:H4'	75:Sa:78:THR:HA	1.94	0.48
52:S2:1316:U:H5	52:S2:1317:C:C4	2.32	0.48
67:SS:133:LEU:HD21	67:SS:176:VAL:HG13	1.96	0.48
84:Sj:20:ARG:NH1	84:Sj:74:MET:HE1	2.28	0.48
6:L5:409:G:OP2	23:LS:2:VAL:N	2.47	0.48
6:L5:4450:C:H2'	6:L5:4451:A:C8	2.49	0.48
16:LK:17:ASP:HB3	16:LK:28:LYS:HB3	1.94	0.48
23:LS:45:THR:HG22	23:LS:49:LYS:HE2	1.94	0.48
52:S2:352:G:O3'	71:SW:139:ARG:NH1	2.47	0.48
52:S2:1537:G:H2'	52:S2:1538:A:C8	2.49	0.48
66:SR:3:LEU:HB3	66:SR:5:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:SER:N	1:E:254:ASP:OD2	2.47	0.48
6:L5:3393:G:H4'	6:L5:3394:A:H5'	1.94	0.48
6:L5:4059:A:OP1	27:LW:92:ARG:NH1	2.47	0.48
15:LJ:230:TYR:HA	15:LJ:233:ILE:HB	1.95	0.48
52:S2:49:C:H2'	52:S2:473:C:H41	1.78	0.48
52:S2:381:G:OP2	68:ST:54:LYS:NZ	2.44	0.48
52:S2:1284:C:H42	72:SX:102:LYS:HD3	1.78	0.48
58:SG:270:LEU:HD21	58:SG:310:TRP:CG	2.49	0.48
63:SO:179:GLN:N	63:SO:179:GLN:OE1	2.46	0.48
83:Si:61:GLN:O	83:Si:62:HY3:N	2.46	0.48
33:Lc:121:ARG:O	33:Lc:124:THR:OG1	2.32	0.48
35:Le:55:LYS:O	35:Le:58:GLN:NE2	2.46	0.48
52:S2:116:OMU:O5'	52:S2:116:OMU:H6	2.14	0.48
52:S2:335:C:H5	66:SR:190:ARG:HH12	1.61	0.48
63:SO:154:ASP:OD1	63:SO:154:ASP:N	2.45	0.48
66:SR:32:MET:HG2	66:SR:100:CYS:HB2	1.95	0.48
78:Sd:34:LYS:HG2	78:Sd:103:LEU:HD23	1.96	0.48
84:Sj:19:GLN:HG3	84:Sj:81:TYR:CG	2.49	0.48
6:L5:755:G:N2	6:L5:800:U:O2	2.38	0.48
6:L5:1072:C:H1'	6:L5:1074:C:C2	2.49	0.48
6:L5:2243:G:H21	40:Lj:6:THR:HG22	1.78	0.48
6:L5:2370:A:OP1	25:LU:38:ARG:NH2	2.40	0.48
11:LF:319:LEU:HD11	14:LI:151:GLU:HA	1.96	0.48
15:LJ:58:PRO:HD2	15:LJ:61:ILE:HG13	1.95	0.48
16:LK:91:LYS:NZ	16:LK:183:GLU:OE1	2.39	0.48
24:LT:119:LYS:HE3	24:LT:121:LEU:HD21	1.96	0.48
40:Lj:41:ALA:O	40:Lj:52:ARG:NH1	2.47	0.48
57:SF:23:CYS:HB3	57:SF:28:ARG:H	1.79	0.48
58:SG:130:LYS:HG2	58:SG:141:THR:HG22	1.95	0.48
63:SO:39:VAL:HG22	63:SO:48:ILE:HG22	1.94	0.48
84:Sj:91:LEU:HD22	84:Sj:96:LEU:HD22	1.96	0.48
2:F:18:U:C4	2:F:73:U:H1'	2.49	0.47
6:L5:697:G:N2	6:L5:698:C:O2	2.47	0.47
6:L5:3834:G:H1'	6:L5:3835:G:C8	2.49	0.47
14:LI:26:GLU:HG2	14:LI:27:LEU:HD22	1.95	0.47
16:LK:12:ILE:HD12	16:LK:18:ILE:HD12	1.96	0.47
25:LU:101:ILE:HD13	25:LU:104:ARG:HH12	1.78	0.47
52:S2:197:U:H2'	52:S2:198:U:C6	2.49	0.47
52:S2:528:C:H2'	52:S2:529:A:C8	2.49	0.47
52:S2:1309:U:O2'	52:S2:1310:C:O4'	2.29	0.47
58:SG:60:ARG:HH22	76:Sb:97:GLN:HB3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SM:68:GLU:HG2	61:SM:83:LYS:HD3	1.95	0.47
6:L5:1572:G:H1'	6:L5:2356:A:N6	2.30	0.47
6:L5:3830:C:H2'	6:L5:3831:C:C6	2.50	0.47
25:LU:23:TRP:HB3	25:LU:51:ILE:HG12	1.96	0.47
33:Lc:36:ARG:NH1	33:Lc:38:TYR:OH	2.46	0.47
52:S2:220:U:H2'	52:S2:221:A:C8	2.49	0.47
52:S2:1741:C:OP1	68:ST:44:HIS:ND1	2.46	0.47
60:SL:118:GLU:OE2	62:SN:65:LYS:N	2.47	0.47
64:SP:100:ARG:HB2	64:SP:114:ILE:HD13	1.95	0.47
65:SQ:120:GLY:O	65:SQ:193:LYS:NZ	2.46	0.47
75:Sa:72:LYS:HD3	75:Sa:93:MET:HE3	1.96	0.47
6:L5:452:A:H62	6:L5:1237:G:H3'	1.78	0.47
6:L5:629:G:H2'	6:L5:630:G:C8	2.50	0.47
10:LE:77:THR:HG21	10:LE:337:VAL:HG22	1.95	0.47
16:LK:150:ASP:HB3	16:LK:153:LEU:HB2	1.95	0.47
52:S2:1787:U:H2'	52:S2:1788:G:C8	2.47	0.47
52:S2:1865:U:OP2	57:SF:4:LYS:NZ	2.35	0.47
54:SC:36:ASP:N	54:SC:36:ASP:OD1	2.43	0.47
58:SG:187:ASN:HB3	63:SO:225:GLU:HG3	1.97	0.47
70:SV:83:LEU:HB3	70:SV:85:LEU:HD23	1.96	0.47
75:Sa:28:MET:HB3	75:Sa:32:GLN:HG3	1.96	0.47
6:L5:1713:C:H2'	6:L5:1714:A:C8	2.50	0.47
6:L5:1743:A:H5'	6:L5:1745:G:O4'	2.14	0.47
6:L5:2499:U:H5''	33:Lc:38:TYR:HB3	1.97	0.47
6:L5:3628:C:O2'	10:LE:268:ARG:NH1	2.45	0.47
9:LD:80:GLU:HB2	9:LD:170:ALA:HA	1.96	0.47
19:LO:78:LEU:HD23	19:LO:100:PRO:HA	1.95	0.47
52:S2:234:C:N4	52:S2:897:U:H3	2.13	0.47
52:S2:660:G:O2'	52:S2:663:G:O2'	2.26	0.47
52:S2:836:C:H41	84:Sj:8:ARG:HD3	1.80	0.47
52:S2:1868:U:O2'	57:SF:38:LYS:HD2	2.15	0.47
58:SG:197:THR:OG1	58:SG:237:ASN:O	2.32	0.47
62:SN:94:ILE:HG21	62:SN:162:ILE:HD12	1.97	0.47
62:SN:248:TYR:OH	81:Sg:10:ASP:OD1	2.23	0.47
76:Sb:30:GLY:N	76:Sb:64:ALA:O	2.48	0.47
6:L5:1375:A:H8	6:L5:1456:C:C5	2.32	0.47
6:L5:1545:C:H4'	6:L5:2700:A:H5'	1.95	0.47
6:L5:2741:G:OP1	25:LU:104:ARG:NH1	2.47	0.47
6:L5:3516:A:O2'	6:L5:3517:A2M:H3'	2.14	0.47
58:SG:22:ALA:HB1	58:SG:71:ILE:HD11	1.95	0.47
85:Sk:58:LEU:HD12	85:Sk:62:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Sk:102:LYS:HA	85:Sk:107:VAL:HG12	1.96	0.47
6:L5:772:C:H2'	6:L5:773:G:C8	2.50	0.47
11:LF:156:ASP:OD1	11:LF:255:SER:N	2.40	0.47
38:Lh:78:LEU:HB3	49:Ls:20:ARG:HD3	1.96	0.47
52:S2:22:A:H4'	69:SU:17:ARG:HA	1.95	0.47
52:S2:616:C:O2	56:SE:85:LYS:NZ	2.46	0.47
55:SD:102:VAL:HG13	72:SX:36:ARG:CZ	2.44	0.47
60:SL:164:ASN:O	60:SL:170:SER:OG	2.31	0.47
64:SP:171:ASP:N	64:SP:171:ASP:OD1	2.45	0.47
81:Sg:1:AME:HT23	81:Sg:1:AME:HA	1.55	0.47
85:Sk:111:ARG:HD3	85:Sk:114:LYS:HE3	1.97	0.47
2:F:51:U:H2'	2:F:52:C:C6	2.50	0.47
6:L5:453:G:H4'	6:L5:454:U:H5'	1.97	0.47
6:L5:2691:G:O2'	6:L5:3570:U:O4	2.30	0.47
6:L5:3443:A:H5''	6:L5:3444:A:N7	2.30	0.47
6:L5:3822:G:H2'	6:L5:3823:G:C8	2.50	0.47
6:L5:4501:G:OP1	39:Li:4:ARG:NH1	2.47	0.47
10:LE:25:HIS:HE1	10:LE:343:ARG:HH11	1.63	0.47
18:LM:44:THR:O	18:LM:78:LYS:NZ	2.48	0.47
18:LM:119:TYR:HB3	78:Sd:12:ILE:HG21	1.96	0.47
26:LV:45:TRP:NE1	26:LV:56:LYS:HG3	2.30	0.47
48:Lr:26:VAL:HG12	48:Lr:30:GLU:HG3	1.96	0.47
52:S2:381:G:N1	52:S2:384:G:OP2	2.33	0.47
52:S2:587:G:H2'	69:SU:172:ARG:HH12	1.78	0.47
52:S2:792:C:H2'	52:S2:793:C:C6	2.49	0.47
52:S2:1061:A:H4'	52:S2:1062:U:H5''	1.96	0.47
55:SD:105:TYR:CD1	55:SD:118:ARG:HG3	2.50	0.47
56:SE:112:TYR:CG	69:SU:33:GLY:HA3	2.50	0.47
58:SG:173:LEU:HD23	58:SG:175:LYS:HZ1	1.80	0.47
65:SQ:201:LYS:HA	65:SQ:204:ARG:HE	1.80	0.47
67:SS:172:THR:O	67:SS:176:VAL:HG12	2.15	0.47
2:F:14:U:H3	2:F:25:G:H1	1.63	0.47
6:L5:707:C:O2	13:LH:133:LYS:NZ	2.47	0.47
6:L5:4060:C:O2'	35:Le:36:ASP:OD1	2.30	0.47
8:L8:102:G:OP2	8:L8:104:A:O2'	2.31	0.47
52:S2:1631:A:H5''	78:Sd:37:GLY:H	1.80	0.47
58:SG:223:GLU:HG3	58:SG:225:LYS:NZ	2.29	0.47
62:SN:121:ARG:HH12	62:SN:123:ARG:HD3	1.80	0.47
74:SZ:16:SER:OG	74:SZ:17:LEU:N	2.46	0.47
81:Sg:53:TYR:OH	81:Sg:76:ASP:OD2	2.27	0.47
82:Sh:115:GLU:HG3	82:Sh:118:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:293:LEU:O	11:LF:299:GLN:NE2	2.37	0.47
23:LS:64:ASN:ND2	23:LS:80:GLN:OE1	2.46	0.47
23:LS:128:ARG:HG3	23:LS:136:ILE:HG23	1.97	0.47
77:Sc:116:ASN:ND2	77:Sc:116:ASN:O	2.46	0.47
80:Sf:20:ILE:HD11	80:Sf:91:LEU:HB2	1.97	0.47
84:Sj:56:PHE:O	84:Sj:74:MET:N	2.46	0.47
2:F:57:G:H2'	2:F:58:A:H8	1.80	0.47
6:L5:1208:C:H2'	6:L5:1209:G:C8	2.49	0.47
6:L5:1701:C:H2'	6:L5:1702:C:C6	2.50	0.47
6:L5:2328:U:H2'	6:L5:2329:G:C8	2.50	0.47
6:L5:4450:C:H2'	6:L5:4451:A:H8	1.80	0.47
9:LD:178:PRO:HD2	48:Lr:26:VAL:HG22	1.97	0.47
10:LE:161:ARG:HG2	10:LE:184:GLN:HA	1.96	0.47
17:LL:44:ASP:OD1	17:LL:44:ASP:N	2.37	0.47
21:LQ:181:HIS:O	21:LQ:195:ARG:NH2	2.42	0.47
52:S2:1607:G:N2	52:S2:1633:G:H1'	2.29	0.47
52:S2:1842:C:H2'	52:S2:1843:4AC:H6	1.97	0.47
58:SG:56:GLN:OE1	58:SG:56:GLN:N	2.48	0.47
63:SO:194:PRO:O	63:SO:201:LYS:NZ	2.47	0.47
79:Se:111:LYS:O	79:Se:126:GLN:NE2	2.45	0.47
80:Sf:38:ASP:O	80:Sf:42:GLY:N	2.43	0.47
3:I:145:C:O2'	3:I:147:C:OP2	2.22	0.46
4:S:1120:U:H2'	4:S:1121:G:C8	2.50	0.46
4:S:1134:C:H2'	4:S:1135:C:H2'	1.96	0.46
6:L5:1288:C:H2'	6:L5:1289:A:C8	2.50	0.46
21:LQ:184:ILE:O	21:LQ:194:ARG:NH1	2.44	0.46
23:LS:115:GLU:HG2	23:LS:151:THR:HG23	1.96	0.46
52:S2:875:G:N3	67:SS:114:GLN:NE2	2.60	0.46
57:SF:44:ILE:O	74:SZ:113:GLN:NE2	2.33	0.46
74:SZ:31:CYS:HA	74:SZ:44:VAL:HA	1.96	0.46
5:B:460:GLU:HG3	5:B:464:HIS:CE1	2.50	0.46
6:L5:279:A:OP2	21:LQ:8:GLN:NE2	2.47	0.46
6:L5:992:C:OP1	6:L5:1106:U:O2'	2.33	0.46
6:L5:1726:A:N3	6:L5:3956:U:O2'	2.48	0.46
6:L5:1947:U:O2'	6:L5:1949:A:N7	2.39	0.46
9:LD:2:GLY:HA2	9:LD:207:VAL:HG23	1.98	0.46
10:LE:80:GLU:HG3	10:LE:326:VAL:HG13	1.97	0.46
16:LK:173:ARG:NH1	46:Lp:125:LYS:O	2.46	0.46
27:LW:4:THR:HG23	27:LW:9:ARG:HD3	1.96	0.46
36:Lf:103:ASP:OD1	36:Lf:103:ASP:N	2.49	0.46
52:S2:17:C:O2'	52:S2:1195:A:N1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1379:A:N6	60:SL:136:GLU:OE2	2.47	0.46
56:SE:109:ARG:HD2	69:SU:124:HIS:CD2	2.50	0.46
65:SQ:42:LYS:HD3	65:SQ:42:LYS:HA	1.81	0.46
66:SR:197:GLN:HA	66:SR:200:LYS:HG2	1.97	0.46
67:SS:117:PRO:HB2	67:SS:120:ARG:HD3	1.96	0.46
70:SV:60:GLU:HB3	70:SV:69:TRP:CD1	2.50	0.46
1:E:228:VAL:N	1:E:301:GLY:O	2.47	0.46
1:E:510:LEU:HA	1:E:575:VAL:HA	1.97	0.46
6:L5:1698:G:N2	6:L5:1712:U:O2	2.35	0.46
6:L5:4198:U:OP2	6:L5:4268:G:N1	2.40	0.46
18:LM:46:GLN:NE2	18:LM:73:THR:O	2.48	0.46
21:LQ:201:HIS:O	21:LQ:204:ARG:NH1	2.46	0.46
33:Lc:9:LYS:HD2	33:Lc:83:THR:O	2.16	0.46
52:S2:339:G:H2'	52:S2:340:A:C8	2.50	0.46
52:S2:1098:G:H4'	60:SL:32:PHE:CD1	2.51	0.46
67:SS:8:ILE:HD13	67:SS:16:PRO:HB3	1.98	0.46
84:Sj:78:SER:OG	84:Sj:80:ASP:OD1	2.25	0.46
6:L5:795:A:H3'	6:L5:796:C:C6	2.51	0.46
13:LH:45:HIS:ND1	13:LH:46:CYS:O	2.46	0.46
16:LK:113:GLU:OE1	16:LK:115:ARG:NH2	2.48	0.46
40:Lj:87:VAL:O	40:Lj:91:ILE:HG12	2.16	0.46
52:S2:1357:G:O3'	62:SN:125:LYS:NZ	2.45	0.46
62:SN:169:TYR:OH	62:SN:175:GLY:O	2.26	0.46
63:SO:14:ASP:OD1	63:SO:15:GLY:N	2.48	0.46
68:ST:42:ARG:HH21	68:ST:59:ARG:HH12	1.63	0.46
77:Sc:29:HIS:O	77:Sc:33:ARG:HG2	2.15	0.46
80:Sf:18:HIS:ND1	80:Sf:95:SER:OG	2.47	0.46
85:Sk:48:VAL:HG22	85:Sk:49:LEU:HD22	1.98	0.46
6:L5:772:C:H2'	6:L5:773:G:H8	1.80	0.46
6:L5:1705:A:H2'	6:L5:1706:A:O4'	2.15	0.46
6:L5:1922:A:H3'	6:L5:1926:C:H41	1.80	0.46
6:L5:2338:U:H2'	6:L5:2339:G:C8	2.51	0.46
10:LE:66:LYS:HZ3	29:LY:13:LYS:HA	1.80	0.46
52:S2:158:A:H61	52:S2:468:G:H1'	1.80	0.46
52:S2:437:OMG:OP2	52:S2:472:G:O2'	2.33	0.46
61:SM:191:ASP:OD1	61:SM:191:ASP:N	2.43	0.46
84:Sj:47:MET:HE2	84:Sj:47:MET:HB2	1.88	0.46
6:L5:521:C:H2'	6:L5:522:U:O4'	2.16	0.46
6:L5:1909:A:H2'	6:L5:1955:C:H42	1.80	0.46
6:L5:2314:G:H5''	15:LJ:59:ARG:HD2	1.98	0.46
6:L5:4012:G:H2'	6:L5:4012:G:N3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LS:8:PRO:HG3	23:LS:149:ILE:HG21	1.97	0.46
52:S2:195:C:H2'	52:S2:196:C:C6	2.51	0.46
52:S2:239:C:O5'	52:S2:892:G:N2	2.49	0.46
52:S2:1754:C:H2'	52:S2:1755:G:C8	2.50	0.46
55:SD:126:CYS:HB2	55:SD:130:VAL:HB	1.97	0.46
58:SG:217:MET:HG2	58:SG:229:THR:HG22	1.98	0.46
67:SS:133:LEU:HD11	67:SS:176:VAL:HG11	1.97	0.46
80:Sf:43:ALA:HB1	80:Sf:48:LEU:HB3	1.98	0.46
82:Sh:36:ARG:HE	82:Sh:110:ILE:HD12	1.80	0.46
2:F:59:C:H2'	2:F:60:A:C8	2.51	0.46
3:I:54:A:H5'	3:I:159:G:N2	2.30	0.46
3:I:175:G:N2	3:I:203:U:OP1	2.49	0.46
6:L5:530:C:H42	6:L5:625:G:H1	1.63	0.46
6:L5:2539:A:H62	44:Ln:35:LYS:NZ	2.14	0.46
12:LG:209:ARG:O	12:LG:213:GLU:HG2	2.16	0.46
31:La:82:THR:HG21	41:Lk:37:THR:HG22	1.97	0.46
49:Ls:26:SER:OG	49:Ls:28:GLU:OE1	2.34	0.46
52:S2:1649:G:O2'	52:S2:1675:G:O6	2.27	0.46
56:SE:108:ARG:O	56:SE:112:TYR:N	2.38	0.46
68:ST:42:ARG:HE	68:ST:59:ARG:NH1	2.14	0.46
80:Sf:32:LEU:HD11	80:Sf:87:ARG:HD3	1.97	0.46
1:E:258:ILE:HG12	1:E:298:LEU:HD11	1.96	0.46
3:I:115:A:H2'	3:I:116:G:H8	1.81	0.46
3:I:150:C:H42	3:I:151:A:N6	2.14	0.46
5:B:697:ASN:OD1	5:B:730:ASN:HB2	2.16	0.46
6:L5:667:C:H2'	6:L5:668:G:C8	2.51	0.46
6:L5:2423:U:P	33:Lc:36:ARG:HH22	2.38	0.46
6:L5:4636:G:C2	6:L5:4637:G:H1'	2.51	0.46
6:L5:4757:C:OP1	68:ST:92:ARG:NH1	2.49	0.46
9:LD:206:PRO:HG3	9:LD:213:GLY:HA3	1.98	0.46
25:LU:106:LEU:HB3	25:LU:120:TYR:HE1	1.80	0.46
52:S2:656:A:H4'	52:S2:657:G:H3'	1.98	0.46
52:S2:1233:PSU:H2'	52:S2:1234:G:H8	1.80	0.46
52:S2:1387:A:OP2	63:SO:160:SER:OG	2.22	0.46
53:SB:67:THR:OG1	53:SB:70:LYS:O	2.34	0.46
58:SG:40:ILE:HB	58:SG:59:LEU:HB2	1.98	0.46
61:SM:70:SER:OG	74:SZ:128:ARG:NH1	2.48	0.46
61:SM:129:THR:OG1	61:SM:131:ASP:OD1	2.27	0.46
72:SX:77:ILE:HD11	72:SX:128:PHE:CZ	2.51	0.46
73:SY:84:LEU:HD13	73:SY:89:TYR:HB2	1.97	0.46
75:Sa:23:ASP:OD1	75:Sa:24:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:1892:U:H2'	6:L5:1893:U:C6	2.51	0.46
6:L5:2372:A:O2'	6:L5:2374:C:OP2	2.34	0.46
10:LE:86:VAL:HG13	10:LE:162:VAL:HG13	1.98	0.46
20:LP:55:MET:O	26:LV:157:ARG:NH2	2.48	0.46
22:LR:125:LYS:HG2	22:LR:129:LEU:HD12	1.98	0.46
38:Lh:108:ARG:NH2	38:Lh:124:ASN:O	2.48	0.46
65:SQ:71:ARG:NH2	65:SQ:148:ASN:OD1	2.48	0.46
73:SY:29:THR:HG23	73:SY:32:ASP:H	1.81	0.46
74:SZ:45:THR:HG22	74:SZ:52:THR:HA	1.98	0.46
76:Sb:16:LYS:HA	76:Sb:16:LYS:HD2	1.80	0.46
76:Sb:86:GLN:NE2	76:Sb:118:THR:O	2.43	0.46
5:B:431:GLN:HB3	52:S2:1291:G:O2'	2.16	0.46
6:L5:3497:G:H21	6:L5:3498:A:N6	2.13	0.46
11:LF:155:GLU:HG2	11:LF:157:LYS:H	1.81	0.46
30:LZ:23:ARG:HH21	30:LZ:27:LYS:HD3	1.80	0.46
52:S2:567:U:H3	52:S2:585:A:H61	1.62	0.46
52:S2:801:U:O4	67:SS:106:ARG:NH1	2.49	0.46
52:S2:1428:C:OP1	79:Se:7:LYS:NZ	2.48	0.46
58:SG:39:THR:HG22	58:SG:60:ARG:HG2	1.98	0.46
61:SM:117:TRP:HB3	61:SM:153:THR:HG22	1.97	0.46
65:SQ:127:ARG:HH22	65:SQ:131:ALA:H	1.63	0.46
70:SV:15:LEU:HD22	70:SV:49:MET:HE1	1.98	0.46
82:Sh:70:ASN:ND2	82:Sh:130:PHE:OXT	2.49	0.46
84:Sj:35:VAL:HG21	84:Sj:40:ILE:HD11	1.97	0.46
4:S:1147:C:H2'	4:S:1148:A:O4'	2.16	0.45
52:S2:115:U:H2'	52:S2:116:OMU:C6	2.46	0.45
52:S2:1099:C:H2'	52:S2:1100:G:C8	2.51	0.45
52:S2:1704:OMC:N3	52:S2:1833:6MZ:H9	2.31	0.45
58:SG:248:LEU:HB3	58:SG:261:LEU:HD21	1.98	0.45
68:ST:135:GLU:O	68:ST:139:LYS:HB2	2.16	0.45
6:L5:108:A:N1	6:L5:333:U:O2'	2.46	0.45
6:L5:1632:PSU:H4'	6:L5:1635:G:N1	2.31	0.45
6:L5:2250:G:OP2	6:L5:2250:G:N2	2.43	0.45
6:L5:2325:C:H2'	6:L5:2326:G:C8	2.51	0.45
6:L5:2721:G:H4'	6:L5:3557:A2M:H5''	1.99	0.45
6:L5:3588:A:H5''	23:LS:83:TRP:O	2.16	0.45
10:LE:357:ARG:O	10:LE:361:GLU:HG3	2.17	0.45
13:LH:182:LEU:HD12	13:LH:186:ARG:HA	1.97	0.45
14:LI:103:LYS:O	14:LI:107:VAL:HG12	2.16	0.45
15:LJ:50:ASP:HA	31:La:40:ILE:HD11	1.98	0.45
30:LZ:93:LYS:HB2	30:LZ:94:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:282:C:N4	52:S2:892:G:H4'	2.31	0.45
72:SX:24:THR:HG22	72:SX:115:GLY:HA3	1.99	0.45
73:SY:93:LYS:HA	73:SY:150:VAL:HG21	1.98	0.45
6:L5:3973:OMU:HM23	6:L5:3973:OMU:H1'	1.73	0.45
6:L5:4657:C:H2'	6:L5:4658:G:O4'	2.17	0.45
12:LG:119:TYR:OH	12:LG:139:PRO:O	2.27	0.45
40:Lj:46:CYS:CB	40:Lj:86:CYS:SG	3.01	0.45
52:S2:65:C:C6	66:SR:174:PRO:HB3	2.51	0.45
52:S2:1266:A:O2'	52:S2:1328:G:OP2	2.21	0.45
52:S2:1751:C:H2'	52:S2:1752:C:O4'	2.16	0.45
55:SD:89:LYS:HE3	55:SD:89:LYS:HB3	1.77	0.45
60:SL:33:GLN:HB3	60:SL:154:LEU:HD12	1.98	0.45
76:Sb:16:LYS:HG3	76:Sb:17:LYS:H	1.82	0.45
78:Sd:125:HIS:CE1	78:Sd:131:VAL:HG11	2.51	0.45
6:L5:522:U:H1'	6:L5:636:G:H22	1.81	0.45
6:L5:1588:G:H5'	6:L5:1589:A:OP1	2.16	0.45
6:L5:2304:G:H2'	6:L5:2305:C:C6	2.51	0.45
6:L5:4073:C:OP1	27:LW:70:HIS:NE2	2.48	0.45
6:L5:4523:G:N2	6:L5:4599:G:N7	2.65	0.45
6:L5:4645:C:H2'	6:L5:4646:G:C8	2.51	0.45
14:LI:237:ASP:OD1	14:LI:237:ASP:N	2.49	0.45
20:LP:27:ILE:HD13	20:LP:38:VAL:HG12	1.98	0.45
47:Lq:34:TYR:O	47:Lq:39:ARG:NH1	2.47	0.45
78:Sd:106:LYS:O	78:Sd:109:GLU:HG2	2.17	0.45
79:Se:82:ARG:NH2	79:Se:90:SER:OG	2.49	0.45
1:E:331:THR:HG23	1:E:350:PHE:H	1.82	0.45
6:L5:2105:G:OP2	49:Ls:98:ARG:NH1	2.50	0.45
6:L5:3593:A:H2'	6:L5:3594:A:C8	2.51	0.45
6:L5:4599:G:H5''	22:LR:169:ARG:NH2	2.32	0.45
17:LL:61:SER:HA	17:LL:126:VAL:HG23	1.99	0.45
32:Lb:50:ARG:HD2	32:Lb:115:ARG:HH11	1.81	0.45
37:Lg:37:GLY:O	37:Lg:41:ARG:HG3	2.17	0.45
52:S2:125:C:OP1	52:S2:127:C:N4	2.49	0.45
52:S2:695:G:C2	52:S2:696:C:H1'	2.52	0.45
52:S2:1857:C:H2'	52:S2:1858:G:C8	2.52	0.45
58:SG:22:ALA:HB3	58:SG:32:LEU:HB2	1.99	0.45
65:SQ:182:LYS:HD2	65:SQ:184:SER:HB2	1.98	0.45
69:SU:114:VAL:HG13	69:SU:126:ALA:HB1	1.97	0.45
75:Sa:93:MET:HE1	75:Sa:106:GLU:HG3	1.98	0.45
83:Si:54:LYS:HD3	83:Si:70:VAL:HG12	1.98	0.45
1:E:338:THR:HG22	1:E:340:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:1138:G:H21	6:L5:1203:G:H2'	1.81	0.45
6:L5:2615:C:H4'	44:Ln:17:ARG:HH12	1.82	0.45
27:LW:18:PRO:HG2	27:LW:21:LYS:HB3	1.97	0.45
34:Ld:100:ILE:HG12	34:Ld:123:ILE:HD12	1.98	0.45
52:S2:220:U:H2'	52:S2:221:A:H8	1.82	0.45
52:S2:1201:A:O2'	52:S2:1358:A:N1	2.49	0.45
52:S2:1663:U:O4	52:S2:1664:A:N6	2.45	0.45
55:SD:129:GLY:HA3	72:SX:40:LYS:HG3	1.99	0.45
58:SG:68:ASP:OD2	58:SG:111:VAL:N	2.40	0.45
60:SL:59:LEU:O	60:SL:63:ARG:HG3	2.17	0.45
68:ST:61:ASP:N	68:ST:61:ASP:OD1	2.50	0.45
82:Sh:118:ARG:HD3	82:Sh:118:ARG:H	1.82	0.45
85:Sk:100:VAL:HB	85:Sk:108:ILE:HB	1.98	0.45
3:I:34:A:C5	3:I:35:U:H1'	2.52	0.45
3:I:66:G:O2'	3:I:67:G:OP1	2.27	0.45
6:L5:991:C:H2'	6:L5:992:C:C6	2.51	0.45
16:LK:103:VAL:HG11	16:LK:144:LEU:HD12	1.99	0.45
21:LQ:90:ASN:O	47:Lq:48:TYR:OH	2.32	0.45
30:LZ:97:LYS:HB2	30:LZ:100:VAL:HG23	1.98	0.45
43:Lm:39:TYR:CG	43:Lm:40:PRO:HA	2.52	0.45
52:S2:467:G:O2'	66:SR:72:ARG:NH2	2.32	0.45
52:S2:903:G:H2'	52:S2:904:A:H8	1.81	0.45
52:S2:1433:U:H5''	52:S2:1434:C:OP2	2.17	0.45
52:S2:1598:C:H4'	52:S2:1604:G:O6	2.17	0.45
52:S2:1743:C:H2'	52:S2:1744:G:O4'	2.17	0.45
58:SG:85:GLY:HA2	58:SG:108:VAL:HG23	1.98	0.45
61:SM:71:LEU:HD11	61:SM:189:ILE:HG23	1.98	0.45
62:SN:121:ARG:HH11	62:SN:145:LYS:NZ	2.15	0.45
65:SQ:14:THR:HB	65:SQ:15:PRO:HD3	1.99	0.45
68:ST:150:ASP:HA	68:ST:153:LYS:HZ3	1.82	0.45
77:Sc:28:PHE:HA	77:Sc:55:THR:HG21	1.99	0.45
1:E:163:MET:N	1:E:163:MET:SD	2.89	0.45
6:L5:2396:A:OP2	6:L5:2417:G:O2'	2.30	0.45
6:L5:3675:A:N6	6:L5:3797:U:O2	2.49	0.45
13:LH:43:LYS:H	13:LH:43:LYS:HD2	1.82	0.45
15:LJ:83:PHE:HA	15:LJ:183:ILE:HD13	1.99	0.45
19:LO:20:ARG:HG3	19:LO:21:ARG:HG3	1.98	0.45
20:LP:24:LEU:HD11	20:LP:86:TRP:CG	2.52	0.45
22:LR:74:ARG:NH1	22:LR:145:VAL:O	2.47	0.45
43:Lm:14:LYS:HE3	45:Lo:51:LEU:O	2.17	0.45
52:S2:98:C:OP2	52:S2:427:A:O2'	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:700:C:N4	52:S2:729:C:H2'	2.32	0.45
58:SG:80:SER:OG	58:SG:90:TRP:NE1	2.39	0.45
58:SG:112:ALA:HB3	58:SG:121:VAL:HG13	1.98	0.45
62:SN:146:GLU:HB3	62:SN:149:THR:HG22	1.98	0.45
73:SY:99:ARG:O	73:SY:103:GLU:HG2	2.16	0.45
75:Sa:96:VAL:HB	75:Sa:120:SER:HB3	1.99	0.45
79:Se:39:LEU:HD21	79:Se:52:TRP:CZ3	2.52	0.45
79:Se:134:ILE:O	79:Se:138:VAL:HG23	2.17	0.45
1:E:428:VAL:O	1:E:448:GLY:N	2.49	0.45
6:L5:693:C:H2'	6:L5:694:G:H8	1.82	0.45
6:L5:1138:G:N2	6:L5:1203:G:H2'	2.32	0.45
6:L5:2404:C:N4	6:L5:2405:G:O6	2.50	0.45
6:L5:2719:OMG:HM23	48:Lr:15:GLY:HA2	1.99	0.45
6:L5:4020:A:H2'	6:L5:4021:G:C8	2.52	0.45
10:LE:19:ARG:HB2	10:LE:234:ARG:NH2	2.32	0.45
14:LI:133:ARG:HA	14:LI:136:GLU:HG2	1.98	0.45
36:Lf:48:LEU:HD21	36:Lf:60:ILE:HG21	1.99	0.45
52:S2:377:A:H2'	52:S2:378:G:O4'	2.17	0.45
52:S2:789:G:H2'	52:S2:790:G:C8	2.52	0.45
52:S2:1524:C:H2'	52:S2:1525:G:H8	1.81	0.45
62:SN:253:PRO:HA	62:SN:256:TRP:CD2	2.52	0.45
1:E:379:TYR:O	1:E:410:GLN:NE2	2.43	0.45
3:I:50:A:H2'	3:I:51:A:H4'	1.98	0.45
5:B:675:LEU:HB3	5:B:747:VAL:HG13	1.99	0.45
5:B:687:ARG:HG2	5:B:721:GLN:CG	2.47	0.45
6:L5:260:C:H2'	6:L5:261:G:C8	2.51	0.45
6:L5:769:C:H2'	6:L5:770:G:H8	1.81	0.45
6:L5:800:U:H2'	6:L5:801:C:C6	2.52	0.45
6:L5:1568:A:H5'	9:LD:183:GLY:HA2	1.98	0.45
6:L5:1758:G:O2'	12:LG:115:MET:SD	2.67	0.45
6:L5:2719:OMG:C8	48:Lr:16:THR:HG22	2.52	0.45
6:L5:4278:PSU:OP2	6:L5:4300:G:N1	2.44	0.45
8:L8:90:C:H2'	8:L8:91:A:C8	2.52	0.45
52:S2:845:U:H2'	52:S2:846:G:H8	1.81	0.45
52:S2:1674:U:O2'	65:SQ:84:GLY:O	2.28	0.45
72:SX:77:ILE:HD11	72:SX:128:PHE:HZ	1.82	0.45
83:Si:52:LEU:HD11	83:Si:73:GLN:HB2	1.99	0.45
6:L5:1105:C:OP2	35:Le:91:ARG:NH1	2.49	0.44
6:L5:2322:G:H2'	6:L5:2323:G:H8	1.82	0.44
6:L5:4006:U:H2'	6:L5:4007:C:C6	2.51	0.44
28:LX:65:ARG:HG2	28:LX:66:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Le:49:HIS:HB3	35:Le:52:LYS:HE3	1.98	0.44
52:S2:5:U:OP2	62:SN:230:THR:OG1	2.24	0.44
52:S2:1590:A:O3'	79:Se:82:ARG:HD2	2.17	0.44
52:S2:1788:G:H2'	52:S2:1789:A:C8	2.50	0.44
60:SL:102:ARG:HA	60:SL:102:ARG:HD2	1.74	0.44
70:SV:63:ALA:HB3	70:SV:68:TYR:HE2	1.82	0.44
77:Sc:81:ARG:HA	77:Sc:81:ARG:HD2	1.64	0.44
78:Sd:36:VAL:HG23	78:Sd:99:LEU:HD22	1.98	0.44
1:E:272:MET:SD	1:E:273:PHE:N	2.90	0.44
4:S:1124:U:O2	4:S:1144:G:O2'	2.36	0.44
6:L5:1651:C:H2'	6:L5:1652:G:O4'	2.16	0.44
6:L5:4005:C:OP2	18:LM:54:ARG:NH2	2.50	0.44
10:LE:92:TYR:HB2	10:LE:159:VAL:HB	1.97	0.44
11:LF:302:LEU:HD21	24:LT:34:PHE:CE2	2.53	0.44
17:LL:30:LYS:HG2	17:LL:63:GLU:HA	1.99	0.44
19:LO:50:PRO:HG3	41:Lk:121:VAL:HG22	1.99	0.44
22:LR:130:LYS:HB2	22:LR:133:ARG:HG2	1.99	0.44
52:S2:17:C:H2'	52:S2:18:C:C6	2.52	0.44
52:S2:913:C:H3'	52:S2:914:A:H5''	1.98	0.44
60:SL:58:LEU:HD21	60:SL:177:MET:HB3	1.99	0.44
62:SN:173:LYS:O	81:Sg:4:ASP:N	2.42	0.44
67:SS:135:PHE:CG	67:SS:136:PRO:HA	2.52	0.44
69:SU:53:ILE:HD13	69:SU:81:LEU:HD21	1.99	0.44
71:SW:104:LYS:HE2	83:Si:8:ARG:NH2	2.27	0.44
73:SY:130:LYS:NZ	73:SY:139:TRP:O	2.42	0.44
78:Sd:48:ALA:HB2	78:Sd:70:ILE:HD12	1.98	0.44
79:Se:82:ARG:HH12	79:Se:84:ARG:HD3	1.82	0.44
1:E:20:LYS:HE3	1:E:95:GLY:HA3	1.99	0.44
6:L5:1353:G:H2'	6:L5:1354:G:C8	2.52	0.44
6:L5:1926:C:H2'	6:L5:1927:G:C8	2.52	0.44
6:L5:4135:C:H2'	6:L5:4136:A:C8	2.52	0.44
8:L8:141:C:H5''	21:LQ:60:VAL:HG11	1.99	0.44
10:LE:78:ILE:HD13	10:LE:332:MET:HG3	1.99	0.44
13:LH:173:SER:OG	13:LH:217:ASP:OD2	2.18	0.44
16:LK:15:ASN:OD1	16:LK:15:ASN:N	2.49	0.44
17:LL:63:GLU:H	17:LL:63:GLU:HG3	1.59	0.44
29:LY:87:SER:HA	29:LY:97:TYR:HB3	1.98	0.44
52:S2:21:U:O2'	69:SU:17:ARG:O	2.29	0.44
52:S2:456:A:O2'	52:S2:1736:A:N3	2.45	0.44
52:S2:1286:G:N1	72:SX:57:ASP:OD1	2.47	0.44
52:S2:1352:G:O2'	52:S2:1379:A:N1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SP:36:HIS:CG	64:SP:85:GLY:HA3	2.51	0.44
6:L5:280:G:OP2	21:LQ:44:ARG:NH2	2.40	0.44
6:L5:811:U:H5	6:L5:814:A:N7	2.14	0.44
6:L5:1347:G:C2	6:L5:1370:G:C2	3.05	0.44
6:L5:2318:G:C2	31:La:50:LYS:HG3	2.52	0.44
10:LE:181:MET:HE3	10:LE:183:ILE:HG13	1.99	0.44
21:LQ:3:ALA:O	21:LQ:7:ILE:HG12	2.18	0.44
22:LR:43:ILE:HD11	22:LR:138:LEU:HD13	1.98	0.44
26:LV:74:ARG:O	26:LV:76:LYS:NZ	2.50	0.44
38:Lh:108:ARG:NH2	38:Lh:127:ALA:HB3	2.32	0.44
52:S2:291:U:O2'	52:S2:293:A:N7	2.43	0.44
52:S2:1374:C:OP1	77:Sc:7:LYS:NZ	2.35	0.44
52:S2:1737:G:H2'	52:S2:1738:G:C8	2.52	0.44
58:SG:55:PRO:HB2	76:Sb:102:GLU:OE2	2.18	0.44
67:SS:130:LEU:HD21	67:SS:156:VAL:HG21	1.98	0.44
77:Sc:90:ALA:O	77:Sc:93:GLN:NE2	2.42	0.44
6:L5:639:G:H2'	6:L5:640:G:H8	1.83	0.44
6:L5:693:C:H2'	6:L5:694:G:C8	2.53	0.44
6:L5:2405:G:N2	6:L5:2407:G:H3'	2.32	0.44
19:LO:104:ASN:O	42:Ll:20:ASN:ND2	2.51	0.44
21:LQ:143:ARG:NH1	41:Lk:95:LEU:HD23	2.32	0.44
24:LT:99:LYS:HE3	24:LT:99:LYS:HB2	1.77	0.44
52:S2:899:U:H2'	52:S2:900:U:C6	2.53	0.44
60:SL:35:GLU:O	60:SL:38:ILE:HG12	2.18	0.44
67:SS:19:PHE:O	67:SS:23:ILE:HG12	2.18	0.44
67:SS:79:LEU:HD22	67:SS:94:PHE:HZ	1.82	0.44
72:SX:63:LYS:HE3	72:SX:63:LYS:HB3	1.84	0.44
78:Sd:104:ASP:OD1	78:Sd:104:ASP:N	2.50	0.44
5:B:438:LYS:C	5:B:440:ASN:H	2.26	0.44
6:L5:1245:C:H2'	6:L5:1246:U:C4	2.53	0.44
6:L5:1776:A:OP1	27:LW:108:ARG:NH2	2.51	0.44
10:LE:231:VAL:HG21	10:LE:251:VAL:HG23	1.99	0.44
16:LK:41:ILE:HG22	16:LK:43:VAL:HG13	2.00	0.44
39:Li:41:PHE:HE1	39:Li:110:ILE:HD13	1.83	0.44
52:S2:698:G:H1'	52:S2:731:C:N3	2.32	0.44
52:S2:1047:PSU:H2'	52:S2:1048:C:O4'	2.17	0.44
57:SF:87:ARG:HB3	57:SF:91:ALA:HB3	1.99	0.44
61:SM:83:LYS:NZ	61:SM:106:THR:HG22	2.32	0.44
62:SN:84:PHE:HA	81:Sg:15:ARG:HH12	1.83	0.44
64:SP:192:ILE:HB	64:SP:243:GLY:HA3	2.00	0.44
65:SQ:42:LYS:HG3	65:SQ:43:GLU:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:ST:110:ARG:NH2	68:ST:123:ARG:HE	2.13	0.44
69:SU:114:VAL:HG21	69:SU:129:LEU:HD11	2.00	0.44
77:Sc:61:ILE:HD13	77:Sc:66:VAL:HG22	1.99	0.44
6:L5:440:U:O2'	39:Li:91:ASN:O	2.32	0.44
6:L5:637:C:H2'	6:L5:638:G:C8	2.53	0.44
6:L5:1284:OMC:HM21	11:LF:106:LYS:HB2	2.00	0.44
6:L5:1342:A:H61	6:L5:1374:G:H2'	1.82	0.44
6:L5:3339:U:H2'	6:L5:3340:A:C8	2.52	0.44
6:L5:4419:PSU:OP2	29:LY:15:ARG:NH2	2.51	0.44
6:L5:4646:G:N2	6:L5:4652:G:H2'	2.33	0.44
10:LE:86:VAL:HG12	10:LE:201:LEU:HD23	1.99	0.44
10:LE:218:ASP:OD2	10:LE:348:ARG:NH2	2.32	0.44
33:Lc:54:THR:HB	33:Lc:57:MET:HE3	2.00	0.44
52:S2:85:A:H2'	52:S2:86:C:C6	2.53	0.44
52:S2:236:A:C6	52:S2:895:G:C6	3.06	0.44
52:S2:1622:U:O2'	52:S2:1623:U:H2'	2.18	0.44
58:SG:150:TRP:HB2	58:SG:170:TRP:CD1	2.53	0.44
61:SM:28:LYS:NZ	74:SZ:51:GLU:OE2	2.37	0.44
61:SM:34:LYS:NZ	61:SM:43:ASN:OD1	2.43	0.44
62:SN:253:PRO:HA	62:SN:256:TRP:CE2	2.53	0.44
65:SQ:127:ARG:HH22	65:SQ:131:ALA:N	2.16	0.44
73:SY:83:ASP:OD1	73:SY:83:ASP:N	2.49	0.44
79:Se:110:LEU:HD22	79:Se:112:MET:HE3	1.99	0.44
82:Sh:30:CYS:SG	82:Sh:31:SER:N	2.89	0.44
2:F:1:G:N2	2:F:87:G:H1'	2.33	0.44
5:B:649:LEU:HD21	5:B:738:LEU:HD23	2.00	0.44
6:L5:1128:C:H2'	6:L5:1129:G:O4'	2.17	0.44
6:L5:4101:G:O6	93:L5:5101:HOH:O	2.20	0.44
9:LD:147:ARG:HH12	9:LD:155:LYS:HD3	1.81	0.44
30:LZ:2:LYS:HE3	30:LZ:2:LYS:HB3	1.84	0.44
52:S2:562:A:O2'	69:SU:132:GLN:OE1	2.33	0.44
52:S2:1356:C:O3'	62:SN:238:LYS:NZ	2.51	0.44
65:SQ:175:ASP:OD1	65:SQ:176:GLU:N	2.51	0.44
78:Sd:84:LEU:HD12	78:Sd:95:TYR:HB3	2.00	0.44
6:L5:1131:G:H1'	6:L5:1209:G:H22	1.83	0.44
6:L5:1248:C:H1'	6:L5:2156:A:H1'	2.00	0.44
28:LX:43:LEU:HD12	28:LX:47:ILE:HD11	2.00	0.44
36:Lf:23:LYS:HE3	36:Lf:23:LYS:HB2	1.84	0.44
52:S2:84:A:H5''	84:Sj:122:LYS:HE3	1.99	0.44
52:S2:449:A:H5''	68:ST:25:ARG:HA	1.99	0.44
64:SP:124:CYS:HB3	64:SP:141:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SQ:40:ALA:HB1	65:SQ:45:TYR:CG	2.53	0.44
68:ST:90:LEU:O	68:ST:95:THR:OG1	2.36	0.44
68:ST:130:THR:OG1	68:ST:132:GLU:OE1	2.32	0.44
68:ST:144:LYS:HA	68:ST:147:LYS:HE2	2.00	0.44
77:Sc:44:LYS:O	77:Sc:48:ASN:ND2	2.51	0.44
79:Se:113:VAL:HG12	79:Se:123:LEU:HD23	2.00	0.44
82:Sh:30:CYS:HB2	82:Sh:61:ILE:HG13	1.99	0.44
3:I:130:G:H2'	3:I:130:G:N3	2.33	0.43
3:I:138:G:H2'	3:I:151:A:N6	2.33	0.43
6:L5:625:G:H2'	6:L5:626:G:C8	2.53	0.43
6:L5:1908:G:H4'	50:Lt:36:GLY:HA2	1.99	0.43
6:L5:2165:G:OP2	38:Lh:34:ASN:ND2	2.50	0.43
6:L5:4780:G:OP2	30:LZ:61:LYS:HD3	2.18	0.43
10:LE:108:GLU:OE2	10:LE:138:GLN:NE2	2.51	0.43
28:LX:28:PRO:HB2	28:LX:34:MET:HG2	2.00	0.43
32:Lb:69:LYS:H	32:Lb:83:GLU:HG2	1.82	0.43
33:Lc:95:VAL:HG13	33:Lc:96:VAL:HG23	2.00	0.43
36:Lf:78:ASN:N	36:Lf:78:ASN:OD1	2.49	0.43
52:S2:1284:C:O2'	52:S2:1314:A:N1	2.48	0.43
58:SG:133:ASN:HB3	58:SG:139:LYS:HE2	1.99	0.43
60:SL:130:ASP:O	60:SL:134:LEU:HG	2.18	0.43
67:SS:21:SER:O	67:SS:25:GLN:HG2	2.18	0.43
72:SX:23:LYS:O	72:SX:27:ILE:HG12	2.18	0.43
84:Sj:56:PHE:HB2	84:Sj:74:MET:HB2	1.99	0.43
6:L5:522:U:O2	6:L5:636:G:N1	2.51	0.43
6:L5:1624:A:P	35:Le:18:ARG:HH12	2.41	0.43
6:L5:2101:C:O2	13:LH:94:THR:OG1	2.30	0.43
6:L5:2346:G:O4'	6:L5:3812:G:N2	2.51	0.43
6:L5:3773:G:N2	6:L5:3775:A:H3'	2.33	0.43
6:L5:4186:G:O3'	17:LL:112:GLN:NE2	2.50	0.43
8:L8:155:C:OP2	15:LJ:89:ARG:NH1	2.51	0.43
18:LM:20:LEU:HD12	18:LM:132:VAL:HB	1.99	0.43
18:LM:118:LYS:HE3	18:LM:118:LYS:HB3	1.79	0.43
22:LR:10:ASP:OD2	22:LR:37:ARG:NH2	2.48	0.43
43:Lm:39:TYR:CD1	43:Lm:40:PRO:HA	2.53	0.43
52:S2:57:U:H5''	52:S2:505:G:H1'	2.00	0.43
52:S2:561:A:H5'	69:SU:174:LYS:HD3	2.00	0.43
52:S2:824:U:H4'	69:SU:140:GLN:OE1	2.17	0.43
55:SD:111:ASN:HD21	55:SD:113:LYS:HG2	1.83	0.43
63:SO:10:LYS:NZ	80:Sf:111:GLU:OE1	2.50	0.43
68:ST:191:GLU:O	71:SW:19:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Sc:10:LYS:O	77:Sc:14:ARG:HD3	2.18	0.43
78:Sd:97:GLN:HG3	78:Sd:99:LEU:HD21	1.99	0.43
6:L5:173:C:P	19:LO:129:ARG:HH12	2.41	0.43
6:L5:681:U:OP1	13:LH:100:GLY:N	2.52	0.43
6:L5:785:G:H2'	6:L5:786:G:H8	1.84	0.43
6:L5:841:C:P	14:LI:241:ARG:HH21	2.41	0.43
6:L5:1068:U:H2'	6:L5:1069:G:C8	2.53	0.43
6:L5:1489:A2M:N3	43:Lm:11:ARG:HB2	2.33	0.43
6:L5:1909:A:H2'	6:L5:1955:C:N4	2.33	0.43
6:L5:3765:C:N4	6:L5:3766:C:O2	2.52	0.43
6:L5:4520:C:H2'	6:L5:4521:C:C6	2.54	0.43
16:LK:16:VAL:HG21	16:LK:81:ILE:HG23	1.99	0.43
25:LU:97:ARG:O	25:LU:101:ILE:HG12	2.19	0.43
28:LX:66:SER:HB3	28:LX:69:LYS:HB2	1.99	0.43
52:S2:78:C:OP1	66:SR:159:ARG:NH1	2.29	0.43
52:S2:794:G:H2'	52:S2:795:A:C8	2.54	0.43
52:S2:907:U:H2'	52:S2:908:G:H8	1.82	0.43
52:S2:1286:G:N2	72:SX:57:ASP:OD1	2.46	0.43
52:S2:1522:C:N4	78:Sd:137:LYS:HD3	2.33	0.43
52:S2:1590:A:H4'	79:Se:82:ARG:HB3	1.99	0.43
55:SD:121:CYS:HB3	55:SD:126:CYS:O	2.19	0.43
60:SL:34:MET:HG2	60:SL:154:LEU:HD11	2.00	0.43
68:ST:92:ARG:HA	68:ST:92:ARG:CZ	2.49	0.43
77:Sc:34:VAL:HG12	77:Sc:38:ILE:HD13	1.99	0.43
77:Sc:51:ALA:O	77:Sc:55:THR:HG23	2.17	0.43
5:B:466:GLN:HB2	5:B:701:ILE:HG13	2.01	0.43
6:L5:3515:A:OP2	6:L5:3540:OMC:N4	2.50	0.43
6:L5:3642:C:H2'	6:L5:3643:C:C6	2.54	0.43
9:LD:247:ARG:HB3	52:S2:1070:U:H4'	2.00	0.43
45:Lo:9:ILE:HD12	45:Lo:51:LEU:HD21	1.99	0.43
52:S2:63:U:H2'	52:S2:64:A:H5''	2.00	0.43
60:SL:210:ILE:HG23	77:Sc:81:ARG:CZ	2.48	0.43
62:SN:254:ASP:OD1	62:SN:254:ASP:N	2.51	0.43
63:SO:133:GLY:HA3	63:SO:156:LEU:O	2.18	0.43
64:SP:79:ASP:OD1	64:SP:79:ASP:N	2.46	0.43
68:ST:124:LYS:HB2	68:ST:124:LYS:HE2	1.72	0.43
73:SY:142:GLU:HB2	73:SY:145:THR:HG22	2.01	0.43
75:Sa:30:TYR:HA	75:Sa:33:LEU:HB2	1.99	0.43
83:Si:40:PRO:HA	83:Si:79:LYS:HD2	2.00	0.43
3:I:115:A:H2'	3:I:116:G:C8	2.53	0.43
4:S:1111:A:H4'	4:S:1112:U:O5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:262:G:H2'	6:L5:263:G:C8	2.52	0.43
6:L5:278:G:O4'	21:LQ:50:ARG:HD2	2.18	0.43
6:L5:2107:C:P	49:Ls:108:MET:HG2	2.58	0.43
6:L5:2118:G:H2'	6:L5:2119:A:C8	2.54	0.43
9:LD:40:TYR:HA	9:LD:91:GLY:HA3	2.00	0.43
32:Lb:31:SER:HA	32:Lb:48:PRO:HA	2.01	0.43
52:S2:192:C:H2'	52:S2:193:C:O4'	2.18	0.43
52:S2:545:G:H2'	52:S2:546:A:C8	2.53	0.43
52:S2:1695:U:HO2'	52:S2:1834:C:HO2'	1.57	0.43
54:SC:37:ASP:N	54:SC:37:ASP:OD1	2.51	0.43
71:SW:13:GLN:HE22	71:SW:35:ARG:HD2	1.82	0.43
3:I:123:G:H1	3:I:163:G:H21	1.66	0.43
6:L5:1350:G:N2	6:L5:1367:G:H1	2.16	0.43
7:L7:120:U:OP2	12:LG:259:ARG:NH2	2.32	0.43
13:LH:177:LEU:HD11	13:LH:189:LEU:HD12	1.99	0.43
32:Lb:2:LYS:HE3	32:Lb:2:LYS:HB3	1.85	0.43
36:Lf:45:LEU:HD21	36:Lf:108:MET:HE3	1.99	0.43
52:S2:1338:4AC:O2'	80:Sf:68:THR:HG22	2.17	0.43
54:SC:13:ARG:HH21	54:SC:53:GLY:HA2	1.83	0.43
55:SD:118:ARG:NE	55:SD:134:SER:OG	2.51	0.43
57:SF:94:ASP:OD1	57:SF:96:THR:HG22	2.18	0.43
58:SG:30:MET:HA	58:SG:43:TRP:O	2.18	0.43
65:SQ:67:PRO:HB2	65:SQ:70:GLU:HG3	2.01	0.43
83:Si:46:HIS:CD2	83:Si:103:ALA:HB2	2.54	0.43
1:E:5:ARG:HD3	1:E:85:LEU:HB2	2.01	0.43
6:L5:367:C:O2'	11:LF:83:GLY:O	2.27	0.43
6:L5:629:G:H2'	6:L5:630:G:H8	1.83	0.43
6:L5:2043:A:N6	6:L5:2044:A:N1	2.66	0.43
6:L5:3689:U:O2'	6:L5:3690:G:H5''	2.18	0.43
6:L5:4203:PSU:H1'	10:LE:252:ALA:HB3	2.00	0.43
6:L5:4364:OMG:H5''	29:LY:15:ARG:HB2	2.00	0.43
6:L5:4371:C:OP1	10:LE:224:LYS:HG3	2.19	0.43
12:LG:60:ILE:HB	12:LG:80:ALA:HB2	1.99	0.43
12:LG:205:ALA:HB2	12:LG:236:MET:HE2	2.01	0.43
13:LH:261:LEU:O	13:LH:265:LYS:HG2	2.18	0.43
52:S2:1:U:O2	52:S2:1:U:H2'	2.18	0.43
52:S2:422:G:OP1	71:SW:98:LYS:HA	2.19	0.43
52:S2:526:A:H2'	52:S2:527:A:C8	2.52	0.43
64:SP:234:PRO:HG2	64:SP:238:LEU:HD21	1.99	0.43
68:ST:81:VAL:HG12	68:ST:91:VAL:HG23	1.99	0.43
69:SU:24:ARG:O	69:SU:28:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SY:70:LYS:O	73:SY:74:ILE:HG12	2.18	0.43
79:Se:96:SER:HB3	79:Se:99:VAL:HG22	1.99	0.43
80:Sf:48:LEU:HD11	80:Sf:93:SER:HB3	2.00	0.43
84:Sj:25:ILE:O	84:Sj:71:GLY:N	2.47	0.43
6:L5:2408:A:C5	6:L5:2409:G:H1'	2.54	0.43
6:L5:3632:G:OP1	6:L5:3633:A:O2'	2.26	0.43
6:L5:3688:G:N2	6:L5:3785:C:O2	2.52	0.43
11:LF:259:LYS:HE2	11:LF:259:LYS:HB3	1.91	0.43
17:LL:70:ILE:HG22	17:LL:74:LYS:HE2	2.01	0.43
17:LL:183:ASP:O	17:LL:187:GLU:HG2	2.19	0.43
52:S2:421:G:O2'	52:S2:661:C:N3	2.49	0.43
58:SG:57:ARG:NH2	58:SG:94:THR:O	2.52	0.43
66:SR:162:LEU:HB3	66:SR:170:ARG:O	2.18	0.43
66:SR:221:LYS:HB3	66:SR:221:LYS:HE3	1.76	0.43
68:ST:107:THR:OG1	68:ST:108:PRO:HD3	2.19	0.43
69:SU:100:LEU:HD13	69:SU:100:LEU:HA	1.86	0.43
69:SU:122:SER:HB3	69:SU:125:HIS:HB3	2.01	0.43
75:Sa:32:GLN:H	75:Sa:32:GLN:HG2	1.67	0.43
75:Sa:41:GLN:OE1	75:Sa:41:GLN:N	2.45	0.43
76:Sb:14:GLY:HA3	76:Sb:86:GLN:HB2	2.01	0.43
76:Sb:32:ILE:HG22	76:Sb:68:ILE:HB	2.00	0.43
1:E:130:CYS:O	1:E:134:GLY:N	2.45	0.43
4:S:1121:G:H1	4:S:1148:A:H2	1.66	0.43
5:B:687:ARG:HG2	5:B:721:GLN:HG3	2.01	0.43
6:L5:1678:G:N3	6:L5:1681:A:N6	2.66	0.43
6:L5:2252:U:H4'	6:L5:2271:A:H4'	2.01	0.43
6:L5:3599:A2M:HM'3	6:L5:3612:G:N2	2.34	0.43
18:LM:136:ARG:HH22	18:LM:161:GLU:CD	2.26	0.43
25:LU:99:MET:HE1	25:LU:127:VAL:HG12	2.00	0.43
49:Ls:94:ARG:HB2	49:Ls:111:ILE:HD11	2.00	0.43
52:S2:229:A:N6	52:S2:888:U:O4	2.50	0.43
52:S2:239:C:H2'	52:S2:240:G:C8	2.54	0.43
52:S2:1124:C:HO2'	61:SM:146:ARG:HH22	1.63	0.43
52:S2:1580:A:O2'	52:S2:1582:C:OP2	2.24	0.43
69:SU:137:VAL:HG22	69:SU:157:ILE:HG12	2.00	0.43
71:SW:22:ARG:HG2	71:SW:26:GLY:HA2	2.00	0.43
75:Sa:34:MET:HB3	75:Sa:42:ARG:HG3	2.00	0.43
78:Sd:120:HIS:CE1	78:Sd:124:ARG:HD2	2.54	0.43
3:I:218:G:O2'	83:Si:61:GLN:NE2	2.49	0.43
6:L5:1922:A:H4'	6:L5:1923:A:N7	2.34	0.43
6:L5:4202:OMC:H1'	6:L5:4202:OMC:HM23	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4516:G:H5''	22:LR:176:ARG:HD3	2.01	0.43
13:LH:164:ARG:O	13:LH:185:ASN:ND2	2.52	0.43
16:LK:95:VAL:HG22	46:Lp:82:LEU:HB3	2.01	0.43
29:LY:21:PRO:HA	29:LY:54:ALA:HA	2.00	0.43
47:Lq:26:TYR:HB3	47:Lq:67:VAL:HG13	2.00	0.43
52:S2:39:A:P	69:SU:7:TRP:HE1	2.41	0.43
52:S2:126:G:OP2	66:SR:198:ARG:NH2	2.38	0.43
52:S2:660:G:H21	83:Si:17:ARG:NH2	2.17	0.43
52:S2:798:C:H2'	52:S2:799:G:C5	2.53	0.43
52:S2:1309:U:O2'	52:S2:1310:C:O5'	2.36	0.43
52:S2:1678:U:H2'	52:S2:1679:A2M:H8	2.01	0.43
55:SD:101:ALA:HB3	72:SX:36:ARG:NH1	2.34	0.43
55:SD:141:CYS:HB3	55:SD:146:LEU:H	1.84	0.43
58:SG:227:LEU:HB3	58:SG:228:TYR:CD2	2.54	0.43
62:SN:254:ASP:HB2	81:Sg:1:AME:HT22	2.01	0.43
67:SS:60:ILE:HB	67:SS:92:VAL:HG22	2.00	0.43
72:SX:132:LYS:HE3	72:SX:132:LYS:HB2	1.89	0.43
73:SY:128:TYR:O	73:SY:131:THR:OG1	2.34	0.43
78:Sd:105:ASN:O	78:Sd:108:ARG:HG2	2.18	0.43
1:E:258:ILE:HG21	1:E:298:LEU:HD11	2.01	0.42
5:B:432:GLN:HG2	52:S2:1291:G:C1'	2.49	0.42
5:B:683:HIS:CD2	5:B:688:LYS:HZ1	2.37	0.42
6:L5:1532:G:O2'	6:L5:1567:G:H4'	2.19	0.42
6:L5:1601:A:O2'	43:Lm:49:TRP:O	2.33	0.42
6:L5:2168:C:OP1	38:Lh:101:HIS:N	2.44	0.42
6:L5:2431:C:OP1	6:L5:2611:C:O2'	2.30	0.42
6:L5:4662:U:H2'	6:L5:4663:C:H6	1.84	0.42
17:LL:193:ASP:OD2	17:LL:198:LYS:HE3	2.19	0.42
25:LU:172:ARG:HH12	52:S2:910:G:P	2.41	0.42
46:Lp:99:CYS:HB2	46:Lp:114:LYS:HD2	2.00	0.42
52:S2:790:G:H2'	52:S2:791:C:O4'	2.19	0.42
52:S2:1381:C:O2'	60:SL:113:GLN:OE1	2.18	0.42
62:SN:75:ILE:HG21	62:SN:81:ILE:HD11	2.01	0.42
62:SN:146:GLU:HG2	63:SO:120:TYR:OH	2.19	0.42
77:Sc:99:ASP:OD1	77:Sc:99:ASP:N	2.44	0.42
3:I:52:A:H3'	3:I:53:U:H5''	2.01	0.42
6:L5:75:G:N7	19:LO:102:ARG:HG3	2.33	0.42
6:L5:92:C:OP2	6:L5:4087:C:O2'	2.30	0.42
6:L5:424:U:OP1	23:LS:34:GLN:NE2	2.53	0.42
6:L5:1352:C:H2'	6:L5:1353:G:C8	2.53	0.42
6:L5:2509:U:OP2	25:LU:124:TYR:OH	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:3359:OMG:HM23	6:L5:3359:OMG:H1'	1.86	0.42
6:L5:3599:A2M:HM'3	6:L5:3612:G:H21	1.84	0.42
6:L5:4261:G:H5''	10:LE:3:HIS:CE1	2.55	0.42
6:L5:4314:A:O2'	6:L5:4720:G:N7	2.52	0.42
6:L5:4792:U:H3'	6:L5:4793:C:C6	2.53	0.42
12:LG:156:GLY:HA2	12:LG:181:PRO:HD3	2.00	0.42
23:LS:111:SER:OG	23:LS:152:GLU:OE1	2.31	0.42
31:La:116:LEU:HD23	31:La:116:LEU:HA	1.91	0.42
32:Lb:47:MET:HE1	32:Lb:118:ILE:HB	2.01	0.42
52:S2:81:U:H2'	52:S2:82:G:O4'	2.19	0.42
52:S2:417:U:H2'	52:S2:418:C:O4'	2.19	0.42
52:S2:982:A:H2'	52:S2:983:G:C8	2.55	0.42
52:S2:1017:U:H5'	73:SY:15:ALA:O	2.18	0.42
60:SL:5:LEU:HD12	60:SL:8:LEU:HD12	2.00	0.42
60:SL:66:VAL:HG21	60:SL:185:MET:HE2	2.01	0.42
70:SV:85:LEU:HD13	70:SV:86:PRO:HD2	2.00	0.42
71:SW:35:ARG:NH1	71:SW:55:TYR:O	2.46	0.42
79:Se:104:LEU:HD13	79:Se:121:ARG:HD2	2.02	0.42
1:E:314:ALA:O	1:E:454:LEU:N	2.47	0.42
2:F:57:G:H2'	2:F:58:A:C8	2.54	0.42
3:I:52:A:H1'	3:I:78:A:C2	2.54	0.42
6:L5:61:A:H5''	21:LQ:164:LEU:HD21	2.02	0.42
6:L5:114:G:N2	6:L5:158:A:H61	2.17	0.42
6:L5:308:G:O6	21:LQ:12:ARG:NH1	2.53	0.42
6:L5:368:C:O4'	11:LF:83:GLY:HA3	2.19	0.42
6:L5:628:U:H2'	6:L5:629:G:C8	2.54	0.42
6:L5:1672:G:N3	6:L5:3960:A:H2'	2.34	0.42
6:L5:1751:C:H5'	35:Le:56:LYS:HD2	2.00	0.42
6:L5:1929:A:H2'	6:L5:1930:A:O4'	2.19	0.42
6:L5:2423:U:H4'	33:Lc:74:VAL:O	2.19	0.42
6:L5:3690:G:H8	6:L5:3774:A:H62	1.68	0.42
29:LY:43:LYS:HG3	29:LY:60:MET:HE3	2.02	0.42
32:Lb:56:GLN:HB3	32:Lb:67:ILE:HD13	2.00	0.42
52:S2:572:U:O3'	84:Sj:60:PHE:HB2	2.19	0.42
52:S2:992:G:C6	52:S2:1135:G:H4'	2.55	0.42
52:S2:1125:C:O2'	77:Sc:126:MET:O	2.37	0.42
52:S2:1602:A:O2'	52:S2:1605:G:O6	2.36	0.42
53:SB:23:ARG:O	82:Sh:60:LYS:NZ	2.52	0.42
62:SN:78:LEU:HA	62:SN:81:ILE:HD13	2.00	0.42
68:ST:98:LYS:HB2	68:ST:178:ARG:HD2	2.00	0.42
78:Sd:86:ARG:HG2	78:Sd:106:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:Se:129:ARG:HB3	79:Se:133:ARG:NH1	2.35	0.42
1:E:351:PHE:CZ	1:E:411:TRP:HB2	2.54	0.42
3:I:77:U:C6	3:I:156:C:HI'	2.54	0.42
6:L5:74:G:H5''	19:LO:59:VAL:HB	2.01	0.42
6:L5:1860:C:C4	20:LP:17:PHE:HB3	2.54	0.42
6:L5:2029:U:OP2	11:LF:307:LYS:NZ	2.49	0.42
23:LS:50:ASP:OD2	23:LS:56:GLN:NE2	2.52	0.42
52:S2:160:U:O2'	52:S2:161:U:H3'	2.20	0.42
52:S2:1321:G:H2'	52:S2:1322:G:O4'	2.19	0.42
52:S2:1411:C:H2'	52:S2:1412:G:C8	2.53	0.42
52:S2:1411:C:H2'	52:S2:1412:G:H8	1.84	0.42
60:SL:149:ASN:OD1	60:SL:150:THR:N	2.46	0.42
66:SR:20:ASP:HB3	66:SR:23:LYS:HD3	2.02	0.42
66:SR:136:LYS:HG3	66:SR:175:LYS:O	2.19	0.42
2:F:59:C:H2'	2:F:60:A:H8	1.85	0.42
6:L5:987:C:H2'	6:L5:988:G:O4'	2.19	0.42
6:L5:1303:G:H4'	21:LQ:203:TYR:HB2	2.02	0.42
6:L5:1458:A:N6	24:LT:87:THR:HG21	2.33	0.42
6:L5:1702:C:H2'	6:L5:1703:G:O4'	2.20	0.42
6:L5:2169:G:H5''	38:Lh:127:ALA:HB2	2.02	0.42
6:L5:2282:G:H5'	6:L5:2621:G:OP2	2.20	0.42
6:L5:3476:OMG:HM23	6:L5:3476:OMG:HI'	1.78	0.42
6:L5:4369:OMG:HM23	6:L5:4369:OMG:HI'	1.81	0.42
87:L7:203:GTP:H5''	12:LG:265:ARG:HH11	1.85	0.42
26:LV:94:TYR:OH	26:LV:132:MET:SD	2.77	0.42
28:LX:24:ASP:HB3	28:LX:111:GLU:HB2	2.02	0.42
33:Lc:28:ASN:HB2	33:Lc:77:TYR:OH	2.20	0.42
52:S2:191:A:C5	52:S2:192:C:HI'	2.54	0.42
55:SD:144:CYS:SG	55:SD:146:LEU:HD13	2.59	0.42
58:SG:114:SER:HB3	58:SG:119:GLN:HB2	2.00	0.42
63:SO:163:PRO:O	63:SO:167:TYR:HB2	2.18	0.42
69:SU:158:ASP:OD1	69:SU:158:ASP:N	2.53	0.42
72:SX:58:GLU:OE1	72:SX:61:TYR:N	2.34	0.42
76:Sb:105:LYS:O	76:Sb:109:LYS:N	2.51	0.42
78:Sd:84:LEU:O	78:Sd:87:GLN:NE2	2.53	0.42
80:Sf:40:ILE:O	80:Sf:44:LYS:HG2	2.20	0.42
1:E:148:ILE:O	1:E:152:PRO:HB3	2.20	0.42
6:L5:398:A2M:HI'	6:L5:398:A2M:HM'3	1.81	0.42
6:L5:3335:G:H2'	6:L5:3336:A:C8	2.54	0.42
6:L5:3834:G:HI'	6:L5:3835:G:H8	1.84	0.42
6:L5:3990:A:H2'	6:L5:3991:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:4282:OMC:HM22	6:L5:4283:C:O4'	2.20	0.42
12:LG:152:ARG:O	12:LG:157:ASN:ND2	2.47	0.42
14:LI:91:VAL:O	14:LI:119:GLY:HA2	2.19	0.42
17:LL:36:LEU:HD12	17:LL:87:ILE:HB	2.01	0.42
17:LL:68:ALA:HB2	17:LL:158:LYS:HB2	2.02	0.42
24:LT:167:VAL:HG12	24:LT:175:GLU:HG3	2.00	0.42
25:LU:157:ASP:OD1	25:LU:158:GLN:N	2.52	0.42
27:LW:120:LYS:HB3	27:LW:120:LYS:HE3	1.74	0.42
32:Lb:67:ILE:O	32:Lb:84:ARG:NH2	2.51	0.42
34:Ld:75:LEU:HD12	34:Ld:75:LEU:HA	1.81	0.42
37:Lg:36:VAL:HG21	37:Lg:44:ARG:HG2	2.02	0.42
52:S2:230:A:H2	52:S2:900:U:H3	1.65	0.42
52:S2:564:G:O2'	52:S2:565:A:H8	2.03	0.42
52:S2:903:G:H2'	52:S2:904:A:C8	2.55	0.42
62:SN:263:LYS:HB3	62:SN:268:GLU:HB3	2.01	0.42
63:SO:69:LEU:O	63:SO:72:VAL:HG12	2.20	0.42
63:SO:74:GLN:OE1	63:SO:81:GLU:HA	2.19	0.42
66:SR:131:ARG:NE	66:SR:132:ARG:H	2.17	0.42
67:SS:36:LEU:HD21	67:SS:78:ARG:HD2	2.02	0.42
68:ST:143:LYS:HG2	68:ST:147:LYS:NZ	2.35	0.42
82:Sh:55:ASP:N	82:Sh:55:ASP:OD1	2.53	0.42
6:L5:519:C:H2'	6:L5:520:G:H8	1.85	0.42
6:L5:2706:G:O2'	25:LU:82:LYS:O	2.33	0.42
6:L5:3625:C:O2'	6:L5:4718:A:N1	2.46	0.42
6:L5:3899:C:H2'	6:L5:3900:G:H8	1.85	0.42
37:Lg:22:THR:OG1	37:Lg:122:VAL:O	2.38	0.42
52:S2:109:PSU:O4	71:SW:71:ARG:NH2	2.53	0.42
52:S2:201:C:N4	52:S2:202:G:N3	2.67	0.42
56:SE:83:VAL:HG22	83:Si:89:GLY:HA2	2.01	0.42
58:SG:99:ARG:HH22	58:SG:136:GLY:HA3	1.85	0.42
64:SP:73:ASP:OD2	64:SP:122:LYS:NZ	2.49	0.42
64:SP:168:LYS:HE3	64:SP:169:ILE:HG12	2.02	0.42
66:SR:56:ASN:HB2	66:SR:108:VAL:HG12	2.01	0.42
70:SV:37:ASP:OD1	70:SV:37:ASP:N	2.53	0.42
73:SY:46:THR:HB	73:SY:86:GLU:HG3	2.02	0.42
80:Sf:42:GLY:O	80:Sf:46:LYS:NZ	2.52	0.42
6:L5:779:G:H2'	6:L5:780:G:H8	1.84	0.42
6:L5:2207:OMG:HM23	6:L5:2207:OMG:H1'	1.78	0.42
6:L5:2687:A:O2'	6:L5:4377:G:H4'	2.19	0.42
6:L5:4047:U:H4'	27:LW:54:HIS:CD2	2.54	0.42
22:LR:62:MET:HE2	22:LR:62:MET:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LT:178:ARG:H	34:Ld:51:GLY:HA2	1.85	0.42
32:Lb:111:LEU:HD12	32:Lb:111:LEU:HA	1.94	0.42
52:S2:400:C:H3'	52:S2:401:C:H5'	2.00	0.42
60:SL:108:PHE:HD2	60:SL:136:GLU:HB3	1.84	0.42
61:SM:52:THR:HG23	61:SM:57:ILE:HA	2.02	0.42
68:ST:17:LYS:HZ3	68:ST:19:LYS:HG2	1.84	0.42
1:E:482:ALA:HA	1:E:488:VAL:HA	2.01	0.42
3:I:123:G:H1	3:I:163:G:N2	2.18	0.42
5:B:628:ARG:C	5:B:630:ARG:H	2.28	0.42
6:L5:2328:U:H2'	6:L5:2329:G:H8	1.85	0.42
6:L5:3573:OMC:HM23	6:L5:3573:OMC:H1'	1.85	0.42
6:L5:3897:G:H2'	6:L5:3898:G:H8	1.85	0.42
6:L5:4445:U:H4'	6:L5:4446:A:OP1	2.20	0.42
7:L7:55:A:H4'	18:LM:155:HIS:HB2	2.00	0.42
10:LE:17:LEU:HD21	10:LE:235:TRP:HH2	1.85	0.42
11:LF:240:LEU:HD12	11:LF:240:LEU:HA	1.89	0.42
15:LJ:111:LYS:HE3	15:LJ:111:LYS:HB3	1.72	0.42
52:S2:236:A:H2'	52:S2:237:C:O4'	2.20	0.42
52:S2:1597:U:O3'	78:Sd:25:LYS:NZ	2.48	0.42
52:S2:1848:G:N7	86:Sl:12:ARG:NH2	2.64	0.42
54:SC:62:GLU:OE1	54:SC:62:GLU:N	2.52	0.42
64:SP:86:PHE:CD2	64:SP:87:MET:HG2	2.55	0.42
64:SP:105:THR:HG23	64:SP:245:ARG:HA	2.02	0.42
64:SP:163:ASP:O	64:SP:167:GLY:N	2.45	0.42
66:SR:49:VAL:HG21	66:SR:115:LYS:HE2	2.01	0.42
69:SU:121:LYS:HE2	69:SU:121:LYS:HB3	1.82	0.42
85:Sk:50:PHE:HZ	85:Sk:58:LEU:HD13	1.84	0.42
6:L5:14:C:H5''	31:La:56:ARG:HG2	2.00	0.42
6:L5:375:G:OP2	43:Lm:52:LYS:NZ	2.40	0.42
6:L5:382:G:H4'	6:L5:407:A:N1	2.35	0.42
6:L5:1089:G:H2'	6:L5:1091:G:C8	2.55	0.42
6:L5:1503:G:O2'	6:L5:2655:A:N3	2.50	0.42
6:L5:1700:G:H1	6:L5:1710:U:H3	1.66	0.42
6:L5:1922:A:H4'	6:L5:1923:A:C8	2.55	0.42
6:L5:2194:OMC:HM23	11:LF:95:MET:HG3	2.02	0.42
6:L5:3767:G:H2'	6:L5:3768:C:O4'	2.20	0.42
6:L5:4204:C:H2'	6:L5:4205:U:C6	2.55	0.42
6:L5:4328:C:O2'	10:LE:99:LEU:O	2.26	0.42
6:L5:4413:C:OP1	10:LE:224:LYS:NZ	2.38	0.42
6:L5:4473:A:H5'	10:LE:130:PHE:H	1.84	0.42
7:L7:74:A:N1	7:L7:100:A:H5''	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LE:54:THR:OG1	10:LE:55:HIS:N	2.52	0.42
11:LF:60:HIS:NE2	11:LF:100:ARG:HD3	2.35	0.42
13:LH:240:LYS:H	13:LH:240:LYS:HD2	1.84	0.42
14:LI:24:PHE:HA	14:LI:27:LEU:HD23	2.01	0.42
19:LO:8:MET:HE2	19:LO:10:LEU:HD21	2.02	0.42
36:Lf:38:ILE:HG21	36:Lf:63:TYR:HB3	2.01	0.42
52:S2:376:U:H2'	52:S2:377:A:C8	2.55	0.42
52:S2:1287:G:N7	72:SX:36:ARG:HG2	2.35	0.42
52:S2:1755:G:H2'	52:S2:1756:C:O4'	2.20	0.42
58:SG:202:PRO:HG2	58:SG:243:PRO:HA	2.02	0.42
60:SL:69:GLU:CD	60:SL:69:GLU:H	2.27	0.42
62:SN:144:SER:HB2	62:SN:150:ALA:HB2	2.02	0.42
85:Sk:74:SER:OG	85:Sk:79:ILE:O	2.32	0.42
6:L5:151:G:H3'	21:LQ:49:ARG:NH2	2.34	0.41
6:L5:1708:G:H2'	6:L5:1709:A:O4'	2.19	0.41
6:L5:1866:U:OP1	6:L5:1888:U:O2'	2.31	0.41
6:L5:1984:G:O6	6:L5:3602:C:O2'	2.35	0.41
6:L5:2321:C:H2'	6:L5:2322:G:O4'	2.20	0.41
6:L5:3465:A:H2'	6:L5:3466:PSU:O4'	2.20	0.41
6:L5:4604:C:H2'	6:L5:4605:C:C6	2.54	0.41
24:LT:178:ARG:N	34:Ld:51:GLY:HA2	2.35	0.41
25:LU:106:LEU:HB3	25:LU:120:TYR:CE1	2.53	0.41
45:Lo:28:TRP:HA	45:Lo:33:ASN:ND2	2.35	0.41
52:S2:384:G:O2'	71:SW:133:PRO:O	2.38	0.41
52:S2:422:G:OP1	71:SW:97:ARG:HD2	2.20	0.41
52:S2:1077:G:P	73:SY:107:LYS:HE3	2.60	0.41
52:S2:1860:A:P	57:SF:10:ARG:HH12	2.43	0.41
58:SG:79:LEU:HD22	58:SG:120:ILE:HD12	2.01	0.41
64:SP:54:TYR:HD1	84:Sj:13:MET:HE1	1.83	0.41
64:SP:124:CYS:HA	64:SP:142:HIS:CE1	2.55	0.41
66:SR:35:GLU:HA	66:SR:51:ARG:HA	2.02	0.41
67:SS:88:SER:OG	67:SS:89:GLY:N	2.52	0.41
67:SS:105:THR:OG1	67:SS:106:ARG:N	2.53	0.41
77:Sc:102:THR:HG23	77:Sc:105:MET:HE2	2.02	0.41
80:Sf:90:ASP:N	80:Sf:90:ASP:OD1	2.53	0.41
5:B:630:ARG:HG2	5:B:632:TYR:CZ	2.55	0.41
6:L5:709:G:OP1	11:LF:321:ASN:ND2	2.45	0.41
6:L5:1346:C:H2'	6:L5:1347:G:C8	2.55	0.41
6:L5:3786:U:H2'	6:L5:3787:C:C6	2.55	0.41
10:LE:369:ASP:OD2	10:LE:373:LYS:NZ	2.54	0.41
18:LM:88:LYS:HE3	18:LM:88:LYS:HB3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Ln:47:ILE:HD11	44:Ln:56:LEU:HD13	2.02	0.41
52:S2:560:G:O2'	52:S2:561:A:H8	2.02	0.41
52:S2:1239:PSU:O2'	75:Sa:126:VAL:HG12	2.19	0.41
52:S2:1629:C:H2'	52:S2:1630:C:C6	2.55	0.41
61:SM:123:ALA:HB2	61:SM:165:ARG:HG3	2.01	0.41
63:SO:197:LYS:HB2	63:SO:197:LYS:HE3	1.88	0.41
66:SR:192:ILE:HD13	66:SR:192:ILE:HA	1.93	0.41
67:SS:100:ILE:HG12	67:SS:125:VAL:HG21	2.02	0.41
6:L5:113:A:H2'	6:L5:114:G:O4'	2.20	0.41
6:L5:520:G:H2'	6:L5:521:C:C6	2.55	0.41
6:L5:1420:G:OP1	35:Le:44:ARG:NH1	2.53	0.41
6:L5:3867:C:H2'	6:L5:3868:C:C6	2.56	0.41
7:L7:2:U:C5'	12:LG:267:ASN:ND2	2.82	0.41
9:LD:14:SER:OG	9:LD:15:VAL:N	2.53	0.41
11:LF:218:VAL:HA	11:LF:229:LEU:HG	2.02	0.41
12:LG:214:GLU:HG2	12:LG:215:ASP:N	2.35	0.41
52:S2:89:C:H2'	52:S2:90:G:C8	2.55	0.41
52:S2:911:G:H2'	52:S2:912:C:O4'	2.20	0.41
52:S2:1595:A:OP2	85:Sk:104:ARG:HG3	2.20	0.41
52:S2:1614:G:OP2	75:Sa:39:ALA:N	2.53	0.41
52:S2:1624:A:N6	78:Sd:132:ARG:HD3	2.35	0.41
52:S2:1855:U:OP1	74:SZ:150:ARG:NH2	2.50	0.41
53:SB:33:MET:HE2	53:SB:48:SER:HA	2.01	0.41
66:SR:50:VAL:HG11	66:SR:111:LEU:HB3	2.01	0.41
66:SR:132:ARG:HB2	66:SR:133:LEU:HD22	2.02	0.41
69:SU:84:ILE:HG13	69:SU:86:VAL:HG23	2.01	0.41
69:SU:103:GLU:HA	69:SU:106:LEU:HD12	2.02	0.41
78:Sd:13:LEU:HB2	78:Sd:20:ILE:HB	2.03	0.41
3:I:174:G:N2	3:I:202:C:O2'	2.48	0.41
6:L5:92:C:C2	34:Ld:55:LYS:HD3	2.56	0.41
6:L5:1130:C:H2'	6:L5:1131:G:O4'	2.20	0.41
6:L5:1952:A:H2'	6:L5:1953:C:C6	2.55	0.41
6:L5:2325:C:H2'	6:L5:2326:G:H8	1.84	0.41
6:L5:3835:G:H2'	6:L5:3836:G:H8	1.84	0.41
6:L5:4270:G:N3	10:LE:252:ALA:HB1	2.35	0.41
6:L5:4512:G:OP1	16:LK:23:ARG:NH1	2.54	0.41
11:LF:186:SER:O	11:LF:188:ARG:NH1	2.51	0.41
52:S2:144:U:H5	66:SR:178:ARG:HD3	1.85	0.41
52:S2:728:G:H2'	52:S2:729:C:C6	2.56	0.41
52:S2:907:U:H2'	52:S2:908:G:C8	2.55	0.41
52:S2:1008:C:H2'	52:S2:1009:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1038:G:H4'	52:S2:1846:A:H4'	2.01	0.41
52:S2:1100:G:H22	52:S2:1134:A:H2	1.68	0.41
52:S2:1247:A:N3	52:S2:1252:A:O2'	2.51	0.41
52:S2:1257:G:O6	80:Sf:65:THR:HG22	2.21	0.41
63:SO:7:LYS:HA	63:SO:7:LYS:HD3	1.91	0.41
69:SU:127:ARG:CZ	69:SU:145:PRO:HG2	2.51	0.41
83:Si:28:LYS:O	83:Si:32:LEU:HB2	2.20	0.41
1:E:336:HIS:CE1	1:E:433:LEU:H	2.39	0.41
5:B:445:GLN:HA	55:SD:147:THR:OG1	2.21	0.41
5:B:691:CYS:SG	5:B:692:ILE:N	2.94	0.41
5:B:771:GLN:O	5:B:775:THR:OG1	2.36	0.41
6:L5:106:A:H2'	6:L5:107:G:O4'	2.19	0.41
6:L5:1930:A:H2'	6:L5:1931:U:O4'	2.21	0.41
6:L5:3385:A:N6	6:L5:3423:G:O2'	2.49	0.41
6:L5:3439:U:H2'	6:L5:3440:C:C6	2.55	0.41
6:L5:4224:G:N2	6:L5:4354:G:O2'	2.54	0.41
18:LM:63:ARG:N	18:LM:66:GLU:OE2	2.44	0.41
18:LM:99:PHE:HB2	18:LM:159:LYS:HE3	2.01	0.41
45:Lo:15:LYS:HE3	45:Lo:15:LYS:HB2	1.82	0.41
52:S2:564:G:O2'	52:S2:565:A:H5''	2.20	0.41
52:S2:897:U:H2'	52:S2:898:U:O4'	2.21	0.41
52:S2:961:U:O2'	52:S2:963:A:N7	2.46	0.41
52:S2:1172:G:O2'	52:S2:1188:G:O6	2.33	0.41
52:S2:1779:C:H2'	52:S2:1780:G:C8	2.56	0.41
55:SD:102:VAL:HA	55:SD:105:TYR:CD2	2.56	0.41
64:SP:63:LYS:O	64:SP:67:GLN:HG2	2.21	0.41
66:SR:121:ILE:HG22	66:SR:124:LEU:H	1.85	0.41
70:SV:14:LEU:H	70:SV:14:LEU:HG	1.62	0.41
71:SW:150:GLY:HA3	73:SY:133:ARG:HH22	1.85	0.41
78:Sd:110:ASP:HA	78:Sd:113:ARG:HG2	2.02	0.41
84:Sj:80:ASP:OD1	84:Sj:81:TYR:N	2.54	0.41
6:L5:1208:C:H2'	6:L5:1209:G:H8	1.85	0.41
6:L5:4237:G:H5''	6:L5:4366:OMU:HM21	2.03	0.41
19:LO:174:LYS:NZ	34:Ld:141:GLY:O	2.53	0.41
52:S2:437:OMG:HM23	52:S2:437:OMG:H1'	1.88	0.41
52:S2:540:C:H2'	52:S2:541:U:C6	2.56	0.41
52:S2:941:U:H2'	52:S2:942:C:C6	2.55	0.41
52:S2:1416:C:O3'	79:Se:129:ARG:HG2	2.21	0.41
52:S2:1776:U:H2'	52:S2:1777:G:C8	2.56	0.41
53:SB:75:GLU:H	53:SB:75:GLU:CD	2.29	0.41
64:SP:62:LYS:HE3	64:SP:62:LYS:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SP:141:THR:OG1	64:SP:145:ARG:HB3	2.21	0.41
71:SW:109:MET:HE2	71:SW:109:MET:HB3	1.90	0.41
78:Sd:64:VAL:O	78:Sd:68:ILE:HG12	2.21	0.41
2:F:49:U:H3	2:F:60:A:H61	1.68	0.41
6:L5:135:G:C6	41:Lk:97:LYS:HD3	2.56	0.41
6:L5:733:C:O5'	20:LP:71:LYS:NZ	2.49	0.41
6:L5:748:C:H42	6:L5:807:G:H1	1.67	0.41
6:L5:1215:G:N3	6:L5:1215:G:H2'	2.36	0.41
6:L5:2281:A:O2'	6:L5:2283:U:OP2	2.29	0.41
6:L5:2478:U:H4'	25:LU:55:VAL:HG11	2.03	0.41
6:L5:4117:G:O2'	6:L5:4118:U:OP2	2.35	0.41
6:L5:4368:A:H4'	10:LE:13:SER:HB2	2.03	0.41
11:LF:268:ARG:CZ	11:LF:268:ARG:HB3	2.49	0.41
14:LI:189:LEU:HD21	14:LI:207:LEU:HD21	2.03	0.41
16:LK:115:ARG:NE	16:LK:123:ILE:HD12	2.35	0.41
19:LO:141:ALA:HA	19:LO:144:LEU:HD23	2.03	0.41
20:LP:126:GLU:HG3	22:LR:185:VAL:HG13	2.03	0.41
21:LQ:146:PRO:HG2	41:Lk:104:THR:HG23	2.02	0.41
24:LT:22:ASP:OD1	24:LT:22:ASP:N	2.54	0.41
24:LT:63:LEU:HD23	24:LT:63:LEU:HA	1.95	0.41
33:Lc:73:LYS:HB3	33:Lc:73:LYS:HE3	1.84	0.41
52:S2:218:PSU:O4	68:ST:184:ARG:NH2	2.51	0.41
52:S2:990:C:OP2	61:SM:155:TYR:OH	2.34	0.41
58:SG:191:HIS:CE1	58:SG:195:LEU:HD11	2.56	0.41
61:SM:103:MET:HE2	61:SM:103:MET:HB2	1.92	0.41
62:SN:271:ASP:OD1	62:SN:271:ASP:N	2.53	0.41
64:SP:68:ARG:HB3	64:SP:76:VAL:HG11	2.02	0.41
64:SP:81:THR:O	64:SP:81:THR:OG1	2.39	0.41
65:SQ:42:LYS:HG3	65:SQ:43:GLU:H	1.86	0.41
72:SX:52:LEU:HD11	72:SX:65:VAL:HG21	2.02	0.41
74:SZ:97:LEU:HD11	74:SZ:112:ALA:HB1	2.01	0.41
80:Sf:34:LYS:HE3	80:Sf:34:LYS:HB3	1.80	0.41
1:E:309:LEU:HD23	1:E:421:THR:HG22	2.03	0.41
6:L5:746:G:H2'	6:L5:747:G:O4'	2.20	0.41
6:L5:1070:U:O2	12:LG:286:SER:OG	2.34	0.41
6:L5:1250:C:H2'	6:L5:1251:A:C8	2.56	0.41
6:L5:1779:G:OP2	14:LI:201:LYS:NZ	2.44	0.41
6:L5:2204:G:O2'	6:L5:3591:G:O6	2.38	0.41
6:L5:2265:OMC:HM23	6:L5:2265:OMC:H1'	1.91	0.41
6:L5:3629:G:OP1	10:LE:250:LYS:HD2	2.20	0.41
6:L5:4383:OMG:H1'	6:L5:4383:OMG:HM23	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LH:210:LYS:HE3	13:LH:210:LYS:HB3	1.93	0.41
15:LJ:165:GLU:CD	21:LQ:11:TRP:HE1	2.28	0.41
23:LS:2:VAL:HB	23:LS:18:ARG:NH1	2.36	0.41
23:LS:15:CYS:SG	23:LS:150:LEU:HB2	2.61	0.41
52:S2:229:A:OP2	52:S2:888:U:H1'	2.20	0.41
52:S2:1590:A:N3	52:S2:1654:U:O2'	2.48	0.41
52:S2:1631:A:H5''	78:Sd:37:GLY:N	2.36	0.41
55:SD:129:GLY:H	72:SX:44:LYS:NZ	2.19	0.41
58:SG:173:LEU:HD11	58:SG:189:ILE:HG12	2.02	0.41
71:SW:33:LEU:HD12	71:SW:34:PRO:HD2	2.02	0.41
73:SY:37:ILE:HD11	73:SY:63:VAL:HG11	2.02	0.41
4:S:1131:C:O2	4:S:1141:G:N2	2.54	0.41
4:S:1134:C:H42	4:S:1137:G:H1'	1.86	0.41
4:S:1139:U:H2'	4:S:1140:G:C8	2.56	0.41
6:L5:82:U:H2'	6:L5:83:C:O4'	2.21	0.41
6:L5:660:G:O2'	11:LF:291:ARG:NH1	2.54	0.41
6:L5:865:G:H2'	14:LI:24:PHE:CE1	2.56	0.41
6:L5:1600:C:OP1	11:LF:80:ARG:NH2	2.47	0.41
6:L5:1658:C:H2'	6:L5:1659:C:O4'	2.21	0.41
6:L5:1694:C:H2'	6:L5:1695:U:O4'	2.21	0.41
6:L5:2688:A:H61	6:L5:3575:C:N4	2.16	0.41
6:L5:3509:G:O2'	6:L5:3547:G:O6	2.33	0.41
6:L5:3698:A:H2'	6:L5:3699:G:O4'	2.21	0.41
6:L5:3788:U:H2'	6:L5:3789:U:C6	2.56	0.41
6:L5:4224:G:O2'	6:L5:4348:A:N1	2.53	0.41
6:L5:4611:G:OP2	20:LP:94:LYS:NZ	2.39	0.41
15:LJ:232:GLU:HA	15:LJ:235:ARG:HG2	2.02	0.41
21:LQ:160:GLU:OE1	21:LQ:160:GLU:N	2.48	0.41
23:LS:14:SER:OG	23:LS:151:THR:HG22	2.21	0.41
26:LV:43:ARG:HA	26:LV:43:ARG:HD2	1.90	0.41
27:LW:110:LYS:HE2	27:LW:110:LYS:HB3	1.90	0.41
32:Lb:116:LYS:O	32:Lb:120:GLU:HG2	2.20	0.41
34:Ld:59:ARG:NH2	47:Lq:36:GLN:OE1	2.40	0.41
52:S2:16:G:H2'	52:S2:17:C:C6	2.56	0.41
52:S2:92:A:C6	52:S2:447:G:C6	3.09	0.41
52:S2:106:C:OP1	52:S2:432:G:O2'	2.31	0.41
52:S2:523:A:H5'	69:SU:144:ILE:HG22	2.02	0.41
52:S2:523:A:H5''	69:SU:145:PRO:HD2	2.02	0.41
52:S2:731:C:N4	52:S2:732:G:O6	2.54	0.41
52:S2:736:C:H2'	52:S2:737:C:C5	2.56	0.41
52:S2:858:U:H2'	52:S2:859:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1465:C:H4'	77:Sc:60:ARG:NH2	2.35	0.41
52:S2:1809:U:H2'	52:S2:1810:A:C8	2.55	0.41
56:SE:105:ARG:HA	69:SU:38:ARG:HA	2.03	0.41
57:SF:47:ALA:O	57:SF:50:VAL:HG12	2.21	0.41
58:SG:57:ARG:HA	76:Sb:102:GLU:OE1	2.21	0.41
58:SG:149:GLU:HG3	58:SG:170:TRP:HB2	2.02	0.41
60:SL:151:ASP:OD1	60:SL:151:ASP:N	2.53	0.41
64:SP:73:ASP:HA	64:SP:164:LEU:HD13	2.02	0.41
64:SP:160:ILE:HD12	64:SP:169:ILE:HG22	2.03	0.41
66:SR:224:ARG:HA	66:SR:227:GLN:HE21	1.85	0.41
67:SS:101:LEU:HD23	67:SS:120:ARG:HG2	2.02	0.41
68:ST:74:ARG:HD3	68:ST:74:ARG:HA	1.92	0.41
68:ST:193:LYS:HD2	68:ST:196:GLU:OE2	2.20	0.41
69:SU:84:ILE:HA	69:SU:150:ARG:HA	2.02	0.41
82:Sh:77:PRO:HD2	82:Sh:79:PHE:CZ	2.56	0.41
1:E:186:ALA:HB3	87:E:1001:GTP:N7	2.36	0.41
6:L5:184:U:H2'	6:L5:188:G:O2'	2.21	0.41
6:L5:443:G:H5''	39:Li:54:LYS:HG2	2.03	0.41
6:L5:888:C:H2'	6:L5:889:C:C6	2.55	0.41
6:L5:1111:G:N1	6:L5:1112:G:N3	2.69	0.41
6:L5:1365:U:H2'	6:L5:1366:C:C6	2.56	0.41
6:L5:3676:OMG:HM23	6:L5:3676:OMG:H1'	1.87	0.41
6:L5:3690:G:H2'	6:L5:3691:U:O4'	2.21	0.41
6:L5:3691:U:H2'	6:L5:3692:A:O4'	2.21	0.41
6:L5:3765:C:H42	6:L5:3778:A:H2	1.68	0.41
11:LF:230:LEU:HD12	11:LF:230:LEU:HA	1.92	0.41
15:LJ:63:LEU:HD12	21:LQ:32:GLN:HB2	2.02	0.41
28:LX:63:ILE:HG13	28:LX:72:VAL:HG22	2.03	0.41
44:Ln:61:PRO:HA	44:Ln:62:PRO:HD3	1.97	0.41
49:Ls:56:ASP:OD1	49:Ls:56:ASP:N	2.53	0.41
52:S2:657:G:H5'	52:S2:663:G:N2	2.36	0.41
52:S2:1447:A:O2'	52:S2:1448:OMG:H5''	2.21	0.41
52:S2:1756:C:H2'	52:S2:1757:C:C6	2.56	0.41
60:SL:111:GLN:H	60:SL:111:GLN:CD	2.29	0.41
62:SN:98:LEU:O	62:SN:102:LEU:HG	2.20	0.41
64:SP:185:GLY:HA2	64:SP:189:LEU:HD12	2.02	0.41
68:ST:3:ILE:HD12	68:ST:3:ILE:H	1.86	0.41
75:Sa:68:PRO:HB2	75:Sa:71:GLU:OE1	2.21	0.41
1:E:164:THR:O	1:E:168:GLN:HG3	2.21	0.40
6:L5:790:G:O2'	6:L5:792:G:O4'	2.37	0.40
6:L5:3706:G:H21	6:L5:3765:C:H5	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:3942:OMG:H1'	6:L5:3942:OMG:HM23	1.81	0.40
7:L7:63:C:H1'	12:LG:280:VAL:HG11	2.03	0.40
7:L7:119:U:P	12:LG:259:ARG:HH21	2.44	0.40
10:LE:238:LYS:HE3	10:LE:238:LYS:HB2	1.94	0.40
14:LI:225:HIS:HB3	14:LI:228:GLU:HG2	2.02	0.40
22:LR:47:PHE:HA	22:LR:136:ALA:HB2	2.02	0.40
26:LV:94:TYR:OH	26:LV:96:GLU:OE2	2.39	0.40
28:LX:101:ARG:HD2	28:LX:115:PHE:CE1	2.57	0.40
30:LZ:19:ARG:NH2	30:LZ:37:GLU:OE2	2.53	0.40
33:Lc:54:THR:O	33:Lc:57:MET:HG2	2.22	0.40
52:S2:3:C:N3	69:SU:17:ARG:NH1	2.69	0.40
52:S2:1026:U:H2'	52:S2:1027:C:O4'	2.22	0.40
52:S2:1649:G:N7	76:Sb:17:LYS:HE2	2.37	0.40
56:SE:85:LYS:O	56:SE:89:GLN:HG3	2.20	0.40
59:SH:5:GLN:N	59:SH:5:GLN:OE1	2.53	0.40
64:SP:11:ARG:NH2	64:SP:20:LEU:HD12	2.37	0.40
67:SS:144:ILE:HD13	67:SS:152:ARG:HH21	1.85	0.40
69:SU:131:ARG:NH1	69:SU:143:ASN:O	2.54	0.40
73:SY:92:ILE:HG23	73:SY:141:TYR:HE1	1.85	0.40
77:Sc:20:TYR:O	77:Sc:24:LEU:HD23	2.21	0.40
85:Sk:79:ILE:HB	85:Sk:83:LEU:HD23	2.02	0.40
5:B:686:LEU:HD12	5:B:688:LYS:NZ	2.37	0.40
6:L5:109:G:OP2	19:LO:74:ARG:NH2	2.54	0.40
6:L5:197:A:N3	6:L5:222:C:O2'	2.53	0.40
6:L5:1806:A:OP1	17:LL:13:LYS:HE2	2.21	0.40
6:L5:1994:G:O6	26:LV:156:HIS:ND1	2.51	0.40
6:L5:3331:A:H2'	6:L5:3332:G:C8	2.56	0.40
6:L5:3657:OMU:HM23	6:L5:3657:OMU:H1'	1.88	0.40
6:L5:3684:A:H2'	6:L5:3685:G:O4'	2.21	0.40
6:L5:4794:G:H2'	6:L5:4795:A:C8	2.56	0.40
12:LG:83:LEU:HB3	12:LG:88:VAL:HB	2.04	0.40
39:Li:50:VAL:HG22	39:Li:69:VAL:HG23	2.03	0.40
49:Ls:17:LEU:HD21	49:Ls:19:LYS:HE3	2.04	0.40
52:S2:145:G:N1	52:S2:146:G:O6	2.53	0.40
52:S2:641:A:H2'	52:S2:642:A:C8	2.56	0.40
52:S2:746:C:H2'	52:S2:747:C:C2	2.56	0.40
52:S2:809:A:H3'	52:S2:810:A:H8	1.85	0.40
52:S2:1306:C:H2'	52:S2:1307:U:C6	2.56	0.40
52:S2:1789:A:N3	52:S2:1789:A:H2'	2.36	0.40
62:SN:60:TRP:NE1	62:SN:92:GLU:OE2	2.55	0.40
65:SQ:74:ASN:HA	65:SQ:77:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SQ:80:GLY:HA2	65:SQ:83:ASN:OD1	2.21	0.40
65:SQ:152:TRP:HE3	65:SQ:153:LEU:HD22	1.87	0.40
66:SR:194:LEU:HD23	66:SR:194:LEU:HA	1.93	0.40
67:SS:65:PRO:HD2	67:SS:68:GLN:HE21	1.86	0.40
69:SU:93:LYS:HE2	69:SU:93:LYS:HB2	1.93	0.40
76:Sb:32:ILE:HD12	76:Sb:39:LEU:HD12	2.03	0.40
85:Sk:90:GLU:O	85:Sk:93:SER:OG	2.32	0.40
3:I:219:A:H1'	52:S2:627:G:O6	2.22	0.40
6:L5:2037:G:OP2	6:L5:2037:G:H8	2.05	0.40
15:LJ:39:PHE:CD1	15:LJ:47:PRO:HD3	2.57	0.40
15:LJ:255:LYS:HE3	15:LJ:255:LYS:HB3	1.84	0.40
52:S2:538:C:H2'	52:S2:539:U:C6	2.57	0.40
52:S2:604:C:N4	52:S2:621:G:O6	2.53	0.40
52:S2:640:C:OP1	56:SE:115:ARG:NH2	2.38	0.40
52:S2:1311:U:H4'	55:SD:143:LYS:HB2	2.04	0.40
52:S2:1311:U:H5''	55:SD:130:VAL:HG13	2.03	0.40
52:S2:1746:A:H1'	66:SR:66:GLY:HA2	2.03	0.40
77:Sc:126:MET:H	77:Sc:126:MET:HG2	1.78	0.40
6:L5:389:A:H1'	32:Lb:91:ASN:HA	2.04	0.40
6:L5:1059:G:C6	6:L5:1085:G:C2	3.09	0.40
6:L5:1109:G:H2'	6:L5:1110:G:C8	2.56	0.40
6:L5:4653:G:OP2	6:L5:4653:G:H8	2.05	0.40
8:L8:15:G:C6	8:L8:16:G:N1	2.90	0.40
8:L8:67:U:H2'	8:L8:68:G:C8	2.57	0.40
9:LD:90:CYS:SG	9:LD:101:VAL:HB	2.61	0.40
14:LI:103:LYS:HE2	14:LI:103:LYS:HB2	1.93	0.40
14:LI:107:VAL:HG23	14:LI:131:MET:HE3	2.04	0.40
17:LL:99:ILE:HG22	17:LL:123:GLN:HB2	2.04	0.40
25:LU:175:GLU:HA	25:LU:178:GLN:HB3	2.04	0.40
28:LX:105:ASN:OD1	28:LX:111:GLU:HB3	2.21	0.40
32:Lb:134:LYS:HE3	32:Lb:134:LYS:HB3	1.88	0.40
46:Lp:78:ILE:HB	46:Lp:83:ARG:HD3	2.04	0.40
52:S2:400:C:C4	71:SW:104:LYS:HD2	2.56	0.40
52:S2:609:C:H2'	52:S2:610:PSU:H6	1.85	0.40
52:S2:888:U:H2'	52:S2:889:U:C6	2.57	0.40
53:SB:42:LYS:NZ	53:SB:57:VAL:HB	2.36	0.40
56:SE:102:ARG:HD3	56:SE:103:THR:N	2.37	0.40
58:SG:44:LYS:NZ	58:SG:56:GLN:HG3	2.36	0.40
59:SH:36:LEU:HD13	59:SH:36:LEU:HA	1.97	0.40
60:SL:33:GLN:OE1	60:SL:154:LEU:HB2	2.21	0.40
65:SQ:44:LYS:HE2	65:SQ:44:LYS:HB2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SS:58:LYS:HB2	67:SS:90:LYS:HG2	2.03	0.40
75:Sa:81:ARG:HB3	75:Sa:117:GLY:HA3	2.03	0.40
77:Sc:9:VAL:HA	77:Sc:50:ILE:HD13	2.04	0.40
78:Sd:102:GLY:HA2	78:Sd:105:ASN:HD22	1.86	0.40
86:Sl:2:ARG:HB3	86:Sl:5:TRP:CD1	2.56	0.40
3:I:45:C:H5'	3:I:84:A:N3	2.37	0.40
3:I:95:U:H2'	3:I:96:G:C6	2.57	0.40
5:B:683:HIS:CE1	5:B:750:PHE:HZ	2.40	0.40
6:L5:223:G:H4'	6:L5:225:G:C8	2.57	0.40
6:L5:2680:OMU:HM23	6:L5:2680:OMU:H1'	1.94	0.40
6:L5:4382:PSU:O2	37:Lg:78:ARG:HD2	2.21	0.40
13:LH:152:ILE:HD12	13:LH:274:LEU:HD11	2.02	0.40
52:S2:445:G:O6	68:ST:26:LYS:HE3	2.21	0.40
52:S2:605:A:N3	52:S2:640:C:O2'	2.53	0.40
52:S2:847:G:C8	64:SP:19:MET:HE1	2.56	0.40
52:S2:1759:G:N1	52:S2:1776:U:O2	2.55	0.40
52:S2:1865:U:OP1	57:SF:86:ASN:ND2	2.47	0.40
60:SL:14:ASP:CG	60:SL:180:ARG:HH22	2.30	0.40
60:SL:81:ASN:HA	60:SL:84:GLN:HG3	2.03	0.40
68:ST:79:ILE:HD12	68:ST:170:LYS:HG3	2.03	0.40
73:SY:3:ARG:HB2	73:SY:6:ALA:HB3	2.04	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	E	509/616 (83%)	460 (90%)	46 (9%)	3 (1%)	21	51
5	B	200/854 (23%)	171 (86%)	28 (14%)	1 (0%)	24	55
9	LD	251/257 (98%)	241 (96%)	10 (4%)	0	100	100
10	LE	395/403 (98%)	386 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	LF	360/413 (87%)	355 (99%)	5 (1%)	0	100	100
12	LG	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
13	LH	226/291 (78%)	220 (97%)	6 (3%)	0	100	100
14	LI	224/247 (91%)	217 (97%)	7 (3%)	0	100	100
15	LJ	229/266 (86%)	227 (99%)	2 (1%)	0	100	100
16	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
17	LL	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
18	LM	168/178 (94%)	162 (96%)	6 (4%)	0	100	100
19	LO	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
20	LP	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
21	LQ	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
22	LR	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
23	LS	157/184 (85%)	153 (98%)	4 (2%)	0	100	100
24	LT	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
25	LU	178/196 (91%)	178 (100%)	0	0	100	100
26	LV	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
27	LW	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
28	LX	97/128 (76%)	94 (97%)	3 (3%)	0	100	100
29	LY	137/140 (98%)	134 (98%)	3 (2%)	0	100	100
30	LZ	89/157 (57%)	89 (100%)	0	0	100	100
31	La	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
32	Lb	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
33	Lc	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
34	Ld	145/148 (98%)	140 (97%)	4 (3%)	1 (1%)	18	47
35	Le	103/245 (42%)	102 (99%)	1 (1%)	0	100	100
36	Lf	106/115 (92%)	106 (100%)	0	0	100	100
37	Lg	105/125 (84%)	105 (100%)	0	0	100	100
38	Lh	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
39	Li	108/110 (98%)	108 (100%)	0	0	100	100
40	Lj	112/117 (96%)	112 (100%)	0	0	100	100
41	Lk	120/123 (98%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Ll	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
43	Lm	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
44	Ln	67/70 (96%)	67 (100%)	0	0	100	100
45	Lo	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
46	Lp	49/128 (38%)	49 (100%)	0	0	100	100
47	Lq	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
48	Lr	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
49	Ls	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
50	Lt	111/318 (35%)	105 (95%)	5 (4%)	1 (1%)	14	41
51	Lx	190/217 (88%)	172 (90%)	17 (9%)	1 (0%)	24	55
53	SB	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
54	SC	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
55	SD	72/156 (46%)	71 (99%)	1 (1%)	0	100	100
56	SE	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
57	SF	99/115 (86%)	99 (100%)	0	0	100	100
58	SG	311/317 (98%)	297 (96%)	14 (4%)	0	100	100
59	SH	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
60	SL	219/295 (74%)	213 (97%)	6 (3%)	0	100	100
61	SM	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
62	SN	218/293 (74%)	216 (99%)	2 (1%)	0	100	100
63	SO	223/281 (79%)	219 (98%)	4 (2%)	0	100	100
64	SP	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
65	SQ	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
66	SR	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
67	SS	188/432 (44%)	183 (97%)	5 (3%)	0	100	100
68	ST	204/208 (98%)	197 (97%)	7 (3%)	0	100	100
69	SU	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
70	SV	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
71	SW	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
72	SX	122/132 (92%)	116 (95%)	6 (5%)	0	100	100
73	SY	148/151 (98%)	146 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	SZ	134/151 (89%)	127 (95%)	6 (4%)	1 (1%)	18	47
75	Sa	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
76	Sb	139/172 (81%)	132 (95%)	7 (5%)	0	100	100
77	Sc	132/135 (98%)	132 (100%)	0	0	100	100
78	Sd	146/152 (96%)	144 (99%)	2 (1%)	0	100	100
79	Se	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
80	Sf	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
81	Sg	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
82	Sh	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
83	Si	137/143 (96%)	136 (99%)	1 (1%)	0	100	100
84	Sj	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
85	Sk	73/124 (59%)	72 (99%)	1 (1%)	0	100	100
86	Sl	23/25 (92%)	23 (100%)	0	0	100	100
All	All	12310/15142 (81%)	11992 (97%)	310 (2%)	8 (0%)	49	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	546	PRO
51	Lx	108	ASP
50	Lt	79	LEU
1	E	297	LEU
5	B	703	SER
34	Ld	15	VAL
74	SZ	138	ASP
1	E	570	GLU

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	E	227/524 (43%)	221 (97%)	6 (3%)	40	75
5	B	102/761 (13%)	99 (97%)	3 (3%)	37	73
9	LD	195/199 (98%)	191 (98%)	4 (2%)	47	79
10	LE	344/347 (99%)	328 (95%)	16 (5%)	23	57
11	LF	302/337 (90%)	297 (98%)	5 (2%)	53	83
12	LG	247/250 (99%)	242 (98%)	5 (2%)	48	80
13	LH	205/251 (82%)	201 (98%)	4 (2%)	48	80
14	LI	197/215 (92%)	191 (97%)	6 (3%)	36	72
15	LJ	199/223 (89%)	196 (98%)	3 (2%)	57	84
16	LK	169/171 (99%)	165 (98%)	4 (2%)	43	77
17	LL	180/181 (99%)	172 (96%)	8 (4%)	25	59
18	LM	143/149 (96%)	139 (97%)	4 (3%)	38	73
19	LO	175/176 (99%)	169 (97%)	6 (3%)	32	68
20	LP	117/161 (73%)	114 (97%)	3 (3%)	40	75
21	LQ	171/172 (99%)	168 (98%)	3 (2%)	51	82
22	LR	171/173 (99%)	171 (100%)	0	100	100
23	LS	139/163 (85%)	138 (99%)	1 (1%)	76	91
24	LT	164/165 (99%)	161 (98%)	3 (2%)	51	82
25	LU	159/175 (91%)	147 (92%)	12 (8%)	12	37
26	LV	154/154 (100%)	149 (97%)	5 (3%)	34	70
27	LW	139/140 (99%)	133 (96%)	6 (4%)	26	60
28	LX	88/113 (78%)	87 (99%)	1 (1%)	65	87
29	LY	106/107 (99%)	106 (100%)	0	100	100
30	LZ	79/126 (63%)	78 (99%)	1 (1%)	61	86
31	La	106/134 (79%)	104 (98%)	2 (2%)	50	81
32	Lb	124/135 (92%)	122 (98%)	2 (2%)	55	83
33	Lc	117/118 (99%)	116 (99%)	1 (1%)	70	89
34	Ld	119/120 (99%)	115 (97%)	4 (3%)	32	68
35	Le	87/183 (48%)	86 (99%)	1 (1%)	65	87
36	Lf	92/98 (94%)	90 (98%)	2 (2%)	45	78
37	Lg	98/110 (89%)	95 (97%)	3 (3%)	35	70
38	Lh	116/121 (96%)	113 (97%)	3 (3%)	40	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Li	89/89 (100%)	86 (97%)	3 (3%)	32	68
40	Lj	98/100 (98%)	97 (99%)	1 (1%)	68	88
41	Lk	109/110 (99%)	106 (97%)	3 (3%)	38	73
42	Ll	86/89 (97%)	85 (99%)	1 (1%)	63	87
43	Lm	73/80 (91%)	70 (96%)	3 (4%)	27	62
44	Ln	64/65 (98%)	63 (98%)	1 (2%)	55	83
45	Lo	47/48 (98%)	47 (100%)	0	100	100
46	Lp	47/115 (41%)	47 (100%)	0	100	100
47	Lq	92/93 (99%)	91 (99%)	1 (1%)	65	87
48	Lr	74/75 (99%)	72 (97%)	2 (3%)	39	74
49	Ls	109/120 (91%)	104 (95%)	5 (5%)	24	58
53	SB	75/76 (99%)	73 (97%)	2 (3%)	39	74
54	SC	56/62 (90%)	53 (95%)	3 (5%)	20	51
55	SD	67/140 (48%)	65 (97%)	2 (3%)	36	72
56	SE	47/106 (44%)	46 (98%)	1 (2%)	47	79
57	SF	88/98 (90%)	87 (99%)	1 (1%)	65	87
58	SG	272/275 (99%)	263 (97%)	9 (3%)	33	69
59	SH	48/49 (98%)	47 (98%)	1 (2%)	47	79
60	SL	182/243 (75%)	178 (98%)	4 (2%)	45	78
61	SM	203/231 (88%)	199 (98%)	4 (2%)	48	80
62	SN	185/223 (83%)	180 (97%)	5 (3%)	39	74
63	SO	189/232 (82%)	184 (97%)	5 (3%)	40	75
64	SP	224/225 (100%)	216 (96%)	8 (4%)	31	66
65	SQ	161/170 (95%)	153 (95%)	8 (5%)	22	54
66	SR	207/218 (95%)	203 (98%)	4 (2%)	50	81
67	SS	170/360 (47%)	163 (96%)	7 (4%)	27	62
68	ST	178/180 (99%)	176 (99%)	2 (1%)	65	87
69	SU	161/168 (96%)	156 (97%)	5 (3%)	35	70
70	SV	87/136 (64%)	84 (97%)	3 (3%)	32	68
71	SW	139/142 (98%)	134 (96%)	5 (4%)	31	66
72	SX	104/108 (96%)	100 (96%)	4 (4%)	29	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	SY	130/131 (99%)	129 (99%)	1 (1%)	73	90
74	SZ	106/119 (89%)	101 (95%)	5 (5%)	23	57
75	Sa	114/130 (88%)	109 (96%)	5 (4%)	25	59
76	Sb	117/140 (84%)	113 (97%)	4 (3%)	32	68
77	Sc	120/121 (99%)	118 (98%)	2 (2%)	53	83
78	Sd	127/131 (97%)	125 (98%)	2 (2%)	55	83
79	Se	112/114 (98%)	110 (98%)	2 (2%)	51	82
80	Sf	94/107 (88%)	91 (97%)	3 (3%)	34	70
81	Sg	67/67 (100%)	64 (96%)	3 (4%)	24	58
82	Sh	112/113 (99%)	110 (98%)	2 (2%)	51	82
83	Si	112/114 (98%)	107 (96%)	5 (4%)	24	58
84	Sj	107/112 (96%)	107 (100%)	0	100	100
85	Sk	66/102 (65%)	64 (97%)	2 (3%)	36	72
86	Sl	24/24 (100%)	24 (100%)	0	100	100
All	All	10170/12403 (82%)	9904 (97%)	266 (3%)	41	75

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	12	VAL
1	E	244	THR
1	E	245	ILE
1	E	277	ILE
1	E	469	VAL
1	E	593	VAL
5	B	674	VAL
5	B	729	LEU
5	B	738	LEU
9	LD	84	THR
9	LD	106	THR
9	LD	157	VAL
9	LD	243	THR
10	LE	94	GLU
10	LE	162	VAL
10	LE	180	LEU
10	LE	182	GLU
10	LE	209	GLN

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Mol	Chain	Res	Type
10	LE	248	LEU
10	LE	298	LEU
10	LE	300	LYS
10	LE	329	ASP
10	LE	344	VAL
10	LE	346	THR
10	LE	347	LEU
10	LE	353	VAL
10	LE	369	ASP
10	LE	370	THR
10	LE	371	THR
11	LF	44	LEU
11	LF	147	VAL
11	LF	174	LEU
11	LF	240	LEU
11	LF	260	LEU
12	LG	36	LEU
12	LG	93	THR
12	LG	143	THR
12	LG	273	LEU
12	LG	288	LEU
13	LH	51	VAL
13	LH	73	ARG
13	LH	103	LYS
13	LH	281	THR
14	LI	24	PHE
14	LI	45	ARG
14	LI	51	GLU
14	LI	82	VAL
14	LI	152	LEU
14	LI	231	ASP
15	LJ	33	GLU
15	LJ	43	GLN
15	LJ	114	LEU
16	LK	55	LEU
16	LK	123	ILE
16	LK	128	MET
16	LK	153	LEU
17	LL	26	VAL
17	LL	36	LEU
17	LL	44	ASP
17	LL	63	GLU

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Mol	Chain	Res	Type
17	LL	126	VAL
17	LL	134	VAL
17	LL	152	LEU
17	LL	191	ILE
18	LM	47	THR
18	LM	57	VAL
18	LM	66	GLU
18	LM	129	ASP
19	LO	67	HIS
19	LO	81	LEU
19	LO	138	ASP
19	LO	144	LEU
19	LO	148	THR
19	LO	160	VAL
20	LP	7	VAL
20	LP	25	VAL
20	LP	48	GLN
21	LQ	36	LEU
21	LQ	126	THR
21	LQ	148	THR
23	LS	115	GLU
24	LT	82	VAL
24	LT	122	THR
24	LT	158	THR
25	LU	4	LEU
25	LU	8	LYS
25	LU	43	LYS
25	LU	44	LEU
25	LU	49	LEU
25	LU	55	VAL
25	LU	57	VAL
25	LU	106	LEU
25	LU	125	LEU
25	LU	145	LEU
25	LU	158	GLN
25	LU	163	ARG
26	LV	17	LEU
26	LV	77	ASN
26	LV	82	LEU
26	LV	158	VAL
26	LV	159	LEU
27	LW	4	THR

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Mol	Chain	Res	Type
27	LW	68	THR
27	LW	76	VAL
27	LW	80	VAL
27	LW	106	LEU
27	LW	141	VAL
28	LX	43	LEU
30	LZ	19	ARG
31	La	50	LYS
31	La	91	GLU
32	Lb	55	VAL
32	Lb	119	LEU
33	Lc	33	THR
34	Ld	63	LEU
34	Ld	75	LEU
34	Ld	95	THR
34	Ld	134	GLU
35	Le	50	ASN
36	Lf	20	LEU
36	Lf	94	LEU
37	Lg	107	THR
37	Lg	119	THR
37	Lg	123	ASP
38	Lh	43	ASN
38	Lh	87	VAL
38	Lh	118	LEU
39	Li	23	GLU
39	Li	25	THR
39	Li	33	VAL
40	Lj	87	VAL
41	Lk	8	ASP
41	Lk	44	LEU
41	Lk	54	ILE
42	Ll	20	ASN
43	Lm	15	THR
43	Lm	18	LEU
43	Lm	64	MET
44	Ln	36	VAL
47	Lq	67	VAL
48	Lr	38	THR
48	Lr	52	VAL
49	Ls	28	GLU
49	Ls	61	VAL

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Mol	Chain	Res	Type
49	Ls	78	VAL
49	Ls	80	THR
49	Ls	108	MET
53	SB	8	LEU
53	SB	18	LYS
54	SC	26	GLN
54	SC	57	THR
54	SC	63	ARG
55	SD	108	VAL
55	SD	144	CYS
56	SE	132	ASN
57	SF	75	VAL
58	SG	18	VAL
58	SG	42	MET
58	SG	64	HIS
58	SG	66	VAL
58	SG	71	ILE
58	SG	107	ASP
58	SG	129	ILE
58	SG	149	GLU
58	SG	166	VAL
59	SH	36	LEU
60	SL	25	LEU
60	SL	197	VAL
60	SL	206	ASP
60	SL	208	GLU
61	SM	9	LEU
61	SM	146	ARG
61	SM	147	ASN
61	SM	175	GLU
62	SN	116	THR
62	SN	122	THR
62	SN	149	THR
62	SN	260	VAL
62	SN	268	GLU
63	SO	11	PHE
63	SO	46	THR
63	SO	115	VAL
63	SO	156	LEU
63	SO	181	VAL
64	SP	20	LEU
64	SP	56	LEU

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Mol	Chain	Res	Type
64	SP	66	MET
64	SP	95	THR
64	SP	106	LYS
64	SP	136	ILE
64	SP	146	THR
64	SP	250	GLU
65	SQ	25	THR
65	SQ	26	ASP
65	SQ	33	ILE
65	SQ	73	THR
65	SQ	123	GLU
65	SQ	153	LEU
65	SQ	171	GLU
65	SQ	187	SER
66	SR	26	THR
66	SR	67	VAL
66	SR	91	GLU
66	SR	147	LEU
67	SS	9	VAL
67	SS	17	ASP
67	SS	29	GLU
67	SS	53	VAL
67	SS	69	LEU
67	SS	99	ARG
67	SS	162	GLN
68	ST	95	THR
68	ST	151	GLU
69	SU	14	VAL
69	SU	61	LEU
69	SU	71	LEU
69	SU	100	LEU
69	SU	144	ILE
70	SV	14	LEU
70	SV	18	GLU
70	SV	40	VAL
71	SW	42	LEU
71	SW	66	VAL
71	SW	83	GLN
71	SW	107	LYS
71	SW	135	SER
72	SX	52	LEU
72	SX	66	GLU

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Mol	Chain	Res	Type
72	SX	119	GLN
72	SX	125	GLU
73	SY	84	LEU
74	SZ	40	THR
74	SZ	44	VAL
74	SZ	119	LEU
74	SZ	133	THR
74	SZ	138	ASP
75	Sa	32	GLN
75	Sa	53	GLN
75	Sa	57	LEU
75	Sa	76	VAL
75	Sa	77	LYS
76	Sb	20	THR
76	Sb	32	ILE
76	Sb	108	ILE
76	Sb	111	ILE
77	Sc	116	ASN
77	Sc	126	MET
78	Sd	45	LEU
78	Sd	104	ASP
79	Se	34	VAL
79	Se	41	LYS
80	Sf	25	THR
80	Sf	51	LYS
80	Sf	78	ASP
81	Sg	36	VAL
81	Sg	49	GLN
81	Sg	70	LEU
82	Sh	57	ARG
82	Sh	105	THR
83	Si	7	LEU
83	Si	32	LEU
83	Si	105	PHE
83	Si	112	VAL
83	Si	125	VAL
85	Sk	58	LEU
85	Sk	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	378	GLN
1	E	452	HIS
1	E	474	HIS
1	E	509	HIS
5	B	656	GLN
5	B	683	HIS
5	B	739	ASN
9	LD	97	ASN
9	LD	205	ASN
10	LE	184	GLN
10	LE	376	HIS
11	LF	38	ASN
11	LF	310	HIS
11	LF	347	HIS
12	LG	45	ASN
12	LG	244	HIS
12	LG	267	ASN
15	LJ	153	GLN
15	LJ	225	ASN
16	LK	39	ASN
16	LK	98	HIS
17	LL	73	ASN
17	LL	166	HIS
18	LM	168	GLN
20	LP	48	GLN
20	LP	70	GLN
21	LQ	8	GLN
21	LQ	15	GLN
23	LS	75	GLN
23	LS	137	ASN
24	LT	45	GLN
24	LT	125	GLN
25	LU	86	ASN
25	LU	118	HIS
27	LW	98	HIS
29	LY	135	ASN
32	Lb	43	ASN
34	Ld	19	HIS
34	Ld	34	ASN
36	Lf	72	HIS
37	Lg	116	ASN
39	Li	78	HIS
41	Lk	107	GLN

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Mol	Chain	Res	Type
47	Lq	3	ASN
48	Lr	72	ASN
49	Ls	121	GLN
53	SB	9	HIS
54	SC	29	GLN
56	SE	89	GLN
57	SF	7	ASN
58	SG	117	ASN
58	SG	178	ASN
60	SL	50	ASN
61	SM	76	ASN
62	SN	267	GLN
64	SP	17	HIS
64	SP	50	ASN
64	SP	197	ASN
66	SR	56	ASN
66	SR	187	HIS
67	SS	33	ASN
67	SS	68	GLN
67	SS	97	GLN
68	ST	165	GLN
68	ST	168	GLN
70	SV	28	HIS
71	SW	39	ASN
71	SW	100	ASN
73	SY	13	GLN
75	Sa	54	HIS
76	Sb	11	GLN
76	Sb	80	GLN
78	Sd	17	ASN
78	Sd	19	ASN
78	Sd	105	ASN
79	Se	11	GLN
79	Se	51	ASN
82	Sh	92	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	89/90 (98%)	26 (29%)	0
3	I	178/1072 (16%)	103 (57%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	S	45/855 (5%)	22 (48%)	1 (2%)
52	S2	1764/1870 (94%)	267 (15%)	1 (0%)
6	L5	3753/4808 (78%)	524 (13%)	3 (0%)
7	L7	118/119 (99%)	8 (6%)	0
8	L8	155/158 (98%)	17 (10%)	0
All	All	6102/8972 (68%)	967 (15%)	6 (0%)

All (967) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	10	A
2	F	12	C
2	F	14	U
2	F	16	A
2	F	19	G
2	F	20	G
2	F	21	U
2	F	22	C
2	F	24	G
2	F	25	G
2	F	28	U
2	F	32	G
2	F	44	G
2	F	46	A
2	F	47	G
2	F	55	G
2	F	57	G
2	F	62	A
2	F	63	G
2	F	65	G
2	F	72	U
2	F	84	G
2	F	85	G
2	F	87	G
2	F	88	C
2	F	90	A
3	I	31	A
3	I	32	A
3	I	35	U
3	I	38	G
3	I	40	U
3	I	41	C

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Mol	Chain	Res	Type
3	I	42	U
3	I	43	U
3	I	44	G
3	I	45	C
3	I	47	U
3	I	48	G
3	I	49	U
3	I	50	A
3	I	51	A
3	I	52	A
3	I	53	U
3	I	54	A
3	I	62	G
3	I	63	A
3	I	67	G
3	I	68	U
3	I	72	U
3	I	73	A
3	I	74	A
3	I	75	A
3	I	76	U
3	I	77	U
3	I	79	C
3	I	80	A
3	I	83	U
3	I	84	A
3	I	87	G
3	I	88	C
3	I	89	U
3	I	91	U
3	I	93	U
3	I	94	U
3	I	96	G
3	I	97	U
3	I	98	A
3	I	101	U
3	I	108	G
3	I	111	A
3	I	112	U
3	I	114	U
3	I	115	A
3	I	120	U

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Mol	Chain	Res	Type
3	I	121	A
3	I	122	C
3	I	123	G
3	I	124	U
3	I	127	C
3	I	129	G
3	I	130	G
3	I	131	A
3	I	132	U
3	I	133	G
3	I	135	C
3	I	138	G
3	I	139	U
3	I	142	C
3	I	143	A
3	I	144	G
3	I	145	C
3	I	146	C
3	I	148	C
3	I	149	A
3	I	150	C
3	I	151	A
3	I	155	U
3	I	156	C
3	I	157	C
3	I	158	A
3	I	160	G
3	I	162	A
3	I	164	C
3	I	167	U
3	I	168	C
3	I	169	U
3	I	171	U
3	I	172	G
3	I	173	C
3	I	174	G
3	I	177	U
3	I	181	C
3	I	182	A
3	I	183	G
3	I	191	A
3	I	199	A

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Mol	Chain	Res	Type
3	I	200	A
3	I	202	C
3	I	203	U
3	I	204	A
3	I	205	A
3	I	206	G
3	I	207	A
3	I	210	U
3	I	212	U
3	I	220	G
3	I	224	U
3	I	225	C
3	I	226	G
4	S	1112	U
4	S	1116	G
4	S	1124	U
4	S	1125	G
4	S	1126	A
4	S	1127	A
4	S	1134	C
4	S	1135	C
4	S	1136	C
4	S	1137	G
4	S	1138	C
4	S	1139	U
4	S	1143	G
4	S	1144	G
4	S	1145	G
4	S	1146	G
4	S	1149	G
4	S	1150	U
4	S	1151	C
4	S	1152	C
4	S	1154	G
4	S	1155	A
6	L5	39	A
6	L5	42	A
6	L5	58	G
6	L5	59	A
6	L5	64	A
6	L5	65	A
6	L5	85	G

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Mol	Chain	Res	Type
6	L5	91	G
6	L5	98	A
6	L5	109	G
6	L5	119	G
6	L5	127	G
6	L5	134	G
6	L5	135	G
6	L5	136	U
6	L5	159	C
6	L5	171	U
6	L5	172	C
6	L5	184	U
6	L5	185	C
6	L5	187	U
6	L5	188	G
6	L5	200	U
6	L5	201	C
6	L5	209	U
6	L5	218	A
6	L5	219	G
6	L5	234	G
6	L5	266	C
6	L5	297	U
6	L5	309	C
6	L5	315	G
6	L5	316	U
6	L5	326	C
6	L5	334	A
6	L5	340	C
6	L5	362	A
6	L5	363	A
6	L5	387	G
6	L5	409	G
6	L5	410	A
6	L5	412	G
6	L5	413	G
6	L5	440	U
6	L5	449	C
6	L5	450	G
6	L5	452	A
6	L5	453	G
6	L5	454	U

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Mol	Chain	Res	Type
6	L5	463	A
6	L5	467	U
6	L5	468	U
6	L5	469	C
6	L5	482	U
6	L5	483	G
6	L5	485	U
6	L5	486	C
6	L5	488	G
6	L5	493	U
6	L5	494	G
6	L5	497	G
6	L5	499	C
6	L5	502	U
6	L5	503	C
6	L5	504	U
6	L5	505	C
6	L5	506	G
6	L5	512	U
6	L5	515	U
6	L5	516	U
6	L5	517	C
6	L5	634	C
6	L5	635	G
6	L5	649	C
6	L5	666	C
6	L5	690	C
6	L5	691	G
6	L5	698	C
6	L5	725	G
6	L5	732	C
6	L5	734	G
6	L5	739	G
6	L5	748	C
6	L5	749	C
6	L5	751	G
6	L5	758	C
6	L5	759	G
6	L5	760	C
6	L5	761	C
6	L5	763	C
6	L5	764	G

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Mol	Chain	Res	Type
6	L5	765	C
6	L5	790	G
6	L5	791	C
6	L5	792	G
6	L5	793	C
6	L5	794	G
6	L5	795	A
6	L5	797	C
6	L5	798	C
6	L5	799	C
6	L5	803	C
6	L5	810	U
6	L5	812	A
6	L5	814	A
6	L5	815	G
6	L5	824	C
6	L5	825	G
6	L5	831	A
6	L5	832	G
6	L5	835	G
6	L5	836	C
6	L5	843	A
6	L5	844	A
6	L5	845	U
6	L5	859	G
6	L5	860	A
6	L5	861	G
6	L5	866	A
6	L5	867	C
6	L5	868	C
6	L5	870	G
6	L5	884	U
6	L5	889	C
6	L5	892	C
6	L5	983	G
6	L5	985	G
6	L5	987	C
6	L5	994	C
6	L5	997	C
6	L5	1016	C
6	L5	1072	C
6	L5	1073	C

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Mol	Chain	Res	Type
6	L5	1074	C
6	L5	1083	C
6	L5	1084	C
6	L5	1085	G
6	L5	1087	G
6	L5	1091	G
6	L5	1102	G
6	L5	1105	C
6	L5	1106	U
6	L5	1124	A
6	L5	1127	G
6	L5	1129	G
6	L5	1133	C
6	L5	1137	C
6	L5	1202	C
6	L5	1204	C
6	L5	1206	C
6	L5	1207	G
6	L5	1208	C
6	L5	1214	A
6	L5	1215	G
6	L5	1217	G
6	L5	1218	A
6	L5	1219	G
6	L5	1228	G
6	L5	1231	G
6	L5	1239	U
6	L5	1240	G
6	L5	1246	U
6	L5	1247	A
6	L5	1270	A2M
6	L5	1281	A
6	L5	1298	A
6	L5	1299	G
6	L5	1303	G
6	L5	1309	C
6	L5	1310	G
6	L5	1321	G
6	L5	1323	C
6	L5	1331	A
6	L5	1341	A
6	L5	1350	G

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Mol	Chain	Res	Type
6	L5	1351	G
6	L5	1352	C
6	L5	1362	C
6	L5	1363	C
6	L5	1365	U
6	L5	1368	U
6	L5	1375	A
6	L5	1376	G
6	L5	1391	C
6	L5	1393	C
6	L5	1395	U
6	L5	1398	A
6	L5	1452	A
6	L5	1453	G
6	L5	1457	G
6	L5	1469	U
6	L5	1471	G
6	L5	1477	OMG
6	L5	1489	A2M
6	L5	1490	C
6	L5	1502	A
6	L5	1521	C
6	L5	1533	U
6	L5	1546	U
6	L5	1551	U
6	L5	1568	A
6	L5	1579	G
6	L5	1580	OMG
6	L5	1586	A
6	L5	1588	G
6	L5	1589	A
6	L5	1593	A
6	L5	1595	C
6	L5	1609	G
6	L5	1616	C
6	L5	1625	G
6	L5	1631	C
6	L5	1632	PSU
6	L5	1646	G
6	L5	1649	C
6	L5	1653	C
6	L5	1657	C

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Mol	Chain	Res	Type
6	L5	1658	C
6	L5	1673	G
6	L5	1694	C
6	L5	1704	A
6	L5	1705	A
6	L5	1709	A
6	L5	1712	U
6	L5	1726	A
6	L5	1743	A
6	L5	1745	G
6	L5	1754	G
6	L5	1774	G
6	L5	1775	G
6	L5	1776	A
6	L5	1781	G
6	L5	1794	G
6	L5	1808	G
6	L5	1836	A
6	L5	1857	U
6	L5	1859	C
6	L5	1860	C
6	L5	1861	G
6	L5	1870	C
6	L5	1871	A
6	L5	1879	G
6	L5	1887	G
6	L5	1890	G
6	L5	1893	U
6	L5	1898	U
6	L5	1899	A
6	L5	1900	G
6	L5	1913	U
6	L5	1914	G
6	L5	1915	G
6	L5	1922	A
6	L5	1923	A
6	L5	1925	U
6	L5	1926	C
6	L5	1936	U
6	L5	1942	G
6	L5	1943	U
6	L5	1960	G

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Mol	Chain	Res	Type
6	L5	1963	G
6	L5	1965	A
6	L5	1985	G
6	L5	1987	U
6	L5	1994	G
6	L5	1995	G
6	L5	2008	A
6	L5	2023	U
6	L5	2032	G
6	L5	2034	A
6	L5	2037	G
6	L5	2041	G
6	L5	2044	A
6	L5	2045	G
6	L5	2046	A
6	L5	2049	G
6	L5	2132	C
6	L5	2143	A
6	L5	2144	G
6	L5	2156	A
6	L5	2159	G
6	L5	2191	G
6	L5	2194	OMC
6	L5	2203	A
6	L5	2238	A
6	L5	2264	G
6	L5	2265	OMC
6	L5	2268	U
6	L5	2269	U
6	L5	2290	U
6	L5	2329	G
6	L5	2332	C
6	L5	2349	G
6	L5	2356	A
6	L5	2372	A
6	L5	2380	A
6	L5	2387	G
6	L5	2388	U
6	L5	2390	G
6	L5	2397	U
6	L5	2407	G
6	L5	2409	G

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Mol	Chain	Res	Type
6	L5	2430	A
6	L5	2432	C
6	L5	2444	A
6	L5	2445	G
6	L5	2470	C
6	L5	2496	C
6	L5	2503	A
6	L5	2512	C
6	L5	2530	U
6	L5	2537	G
6	L5	2538	A
6	L5	2539	A
6	L5	2546	G
6	L5	2550	U
6	L5	2551	U
6	L5	2552	C
6	L5	2554	G
6	L5	2569	G
6	L5	2578	G
6	L5	2586	A
6	L5	2606	U
6	L5	2612	U
6	L5	2631	U
6	L5	2633	U
6	L5	2641	A
6	L5	2657	C
6	L5	2658	A2M
6	L5	2669	U
6	L5	2670	G
6	L5	2672	U
6	L5	2698	G
6	L5	2745	G
6	L5	3350	C
6	L5	3358	G
6	L5	3362	A
6	L5	3367	A
6	L5	3380	A
6	L5	3385	A
6	L5	3394	A
6	L5	3405	C
6	L5	3412	U
6	L5	3428	C

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Mol	Chain	Res	Type
6	L5	3443	A
6	L5	3444	A
6	L5	3485	G
6	L5	3492	A2M
6	L5	3493	C
6	L5	3494	PSU
6	L5	3498	A
6	L5	3508	G
6	L5	3509	G
6	L5	3515	A
6	L5	3516	A
6	L5	3543	G
6	L5	3544	C
6	L5	3546	U
6	L5	3549	A
6	L5	3550	U
6	L5	3551	G
6	L5	3570	U
6	L5	3572	U
6	L5	3609	A
6	L5	3610	C
6	L5	3611	G
6	L5	3629	G
6	L5	3633	A
6	L5	3638	A
6	L5	3639	G
6	L5	3640	A
6	L5	3647	U
6	L5	3670	G
6	L5	3674	A
6	L5	3679	A
6	L5	3688	G
6	L5	3689	U
6	L5	3694	A
6	L5	3697	A
6	L5	3698	A
6	L5	3702	G
6	L5	3704	A
6	L5	3708	C
6	L5	3765	C
6	L5	3766	C
6	L5	3767	G

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Mol	Chain	Res	Type
6	L5	3777	U
6	L5	3778	A
6	L5	3783	U
6	L5	3797	U
6	L5	3798	U
6	L5	3804	G
6	L5	3824	C
6	L5	3825	G
6	L5	3832	G
6	L5	3833	A
6	L5	3834	G
6	L5	3841	U
6	L5	3842	C
6	L5	3846	U
6	L5	3847	C
6	L5	3850	G
6	L5	3855	A
6	L5	3862	G
6	L5	3873	G
6	L5	3875	C
6	L5	3891	C
6	L5	3892	G
6	L5	3904	C
6	L5	3908	C
6	L5	3909	U
6	L5	3916	A
6	L5	3929	G
6	L5	3930	G
6	L5	3937	G
6	L5	3949	A
6	L5	3971	G
6	L5	3975	U
6	L5	3979	A
6	L5	3997	A
6	L5	4000	G
6	L5	4012	G
6	L5	4014	A
6	L5	4017	A
6	L5	4019	A
6	L5	4027	A
6	L5	4035	U
6	L5	4037	G

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Mol	Chain	Res	Type
6	L5	4050	A
6	L5	4051	G
6	L5	4060	C
6	L5	4076	G
6	L5	4078	C
6	L5	4085	A
6	L5	4096	C
6	L5	4100	U
6	L5	4119	G
6	L5	4123	G
6	L5	4124	A
6	L5	4126	A
6	L5	4133	C
6	L5	4139	G
6	L5	4140	A
6	L5	4161	A
6	L5	4168	A
6	L5	4170	A
6	L5	4194	G
6	L5	4210	A
6	L5	4212	C
6	L5	4221	G
6	L5	4258	U
6	L5	4259	A
6	L5	4261	G
6	L5	4268	G
6	L5	4270	G
6	L5	4294	A
6	L5	4306	C
6	L5	4313	G
6	L5	4316	G
6	L5	4321	G
6	L5	4336	A2M
6	L5	4382	PSU
6	L5	4383	OMG
6	L5	4402	A
6	L5	4416	C
6	L5	4418	A
6	L5	4437	A
6	L5	4446	A
6	L5	4454	A
6	L5	4455	U

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Mol	Chain	Res	Type
6	L5	4465	G
6	L5	4475	A
6	L5	4476	C
6	L5	4477	G
6	L5	4478	G
6	L5	4479	C
6	L5	4486	G
6	L5	4487	A
6	L5	4488	A
6	L5	4489	G
6	L5	4490	G
6	L5	4501	G
6	L5	4504	C
6	L5	4506	C
6	L5	4508	G
6	L5	4512	G
6	L5	4518	C
6	L5	4609	G
6	L5	4610	C
6	L5	4614	G
6	L5	4621	U
6	L5	4622	C
6	L5	4637	G
6	L5	4638	G
6	L5	4639	C
6	L5	4640	G
6	L5	4641	C
6	L5	4644	C
6	L5	4645	C
6	L5	4646	G
6	L5	4649	A
6	L5	4651	G
6	L5	4658	G
6	L5	4665	C
6	L5	4705	A
6	L5	4715	U
6	L5	4724	U
6	L5	4728	U
6	L5	4729	C
6	L5	4730	U
6	L5	4753	A
6	L5	4756	G

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Mol	Chain	Res	Type
6	L5	4761	U
6	L5	4762	C
6	L5	4763	C
6	L5	4764	C
6	L5	4765	U
6	L5	4766	C
6	L5	4780	G
6	L5	4789	C
6	L5	4793	C
6	L5	4797	A
6	L5	4800	A
6	L5	4801	G
6	L5	4808	U
7	L7	7	G
7	L7	11	A
7	L7	50	A
7	L7	53	U
7	L7	54	A
7	L7	64	G
7	L7	110	G
7	L7	120	U
8	L8	34	U
8	L8	35	C
8	L8	59	A
8	L8	62	A
8	L8	63	U
8	L8	81	C
8	L8	84	A
8	L8	87	G
8	L8	94	G
8	L8	103	A
8	L8	105	C
8	L8	110	U
8	L8	111	U
8	L8	114	G
8	L8	123	U
8	L8	127	U
8	L8	153	C
52	S2	3	C
52	S2	33	G
52	S2	41	G
52	S2	46	A

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Mol	Chain	Res	Type
52	S2	56	G
52	S2	58	C
52	S2	67	C
52	S2	68	A
52	S2	73	C
52	S2	74	G
52	S2	77	A
52	S2	79	A
52	S2	103	A
52	S2	113	G
52	S2	115	U
52	S2	120	U
52	S2	124	U
52	S2	126	G
52	S2	130	G
52	S2	142	C
52	S2	143	U
52	S2	147	A
52	S2	155	G
52	S2	162	C
52	S2	163	U
52	S2	168	C
52	S2	175	A
52	S2	178	C
52	S2	180	G
52	S2	184	G
52	S2	188	C
52	S2	192	C
52	S2	226	A
52	S2	227	U
52	S2	228	C
52	S2	229	A
52	S2	234	C
52	S2	236	A
52	S2	241	G
52	S2	282	C
52	S2	306	U
52	S2	307	C
52	S2	310	G
52	S2	313	G
52	S2	320	C
52	S2	324	C

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Mol	Chain	Res	Type
52	S2	325	U
52	S2	326	C
52	S2	327	C
52	S2	328	G
52	S2	336	G
52	S2	348	G
52	S2	363	C
52	S2	365	A
52	S2	369	U
52	S2	370	C
52	S2	386	G
52	S2	387	C
52	S2	401	C
52	S2	410	C
52	S2	422	G
52	S2	439	G
52	S2	449	A
52	S2	451	C
52	S2	453	G
52	S2	465	A
52	S2	466	A
52	S2	471	G
52	S2	473	C
52	S2	474	A
52	S2	475	G
52	S2	483	G
52	S2	488	U
52	S2	493	C
52	S2	502	C
52	S2	509	A
52	S2	510	OMG
52	S2	518	OMC
52	S2	536	G
52	S2	549	C
52	S2	560	G
52	S2	569	C
52	S2	584	A
52	S2	588	A
52	S2	590	G
52	S2	592	U
52	S2	607	G
52	S2	609	C

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Mol	Chain	Res	Type
52	S2	615	C
52	S2	628	OMU
52	S2	629	A
52	S2	632	U
52	S2	633	C
52	S2	644	A
52	S2	645	OMG
52	S2	656	A
52	S2	661	C
52	S2	669	A2M
52	S2	670	A
52	S2	672	A
52	S2	673	A
52	S2	674	G
52	S2	684	OMG
52	S2	690	U
52	S2	697	G
52	S2	698	G
52	S2	728	G
52	S2	730	C
52	S2	735	C
52	S2	737	C
52	S2	747	C
52	S2	748	U
52	S2	750	U
52	S2	754	C
52	S2	755	G
52	S2	756	C
52	S2	757	C
52	S2	796	A
52	S2	798	C
52	S2	799	G
52	S2	800	U
52	S2	802	PSU
52	S2	810	A
52	S2	812	A
52	S2	822	G
52	S2	823	PSU
52	S2	828	A
52	S2	831	A
52	S2	832	G
52	S2	837	G

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Mol	Chain	Res	Type
52	S2	838	A
52	S2	839	G
52	S2	840	C
52	S2	841	C
52	S2	842	G
52	S2	848	A
52	S2	871	A
52	S2	873	A
52	S2	879	G
52	S2	892	G
52	S2	893	U
52	S2	896	G
52	S2	901	C
52	S2	906	C
52	S2	910	G
52	S2	914	A
52	S2	915	U
52	S2	921	A
52	S2	923	A
52	S2	931	C
52	S2	934	G
52	S2	944	U
52	S2	956	A
52	S2	964	A
52	S2	972	G
52	S2	991	A
52	S2	993	A
52	S2	1000	G
52	S2	1018	U
52	S2	1024	A
52	S2	1061	A
52	S2	1062	U
52	S2	1063	A
52	S2	1084	A
52	S2	1086	C
52	S2	1116	U
52	S2	1117	C
52	S2	1118	C
52	S2	1119	C
52	S2	1122	G
52	S2	1124	C
52	S2	1134	A

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Mol	Chain	Res	Type
52	S2	1145	A
52	S2	1150	A
52	S2	1151	A
52	S2	1154	C
52	S2	1155	U
52	S2	1196	A
52	S2	1208	G
52	S2	1216	C
52	S2	1222	G
52	S2	1225	G
52	S2	1243	U
52	S2	1249	U
52	S2	1252	A
52	S2	1254	A
52	S2	1257	G
52	S2	1258	G
52	S2	1260	A
52	S2	1266	A
52	S2	1275	G
52	S2	1276	G
52	S2	1283	A
52	S2	1286	G
52	S2	1287	G
52	S2	1292	A
52	S2	1294	A
52	S2	1296	A
52	S2	1303	G
52	S2	1304	C
52	S2	1305	U
52	S2	1316	U
52	S2	1343	U
52	S2	1359	U
52	S2	1372	U
52	S2	1373	U
52	S2	1379	A
52	S2	1398	U
52	S2	1406	A
52	S2	1407	G
52	S2	1419	C
52	S2	1420	C
52	S2	1422	A
52	S2	1423	G

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Mol	Chain	Res	Type
52	S2	1424	C
52	S2	1436	C
52	S2	1438	C
52	S2	1448	OMG
52	S2	1455	A
52	S2	1463	U
52	S2	1464	U
52	S2	1481	A
52	S2	1488	A
52	S2	1490	A
52	S2	1491	OMG
52	S2	1498	G
52	S2	1510	U
52	S2	1522	C
52	S2	1523	A
52	S2	1534	A
52	S2	1553	G
52	S2	1571	G
52	S2	1579	U
52	S2	1581	A
52	S2	1586	U
52	S2	1587	U
52	S2	1589	A
52	S2	1602	A
52	S2	1622	U
52	S2	1624	A
52	S2	1655	G
52	S2	1662	A
52	S2	1666	G
52	S2	1699	C
52	S2	1700	A
52	S2	1722	U
52	S2	1723	G
52	S2	1765	G
52	S2	1780	G
52	S2	1782	A
52	S2	1783	G
52	S2	1784	C
52	S2	1785	G
52	S2	1787	U
52	S2	1825	A
52	S2	1827	G

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Mol	Chain	Res	Type
52	S2	1830	G
52	S2	1836	A
52	S2	1837	G
52	S2	1839	U
52	S2	1850	G
52	S2	1852	MA6
52	S2	1862	G
52	S2	1863	G
52	S2	1864	A
52	S2	1865	U
52	S2	1866	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	I	66	G
4	S	1111	A
6	L5	1588	G
6	L5	1892	U
6	L5	4445	U
52	S2	1265	C

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

218 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
6	A2M	L5	3557	6	22,25,26	1.72	7 (31%)	31,36,39	2.43	13 (41%)
6	OMU	L5	2680	6	19,22,23	0.99	2 (10%)	26,31,34	1.82	6 (23%)
52	OMC	S2	174	52	19,22,23	1.20	3 (15%)	26,31,34	0.88	0
52	PSU	S2	682	52	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
52	OMU	S2	121	52	19,22,23	0.99	2 (10%)	26,31,34	1.75	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	L5	2351	6	18,21,22	1.34	3 (16%)	22,30,33	1.86	4 (18%)
6	OMC	L5	2194	6	19,22,23	1.11	2 (10%)	26,31,34	0.95	1 (3%)
52	OMU	S2	355	71,52	19,22,23	0.98	2 (10%)	26,31,34	1.83	5 (19%)
6	A2M	L5	398	6	22,25,26	1.71	7 (31%)	31,36,39	2.41	14 (45%)
6	OMC	L5	3433	6,90	19,22,23	1.16	2 (10%)	26,31,34	0.92	1 (3%)
52	OMG	S2	510	52,89	23,26,27	1.17	2 (8%)	33,38,41	1.89	10 (30%)
6	OMG	L5	1260	6	23,26,27	1.22	4 (17%)	33,38,41	1.92	10 (30%)
6	PSU	L5	1720	6	18,21,22	1.36	3 (16%)	22,30,33	1.82	5 (22%)
52	PSU	S2	823	52	18,21,22	1.40	3 (16%)	22,30,33	1.80	4 (18%)
6	PSU	L5	4246	6	18,21,22	1.39	3 (16%)	22,30,33	1.88	5 (22%)
6	PSU	L5	4740	6	18,21,22	1.38	3 (16%)	22,30,33	1.78	3 (13%)
6	PSU	L5	3490	6	18,21,22	1.35	3 (16%)	22,30,33	1.81	4 (18%)
6	PSU	L5	1638	6,90	18,21,22	1.34	3 (16%)	22,30,33	1.87	5 (22%)
52	PSU	S2	610	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	4 (18%)
6	OMC	L5	2208	6,89	19,22,23	1.13	2 (10%)	26,31,34	0.91	1 (3%)
6	PSU	L5	3447	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	4 (18%)
6	OMC	L5	3601	6	19,22,23	1.16	2 (10%)	26,31,34	0.89	0
6	PSU	L5	4435	6	18,21,22	1.35	3 (16%)	22,30,33	1.84	4 (18%)
52	A2M	S2	669	52,89	22,25,26	1.74	8 (36%)	31,36,39	2.61	15 (48%)
6	PSU	L5	1718	6	18,21,22	1.35	3 (16%)	22,30,33	1.82	4 (18%)
47	MLZ	Lq	53	47	8,9,10	0.46	0	4,9,11	0.08	0
6	PSU	L5	3652	6,89	18,21,22	1.31	3 (16%)	22,30,33	1.86	4 (18%)
52	PSU	S2	1005	52	18,21,22	1.63	5 (27%)	22,30,33	2.85	6 (27%)
52	PSU	S2	1178	52	18,21,22	1.39	3 (16%)	22,30,33	1.80	4 (18%)
6	PSU	L5	3371	6	18,21,22	1.33	3 (16%)	22,30,33	1.82	5 (22%)
52	OMG	S2	602	52	23,26,27	1.17	3 (13%)	33,38,41	1.86	10 (30%)
6	PSU	L5	3585	6,89	18,21,22	1.32	3 (16%)	22,30,33	1.83	4 (18%)
6	OMG	L5	4138	6	23,26,27	1.19	3 (13%)	33,38,41	1.89	10 (30%)
6	OMG	L5	2719	6	23,26,27	1.17	2 (8%)	33,38,41	2.04	12 (36%)
6	OMG	L5	4116	6	23,26,27	1.19	3 (13%)	33,38,41	1.87	10 (30%)
6	PSU	L5	4217	6	18,21,22	1.34	3 (16%)	22,30,33	1.81	5 (22%)
52	OMG	S2	1491	52,89	23,26,27	1.18	3 (13%)	33,38,41	1.88	9 (27%)
6	PSU	L5	3554	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	5 (22%)
6	A2M	L5	3562	6	22,25,26	1.71	7 (31%)	31,36,39	2.44	14 (45%)
6	A2M	L5	400	6	22,25,26	1.75	7 (31%)	31,36,39	2.51	14 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	S2	1082	52	18,21,22	1.33	3 (16%)	22,30,33	1.82	4 (18%)
52	OMU	S2	1443	52,89	19,22,23	0.99	2 (10%)	26,31,34	1.74	4 (15%)
6	OMU	L5	4244	6	19,22,23	1.00	2 (10%)	26,31,34	1.83	5 (19%)
6	OMG	L5	4364	6	23,26,27	1.18	3 (13%)	33,38,41	1.88	10 (30%)
52	PSU	S2	407	52	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
6	OMG	L5	4383	6,90	23,26,27	1.20	3 (13%)	33,38,41	1.87	10 (30%)
52	OMG	S2	645	52	23,26,27	1.17	3 (13%)	33,38,41	1.92	10 (30%)
52	PSU	S2	1057	52	18,21,22	1.37	3 (16%)	22,30,33	1.84	5 (22%)
6	OMU	L5	2258	6	19,22,23	0.99	2 (10%)	26,31,34	1.77	5 (19%)
6	A2M	L5	1270	6	22,25,26	1.74	7 (31%)	31,36,39	2.56	16 (51%)
52	PSU	S2	119	52	18,21,22	1.41	3 (16%)	22,30,33	1.78	4 (18%)
52	PSU	S2	1239	52	18,21,22	1.37	3 (16%)	22,30,33	1.83	5 (22%)
11	AYA	LF	2	11	6,7,8	0.75	0	5,8,10	0.25	0
6	PSU	L5	4169	6	18,21,22	1.37	3 (16%)	22,30,33	1.85	5 (22%)
52	A2M	S2	591	52	22,25,26	1.72	6 (27%)	31,36,39	2.58	15 (48%)
35	MLZ	Le	5	35	8,9,10	0.47	0	4,9,11	0.13	0
52	PSU	S2	864	52	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
52	OMU	S2	172	52	19,22,23	0.99	2 (10%)	26,31,34	1.85	7 (26%)
52	OMC	S2	518	52	19,22,23	1.15	2 (10%)	26,31,34	0.91	1 (3%)
52	MA6	S2	1852	52	23,26,27	1.45	4 (17%)	34,38,41	2.33	13 (38%)
46	M3L	Lp	98	46	10,11,12	0.51	0	9,14,16	0.47	0
6	A2M	L5	3517	6	22,25,26	1.71	7 (31%)	31,36,39	2.62	15 (48%)
6	OMU	L5	4052	6	19,22,23	1.00	2 (10%)	26,31,34	1.74	4 (15%)
52	OMU	S2	429	52	19,22,23	1.02	2 (10%)	26,31,34	1.79	5 (19%)
6	OMC	L5	4202	6	19,22,23	1.14	2 (10%)	26,31,34	0.93	1 (3%)
8	PSU	L8	55	8	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
52	MA6	S2	1851	52	23,26,27	1.47	4 (17%)	34,38,41	2.33	13 (38%)
6	PSU	L5	3466	6	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
6	PSU	L5	1491	6	18,21,22	1.34	3 (16%)	22,30,33	1.85	4 (18%)
52	PSU	S2	816	52	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
6	PSU	L5	3583	6	18,21,22	1.33	3 (16%)	22,30,33	1.90	5 (22%)
6	PSU	L5	4039	6	18,21,22	1.35	3 (16%)	22,30,33	1.87	5 (22%)
6	PSU	L5	4045	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	4 (18%)
6	6MZ	L5	3966	6	22,25,26	1.39	4 (18%)	30,36,39	2.16	10 (33%)
6	OMC	L5	3619	6,22	19,22,23	1.14	2 (10%)	26,31,34	0.93	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	L5	3500	6	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
52	OMU	S2	628	52	19,22,23	1.01	2 (10%)	26,31,34	1.82	6 (23%)
6	OMU	L5	4366	6	19,22,23	1.00	2 (10%)	26,31,34	1.81	6 (23%)
52	4AC	S2	1338	52	21,24,25	1.12	2 (9%)	29,34,37	1.21	3 (10%)
52	OMU	S2	1327	52,89	19,22,23	1.00	2 (10%)	26,31,34	1.79	5 (19%)
52	PSU	S2	218	52	18,21,22	1.38	3 (16%)	22,30,33	1.81	4 (18%)
6	OMG	L5	3524	6	23,26,27	1.19	3 (13%)	33,38,41	1.89	10 (30%)
6	PSU	L5	4099	6	18,21,22	1.35	3 (16%)	22,30,33	1.90	5 (22%)
6	OMG	L5	3942	6	23,26,27	1.18	3 (13%)	33,38,41	1.88	9 (27%)
52	OMG	S2	1448	52	23,26,27	1.18	3 (13%)	33,38,41	1.85	9 (27%)
6	PSU	L5	3502	6	18,21,22	1.39	3 (16%)	22,30,33	1.83	4 (18%)
52	A2M	S2	469	52	22,25,26	1.71	7 (31%)	31,36,39	2.47	15 (48%)
6	A2M	L5	2244	6	22,25,26	1.74	7 (31%)	31,36,39	2.51	15 (48%)
52	PSU	S2	36	52	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
6	PSU	L5	4382	6	18,21,22	1.42	4 (22%)	22,30,33	2.01	3 (13%)
6	A2M	L5	3450	6	22,25,26	1.72	7 (31%)	31,36,39	2.42	14 (45%)
6	OMC	L5	2667	6	19,22,23	1.14	2 (10%)	26,31,34	0.87	0
6	OMG	L5	3676	6	23,26,27	1.15	2 (8%)	33,38,41	1.87	9 (27%)
6	PSU	L5	4322	6	18,21,22	1.39	3 (16%)	22,30,33	1.79	5 (22%)
6	PSU	L5	4267	6,89	18,21,22	1.33	3 (16%)	22,30,33	1.93	4 (18%)
52	OMU	S2	1805	52	19,22,23	0.98	2 (10%)	26,31,34	1.80	5 (19%)
6	PSU	L5	3427	6	18,21,22	1.36	3 (16%)	22,30,33	1.81	5 (22%)
52	PSU	S2	34	52	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
52	6MZ	S2	1833	52,89	22,25,26	1.41	4 (18%)	30,36,39	2.17	9 (30%)
6	PSU	L5	3496	6	18,21,22	1.37	3 (16%)	22,30,33	1.84	5 (22%)
6	OMG	L5	4369	6	23,26,27	1.19	2 (8%)	33,38,41	1.87	9 (27%)
6	A2M	L5	3599	6	22,25,26	1.75	7 (31%)	31,36,39	2.52	16 (51%)
6	OMU	L5	3973	6	19,22,23	1.00	2 (10%)	26,31,34	1.83	6 (23%)
52	PSU	S2	802	52	18,21,22	1.40	3 (16%)	22,30,33	1.77	4 (18%)
6	PSU	L5	4058	6	18,21,22	1.37	3 (16%)	22,30,33	1.80	5 (22%)
52	A2M	S2	159	52	22,25,26	1.70	6 (27%)	31,36,39	2.40	14 (45%)
52	PSU	S2	1245	52	18,21,22	1.36	3 (16%)	22,30,33	1.85	4 (18%)
81	AME	Sg	1	81	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
52	PSU	S2	687	52	18,21,22	1.41	3 (16%)	22,30,33	1.84	5 (22%)
6	OMC	L5	2265	6,89	19,22,23	1.12	2 (10%)	26,31,34	0.90	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	L5	1537	6	18,21,22	1.38	3 (16%)	22,30,33	1.81	4 (18%)
6	OMC	L5	2647	6	19,22,23	1.14	2 (10%)	26,31,34	0.88	1 (3%)
6	PSU	L5	3462	6	18,21,22	1.38	3 (16%)	22,30,33	1.80	5 (22%)
6	PSU	L5	3369	6,90,89	18,21,22	1.29	3 (16%)	22,30,33	1.87	4 (18%)
52	A2M	S2	577	52	22,25,26	1.71	7 (31%)	31,36,39	2.46	16 (51%)
83	HY3	Si	62	83	6,8,9	1.32	1 (16%)	5,10,12	1.43	1 (20%)
6	OMG	L5	3631	6	23,26,27	1.21	4 (17%)	33,38,41	1.90	10 (30%)
6	PSU	L5	1632	6	18,21,22	1.41	3 (16%)	22,30,33	1.74	4 (18%)
52	PSU	S2	1047	52	18,21,22	1.39	3 (16%)	22,30,33	1.79	4 (18%)
6	PSU	L5	1731	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	3576	6	18,21,22	1.36	3 (16%)	22,30,33	1.77	4 (18%)
6	A2M	L5	4336	6	22,25,26	1.74	7 (31%)	31,36,39	2.51	15 (48%)
52	A2M	S2	1384	52	22,25,26	1.74	7 (31%)	31,36,39	2.46	15 (48%)
6	PSU	L5	3494	6	18,21,22	1.39	3 (16%)	22,30,33	1.78	5 (22%)
10	HIC	LE	245	10	10,11,12	0.55	0	8,14,16	0.48	0
52	PSU	S2	1368	52	18,21,22	1.41	3 (16%)	22,30,33	1.85	5 (22%)
52	PSU	S2	1046	52	18,21,22	1.35	3 (16%)	22,30,33	1.88	4 (18%)
6	PSU	L5	4374	6	18,21,22	1.36	3 (16%)	22,30,33	1.82	5 (22%)
52	PSU	S2	1644	52,89	18,21,22	1.36	3 (16%)	22,30,33	1.83	4 (18%)
52	PSU	S2	93	52	18,21,22	1.42	3 (16%)	22,30,33	1.76	3 (13%)
52	PSU	S2	109	52	18,21,22	1.42	3 (16%)	22,30,33	1.80	5 (22%)
52	A2M	S2	485	52	22,25,26	1.73	7 (31%)	31,36,39	2.54	15 (48%)
6	A2M	L5	3492	6,89	22,25,26	1.74	7 (31%)	31,36,39	2.47	14 (45%)
52	PSU	S2	1693	52	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
6	OMU	L5	3657	6	19,22,23	1.01	2 (10%)	26,31,34	1.82	5 (19%)
6	5MC	L5	4193	6	18,22,23	1.24	3 (16%)	26,32,35	1.53	3 (11%)
52	OMC	S2	1392	52	19,22,23	1.16	2 (10%)	26,31,34	0.94	1 (3%)
52	PSU	S2	652	52	18,21,22	1.39	3 (16%)	22,30,33	1.84	4 (18%)
52	PSU	S2	1348	52	18,21,22	1.38	3 (16%)	22,30,33	1.81	3 (13%)
52	OMU	S2	116	52	19,22,23	1.01	2 (10%)	26,31,34	1.80	6 (23%)
52	PSU	S2	1233	52	18,21,22	1.37	3 (16%)	22,30,33	1.81	5 (22%)
52	PSU	S2	573	52	18,21,22	1.43	3 (16%)	22,30,33	1.84	4 (18%)
6	PSU	L5	4166	6	18,21,22	1.38	3 (16%)	22,30,33	1.79	4 (18%)
6	PSU	L5	4177	6	18,21,22	1.33	3 (16%)	22,30,33	1.86	5 (22%)
52	OMC	S2	1704	52,89	19,22,23	1.13	2 (10%)	26,31,34	0.89	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMG	L5	3476	6	23,26,27	1.19	3 (13%)	33,38,41	1.87	9 (27%)
6	OMG	L5	4240	6	23,26,27	1.20	3 (13%)	33,38,41	1.87	10 (30%)
52	A2M	S2	27	52	22,25,26	1.74	7 (31%)	31,36,39	2.46	14 (45%)
6	UR3	L5	4276	6	19,22,23	1.30	3 (15%)	26,32,35	1.20	2 (7%)
6	OMC	L5	3540	6	19,22,23	1.10	2 (10%)	26,31,34	0.89	2 (7%)
52	OMG	S2	684	52	23,26,27	1.18	3 (13%)	33,38,41	1.90	10 (30%)
52	OMG	S2	868	52	23,26,27	1.16	2 (8%)	33,38,41	1.87	9 (27%)
6	OMG	L5	1477	6	23,26,27	1.21	3 (13%)	33,38,41	1.95	10 (30%)
6	PSU	L5	4203	6	18,21,22	1.33	3 (16%)	22,30,33	1.81	4 (18%)
52	PSU	S2	105	52	18,21,22	1.39	3 (16%)	22,30,33	1.81	4 (18%)
6	OMC	L5	1820	6,89	19,22,23	1.15	2 (10%)	26,31,34	0.89	0
6	A2M	L5	3456	6	22,25,26	1.71	7 (31%)	31,36,39	2.41	13 (41%)
52	A2M	S2	1679	52	22,25,26	1.71	7 (31%)	31,36,39	2.43	13 (41%)
6	PSU	L5	1799	6	18,21,22	1.38	3 (16%)	22,30,33	1.86	5 (22%)
6	PSU	L5	1801	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	3 (13%)
6	A2M	L5	2658	6,89	22,25,26	1.74	7 (31%)	31,36,39	2.49	15 (48%)
6	PSU	L5	4149	6	18,21,22	1.33	3 (16%)	22,30,33	1.93	5 (22%)
52	PSU	S2	1446	52	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
6	PSU	L5	1721	6	18,21,22	1.35	3 (16%)	22,30,33	1.83	5 (22%)
6	PSU	L5	4188	6	18,21,22	1.33	3 (16%)	22,30,33	1.93	4 (18%)
6	PSU	L5	4107	6	18,21,22	1.33	3 (16%)	22,30,33	1.79	3 (13%)
6	OMC	L5	2704	6	19,22,23	1.14	2 (10%)	26,31,34	0.86	0
6	PSU	L5	4711	6	18,21,22	1.35	3 (16%)	22,30,33	1.82	5 (22%)
6	1MA	L5	1266	6,89	21,25,26	1.82	5 (23%)	31,37,40	1.92	5 (16%)
6	A2M	L5	1810	6,89	22,25,26	1.76	7 (31%)	31,36,39	2.52	15 (48%)
6	OMG	L5	3359	6	23,26,27	1.19	3 (13%)	33,38,41	1.89	10 (30%)
6	PSU	L5	4749	6	18,21,22	1.39	3 (16%)	22,30,33	1.84	4 (18%)
6	A2M	L5	2630	6	22,25,26	1.75	7 (31%)	31,36,39	2.63	17 (54%)
52	A2M	S2	513	52	22,25,26	1.72	7 (31%)	31,36,39	2.43	13 (41%)
52	PSU	S2	650	52	18,21,22	1.38	3 (16%)	22,30,33	1.83	4 (18%)
52	PSU	S2	1626	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	5 (22%)
6	PSU	L5	4419	6	18,21,22	1.34	3 (16%)	22,30,33	1.84	5 (22%)
52	A2M	S2	1032	52	22,25,26	1.71	7 (31%)	31,36,39	2.46	14 (45%)
8	PSU	L8	69	8	18,21,22	1.36	3 (16%)	22,30,33	1.90	5 (22%)
6	A2M	L5	4317	6	22,25,26	1.75	7 (31%)	31,36,39	2.46	14 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	OMC	S2	463	52	19,22,23	1.16	2 (10%)	26,31,34	0.90	0
6	OMC	L5	3573	6	19,22,23	1.13	2 (10%)	26,31,34	0.89	2 (7%)
52	OMU	S2	1289	52,55	19,22,23	0.97	1 (5%)	26,31,34	1.76	5 (19%)
52	A2M	S2	99	52,89	22,25,26	1.71	6 (27%)	31,36,39	2.40	13 (41%)
6	5MC	L5	3514	6,89	18,22,23	1.27	3 (16%)	26,32,35	1.26	4 (15%)
6	OMG	L5	4245	6	23,26,27	1.20	4 (17%)	33,38,41	1.87	10 (30%)
52	PSU	S2	815	52	18,21,22	1.38	3 (16%)	22,30,33	1.83	4 (18%)
6	PSU	L5	4325	6	18,21,22	1.35	3 (16%)	22,30,33	1.85	5 (22%)
52	7MG	S2	1640	52	22,26,27	1.22	2 (9%)	29,39,42	2.14	9 (31%)
6	OMG	L5	2267	6	23,26,27	1.19	2 (8%)	33,38,41	1.85	9 (27%)
52	PSU	S2	967	52	18,21,22	1.40	3 (16%)	22,30,33	1.79	4 (18%)
52	A2M	S2	166	52	22,25,26	1.71	6 (27%)	31,36,39	2.46	15 (48%)
6	PSU	L5	1683	6,90	18,21,22	1.36	3 (16%)	22,30,33	1.82	4 (18%)
6	OMG	L5	3974	6	23,26,27	1.19	3 (13%)	33,38,41	1.86	9 (27%)
6	PSU	L5	2475	6	18,21,22	1.37	3 (16%)	22,30,33	1.82	5 (22%)
6	OMC	L5	4282	6	19,22,23	1.15	2 (10%)	26,31,34	0.91	1 (3%)
6	A2M	L5	4269	6,89	22,25,26	1.74	7 (31%)	31,36,39	2.45	14 (45%)
52	4AC	S2	1843	52,86	21,24,25	1.15	2 (9%)	29,34,37	1.10	2 (6%)
8	OMG	L8	75	8	23,26,27	1.19	3 (13%)	33,38,41	1.85	9 (27%)
52	PSU	S2	867	52	18,21,22	1.44	3 (16%)	22,30,33	1.81	4 (18%)
6	A2M	L5	1479	6	22,25,26	1.72	7 (31%)	31,36,39	2.54	14 (45%)
6	OMG	L5	2207	6	23,26,27	1.18	3 (13%)	33,38,41	2.01	10 (30%)
6	PSU	L5	4278	6	18,21,22	1.38	3 (16%)	22,30,33	1.79	4 (18%)
52	PSU	S2	210	52	18,21,22	1.45	3 (16%)	22,30,33	1.84	4 (18%)
49	SAC	Ls	2	49	7,8,9	0.53	0	8,9,11	0.84	1 (12%)
6	PSU	L5	4298	6	18,21,22	1.34	3 (16%)	22,30,33	1.83	4 (18%)
78	SAC	Sd	2	78	7,8,9	0.52	0	8,9,11	0.90	1 (12%)
52	PSU	S2	1175	52	18,21,22	1.36	3 (16%)	22,30,33	1.84	5 (22%)
52	OMG	S2	1329	52	23,26,27	1.17	2 (8%)	33,38,41	1.86	10 (30%)
79	NMM	Se	67	79	9,11,12	1.56	1 (11%)	6,12,14	3.48	2 (33%)
6	A2M	L5	2206	6,89	22,25,26	1.76	7 (31%)	31,36,39	2.47	15 (48%)
6	OMC	L5	1284	6	19,22,23	1.16	2 (10%)	26,31,34	0.86	0
6	PSU	L5	4042	6	18,21,22	1.36	3 (16%)	22,30,33	1.87	4 (18%)
52	OMG	S2	437	52	23,26,27	1.16	2 (8%)	33,38,41	1.88	9 (27%)
60	SAC	SL	2	60	7,8,9	0.53	0	8,9,11	0.86	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A2M	L5	1489	6,89	22,25,26	1.75	7 (31%)	31,36,39	2.42	12 (38%)
6	PSU	L5	3616	6	18,21,22	1.34	3 (16%)	22,30,33	1.86	5 (22%)
6	OMG	L5	1580	6	23,26,27	1.20	3 (13%)	33,38,41	1.93	10 (30%)

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
6	A2M	L5	3557	6	-	0/9/27/28	0/3/3/3
6	OMU	L5	2680	6	-	0/9/27/28	0/2/2/2
52	OMC	S2	174	52	-	0/9/27/28	0/2/2/2
52	PSU	S2	682	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	121	52	-	0/9/27/28	0/2/2/2
6	PSU	L5	2351	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	2194	6	-	1/9/27/28	0/2/2/2
52	OMU	S2	355	71,52	-	0/9/27/28	0/2/2/2
6	A2M	L5	398	6	-	0/9/27/28	0/3/3/3
6	OMC	L5	3433	6,90	-	4/9/27/28	0/2/2/2
52	OMG	S2	510	52,89	-	2/9/27/28	0/3/3/3
6	OMG	L5	1260	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	1720	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	823	52	-	2/7/25/26	0/2/2/2
6	PSU	L5	4246	6	-	1/7/25/26	0/2/2/2
6	PSU	L5	4740	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3490	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1638	6,90	-	0/7/25/26	0/2/2/2
52	PSU	S2	610	52	-	0/7/25/26	0/2/2/2
6	OMC	L5	2208	6,89	-	0/9/27/28	0/2/2/2
6	PSU	L5	3447	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	3601	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	4435	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	669	52,89	-	2/9/27/28	0/3/3/3
6	PSU	L5	1718	6	-	0/7/25/26	0/2/2/2
47	MLZ	Lq	53	47	-	0/7/8/10	-
6	PSU	L5	3652	6,89	-	0/7/25/26	0/2/2/2
52	PSU	S2	1005	52	-	1/7/25/26	0/2/2/2
52	PSU	S2	1178	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	3371	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	602	52	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L5	3585	6,89	-	0/7/25/26	0/2/2/2
6	OMG	L5	4138	6	-	0/9/27/28	0/3/3/3
6	OMG	L5	2719	6	-	1/9/27/28	0/3/3/3
6	OMG	L5	4116	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4217	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	1491	52,89	-	1/9/27/28	0/3/3/3
6	PSU	L5	3554	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	3562	6	-	0/9/27/28	0/3/3/3
6	A2M	L5	400	6	-	0/9/27/28	0/3/3/3
52	PSU	S2	1082	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	1443	52,89	-	0/9/27/28	0/2/2/2
6	OMU	L5	4244	6	-	0/9/27/28	0/2/2/2
6	OMG	L5	4364	6	-	0/9/27/28	0/3/3/3
52	PSU	S2	407	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	4383	6,90	-	0/9/27/28	0/3/3/3
52	OMG	S2	645	52	-	3/9/27/28	0/3/3/3
52	PSU	S2	1057	52	-	0/7/25/26	0/2/2/2
6	OMU	L5	2258	6	-	0/9/27/28	0/2/2/2
6	A2M	L5	1270	6	-	1/9/27/28	0/3/3/3
52	PSU	S2	119	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1239	52	-	0/7/25/26	0/2/2/2
11	AYA	LF	2	11	-	2/4/6/8	-
6	PSU	L5	4169	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	591	52	-	1/9/27/28	0/3/3/3
35	MLZ	Le	5	35	-	2/7/8/10	-
52	PSU	S2	864	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	172	52	-	0/9/27/28	0/2/2/2
52	OMC	S2	518	52	-	2/9/27/28	0/2/2/2
52	MA6	S2	1852	52	-	2/11/29/30	0/3/3/3
46	M3L	Lp	98	46	-	0/9/10/12	-
6	A2M	L5	3517	6	-	3/9/27/28	0/3/3/3
6	OMU	L5	4052	6	-	0/9/27/28	0/2/2/2
52	OMU	S2	429	52	-	4/9/27/28	0/2/2/2
6	OMC	L5	4202	6	-	0/9/27/28	0/2/2/2
8	PSU	L8	55	8	-	0/7/25/26	0/2/2/2
52	MA6	S2	1851	52	-	2/11/29/30	0/3/3/3
6	PSU	L5	3466	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1491	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	816	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	3583	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L5	4039	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4045	6	-	0/7/25/26	0/2/2/2
6	6MZ	L5	3966	6	-	0/9/27/28	0/3/3/3
6	OMC	L5	3619	6,22	-	2/9/27/28	0/2/2/2
6	PSU	L5	3500	6	-	0/7/25/26	0/2/2/2
52	OMU	S2	628	52	-	6/9/27/28	0/2/2/2
6	OMU	L5	4366	6	-	0/9/27/28	0/2/2/2
52	4AC	S2	1338	52	-	4/11/29/30	0/2/2/2
52	OMU	S2	1327	52,89	-	0/9/27/28	0/2/2/2
52	PSU	S2	218	52	-	0/7/25/26	0/2/2/2
6	OMG	L5	3524	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4099	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	3942	6	-	0/9/27/28	0/3/3/3
52	OMG	S2	1448	52	-	3/9/27/28	0/3/3/3
6	PSU	L5	3502	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	469	52	-	0/9/27/28	0/3/3/3
6	A2M	L5	2244	6	-	1/9/27/28	0/3/3/3
52	PSU	S2	36	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4382	6	-	2/7/25/26	0/2/2/2
6	A2M	L5	3450	6	-	0/9/27/28	0/3/3/3
6	OMC	L5	2667	6	-	0/9/27/28	0/2/2/2
6	OMG	L5	3676	6	-	1/9/27/28	0/3/3/3
6	PSU	L5	4322	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4267	6,89	-	0/7/25/26	0/2/2/2
52	OMU	S2	1805	52	-	0/9/27/28	0/2/2/2
6	PSU	L5	3427	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	34	52	-	0/7/25/26	0/2/2/2
52	6MZ	S2	1833	52,89	-	1/9/27/28	0/3/3/3
6	PSU	L5	3496	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4369	6	-	2/9/27/28	0/3/3/3
6	A2M	L5	3599	6	-	0/9/27/28	0/3/3/3
6	OMU	L5	3973	6	-	0/9/27/28	0/2/2/2
52	PSU	S2	802	52	-	3/7/25/26	0/2/2/2
6	PSU	L5	4058	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	159	52	-	0/9/27/28	0/3/3/3
52	PSU	S2	1245	52	-	0/7/25/26	0/2/2/2
81	AME	Sg	1	81	-	2/9/10/12	-
52	PSU	S2	687	52	-	0/7/25/26	0/2/2/2
6	OMC	L5	2265	6,89	-	2/9/27/28	0/2/2/2
6	PSU	L5	1537	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMC	L5	2647	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	3462	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3369	6,90,89	-	0/7/25/26	0/2/2/2
52	A2M	S2	577	52	-	1/9/27/28	0/3/3/3
83	HY3	Si	62	83	-	1/1/12/14	0/1/1/1
6	OMG	L5	3631	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	1632	6	-	1/7/25/26	0/2/2/2
52	PSU	S2	1047	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	1731	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3576	6	-	1/7/25/26	0/2/2/2
6	A2M	L5	4336	6	-	2/9/27/28	0/3/3/3
52	A2M	S2	1384	52	-	0/9/27/28	0/3/3/3
6	PSU	L5	3494	6	-	2/7/25/26	0/2/2/2
10	HIC	LE	245	10	-	2/5/6/8	0/1/1/1
52	PSU	S2	1368	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1046	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4374	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1644	52,89	-	0/7/25/26	0/2/2/2
52	PSU	S2	93	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	109	52	-	0/7/25/26	0/2/2/2
52	A2M	S2	485	52	-	1/9/27/28	0/3/3/3
6	A2M	L5	3492	6,89	-	3/9/27/28	0/3/3/3
52	PSU	S2	1693	52	-	0/7/25/26	0/2/2/2
6	OMU	L5	3657	6	-	0/9/27/28	0/2/2/2
6	5MC	L5	4193	6	-	3/7/25/26	0/2/2/2
52	OMC	S2	1392	52	-	2/9/27/28	0/2/2/2
52	PSU	S2	652	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1348	52	-	0/7/25/26	0/2/2/2
52	OMU	S2	116	52	-	0/9/27/28	0/2/2/2
52	PSU	S2	1233	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	573	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4166	6	-	2/7/25/26	0/2/2/2
6	PSU	L5	4177	6	-	0/7/25/26	0/2/2/2
52	OMC	S2	1704	52,89	-	0/9/27/28	0/2/2/2
6	OMG	L5	3476	6	-	0/9/27/28	0/3/3/3
6	OMG	L5	4240	6	-	1/9/27/28	0/3/3/3
52	A2M	S2	27	52	-	0/9/27/28	0/3/3/3
6	UR3	L5	4276	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	3540	6	-	0/9/27/28	0/2/2/2
52	OMG	S2	684	52	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	OMG	S2	868	52	-	0/9/27/28	0/3/3/3
6	OMG	L5	1477	6	-	3/9/27/28	0/3/3/3
6	PSU	L5	4203	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	105	52	-	0/7/25/26	0/2/2/2
6	OMC	L5	1820	6,89	-	0/9/27/28	0/2/2/2
6	A2M	L5	3456	6	-	0/9/27/28	0/3/3/3
52	A2M	S2	1679	52	-	0/9/27/28	0/3/3/3
6	PSU	L5	1799	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1801	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	2658	6,89	-	1/9/27/28	0/3/3/3
6	PSU	L5	4149	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	1446	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	1721	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4188	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4107	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	2704	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	4711	6	-	0/7/25/26	0/2/2/2
6	1MA	L5	1266	6,89	-	2/7/25/26	0/3/3/3
6	A2M	L5	1810	6,89	-	0/9/27/28	0/3/3/3
6	OMG	L5	3359	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4749	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	2630	6	-	3/9/27/28	0/3/3/3
52	A2M	S2	513	52	-	0/9/27/28	0/3/3/3
52	PSU	S2	650	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1626	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4419	6	-	0/7/25/26	0/2/2/2
52	A2M	S2	1032	52	-	0/9/27/28	0/3/3/3
8	PSU	L8	69	8	-	0/7/25/26	0/2/2/2
6	A2M	L5	4317	6	-	0/9/27/28	0/3/3/3
52	OMC	S2	463	52	-	0/9/27/28	0/2/2/2
6	OMC	L5	3573	6	-	0/9/27/28	0/2/2/2
52	OMU	S2	1289	52,55	-	0/9/27/28	0/2/2/2
52	A2M	S2	99	52,89	-	1/9/27/28	0/3/3/3
6	5MC	L5	3514	6,89	-	0/7/25/26	0/2/2/2
6	OMG	L5	4245	6	-	0/9/27/28	0/3/3/3
52	PSU	S2	815	52	-	0/7/25/26	0/2/2/2
6	PSU	L5	4325	6	-	0/7/25/26	0/2/2/2
52	7MG	S2	1640	52	-	0/7/37/38	0/3/3/3
6	OMG	L5	2267	6	-	0/9/27/28	0/3/3/3
52	PSU	S2	967	52	-	0/7/25/26	0/2/2/2
52	A2M	S2	166	52	-	0/9/27/28	0/3/3/3
6	PSU	L5	1683	6,90	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	L5	3974	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	2475	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	4282	6	-	0/9/27/28	0/2/2/2
6	A2M	L5	4269	6,89	-	0/9/27/28	0/3/3/3
52	4AC	S2	1843	52,86	-	2/11/29/30	0/2/2/2
8	OMG	L8	75	8	-	0/9/27/28	0/3/3/3
52	PSU	S2	867	52	-	0/7/25/26	0/2/2/2
6	A2M	L5	1479	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	2207	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4278	6	-	0/7/25/26	0/2/2/2
52	PSU	S2	210	52	-	0/7/25/26	0/2/2/2
49	SAC	Ls	2	49	-	0/7/8/10	-
6	PSU	L5	4298	6	-	0/7/25/26	0/2/2/2
78	SAC	Sd	2	78	-	0/7/8/10	-
52	PSU	S2	1175	52	-	0/7/25/26	0/2/2/2
52	OMG	S2	1329	52	-	0/9/27/28	0/3/3/3
79	NMM	Se	67	79	-	3/9/11/13	-
6	A2M	L5	2206	6,89	-	0/9/27/28	0/3/3/3
6	OMC	L5	1284	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	4042	6	-	0/7/25/26	0/2/2/2
52	OMG	S2	437	52	-	0/9/27/28	0/3/3/3
60	SAC	SL	2	60	-	1/7/8/10	-
6	A2M	L5	1489	6,89	-	2/9/27/28	0/3/3/3
6	PSU	L5	3616	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	1580	6	-	1/9/27/28	0/3/3/3

All (716) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1266	1MA	C2-N3	4.79	1.39	1.30
52	S2	1851	MA6	C5-C4	4.52	1.47	1.39
52	S2	1852	MA6	C5-C4	4.44	1.47	1.39
52	S2	1833	6MZ	C5-C4	4.31	1.47	1.39
79	Se	67	NMM	CZ-NH2	4.23	1.44	1.34
6	L5	3966	6MZ	C5-C4	4.21	1.46	1.39
6	L5	1266	1MA	C5-C6	-3.98	1.33	1.43
52	S2	867	PSU	C6-C5	3.76	1.39	1.35
52	S2	573	PSU	C6-C5	3.71	1.39	1.35
52	S2	816	PSU	C6-C5	3.71	1.39	1.35
52	S2	864	PSU	C6-C5	3.71	1.39	1.35
52	S2	687	PSU	C6-C5	3.70	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	109	PSU	C6-C5	3.69	1.39	1.35
52	S2	1368	PSU	C6-C5	3.68	1.39	1.35
52	S2	1626	PSU	C6-C5	3.67	1.39	1.35
52	S2	93	PSU	C6-C5	3.67	1.39	1.35
52	S2	210	PSU	C6-C5	3.66	1.39	1.35
52	S2	1640	7MG	C5-C6	-3.64	1.34	1.43
52	S2	1640	7MG	C4-N9	-3.63	1.33	1.37
52	S2	610	PSU	C6-C5	3.63	1.39	1.35
52	S2	802	PSU	C6-C5	3.63	1.39	1.35
52	S2	119	PSU	C6-C5	3.59	1.39	1.35
52	S2	36	PSU	C6-C5	3.58	1.39	1.35
6	L5	3502	PSU	C6-C5	3.58	1.39	1.35
52	S2	105	PSU	C6-C5	3.58	1.39	1.35
52	S2	1348	PSU	C6-C5	3.57	1.39	1.35
6	L5	1632	PSU	C6-C5	3.57	1.39	1.35
52	S2	967	PSU	C6-C5	3.56	1.39	1.35
52	S2	823	PSU	C6-C5	3.55	1.39	1.35
52	S2	1446	PSU	C6-C5	3.55	1.39	1.35
52	S2	34	PSU	C6-C5	3.54	1.39	1.35
6	L5	3466	PSU	C6-C5	3.53	1.39	1.35
6	L5	3494	PSU	C6-C5	3.53	1.39	1.35
6	L5	4749	PSU	C6-C5	3.52	1.39	1.35
52	S2	1233	PSU	C6-C5	3.52	1.39	1.35
6	L5	4278	PSU	C6-C5	3.52	1.39	1.35
52	S2	407	PSU	C6-C5	3.51	1.39	1.35
6	L5	4322	PSU	C6-C5	3.51	1.39	1.35
6	L5	1683	PSU	C6-C5	3.51	1.39	1.35
6	L5	3462	PSU	C6-C5	3.51	1.39	1.35
52	S2	650	PSU	C6-C5	3.50	1.39	1.35
52	S2	1047	PSU	C6-C5	3.50	1.39	1.35
52	S2	652	PSU	C6-C5	3.50	1.39	1.35
6	L5	4740	PSU	C6-C5	3.49	1.39	1.35
6	L5	4246	PSU	C6-C5	3.49	1.39	1.35
52	S2	218	PSU	C6-C5	3.48	1.39	1.35
52	S2	1178	PSU	C6-C5	3.48	1.39	1.35
6	L5	1799	PSU	C6-C5	3.47	1.39	1.35
52	S2	1239	PSU	C6-C5	3.47	1.39	1.35
8	L8	55	PSU	C6-C5	3.47	1.39	1.35
52	S2	815	PSU	C6-C5	3.46	1.39	1.35
52	S2	1175	PSU	C6-C5	3.46	1.39	1.35
52	S2	1245	PSU	C6-C5	3.45	1.39	1.35
6	L5	3496	PSU	C6-C5	3.44	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3490	PSU	C6-C5	3.44	1.39	1.35
6	L5	3576	PSU	C6-C5	3.44	1.39	1.35
6	L5	1718	PSU	C6-C5	3.44	1.39	1.35
6	L5	3500	PSU	C6-C5	3.44	1.39	1.35
52	S2	1057	PSU	C6-C5	3.42	1.39	1.35
6	L5	4169	PSU	C6-C5	3.42	1.39	1.35
52	S2	1644	PSU	C6-C5	3.41	1.39	1.35
6	L5	3447	PSU	C6-C5	3.41	1.39	1.35
6	L5	2475	PSU	C6-C5	3.41	1.39	1.35
6	L5	4374	PSU	C6-C5	3.41	1.39	1.35
6	L5	3554	PSU	C6-C5	3.41	1.39	1.35
52	S2	1693	PSU	C6-C5	3.41	1.39	1.35
6	L5	1801	PSU	C6-C5	3.40	1.39	1.35
52	S2	1046	PSU	C6-C5	3.40	1.39	1.35
6	L5	3427	PSU	C6-C5	3.39	1.39	1.35
6	L5	1720	PSU	C6-C5	3.39	1.39	1.35
6	L5	4039	PSU	C6-C5	3.39	1.39	1.35
8	L8	69	PSU	C6-C5	3.39	1.39	1.35
52	S2	682	PSU	C6-C5	3.39	1.39	1.35
6	L5	4711	PSU	C6-C5	3.38	1.39	1.35
6	L5	4166	PSU	C6-C5	3.38	1.39	1.35
6	L5	4435	PSU	C6-C5	3.38	1.39	1.35
6	L5	1721	PSU	C6-C5	3.37	1.39	1.35
6	L5	4058	PSU	C6-C5	3.37	1.39	1.35
6	L5	4042	PSU	C6-C5	3.37	1.39	1.35
6	L5	4298	PSU	C6-C5	3.36	1.39	1.35
6	L5	1537	PSU	C6-C5	3.36	1.39	1.35
6	L5	4045	PSU	C6-C5	3.36	1.39	1.35
6	L5	1731	PSU	C6-C5	3.35	1.39	1.35
6	L5	4217	PSU	C6-C5	3.34	1.39	1.35
6	L5	4099	PSU	C6-C5	3.33	1.39	1.35
6	L5	4325	PSU	C6-C5	3.32	1.39	1.35
6	L5	4107	PSU	C6-C5	3.32	1.39	1.35
6	L5	3616	PSU	C6-C5	3.32	1.39	1.35
52	S2	1843	4AC	C4-N4	-3.31	1.34	1.39
52	S2	166	A2M	C2-N3	3.31	1.40	1.33
6	L5	1638	PSU	C6-C5	3.30	1.39	1.35
6	L5	2630	A2M	C5-C4	-3.30	1.32	1.39
6	L5	4419	PSU	C6-C5	3.29	1.39	1.35
6	L5	1491	PSU	C6-C5	3.28	1.39	1.35
52	S2	1384	A2M	C2-N3	3.27	1.40	1.33
52	S2	1082	PSU	C6-C5	3.27	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	27	A2M	C2-N3	3.27	1.40	1.33
6	L5	4177	PSU	C6-C5	3.27	1.39	1.35
6	L5	4382	PSU	C6-C5	3.27	1.39	1.35
6	L5	2351	PSU	C6-C5	3.26	1.39	1.35
6	L5	3583	PSU	C6-C5	3.26	1.39	1.35
52	S2	469	A2M	C2-N3	3.25	1.40	1.33
52	S2	159	A2M	C2-N3	3.25	1.40	1.33
6	L5	1489	A2M	C5-N7	-3.24	1.32	1.39
52	S2	577	A2M	C2-N1	3.24	1.39	1.33
6	L5	3517	A2M	C5-N7	-3.24	1.32	1.39
52	S2	591	A2M	C2-N3	3.24	1.39	1.33
6	L5	4317	A2M	C2-N3	3.23	1.39	1.33
52	S2	513	A2M	C2-N3	3.23	1.39	1.33
6	L5	4188	PSU	C6-C5	3.23	1.39	1.35
52	S2	1679	A2M	C2-N3	3.23	1.39	1.33
6	L5	3456	A2M	C2-N3	3.22	1.39	1.33
6	L5	4149	PSU	C6-C5	3.22	1.39	1.35
52	S2	99	A2M	C2-N3	3.22	1.39	1.33
52	S2	469	A2M	C2-N1	3.22	1.39	1.33
6	L5	4203	PSU	C6-C5	3.22	1.39	1.35
6	L5	2207	OMG	C5-C6	-3.21	1.32	1.44
52	S2	513	A2M	C2-N1	3.20	1.39	1.33
6	L5	400	A2M	C2-N3	3.20	1.39	1.33
6	L5	3371	PSU	C6-C5	3.20	1.39	1.35
6	L5	1580	OMG	C5-N7	-3.20	1.32	1.39
52	S2	577	A2M	C2-N3	3.20	1.39	1.33
6	L5	3492	A2M	C2-N3	3.20	1.39	1.33
52	S2	27	A2M	C2-N1	3.19	1.39	1.33
52	S2	159	A2M	C2-N1	3.19	1.39	1.33
6	L5	3450	A2M	C5-N7	-3.19	1.33	1.39
6	L5	1810	A2M	C5-N7	-3.19	1.33	1.39
6	L5	1477	OMG	C5-N7	-3.18	1.32	1.39
6	L5	400	A2M	C5-N7	-3.18	1.33	1.39
52	S2	485	A2M	C2-N3	3.18	1.39	1.33
52	S2	485	A2M	C2-N1	3.18	1.39	1.33
6	L5	2206	A2M	C5-N7	-3.17	1.33	1.39
6	L5	1810	A2M	C5-C4	-3.17	1.33	1.39
6	L5	4267	PSU	C6-C5	3.17	1.39	1.35
6	L5	3585	PSU	C6-C5	3.17	1.39	1.35
6	L5	3557	A2M	C5-N7	-3.17	1.33	1.39
6	L5	4317	A2M	C2-N1	3.17	1.39	1.33
6	L5	3492	A2M	C2-N1	3.16	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	166	A2M	C2-N1	3.16	1.39	1.33
6	L5	4336	A2M	C2-N3	3.16	1.39	1.33
6	L5	3492	A2M	C5-N7	-3.16	1.33	1.39
52	S2	1384	A2M	C2-N1	3.16	1.39	1.33
6	L5	1489	A2M	C2-N3	3.16	1.39	1.33
52	S2	591	A2M	C2-N1	3.16	1.39	1.33
6	L5	4269	A2M	C5-N7	-3.15	1.33	1.39
6	L5	2719	OMG	C5-N7	-3.15	1.33	1.39
6	L5	2267	OMG	C5-N7	-3.15	1.33	1.39
52	S2	99	A2M	C5-N7	-3.15	1.33	1.39
6	L5	2244	A2M	C5-N7	-3.15	1.33	1.39
6	L5	2630	A2M	C5-N7	-3.14	1.33	1.39
6	L5	3517	A2M	C2-N3	3.14	1.39	1.33
6	L5	4269	A2M	C5-C4	-3.14	1.33	1.39
6	L5	3652	PSU	C6-C5	3.14	1.39	1.35
6	L5	3631	OMG	C5-C6	-3.14	1.33	1.44
52	S2	591	A2M	C5-N7	-3.13	1.33	1.39
6	L5	3524	OMG	C5-N7	-3.13	1.33	1.39
6	L5	398	A2M	C5-N7	-3.13	1.33	1.39
6	L5	1270	A2M	C5-C4	-3.13	1.33	1.39
6	L5	398	A2M	C2-N3	3.13	1.39	1.33
6	L5	2207	OMG	C5-N7	-3.13	1.33	1.39
6	L5	2658	A2M	C2-N3	3.13	1.39	1.33
6	L5	4138	OMG	C5-C6	-3.13	1.33	1.44
6	L5	4240	OMG	C5-N7	-3.12	1.33	1.39
6	L5	1270	A2M	C5-N7	-3.12	1.33	1.39
6	L5	2658	A2M	C5-N7	-3.12	1.33	1.39
6	L5	1479	A2M	C5-N7	-3.12	1.33	1.39
6	L5	4369	OMG	C5-N7	-3.11	1.33	1.39
52	S2	1384	A2M	C5-N7	-3.11	1.33	1.39
6	L5	3369	PSU	C6-C5	3.11	1.39	1.35
6	L5	2267	OMG	C5-C6	-3.11	1.33	1.44
8	L8	75	OMG	C5-C6	-3.11	1.33	1.44
6	L5	4240	OMG	C5-C6	-3.11	1.33	1.44
6	L5	3456	A2M	C2-N1	3.11	1.39	1.33
6	L5	2630	A2M	C2-N3	3.11	1.39	1.33
6	L5	3599	A2M	C5-N7	-3.11	1.33	1.39
6	L5	2206	A2M	C5-C4	-3.11	1.33	1.39
6	L5	3974	OMG	C5-C6	-3.11	1.33	1.44
6	L5	1260	OMG	C5-C6	-3.11	1.33	1.44
6	L5	3476	OMG	C5-C6	-3.11	1.33	1.44
52	S2	1491	OMG	C5-C6	-3.10	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3456	A2M	C5-N7	-3.10	1.33	1.39
6	L5	2719	OMG	C5-C6	-3.10	1.33	1.44
6	L5	3524	OMG	C5-C6	-3.10	1.33	1.44
6	L5	1260	OMG	C5-N7	-3.10	1.33	1.39
6	L5	4138	OMG	C5-N7	-3.10	1.33	1.39
6	L5	1580	OMG	C5-C6	-3.10	1.33	1.44
6	L5	4269	A2M	C2-N3	3.10	1.39	1.33
6	L5	4245	OMG	C5-C6	-3.10	1.33	1.44
52	S2	669	A2M	C5-C4	-3.09	1.33	1.39
6	L5	3599	A2M	C2-N3	3.09	1.39	1.33
6	L5	3562	A2M	C5-C4	-3.09	1.33	1.39
6	L5	4317	A2M	C5-N7	-3.09	1.33	1.39
6	L5	4245	OMG	C5-N7	-3.09	1.33	1.39
52	S2	602	OMG	C5-C6	-3.09	1.33	1.44
52	S2	669	A2M	C2-N3	3.09	1.39	1.33
6	L5	3476	OMG	C5-N7	-3.09	1.33	1.39
6	L5	2658	A2M	C5-C4	-3.08	1.33	1.39
6	L5	4336	A2M	C5-N7	-3.08	1.33	1.39
6	L5	4383	OMG	C5-N7	-3.08	1.33	1.39
6	L5	2244	A2M	C2-N3	3.08	1.39	1.33
6	L5	4116	OMG	C5-N7	-3.08	1.33	1.39
52	S2	669	A2M	C5-N7	-3.08	1.33	1.39
52	S2	510	OMG	C5-C6	-3.07	1.33	1.44
6	L5	398	A2M	C2-N1	3.07	1.39	1.33
52	S2	1338	4AC	C4-N4	-3.07	1.35	1.39
6	L5	3942	OMG	C5-N7	-3.07	1.33	1.39
52	S2	1032	A2M	C5-N7	-3.07	1.33	1.39
8	L8	75	OMG	C5-N7	-3.07	1.33	1.39
6	L5	4116	OMG	C5-C6	-3.07	1.33	1.44
6	L5	1489	A2M	C5-C4	-3.07	1.33	1.39
52	S2	1679	A2M	C2-N1	3.07	1.39	1.33
6	L5	3517	A2M	C5-C4	-3.07	1.33	1.39
52	S2	1491	OMG	C5-N7	-3.07	1.33	1.39
6	L5	4364	OMG	C5-C6	-3.07	1.33	1.44
6	L5	3599	A2M	C5-C4	-3.07	1.33	1.39
52	S2	1032	A2M	C2-N3	3.07	1.39	1.33
6	L5	1489	A2M	C2-N1	3.07	1.39	1.33
6	L5	4369	OMG	C5-C6	-3.07	1.33	1.44
6	L5	3562	A2M	C5-N7	-3.07	1.33	1.39
52	S2	1448	OMG	C5-N7	-3.06	1.33	1.39
52	S2	437	OMG	C5-C6	-3.06	1.33	1.44
6	L5	4364	OMG	C5-N7	-3.06	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1477	OMG	C5-C6	-3.06	1.33	1.44
6	L5	4336	A2M	C2-N1	3.06	1.39	1.33
6	L5	3557	A2M	C2-N3	3.06	1.39	1.33
52	S2	27	A2M	C5-N7	-3.06	1.33	1.39
52	S2	1032	A2M	C5-C4	-3.06	1.33	1.39
6	L5	3359	OMG	C5-C6	-3.06	1.33	1.44
6	L5	1479	A2M	C2-N3	3.06	1.39	1.33
6	L5	3450	A2M	C2-N1	3.06	1.39	1.33
6	L5	4383	OMG	C5-C6	-3.05	1.33	1.44
6	L5	2206	A2M	C2-N3	3.05	1.39	1.33
52	S2	1448	OMG	C5-C6	-3.05	1.33	1.44
6	L5	3942	OMG	C5-C6	-3.05	1.33	1.44
6	L5	2244	A2M	C5-C4	-3.05	1.33	1.39
52	S2	684	OMG	C5-C6	-3.05	1.33	1.44
6	L5	3974	OMG	C5-N7	-3.05	1.33	1.39
6	L5	1479	A2M	C5-C4	-3.05	1.33	1.39
6	L5	3557	A2M	C5-C4	-3.04	1.33	1.39
52	S2	510	OMG	C5-N7	-3.04	1.33	1.39
6	L5	3450	A2M	C5-C4	-3.04	1.33	1.39
52	S2	513	A2M	C5-N7	-3.04	1.33	1.39
52	S2	1329	OMG	C5-C6	-3.04	1.33	1.44
52	S2	602	OMG	C5-N7	-3.04	1.33	1.39
52	S2	645	OMG	C5-C6	-3.04	1.33	1.44
6	L5	400	A2M	C2-N1	3.04	1.39	1.33
6	L5	3450	A2M	C2-N3	3.04	1.39	1.33
52	S2	1679	A2M	C5-N7	-3.03	1.33	1.39
6	L5	3359	OMG	C5-N7	-3.03	1.33	1.39
52	S2	99	A2M	C2-N1	3.03	1.39	1.33
52	S2	27	A2M	C5-C4	-3.03	1.33	1.39
6	L5	3562	A2M	C2-N1	3.03	1.39	1.33
52	S2	868	OMG	C5-C6	-3.03	1.33	1.44
6	L5	2658	A2M	C2-N1	3.02	1.39	1.33
52	S2	1329	OMG	C5-N7	-3.02	1.33	1.39
52	S2	669	A2M	C2-N1	3.02	1.39	1.33
52	S2	684	OMG	C5-N7	-3.02	1.33	1.39
52	S2	485	A2M	C5-N7	-3.02	1.33	1.39
6	L5	3676	OMG	C5-N7	-3.02	1.33	1.39
6	L5	3631	OMG	C5-N7	-3.01	1.33	1.39
6	L5	4336	A2M	C5-C4	-3.01	1.33	1.39
6	L5	3676	OMG	C5-C6	-3.01	1.33	1.44
6	L5	1270	A2M	C5-C6	-3.01	1.32	1.41
6	L5	400	A2M	C5-C4	-3.01	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	166	A2M	C5-N7	-3.01	1.33	1.39
6	L5	4317	A2M	C5-C4	-3.01	1.33	1.39
6	L5	1270	A2M	C2-N3	3.00	1.39	1.33
6	L5	1810	A2M	C2-N1	3.00	1.39	1.33
52	S2	1005	PSU	C2-N3	3.00	1.42	1.37
6	L5	3562	A2M	C2-N3	2.99	1.39	1.33
6	L5	1266	1MA	C5-N7	-2.99	1.33	1.39
6	L5	3456	A2M	C5-C4	-2.98	1.33	1.39
52	S2	577	A2M	C5-N7	-2.98	1.33	1.39
52	S2	159	A2M	C5-N7	-2.98	1.33	1.39
6	L5	1810	A2M	C5-C6	-2.98	1.32	1.41
52	S2	1679	A2M	C5-C4	-2.98	1.33	1.39
6	L5	1810	A2M	C2-N3	2.98	1.39	1.33
52	S2	437	OMG	C5-N7	-2.98	1.33	1.39
52	S2	645	OMG	C5-N7	-2.97	1.33	1.39
6	L5	3517	A2M	C5-C6	-2.97	1.33	1.41
6	L5	3562	A2M	C5-C6	-2.97	1.33	1.41
6	L5	398	A2M	C5-C4	-2.97	1.33	1.39
6	L5	3557	A2M	C5-C6	-2.97	1.33	1.41
52	S2	1032	A2M	C2-N1	2.97	1.39	1.33
6	L5	3557	A2M	C2-N1	2.97	1.39	1.33
52	S2	469	A2M	C5-N7	-2.97	1.33	1.39
52	S2	485	A2M	C5-C4	-2.96	1.33	1.39
6	L5	4269	A2M	C2-N1	2.96	1.39	1.33
52	S2	1384	A2M	C5-C4	-2.96	1.33	1.39
6	L5	4276	UR3	C2-N1	-2.96	1.34	1.38
6	L5	2206	A2M	C2-N1	2.96	1.39	1.33
52	S2	99	A2M	C5-C4	-2.95	1.33	1.39
6	L5	3599	A2M	C2-N1	2.94	1.39	1.33
52	S2	1032	A2M	C5-C6	-2.94	1.33	1.41
6	L5	1479	A2M	C2-N1	2.94	1.39	1.33
52	S2	868	OMG	C5-N7	-2.94	1.33	1.39
6	L5	1270	A2M	C2-N1	2.94	1.39	1.33
6	L5	2244	A2M	C5-C6	-2.93	1.33	1.41
6	L5	4336	A2M	C5-C6	-2.93	1.33	1.41
6	L5	4276	UR3	C4-N3	-2.93	1.34	1.40
52	S2	513	A2M	C5-C4	-2.92	1.33	1.39
6	L5	3492	A2M	C5-C4	-2.92	1.33	1.39
6	L5	3517	A2M	C2-N1	2.92	1.39	1.33
6	L5	4193	5MC	C6-C5	2.92	1.39	1.34
6	L5	1489	A2M	C5-C6	-2.92	1.33	1.41
6	L5	400	A2M	C5-C6	-2.92	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	4269	A2M	C5-C6	-2.92	1.33	1.41
6	L5	2206	A2M	C5-C6	-2.92	1.33	1.41
6	L5	3450	A2M	C5-C6	-2.92	1.33	1.41
6	L5	2244	A2M	C2-N1	2.92	1.39	1.33
6	L5	3514	5MC	C4-N3	2.92	1.39	1.34
52	S2	1005	PSU	C6-C5	2.91	1.38	1.35
6	L5	3599	A2M	C5-C6	-2.90	1.33	1.41
6	L5	2630	A2M	C5-C6	-2.90	1.33	1.41
52	S2	469	A2M	C5-C4	-2.90	1.33	1.39
52	S2	166	A2M	C5-C4	-2.89	1.33	1.39
6	L5	3492	A2M	C5-C6	-2.89	1.33	1.41
6	L5	4317	A2M	C5-C6	-2.89	1.33	1.41
6	L5	1479	A2M	C5-C6	-2.89	1.33	1.41
52	S2	27	A2M	C5-C6	-2.88	1.33	1.41
6	L5	2630	A2M	C2-N1	2.88	1.39	1.33
52	S2	669	A2M	C5-C6	-2.88	1.33	1.41
52	S2	159	A2M	C5-C4	-2.88	1.33	1.39
6	L5	2658	A2M	C5-C6	-2.88	1.33	1.41
52	S2	1679	A2M	C5-C6	-2.87	1.33	1.41
52	S2	1384	A2M	C5-C6	-2.87	1.33	1.41
52	S2	577	A2M	C5-C4	-2.87	1.33	1.39
52	S2	159	A2M	C5-C6	-2.86	1.33	1.41
52	S2	591	A2M	C5-C4	-2.86	1.33	1.39
6	L5	398	A2M	C5-C6	-2.86	1.33	1.41
52	S2	99	A2M	C5-C6	-2.85	1.33	1.41
52	S2	485	A2M	C5-C6	-2.85	1.33	1.41
52	S2	1851	MA6	C5-C6	2.84	1.49	1.41
6	L5	3456	A2M	C5-C6	-2.84	1.33	1.41
52	S2	210	PSU	C2-N1	2.84	1.40	1.36
52	S2	513	A2M	C5-C6	-2.81	1.33	1.41
52	S2	591	A2M	C5-C6	-2.81	1.33	1.41
52	S2	577	A2M	C5-C6	-2.80	1.33	1.41
52	S2	1005	PSU	C4-N3	2.79	1.44	1.38
6	L5	1284	OMC	C2-N1	-2.79	1.33	1.40
6	L5	3657	OMU	C2-N1	-2.76	1.34	1.38
6	L5	3433	OMC	C2-N1	-2.76	1.34	1.40
6	L5	3514	5MC	C6-C5	2.75	1.39	1.34
52	S2	469	A2M	C5-C6	-2.75	1.33	1.41
6	L5	4282	OMC	C2-N1	-2.75	1.34	1.40
52	S2	1852	MA6	C5-C6	2.75	1.48	1.41
6	L5	1820	OMC	C2-N1	-2.74	1.34	1.40
52	S2	166	A2M	C5-C6	-2.74	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	4244	OMU	C2-N1	-2.74	1.34	1.38
52	S2	1005	PSU	C6-N1	-2.73	1.31	1.36
6	L5	2647	OMC	C2-N1	-2.72	1.34	1.40
52	S2	34	PSU	C2-N1	2.71	1.40	1.36
83	Si	62	HY3	C3-CA	-2.71	1.52	1.55
6	L5	2208	OMC	C2-N1	-2.71	1.34	1.40
52	S2	1704	OMC	C2-N1	-2.70	1.34	1.40
6	L5	3619	OMC	C2-N1	-2.70	1.34	1.40
52	S2	174	OMC	C4-N3	2.69	1.40	1.34
52	S2	1446	PSU	C2-N1	2.68	1.40	1.36
6	L5	3466	PSU	C2-N1	2.67	1.40	1.36
52	S2	1327	OMU	C2-N1	-2.67	1.34	1.38
52	S2	573	PSU	C2-N1	2.66	1.40	1.36
6	L5	3973	OMU	C2-N1	-2.66	1.34	1.38
6	L5	4366	OMU	C2-N1	-2.66	1.34	1.38
6	L5	4202	OMC	C2-N1	-2.65	1.34	1.40
6	L5	4193	5MC	C2-N1	-2.65	1.34	1.40
6	L5	4166	PSU	C2-N1	2.64	1.40	1.36
52	S2	628	OMU	C2-N1	-2.64	1.34	1.38
6	L5	3573	OMC	C2-N1	-2.63	1.34	1.40
6	L5	3601	OMC	C2-N1	-2.63	1.34	1.40
52	S2	815	PSU	C2-N1	2.62	1.40	1.36
52	S2	218	PSU	C2-N1	2.62	1.40	1.36
6	L5	1270	A2M	C8-N9	-2.61	1.32	1.37
6	L5	2194	OMC	C2-N1	-2.60	1.34	1.40
6	L5	2704	OMC	C2-N1	-2.60	1.34	1.40
52	S2	36	PSU	C2-N1	2.60	1.40	1.36
6	L5	3517	A2M	C8-N9	-2.59	1.32	1.37
6	L5	2680	OMU	C2-N1	-2.59	1.34	1.38
6	L5	2667	OMC	C2-N1	-2.59	1.34	1.40
52	S2	816	PSU	C2-N1	2.59	1.40	1.36
6	L5	3599	A2M	C8-N9	-2.59	1.32	1.37
6	L5	1489	A2M	C8-N9	-2.59	1.32	1.37
52	S2	518	OMC	C4-N3	2.59	1.39	1.34
52	S2	463	OMC	C4-N3	2.58	1.39	1.34
52	S2	1005	PSU	C2-N1	2.58	1.40	1.36
52	S2	429	OMU	C2-N1	-2.58	1.34	1.38
52	S2	652	PSU	C2-N1	2.57	1.40	1.36
6	L5	4042	PSU	C2-N1	2.57	1.40	1.36
6	L5	4382	PSU	C6-N1	-2.57	1.32	1.36
6	L5	2658	A2M	C8-N9	-2.57	1.32	1.37
52	S2	867	PSU	C2-N1	2.56	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	2258	OMU	C2-N1	-2.55	1.34	1.38
6	L5	1810	A2M	C8-N9	-2.55	1.32	1.37
6	L5	4749	PSU	C2-N1	2.54	1.40	1.36
6	L5	3540	OMC	C2-N1	-2.54	1.34	1.40
6	L5	4052	OMU	C2-N1	-2.54	1.34	1.38
6	L5	2206	A2M	C8-N9	-2.54	1.33	1.37
6	L5	4435	PSU	C6-N1	-2.54	1.32	1.36
52	S2	1392	OMC	C4-N3	2.53	1.39	1.34
52	S2	967	PSU	C2-N1	2.53	1.40	1.36
6	L5	1537	PSU	C2-N1	2.53	1.40	1.36
52	S2	174	OMC	C2-N1	-2.53	1.34	1.40
52	S2	1047	PSU	C2-N1	2.53	1.40	1.36
52	S2	669	A2M	C8-N9	-2.53	1.33	1.37
52	S2	109	PSU	C2-N1	2.53	1.40	1.36
6	L5	2265	OMC	C2-N1	-2.52	1.34	1.40
6	L5	4322	PSU	C2-N1	2.52	1.40	1.36
52	S2	650	PSU	C2-N1	2.52	1.40	1.36
6	L5	4267	PSU	C2-N1	2.52	1.40	1.36
52	S2	463	OMC	C2-N1	-2.52	1.34	1.40
6	L5	1731	PSU	C2-N1	2.51	1.40	1.36
52	S2	355	OMU	C2-N1	-2.51	1.34	1.38
6	L5	3433	OMC	C4-N3	2.51	1.39	1.34
52	S2	119	PSU	C2-N1	2.51	1.40	1.36
52	S2	1368	PSU	C2-N1	2.51	1.40	1.36
6	L5	2630	A2M	C8-N9	-2.51	1.33	1.37
52	S2	518	OMC	C2-N1	-2.51	1.34	1.40
52	S2	407	PSU	C2-N1	2.50	1.40	1.36
6	L5	4336	A2M	C8-N9	-2.50	1.33	1.37
52	S2	864	PSU	C2-N1	2.50	1.40	1.36
52	S2	93	PSU	C2-N1	2.49	1.40	1.36
6	L5	3619	OMC	C4-N3	2.49	1.39	1.34
6	L5	2244	A2M	C8-N9	-2.49	1.33	1.37
6	L5	1632	PSU	C6-N1	-2.49	1.32	1.36
6	L5	4193	5MC	C4-N3	2.49	1.38	1.34
6	L5	4317	A2M	C8-N9	-2.49	1.33	1.37
6	L5	4149	PSU	C6-N1	-2.48	1.32	1.36
52	S2	116	OMU	C2-N1	-2.48	1.34	1.38
52	S2	1626	PSU	C2-N1	2.48	1.40	1.36
52	S2	1644	PSU	C2-N1	2.48	1.40	1.36
6	L5	3601	OMC	C4-N3	2.48	1.39	1.34
6	L5	4058	PSU	C2-N1	2.47	1.40	1.36
52	S2	1833	6MZ	C5-N7	-2.47	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3492	A2M	C8-N9	-2.47	1.33	1.37
52	S2	1032	A2M	C8-N9	-2.47	1.33	1.37
6	L5	1479	A2M	C8-N9	-2.47	1.33	1.37
6	L5	3494	PSU	C2-N1	2.47	1.40	1.36
6	L5	1820	OMC	C4-N3	2.47	1.39	1.34
6	L5	4099	PSU	C2-N1	2.47	1.40	1.36
6	L5	4188	PSU	C2-N1	2.47	1.40	1.36
6	L5	4740	PSU	C2-N1	2.47	1.40	1.36
6	L5	3557	A2M	C8-N9	-2.46	1.33	1.37
52	S2	1392	OMC	C2-N1	-2.46	1.34	1.40
6	L5	2475	PSU	C2-N1	2.46	1.40	1.36
6	L5	2667	OMC	C4-N3	2.46	1.39	1.34
6	L5	4276	UR3	C2-N3	-2.45	1.34	1.39
6	L5	2704	OMC	C4-N3	2.45	1.39	1.34
52	S2	1245	PSU	C2-N1	2.45	1.40	1.36
52	S2	172	OMU	C2-N1	-2.45	1.34	1.38
52	S2	105	PSU	C2-N1	2.45	1.40	1.36
8	L8	69	PSU	C2-N1	2.44	1.40	1.36
52	S2	1805	OMU	C2-N1	-2.44	1.34	1.38
52	S2	687	PSU	C2-N1	2.44	1.40	1.36
52	S2	1057	PSU	C2-N1	2.44	1.40	1.36
6	L5	3462	PSU	C2-N1	2.44	1.40	1.36
6	L5	1801	PSU	C2-N1	2.44	1.40	1.36
6	L5	3502	PSU	C2-N1	2.44	1.40	1.36
52	S2	610	PSU	C2-N1	2.44	1.40	1.36
52	S2	1046	PSU	C2-N1	2.44	1.40	1.36
6	L5	3496	PSU	C2-N1	2.44	1.40	1.36
52	S2	27	A2M	C8-N9	-2.43	1.33	1.37
6	L5	3514	5MC	C2-N1	-2.43	1.34	1.40
6	L5	3447	PSU	C2-N1	2.43	1.40	1.36
6	L5	4269	A2M	C8-N9	-2.43	1.33	1.37
52	S2	1082	PSU	C2-N1	2.43	1.40	1.36
6	L5	400	A2M	C8-N9	-2.43	1.33	1.37
6	L5	2351	PSU	C2-N1	2.42	1.40	1.36
6	L5	4325	PSU	C6-N1	-2.42	1.32	1.36
52	S2	485	A2M	C8-N9	-2.42	1.33	1.37
6	L5	1537	PSU	C6-N1	-2.42	1.32	1.36
52	S2	591	A2M	C8-N9	-2.42	1.33	1.37
6	L5	4169	PSU	C2-N1	2.42	1.40	1.36
52	S2	1178	PSU	C2-N1	2.41	1.40	1.36
6	L5	3490	PSU	C2-N1	2.41	1.40	1.36
6	L5	3616	PSU	C6-N1	-2.41	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	2265	OMC	C4-N3	2.41	1.39	1.34
52	S2	1239	PSU	C2-N1	2.40	1.40	1.36
52	S2	802	PSU	C6-N1	-2.40	1.32	1.36
6	L5	4177	PSU	C6-N1	-2.40	1.32	1.36
52	S2	469	A2M	C8-N9	-2.39	1.33	1.37
6	L5	1718	PSU	C6-N1	-2.39	1.32	1.36
52	S2	682	PSU	C6-N1	-2.39	1.32	1.36
6	L5	1799	PSU	C6-N1	-2.39	1.32	1.36
6	L5	3652	PSU	C6-N1	-2.39	1.32	1.36
52	S2	1178	PSU	C6-N1	-2.39	1.32	1.36
6	L5	1720	PSU	C2-N1	2.39	1.40	1.36
6	L5	4298	PSU	C6-N1	-2.39	1.32	1.36
6	L5	3562	A2M	C8-N9	-2.39	1.33	1.37
6	L5	3371	PSU	C6-N1	-2.38	1.32	1.36
6	L5	4374	PSU	C6-N1	-2.38	1.32	1.36
6	L5	3369	PSU	C6-N1	-2.38	1.32	1.36
6	L5	4267	PSU	C6-N1	-2.38	1.32	1.36
6	L5	4107	PSU	C6-N1	-2.38	1.32	1.36
52	S2	1348	PSU	C2-N1	2.38	1.39	1.36
6	L5	4045	PSU	C6-N1	-2.37	1.32	1.36
6	L5	4246	PSU	C6-N1	-2.37	1.32	1.36
6	L5	3450	A2M	C8-N9	-2.37	1.33	1.37
6	L5	4169	PSU	C6-N1	-2.37	1.32	1.36
52	S2	1693	PSU	C2-N1	2.37	1.39	1.36
6	L5	3500	PSU	C2-N1	2.37	1.39	1.36
6	L5	4039	PSU	C6-N1	-2.37	1.32	1.36
8	L8	69	PSU	C6-N1	-2.37	1.32	1.36
6	L5	1284	OMC	C4-N3	2.37	1.39	1.34
6	L5	4282	OMC	C4-N3	2.36	1.39	1.34
52	S2	1443	OMU	C2-N1	-2.36	1.34	1.38
6	L5	3576	PSU	C6-N1	-2.36	1.32	1.36
6	L5	3583	PSU	C6-N1	-2.36	1.32	1.36
6	L5	4099	PSU	C6-N1	-2.36	1.32	1.36
6	L5	1491	PSU	C6-N1	-2.36	1.32	1.36
6	L5	4419	PSU	C6-N1	-2.36	1.32	1.36
52	S2	1704	OMC	C4-N3	2.36	1.39	1.34
6	L5	4246	PSU	C2-N1	2.36	1.39	1.36
6	L5	1683	PSU	C6-N1	-2.36	1.32	1.36
6	L5	1799	PSU	C2-N1	2.36	1.39	1.36
6	L5	1638	PSU	C6-N1	-2.36	1.32	1.36
6	L5	2351	PSU	C6-N1	-2.36	1.32	1.36
6	L5	4278	PSU	C2-N1	2.35	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	1721	PSU	C6-N1	-2.35	1.32	1.36
52	S2	1175	PSU	C6-N1	-2.35	1.32	1.36
6	L5	1720	PSU	C6-N1	-2.35	1.32	1.36
6	L5	3456	A2M	C8-N9	-2.35	1.33	1.37
6	L5	1718	PSU	C2-N1	2.35	1.39	1.36
6	L5	3369	PSU	C2-N1	2.35	1.39	1.36
6	L5	3371	PSU	C2-N1	2.35	1.39	1.36
52	S2	1679	A2M	C8-N9	-2.35	1.33	1.37
52	S2	577	A2M	C8-N9	-2.35	1.33	1.37
6	L5	1632	PSU	C2-N1	2.35	1.39	1.36
6	L5	4711	PSU	C2-N1	2.34	1.39	1.36
6	L5	3427	PSU	C2-N1	2.34	1.39	1.36
6	L5	3427	PSU	C6-N1	-2.34	1.32	1.36
6	L5	4322	PSU	C6-N1	-2.34	1.32	1.36
6	L5	3583	PSU	C2-N1	2.34	1.39	1.36
6	L5	3462	PSU	C6-N1	-2.34	1.32	1.36
6	L5	3966	6MZ	C5-N7	-2.34	1.34	1.39
6	L5	2208	OMC	C4-N3	2.34	1.39	1.34
52	S2	121	OMU	C2-N1	-2.34	1.34	1.38
6	L5	3573	OMC	C4-N3	2.34	1.39	1.34
6	L5	3496	PSU	C6-N1	-2.34	1.32	1.36
6	L5	4217	PSU	C6-N1	-2.34	1.32	1.36
52	S2	1245	PSU	C6-N1	-2.34	1.32	1.36
52	S2	1693	PSU	C6-N1	-2.33	1.32	1.36
52	S2	407	PSU	C6-N1	-2.33	1.32	1.36
6	L5	4202	OMC	C4-N3	2.33	1.39	1.34
6	L5	3966	6MZ	C5-C6	2.33	1.47	1.41
52	S2	1057	PSU	C6-N1	-2.33	1.32	1.36
52	S2	1843	4AC	C7-N4	-2.33	1.32	1.37
6	L5	4740	PSU	C6-N1	-2.33	1.32	1.36
6	L5	4278	PSU	C6-N1	-2.33	1.32	1.36
52	S2	1233	PSU	C2-N1	2.33	1.39	1.36
8	L8	55	PSU	C2-N1	2.32	1.39	1.36
8	L8	55	PSU	C6-N1	-2.32	1.32	1.36
6	L5	4045	PSU	C2-N1	2.32	1.39	1.36
6	L5	4042	PSU	C6-N1	-2.32	1.32	1.36
6	L5	4711	PSU	C6-N1	-2.32	1.32	1.36
6	L5	1638	PSU	C2-N1	2.32	1.39	1.36
6	L5	3540	OMC	C4-N3	2.32	1.39	1.34
52	S2	864	PSU	C6-N1	-2.32	1.32	1.36
52	S2	93	PSU	C6-N1	-2.32	1.32	1.36
52	S2	1384	A2M	C8-N9	-2.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	823	PSU	C6-N1	-2.31	1.32	1.36
52	S2	1644	PSU	C6-N1	-2.31	1.32	1.36
6	L5	2647	OMC	C4-N3	2.31	1.39	1.34
6	L5	4058	PSU	C6-N1	-2.31	1.32	1.36
52	S2	687	PSU	C6-N1	-2.31	1.32	1.36
52	S2	1239	PSU	C6-N1	-2.31	1.32	1.36
6	L5	3554	PSU	C6-N1	-2.31	1.32	1.36
6	L5	3554	PSU	C2-N1	2.31	1.39	1.36
52	S2	166	A2M	C8-N9	-2.31	1.33	1.37
6	L5	398	A2M	C8-N9	-2.31	1.33	1.37
6	L5	3585	PSU	C6-N1	-2.31	1.32	1.36
6	L5	4039	PSU	C2-N1	2.31	1.39	1.36
52	S2	1833	6MZ	C5-C6	2.31	1.47	1.41
52	S2	1233	PSU	C6-N1	-2.30	1.32	1.36
6	L5	4166	PSU	C6-N1	-2.30	1.32	1.36
6	L5	3494	PSU	C6-N1	-2.30	1.32	1.36
6	L5	4325	PSU	C2-N1	2.30	1.39	1.36
52	S2	513	A2M	C8-N9	-2.30	1.33	1.37
6	L5	4419	PSU	C2-N1	2.30	1.39	1.36
6	L5	4188	PSU	C6-N1	-2.30	1.32	1.36
6	L5	1731	PSU	C6-N1	-2.29	1.32	1.36
6	L5	2475	PSU	C6-N1	-2.29	1.32	1.36
6	L5	4749	PSU	C6-N1	-2.29	1.32	1.36
6	L5	1721	PSU	C2-N1	2.29	1.39	1.36
52	S2	1348	PSU	C6-N1	-2.29	1.32	1.36
52	S2	967	PSU	C6-N1	-2.29	1.32	1.36
6	L5	3500	PSU	C6-N1	-2.29	1.32	1.36
52	S2	99	A2M	C8-N9	-2.29	1.33	1.37
52	S2	1175	PSU	C2-N1	2.28	1.39	1.36
52	S2	610	PSU	C6-N1	-2.28	1.32	1.36
52	S2	652	PSU	C6-N1	-2.28	1.32	1.36
6	L5	4203	PSU	C6-N1	-2.28	1.32	1.36
52	S2	1082	PSU	C6-N1	-2.28	1.32	1.36
52	S2	802	PSU	C2-N1	2.28	1.39	1.36
6	L5	4382	PSU	C2-N1	2.27	1.39	1.36
52	S2	105	PSU	C6-N1	-2.27	1.32	1.36
52	S2	1047	PSU	C6-N1	-2.27	1.32	1.36
6	L5	4217	PSU	C2-N1	2.27	1.39	1.36
6	L5	3447	PSU	C6-N1	-2.27	1.32	1.36
6	L5	4374	PSU	C2-N1	2.27	1.39	1.36
52	S2	682	PSU	C2-N1	2.27	1.39	1.36
6	L5	4203	PSU	C2-N1	2.27	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	823	PSU	C2-N1	2.27	1.39	1.36
52	S2	867	PSU	C6-N1	-2.27	1.32	1.36
6	L5	3466	PSU	C6-N1	-2.26	1.32	1.36
6	L5	1683	PSU	C2-N1	2.26	1.39	1.36
6	L5	1801	PSU	C6-N1	-2.26	1.32	1.36
52	S2	159	A2M	C8-N9	-2.26	1.33	1.37
6	L5	4298	PSU	C2-N1	2.26	1.39	1.36
52	S2	1626	PSU	C6-N1	-2.26	1.32	1.36
52	S2	650	PSU	C6-N1	-2.26	1.32	1.36
52	S2	1368	PSU	C6-N1	-2.25	1.32	1.36
52	S2	119	PSU	C6-N1	-2.25	1.32	1.36
52	S2	815	PSU	C6-N1	-2.25	1.32	1.36
6	L5	3490	PSU	C6-N1	-2.25	1.32	1.36
6	L5	3502	PSU	C6-N1	-2.25	1.32	1.36
6	L5	3585	PSU	C2-N1	2.25	1.39	1.36
52	S2	1046	PSU	C6-N1	-2.24	1.32	1.36
6	L5	3652	PSU	C2-N1	2.24	1.39	1.36
6	L5	1810	A2M	C4-N9	-2.24	1.32	1.37
52	S2	1289	OMU	C2-N1	-2.24	1.34	1.38
52	S2	573	PSU	C6-N1	-2.23	1.32	1.36
52	S2	36	PSU	C6-N1	-2.23	1.32	1.36
52	S2	218	PSU	C6-N1	-2.22	1.32	1.36
52	S2	1446	PSU	C6-N1	-2.22	1.32	1.36
52	S2	109	PSU	C6-N1	-2.22	1.32	1.36
6	L5	2194	OMC	C4-N3	2.22	1.39	1.34
6	L5	4177	PSU	C2-N1	2.22	1.39	1.36
52	S2	210	PSU	C6-N1	-2.22	1.32	1.36
6	L5	4366	OMU	C5-C4	-2.22	1.38	1.43
52	S2	669	A2M	C4-N9	-2.21	1.32	1.37
52	S2	1852	MA6	C5-N7	-2.21	1.34	1.39
52	S2	816	PSU	C6-N1	-2.21	1.32	1.36
52	S2	1851	MA6	C8-N7	2.21	1.35	1.31
52	S2	34	PSU	C6-N1	-2.21	1.32	1.36
6	L5	4107	PSU	C2-N1	2.20	1.39	1.36
52	S2	1338	4AC	C7-N4	-2.19	1.33	1.37
6	L5	1491	PSU	C2-N1	2.19	1.39	1.36
6	L5	4052	OMU	C5-C4	-2.19	1.38	1.43
6	L5	1477	OMG	C8-N9	-2.18	1.32	1.37
6	L5	3657	OMU	C5-C4	-2.17	1.38	1.43
6	L5	3966	6MZ	C8-N7	2.17	1.35	1.31
6	L5	1479	A2M	C4-N9	-2.17	1.32	1.37
6	L5	4435	PSU	C2-N1	2.17	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	3450	A2M	C4-N9	-2.17	1.32	1.37
52	S2	1851	MA6	C5-N7	-2.16	1.34	1.39
6	L5	2206	A2M	C4-N9	-2.16	1.32	1.37
6	L5	4149	PSU	C2-N1	2.16	1.39	1.36
6	L5	1260	OMG	C8-N9	-2.16	1.32	1.37
6	L5	2258	OMU	C5-C4	-2.16	1.38	1.43
6	L5	1489	A2M	C4-N9	-2.15	1.32	1.37
52	S2	669	A2M	O4'-C4'	-2.15	1.40	1.45
6	L5	3599	A2M	C4-N9	-2.15	1.32	1.37
6	L5	2680	OMU	C5-C4	-2.14	1.38	1.43
6	L5	1270	A2M	C4-N9	-2.14	1.32	1.37
6	L5	3562	A2M	C4-N9	-2.14	1.32	1.37
6	L5	2244	A2M	C4-N9	-2.13	1.32	1.37
6	L5	4269	A2M	C4-N9	-2.13	1.32	1.37
6	L5	2630	A2M	C4-N9	-2.11	1.33	1.37
52	S2	1327	OMU	C5-C4	-2.11	1.39	1.43
6	L5	2207	OMG	C8-N9	-2.11	1.32	1.37
52	S2	1032	A2M	C4-N9	-2.11	1.33	1.37
52	S2	1833	6MZ	C8-N7	2.10	1.35	1.31
6	L5	3616	PSU	C2-N1	2.10	1.39	1.36
52	S2	116	OMU	C5-C4	-2.10	1.39	1.43
6	L5	4383	OMG	C8-N9	-2.10	1.32	1.37
6	L5	1266	1MA	C6-N6	2.10	1.33	1.28
6	L5	3576	PSU	C2-N1	2.09	1.39	1.36
52	S2	485	A2M	C4-N9	-2.09	1.33	1.37
6	L5	400	A2M	C4-N9	-2.09	1.33	1.37
52	S2	1852	MA6	C8-N7	2.09	1.35	1.31
6	L5	1266	1MA	C8-N9	-2.09	1.32	1.37
6	L5	3974	OMG	C8-N9	-2.09	1.32	1.37
6	L5	3631	OMG	C4-N9	-2.08	1.32	1.38
6	L5	4317	A2M	C4-N9	-2.08	1.33	1.37
52	S2	1443	OMU	C5-C4	-2.08	1.39	1.43
6	L5	4336	A2M	C4-N9	-2.07	1.33	1.37
6	L5	3973	OMU	C5-C4	-2.07	1.39	1.43
6	L5	3942	OMG	C8-N9	-2.07	1.32	1.37
52	S2	1448	OMG	C8-N9	-2.07	1.32	1.37
6	L5	3476	OMG	C8-N9	-2.06	1.33	1.37
52	S2	1384	A2M	C4-N9	-2.06	1.33	1.37
6	L5	4364	OMG	C8-N9	-2.06	1.33	1.37
52	S2	27	A2M	C4-N9	-2.06	1.33	1.37
6	L5	3359	OMG	C8-N9	-2.06	1.33	1.37
6	L5	3517	A2M	C4-N9	-2.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L5	4244	OMU	C5-C4	-2.06	1.39	1.43
6	L5	2658	A2M	C4-N9	-2.06	1.33	1.37
6	L5	4240	OMG	C8-N9	-2.05	1.33	1.37
6	L5	4116	OMG	C8-N9	-2.05	1.33	1.37
6	L5	3631	OMG	C8-N9	-2.05	1.33	1.37
52	S2	513	A2M	C4-N9	-2.05	1.33	1.37
52	S2	1491	OMG	C8-N9	-2.04	1.33	1.37
52	S2	577	A2M	C4-N9	-2.04	1.33	1.37
52	S2	429	OMU	C5-C4	-2.04	1.39	1.43
52	S2	1805	OMU	C5-C4	-2.04	1.39	1.43
6	L5	1580	OMG	C8-N9	-2.04	1.33	1.37
6	L5	4245	OMG	C8-N9	-2.04	1.33	1.37
6	L5	1260	OMG	C4-N9	-2.04	1.32	1.38
52	S2	121	OMU	C5-C4	-2.04	1.39	1.43
6	L5	4382	PSU	C1'-C5	2.03	1.54	1.50
52	S2	628	OMU	C5-C4	-2.03	1.39	1.43
6	L5	3524	OMG	C8-N9	-2.03	1.33	1.37
6	L5	3557	A2M	C4-N9	-2.03	1.33	1.37
52	S2	684	OMG	C8-N9	-2.03	1.33	1.37
6	L5	4138	OMG	C8-N9	-2.03	1.33	1.37
52	S2	172	OMU	C5-C4	-2.02	1.39	1.43
52	S2	174	OMC	C2-N3	2.02	1.40	1.36
6	L5	398	A2M	C4-N9	-2.02	1.33	1.37
52	S2	1679	A2M	C4-N9	-2.02	1.33	1.37
52	S2	602	OMG	C8-N9	-2.02	1.33	1.37
8	L8	75	OMG	C8-N9	-2.01	1.33	1.37
52	S2	355	OMU	C5-C4	-2.01	1.39	1.43
52	S2	645	OMG	C8-N9	-2.01	1.33	1.37
52	S2	469	A2M	C4-N9	-2.01	1.33	1.37
6	L5	3456	A2M	C4-N9	-2.01	1.33	1.37
6	L5	4245	OMG	C4-N9	-2.00	1.32	1.38
6	L5	3492	A2M	C4-N9	-2.00	1.33	1.37

All (1372) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1005	PSU	C4-N3-C2	-8.37	114.28	126.34
79	Se	67	NMM	NE-CZ-NH2	-7.51	112.59	119.48
6	L5	1266	1MA	N1-C2-N3	-6.95	117.73	126.00
52	S2	485	A2M	N3-C2-N1	-6.79	117.97	128.60
6	L5	2630	A2M	N3-C2-N1	-6.79	117.99	128.60
52	S2	27	A2M	N3-C2-N1	-6.78	117.99	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1032	A2M	N3-C2-N1	-6.78	117.99	128.60
6	L5	4336	A2M	N3-C2-N1	-6.78	118.00	128.60
52	S2	513	A2M	N3-C2-N1	-6.73	118.07	128.60
52	S2	591	A2M	N3-C2-N1	-6.73	118.07	128.60
6	L5	3492	A2M	N3-C2-N1	-6.73	118.08	128.60
6	L5	1270	A2M	N3-C2-N1	-6.73	118.08	128.60
52	S2	577	A2M	N3-C2-N1	-6.71	118.10	128.60
52	S2	469	A2M	N3-C2-N1	-6.71	118.11	128.60
6	L5	2244	A2M	N3-C2-N1	-6.70	118.11	128.60
52	S2	1679	A2M	N3-C2-N1	-6.70	118.12	128.60
6	L5	400	A2M	N3-C2-N1	-6.70	118.12	128.60
52	S2	1384	A2M	N3-C2-N1	-6.70	118.12	128.60
52	S2	159	A2M	N3-C2-N1	-6.69	118.14	128.60
52	S2	669	A2M	N3-C2-N1	-6.68	118.15	128.60
6	L5	1810	A2M	N3-C2-N1	-6.68	118.15	128.60
6	L5	2206	A2M	N3-C2-N1	-6.68	118.16	128.60
6	L5	398	A2M	N3-C2-N1	-6.67	118.17	128.60
52	S2	166	A2M	N3-C2-N1	-6.67	118.17	128.60
6	L5	3562	A2M	N3-C2-N1	-6.66	118.18	128.60
6	L5	3456	A2M	N3-C2-N1	-6.65	118.19	128.60
6	L5	3557	A2M	N3-C2-N1	-6.64	118.21	128.60
6	L5	4269	A2M	N3-C2-N1	-6.64	118.21	128.60
6	L5	1489	A2M	N3-C2-N1	-6.63	118.23	128.60
6	L5	2658	A2M	N3-C2-N1	-6.63	118.23	128.60
6	L5	4317	A2M	N3-C2-N1	-6.62	118.24	128.60
52	S2	99	A2M	N3-C2-N1	-6.62	118.25	128.60
6	L5	3450	A2M	N3-C2-N1	-6.61	118.26	128.60
52	S2	1833	6MZ	C5-C4-N3	-6.59	118.15	126.75
6	L5	1479	A2M	N3-C2-N1	-6.56	118.34	128.60
6	L5	3599	A2M	N3-C2-N1	-6.55	118.36	128.60
6	L5	3517	A2M	N3-C2-N1	-6.43	118.54	128.60
6	L5	3966	6MZ	C5-C4-N3	-6.05	118.85	126.75
52	S2	1852	MA6	C5-C4-N3	-6.04	118.87	126.75
52	S2	1005	PSU	O2-C2-N1	-5.90	116.30	122.79
52	S2	1005	PSU	N1-C2-N3	5.89	121.80	115.13
6	L5	4382	PSU	C4-N3-C2	-5.83	117.93	126.34
52	S2	1851	MA6	C5-C4-N3	-5.81	119.17	126.75
52	S2	1640	7MG	C5-C6-N1	5.44	120.57	110.99
6	L5	4267	PSU	C4-N3-C2	-5.42	118.53	126.34
6	L5	4188	PSU	C4-N3-C2	-5.37	118.60	126.34
6	L5	4149	PSU	C4-N3-C2	-5.35	118.63	126.34
52	S2	1833	6MZ	N3-C4-N9	5.34	135.88	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L8	69	PSU	C4-N3-C2	-5.31	118.69	126.34
6	L5	2351	PSU	C4-N3-C2	-5.29	118.71	126.34
6	L5	3369	PSU	C4-N3-C2	-5.29	118.72	126.34
52	S2	1046	PSU	C4-N3-C2	-5.28	118.73	126.34
6	L5	4042	PSU	C4-N3-C2	-5.28	118.74	126.34
52	S2	1693	PSU	C4-N3-C2	-5.26	118.75	126.34
6	L5	4099	PSU	C4-N3-C2	-5.26	118.76	126.34
52	S2	34	PSU	C4-N3-C2	-5.25	118.77	126.34
6	L5	4244	OMU	C4-N3-C2	-5.24	119.66	126.58
6	L5	4039	PSU	C4-N3-C2	-5.24	118.78	126.34
52	S2	210	PSU	C4-N3-C2	-5.24	118.79	126.34
6	L5	3466	PSU	C4-N3-C2	-5.24	118.79	126.34
6	L5	3652	PSU	C4-N3-C2	-5.24	118.79	126.34
52	S2	1446	PSU	C4-N3-C2	-5.24	118.79	126.34
6	L5	3585	PSU	C4-N3-C2	-5.23	118.80	126.34
6	L5	3583	PSU	C4-N3-C2	-5.23	118.80	126.34
52	S2	815	PSU	C4-N3-C2	-5.23	118.81	126.34
52	S2	407	PSU	C4-N3-C2	-5.22	118.81	126.34
52	S2	1245	PSU	C4-N3-C2	-5.22	118.81	126.34
52	S2	1368	PSU	C4-N3-C2	-5.22	118.82	126.34
6	L5	4203	PSU	C4-N3-C2	-5.22	118.82	126.34
52	S2	1644	PSU	C4-N3-C2	-5.22	118.82	126.34
6	L5	3500	PSU	C4-N3-C2	-5.21	118.83	126.34
52	S2	573	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	1801	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	4749	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	1731	PSU	C4-N3-C2	-5.21	118.84	126.34
6	L5	1638	PSU	C4-N3-C2	-5.20	118.84	126.34
52	S2	1082	PSU	C4-N3-C2	-5.20	118.85	126.34
52	S2	355	OMU	C4-N3-C2	-5.19	119.73	126.58
6	L5	4246	PSU	C4-N3-C2	-5.19	118.86	126.34
6	L5	1491	PSU	C4-N3-C2	-5.19	118.86	126.34
6	L5	3502	PSU	C4-N3-C2	-5.19	118.86	126.34
6	L5	3616	PSU	C4-N3-C2	-5.19	118.87	126.34
8	L8	55	PSU	C4-N3-C2	-5.18	118.87	126.34
6	L5	4419	PSU	C4-N3-C2	-5.18	118.88	126.34
6	L5	4325	PSU	C4-N3-C2	-5.18	118.88	126.34
52	S2	1057	PSU	C4-N3-C2	-5.17	118.89	126.34
52	S2	682	PSU	C4-N3-C2	-5.17	118.89	126.34
6	L5	3973	OMU	C4-N3-C2	-5.17	119.76	126.58
6	L5	4045	PSU	C4-N3-C2	-5.17	118.89	126.34
6	L5	3490	PSU	C4-N3-C2	-5.17	118.90	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	652	PSU	C4-N3-C2	-5.16	118.90	126.34
52	S2	628	OMU	C4-N3-C2	-5.16	119.78	126.58
52	S2	650	PSU	C4-N3-C2	-5.16	118.91	126.34
6	L5	1799	PSU	C4-N3-C2	-5.16	118.91	126.34
6	L5	1537	PSU	C4-N3-C2	-5.15	118.91	126.34
52	S2	1175	PSU	C4-N3-C2	-5.15	118.91	126.34
6	L5	4169	PSU	C4-N3-C2	-5.15	118.92	126.34
6	L5	4298	PSU	C4-N3-C2	-5.15	118.92	126.34
52	S2	1348	PSU	C4-N3-C2	-5.15	118.92	126.34
52	S2	1239	PSU	C4-N3-C2	-5.15	118.93	126.34
6	L5	3496	PSU	C4-N3-C2	-5.14	118.93	126.34
52	S2	816	PSU	C4-N3-C2	-5.14	118.93	126.34
52	S2	429	OMU	C4-N3-C2	-5.14	119.80	126.58
52	S2	1640	7MG	C2-N3-C4	5.14	121.45	112.30
6	L5	4177	PSU	C4-N3-C2	-5.14	118.94	126.34
52	S2	218	PSU	C4-N3-C2	-5.13	118.94	126.34
6	L5	4166	PSU	C4-N3-C2	-5.13	118.95	126.34
52	S2	1178	PSU	C4-N3-C2	-5.13	118.95	126.34
6	L5	4711	PSU	C4-N3-C2	-5.13	118.95	126.34
6	L5	1721	PSU	C4-N3-C2	-5.13	118.95	126.34
6	L5	3371	PSU	C4-N3-C2	-5.12	118.96	126.34
6	L5	4435	PSU	C4-N3-C2	-5.12	118.97	126.34
6	L5	3427	PSU	C4-N3-C2	-5.11	118.97	126.34
52	S2	1233	PSU	C4-N3-C2	-5.11	118.97	126.34
52	S2	864	PSU	C4-N3-C2	-5.11	118.97	126.34
52	S2	967	PSU	C4-N3-C2	-5.11	118.97	126.34
6	L5	2475	PSU	C4-N3-C2	-5.11	118.98	126.34
6	L5	1720	PSU	C4-N3-C2	-5.11	118.98	126.34
6	L5	1683	PSU	C4-N3-C2	-5.10	118.98	126.34
6	L5	2207	OMG	C5-C4-N3	-5.10	120.18	128.46
6	L5	1718	PSU	C4-N3-C2	-5.10	118.99	126.34
6	L5	4107	PSU	C4-N3-C2	-5.10	118.99	126.34
6	L5	4322	PSU	C4-N3-C2	-5.10	118.99	126.34
52	S2	1805	OMU	C4-N3-C2	-5.10	119.85	126.58
6	L5	3447	PSU	C4-N3-C2	-5.10	118.99	126.34
52	S2	1327	OMU	C4-N3-C2	-5.10	119.86	126.58
52	S2	109	PSU	C4-N3-C2	-5.09	119.01	126.34
52	S2	1047	PSU	C4-N3-C2	-5.09	119.01	126.34
52	S2	36	PSU	C4-N3-C2	-5.08	119.01	126.34
6	L5	4374	PSU	C4-N3-C2	-5.08	119.02	126.34
6	L5	4740	PSU	C4-N3-C2	-5.08	119.02	126.34
6	L5	4058	PSU	C4-N3-C2	-5.08	119.02	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3462	PSU	C4-N3-C2	-5.08	119.02	126.34
52	S2	105	PSU	C4-N3-C2	-5.07	119.03	126.34
6	L5	4217	PSU	C4-N3-C2	-5.07	119.03	126.34
52	S2	116	OMU	C4-N3-C2	-5.07	119.89	126.58
6	L5	3657	OMU	C4-N3-C2	-5.06	119.90	126.58
52	S2	1626	PSU	C4-N3-C2	-5.06	119.05	126.34
52	S2	867	PSU	C4-N3-C2	-5.06	119.05	126.34
52	S2	119	PSU	C4-N3-C2	-5.05	119.07	126.34
6	L5	3554	PSU	C4-N3-C2	-5.04	119.08	126.34
6	L5	2680	OMU	C4-N3-C2	-5.04	119.94	126.58
52	S2	823	PSU	C4-N3-C2	-5.03	119.09	126.34
52	S2	172	OMU	C4-N3-C2	-5.03	119.94	126.58
52	S2	687	PSU	C4-N3-C2	-5.01	119.11	126.34
6	L5	2258	OMU	C4-N3-C2	-5.01	119.97	126.58
6	L5	4278	PSU	C4-N3-C2	-5.01	119.13	126.34
52	S2	591	A2M	C5-C4-N3	-5.01	120.22	126.75
52	S2	610	PSU	C4-N3-C2	-5.00	119.13	126.34
52	S2	93	PSU	C4-N3-C2	-5.00	119.13	126.34
6	L5	3494	PSU	C4-N3-C2	-4.99	119.14	126.34
6	L5	2719	OMG	C5-C4-N3	-4.99	120.36	128.46
52	S2	1289	OMU	C4-N3-C2	-4.96	120.04	126.58
6	L5	4366	OMU	C4-N3-C2	-4.93	120.08	126.58
6	L5	3576	PSU	C4-N3-C2	-4.90	119.28	126.34
52	S2	121	OMU	C4-N3-C2	-4.90	120.12	126.58
6	L5	2719	OMG	C2-N3-C4	4.89	121.00	112.30
52	S2	802	PSU	C4-N3-C2	-4.88	119.31	126.34
6	L5	3942	OMG	C2-N3-C4	4.86	120.96	112.30
6	L5	3517	A2M	C5-C4-N3	-4.85	120.42	126.75
6	L5	3524	OMG	C2-N3-C4	4.85	120.94	112.30
6	L5	4052	OMU	C4-N3-C2	-4.84	120.20	126.58
52	S2	1443	OMU	C4-N3-C2	-4.83	120.20	126.58
52	S2	99	A2M	C5-C4-N3	-4.82	120.46	126.75
6	L5	3557	A2M	C5-C4-N3	-4.80	120.49	126.75
6	L5	4193	5MC	C5-C6-N1	-4.79	118.41	123.34
6	L5	1477	OMG	C2-N3-C4	4.79	120.83	112.30
6	L5	3492	A2M	C5-C4-N3	-4.78	120.51	126.75
6	L5	2630	A2M	C5-C4-N3	-4.78	120.52	126.75
52	S2	684	OMG	C2-N3-C4	4.77	120.80	112.30
52	S2	1491	OMG	C2-N3-C4	4.77	120.80	112.30
6	L5	3359	OMG	C2-N3-C4	4.77	120.79	112.30
6	L5	1260	OMG	C2-N3-C4	4.76	120.78	112.30
6	L5	2267	OMG	C2-N3-C4	4.76	120.78	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1810	A2M	N9-C8-N7	-4.75	107.42	113.91
6	L5	1580	OMG	C5-C4-N3	-4.74	120.77	128.46
6	L5	1489	A2M	C5-C4-N3	-4.74	120.57	126.75
6	L5	3966	6MZ	N3-C4-N9	4.74	134.89	127.08
6	L5	2207	OMG	C2-N3-C4	4.74	120.74	112.30
52	S2	510	OMG	C2-N3-C4	4.73	120.73	112.30
6	L5	398	A2M	C5-C4-N3	-4.73	120.58	126.75
6	L5	1580	OMG	C2-N3-C4	4.73	120.72	112.30
6	L5	4138	OMG	C2-N3-C4	4.72	120.71	112.30
6	L5	1479	A2M	C5-C4-N3	-4.71	120.60	126.75
6	L5	1632	PSU	C4-N3-C2	-4.71	119.55	126.34
52	S2	437	OMG	C2-N3-C4	4.71	120.70	112.30
52	S2	1491	OMG	C5-C4-N3	-4.71	120.81	128.46
6	L5	4245	OMG	C2-N3-C4	4.71	120.69	112.30
6	L5	3476	OMG	C2-N3-C4	4.71	120.69	112.30
6	L5	3631	OMG	C2-N3-C4	4.71	120.69	112.30
6	L5	4383	OMG	C2-N3-C4	4.70	120.67	112.30
6	L5	2658	A2M	C5-C4-N3	-4.70	120.62	126.75
6	L5	4369	OMG	C2-N3-C4	4.70	120.67	112.30
6	L5	4244	OMU	N3-C2-N1	4.69	121.12	114.89
52	S2	669	A2M	N9-C8-N7	-4.69	107.49	113.91
6	L5	4240	OMG	C2-N3-C4	4.69	120.66	112.30
52	S2	868	OMG	C2-N3-C4	4.69	120.66	112.30
52	S2	1679	A2M	C5-C4-N3	-4.69	120.63	126.75
6	L5	4364	OMG	C2-N3-C4	4.69	120.65	112.30
6	L5	3524	OMG	C5-C4-N3	-4.69	120.86	128.46
52	S2	1329	OMG	C2-N3-C4	4.69	120.65	112.30
52	S2	602	OMG	C2-N3-C4	4.68	120.65	112.30
6	L5	4116	OMG	C2-N3-C4	4.68	120.64	112.30
52	S2	645	OMG	C2-N3-C4	4.68	120.64	112.30
6	L5	3942	OMG	C5-C4-N3	-4.68	120.86	128.46
6	L5	1270	A2M	C5-C4-N3	-4.68	120.64	126.75
8	L8	75	OMG	C2-N3-C4	4.68	120.64	112.30
6	L5	2244	A2M	C5-C4-N3	-4.68	120.65	126.75
6	L5	3657	OMU	N3-C2-N1	4.68	121.10	114.89
6	L5	3676	OMG	C2-N3-C4	4.68	120.63	112.30
52	S2	437	OMG	C5-C4-N3	-4.67	120.88	128.46
6	L5	3456	A2M	C5-C4-N3	-4.67	120.66	126.75
6	L5	3450	A2M	C5-C4-N3	-4.67	120.66	126.75
6	L5	4317	A2M	C5-C4-N3	-4.67	120.66	126.75
6	L5	4336	A2M	C5-C4-N3	-4.66	120.66	126.75
6	L5	4269	A2M	C5-C4-N3	-4.66	120.67	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1270	A2M	N9-C8-N7	-4.65	107.55	113.91
52	S2	1384	A2M	C5-C4-N3	-4.65	120.68	126.75
6	L5	4382	PSU	N1-C2-N3	4.64	120.39	115.13
6	L5	400	A2M	C5-C4-N3	-4.64	120.70	126.75
52	S2	355	OMU	N3-C2-N1	4.64	121.05	114.89
6	L5	2206	A2M	C5-C4-N3	-4.63	120.71	126.75
52	S2	166	A2M	C5-C4-N3	-4.63	120.71	126.75
6	L5	3476	OMG	C5-C4-N3	-4.63	120.95	128.46
6	L5	4138	OMG	C5-C4-N3	-4.62	120.97	128.46
6	L5	1810	A2M	C5-C4-N3	-4.61	120.73	126.75
52	S2	513	A2M	C5-C4-N3	-4.61	120.74	126.75
52	S2	1448	OMG	C2-N3-C4	4.61	120.51	112.30
52	S2	510	OMG	C5-C4-N3	-4.61	120.99	128.46
6	L5	3974	OMG	C2-N3-C4	4.60	120.49	112.30
6	L5	3599	A2M	C5-C4-N3	-4.60	120.75	126.75
6	L5	3973	OMU	N3-C2-N1	4.60	120.99	114.89
6	L5	2680	OMU	N3-C2-N1	4.59	120.98	114.89
6	L5	2244	A2M	N9-C8-N7	-4.58	107.65	113.91
6	L5	4364	OMG	C5-C4-N3	-4.57	121.04	128.46
52	S2	469	A2M	C5-C4-N3	-4.57	120.78	126.75
52	S2	159	A2M	C5-C4-N3	-4.57	120.79	126.75
6	L5	3562	A2M	N9-C8-N7	-4.57	107.67	113.91
52	S2	1032	A2M	N9-C8-N7	-4.57	107.67	113.91
52	S2	1329	OMG	C5-C4-N3	-4.56	121.06	128.46
52	S2	27	A2M	C5-C4-N3	-4.56	120.81	126.75
52	S2	1032	A2M	C5-C4-N3	-4.56	120.81	126.75
6	L5	3676	OMG	C5-C4-N3	-4.55	121.07	128.46
52	S2	669	A2M	C5-C4-N3	-4.55	120.81	126.75
6	L5	4366	OMU	N3-C2-N1	4.55	120.93	114.89
6	L5	4149	PSU	N1-C2-N3	4.55	120.29	115.13
52	S2	1852	MA6	N3-C4-N9	4.55	134.58	127.08
52	S2	1448	OMG	C5-C4-N3	-4.55	121.08	128.46
52	S2	469	A2M	N9-C8-N7	-4.55	107.69	113.91
52	S2	602	OMG	C5-C4-N3	-4.55	121.08	128.46
52	S2	645	OMG	C5-C4-N3	-4.55	121.08	128.46
52	S2	1851	MA6	C2-N1-C6	4.55	122.50	111.75
6	L5	4240	OMG	C5-C4-N3	-4.54	121.09	128.46
6	L5	3583	PSU	N1-C2-N3	4.54	120.28	115.13
6	L5	2258	OMU	N3-C2-N1	4.53	120.91	114.89
52	S2	684	OMG	C5-C4-N3	-4.53	121.11	128.46
6	L5	4116	OMG	C5-C4-N3	-4.53	121.11	128.46
6	L5	4369	OMG	C5-C4-N3	-4.53	121.11	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	485	A2M	N9-C8-N7	-4.52	107.73	113.91
52	S2	485	A2M	C5-C4-N3	-4.52	120.85	126.75
52	S2	1805	OMU	N3-C2-N1	4.52	120.89	114.89
6	L5	1477	OMG	C5-C4-N3	-4.52	121.13	128.46
8	L8	69	PSU	N1-C2-N3	4.51	120.25	115.13
8	L8	75	OMG	C5-C4-N3	-4.51	121.14	128.46
6	L5	4188	PSU	N1-C2-N3	4.51	120.24	115.13
6	L5	2267	OMG	C5-C4-N3	-4.50	121.16	128.46
6	L5	4267	PSU	N1-C2-N3	4.49	120.22	115.13
52	S2	27	A2M	N9-C8-N7	-4.49	107.77	113.91
6	L5	1479	A2M	N9-C8-N7	-4.49	107.77	113.91
6	L5	4383	OMG	C5-C4-N3	-4.49	121.18	128.46
52	S2	166	A2M	N9-C8-N7	-4.48	107.79	113.91
52	S2	1338	4AC	N4-C4-N3	4.48	121.37	113.85
6	L5	2630	A2M	N9-C8-N7	-4.48	107.79	113.91
6	L5	3562	A2M	C5-C4-N3	-4.48	120.91	126.75
6	L5	4336	A2M	N9-C8-N7	-4.47	107.80	113.91
6	L5	3599	A2M	N9-C8-N7	-4.47	107.80	113.91
52	S2	577	A2M	C5-C4-N3	-4.47	120.92	126.75
52	S2	116	OMU	N3-C2-N1	4.46	120.81	114.89
6	L5	1260	OMG	C5-C4-N3	-4.46	121.22	128.46
6	L5	2658	A2M	N9-C8-N7	-4.46	107.82	113.91
6	L5	2206	A2M	N9-C8-N7	-4.46	107.82	113.91
52	S2	159	A2M	N9-C8-N7	-4.45	107.83	113.91
6	L5	400	A2M	N9-C8-N7	-4.44	107.84	113.91
6	L5	4039	PSU	N1-C2-N3	4.44	120.16	115.13
6	L5	3974	OMG	C5-C4-N3	-4.44	121.26	128.46
6	L5	4245	OMG	C5-C4-N3	-4.44	121.26	128.46
52	S2	577	A2M	N9-C8-N7	-4.44	107.84	113.91
6	L5	4246	PSU	N1-C2-N3	4.42	120.14	115.13
6	L5	4099	PSU	N1-C2-N3	4.42	120.14	115.13
6	L5	3359	OMG	C5-C4-N3	-4.42	121.29	128.46
6	L5	1266	1MA	C5-C4-N3	-4.41	120.68	127.26
6	L5	4269	A2M	N9-C8-N7	-4.41	107.88	113.91
6	L5	3369	PSU	N1-C2-N3	4.41	120.13	115.13
6	L5	3616	PSU	N1-C2-N3	4.41	120.12	115.13
52	S2	1679	A2M	N9-C8-N7	-4.41	107.89	113.91
52	S2	868	OMG	C5-C4-N3	-4.39	121.34	128.46
52	S2	513	A2M	N9-C8-N7	-4.39	107.91	113.91
6	L5	3652	PSU	N1-C2-N3	4.39	120.10	115.13
52	S2	1443	OMU	N3-C2-N1	4.39	120.71	114.89
52	S2	1693	PSU	N1-C2-N3	4.39	120.10	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1638	PSU	N1-C2-N3	4.38	120.09	115.13
6	L5	3517	A2M	O4'-C1'-C2'	-4.38	98.89	106.57
6	L5	1799	PSU	N1-C2-N3	4.37	120.08	115.13
6	L5	3631	OMG	C5-C4-N3	-4.37	121.37	128.46
6	L5	4177	PSU	N1-C2-N3	4.37	120.08	115.13
52	S2	1384	A2M	N9-C8-N7	-4.37	107.94	113.91
6	L5	1491	PSU	N1-C2-N3	4.37	120.08	115.13
52	S2	121	OMU	N3-C2-N1	4.36	120.68	114.89
6	L5	4052	OMU	N3-C2-N1	4.36	120.68	114.89
52	S2	1046	PSU	N1-C2-N3	4.36	120.07	115.13
6	L5	4325	PSU	N1-C2-N3	4.36	120.07	115.13
6	L5	4435	PSU	N1-C2-N3	4.35	120.05	115.13
6	L5	4419	PSU	N1-C2-N3	4.35	120.05	115.13
52	S2	1852	MA6	C2-N1-C6	4.34	122.01	111.75
52	S2	34	PSU	N1-C2-N3	4.34	120.04	115.13
6	L5	4317	A2M	N9-C8-N7	-4.33	107.99	113.91
52	S2	682	PSU	N1-C2-N3	4.33	120.04	115.13
6	L5	4045	PSU	N1-C2-N3	4.33	120.04	115.13
6	L5	3456	A2M	N9-C8-N7	-4.33	107.99	113.91
6	L5	3496	PSU	N1-C2-N3	4.33	120.03	115.13
52	S2	1368	PSU	N1-C2-N3	4.33	120.03	115.13
6	L5	3492	A2M	N9-C8-N7	-4.33	108.00	113.91
52	S2	1852	MA6	C9-N6-C6	-4.33	109.18	120.40
6	L5	3585	PSU	N1-C2-N3	4.32	120.02	115.13
6	L5	4169	PSU	N1-C2-N3	4.32	120.02	115.13
52	S2	1175	PSU	N1-C2-N3	4.32	120.02	115.13
6	L5	4217	PSU	N1-C2-N3	4.32	120.02	115.13
6	L5	3371	PSU	N1-C2-N3	4.31	120.02	115.13
52	S2	1644	PSU	N1-C2-N3	4.31	120.02	115.13
6	L5	3466	PSU	N1-C2-N3	4.31	120.01	115.13
6	L5	1489	A2M	N9-C8-N7	-4.31	108.02	113.91
52	S2	1851	MA6	N3-C4-N9	4.31	134.18	127.08
6	L5	3450	A2M	N9-C8-N7	-4.30	108.03	113.91
52	S2	407	PSU	N1-C2-N3	4.30	120.00	115.13
6	L5	3517	A2M	N9-C8-N7	-4.30	108.04	113.91
6	L5	398	A2M	N9-C8-N7	-4.29	108.04	113.91
6	L5	4374	PSU	N1-C2-N3	4.29	119.99	115.13
52	S2	1082	PSU	N1-C2-N3	4.29	119.99	115.13
6	L5	4203	PSU	N1-C2-N3	4.28	119.98	115.13
52	S2	1245	PSU	N1-C2-N3	4.28	119.98	115.13
6	L5	1721	PSU	N1-C2-N3	4.28	119.98	115.13
52	S2	687	PSU	N1-C2-N3	4.28	119.98	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1446	PSU	N1-C2-N3	4.28	119.98	115.13
6	L5	4298	PSU	N1-C2-N3	4.28	119.98	115.13
6	L5	4278	PSU	N1-C2-N3	4.28	119.98	115.13
52	S2	1057	PSU	N1-C2-N3	4.27	119.97	115.13
8	L8	55	PSU	N1-C2-N3	4.27	119.97	115.13
6	L5	3554	PSU	N1-C2-N3	4.27	119.97	115.13
6	L5	3557	A2M	N9-C8-N7	-4.27	108.07	113.91
6	L5	4042	PSU	N1-C2-N3	4.27	119.96	115.13
52	S2	172	OMU	N3-C2-N1	4.26	120.55	114.89
52	S2	652	PSU	N1-C2-N3	4.26	119.95	115.13
6	L5	4711	PSU	N1-C2-N3	4.26	119.95	115.13
52	S2	823	PSU	N1-C2-N3	4.26	119.95	115.13
6	L5	2351	PSU	N1-C2-N3	4.26	119.95	115.13
52	S2	1289	OMU	N3-C2-N1	4.25	120.54	114.89
6	L5	3427	PSU	N1-C2-N3	4.25	119.95	115.13
6	L5	3500	PSU	N1-C2-N3	4.25	119.95	115.13
6	L5	2475	PSU	N1-C2-N3	4.25	119.94	115.13
52	S2	1239	PSU	N1-C2-N3	4.25	119.94	115.13
52	S2	1851	MA6	C9-N6-C6	-4.24	109.39	120.40
6	L5	1683	PSU	N1-C2-N3	4.24	119.94	115.13
6	L5	4749	PSU	N1-C2-N3	4.24	119.94	115.13
6	L5	3502	PSU	N1-C2-N3	4.24	119.94	115.13
6	L5	1731	PSU	N1-C2-N3	4.24	119.93	115.13
52	S2	1233	PSU	N1-C2-N3	4.24	119.93	115.13
52	S2	573	PSU	N1-C2-N3	4.23	119.93	115.13
6	L5	1537	PSU	N1-C2-N3	4.23	119.92	115.13
6	L5	1479	A2M	O4'-C4'-C3'	-4.23	96.75	105.11
6	L5	1720	PSU	N1-C2-N3	4.23	119.92	115.13
52	S2	816	PSU	N1-C2-N3	4.23	119.92	115.13
52	S2	1178	PSU	N1-C2-N3	4.22	119.92	115.13
6	L5	1801	PSU	N1-C2-N3	4.22	119.91	115.13
52	S2	802	PSU	N1-C2-N3	4.22	119.91	115.13
52	S2	99	A2M	N9-C8-N7	-4.22	108.15	113.91
6	L5	4107	PSU	N1-C2-N3	4.21	119.91	115.13
6	L5	4740	PSU	N1-C2-N3	4.21	119.90	115.13
6	L5	1632	PSU	N1-C2-N3	4.20	119.89	115.13
52	S2	815	PSU	N1-C2-N3	4.20	119.89	115.13
52	S2	218	PSU	N1-C2-N3	4.20	119.89	115.13
6	L5	3447	PSU	N1-C2-N3	4.20	119.89	115.13
52	S2	628	OMU	N3-C2-N1	4.20	120.46	114.89
6	L5	3494	PSU	N1-C2-N3	4.20	119.88	115.13
6	L5	1718	PSU	N1-C2-N3	4.19	119.88	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3490	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	1348	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	105	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	36	PSU	N1-C2-N3	4.19	119.88	115.13
52	S2	864	PSU	N1-C2-N3	4.19	119.87	115.13
52	S2	1047	PSU	N1-C2-N3	4.18	119.87	115.13
6	L5	4322	PSU	N1-C2-N3	4.18	119.87	115.13
52	S2	650	PSU	N1-C2-N3	4.18	119.86	115.13
52	S2	610	PSU	N1-C2-N3	4.18	119.86	115.13
52	S2	210	PSU	N1-C2-N3	4.18	119.86	115.13
52	S2	867	PSU	N1-C2-N3	4.17	119.85	115.13
52	S2	109	PSU	N1-C2-N3	4.17	119.85	115.13
6	L5	4058	PSU	N1-C2-N3	4.16	119.85	115.13
52	S2	1626	PSU	N1-C2-N3	4.16	119.84	115.13
6	L5	3462	PSU	N1-C2-N3	4.16	119.84	115.13
52	S2	429	OMU	N3-C2-N1	4.16	120.41	114.89
6	L5	4166	PSU	N1-C2-N3	4.16	119.84	115.13
6	L5	3576	PSU	N1-C2-N3	4.16	119.84	115.13
52	S2	967	PSU	N1-C2-N3	4.14	119.82	115.13
52	S2	119	PSU	N1-C2-N3	4.11	119.79	115.13
52	S2	591	A2M	N9-C8-N7	-4.09	108.32	113.91
52	S2	1327	OMU	N3-C2-N1	4.08	120.31	114.89
52	S2	93	PSU	N1-C2-N3	4.08	119.75	115.13
52	S2	1851	MA6	C4-C5-N7	-3.93	105.84	110.62
52	S2	1833	6MZ	C2-N3-C4	3.90	120.96	111.75
6	L5	1266	1MA	C2-N3-C4	3.88	120.04	112.41
6	L5	2719	OMG	C2-N1-C6	-3.86	118.06	125.10
6	L5	1580	OMG	C2-N1-C6	-3.86	118.07	125.10
79	Se	67	NMM	NE-CZ-NH1	3.84	127.46	120.26
52	S2	1852	MA6	C2-N3-C4	3.84	120.81	111.75
52	S2	1329	OMG	C2-N1-C6	-3.82	118.13	125.10
52	S2	437	OMG	C2-N1-C6	-3.82	118.13	125.10
6	L5	3966	6MZ	C2-N3-C4	3.82	120.77	111.75
52	S2	1843	4AC	N4-C4-N3	3.81	120.25	113.85
52	S2	1851	MA6	C2-N3-C4	3.81	120.75	111.75
6	L5	3676	OMG	C2-N1-C6	-3.81	118.16	125.10
6	L5	4138	OMG	C2-N1-C6	-3.80	118.17	125.10
52	S2	669	A2M	C4'-O4'-C1'	-3.79	101.11	109.47
52	S2	510	OMG	C2-N1-C6	-3.78	118.20	125.10
52	S2	1640	7MG	C5-C4-N3	-3.78	120.93	128.13
52	S2	1491	OMG	C2-N1-C6	-3.78	118.21	125.10
52	S2	645	OMG	C2-N1-C6	-3.78	118.21	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	2267	OMG	C2-N1-C6	-3.77	118.22	125.10
52	S2	1448	OMG	C2-N1-C6	-3.77	118.22	125.10
6	L5	4116	OMG	C2-N1-C6	-3.77	118.23	125.10
6	L5	4364	OMG	C2-N1-C6	-3.76	118.24	125.10
52	S2	684	OMG	C2-N1-C6	-3.76	118.25	125.10
6	L5	3942	OMG	C2-N1-C6	-3.75	118.25	125.10
6	L5	4383	OMG	C2-N1-C6	-3.75	118.25	125.10
6	L5	3476	OMG	C2-N1-C6	-3.74	118.27	125.10
6	L5	4369	OMG	C2-N1-C6	-3.74	118.28	125.10
52	S2	1005	PSU	C6-C5-C4	3.72	120.80	118.20
52	S2	1640	7MG	C2-N1-C6	-3.72	118.32	125.10
52	S2	1852	MA6	C4-C5-N7	-3.72	106.09	110.62
8	L8	75	OMG	C2-N1-C6	-3.70	118.35	125.10
52	S2	602	OMG	C2-N1-C6	-3.70	118.35	125.10
6	L5	1477	OMG	C2-N1-C6	-3.70	118.35	125.10
6	L5	4245	OMG	C2-N1-C6	-3.69	118.38	125.10
6	L5	1260	OMG	C2-N1-C6	-3.67	118.41	125.10
6	L5	3974	OMG	C2-N1-C6	-3.67	118.41	125.10
6	L5	3631	OMG	C2-N1-C6	-3.65	118.44	125.10
6	L5	3359	OMG	C2-N1-C6	-3.65	118.44	125.10
52	S2	868	OMG	C2-N1-C6	-3.65	118.45	125.10
6	L5	4240	OMG	C2-N1-C6	-3.64	118.46	125.10
6	L5	3524	OMG	C2-N1-C6	-3.64	118.47	125.10
52	S2	669	A2M	O4'-C4'-C3'	-3.63	97.92	105.11
6	L5	2630	A2M	O4'-C1'-N9	-3.62	100.93	108.06
6	L5	2207	OMG	N9-C4-N3	3.57	133.11	125.94
6	L5	4276	UR3	C4-N3-C2	-3.55	121.22	124.56
6	L5	2207	OMG	C2-N1-C6	-3.55	118.63	125.10
52	S2	591	A2M	C2-N3-C4	3.53	120.09	111.75
6	L5	4382	PSU	O2-C2-N1	-3.52	118.92	122.79
6	L5	2630	A2M	C2-N3-C4	3.49	120.00	111.75
6	L5	400	A2M	O4'-C1'-N9	-3.47	101.21	108.06
6	L5	3517	A2M	C5-C6-N6	-3.45	115.91	123.43
6	L5	3492	A2M	C2-N3-C4	3.44	119.89	111.75
6	L5	4336	A2M	C2-N3-C4	3.44	119.87	111.75
6	L5	1810	A2M	C5-N7-C8	3.43	108.39	103.51
6	L5	3557	A2M	C5-C6-N6	-3.43	115.97	123.43
6	L5	398	A2M	C2-N3-C4	3.42	119.84	111.75
52	S2	1679	A2M	C2-N3-C4	3.42	119.83	111.75
6	L5	400	A2M	C5-C6-N6	-3.41	116.00	123.43
6	L5	2244	A2M	C2-N3-C4	3.41	119.81	111.75
6	L5	1489	A2M	C2-N3-C4	3.41	119.81	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	99	A2M	C2-N3-C4	3.41	119.81	111.75
52	S2	513	A2M	C2-N3-C4	3.41	119.80	111.75
6	L5	3557	A2M	C2-N3-C4	3.40	119.79	111.75
52	S2	469	A2M	C2-N3-C4	3.40	119.78	111.75
6	L5	2206	A2M	C2-N3-C4	3.39	119.77	111.75
52	S2	485	A2M	C2-N3-C4	3.39	119.77	111.75
6	L5	1270	A2M	C5-N7-C8	3.39	108.33	103.51
52	S2	166	A2M	C2-N3-C4	3.39	119.75	111.75
6	L5	3450	A2M	C2-N3-C4	3.39	119.75	111.75
6	L5	1479	A2M	C4'-O4'-C1'	-3.39	102.00	109.47
52	S2	27	A2M	C2-N3-C4	3.38	119.75	111.75
6	L5	1810	A2M	C2-N3-C4	3.38	119.74	111.75
6	L5	1270	A2M	C2-N3-C4	3.38	119.74	111.75
6	L5	4269	A2M	C2-N3-C4	3.38	119.74	111.75
52	S2	1384	A2M	C2-N3-C4	3.38	119.73	111.75
6	L5	2658	A2M	C2-N3-C4	3.38	119.73	111.75
6	L5	1479	A2M	C2-N3-C4	3.37	119.72	111.75
52	S2	1679	A2M	C5-C6-N6	-3.37	116.09	123.43
6	L5	3456	A2M	C2-N3-C4	3.37	119.72	111.75
6	L5	400	A2M	C2-N3-C4	3.37	119.71	111.75
52	S2	669	A2M	C2-N3-C4	3.37	119.71	111.75
6	L5	2630	A2M	C5-N7-C8	3.37	108.30	103.51
6	L5	1270	A2M	O4'-C1'-N9	-3.36	101.44	108.06
52	S2	27	A2M	C5-C6-N6	-3.36	116.12	123.43
52	S2	159	A2M	C2-N3-C4	3.36	119.69	111.75
52	S2	669	A2M	C5-N7-C8	3.36	108.28	103.51
6	L5	4317	A2M	C2-N3-C4	3.36	119.69	111.75
6	L5	4336	A2M	C5-C6-N6	-3.36	116.12	123.43
52	S2	1032	A2M	C2-N3-C4	3.35	119.67	111.75
6	L5	4269	A2M	C5-C6-N6	-3.35	116.14	123.43
52	S2	166	A2M	C5-N7-C8	3.34	108.26	103.51
6	L5	4317	A2M	C5-C6-N6	-3.34	116.17	123.43
52	S2	99	A2M	C5-C6-N6	-3.33	116.17	123.43
52	S2	577	A2M	C2-N3-C4	3.33	119.62	111.75
6	L5	3517	A2M	C2-N3-C4	3.33	119.62	111.75
52	S2	669	A2M	O4'-C1'-N9	-3.33	101.50	108.06
6	L5	2244	A2M	C5-C6-N6	-3.33	116.19	123.43
6	L5	3562	A2M	C2-N3-C4	3.32	119.60	111.75
6	L5	2206	A2M	C5-C6-N6	-3.32	116.20	123.43
6	L5	3599	A2M	C2-N3-C4	3.32	119.60	111.75
6	L5	3562	A2M	C5-C6-N6	-3.32	116.20	123.43
52	S2	591	A2M	C2'-C3'-C4'	-3.32	94.78	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	398	A2M	C5-C6-N6	-3.32	116.22	123.43
6	L5	1810	A2M	C5-C6-N6	-3.32	116.22	123.43
52	S2	1032	A2M	C5-N7-C8	3.31	108.22	103.51
6	L5	2244	A2M	C5-N7-C8	3.31	108.22	103.51
6	L5	3599	A2M	C5-C6-N6	-3.31	116.22	123.43
52	S2	469	A2M	C5-N7-C8	3.31	108.21	103.51
6	L5	1489	A2M	C5-C6-N6	-3.31	116.22	123.43
52	S2	1384	A2M	C5-C6-N6	-3.31	116.23	123.43
6	L5	3966	6MZ	C6-C5-N7	3.31	135.97	132.39
6	L5	3450	A2M	C5-C6-N6	-3.31	116.24	123.43
52	S2	513	A2M	C5-C6-N6	-3.30	116.24	123.43
6	L5	2630	A2M	C4-N9-C1'	-3.30	118.73	126.59
6	L5	1479	A2M	C5-C6-N6	-3.30	116.25	123.43
52	S2	159	A2M	C5-C6-N6	-3.30	116.25	123.43
52	S2	469	A2M	C2'-C3'-C4'	-3.30	94.83	101.99
52	S2	485	A2M	O4'-C1'-N9	-3.30	101.56	108.06
6	L5	1270	A2M	C5-C6-N6	-3.29	116.26	123.43
52	S2	669	A2M	C5-C6-N6	-3.29	116.27	123.43
52	S2	485	A2M	C5-C6-N6	-3.29	116.27	123.43
52	S2	166	A2M	C5-C6-N6	-3.29	116.28	123.43
52	S2	591	A2M	C5-C6-N6	-3.29	116.28	123.43
6	L5	2658	A2M	C5-N7-C8	3.29	108.18	103.51
6	L5	3562	A2M	C5-N7-C8	3.27	108.16	103.51
6	L5	3456	A2M	C5-C6-N6	-3.27	116.31	123.43
52	S2	1327	OMU	C5-C4-N3	3.27	119.73	114.84
52	S2	1032	A2M	C5-C6-N6	-3.27	116.31	123.43
52	S2	1851	MA6	N1-C2-N3	-3.27	123.49	128.60
52	S2	577	A2M	C5-N7-C8	3.27	108.15	103.51
52	S2	577	A2M	C5-C6-N6	-3.26	116.33	123.43
6	L5	3492	A2M	C5-C6-N6	-3.26	116.33	123.43
52	S2	27	A2M	C5-N7-C8	3.26	108.14	103.51
6	L5	2630	A2M	C5-C6-N6	-3.26	116.34	123.43
6	L5	2658	A2M	C5-C6-N6	-3.26	116.34	123.43
6	L5	4336	A2M	C2'-C3'-C4'	-3.26	94.92	101.99
52	S2	469	A2M	C5-C6-N6	-3.26	116.34	123.43
52	S2	577	A2M	C2'-C3'-C4'	-3.26	94.92	101.99
6	L5	2206	A2M	C5-N7-C8	3.25	108.13	103.51
6	L5	4336	A2M	C5-N7-C8	3.24	108.12	103.51
52	S2	159	A2M	C5-N7-C8	3.24	108.11	103.51
6	L5	4269	A2M	C5-N7-C8	3.24	108.11	103.51
6	L5	398	A2M	C5-N7-C8	3.23	108.11	103.51
52	S2	591	A2M	O4'-C4'-C3'	-3.23	98.71	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3966	6MZ	C9-N6-C6	-3.23	120.09	122.87
52	S2	1679	A2M	C5-N7-C8	3.23	108.10	103.51
52	S2	485	A2M	C5-N7-C8	3.23	108.09	103.51
52	S2	1384	A2M	C5-N7-C8	3.22	108.09	103.51
6	L5	1479	A2M	C5-N7-C8	3.22	108.09	103.51
6	L5	3514	5MC	C5-C6-N1	-3.22	120.02	123.34
6	L5	3456	A2M	C5-N7-C8	3.22	108.08	103.51
52	S2	429	OMU	C5-C4-N3	3.22	119.66	114.84
52	S2	1289	OMU	C5-C4-N3	3.21	119.64	114.84
6	L5	400	A2M	C5-N7-C8	3.21	108.07	103.51
52	S2	513	A2M	C5-N7-C8	3.20	108.06	103.51
6	L5	3599	A2M	O4'-C1'-N9	-3.20	101.75	108.06
6	L5	4193	5MC	C5-C4-N4	-3.20	116.69	121.48
6	L5	3492	A2M	C5-N7-C8	3.20	108.05	103.51
6	L5	3450	A2M	C5-N7-C8	3.20	108.05	103.51
52	S2	628	OMU	C5-C4-N3	3.19	119.62	114.84
52	S2	99	A2M	C5-N7-C8	3.19	108.04	103.51
52	S2	1851	MA6	C5-N7-C8	3.19	108.04	103.51
52	S2	116	OMU	C5-C4-N3	3.19	119.61	114.84
6	L5	3599	A2M	C5-N7-C8	3.19	108.04	103.51
6	L5	1489	A2M	C5-N7-C8	3.19	108.04	103.51
52	S2	355	OMU	C5-C4-N3	3.18	119.60	114.84
52	S2	1805	OMU	C5-C4-N3	3.18	119.60	114.84
6	L5	2258	OMU	C5-C4-N3	3.17	119.58	114.84
6	L5	4244	OMU	C5-C4-N3	3.17	119.58	114.84
6	L5	2719	OMG	C1'-N9-C8	-3.16	117.70	126.70
6	L5	3557	A2M	C5-N7-C8	3.16	107.99	103.51
6	L5	3966	6MZ	N1-C2-N3	-3.15	123.67	128.60
6	L5	4317	A2M	C5-N7-C8	3.15	107.99	103.51
6	L5	3966	6MZ	C4-C5-N7	-3.15	106.78	110.62
52	S2	513	A2M	C2'-C3'-C4'	-3.14	95.17	101.99
52	S2	1640	7MG	C5-C4-N9	3.14	110.42	106.35
6	L5	4366	OMU	C5-C4-N3	3.14	119.53	114.84
52	S2	1852	MA6	N1-C2-N3	-3.13	123.70	128.60
6	L5	4052	OMU	C5-C4-N3	3.13	119.52	114.84
52	S2	172	OMU	C5-C4-N3	3.12	119.51	114.84
6	L5	2680	OMU	C5-C4-N3	3.12	119.50	114.84
6	L5	1260	OMG	N9-C8-N7	-3.11	107.53	113.39
6	L5	3517	A2M	C5-N7-C8	3.11	107.93	103.51
6	L5	3973	OMU	C5-C4-N3	3.11	119.49	114.84
52	S2	591	A2M	C5-N7-C8	3.11	107.92	103.51
52	S2	121	OMU	C5-C4-N3	3.09	119.47	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	645	OMG	N9-C8-N7	-3.09	107.57	113.39
52	S2	1443	OMU	C5-C4-N3	3.08	119.44	114.84
6	L5	3657	OMU	C5-C4-N3	3.07	119.44	114.84
52	S2	485	A2M	O4'-C4'-C3'	-3.07	99.03	105.11
52	S2	868	OMG	N9-C8-N7	-3.07	107.62	113.39
6	L5	3517	A2M	N3-C4-N9	3.06	132.13	127.08
6	L5	4245	OMG	N9-C8-N7	-3.03	107.68	113.39
6	L5	4188	PSU	C6-C5-C4	3.02	120.31	118.20
6	L5	1266	1MA	N9-C8-N7	-3.02	107.71	113.39
52	S2	1852	MA6	C5-N7-C8	3.02	107.79	103.51
6	L5	3631	OMG	N9-C8-N7	-3.01	107.72	113.39
6	L5	2244	A2M	C2'-C3'-C4'	-3.01	95.47	101.99
6	L5	2719	OMG	N9-C4-N3	3.00	131.97	125.94
52	S2	1833	6MZ	N1-C2-N3	-2.99	123.93	128.60
6	L5	3359	OMG	N9-C8-N7	-2.99	107.76	113.39
6	L5	4116	OMG	N9-C8-N7	-2.98	107.77	113.39
6	L5	4383	OMG	N9-C8-N7	-2.98	107.78	113.39
6	L5	3974	OMG	N9-C8-N7	-2.97	107.79	113.39
6	L5	3514	5MC	C5-C4-N4	-2.97	117.04	121.48
6	L5	3599	A2M	C2'-C3'-C4'	-2.97	95.54	101.99
52	S2	684	OMG	N9-C8-N7	-2.96	107.82	113.39
6	L5	4317	A2M	O4'-C1'-N9	-2.96	102.23	108.06
6	L5	3562	A2M	C2'-C3'-C4'	-2.95	95.58	101.99
52	S2	602	OMG	N9-C8-N7	-2.95	107.83	113.39
52	S2	591	A2M	N3-C4-N9	2.95	131.94	127.08
6	L5	1810	A2M	C2'-C3'-C4'	-2.94	95.61	101.99
6	L5	4138	OMG	N9-C8-N7	-2.94	107.85	113.39
6	L5	4240	OMG	N9-C8-N7	-2.93	107.87	113.39
6	L5	4364	OMG	N9-C8-N7	-2.93	107.88	113.39
6	L5	1477	OMG	N9-C8-N7	-2.92	107.88	113.39
52	S2	166	A2M	C2'-C3'-C4'	-2.92	95.66	101.99
52	S2	1327	OMU	O4-C4-C5	-2.92	120.03	125.16
6	L5	4267	PSU	C6-C5-C4	2.91	120.23	118.20
52	S2	1852	MA6	C10-N6-C6	-2.91	112.86	120.40
52	S2	1329	OMG	N9-C8-N7	-2.91	107.92	113.39
52	S2	1833	6MZ	C4-C5-N7	-2.91	107.08	110.62
6	L5	2267	OMG	N9-C8-N7	-2.90	107.93	113.39
6	L5	4336	A2M	O4'-C4'-C3'	-2.89	99.39	105.11
52	S2	1851	MA6	C10-N6-C6	-2.89	112.91	120.40
8	L8	75	OMG	N9-C8-N7	-2.89	107.95	113.39
6	L5	3476	OMG	N9-C8-N7	-2.89	107.95	113.39
6	L5	2658	A2M	O4'-C1'-N9	-2.88	102.38	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3524	OMG	N9-C8-N7	-2.88	107.96	113.39
6	L5	3942	OMG	N9-C8-N7	-2.88	107.97	113.39
6	L5	4369	OMG	N9-C8-N7	-2.87	107.98	113.39
52	S2	1384	A2M	C2'-C3'-C4'	-2.87	95.76	101.99
6	L5	4269	A2M	C2'-C3'-C4'	-2.87	95.76	101.99
52	S2	823	PSU	O2-C2-N1	-2.87	119.63	122.79
6	L5	3517	A2M	C6-C5-C4	2.87	121.04	117.18
52	S2	510	OMG	N9-C8-N7	-2.86	108.00	113.39
6	L5	3492	A2M	N3-C4-N9	2.86	131.80	127.08
6	L5	3517	A2M	C2'-C1'-N9	-2.85	108.72	113.53
6	L5	3676	OMG	N9-C8-N7	-2.85	108.02	113.39
6	L5	3456	A2M	C2'-C3'-C4'	-2.85	95.81	101.99
6	L5	4099	PSU	C6-C5-C4	2.84	120.18	118.20
6	L5	2207	OMG	N9-C8-N7	-2.83	108.06	113.39
52	S2	591	A2M	C6-C5-C4	2.83	120.99	117.18
52	S2	429	OMU	O4-C4-C5	-2.83	120.18	125.16
52	S2	1491	OMG	N9-C8-N7	-2.83	108.07	113.39
52	S2	437	OMG	N9-C8-N7	-2.82	108.08	113.39
52	S2	172	OMU	O4-C4-C5	-2.82	120.20	125.16
52	S2	116	OMU	O4-C4-C5	-2.82	120.21	125.16
6	L5	1580	OMG	N9-C8-N7	-2.82	108.09	113.39
6	L5	1580	OMG	N9-C4-N3	2.81	131.59	125.94
6	L5	400	A2M	N3-C4-N9	2.81	131.71	127.08
52	S2	591	A2M	C1'-N9-C8	-2.81	120.80	127.14
52	S2	628	OMU	O4-C4-C5	-2.80	120.23	125.16
6	L5	3557	A2M	N3-C4-N9	2.80	131.69	127.08
52	S2	485	A2M	CM'-O2'-C2'	-2.80	107.19	114.52
6	L5	2680	OMU	O4-C4-C5	-2.80	120.24	125.16
52	S2	1032	A2M	C2'-C3'-C4'	-2.80	95.92	101.99
6	L5	3492	A2M	C2'-C3'-C4'	-2.79	95.93	101.99
6	L5	1489	A2M	C3'-C2'-C1'	-2.79	97.65	102.89
6	L5	1270	A2M	N3-C4-N9	2.78	131.67	127.08
52	S2	1805	OMU	O4-C4-C5	-2.78	120.27	125.16
6	L5	3583	PSU	C6-C5-C4	2.78	120.14	118.20
52	S2	1679	A2M	C2'-C3'-C4'	-2.77	95.99	101.99
6	L5	3973	OMU	O4-C4-C5	-2.76	120.30	125.16
52	S2	437	OMG	N9-C4-N3	2.76	131.49	125.94
6	L5	3524	OMG	N9-C4-N3	2.76	131.49	125.94
52	S2	1443	OMU	O4-C4-C5	-2.76	120.31	125.16
6	L5	1489	A2M	C6-C5-C4	2.75	120.88	117.18
6	L5	3557	A2M	C6-C5-C4	2.75	120.88	117.18
6	L5	4317	A2M	C6-C5-C4	2.75	120.88	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1448	OMG	N9-C8-N7	-2.74	108.22	113.39
6	L5	1810	A2M	CM'-O2'-C2'	-2.74	107.33	114.52
52	S2	99	A2M	C6-C5-C4	2.74	120.87	117.18
6	L5	3517	A2M	C1'-N9-C8	-2.74	120.95	127.14
6	L5	2630	A2M	C1'-N9-C8	2.74	133.32	127.14
6	L5	1479	A2M	N3-C4-N9	2.74	131.59	127.08
6	L5	2244	A2M	N3-C4-N9	2.73	131.59	127.08
6	L5	3657	OMU	O4-C4-C5	-2.73	120.35	125.16
52	S2	1679	A2M	N3-C4-N9	2.73	131.58	127.08
6	L5	4149	PSU	O2-C2-N1	-2.73	119.79	122.79
6	L5	4244	OMU	O4-C4-C5	-2.72	120.37	125.16
6	L5	2658	A2M	N3-C4-N9	2.72	131.57	127.08
6	L5	3599	A2M	N3-C4-N9	2.72	131.57	127.08
6	L5	3557	A2M	C2'-C3'-C4'	-2.72	96.08	101.99
6	L5	1479	A2M	C6-C5-C4	2.72	120.84	117.18
6	L5	1270	A2M	C6-C5-C4	2.72	120.84	117.18
6	L5	2658	A2M	C6-C5-C4	2.72	120.84	117.18
6	L5	3492	A2M	C6-C5-C4	2.72	120.83	117.18
8	L8	69	PSU	C6-C5-C4	2.71	120.09	118.20
6	L5	2258	OMU	O4-C4-C5	-2.70	120.40	125.16
6	L5	3456	A2M	C6-C5-C4	2.70	120.81	117.18
6	L5	398	A2M	C6-C5-C4	2.70	120.81	117.18
52	S2	1491	OMG	N9-C4-N3	2.69	131.35	125.94
6	L5	3450	A2M	C6-C5-C4	2.69	120.80	117.18
6	L5	4317	A2M	N3-C4-N9	2.69	131.52	127.08
6	L5	2719	OMG	N9-C8-N7	-2.69	108.33	113.39
52	S2	27	A2M	N3-C4-N9	2.69	131.51	127.08
52	S2	34	PSU	C6-C5-C4	2.69	120.08	118.20
52	S2	1384	A2M	C6-C5-C4	2.69	120.79	117.18
52	S2	99	A2M	N3-C4-N9	2.69	131.51	127.08
6	L5	2206	A2M	C2'-C3'-C4'	-2.68	96.16	101.99
6	L5	1489	A2M	N3-C4-N9	2.68	131.50	127.08
6	L5	4336	A2M	N3-C4-N9	2.68	131.50	127.08
6	L5	1270	A2M	C2'-C3'-C4'	-2.68	96.18	101.99
6	L5	4052	OMU	O4-C4-C5	-2.68	120.45	125.16
6	L5	3942	OMG	N9-C4-N3	2.68	131.31	125.94
52	S2	1032	A2M	C6-C5-C4	2.67	120.78	117.18
6	L5	4269	A2M	C6-C5-C4	2.67	120.78	117.18
52	S2	121	OMU	O4-C4-C5	-2.67	120.47	125.16
6	L5	400	A2M	C6-C5-C4	2.67	120.77	117.18
52	S2	99	A2M	C2'-C3'-C4'	-2.66	96.21	101.99
6	L5	2719	OMG	C1'-N9-C4	2.66	134.41	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1640	7MG	C4-C5-N7	2.66	109.22	105.53
6	L5	2630	A2M	C6-C5-C4	2.66	120.76	117.18
52	S2	1289	OMU	O4-C4-C5	-2.66	120.49	125.16
6	L5	4202	OMC	CM2-O2'-C2'	-2.66	107.55	114.52
6	L5	4366	OMU	O4-C4-C5	-2.65	120.49	125.16
52	S2	1851	MA6	C4-N9-C8	2.65	108.60	105.73
6	L5	1810	A2M	C6-C5-C4	2.65	120.75	117.18
52	S2	1005	PSU	O4-C4-C5	-2.65	117.12	124.05
6	L5	1270	A2M	O4'-C4'-C3'	-2.65	99.88	105.11
6	L5	4138	OMG	C5-C6-N1	2.64	119.90	113.19
6	L5	3456	A2M	N3-C4-N9	2.64	131.43	127.08
52	S2	591	A2M	C4'-O4'-C1'	-2.64	103.65	109.47
52	S2	1679	A2M	C6-C5-C4	2.64	120.73	117.18
6	L5	1810	A2M	N3-C4-N9	2.64	131.43	127.08
6	L5	4246	PSU	O2-C2-N1	-2.64	119.89	122.79
6	L5	3966	6MZ	C5-N7-C8	2.64	107.25	103.51
52	S2	27	A2M	CM'-O2'-C2'	-2.63	107.61	114.52
52	S2	355	OMU	O4-C4-C5	-2.63	120.53	125.16
6	L5	4317	A2M	CM'-O2'-C2'	-2.63	107.62	114.52
6	L5	3599	A2M	C6-C5-C4	2.63	120.72	117.18
52	S2	687	PSU	O2-C2-N1	-2.63	119.89	122.79
6	L5	3619	OMC	CM2-O2'-C2'	-2.63	107.62	114.52
6	L5	2206	A2M	N3-C4-N9	2.63	131.41	127.08
6	L5	2207	OMG	C5-C6-N1	2.63	119.86	113.19
52	S2	1032	A2M	N3-C4-N9	2.63	131.41	127.08
52	S2	1446	PSU	C6-C5-C4	2.63	120.03	118.20
6	L5	4269	A2M	N3-C4-N9	2.63	131.41	127.08
6	L5	2244	A2M	C6-C5-C4	2.62	120.71	117.18
6	L5	1270	A2M	C4-N9-C8	2.62	108.57	105.73
6	L5	4149	PSU	C6-C5-C4	2.62	120.03	118.20
6	L5	398	A2M	N3-C4-N9	2.62	131.40	127.08
52	S2	166	A2M	C6-C5-C4	2.62	120.70	117.18
52	S2	159	A2M	N3-C4-N9	2.62	131.40	127.08
52	S2	159	A2M	C6-C5-C4	2.62	120.70	117.18
52	S2	210	PSU	C6-C5-C4	2.62	120.03	118.20
6	L5	2244	A2M	O4'-C4'-C3'	-2.61	99.94	105.11
52	S2	469	A2M	N3-C4-N9	2.61	131.39	127.08
52	S2	513	A2M	N3-C4-N9	2.61	131.39	127.08
52	S2	1491	OMG	C5-C6-N1	2.61	119.82	113.19
52	S2	513	A2M	C6-C5-C4	2.61	120.69	117.18
6	L5	2719	OMG	C5-C6-N1	2.61	119.82	113.19
6	L5	2267	OMG	C5-C6-N1	2.61	119.81	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3450	A2M	C2'-C3'-C4'	-2.61	96.33	101.99
6	L5	1810	A2M	C4-N9-C8	2.61	108.55	105.73
52	S2	27	A2M	C6-C5-C4	2.60	120.68	117.18
52	S2	669	A2M	C4-N9-C8	2.60	108.55	105.73
52	S2	485	A2M	N3-C4-N9	2.60	131.37	127.08
52	S2	684	OMG	C5-C6-N1	2.60	119.79	113.19
6	L5	3557	A2M	CM'-O2'-C2'	-2.60	107.70	114.52
6	L5	4269	A2M	CM'-O2'-C2'	-2.60	107.71	114.52
6	L5	3524	OMG	C5-C6-N1	2.60	119.79	113.19
6	L5	3476	OMG	N9-C4-N3	2.59	131.15	125.94
6	L5	3942	OMG	C5-C6-N1	2.59	119.77	113.19
52	S2	1032	A2M	CM'-O2'-C2'	-2.59	107.73	114.52
6	L5	1260	OMG	C5-C6-N1	2.59	119.76	113.19
52	S2	1384	A2M	N3-C4-N9	2.59	131.34	127.08
6	L5	4336	A2M	C6-C5-C4	2.59	120.66	117.18
52	S2	573	PSU	O2-C2-N1	-2.58	119.94	122.79
52	S2	469	A2M	C6-C5-C4	2.58	120.66	117.18
6	L5	3966	6MZ	C4-N9-C8	2.58	108.53	105.73
6	L5	4383	OMG	C5-C6-N1	2.58	119.74	113.19
52	S2	166	A2M	N3-C4-N9	2.58	131.33	127.08
6	L5	3476	OMG	C5-C6-N1	2.58	119.73	113.19
8	L8	75	OMG	N9-C4-N3	2.57	131.11	125.94
6	L5	1477	OMG	C5-C6-N1	2.57	119.73	113.19
6	L5	4374	PSU	O2-C2-N1	-2.57	119.96	122.79
6	L5	398	A2M	C2'-C3'-C4'	-2.57	96.41	101.99
52	S2	510	OMG	N9-C4-N3	2.57	131.10	125.94
52	S2	669	A2M	N3-C4-N9	2.57	131.32	127.08
52	S2	669	A2M	C6-C5-C4	2.57	120.64	117.18
6	L5	2207	OMG	C1'-N9-C8	-2.57	119.38	126.70
52	S2	645	OMG	N9-C4-N3	2.57	131.10	125.94
52	S2	27	A2M	O4'-C1'-N9	-2.57	103.00	108.06
6	L5	3562	A2M	C6-C5-C4	2.57	120.64	117.18
52	S2	577	A2M	C6-C5-C4	2.57	120.64	117.18
52	S2	1448	OMG	N9-C4-N3	2.57	131.09	125.94
52	S2	645	OMG	C5-C6-N1	2.57	119.71	113.19
6	L5	4245	OMG	C5-C6-N1	2.56	119.70	113.19
52	S2	1329	OMG	C5-C6-N1	2.56	119.70	113.19
6	L5	4364	OMG	N9-C4-N3	2.56	131.08	125.94
6	L5	3676	OMG	N9-C4-N3	2.56	131.08	125.94
52	S2	437	OMG	C5-C6-N1	2.56	119.69	113.19
6	L5	4364	OMG	C5-C6-N1	2.56	119.69	113.19
6	L5	4369	OMG	C5-C6-N1	2.56	119.69	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	602	OMG	N9-C4-N3	2.56	131.07	125.94
6	L5	4116	OMG	C5-C6-N1	2.56	119.68	113.19
52	S2	485	A2M	C6-C5-C4	2.56	120.62	117.18
6	L5	4240	OMG	N9-C4-N3	2.55	131.07	125.94
6	L5	3676	OMG	C5-C6-N1	2.55	119.68	113.19
6	L5	2206	A2M	C6-C5-C4	2.55	120.61	117.18
6	L5	1580	OMG	C5-C6-N1	2.55	119.66	113.19
52	S2	510	OMG	C5-C6-N1	2.55	119.66	113.19
6	L5	4246	PSU	C6-C5-C4	2.55	119.98	118.20
8	L8	75	OMG	C5-C6-N1	2.54	119.65	113.19
6	L5	3631	OMG	C5-C6-N1	2.54	119.65	113.19
6	L5	4244	OMU	O2-C2-N1	-2.54	119.41	122.79
6	L5	3562	A2M	N3-C4-N9	2.54	131.27	127.08
52	S2	684	OMG	CM2-O2'-C2'	-2.54	107.87	114.52
52	S2	602	OMG	C5-C6-N1	2.54	119.63	113.19
52	S2	1245	PSU	O2-C2-N1	-2.53	120.00	122.79
52	S2	802	PSU	O2-C2-N1	-2.53	120.00	122.79
6	L5	3359	OMG	C5-C6-N1	2.53	119.62	113.19
81	Sg	1	AME	O-C-CA	-2.53	118.14	124.78
6	L5	4369	OMG	N9-C4-N3	2.53	131.02	125.94
6	L5	3554	PSU	O2-C2-N1	-2.53	120.01	122.79
52	S2	684	OMG	N9-C4-N3	2.53	131.01	125.94
6	L5	3974	OMG	N9-C4-N3	2.52	131.01	125.94
52	S2	27	A2M	C2'-C3'-C4'	-2.52	96.51	101.99
52	S2	119	PSU	O2-C2-N1	-2.52	120.02	122.79
6	L5	3652	PSU	C6-C5-C4	2.52	119.96	118.20
6	L5	4240	OMG	C5-C6-N1	2.52	119.59	113.19
6	L5	4116	OMG	N9-C4-N3	2.52	131.00	125.94
6	L5	3974	OMG	C5-C6-N1	2.51	119.57	113.19
6	L5	4138	OMG	N9-C4-N3	2.51	130.99	125.94
52	S2	1368	PSU	O2-C2-N1	-2.51	120.03	122.79
52	S2	1693	PSU	O2-C2-N1	-2.51	120.03	122.79
52	S2	1833	6MZ	C5-N7-C8	2.51	107.07	103.51
6	L5	4169	PSU	C6-C5-C4	2.51	119.95	118.20
52	S2	1833	6MZ	C6-C5-N7	2.51	135.10	132.39
6	L5	3599	A2M	C4-N9-C8	2.51	108.45	105.73
52	S2	577	A2M	N3-C4-N9	2.51	131.21	127.08
52	S2	1329	OMG	N9-C4-N3	2.51	130.97	125.94
52	S2	868	OMG	C5-C6-N1	2.51	119.55	113.19
6	L5	2658	A2M	C2'-C3'-C4'	-2.50	96.55	101.99
52	S2	1852	MA6	C4-N9-C8	2.50	108.44	105.73
6	L5	1270	A2M	CM'-O2'-C2'	-2.50	107.95	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	1799	PSU	O2-C2-N1	-2.50	120.03	122.79
6	L5	4177	PSU	O2-C2-N1	-2.50	120.03	122.79
6	L5	2206	A2M	CM'-O2'-C2'	-2.50	107.96	114.52
52	S2	1046	PSU	C6-C5-C4	2.50	119.95	118.20
52	S2	159	A2M	C2'-C3'-C4'	-2.50	96.56	101.99
52	S2	816	PSU	O2-C2-N1	-2.50	120.04	122.79
52	S2	1851	MA6	C10-N6-C9	-2.50	108.07	116.12
6	L5	3466	PSU	C6-C5-C4	2.50	119.94	118.20
6	L5	4383	OMG	N9-C4-N3	2.50	130.95	125.94
6	L5	3576	PSU	O2-C2-N1	-2.49	120.04	122.79
6	L5	400	A2M	CM'-O2'-C2'	-2.49	107.99	114.52
52	S2	1239	PSU	O2-C2-N1	-2.49	120.05	122.79
6	L5	3450	A2M	N3-C4-N9	2.49	131.18	127.08
6	L5	1491	PSU	O2-C2-N1	-2.49	120.05	122.79
52	S2	868	OMG	N9-C4-N3	2.49	130.93	125.94
6	L5	1683	PSU	O2-C2-N1	-2.49	120.05	122.79
6	L5	2244	A2M	C4-N9-C8	2.49	108.42	105.73
6	L5	4099	PSU	O2-C2-N1	-2.49	120.05	122.79
52	S2	485	A2M	C4-N9-C8	2.48	108.42	105.73
52	S2	1032	A2M	C4-N9-C8	2.48	108.42	105.73
6	L5	1260	OMG	N9-C4-N3	2.48	130.92	125.94
6	L5	4166	PSU	C6-C5-C4	2.48	119.93	118.20
52	S2	867	PSU	O2-C2-N1	-2.48	120.06	122.79
52	S2	1448	OMG	C5-C6-N1	2.48	119.48	113.19
52	S2	610	PSU	O2-C2-N1	-2.48	120.06	122.79
6	L5	3500	PSU	O2-C2-N1	-2.47	120.07	122.79
6	L5	4419	PSU	O2-C2-N1	-2.47	120.07	122.79
52	S2	469	A2M	C4-N9-C8	2.47	108.41	105.73
6	L5	4325	PSU	O2-C2-N1	-2.47	120.07	122.79
52	S2	105	PSU	O2-C2-N1	-2.47	120.08	122.79
6	L5	4435	PSU	O2-C2-N1	-2.47	120.08	122.79
6	L5	1632	PSU	C6-N1-C2	-2.47	120.16	122.68
6	L5	2630	A2M	N3-C4-N9	2.46	131.14	127.08
52	S2	1833	6MZ	C9-N6-C6	-2.46	120.75	122.87
6	L5	3496	PSU	O2-C2-N1	-2.46	120.08	122.79
52	S2	682	PSU	O2-C2-N1	-2.46	120.09	122.79
52	S2	27	A2M	C4-N9-C8	2.45	108.39	105.73
6	L5	2630	A2M	C4-C5-N7	-2.45	107.63	110.62
6	L5	1721	PSU	O2-C2-N1	-2.45	120.09	122.79
52	S2	210	PSU	O2-C2-N1	-2.45	120.10	122.79
52	S2	864	PSU	O2-C2-N1	-2.45	120.10	122.79
6	L5	4240	OMG	CM2-O2'-C2'	-2.45	108.10	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	Si	62	HY3	O-C-CA	-2.45	118.01	124.83
6	L5	3599	A2M	C4'-O4'-C1'	-2.45	104.08	109.47
6	L5	3562	A2M	C4-N9-C8	2.45	108.38	105.73
6	L5	3494	PSU	O2-C2-N1	-2.45	120.10	122.79
6	L5	1720	PSU	O2-C2-N1	-2.44	120.10	122.79
6	L5	2267	OMG	N9-C4-N3	2.44	130.84	125.94
6	L5	4267	PSU	O2-C2-N1	-2.44	120.10	122.79
8	L8	69	PSU	O2-C2-N1	-2.44	120.10	122.79
6	L5	2658	A2M	CM'-O2'-C2'	-2.44	108.12	114.52
6	L5	4269	A2M	O4'-C4'-C3'	-2.44	100.29	105.11
52	S2	36	PSU	O2-C2-N1	-2.44	120.11	122.79
6	L5	3450	A2M	CM'-O2'-C2'	-2.43	108.14	114.52
52	S2	652	PSU	C6-C5-C4	2.43	119.90	118.20
6	L5	3583	PSU	O2-C2-N1	-2.43	120.11	122.79
52	S2	99	A2M	C3'-C2'-C1'	-2.43	98.32	102.89
52	S2	1175	PSU	O2-C2-N1	-2.43	120.11	122.79
6	L5	3599	A2M	CM'-O2'-C2'	-2.43	108.14	114.52
6	L5	1718	PSU	O2-C2-N1	-2.43	120.12	122.79
52	S2	815	PSU	C6-C5-C4	2.43	119.90	118.20
52	S2	1852	MA6	N1-C6-N6	2.43	119.74	117.08
6	L5	3562	A2M	CM'-O2'-C2'	-2.43	108.16	114.52
6	L5	4169	PSU	O2-C2-N1	-2.43	120.12	122.79
6	L5	1479	A2M	C4-N9-C8	2.43	108.36	105.73
6	L5	4042	PSU	C6-C5-C4	2.42	119.89	118.20
52	S2	172	OMU	CM2-O2'-C2'	-2.42	108.17	114.52
6	L5	3447	PSU	O2-C2-N1	-2.42	120.13	122.79
6	L5	4711	PSU	O2-C2-N1	-2.42	120.13	122.79
52	S2	407	PSU	O2-C2-N1	-2.42	120.13	122.79
6	L5	4245	OMG	N9-C4-N3	2.41	130.79	125.94
52	S2	166	A2M	CM'-O2'-C2'	-2.41	108.19	114.52
78	Sd	2	SAC	O-C-CA	-2.41	118.45	124.78
8	L8	55	PSU	O2-C2-N1	-2.41	120.14	122.79
6	L5	400	A2M	C4-N9-C8	2.41	108.34	105.73
6	L5	3616	PSU	O2-C2-N1	-2.41	120.14	122.79
52	S2	1833	6MZ	C4-N9-C8	2.41	108.34	105.73
52	S2	116	OMU	O2-C2-N1	-2.41	119.59	122.79
52	S2	218	PSU	O2-C2-N1	-2.41	120.14	122.79
6	L5	3657	OMU	O2-C2-N1	-2.40	119.59	122.79
52	S2	1392	OMC	CM2-O2'-C2'	-2.40	108.22	114.52
6	L5	4138	OMG	CM2-O2'-C2'	-2.40	108.22	114.52
6	L5	2475	PSU	O2-C2-N1	-2.40	120.15	122.79
52	S2	1047	PSU	O2-C2-N1	-2.40	120.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3973	OMU	O2-C2-N1	-2.40	119.60	122.79
6	L5	3599	A2M	O4'-C4'-C3'	-2.40	100.37	105.11
52	S2	469	A2M	O4'-C4'-C3'	-2.39	100.38	105.11
52	S2	1046	PSU	O2-C2-N1	-2.39	120.16	122.79
6	L5	1479	A2M	CM'-O2'-C2'	-2.39	108.25	114.52
6	L5	4336	A2M	C4-N9-C8	2.39	108.32	105.73
52	S2	1289	OMU	CM2-O2'-C2'	-2.39	108.25	114.52
52	S2	1640	7MG	O6-C6-C5	-2.39	121.68	127.54
52	S2	1338	4AC	C5-C4-N4	-2.39	118.77	122.92
6	L5	2351	PSU	O2-C2-N1	-2.38	120.17	122.79
52	S2	109	PSU	O2-C2-N1	-2.38	120.17	122.79
52	S2	1644	PSU	O2-C2-N1	-2.38	120.17	122.79
6	L5	4039	PSU	C6-C5-C4	2.38	119.86	118.20
52	S2	650	PSU	O2-C2-N1	-2.38	120.18	122.79
6	L5	3371	PSU	O2-C2-N1	-2.38	120.18	122.79
52	S2	1338	4AC	C6-C5-C4	2.37	119.86	116.96
52	S2	628	OMU	O2-C2-N1	-2.37	119.64	122.79
52	S2	650	PSU	C6-C5-C4	2.37	119.86	118.20
6	L5	3517	A2M	C4-N9-C8	2.37	108.30	105.73
52	S2	687	PSU	C6-C5-C4	2.37	119.85	118.20
52	S2	1245	PSU	C6-C5-C4	2.37	119.85	118.20
52	S2	1057	PSU	O2-C2-N1	-2.37	120.19	122.79
6	L5	1638	PSU	O2-C2-N1	-2.37	120.19	122.79
6	L5	2658	A2M	C4-N9-C8	2.36	108.29	105.73
52	S2	407	PSU	C6-C5-C4	2.36	119.85	118.20
6	L5	3585	PSU	O2-C2-N1	-2.36	120.19	122.79
52	S2	1233	PSU	O2-C2-N1	-2.36	120.20	122.79
6	L5	3496	PSU	C6-C5-C4	2.35	119.84	118.20
6	L5	3359	OMG	N9-C4-N3	2.35	130.66	125.94
52	S2	577	A2M	O4'-C4'-C3'	-2.35	100.46	105.11
6	L5	3462	PSU	O2-C2-N1	-2.35	120.20	122.79
6	L5	4276	UR3	C6-N1-C2	-2.35	119.68	121.79
6	L5	3631	OMG	CM2-O2'-C2'	-2.35	108.36	114.52
52	S2	652	PSU	O2-C2-N1	-2.35	120.20	122.79
6	L5	2244	A2M	CM'-O2'-C2'	-2.35	108.36	114.52
6	L5	398	A2M	C3'-C2'-C1'	-2.35	98.47	102.89
52	S2	645	OMG	CM2-O2'-C2'	-2.35	108.37	114.52
52	S2	577	A2M	C4-N9-C8	2.34	108.27	105.73
6	L5	3369	PSU	C6-C5-C4	2.34	119.83	118.20
52	S2	355	OMU	O2-C2-N1	-2.34	119.68	122.79
52	S2	1446	PSU	O2-C2-N1	-2.34	120.22	122.79
6	L5	1801	PSU	O2-C2-N1	-2.33	120.22	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4740	PSU	O2-C2-N1	-2.33	120.22	122.79
6	L5	2351	PSU	C6-C5-C4	2.33	119.83	118.20
6	L5	1477	OMG	N9-C4-N3	2.33	130.62	125.94
6	L5	4039	PSU	O2-C2-N1	-2.33	120.23	122.79
52	S2	218	PSU	C6-C5-C4	2.33	119.83	118.20
6	L5	2206	A2M	C4-N9-C8	2.33	108.25	105.73
6	L5	3502	PSU	O2-C2-N1	-2.33	120.23	122.79
52	S2	159	A2M	C4-N9-C8	2.32	108.24	105.73
52	S2	1626	PSU	O2-C2-N1	-2.32	120.23	122.79
52	S2	1239	PSU	C6-C5-C4	2.32	119.82	118.20
6	L5	1810	A2M	O4'-C4'-C3'	-2.32	100.53	105.11
52	S2	669	A2M	C4-C5-N7	-2.31	107.80	110.62
52	S2	645	OMG	C8-N7-C5	2.31	108.43	104.24
6	L5	3652	PSU	O2-C2-N1	-2.31	120.24	122.79
6	L5	2208	OMC	CM2-O2'-C2'	-2.31	108.45	114.52
6	L5	1810	A2M	C4-C5-N7	-2.31	107.80	110.62
52	S2	816	PSU	C6-C5-C4	2.31	119.81	118.20
52	S2	1644	PSU	C6-C5-C4	2.31	119.81	118.20
6	L5	2475	PSU	C6-C5-C4	2.31	119.81	118.20
6	L5	4217	PSU	O2-C2-N1	-2.31	120.25	122.79
6	L5	1731	PSU	C6-C5-C4	2.31	119.81	118.20
6	L5	4193	5MC	N4-C4-N3	2.30	122.67	118.48
52	S2	1851	MA6	C6-C5-N7	2.30	137.15	133.28
52	S2	682	PSU	C6-C5-C4	2.30	119.81	118.20
52	S2	166	A2M	C4-C5-N7	-2.30	107.82	110.62
6	L5	3631	OMG	N9-C4-N3	2.30	130.56	125.94
52	S2	1057	PSU	C6-C5-C4	2.30	119.81	118.20
6	L5	3517	A2M	C4'-O4'-C1'	-2.30	104.40	109.47
6	L5	4203	PSU	O2-C2-N1	-2.30	120.26	122.79
6	L5	4749	PSU	C6-C5-C4	2.30	119.80	118.20
52	S2	1679	A2M	C4-N9-C8	2.29	108.22	105.73
6	L5	1477	OMG	C1'-N9-C4	-2.29	119.69	126.50
6	L5	2194	OMC	O2-C2-N3	-2.29	118.60	122.33
6	L5	3492	A2M	O2'-C2'-C1'	2.29	113.55	109.08
52	S2	1047	PSU	C6-C5-C4	2.29	119.80	118.20
6	L5	2206	A2M	O4'-C4'-C3'	-2.29	100.58	105.11
6	L5	1270	A2M	C4'-O4'-C1'	-2.29	104.42	109.47
6	L5	3490	PSU	O2-C2-N1	-2.29	120.27	122.79
6	L5	3492	A2M	C3'-C2'-C1'	-2.28	98.60	102.89
52	S2	429	OMU	O2-C2-N1	-2.28	119.75	122.79
6	L5	4336	A2M	C4'-O4'-C1'	-2.28	104.43	109.47
52	S2	802	PSU	C6-N1-C2	-2.28	120.35	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L8	55	PSU	C6-C5-C4	2.28	119.79	118.20
52	S2	1327	OMU	O2-C2-N1	-2.28	119.75	122.79
6	L5	2719	OMG	O6-C6-C5	-2.28	120.55	126.60
6	L5	4188	PSU	O2-C2-N1	-2.28	120.28	122.79
6	L5	2207	OMG	N1-C2-N3	-2.28	119.07	123.32
60	SL	2	SAC	O-C-CA	-2.28	118.81	124.78
52	S2	1348	PSU	O2-C2-N1	-2.28	120.28	122.79
6	L5	4298	PSU	O2-C2-N1	-2.28	120.28	122.79
52	S2	577	A2M	C3'-C2'-C1'	-2.28	98.61	102.89
6	L5	3492	A2M	C4-N9-C8	2.27	108.19	105.73
6	L5	400	A2M	O4'-C4'-C3'	-2.27	100.62	105.11
6	L5	2719	OMG	CM2-O2'-C2'	-2.27	108.56	114.52
52	S2	34	PSU	O2-C2-N1	-2.27	120.29	122.79
6	L5	2206	A2M	O4'-C1'-N9	-2.27	103.58	108.06
6	L5	1632	PSU	O2-C2-N1	-2.27	120.29	122.79
6	L5	4317	A2M	C4-N9-C8	2.27	108.19	105.73
6	L5	3427	PSU	O2-C2-N1	-2.27	120.29	122.79
52	S2	1640	7MG	N1-C2-N3	-2.27	119.09	123.32
6	L5	1260	OMG	C8-N7-C5	2.27	108.34	104.24
52	S2	1178	PSU	O2-C2-N1	-2.27	120.30	122.79
6	L5	1537	PSU	C6-C5-C4	2.26	119.78	118.20
52	S2	469	A2M	C4-C5-N7	-2.26	107.86	110.62
52	S2	469	A2M	C4'-O4'-C1'	-2.26	104.48	109.47
6	L5	2647	OMC	CM2-O2'-C2'	-2.26	108.59	114.52
6	L5	1580	OMG	O6-C6-C5	-2.26	120.60	126.60
52	S2	1491	OMG	O6-C6-C5	-2.26	120.61	126.60
6	L5	1270	A2M	C4-C5-N7	-2.26	107.87	110.62
52	S2	815	PSU	O2-C2-N1	-2.26	120.31	122.79
6	L5	4366	OMU	CM2-O2'-C2'	-2.26	108.60	114.52
52	S2	166	A2M	C4-N9-C8	2.26	108.17	105.73
6	L5	3585	PSU	C6-C5-C4	2.26	119.78	118.20
52	S2	577	A2M	C4-C5-N7	-2.26	107.87	110.62
6	L5	3450	A2M	C4-C5-N7	-2.26	107.87	110.62
6	L5	4322	PSU	O2-C2-N1	-2.25	120.31	122.79
6	L5	2630	A2M	C2'-C3'-C4'	-2.25	97.10	101.99
6	L5	2244	A2M	C4'-O4'-C1'	-2.25	104.50	109.47
6	L5	3576	PSU	C6-N1-C2	-2.25	120.38	122.68
52	S2	513	A2M	C3'-C2'-C1'	-2.25	98.66	102.89
52	S2	513	A2M	C4-N9-C8	2.25	108.16	105.73
49	Ls	2	SAC	O-C-CA	-2.25	118.89	124.78
6	L5	4298	PSU	C6-C5-C4	2.25	119.77	118.20
52	S2	1082	PSU	O2-C2-N1	-2.24	120.32	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4045	PSU	O2-C2-N1	-2.24	120.32	122.79
6	L5	2680	OMU	O2-C2-N1	-2.24	119.81	122.79
6	L5	1638	PSU	C6-C5-C4	2.24	119.77	118.20
6	L5	3524	OMG	N1-C2-N3	-2.24	119.14	123.32
8	L8	75	OMG	O6-C6-C5	-2.24	120.67	126.60
6	L5	1477	OMG	C8-N7-C5	2.24	108.29	104.24
52	S2	437	OMG	O6-C6-C5	-2.24	120.67	126.60
6	L5	3676	OMG	O6-C6-C5	-2.24	120.67	126.60
6	L5	1491	PSU	C6-N1-C2	-2.23	120.40	122.68
6	L5	4246	PSU	C6-N1-C2	-2.23	120.40	122.68
52	S2	1851	MA6	N9-C8-N7	-2.23	110.86	113.91
6	L5	1260	OMG	N1-C2-N3	-2.23	119.16	123.32
6	L5	4107	PSU	O2-C2-N1	-2.23	120.33	122.79
6	L5	2267	OMG	O6-C6-C5	-2.23	120.69	126.60
6	L5	1537	PSU	O2-C2-N1	-2.23	120.34	122.79
6	L5	4317	A2M	C2'-C3'-C4'	-2.23	97.15	101.99
6	L5	3524	OMG	CM2-O2'-C2'	-2.23	108.68	114.52
6	L5	2658	A2M	C4-C5-N7	-2.23	107.91	110.62
52	S2	510	OMG	O6-C6-C5	-2.22	120.70	126.60
6	L5	3466	PSU	O2-C2-N1	-2.22	120.34	122.79
6	L5	1799	PSU	C6-N1-C2	-2.22	120.41	122.68
6	L5	3476	OMG	O6-C6-C5	-2.22	120.70	126.60
6	L5	4245	OMG	C8-N7-C5	2.22	108.26	104.24
52	S2	1704	OMC	CM2-O2'-C2'	-2.22	108.69	114.52
52	S2	1032	A2M	C4-C5-N7	-2.22	107.91	110.62
52	S2	868	OMG	O6-C6-C5	-2.22	120.71	126.60
52	S2	1448	OMG	O6-C6-C5	-2.22	120.71	126.60
6	L5	3631	OMG	N1-C2-N3	-2.22	119.18	123.32
6	L5	1266	1MA	C8-N7-C5	2.22	108.26	104.24
6	L5	2207	OMG	O6-C6-C5	-2.22	120.72	126.60
6	L5	3973	OMU	CM2-O2'-C2'	-2.22	108.71	114.52
6	L5	4278	PSU	C6-N1-C2	-2.22	120.42	122.68
6	L5	398	A2M	C4-C5-N7	-2.22	107.92	110.62
6	L5	2206	A2M	C4-C5-N7	-2.22	107.92	110.62
6	L5	3359	OMG	N1-C2-N3	-2.21	119.19	123.32
6	L5	4138	OMG	C8-N7-C5	2.21	108.25	104.24
52	S2	36	PSU	C6-C5-C4	2.21	119.75	118.20
52	S2	868	OMG	C8-N7-C5	2.21	108.24	104.24
6	L5	4058	PSU	O2-C2-N1	-2.21	120.36	122.79
6	L5	4278	PSU	O2-C2-N1	-2.21	120.36	122.79
6	L5	4325	PSU	C6-C5-C4	2.21	119.74	118.20
52	S2	645	OMG	O6-C6-C5	-2.21	120.74	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4435	PSU	C6-N1-C2	-2.21	120.42	122.68
6	L5	4269	A2M	C4-N9-C8	2.21	108.12	105.73
6	L5	4336	A2M	C4-C5-N7	-2.21	107.93	110.62
6	L5	2206	A2M	C5-C6-N1	2.21	122.13	117.39
6	L5	4383	OMG	O6-C6-C5	-2.21	120.75	126.60
6	L5	4177	PSU	C6-N1-C2	-2.21	120.43	122.68
6	L5	1489	A2M	C4-C5-N7	-2.21	107.93	110.62
52	S2	577	A2M	C4'-O4'-C1'	-2.20	104.61	109.47
6	L5	2258	OMU	O2-C2-N1	-2.20	119.86	122.79
52	S2	868	OMG	N1-C2-N3	-2.20	119.22	123.32
6	L5	4116	OMG	C8-N7-C5	2.20	108.22	104.24
6	L5	4749	PSU	O2-C2-N1	-2.20	120.37	122.79
52	S2	518	OMC	CM2-O2'-C2'	-2.20	108.75	114.52
6	L5	2630	A2M	C5-C4-N9	2.20	108.34	105.78
6	L5	2244	A2M	C4-C5-N7	-2.20	107.94	110.62
6	L5	4366	OMU	O2-C2-N1	-2.20	119.86	122.79
52	S2	967	PSU	O2-C2-N1	-2.20	120.37	122.79
52	S2	602	OMG	O6-C6-C5	-2.20	120.77	126.60
6	L5	2630	A2M	C5-C6-N1	2.20	122.11	117.39
52	S2	823	PSU	C6-N1-C2	-2.20	120.44	122.68
6	L5	4166	PSU	O2-C2-N1	-2.20	120.37	122.79
6	L5	4282	OMC	CM2-O2'-C2'	-2.19	108.77	114.52
6	L5	4116	OMG	O6-C6-C5	-2.19	120.78	126.60
52	S2	1384	A2M	C4-C5-N7	-2.19	107.95	110.62
6	L5	4336	A2M	C5-C6-N1	2.19	122.10	117.39
6	L5	4245	OMG	N1-C2-N3	-2.19	119.23	123.32
52	S2	602	OMG	C8-N7-C5	2.19	108.21	104.24
6	L5	4042	PSU	O2-C2-N1	-2.19	120.38	122.79
6	L5	4245	OMG	O6-C6-C5	-2.19	120.79	126.60
52	S2	573	PSU	C6-C5-C4	2.19	119.73	118.20
6	L5	1731	PSU	O2-C2-N1	-2.19	120.38	122.79
6	L5	3616	PSU	C6-N1-C2	-2.19	120.44	122.68
6	L5	1477	OMG	N1-C2-N3	-2.19	119.24	123.32
6	L5	2658	A2M	O4'-C4'-C3'	-2.19	100.79	105.11
6	L5	4383	OMG	C8-N7-C5	2.19	108.19	104.24
6	L5	4269	A2M	C4-C5-N7	-2.18	107.96	110.62
6	L5	3974	OMG	O6-C6-C5	-2.18	120.81	126.60
52	S2	864	PSU	C6-C5-C4	2.18	119.72	118.20
52	S2	684	OMG	C8-N7-C5	2.18	108.19	104.24
6	L5	4240	OMG	C8-N7-C5	2.18	108.18	104.24
6	L5	4177	PSU	C6-C5-C4	2.18	119.72	118.20
6	L5	3524	OMG	O6-C6-C5	-2.18	120.83	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	99	A2M	C4-C5-N7	-2.18	107.97	110.62
52	S2	1329	OMG	C8-N7-C5	2.17	108.18	104.24
6	L5	3554	PSU	C6-N1-C2	-2.17	120.46	122.68
6	L5	2267	OMG	N1-C2-N3	-2.17	119.27	123.32
52	S2	159	A2M	CM'-O2'-C2'	-2.17	108.82	114.52
6	L5	3562	A2M	C3'-C2'-C1'	-2.17	98.81	102.89
6	L5	4369	OMG	O6-C6-C5	-2.17	120.84	126.60
52	S2	687	PSU	C6-N1-C2	-2.17	120.46	122.68
6	L5	3562	A2M	C4-C5-N7	-2.17	107.97	110.62
6	L5	1489	A2M	C4-N9-C8	2.17	108.08	105.73
6	L5	4364	OMG	C8-N7-C5	2.17	108.17	104.24
52	S2	669	A2M	CM'-O2'-C2'	-2.17	108.83	114.52
52	S2	485	A2M	C4-C5-N7	-2.17	107.98	110.62
52	S2	1679	A2M	C5-C6-N1	2.17	122.05	117.39
6	L5	3359	OMG	O6-C6-C5	-2.17	120.85	126.60
6	L5	3942	OMG	N1-C2-N3	-2.17	119.28	123.32
6	L5	3456	A2M	C4-C5-N7	-2.17	107.98	110.62
52	S2	684	OMG	O6-C6-C5	-2.17	120.85	126.60
6	L5	3517	A2M	C5-C6-N1	2.17	122.04	117.39
6	L5	4325	PSU	C6-N1-C2	-2.17	120.47	122.68
6	L5	4045	PSU	C6-C5-C4	2.17	119.71	118.20
6	L5	1479	A2M	C4-C5-N7	-2.17	107.98	110.62
6	L5	3359	OMG	C8-N7-C5	2.16	108.16	104.24
52	S2	27	A2M	C5-C6-N1	2.16	122.03	117.39
6	L5	4374	PSU	C6-N1-C2	-2.16	120.47	122.68
6	L5	3427	PSU	C6-C5-C4	2.16	119.71	118.20
6	L5	3514	5MC	N4-C4-N3	2.16	122.42	118.48
6	L5	3554	PSU	C6-C5-C4	2.16	119.71	118.20
6	L5	3942	OMG	O6-C6-C5	-2.16	120.87	126.60
52	S2	159	A2M	C4-C5-N7	-2.16	107.99	110.62
52	S2	510	OMG	CM2-O2'-C2'	-2.16	108.86	114.52
52	S2	99	A2M	C5-C6-N1	2.16	122.02	117.39
6	L5	4240	OMG	O6-C6-C5	-2.16	120.88	126.60
52	S2	513	A2M	C4-C5-N7	-2.16	107.99	110.62
6	L5	1489	A2M	C5-C6-N1	2.16	122.02	117.39
6	L5	1260	OMG	O6-C6-C5	-2.16	120.88	126.60
52	S2	684	OMG	N1-C2-N3	-2.16	119.30	123.32
6	L5	4240	OMG	N1-C2-N3	-2.16	119.30	123.32
52	S2	159	A2M	C3'-C2'-C1'	-2.16	98.84	102.89
52	S2	1693	PSU	C6-C5-C4	2.16	119.70	118.20
6	L5	3492	A2M	C5-C6-N1	2.16	122.02	117.39
6	L5	4149	PSU	C6-N1-C2	-2.15	120.48	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3631	OMG	O6-C6-C5	-2.15	120.88	126.60
6	L5	3494	PSU	C6-N1-C2	-2.15	120.48	122.68
6	L5	4138	OMG	O6-C6-C5	-2.15	120.89	126.60
6	L5	4364	OMG	O6-C6-C5	-2.15	120.89	126.60
52	S2	1329	OMG	O6-C6-C5	-2.15	120.90	126.60
6	L5	3974	OMG	C8-N7-C5	2.15	108.13	104.24
52	S2	93	PSU	O2-C2-N1	-2.15	120.42	122.79
6	L5	1810	A2M	C3'-C2'-C1'	-2.15	98.85	102.89
52	S2	109	PSU	C6-C5-C4	2.15	119.70	118.20
6	L5	3599	A2M	C5-C6-N1	2.15	122.00	117.39
6	L5	3514	5MC	O2-C2-N3	-2.15	118.84	122.33
6	L5	4269	A2M	C5-C6-N1	2.15	122.00	117.39
52	S2	166	A2M	C3'-C2'-C1'	-2.15	98.86	102.89
6	L5	3583	PSU	C6-N1-C2	-2.14	120.49	122.68
52	S2	669	A2M	C5-C6-N1	2.14	121.99	117.39
6	L5	3447	PSU	C6-C5-C4	2.14	119.70	118.20
6	L5	1260	OMG	CM2-O2'-C2'	-2.14	108.90	114.52
6	L5	1721	PSU	C6-C5-C4	2.14	119.70	118.20
52	S2	1384	A2M	C4-N9-C8	2.14	108.05	105.73
52	S2	1679	A2M	C4-C5-N7	-2.14	108.01	110.62
6	L5	1799	PSU	C6-C5-C4	2.14	119.69	118.20
6	L5	4369	OMG	C8-N7-C5	2.14	108.11	104.24
52	S2	1384	A2M	C5-C6-N1	2.14	121.99	117.39
6	L5	3557	A2M	C5-C6-N1	2.14	121.98	117.39
6	L5	3676	OMG	C8-N7-C5	2.14	108.11	104.24
6	L5	1810	A2M	C5-C6-N1	2.14	121.98	117.39
6	L5	3557	A2M	C4-N9-C8	2.14	108.05	105.73
6	L5	4317	A2M	C5-C6-N1	2.14	121.98	117.39
52	S2	510	OMG	C8-N7-C5	2.14	108.11	104.24
52	S2	116	OMU	CM2-O2'-C2'	-2.14	108.91	114.52
6	L5	2244	A2M	C5-C6-N1	2.14	121.98	117.39
8	L8	75	OMG	N1-C2-N3	-2.14	119.33	123.32
6	L5	3631	OMG	C8-N7-C5	2.14	108.11	104.24
6	L5	3517	A2M	C3'-C2'-C1'	-2.14	98.87	102.89
6	L5	3371	PSU	C6-C5-C4	2.14	119.69	118.20
6	L5	4711	PSU	C6-C5-C4	2.14	119.69	118.20
6	L5	4317	A2M	C4-C5-N7	-2.13	108.02	110.62
6	L5	4419	PSU	C6-N1-C2	-2.13	120.50	122.68
6	L5	4336	A2M	CM'-O2'-C2'	-2.13	108.92	114.52
52	S2	591	A2M	C5-C6-N1	2.13	121.97	117.39
6	L5	2207	OMG	C8-N7-C5	2.13	108.10	104.24
6	L5	3942	OMG	C8-N7-C5	2.13	108.10	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	166	A2M	C5-C6-N1	2.13	121.97	117.39
6	L5	400	A2M	C5-C6-N1	2.13	121.97	117.39
52	S2	513	A2M	C5-C6-N1	2.13	121.97	117.39
52	S2	1491	OMG	N1-C2-N3	-2.13	119.34	123.32
52	S2	159	A2M	C5-C6-N1	2.13	121.97	117.39
52	S2	1843	4AC	C6-C5-C4	2.13	119.57	116.96
6	L5	2267	OMG	C8-N7-C5	2.13	108.09	104.24
6	L5	3456	A2M	C4-N9-C8	2.13	108.03	105.73
52	S2	27	A2M	C4-C5-N7	-2.13	108.03	110.62
6	L5	3500	PSU	C6-C5-C4	2.13	119.69	118.20
52	S2	602	OMG	N1-C2-N3	-2.13	119.35	123.32
6	L5	4374	PSU	C6-C5-C4	2.13	119.68	118.20
52	S2	1491	OMG	C8-N7-C5	2.12	108.09	104.24
6	L5	3476	OMG	C8-N7-C5	2.12	108.09	104.24
6	L5	4058	PSU	C6-C5-C4	2.12	119.68	118.20
6	L5	2658	A2M	C5-C6-N1	2.12	121.95	117.39
6	L5	3562	A2M	C5-C6-N1	2.12	121.95	117.39
52	S2	36	PSU	C6-N1-C2	-2.12	120.51	122.68
6	L5	1638	PSU	C6-N1-C2	-2.12	120.51	122.68
52	S2	469	A2M	C5-C6-N1	2.12	121.95	117.39
6	L5	3502	PSU	C6-C5-C4	2.12	119.68	118.20
6	L5	4383	OMG	N1-C2-N3	-2.12	119.36	123.32
52	S2	1032	A2M	O4'-C1'-N9	-2.12	103.88	108.06
6	L5	3599	A2M	C4-C5-N7	-2.12	108.03	110.62
6	L5	3450	A2M	C5-C6-N1	2.12	121.94	117.39
6	L5	3456	A2M	C5-C6-N1	2.12	121.94	117.39
52	S2	1175	PSU	C6-N1-C2	-2.12	120.52	122.68
6	L5	3476	OMG	N1-C2-N3	-2.12	119.37	123.32
6	L5	398	A2M	C5-C6-N1	2.12	121.94	117.39
52	S2	628	OMU	CM2-O2'-C2'	-2.12	108.97	114.52
6	L5	1477	OMG	O6-C6-C5	-2.12	120.98	126.60
52	S2	1640	7MG	N9-C4-N3	2.12	128.63	125.47
6	L5	4217	PSU	C6-N1-C2	-2.12	120.52	122.68
52	S2	485	A2M	C5-C6-N1	2.11	121.93	117.39
6	L5	1718	PSU	C6-C5-C4	2.11	119.67	118.20
52	S2	867	PSU	C6-N1-C2	-2.11	120.52	122.68
6	L5	1720	PSU	C6-C5-C4	2.11	119.67	118.20
6	L5	3494	PSU	C6-C5-C4	2.11	119.67	118.20
6	L5	4039	PSU	C6-N1-C2	-2.11	120.53	122.68
6	L5	1721	PSU	C6-N1-C2	-2.11	120.53	122.68
52	S2	1178	PSU	C6-N1-C2	-2.11	120.53	122.68
6	L5	3371	PSU	C6-N1-C2	-2.10	120.53	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	121	OMU	CM2-O2'-C2'	-2.10	109.00	114.52
6	L5	2265	OMC	O2-C2-N3	-2.10	118.91	122.33
6	L5	3524	OMG	C8-N7-C5	2.10	108.05	104.24
8	L8	75	OMG	C8-N7-C5	2.10	108.05	104.24
6	L5	1479	A2M	C5-C6-N1	2.10	121.90	117.39
6	L5	3974	OMG	N1-C2-N3	-2.10	119.40	123.32
6	L5	4217	PSU	C6-C5-C4	2.10	119.67	118.20
52	S2	172	OMU	O2'-C2'-C1'	2.10	113.17	109.08
52	S2	510	OMG	N1-C2-N3	-2.10	119.41	123.32
6	L5	2475	PSU	C6-N1-C2	-2.10	120.54	122.68
6	L5	4383	OMG	CM2-O2'-C2'	-2.10	109.02	114.52
6	L5	4245	OMG	CM2-O2'-C2'	-2.10	109.02	114.52
52	S2	166	A2M	O4'-C4'-C3'	-2.10	100.97	105.11
52	S2	577	A2M	CM'-O2'-C2'	-2.09	109.03	114.52
52	S2	1384	A2M	C3'-C2'-C1'	-2.09	98.95	102.89
6	L5	4419	PSU	C6-C5-C4	2.09	119.66	118.20
6	L5	4369	OMG	N1-C2-N3	-2.09	119.42	123.32
6	L5	3492	A2M	C4-C5-N7	-2.09	108.07	110.62
6	L5	1580	OMG	C8-N7-C5	2.09	108.03	104.24
52	S2	645	OMG	N1-C2-N3	-2.09	119.42	123.32
6	L5	4116	OMG	N1-C2-N3	-2.09	119.42	123.32
6	L5	1720	PSU	C6-N1-C2	-2.09	120.55	122.68
52	S2	1384	A2M	O4'-C4'-C3'	-2.09	100.98	105.11
6	L5	3490	PSU	C6-C5-C4	2.09	119.66	118.20
6	L5	1270	A2M	C5-C6-N1	2.09	121.88	117.39
6	L5	4169	PSU	C6-N1-C2	-2.09	120.55	122.68
6	L5	4711	PSU	C6-N1-C2	-2.09	120.55	122.68
6	L5	3557	A2M	C4-C5-N7	-2.09	108.08	110.62
52	S2	610	PSU	C6-N1-C2	-2.09	120.55	122.68
6	L5	2265	OMC	CM2-O2'-C2'	-2.09	109.05	114.52
6	L5	2719	OMG	C8-N7-C5	2.08	108.01	104.24
6	L5	2719	OMG	N1-C2-N3	-2.08	119.44	123.32
6	L5	4138	OMG	N1-C2-N3	-2.08	119.44	123.32
8	L8	69	PSU	C6-N1-C2	-2.08	120.56	122.68
52	S2	172	OMU	O2-C2-N1	-2.08	120.02	122.79
52	S2	591	A2M	C4-C5-N7	-2.08	108.08	110.62
52	S2	1679	A2M	CM'-O2'-C2'	-2.08	109.07	114.52
52	S2	1368	PSU	C6-C5-C4	2.08	119.65	118.20
52	S2	437	OMG	C8-N7-C5	2.08	108.00	104.24
52	S2	1805	OMU	O2-C2-N1	-2.08	120.03	122.79
6	L5	4364	OMG	N1-C2-N3	-2.08	119.45	123.32
52	S2	577	A2M	C5-C6-N1	2.07	121.84	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	3369	PSU	O2-C2-N1	-2.07	120.51	122.79
52	S2	1448	OMG	C8-N7-C5	2.07	107.99	104.24
6	L5	3676	OMG	N1-C2-N3	-2.07	119.46	123.32
6	L5	3427	PSU	C6-N1-C2	-2.07	120.57	122.68
52	S2	1233	PSU	C6-C5-C4	2.07	119.64	118.20
52	S2	1175	PSU	C6-C5-C4	2.06	119.64	118.20
52	S2	1626	PSU	C6-C5-C4	2.06	119.64	118.20
6	L5	4322	PSU	C6-C5-C4	2.06	119.64	118.20
6	L5	3496	PSU	C6-N1-C2	-2.06	120.58	122.68
6	L5	1683	PSU	C6-N1-C2	-2.06	120.58	122.68
6	L5	1580	OMG	C1'-N9-C8	-2.05	120.85	126.70
52	S2	119	PSU	C6-N1-C2	-2.05	120.58	122.68
52	S2	1082	PSU	C6-C5-C4	2.05	119.63	118.20
52	S2	1329	OMG	CM2-O2'-C2'	-2.05	109.14	114.52
52	S2	967	PSU	C6-N1-C2	-2.05	120.59	122.68
52	S2	485	A2M	C4'-O4'-C1'	-2.05	104.95	109.47
52	S2	1329	OMG	N1-C2-N3	-2.05	119.50	123.32
6	L5	3462	PSU	C6-C5-C4	2.05	119.63	118.20
52	S2	682	PSU	C6-N1-C2	-2.05	120.59	122.68
6	L5	398	A2M	CM'-O2'-C2'	-2.05	109.15	114.52
52	S2	1693	PSU	C6-N1-C2	-2.05	120.59	122.68
6	L5	3540	OMC	CM2-O2'-C2'	-2.04	109.16	114.52
52	S2	1368	PSU	C6-N1-C2	-2.04	120.59	122.68
6	L5	4116	OMG	CM2-O2'-C2'	-2.04	109.16	114.52
52	S2	1852	MA6	N9-C8-N7	-2.04	111.12	113.91
52	S2	99	A2M	CM'-O2'-C2'	-2.04	109.17	114.52
6	L5	4203	PSU	C6-N1-C2	-2.04	120.60	122.68
6	L5	3450	A2M	C5-C4-N9	2.04	108.16	105.78
6	L5	3616	PSU	C6-C5-C4	2.04	119.62	118.20
6	L5	2630	A2M	C4-N9-C8	2.04	107.94	105.73
52	S2	437	OMG	N1-C2-N3	-2.04	119.52	123.32
6	L5	1580	OMG	N1-C2-N3	-2.04	119.53	123.32
6	L5	3540	OMC	O2-C2-N3	-2.03	119.02	122.33
52	S2	1233	PSU	C6-N1-C2	-2.03	120.60	122.68
6	L5	4322	PSU	C6-N1-C2	-2.03	120.60	122.68
52	S2	1384	A2M	C4'-O4'-C1'	-2.03	104.99	109.47
6	L5	3433	OMC	CM2-O2'-C2'	-2.03	109.19	114.52
52	S2	469	A2M	CM'-O2'-C2'	-2.03	109.19	114.52
6	L5	3456	A2M	CM'-O2'-C2'	-2.03	109.20	114.52
52	S2	1852	MA6	C6-C5-N7	2.03	136.68	133.28
52	S2	105	PSU	C6-N1-C2	-2.03	120.61	122.68
52	S2	1005	PSU	C5-C4-N3	2.02	121.16	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L5	4099	PSU	C6-N1-C2	-2.02	120.61	122.68
6	L5	3573	OMC	O2-C2-N3	-2.02	119.04	122.33
6	L5	400	A2M	C4-C5-N7	-2.02	108.16	110.62
52	S2	602	OMG	CM2-O2'-C2'	-2.02	109.23	114.52
6	L5	398	A2M	C4-N9-C8	2.01	107.91	105.73
6	L5	2630	A2M	CM'-O2'-C2'	-2.01	109.24	114.52
52	S2	816	PSU	C6-N1-C2	-2.01	120.63	122.68
6	L5	3359	OMG	CM2-O2'-C2'	-2.01	109.25	114.52
6	L5	4058	PSU	C6-N1-C2	-2.01	120.63	122.68
6	L5	2680	OMU	CM2-O2'-C2'	-2.01	109.25	114.52
52	S2	1448	OMG	N1-C2-N3	-2.01	119.58	123.32
52	S2	1239	PSU	C6-N1-C2	-2.01	120.63	122.68
52	S2	1626	PSU	C6-N1-C2	-2.01	120.63	122.68
52	S2	1057	PSU	C6-N1-C2	-2.01	120.63	122.68
52	S2	1032	A2M	C5-C6-N1	2.00	121.69	117.39
6	L5	3462	PSU	C6-N1-C2	-2.00	120.63	122.68
52	S2	591	A2M	C4-N9-C1'	2.00	131.36	126.59
6	L5	3966	6MZ	N9-C8-N7	-2.00	111.18	113.91
6	L5	3450	A2M	C4-N9-C8	2.00	107.90	105.73
52	S2	109	PSU	C6-N1-C2	-2.00	120.64	122.68
6	L5	3573	OMC	CM2-O2'-C2'	-2.00	109.27	114.52
6	L5	4364	OMG	CM2-O2'-C2'	-2.00	109.28	114.52

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	LF	2	AYA	OT-CT-N-CA
11	LF	2	AYA	CM-CT-N-CA
35	Le	5	MLZ	N-CA-CB-CG
35	Le	5	MLZ	C-CA-CB-CG
52	S2	429	OMU	C2'-C1'-N1-C2
52	S2	429	OMU	C2'-C1'-N1-C6
52	S2	645	OMG	O4'-C4'-C5'-O5'
52	S2	684	OMG	O4'-C4'-C5'-O5'
52	S2	684	OMG	C3'-C4'-C5'-O5'
52	S2	802	PSU	C3'-C4'-C5'-O5'
52	S2	1448	OMG	C3'-C4'-C5'-O5'
52	S2	1833	6MZ	N1-C6-N6-C9
52	S2	1851	MA6	C5-C6-N6-C10
79	Se	67	NMM	N-CA-CB-CG
83	Si	62	HY3	O-C-CA-C3

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Mol	Chain	Res	Type	Atoms
6	L5	1632	PSU	C2'-C1'-C5-C4
6	L5	3433	OMC	C2'-C1'-N1-C6
6	L5	3492	A2M	C1'-C2'-O2'-CM'
6	L5	3494	PSU	C3'-C4'-C5'-O5'
6	L5	3494	PSU	O4'-C4'-C5'-O5'
6	L5	3517	A2M	O4'-C4'-C5'-O5'
6	L5	4382	PSU	C3'-C4'-C5'-O5'
6	L5	4382	PSU	O4'-C4'-C5'-O5'
52	S2	1338	4AC	N3-C4-N4-C7
52	S2	1338	4AC	C5-C4-N4-C7
52	S2	1338	4AC	O7-C7-N4-C4
52	S2	1338	4AC	CM7-C7-N4-C4
52	S2	1843	4AC	N3-C4-N4-C7
52	S2	1843	4AC	C5-C4-N4-C7
6	L5	3433	OMC	C2'-C1'-N1-C2
52	S2	518	OMC	C3'-C4'-C5'-O5'
52	S2	645	OMG	C3'-C4'-C5'-O5'
6	L5	1477	OMG	O4'-C4'-C5'-O5'
6	L5	1477	OMG	C3'-C4'-C5'-O5'
6	L5	3517	A2M	C3'-C4'-C5'-O5'
6	L5	4166	PSU	C3'-C4'-C5'-O5'
81	Sg	1	AME	CT2-CT1-N-CA
81	Sg	1	AME	OT-CT1-N-CA
79	Se	67	NMM	NE-CD-CG-CB
6	L5	4336	A2M	C4'-C5'-O5'-P
52	S2	518	OMC	O4'-C4'-C5'-O5'
52	S2	669	A2M	C3'-C4'-C5'-O5'
52	S2	1448	OMG	O4'-C4'-C5'-O5'
6	L5	2265	OMC	C3'-C4'-C5'-O5'
6	L5	2265	OMC	O4'-C4'-C5'-O5'
6	L5	4166	PSU	O4'-C4'-C5'-O5'
6	L5	2630	A2M	C2'-C1'-N9-C4
6	L5	2630	A2M	C2'-C1'-N9-C8
6	L5	1580	OMG	C3'-C2'-O2'-CM2
52	S2	628	OMU	C2'-C1'-N1-C6
52	S2	802	PSU	O4'-C4'-C5'-O5'
52	S2	823	PSU	C3'-C4'-C5'-O5'
52	S2	1392	OMC	C3'-C4'-C5'-O5'
52	S2	99	A2M	O4'-C4'-C5'-O5'
52	S2	628	OMU	O4'-C4'-C5'-O5'
52	S2	823	PSU	O4'-C4'-C5'-O5'
52	S2	1851	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
52	S2	1852	MA6	C5-C6-N6-C10
6	L5	1489	A2M	C4'-C5'-O5'-P
52	S2	1392	OMC	O4'-C4'-C5'-O5'
6	L5	4246	PSU	C4'-C5'-O5'-P
52	S2	510	OMG	O4'-C4'-C5'-O5'
52	S2	628	OMU	C3'-C4'-C5'-O5'
52	S2	628	OMU	C2'-C1'-N1-C2
10	LE	245	HIC	CA-CB-CG-ND1
6	L5	1479	A2M	O4'-C1'-N9-C4
52	S2	628	OMU	O4'-C1'-N1-C6
6	L5	1270	A2M	C4'-C5'-O5'-P
6	L5	1477	OMG	C4'-C5'-O5'-P
6	L5	3576	PSU	C4'-C5'-O5'-P
6	L5	3433	OMC	O4'-C1'-N1-C2
6	L5	3433	OMC	O4'-C1'-N1-C6
52	S2	577	A2M	C3'-C4'-C5'-O5'
6	L5	3619	OMC	C3'-C4'-C5'-O5'
79	Se	67	NMM	C-CA-CB-CG
6	L5	3517	A2M	C2'-C1'-N9-C8
6	L5	1266	1MA	C2'-C1'-N9-C8
52	S2	628	OMU	O4'-C1'-N1-C2
52	S2	645	OMG	C4'-C5'-O5'-P
6	L5	4336	A2M	C3'-C4'-C5'-O5'
52	S2	429	OMU	O4'-C1'-N1-C6
6	L5	4193	5MC	O4'-C1'-N1-C6
6	L5	1479	A2M	O4'-C1'-N9-C8
52	S2	1491	OMG	C4'-C5'-O5'-P
52	S2	1852	MA6	C4'-C5'-O5'-P
6	L5	4240	OMG	C3'-C2'-O2'-CM2
52	S2	1448	OMG	C4'-C5'-O5'-P
6	L5	2658	A2M	C4'-C5'-O5'-P
6	L5	3676	OMG	C3'-C4'-C5'-O5'
52	S2	429	OMU	O4'-C1'-N1-C2
52	S2	1005	PSU	O4'-C1'-C5-C4
6	L5	2719	OMG	C3'-C2'-O2'-CM2
6	L5	1266	1MA	C2'-C1'-N9-C4
6	L5	4193	5MC	C2'-C1'-N1-C6
6	L5	3492	A2M	O4'-C4'-C5'-O5'
6	L5	4193	5MC	O4'-C1'-N1-C2
6	L5	2194	OMC	O4'-C4'-C5'-O5'
52	S2	591	A2M	O4'-C1'-N9-C8
6	L5	2630	A2M	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
52	S2	510	OMG	C3'-C4'-C5'-O5'
52	S2	669	A2M	O4'-C4'-C5'-O5'
6	L5	2244	A2M	C3'-C4'-C5'-O5'
6	L5	3492	A2M	C3'-C4'-C5'-O5'
10	LE	245	HIC	CA-CB-CG-CD2
52	S2	485	A2M	O4'-C4'-C5'-O5'
6	L5	4369	OMG	O4'-C4'-C5'-O5'
6	L5	4369	OMG	C3'-C4'-C5'-O5'
6	L5	1489	A2M	O4'-C4'-C5'-O5'
60	SL	2	SAC	C-CA-N-C1A
52	S2	802	PSU	C4'-C5'-O5'-P
6	L5	3619	OMC	C4'-C5'-O5'-P

There are no ring outliers.

67 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L5	3557	A2M	1	0
6	L5	2680	OMU	1	0
52	S2	682	PSU	1	0
6	L5	2194	OMC	2	0
6	L5	398	A2M	1	0
52	S2	610	PSU	1	0
6	L5	4138	OMG	1	0
6	L5	2719	OMG	2	0
6	L5	400	A2M	1	0
6	L5	4364	OMG	1	0
6	L5	4383	OMG	1	0
6	L5	1270	A2M	1	0
52	S2	1239	PSU	1	0
35	Le	5	MLZ	1	0
52	S2	172	OMU	1	0
52	S2	1852	MA6	1	0
6	L5	3517	A2M	1	0
6	L5	4202	OMC	1	0
52	S2	1851	MA6	1	0
6	L5	3466	PSU	1	0
6	L5	4366	OMU	2	0
52	S2	1338	4AC	4	0
52	S2	218	PSU	1	0
6	L5	3942	OMG	1	0
52	S2	1448	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L5	4382	PSU	2	0
6	L5	3676	OMG	1	0
52	S2	1833	6MZ	1	0
6	L5	4369	OMG	2	0
6	L5	3599	A2M	2	0
6	L5	3973	OMU	2	0
81	Sg	1	AME	2	0
6	L5	2265	OMC	1	0
83	Si	62	HY3	1	0
6	L5	3631	OMG	1	0
6	L5	1632	PSU	1	0
52	S2	1047	PSU	2	0
52	S2	1046	PSU	1	0
6	L5	4374	PSU	1	0
52	S2	109	PSU	1	0
6	L5	3657	OMU	1	0
6	L5	4193	5MC	2	0
52	S2	116	OMU	2	0
52	S2	1233	PSU	2	0
52	S2	1704	OMC	1	0
6	L5	3476	OMG	1	0
6	L5	3540	OMC	1	0
6	L5	1477	OMG	2	0
6	L5	4203	PSU	1	0
52	S2	1679	A2M	1	0
6	L5	3359	OMG	1	0
52	S2	513	A2M	1	0
6	L5	4419	PSU	1	0
52	S2	1032	A2M	1	0
6	L5	3573	OMC	1	0
6	L5	3514	5MC	1	0
52	S2	1640	7MG	1	0
6	L5	4282	OMC	1	0
52	S2	1843	4AC	1	0
8	L8	75	OMG	1	0
6	L5	2207	OMG	2	0
6	L5	4278	PSU	1	0
6	L5	1284	OMC	1	0
52	S2	437	OMG	2	0
60	SL	2	SAC	1	0
6	L5	1489	A2M	1	0
6	L5	1580	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 256 ligands modelled in this entry, 253 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
88	SER	F	101	2	4,5,6	0.57	0	0,5,7	-	-
87	GTP	E	1001	-	30,34,34	0.84	1 (3%)	46,54,54	1.68	10 (21%)
87	GTP	L7	203	7	30,34,34	1.11	4 (13%)	46,54,54	1.81	9 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SER	F	101	2	-	0/2/4/6	-
87	GTP	E	1001	-	-	6/22/38/38	0/3/3/3
87	GTP	L7	203	7	-	0/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L7	203	GTP	C5-N7	-2.60	1.34	1.39
87	L7	203	GTP	C5-C4	2.54	1.45	1.38
87	L7	203	GTP	C6-N1	-2.42	1.34	1.38
87	L7	203	GTP	C4-N9	-2.21	1.32	1.38
87	E	1001	GTP	C2-N3	2.15	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L7	203	GTP	C5-C4-N3	-5.40	119.70	128.46
87	E	1001	GTP	C5-C4-N3	-4.96	120.41	128.46
87	L7	203	GTP	N9-C4-N3	4.95	135.87	125.94
87	L7	203	GTP	C2-N3-C4	4.69	120.66	112.30
87	E	1001	GTP	C2-N3-C4	4.41	120.15	112.30
87	L7	203	GTP	PB-O3B-PG	-3.61	120.43	132.83
87	L7	203	GTP	PA-O3A-PB	-3.61	120.44	132.83
87	E	1001	GTP	N9-C4-N3	3.32	132.61	125.94
87	E	1001	GTP	PA-O3A-PB	-2.94	122.75	132.83
87	E	1001	GTP	C2-N1-C6	-2.82	119.96	125.10
87	E	1001	GTP	O6-C6-C5	-2.56	119.81	126.60
87	E	1001	GTP	C5-C6-N1	2.41	119.32	113.19
87	E	1001	GTP	C8-N7-C5	2.35	108.49	104.24
87	E	1001	GTP	N9-C8-N7	-2.34	108.99	113.39
87	L7	203	GTP	O6-C6-C5	-2.21	120.74	126.60
87	L7	203	GTP	C6-C5-N7	2.13	134.21	130.25
87	E	1001	GTP	C3'-C2'-C1'	2.11	105.44	101.43
87	L7	203	GTP	C5-C6-N1	2.06	118.43	113.19
87	L7	203	GTP	C2'-C1'-N9	-2.03	107.45	113.22

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	E	1001	GTP	C5'-O5'-PA-O3A
87	E	1001	GTP	O4'-C4'-C5'-O5'
87	E	1001	GTP	C3'-C4'-C5'-O5'
87	E	1001	GTP	C5'-O5'-PA-O1A
87	E	1001	GTP	C5'-O5'-PA-O2A
87	E	1001	GTP	C4'-C5'-O5'-PA

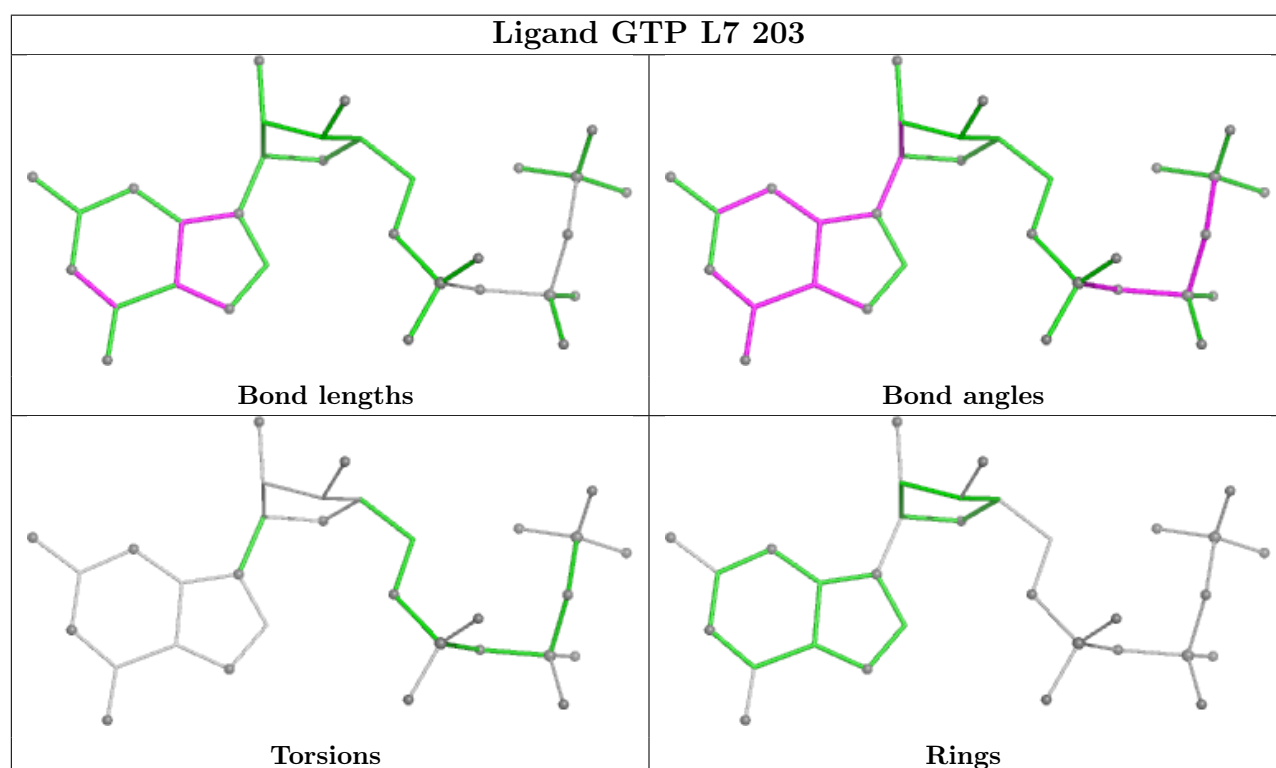
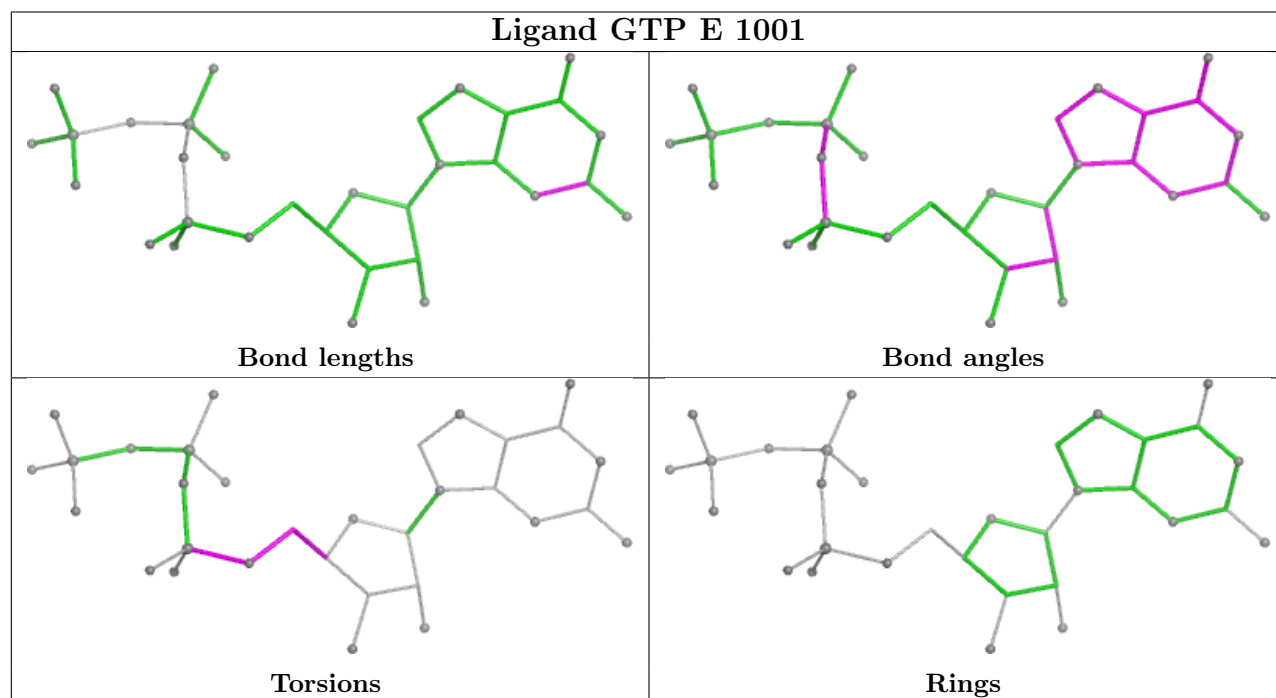
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	E	1001	GTP	1	0
87	L7	203	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
83	Si	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Si	61:GLN	C	62:HY3	N	3.10

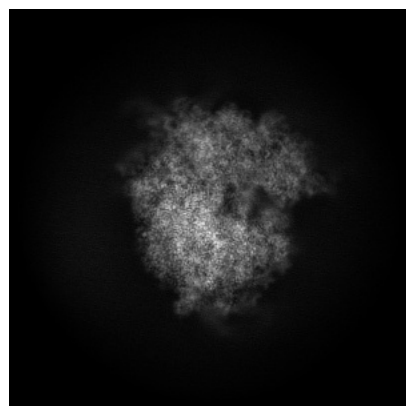
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14751. These allow visual inspection of the internal detail of the map and identification of artifacts.

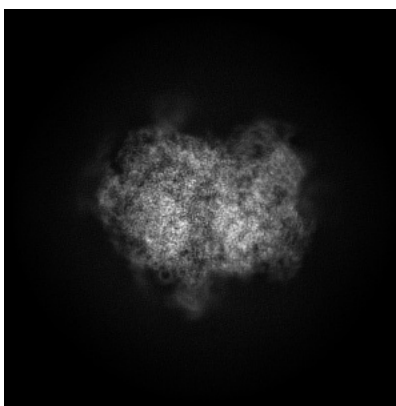
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

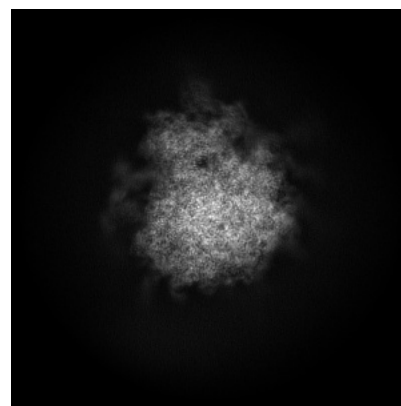
6.1.1 Primary map



X

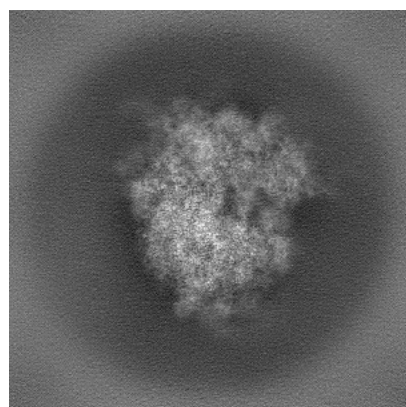


Y

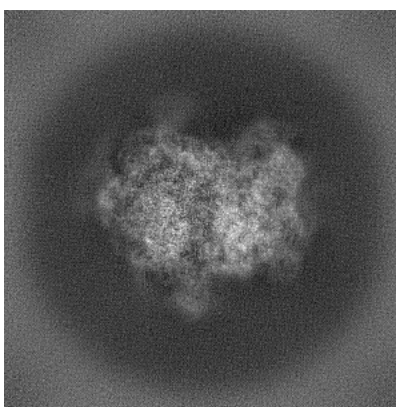


Z

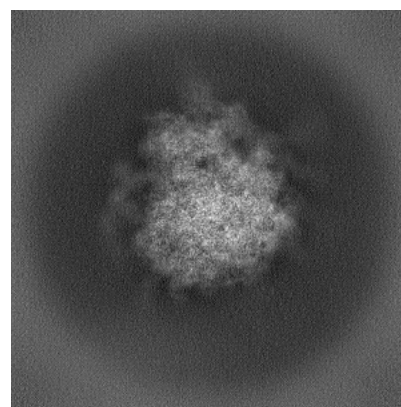
6.1.2 Raw map



X



Y

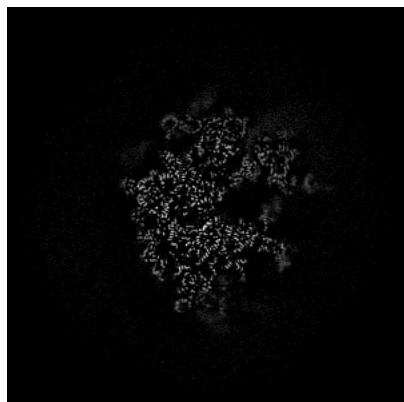


Z

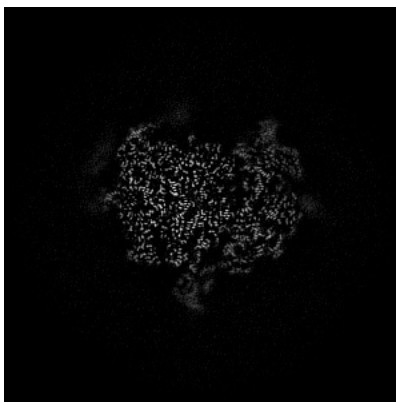
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

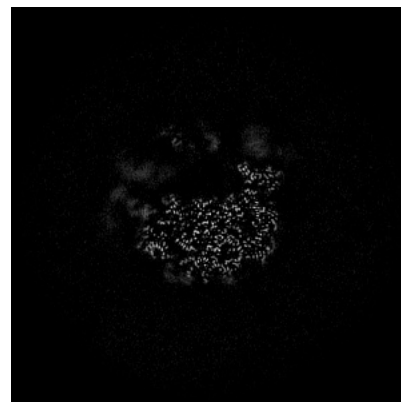
6.2.1 Primary map



X Index: 256

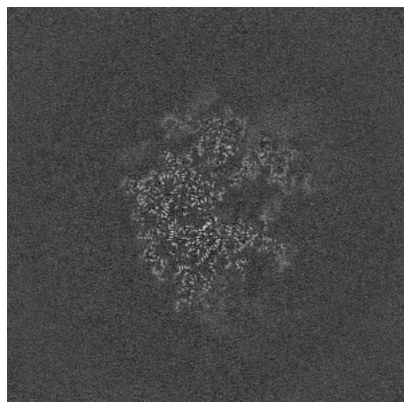


Y Index: 256

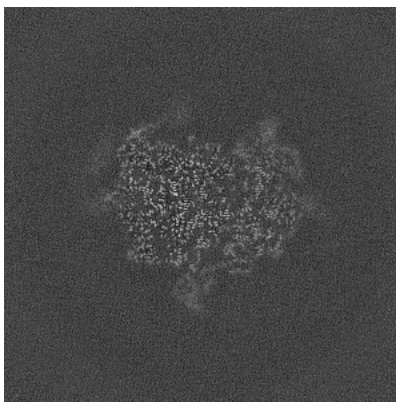


Z Index: 256

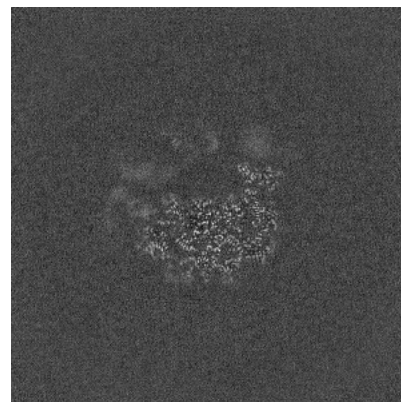
6.2.2 Raw map



X Index: 256



Y Index: 256

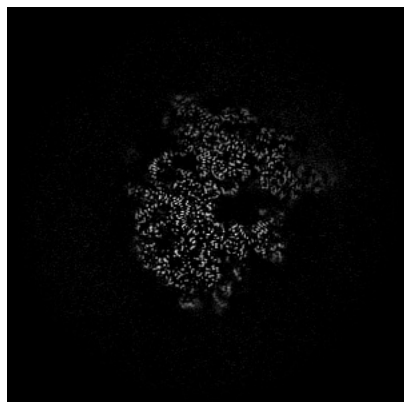


Z Index: 256

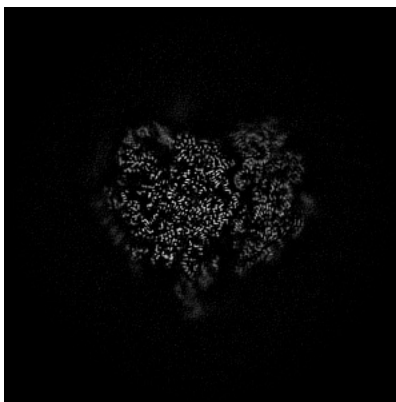
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

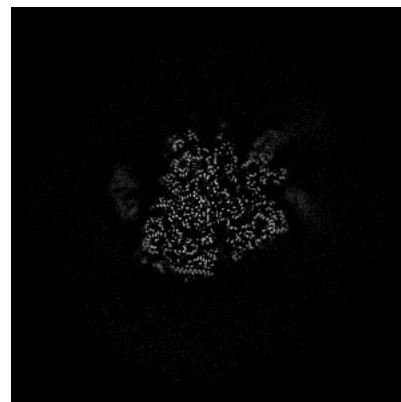
6.3.1 Primary map



X Index: 240

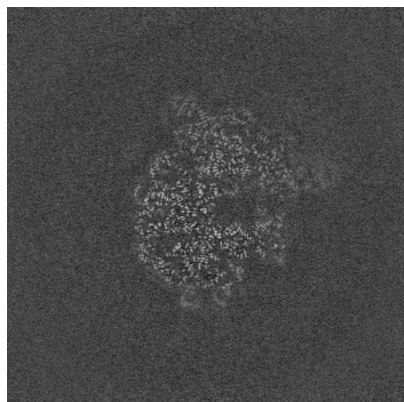


Y Index: 246

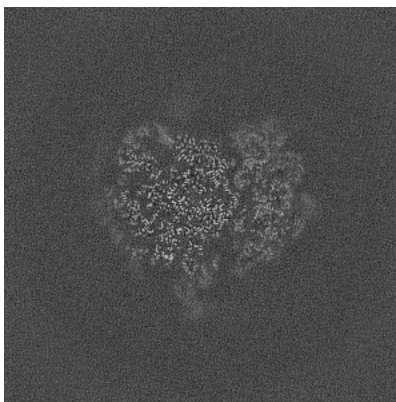


Z Index: 223

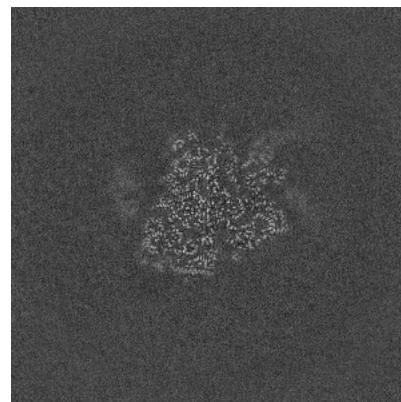
6.3.2 Raw map



X Index: 238



Y Index: 246

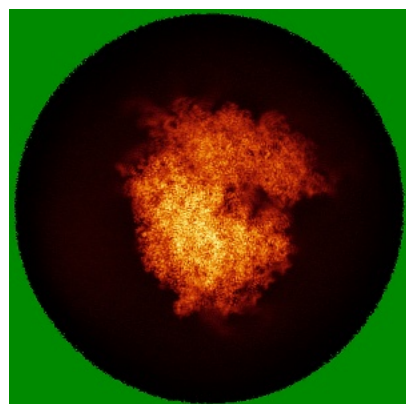


Z Index: 223

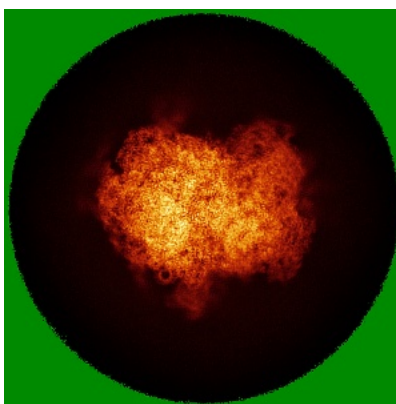
The images above show the largest variance slices of the map in three orthogonal directions.

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

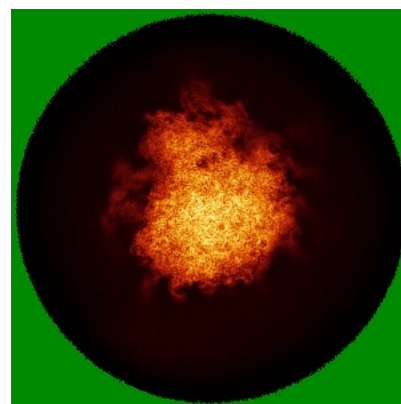
6.4.1 Primary map



X

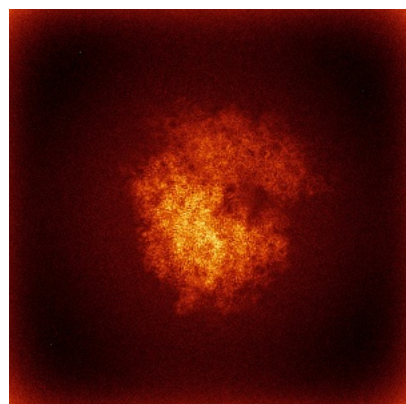


Y

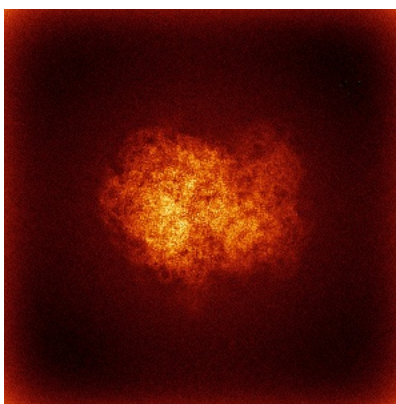


Z

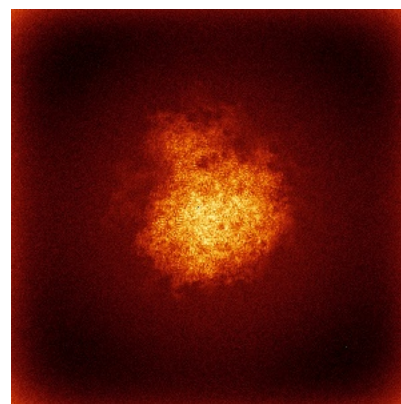
6.4.2 Raw map



X



Y

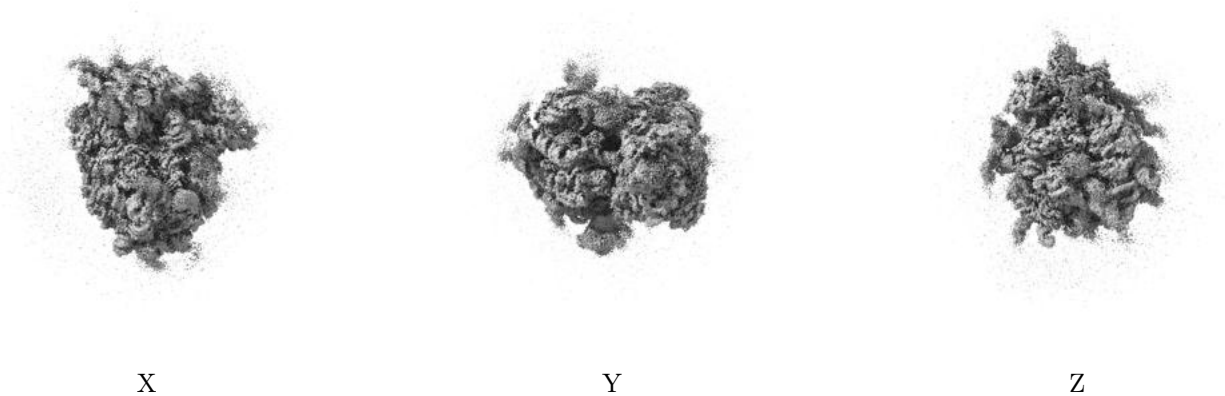


Z

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

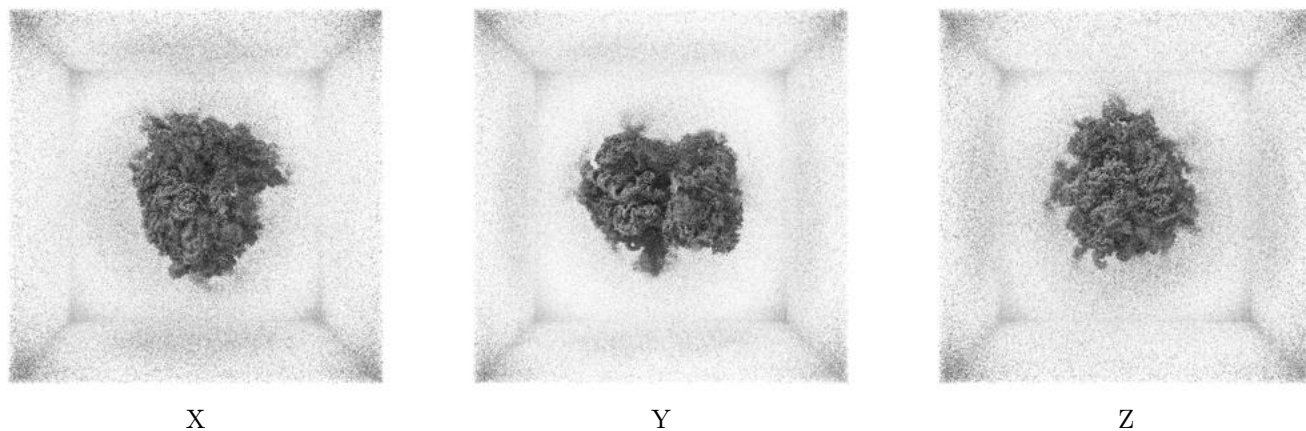
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

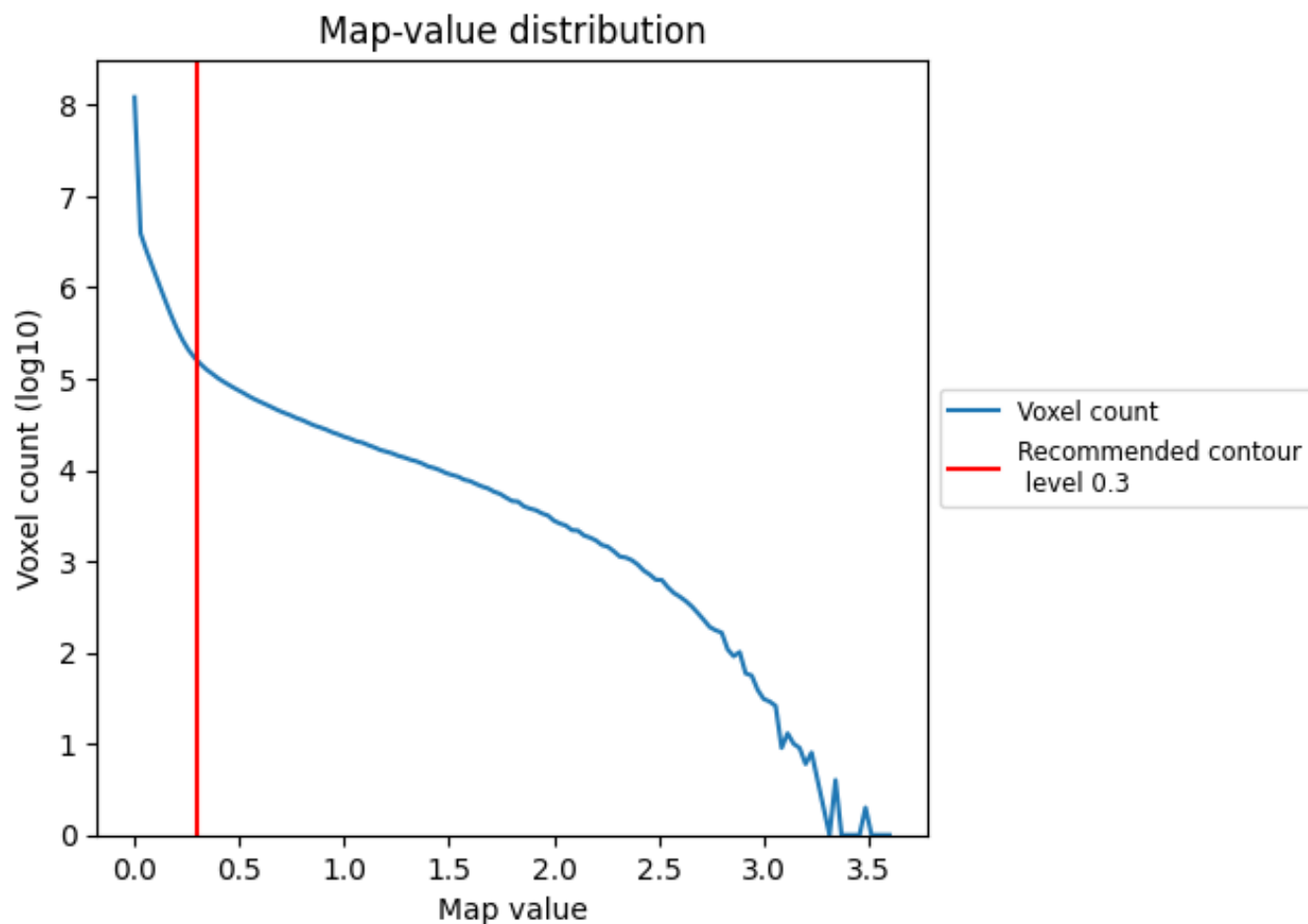
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

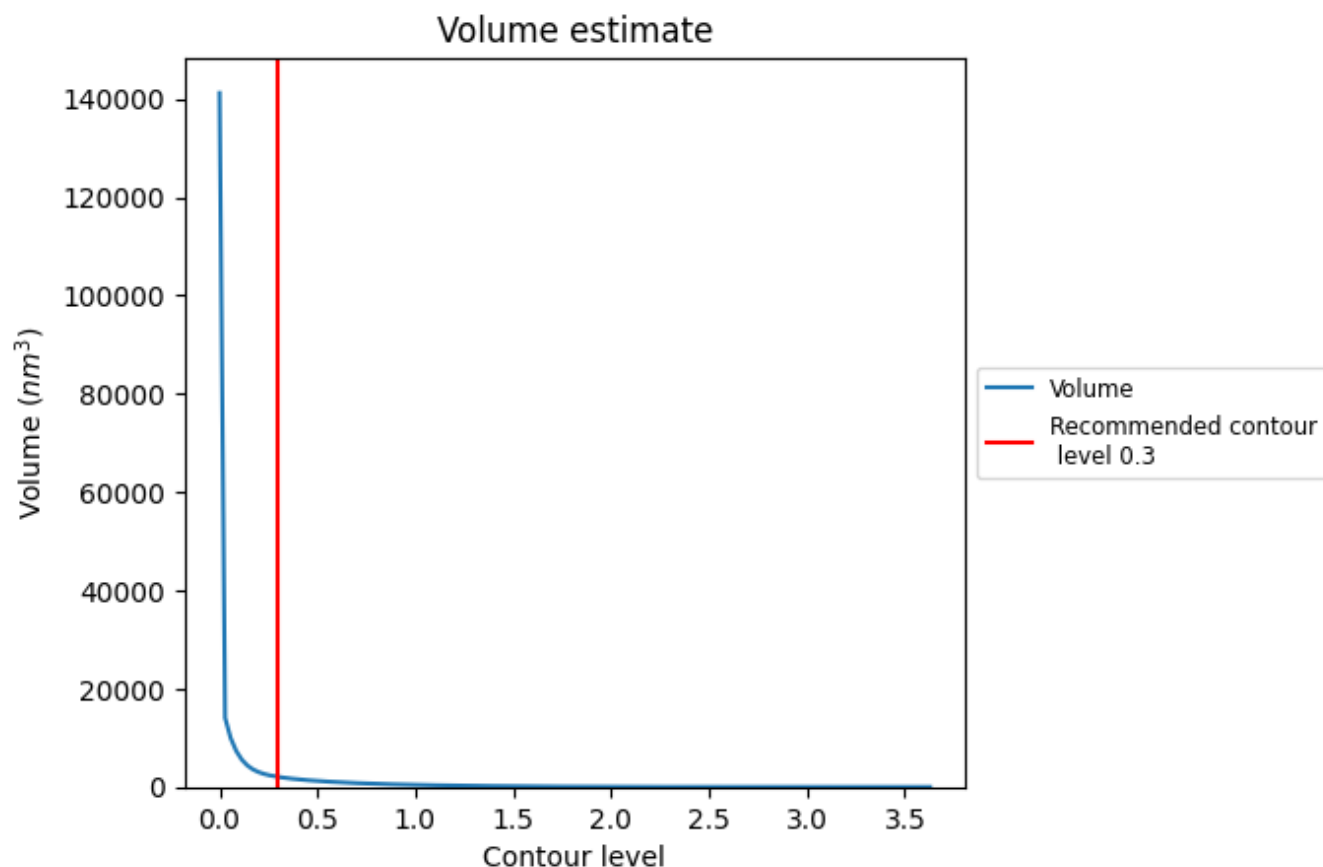
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

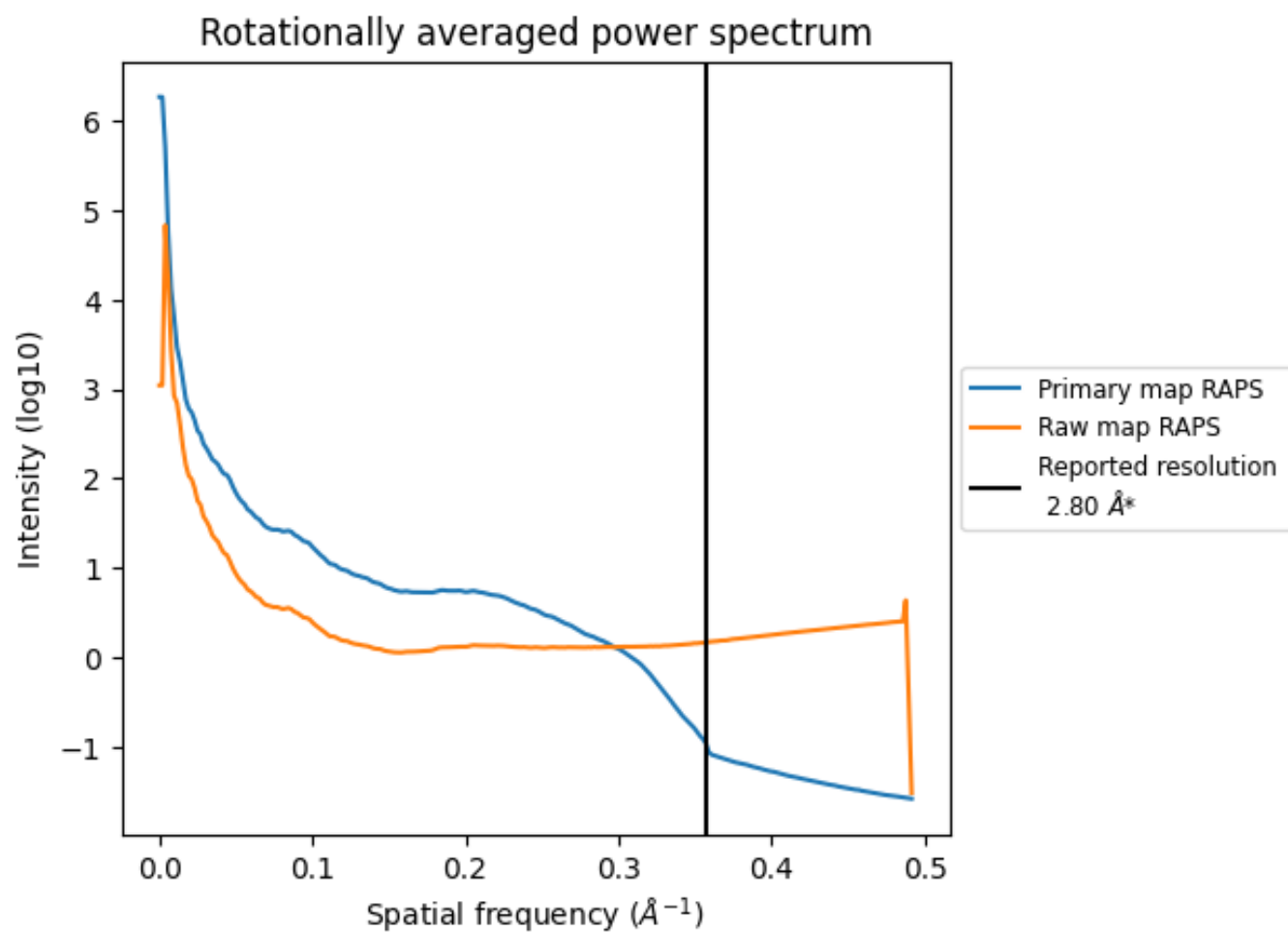
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2046 nm^3 ; this corresponds to an approximate mass of 1848 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 [i](#)

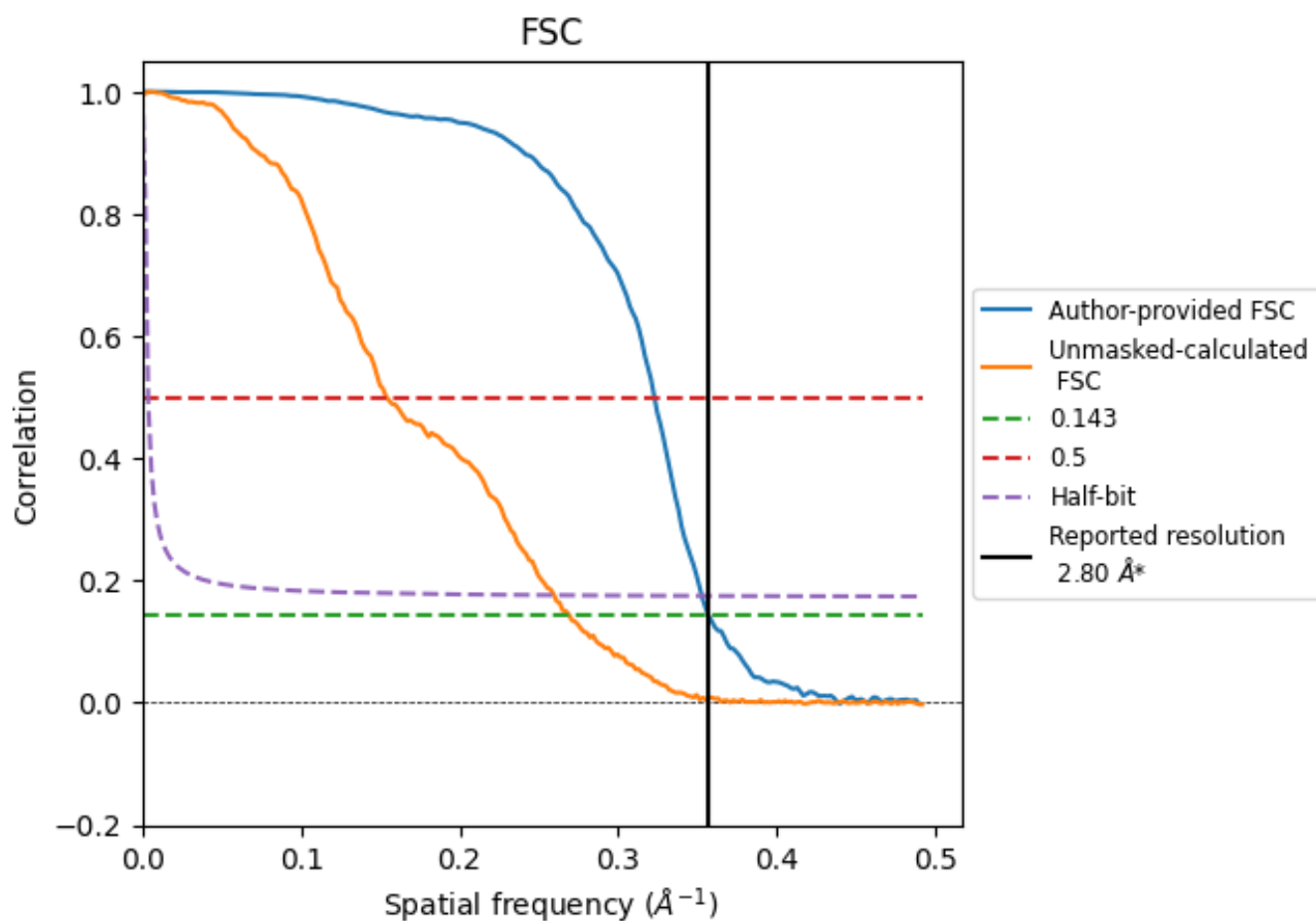


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

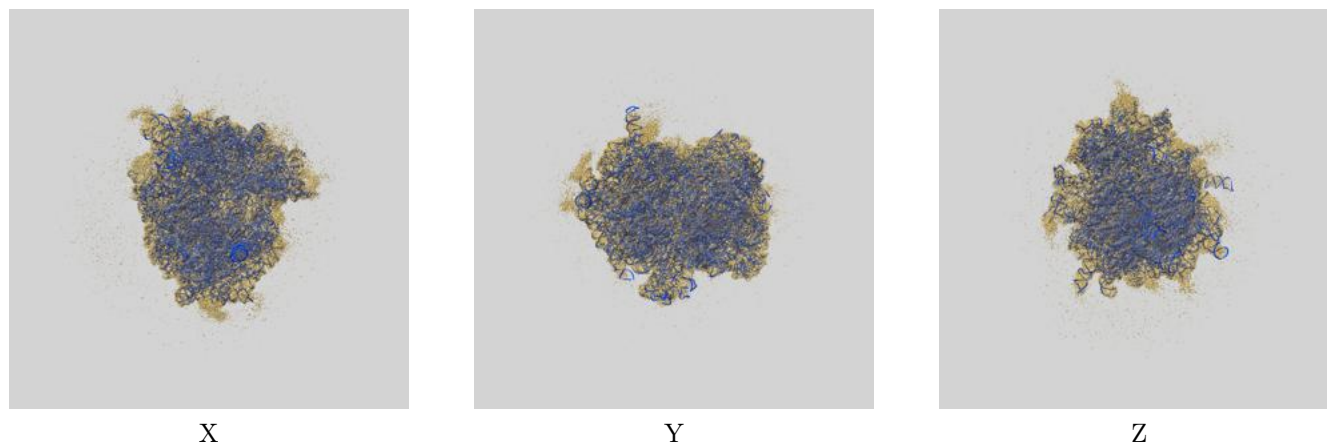
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.10	2.83
Unmasked-calculated*	3.72	6.49	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.72 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

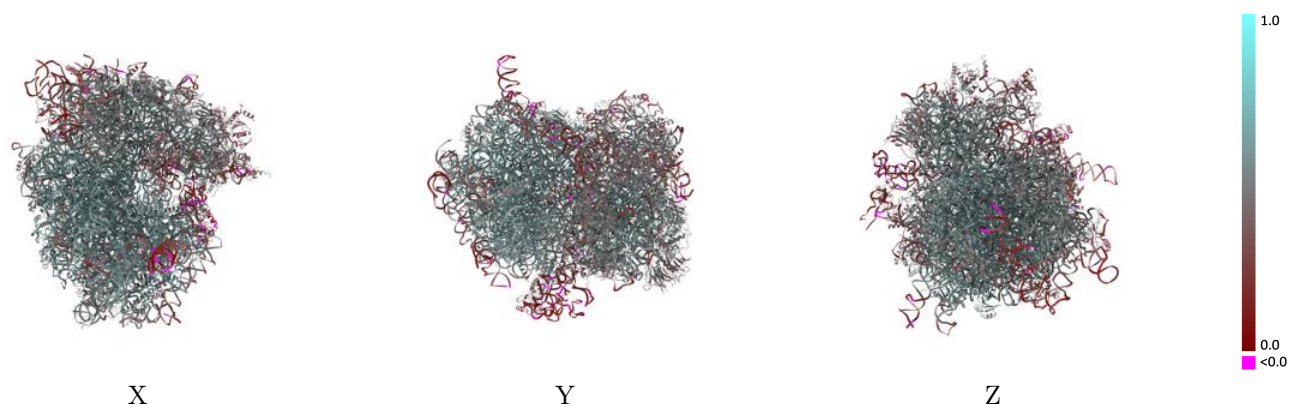
This section contains information regarding the fit between EMDB map EMD-14751 and PDB model 7ZJW. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



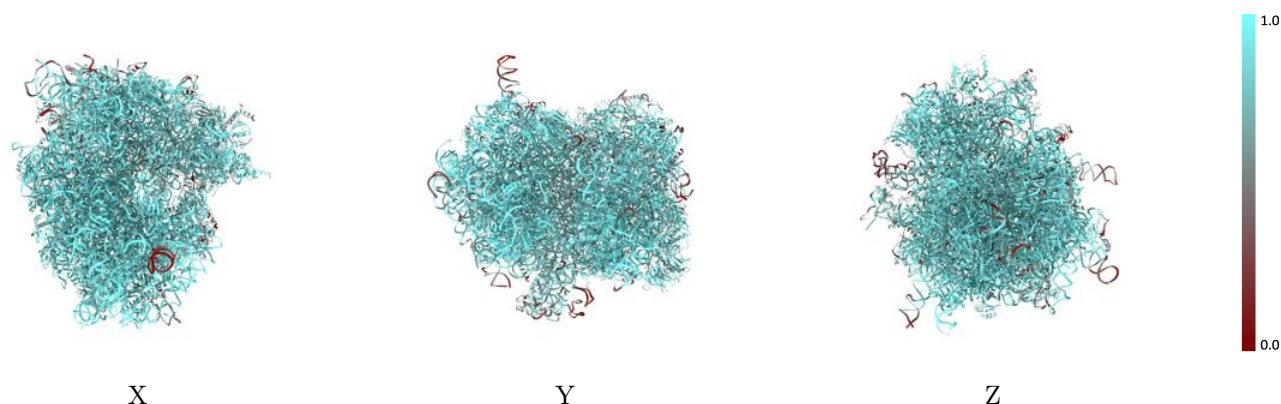
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



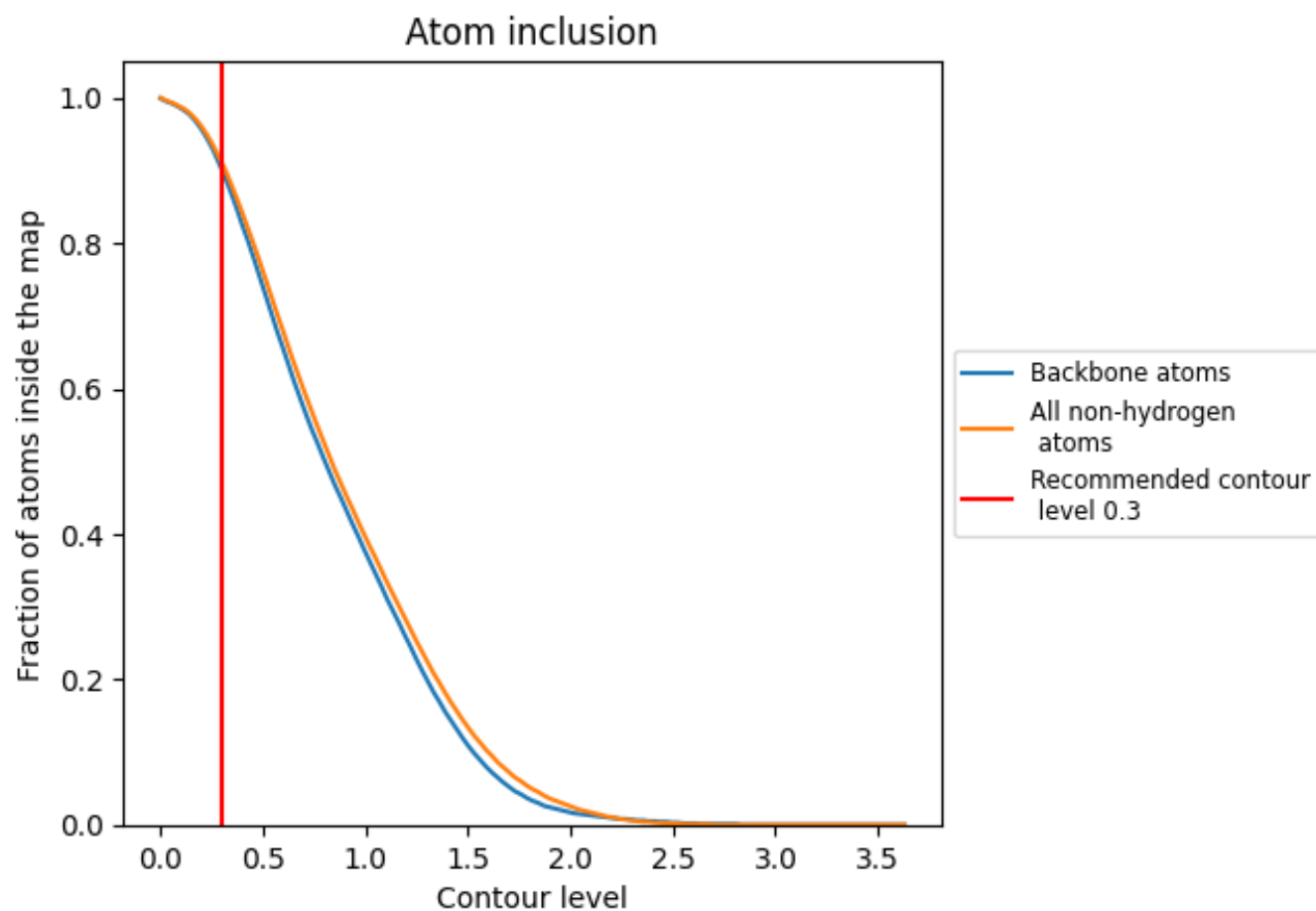
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.5140
B	 0.8170	 0.4050
E	 0.7650	 0.3700
F	 0.7450	 0.3280
I	 0.6340	 0.2040
L5	 0.9540	 0.5340
L7	 0.9970	 0.5910
L8	 0.9790	 0.5740
LD	 0.9440	 0.5950
LE	 0.9460	 0.5830
LF	 0.9480	 0.5850
LG	 0.9410	 0.5540
LH	 0.9140	 0.5460
LI	 0.9430	 0.5850
LJ	 0.8990	 0.5380
LK	 0.9230	 0.5660
LL	 0.9030	 0.5590
LM	 0.9110	 0.5300
LO	 0.9160	 0.5610
LP	 0.9340	 0.5650
LQ	 0.9700	 0.6080
LR	 0.9490	 0.5870
LS	 0.9220	 0.5770
LT	 0.9480	 0.5860
LU	 0.9150	 0.5480
LV	 0.9610	 0.5940
LW	 0.9200	 0.5650
LX	 0.9210	 0.5110
LY	 0.9000	 0.5750
LZ	 0.8160	 0.4910
La	 0.9320	 0.5610
Lb	 0.9310	 0.5730
Lc	 0.9430	 0.5590
Ld	 0.9630	 0.5940
Le	 0.8330	 0.4890



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Chain	Atom inclusion	Q-score
Lf	 0.8520	 0.5250
Lg	 0.9360	 0.5700
Lh	 0.9430	 0.5910
Li	 0.9520	 0.5940
Lj	 0.9280	 0.5670
Lk	 0.9250	 0.5620
Ll	 0.9250	 0.5570
Lm	 0.9670	 0.6070
Ln	 0.8760	 0.5360
Lo	 0.9370	 0.5810
Lp	 0.9310	 0.5710
Lq	 0.9190	 0.5790
Lr	 0.9270	 0.5760
Ls	 0.9540	 0.5850
Lt	 0.6190	 0.2220
Lx	 0.6990	 0.2950
S	 0.8890	 0.2700
S2	 0.9330	 0.4940
SB	 0.8230	 0.5070
SC	 0.8070	 0.4900
SD	 0.6820	 0.3590
SE	 0.7160	 0.4180
SF	 0.8980	 0.5410
SG	 0.8230	 0.4210
SH	 0.9050	 0.5370
SL	 0.8620	 0.5140
SM	 0.8600	 0.5110
SN	 0.8820	 0.5300
SO	 0.8300	 0.4860
SP	 0.8270	 0.4790
SQ	 0.8430	 0.4820
SR	 0.8170	 0.4060
SS	 0.7670	 0.4550
ST	 0.8380	 0.4760
SU	 0.8260	 0.4680
SV	 0.8490	 0.4690
SW	 0.7760	 0.4980
SX	 0.6610	 0.3040
SY	 0.8800	 0.5410
SZ	 0.8760	 0.5310
Sa	 0.7780	 0.4480
Sb	 0.8620	 0.5000

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Chain	Atom inclusion	Q-score
Sc	 0.8050	 0.4680
Sd	 0.8620	 0.4840
Se	 0.8730	 0.4940
Sf	 0.8160	 0.4630
Sg	 0.8670	 0.5210
Sh	 0.9120	 0.5560
Si	 0.8980	 0.5470
Sj	 0.8500	 0.4590
Sk	 0.8080	 0.4450
Sl	 0.9270	 0.5970