



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 07:51 am BST

PDB ID : 7ZJX / pdb_00007zjx
EMDB ID : EMD-14752
Title : Rabbit 80S ribosome programmed with SECIS and SBP2
Authors : Hilal, T.; Simonovic, M.; Spahn, C.M.T.
Deposited on : 2022-04-12
Resolution : 3.10 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
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

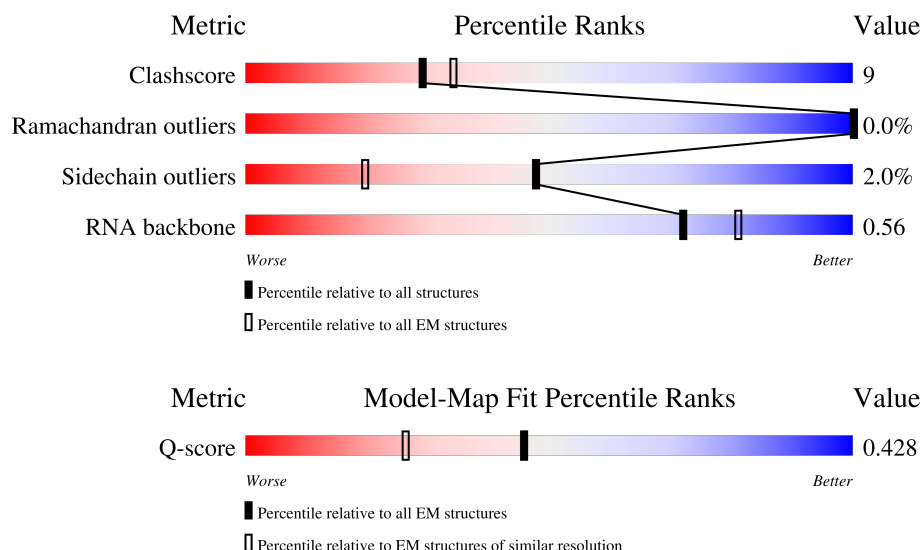
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



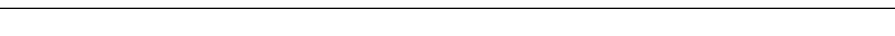
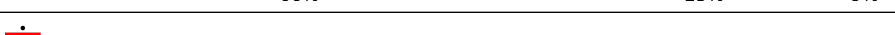
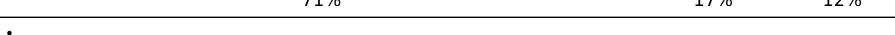
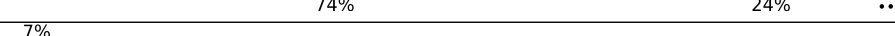
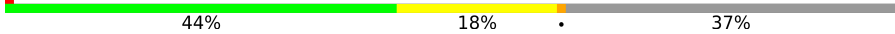
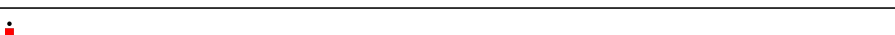
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	B	854	9% 18% 6% 76%
2	I	163	22% 22% 48% 30%
3	L5	4808	46% 26% 5% 22%

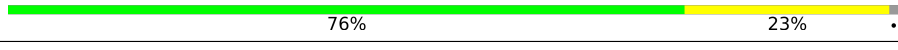
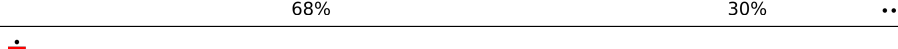
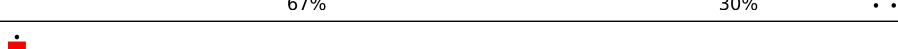
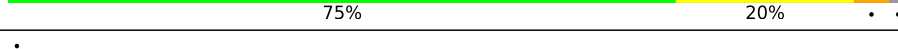
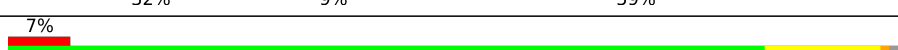
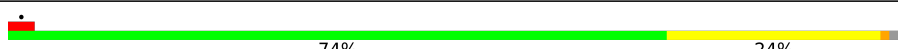
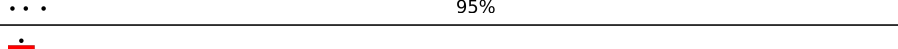
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	158	
6	LD	257	
7	LE	403	
8	LF	413	
9	LG	297	
10	LH	291	
11	LI	247	
12	LJ	266	
13	LK	192	
14	LL	214	
15	LM	178	
16	LO	211	
17	LP	218	
18	LQ	204	
19	LR	203	
20	LS	184	
21	LT	188	
22	LU	196	
23	LV	176	
24	LW	160	
25	LX	128	
26	LY	140	
27	LZ	157	
28	La	156	

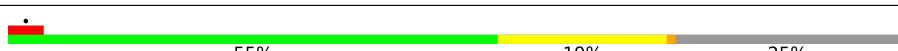
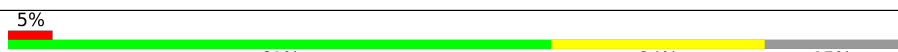
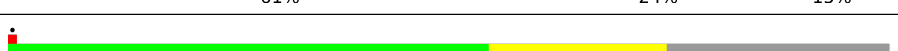
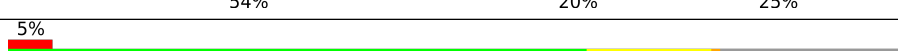
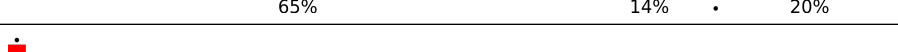
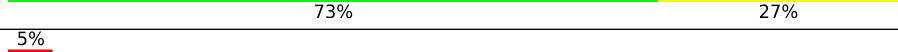
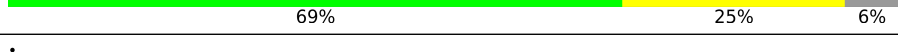
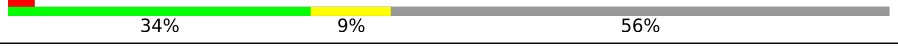
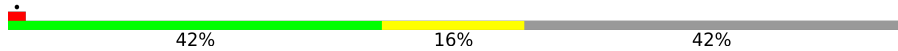
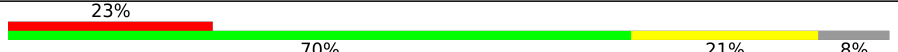
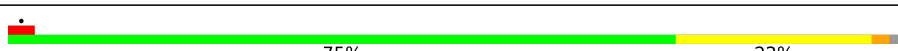
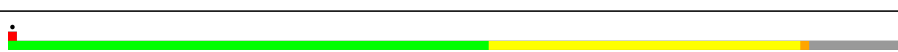
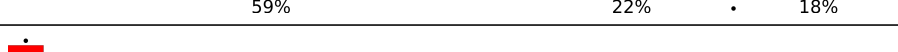
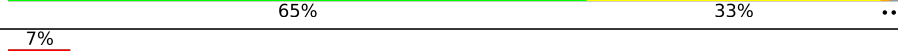
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Mol	Chain	Length	Quality of chain
29	Lb	145	
30	Lc	136	
31	Ld	148	
32	Le	245	
33	Lf	115	
34	Lg	125	
35	Lh	135	
36	Li	110	
37	Lj	117	
38	Lk	123	
39	Ll	105	
40	Lm	97	
41	Ln	70	
42	Lo	51	
43	Lp	128	
44	Lq	106	
45	Lr	92	
46	Ls	137	
47	Lx	217	
48	S	855	
49	S2	1870	
50	SB	84	
51	SC	69	
52	SD	156	
53	SE	133	

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Mol	Chain	Length	Quality of chain
54	SF	115	
55	SG	317	
56	SH	56	
57	SL	295	
58	SM	264	
59	SN	293	
60	SO	281	
61	SP	263	
62	SQ	204	
63	SR	249	
64	SS	432	
65	ST	208	
66	SU	194	
67	SV	165	
68	SW	158	
69	SX	132	
70	SY	151	
71	SZ	151	
72	Sa	145	
73	Sb	172	
74	Sc	135	
75	Sd	152	
76	Se	145	
77	Sf	119	
78	Sg	83	

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Mol	Chain	Length	Quality of chain
79	Sh	130	69% 30%
80	Si	143	74% 23%
81	Sj	130	73% 22%
82	Sk	124	34% 25% 40%
83	Sl	25	88% 12%

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 222755 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 Selenocysteine insertion sequence-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	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 2 is a RNA chain called CrPV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	163	Total	C	N	O	P	0	0
			3447	1544	588	1152	163		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3732	Total	C	N	O	P	0	0
			80089	35700	14644	26013	3732		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

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

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

- Molecule 6 is a protein called 60S ribosomal protein uL2.

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

- Molecule 7 is a protein called 60S ribosomal protein uL3.

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

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

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

- Molecule 9 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	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 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LH	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 11 is a protein called 60S ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	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 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called Ribosomal protein L10.

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

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

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

- Molecule 16 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	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

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

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

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

- Molecule 18 is a protein called Ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	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 20 is a protein called 60S ribosomal protein uL22.

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

- Molecule 21 is a protein called 60S ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	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 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	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 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	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 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

- Molecule 28 is a protein called Ribosomal_L23eN domain-containing protein.

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

- Molecule 29 is a protein called Ribosomal protein L26.

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

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

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ld	147	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

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

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

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

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

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

- Molecule 35 is a protein called Ribosomal protein L32.

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

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

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

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

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

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

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

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

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

- Molecule 40 is a protein called Ribosomal protein L37.

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

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

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

- Molecule 42 is a protein called 60S ribosomal protein eL39.

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

- Molecule 43 is a protein called 60S ribosomal protein L40.

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

- Molecule 44 is a protein called 60S ribosomal protein eL42.

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

- Molecule 45 is a protein called 60S ribosomal protein eL43.

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

- Molecule 46 is a protein called 60S ribosomal protein eL28.

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

- Molecule 47 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lx	169	Total	C	N	O		0	0
			840	502	169	169			

- Molecule 48 is a RNA chain called GPX4 SECIS element.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	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 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	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 50 is a protein called 40S ribosomal protein S27.

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

- Molecule 51 is a protein called 40S ribosomal protein S28.

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

- Molecule 52 is a protein called Ubiquitin carboxyl extension protein 80.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SD	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 53 is a protein called 40S ribosomal protein S30.

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

- Molecule 54 is a protein called 40S ribosomal protein eS26.

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

- Molecule 55 is a protein called Guanine nucleotide-binding protein subunit beta-2-like 1.

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

- Molecule 56 is a protein called 40S ribosomal protein S29.

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

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

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

- Molecule 58 is a protein called 40S ribosomal protein S3a.

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

- Molecule 59 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	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 60 is a protein called 40S ribosomal protein S3.

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

- Molecule 61 is a protein called 40S ribosomal protein S4.

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

- Molecule 62 is a protein called Ribosomal protein S5.

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

- Molecule 63 is a protein called 40S ribosomal protein S6.

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

- Molecule 64 is a protein called 40S ribosomal protein S7.

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

- Molecule 65 is a protein called 40S ribosomal protein S8.

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

- Molecule 66 is a protein called 40S ribosomal protein S9.

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

- Molecule 67 is a protein called S10_ plectin domain-containing protein.

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

- Molecule 68 is a protein called 40S ribosomal protein S11.

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

- Molecule 69 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SX	121	Total	C	N	O	S	0	0
			943	591	167	176	9		

- Molecule 70 is a protein called 40S ribosomal protein S13.

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

- Molecule 71 is a protein called 40S ribosomal protein uS11.

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

- Molecule 72 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sa	127	Total	C	N	O	S	0	0
			1042	662	196	177	7		

- Molecule 73 is a protein called 40S ribosomal protein uS9.

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

- Molecule 74 is a protein called 40S ribosomal protein S17.

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

- Molecule 75 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sd	141	Total	C	N	O	S	0	0
			1171	736	235	199	1		

- Molecule 76 is a protein called 40S Ribosomal protein eS19.

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

- Molecule 77 is a protein called 40S ribosomal protein S20.

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

- Molecule 78 is a protein called 40S ribosomal protein eS21.

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

- Molecule 79 is a protein called 40S ribosomal protein S15a.

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

- Molecule 80 is a protein called 40S ribosomal protein S23.

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

- Molecule 81 is a protein called 40S ribosomal protein S24.

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

- Molecule 82 is a protein called 40S ribosomal protein S25.

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

- Molecule 83 is a protein called 60S ribosomal protein L41.

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

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Lj	1	Total	Zn	0
			1	1	
84	Lm	1	Total	Zn	0
			1	1	
84	Lp	1	Total	Zn	0
			1	1	
84	Lq	1	Total	Zn	0
			1	1	
84	Lr	1	Total	Zn	0
			1	1	
84	SD	1	Total	Zn	0
			1	1	

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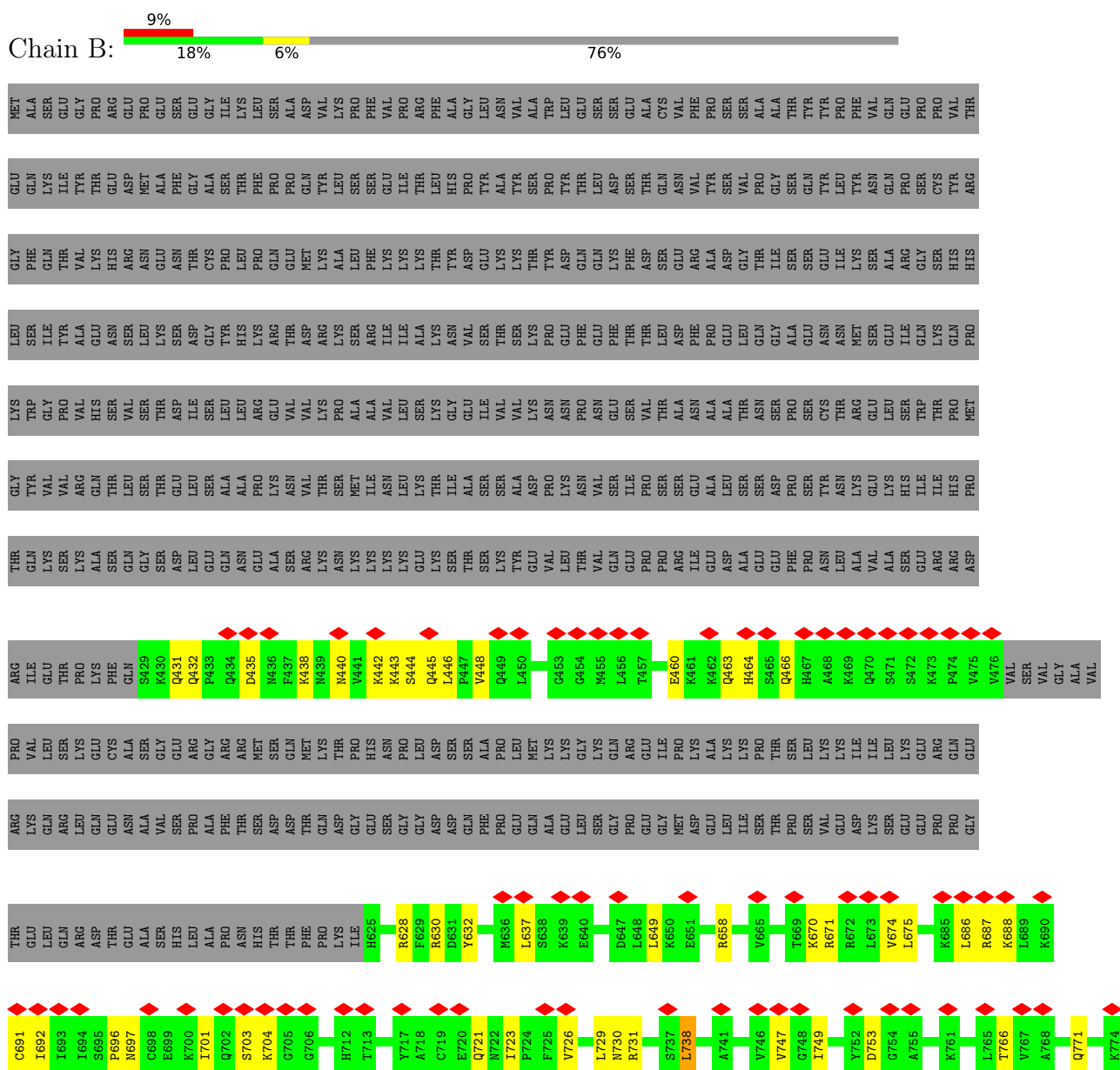
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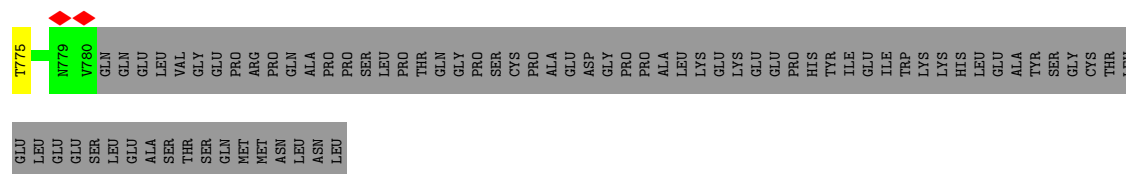
Mol	Chain	Residues	Atoms		AltConf
84	SF	1	Total 1	Zn 1	0
84	SH	1	Total 1	Zn 1	0

3 Residue-property plots

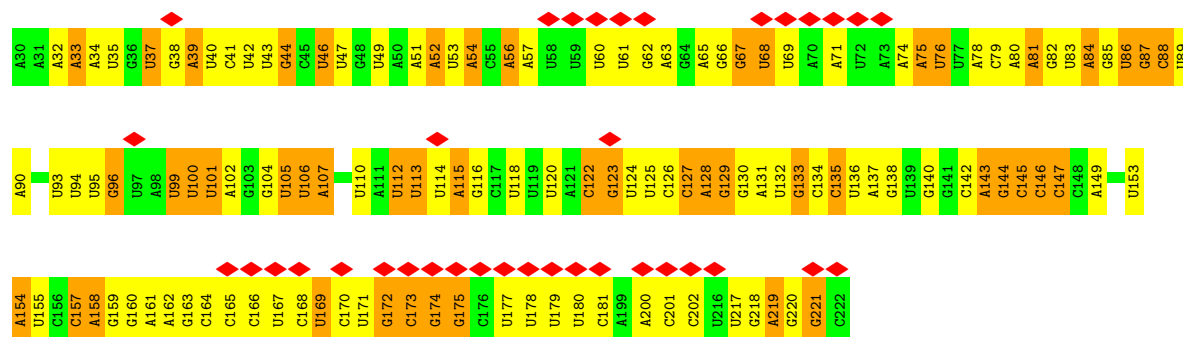
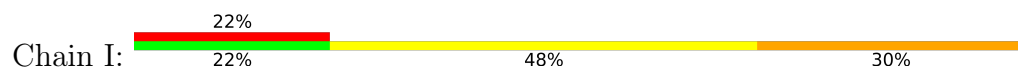
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Selenocysteine insertion sequence-binding protein 2

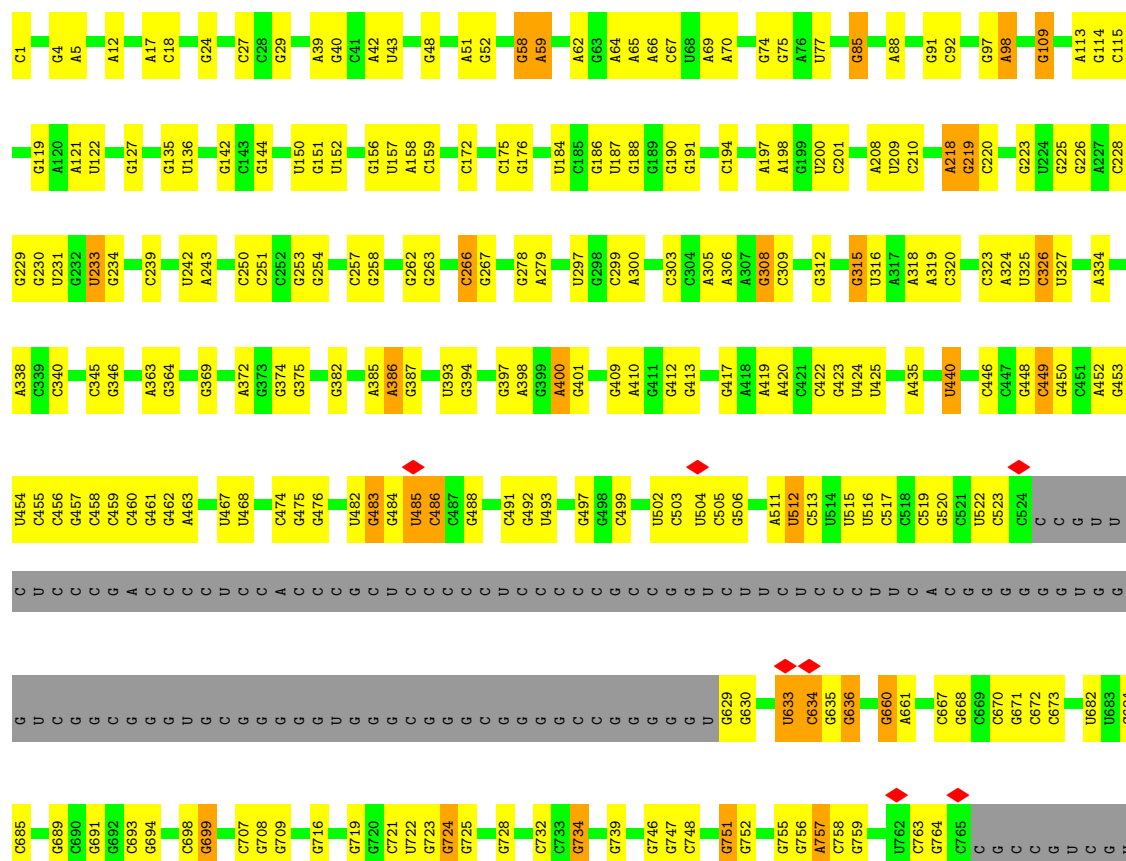




• Molecule 2: CrPV IRES



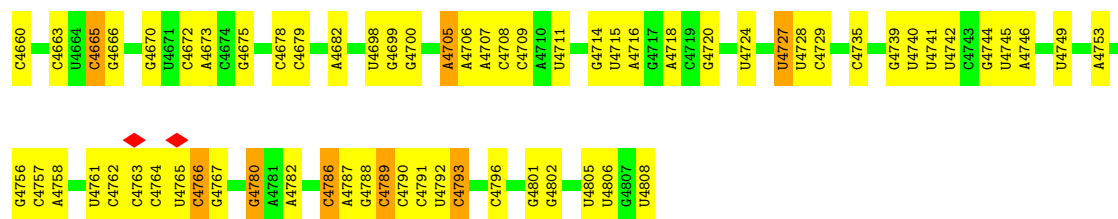
• Molecule 3: 28S rRNA











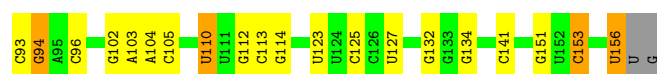
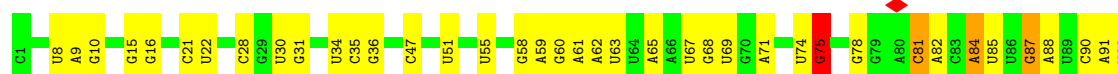
- Molecule 4: 5S rRNA

Chain L7: 70% 27%



- Molecule 5: 5.8S rRNA

Chain L8: 61% 32%



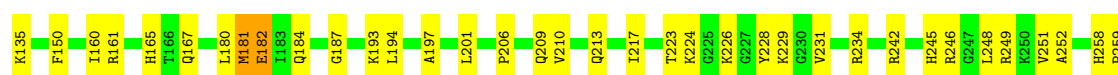
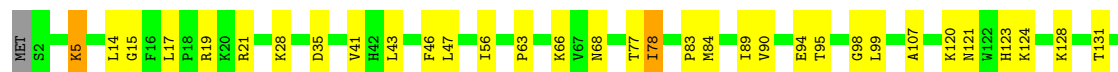
- Molecule 6: 60S ribosomal protein uL2

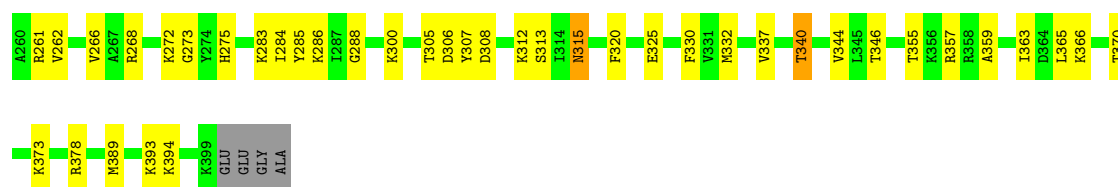
Chain LD: 68% 30%



- Molecule 7: 60S ribosomal protein uL3

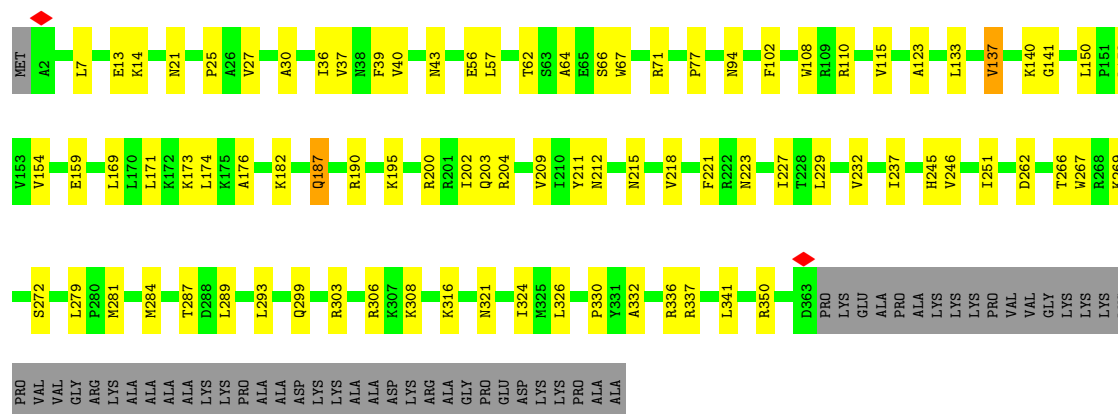
Chain LE: 72% 26%





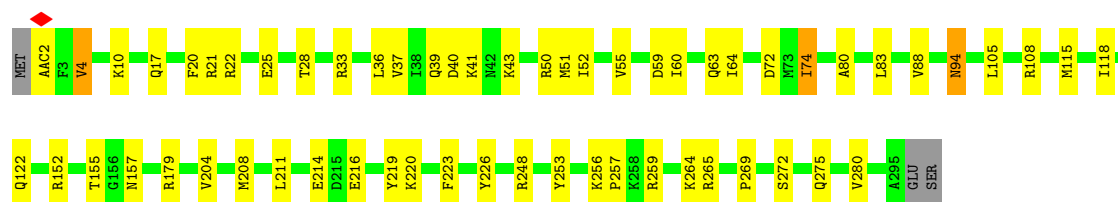
• Molecule 8: 60S ribosomal protein L4

Chain LF: 67% 20% 12%



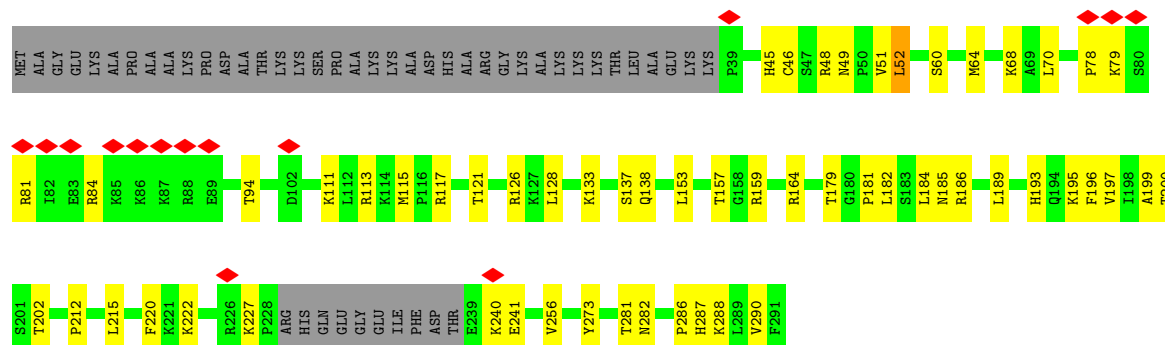
• Molecule 9: Ribosomal_L18_c domain-containing protein

Chain LG: 79% 19% ..



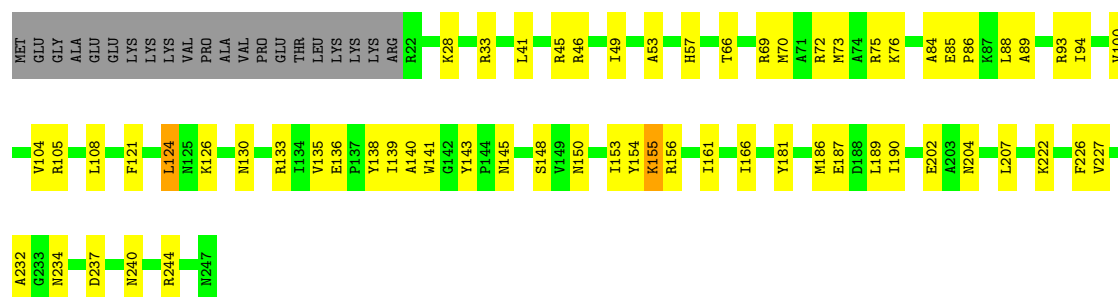
• Molecule 10: 60S ribosomal protein L6

Chain LH: 5% 64% 20% 16%



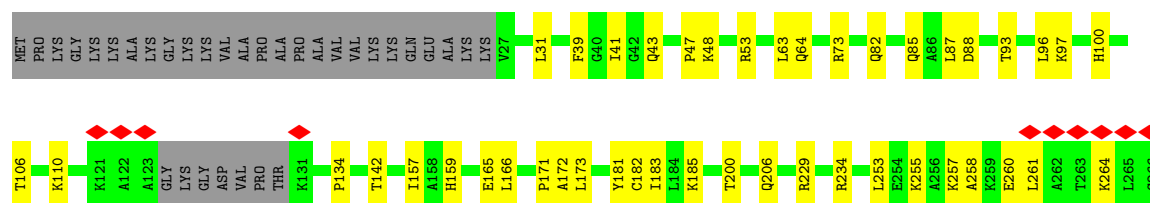
• Molecule 11: 60S ribosomal Protein uL30

Chain LI:  66% 25% 9%



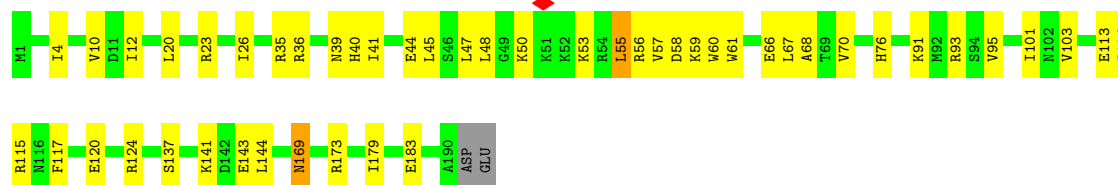
- Molecule 12: 60S ribosomal protein eL8

Chain LJ:  71% 17% 12%



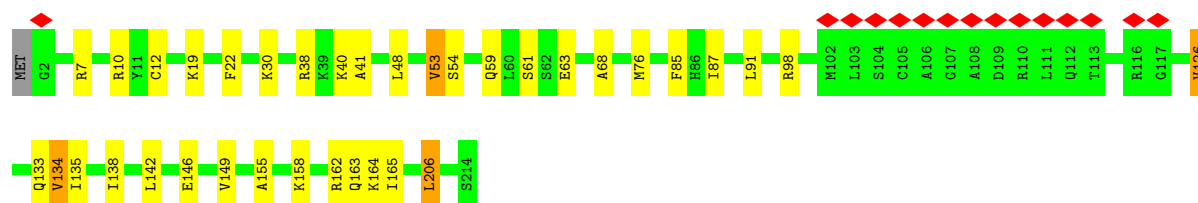
- Molecule 13: 60S ribosomal protein L9

Chain LK:  74% 24% 2%



- Molecule 14: Ribosomal protein L10

Chain LL:  7% 83% 15%



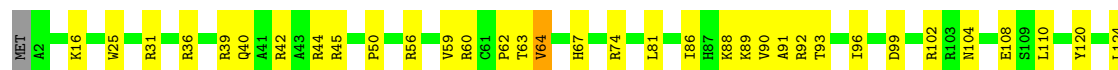
- Molecule 15: 60S ribosomal protein L11

Chain LM:  69% 27% 4%

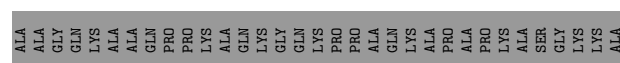
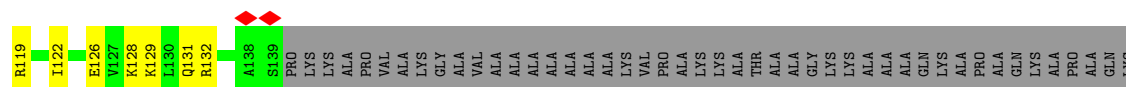




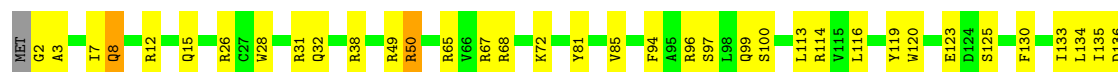
- Molecule 16: 60S ribosomal protein eL13



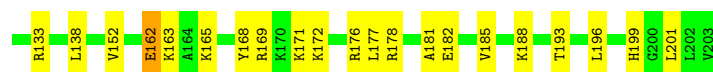
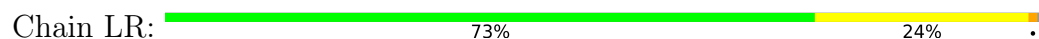
- Molecule 17: 60S ribosomal protein L14



- Molecule 18: Ribosomal protein L15

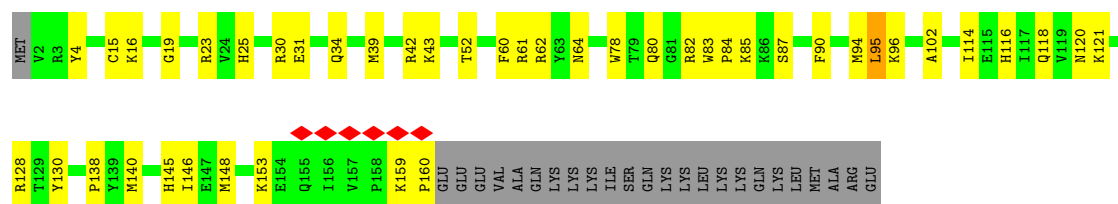


- Molecule 19: 60S ribosomal protein uL13



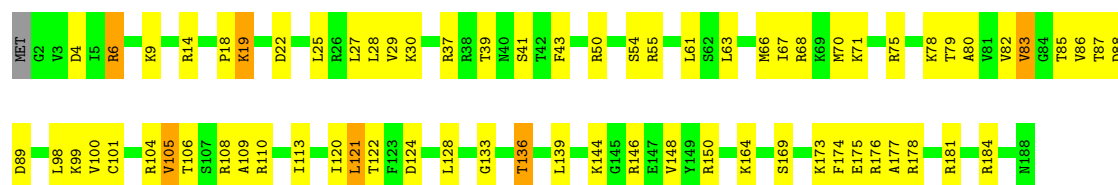
- Molecule 20: 60S ribosomal protein uL22

Chain LS: 



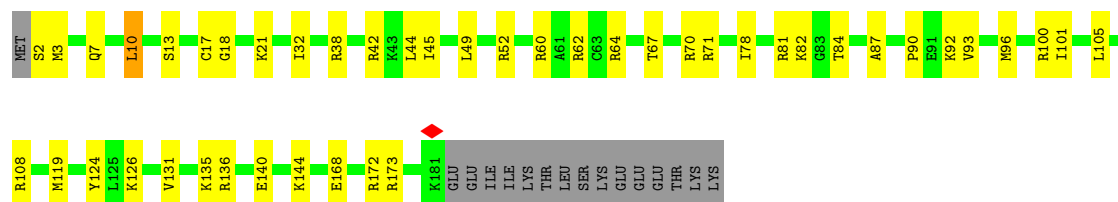
- Molecule 21: 60S ribosomal Protein eL18

Chain LT: 



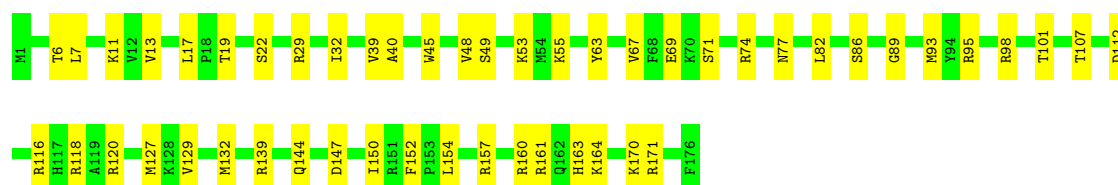
- Molecule 22: 60S ribosomal protein L19

Chain LU: 



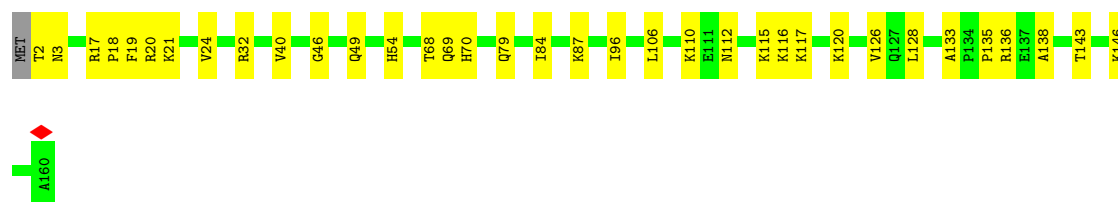
- Molecule 23: 60S ribosomal protein eL20

Chain LV: 



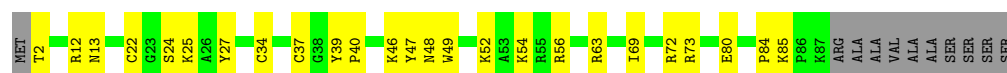
- Molecule 24: 60S ribosomal protein L21

Chain LW: 



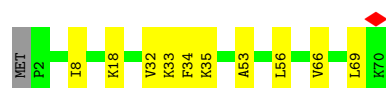
- | | | | | | | | | | | | | |
|----|----|----|----|------|------|------|------|------|------|------|------|------|
| M1 | K2 | F3 | T8 | R11 | S12 | K13 | K23 | S31 | L34 | L33 | R39 | N43 | R45 | S46 | M47 | R50 | I67 | Q72 | V73 | Y74 | R75 | K76 | K77 | I80 | R84 | V85 | Q86 | T94 | I99 | H100 | K103 | R115 | R121 | K122 | A123 | R126 | Q127 | K134 |
|----|----|----|----|------|------|------|------|------|------|------|------|------|

Chain Lm:  63% 26% 11%



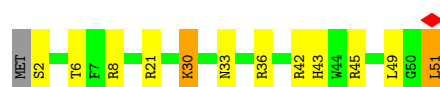
- Molecule 41: 60S ribosomal protein L38

Chain Ln:  84% 14%



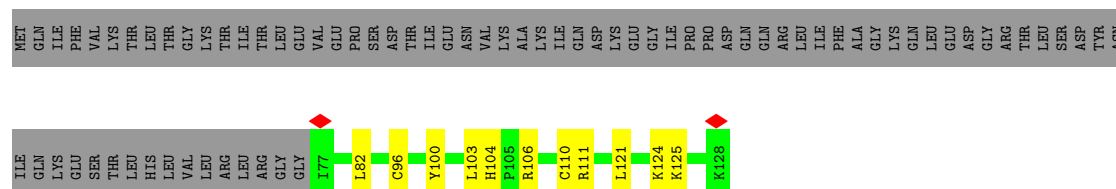
- Molecule 42: 60S ribosomal protein eL39

Chain Lo:  75% 20%



- Molecule 43: 60S ribosomal protein L40

Chain Lp:  32% 9% 59%



- Molecule 44: 60S ribosomal protein eL42

Chain Lq:  7% 85% 13%



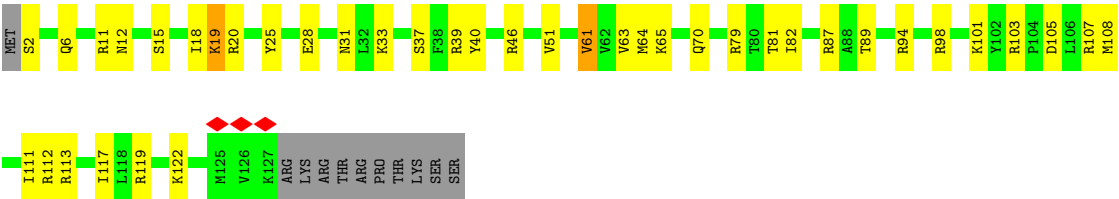
- Molecule 45: 60S ribosomal protein eL43

Chain Lr:  74% 24%

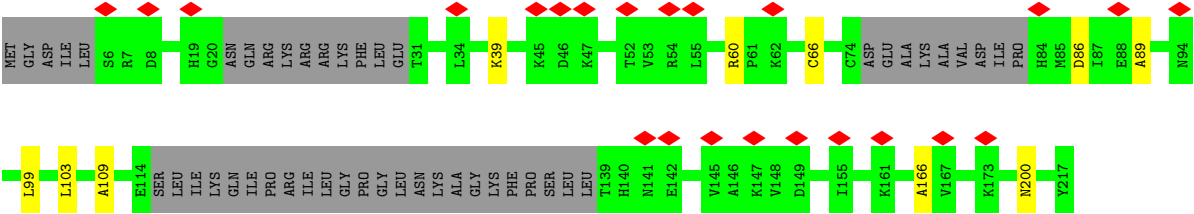
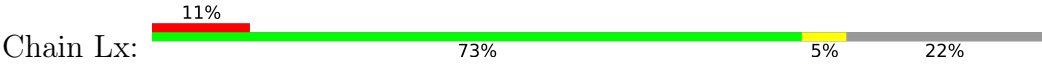


- Molecule 46: 60S ribosomal protein eL28

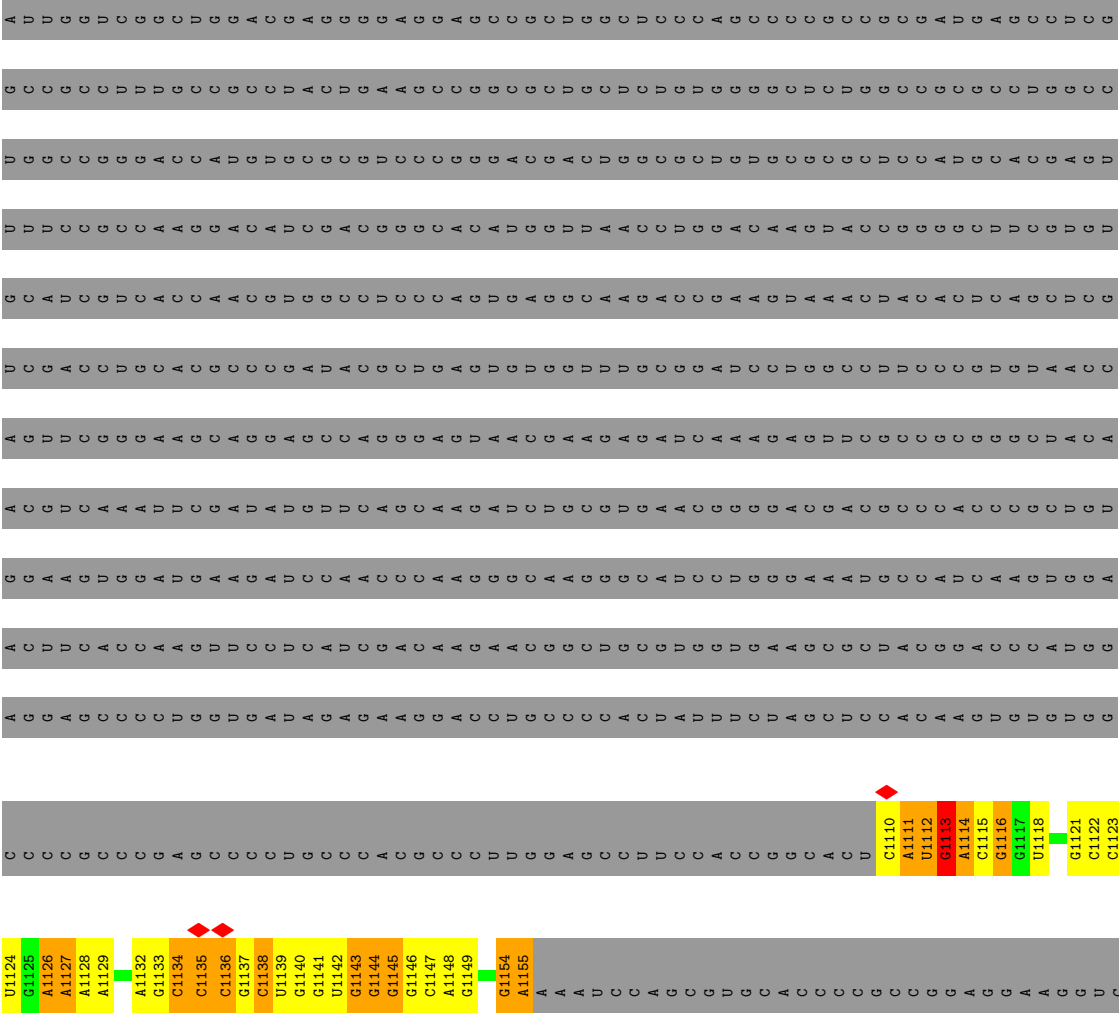
Chain Ls:  63% 28% 8%



• Molecule 47: Ribosomal protein

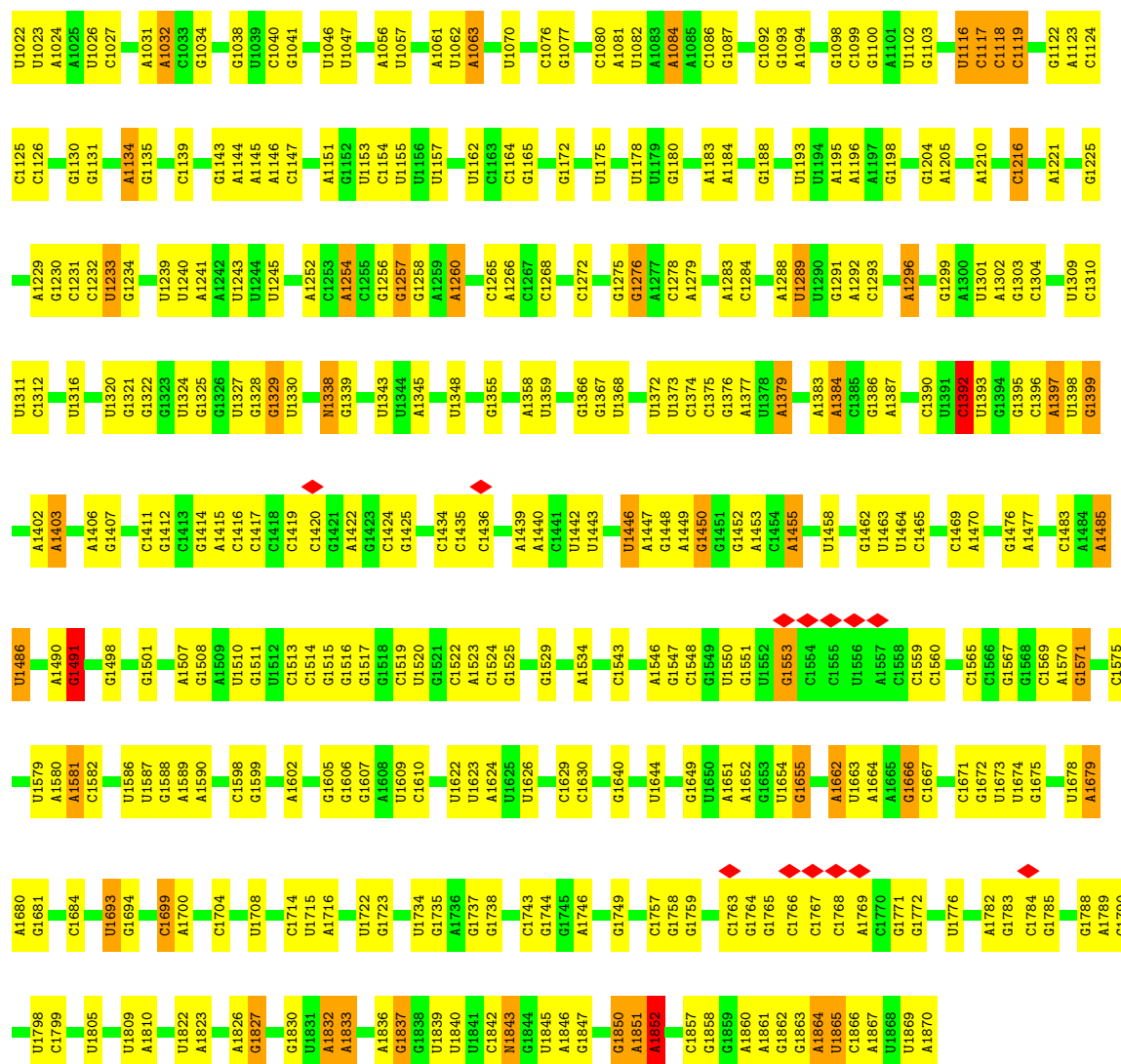


• Molecule 48: GPX4 SECIS element

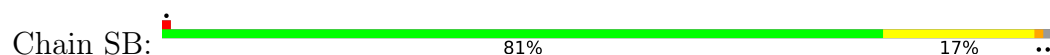


Chain S2: 54% 35% 6% 5%





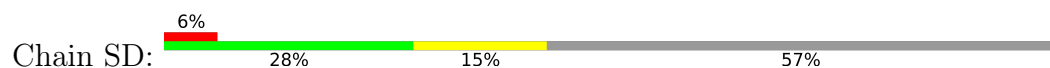
• Molecule 50: 40S ribosomal protein S27



• Molecule 51: 40S ribosomal protein S28

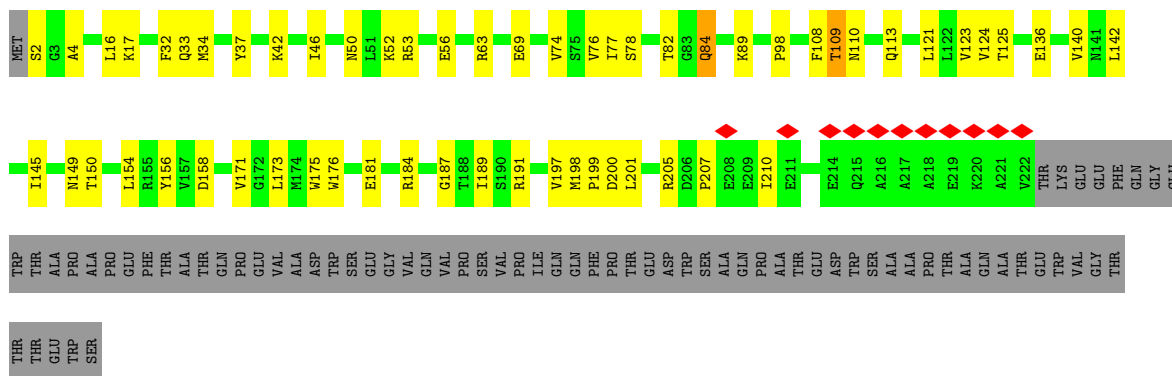


• Molecule 52: Ubiquitin carboxyl extension protein 80

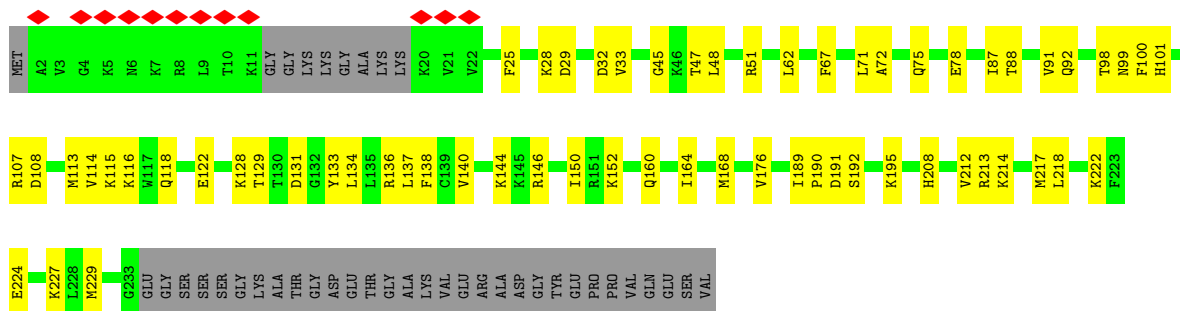




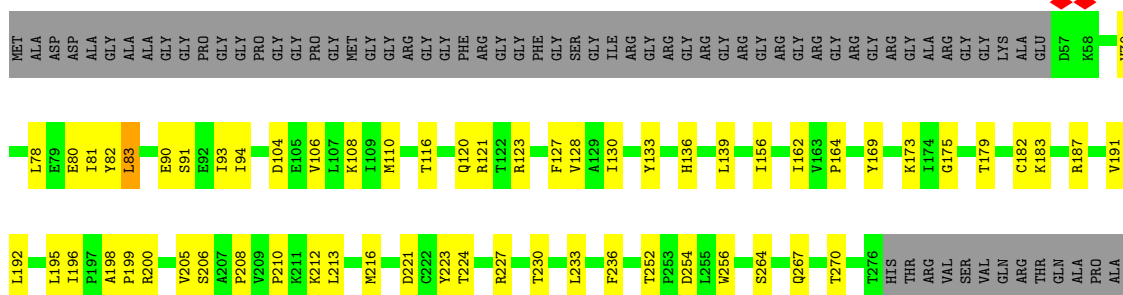
Chain SL: 55% 19% 25%

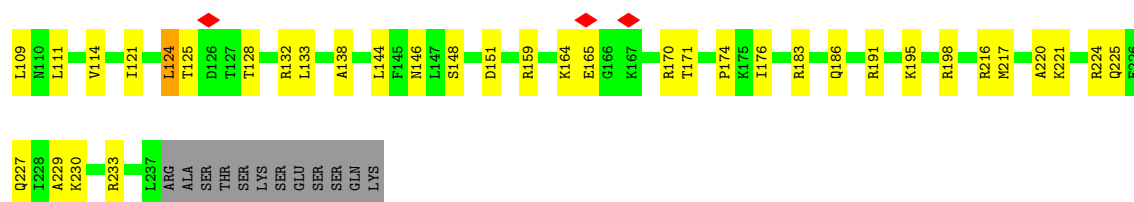


Chain SM:

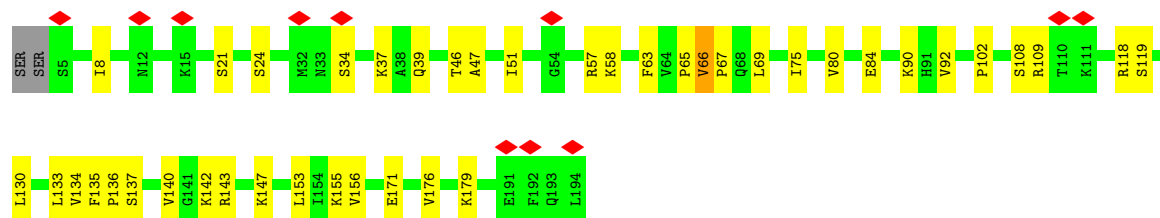
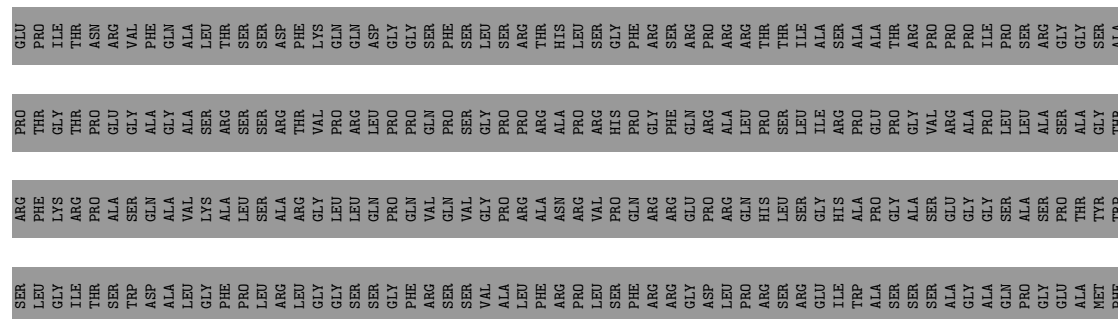
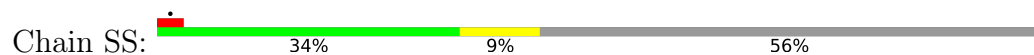


Chain SN:

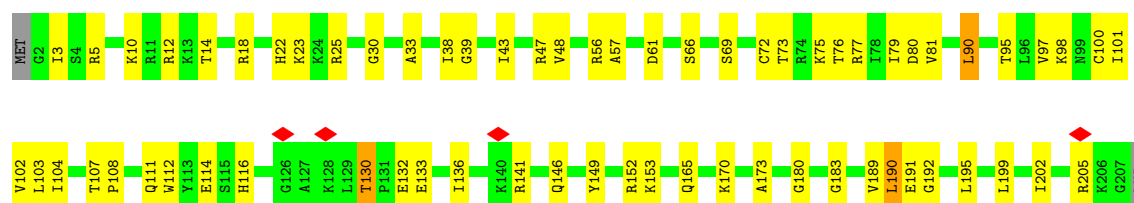




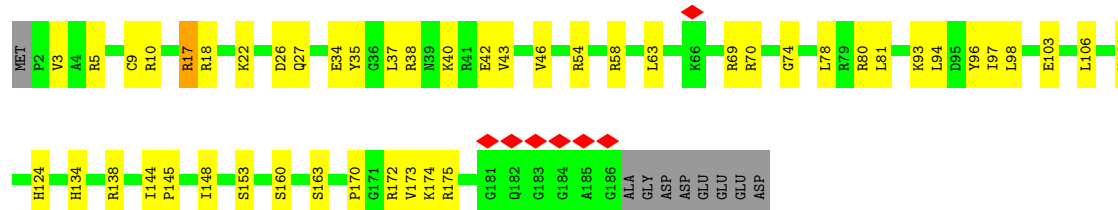
• Molecule 64: 40S ribosomal protein S7



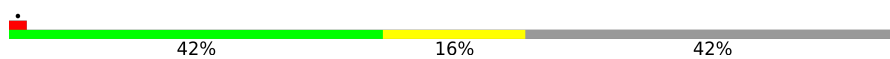
• Molecule 65: 40S ribosomal protein S8

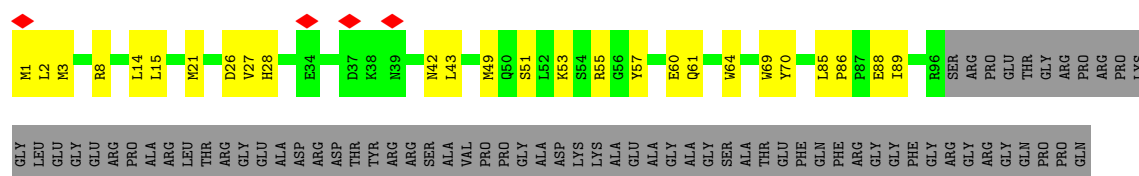


• Molecule 66: 40S ribosomal protein S9



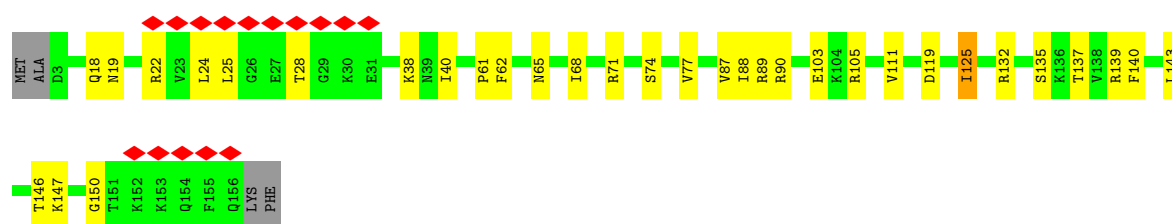
• Molecule 67: S10_ plectin domain-containing protein

Chain SV: 



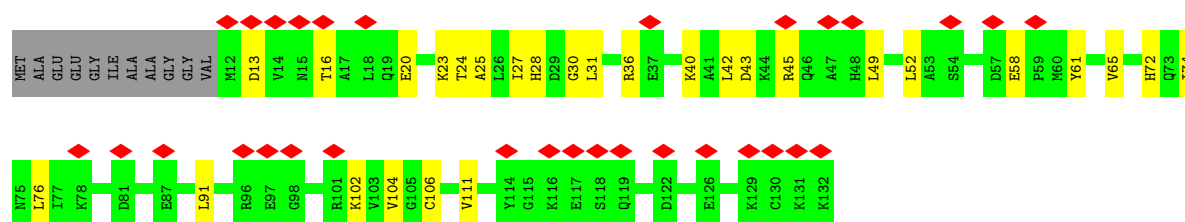
- Molecule 68: 40S ribosomal protein S11

Chain SW: 



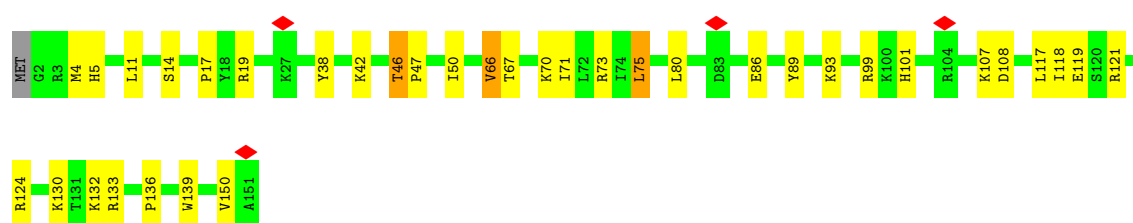
- Molecule 69: 40S ribosomal protein S12

Chain SX: 



- Molecule 70: 40S ribosomal protein S13

Chain SY: 



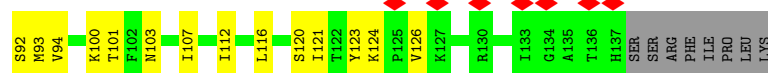
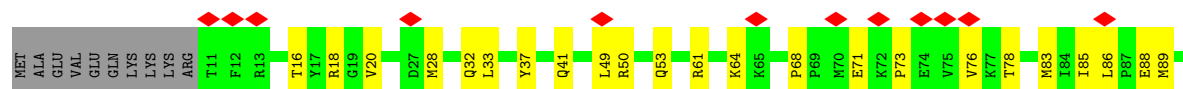
- Molecule 71: 40S ribosomal protein uS11

Chain SZ: 

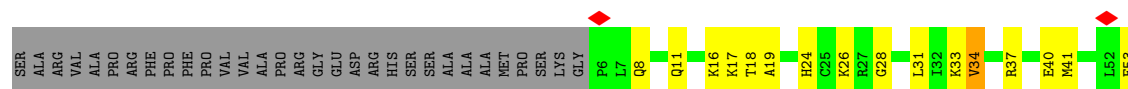




- Molecule 72: 40S ribosomal protein S15



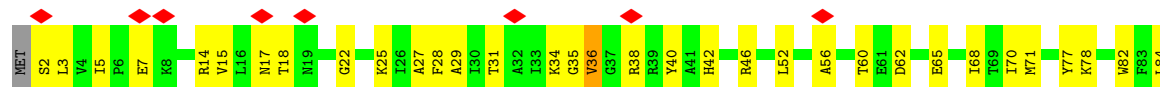
- Molecule 73: 40S ribosomal protein uS9



- Molecule 74: 40S ribosomal protein S17

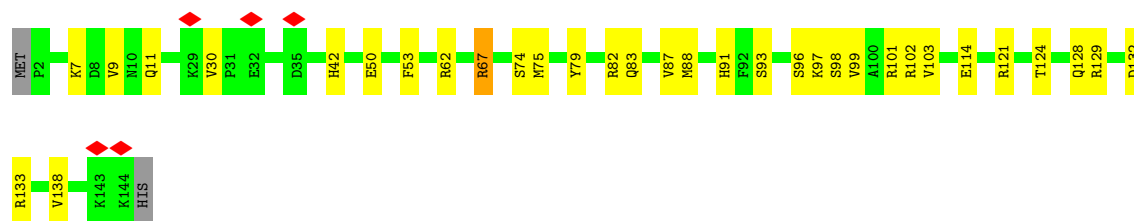


- Molecule 75: 40S ribosomal protein S18



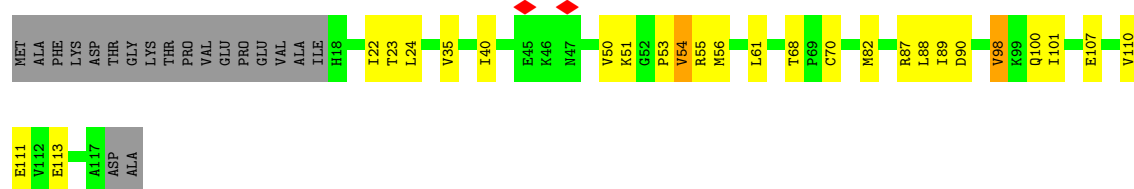
- Molecule 76: 40S Ribosomal protein eS19

Chain Se:  76% 22% ..



- Molecule 77: 40S ribosomal protein S20

Chain Sf:  62% 20% 16%



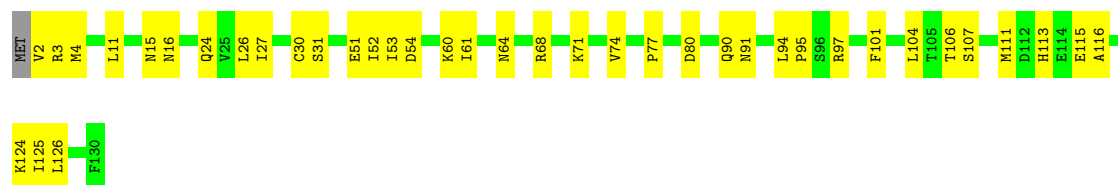
- Molecule 78: 40S ribosomal protein eS21

Chain Sg:  72% 27%



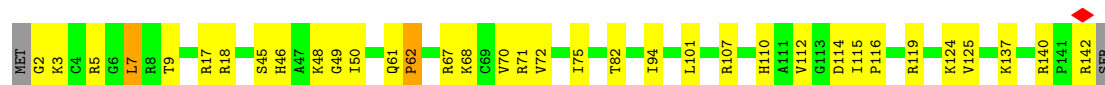
- Molecule 79: 40S ribosomal protein S15a

Chain Sh:  69% 30%



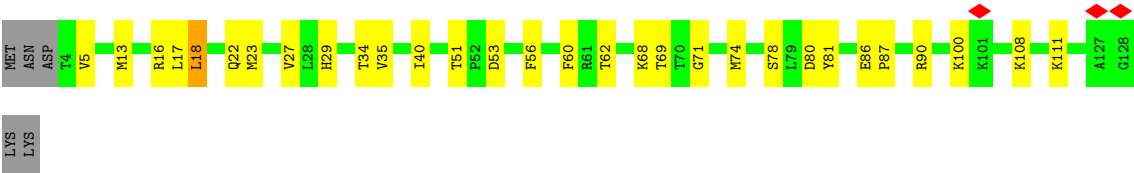
- Molecule 80: 40S ribosomal protein S23

Chain Si:  74% 23% ..

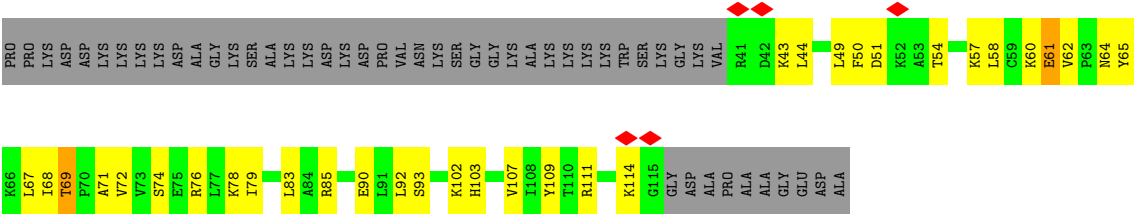
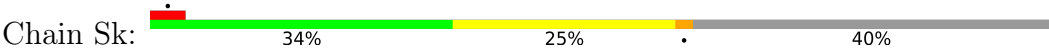


- Molecule 81: 40S ribosomal protein S24

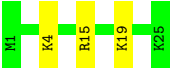
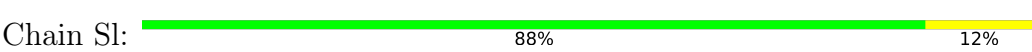
Chain Sj:  73% 22%



• Molecule 82: 40S ribosomal protein S25



• Molecule 83: 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	39295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.751	Depositor
Minimum map value	0.000	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	409.2, 409.2, 409.2	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.15	0/1398	0.34	1/1905 (0.1%)
2	I	0.10	0/3847	0.30	2/5981 (0.0%)
3	L5	0.14	0/86665	0.15	0/135207
4	L7	0.13	0/2835	0.16	0/4418
5	L8	0.12	0/3635	0.14	0/5661
6	LD	0.13	0/1977	0.26	0/2651
7	LE	0.13	0/3261	0.26	0/4364
8	LF	0.13	0/2932	0.24	0/3939
9	LG	0.12	0/2437	0.25	0/3264
10	LH	0.13	0/1998	0.27	0/2673
11	LI	0.13	0/1922	0.26	0/2563
12	LJ	0.11	0/1908	0.24	0/2566
13	LK	0.12	0/1535	0.24	0/2063
14	LL	0.13	0/1756	0.26	0/2346
15	LM	0.11	0/1385	0.26	0/1852
16	LO	0.12	0/1733	0.26	0/2316
17	LP	0.12	0/1158	0.26	0/1547
18	LQ	0.14	0/1746	0.26	0/2338
19	LR	0.13	0/1662	0.24	0/2222
20	LS	0.13	0/1315	0.24	0/1763
21	LT	0.13	0/1539	0.26	0/2054
22	LU	0.11	0/1524	0.21	0/2013
23	LV	0.14	0/1497	0.26	0/2008
24	LW	0.13	0/1326	0.26	0/1770
25	LX	0.10	0/820	0.24	0/1100
26	LY	0.13	0/1048	0.27	0/1402
27	LZ	0.12	0/779	0.24	0/1034
28	La	0.11	0/984	0.23	0/1323
29	Lb	0.12	0/1132	0.25	0/1504
30	Lc	0.11	0/1130	0.21	0/1507
31	Ld	0.13	0/1188	0.27	0/1587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Le	0.11	0/884	0.23	0/1169
33	Lf	0.12	0/847	0.26	0/1134
34	Lg	0.12	0/903	0.23	0/1216
35	Lh	0.13	0/1088	0.25	0/1451
36	Li	0.14	0/903	0.26	0/1208
37	Lj	0.12	0/916	0.26	0/1220
38	Lk	0.10	0/1021	0.23	0/1348
39	Ll	0.11	0/841	0.25	0/1112
40	Lm	0.12	0/720	0.26	0/952
41	Ln	0.10	0/575	0.22	0/761
42	Lo	0.12	0/459	0.27	0/608
43	Lp	0.13	0/426	0.28	0/564
44	Lq	0.11	0/866	0.26	0/1141
45	Lr	0.13	0/718	0.27	0/953
46	Ls	0.12	0/1020	0.26	0/1366
47	Lx	0.10	0/836	0.32	0/1161
48	S	0.18	0/1098	0.40	1/1710 (0.1%)
49	S2	0.15	0/40365	0.16	0/62915
50	SB	0.11	0/665	0.27	0/891
51	SC	0.10	0/497	0.23	0/666
52	SD	0.08	0/560	0.24	0/745
53	SE	0.10	0/462	0.26	0/607
54	SF	0.11	0/828	0.23	0/1109
55	SG	0.09	0/2493	0.24	0/3394
56	SH	0.11	0/470	0.25	0/623
57	SL	0.11	0/1771	0.24	0/2406
58	SM	0.11	0/1841	0.26	0/2459
59	SN	0.11	0/1742	0.25	0/2354
60	SO	0.10	0/1779	0.25	0/2395
61	SP	0.10	0/2118	0.25	0/2849
62	SQ	0.10	0/1531	0.25	0/2059
63	SR	0.09	0/1946	0.24	0/2590
64	SS	0.09	0/1552	0.25	0/2079
65	ST	0.12	0/1715	0.24	0/2287
66	SU	0.10	0/1550	0.25	0/2069
67	SV	0.10	0/834	0.27	0/1125
68	SW	0.10	0/1284	0.25	0/1717
69	SX	0.10	0/953	0.29	0/1276
70	SY	0.11	0/1232	0.25	0/1656
71	SZ	0.11	0/1029	0.27	0/1380
72	Sa	0.09	0/1063	0.24	0/1421
73	Sb	0.10	0/1142	0.28	0/1528
74	Sc	0.10	0/1094	0.23	0/1469

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sd	0.08	0/1180	0.23	0/1581
76	Se	0.08	0/1119	0.21	0/1498
77	Sf	0.10	0/805	0.23	0/1081
78	Sg	0.13	0/636	0.24	0/852
79	Sh	0.12	0/1051	0.26	0/1406
80	Si	0.11	0/1107	0.25	0/1475
81	Sj	0.10	0/1032	0.25	0/1371
82	Sk	0.09	0/604	0.28	0/810
83	Sl	0.10	0/240	0.17	0/305
All	All	0.13	0/234483	0.20	4/344463 (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
47	Lx	0	1
80	Si	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	219	A	OP1-P-O3'	-8.72	81.84	108.00
2	I	219	A	OP2-P-O3'	-8.68	81.96	108.00
48	S	1113	G	C5'-C4'-C3'	8.21	127.51	115.20
1	B	704	LYS	CB-CA-C	-5.27	110.48	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	Lx	60	ARG	Peptide
80	Si	61	GLN	Peptide,Mainchain
80	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	B	1379	0	1207	78	0
2	I	3447	0	1741	75	0
3	L5	80089	0	40554	964	0
4	L7	2570	0	1295	26	0
5	L8	3319	0	1684	46	0
6	LD	1939	0	2036	59	0
7	LE	3206	0	3353	91	0
8	LF	2886	0	3057	65	0
9	LG	2398	0	2430	46	0
10	LH	1960	0	2153	47	0
11	LI	1886	0	2008	50	0
12	LJ	1877	0	2023	30	0
13	LK	1516	0	1597	35	0
14	LL	1717	0	1764	28	0
15	LM	1362	0	1399	34	0
16	LO	1702	0	1820	45	0
17	LP	1137	0	1211	38	0
18	LQ	1701	0	1749	51	0
19	LR	1630	0	1777	47	0
20	LS	1288	0	1326	31	0
21	LT	1515	0	1634	55	0
22	LU	1508	0	1664	39	0
23	LV	1457	0	1492	34	0
24	LW	1298	0	1366	29	0
25	LX	806	0	827	15	0
26	LY	1034	0	1097	18	0
27	LZ	766	0	794	19	0
28	La	967	0	1040	20	0
29	Lb	1115	0	1205	28	0
30	Lc	1107	0	1182	19	0
31	Ld	1159	0	1202	38	0
32	Le	881	0	957	33	0
33	Lf	836	0	888	14	0
34	Lg	888	0	930	16	0
35	Lh	1070	0	1165	34	0
36	Li	884	0	924	18	0
37	Lj	906	0	998	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lk	1013	0	1147	31	0
39	Ll	830	0	916	20	0
40	Lm	705	0	737	25	0
41	Ln	569	0	637	6	0
42	Lo	447	0	480	15	0
43	Lp	432	0	470	11	0
44	Lq	863	0	927	12	0
45	Lr	708	0	756	20	0
46	Ls	1014	0	1083	28	0
47	Lx	840	0	365	6	0
48	S	983	0	499	32	0
49	S2	37825	0	19178	490	0
50	SB	651	0	672	9	0
51	SC	495	0	523	13	0
52	SD	548	0	554	50	0
53	SE	457	0	502	8	0
54	SF	814	0	863	25	0
55	SG	2436	0	2393	95	0
56	SH	459	0	449	15	0
57	SL	1743	0	1748	43	0
58	SM	1815	0	1908	45	0
59	SN	1706	0	1796	39	0
60	SO	1751	0	1846	28	0
61	SP	2076	0	2177	50	0
62	SQ	1509	0	1563	42	0
63	SR	1923	0	2089	51	0
64	SS	1529	0	1627	27	0
65	ST	1686	0	1772	47	0
66	SU	1525	0	1640	38	0
67	SV	810	0	836	17	0
68	SW	1262	0	1335	23	0
69	SX	943	0	978	17	0
70	SY	1208	0	1294	25	0
71	SZ	1016	0	1039	36	0
72	Sa	1042	0	1088	23	0
73	Sb	1124	0	1193	28	0
74	Sc	1080	0	1135	38	0
75	Sd	1171	0	1230	33	0
76	Se	1113	0	1145	33	0
77	Sf	795	0	862	15	0
78	Sg	640	0	632	20	0
79	Sh	1034	0	1080	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Si	1099	0	1162	26	0
81	Sj	1015	0	1086	23	0
82	Sk	598	0	656	24	0
83	Sl	239	0	289	3	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Lq	1	0	0	0	0
84	Lr	1	0	0	0	0
84	SD	1	0	0	0	0
84	SF	1	0	0	0	0
84	SH	1	0	0	0	0
All	All	222755	0	163906	3197	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 9.

All (3197) 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)
1:B:448:VAL:HG22	52:SD:148:TYR:CB	1.57	1.33
1:B:448:VAL:CG2	52:SD:148:TYR:HB3	1.64	1.28
1:B:658:ARG:HH12	49:S2:1575:C:P	1.61	1.24
1:B:446:LEU:HD21	52:SD:146:LEU:HD23	1.17	1.17
1:B:446:LEU:HD21	52:SD:146:LEU:CD2	1.78	1.11
1:B:446:LEU:HD11	52:SD:146:LEU:CD2	1.81	1.10
1:B:446:LEU:CD2	52:SD:146:LEU:HD23	1.81	1.10
1:B:445:GLN:HA	52:SD:147:THR:OG1	1.55	1.06
1:B:446:LEU:HD11	52:SD:146:LEU:HD21	1.43	1.01
49:S2:1034:G:H1	49:S2:1081:A:HO2'	1.04	0.97
49:S2:1092:C:HO2'	79:Sh:2:VAL:N	1.60	0.97
5:L8:81:C:HO2'	38:Lk:2:ALA:N	1.62	0.96
1:B:446:LEU:O	52:SD:147:THR:O	1.87	0.91
3:L5:4254:C:H5'	26:LY:62:MET:HE1	1.56	0.88
3:L5:3374:A:HO2'	40:Lm:2:THR:N	1.69	0.87
1:B:432:GLN:HG2	49:S2:1291:G:H1'	1.55	0.86
1:B:658:ARG:NH1	49:S2:1575:C:P	2.47	0.86
1:B:658:ARG:NH2	49:S2:1575:C:OP2	2.08	0.85
1:B:448:VAL:CG1	52:SD:119:ARG:HH12	1.90	0.84
1:B:446:LEU:CD1	52:SD:146:LEU:CD2	2.56	0.83
55:SG:87:LEU:HB2	55:SG:101:PHE:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLN:CD	52:SD:147:THR:OG1	2.22	0.82
1:B:445:GLN:HA	52:SD:147:THR:HG1	1.40	0.82
3:L5:755:G:H22	3:L5:800:U:H3	1.28	0.82
1:B:445:GLN:OE1	52:SD:147:THR:OG1	1.98	0.82
3:L5:1:C:H42	5:L8:156:U:H3	1.28	0.82
1:B:658:ARG:NH1	49:S2:1575:C:OP2	2.12	0.82
49:S2:695:G:H1	49:S2:733:U:H3	1.28	0.81
49:S2:928:C:O2	50:SB:51:GLN:NE2	2.13	0.81
43:Lp:103:LEU:HD21	43:Lp:110:CYS:HA	1.61	0.81
1:B:448:VAL:HG13	52:SD:119:ARG:HH12	1.45	0.80
81:Sj:87:PRO:HD2	81:Sj:90:ARG:HE	1.48	0.79
1:B:443:LYS:H	52:SD:145:CYS:HB2	1.48	0.79
3:L5:1611:U:OP2	31:Ld:26:ARG:NH2	2.16	0.79
10:LH:273:TYR:OH	17:LP:106:ASP:OD2	2.00	0.78
58:SM:107:ARG:NH1	71:SZ:133:THR:O	2.16	0.77
3:L5:1509:A:H4'	45:Lr:10:ILE:HG12	1.67	0.77
2:I:140:G:OP2	2:I:143:A:N6	2.17	0.77
55:SG:245:ARG:HH22	55:SG:312:VAL:HG21	1.50	0.77
1:B:431:GLN:HB3	49:S2:1291:G:O2'	1.85	0.76
48:S:1145:G:H21	52:SD:137:ASP:HB3	1.49	0.76
57:SL:123:VAL:HG12	57:SL:145:ILE:HB	1.66	0.76
1:B:445:GLN:OE1	52:SD:147:THR:CB	2.34	0.75
2:I:56:A:N7	2:I:161:A:O2'	2.20	0.75
3:L5:4098:U:H1'	31:Ld:58:MET:HE1	1.67	0.75
6:LD:117:GLU:HG3	6:LD:124:GLY:H	1.51	0.74
42:Lo:30:LYS:HB2	42:Lo:33:ASN:HB2	1.67	0.74
1:B:658:ARG:NH1	49:S2:1575:C:OP1	2.20	0.74
3:L5:4612:G:H22	19:LR:176:ARG:HH22	1.35	0.74
3:L5:1137:C:H42	3:L5:1204:C:H42	1.34	0.74
71:SZ:34:PHE:HB3	71:SZ:41:PHE:HB2	1.70	0.74
18:LQ:114:ARG:HG2	18:LQ:137:PRO:HG3	1.70	0.74
49:S2:304:C:H5''	65:ST:75:LYS:HE3	1.69	0.74
1:B:675:LEU:O	48:S:1113:G:O6	2.06	0.74
3:L5:4445:U:OP2	43:Lp:111:ARG:NH1	2.19	0.74
49:S2:151:C:O2	63:SR:132:ARG:NH2	2.21	0.74
59:SN:256:TRP:HB3	79:Sh:68:ARG:HH21	1.51	0.74
9:LG:41:LYS:NZ	24:LW:32:ARG:O	2.19	0.73
55:SG:129:ILE:HD11	55:SG:151:VAL:HG11	1.69	0.73
3:L5:320:C:OP1	39:Ll:84:LYS:NZ	2.21	0.73
4:L7:5:A:OP1	15:LM:147:ARG:NH2	2.21	0.73
64:SS:46:THR:HG23	64:SS:65:PRO:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SG:256:ILE:HB	55:SG:270:LEU:HB2	1.70	0.73
3:L5:1897:A:O2'	3:L5:1964:A:N1	2.19	0.73
3:L5:3628:C:O2'	7:LE:268:ARG:NH2	2.20	0.73
57:SL:184:ARG:O	78:Sg:45:ARG:NH2	2.21	0.73
5:L8:51:U:H4'	42:Lo:21:ARG:HH22	1.54	0.73
49:S2:1399:G:O5'	55:SG:61:GLY:HA2	1.89	0.73
48:S:1112:U:H5'	48:S:1112:U:O2	1.89	0.72
49:S2:1210:A:O3'	54:SF:82:LYS:NZ	2.23	0.72
49:S2:926:G:H1	49:S2:1018:U:H3	1.33	0.72
16:LO:104:ASN:HD21	16:LO:110:LEU:HB2	1.54	0.72
49:S2:165:G:OP2	49:S2:165:G:N2	2.22	0.72
49:S2:353:U:O2	68:SW:71:ARG:NH1	2.21	0.72
30:Lc:89:ILE:HD11	30:Lc:117:LYS:HB3	1.72	0.72
3:L5:3373:U:OP2	3:L5:3378:A:N6	2.22	0.72
49:S2:3:C:O2	66:SU:18:ARG:NH2	2.22	0.72
3:L5:413:G:OP2	42:Lo:36:ARG:NH1	2.23	0.72
20:LS:94:MET:HE2	20:LS:148:MET:HG2	1.72	0.72
3:L5:719:G:OP2	8:LF:350:ARG:NH2	2.22	0.72
49:S2:483:G:N1	49:S2:486:A:OP2	2.23	0.72
3:L5:2293:G:OP1	6:LD:17:ARG:NH1	2.22	0.71
63:SR:2:LYS:HB2	63:SR:108:VAL:HG12	1.73	0.71
3:L5:266:C:H1'	38:Lk:109:ARG:HH12	1.55	0.71
71:SZ:62:VAL:HG11	71:SZ:67:ASP:HB2	1.72	0.71
79:Sh:27:ILE:HB	79:Sh:61:ILE:HB	1.72	0.71
3:L5:660:G:N3	46:Ls:46:ARG:NH1	2.38	0.71
1:B:446:LEU:CD2	52:SD:146:LEU:CD2	2.53	0.71
59:SN:183:LYS:NZ	79:Sh:91:ASN:O	2.24	0.71
23:LV:19:THR:HG23	23:LV:22:SER:H	1.56	0.71
64:SS:51:ILE:HG12	64:SS:179:LYS:HG3	1.72	0.71
5:L8:75:OMG:OP2	29:Lb:74:TYR:OH	2.08	0.70
5:L8:110:U:OP2	42:Lo:8:ARG:NH2	2.24	0.70
27:LZ:102:LYS:HA	27:LZ:105:ARG:HB3	1.72	0.70
48:S:1111:A:H4'	48:S:1113:G:H5'	1.73	0.70
2:I:110:U:OP2	71:SZ:63:LYS:NZ	2.23	0.70
3:L5:4627:C:O2	3:L5:4670:G:N2	2.22	0.70
11:LI:126:LYS:O	11:LI:130:ASN:ND2	2.24	0.70
3:L5:40:G:N2	3:L5:4126:A:N7	2.40	0.70
3:L5:633:U:H5''	3:L5:634:C:H2'	1.73	0.70
55:SG:42:MET:O	55:SG:56:GLN:N	2.23	0.70
62:SQ:155:CYS:SG	62:SQ:159:ARG:NH2	2.65	0.70
49:S2:629:A:N6	60:SO:178:ARG:O	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sk:69:THR:HG22	82:Sk:72:VAL:HG22	1.74	0.70
3:L5:3541:G:OP2	3:L5:3541:G:N2	2.24	0.70
59:SN:182:CYS:HB2	79:Sh:95:PRO:HB2	1.74	0.70
49:S2:679:U:OP2	49:S2:1027:C:N4	2.25	0.70
11:LI:45:ARG:HG2	32:Le:100:ALA:HB1	1.73	0.70
4:L7:7:G:O3'	9:LG:33:ARG:NH1	2.24	0.70
4:L7:66:G:OP1	9:LG:10:LYS:NZ	2.25	0.70
49:S2:1843:4AC:O7	83:Sl:4:LYS:NZ	2.24	0.70
65:ST:165:GLN:HE22	65:ST:195:LEU:HD11	1.56	0.70
1:B:448:VAL:HA	52:SD:148:TYR:CD1	2.27	0.69
61:SP:122:LYS:NZ	61:SP:124:CYS:SG	2.63	0.69
1:B:446:LEU:HD11	52:SD:146:LEU:HD22	1.69	0.69
7:LE:224:LYS:HG2	7:LE:340:THR:HG22	1.74	0.69
27:LZ:44:ARG:HD3	27:LZ:49:ILE:HD11	1.73	0.69
49:S2:189:U:O2	49:S2:211:G:N1	2.17	0.69
55:SG:129:ILE:HB	55:SG:142:VAL:HB	1.74	0.69
3:L5:2579:G:OP2	45:Lr:48:LYS:NZ	2.25	0.69
13:LK:23:ARG:HE	13:LK:39:ASN:HA	1.57	0.69
26:LY:71:GLU:O	26:LY:75:LYS:NZ	2.25	0.69
61:SP:45:ILE:HA	61:SP:61:VAL:HG11	1.75	0.69
3:L5:724:G:N7	11:LI:76:LYS:NZ	2.37	0.69
15:LM:32:ARG:HD2	15:LM:35:ARG:HH22	1.57	0.69
3:L5:4073:C:OP1	24:LW:70:HIS:NE2	2.24	0.69
49:S2:819:A:OP1	66:SU:80:ARG:NH2	2.26	0.69
3:L5:755:G:N2	3:L5:801:C:N3	2.40	0.69
49:S2:1678:U:H2'	49:S2:1679:A2M:H8	1.74	0.69
70:SY:136:PRO:HG2	70:SY:139:TRP:HB2	1.74	0.69
3:L5:1983:U:O3'	19:LR:63:ASN:ND2	2.25	0.69
49:S2:1022:U:OP1	70:SY:132:LYS:NZ	2.26	0.69
49:S2:1651:A:N1	62:SQ:83:ASN:ND2	2.40	0.69
3:L5:4366:OMU:OP2	3:L5:4416:C:N4	2.25	0.69
8:LF:303:ARG:NH1	21:LT:37:ARG:O	2.24	0.69
3:L5:3909:U:H5'	3:L5:3910:C:H5''	1.74	0.68
5:L8:94:G:OP2	40:Lm:72:ARG:NH1	2.26	0.68
7:LE:63:PRO:HA	7:LE:68:ASN:HD21	1.56	0.68
49:S2:385:U:O4	65:ST:5:ARG:NH2	2.25	0.68
49:S2:1465:C:H5'	74:Sc:60:ARG:HH22	1.57	0.68
35:Lh:43:ASN:HB3	35:Lh:46:ARG:HG2	1.75	0.68
49:S2:126:G:N2	49:S2:180:G:N3	2.41	0.68
49:S2:507:G:OP1	81:Sj:108:LYS:NZ	2.25	0.68
49:S2:745:G:O2'	64:SS:109:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1021:A:N7	70:SY:70:LYS:NZ	2.40	0.68
49:S2:700:C:H42	49:S2:728:G:H22	1.39	0.68
3:L5:1338:G:H5'	16:LO:186:ARG:HH11	1.59	0.68
3:L5:3805:A:N1	3:L5:3917:C:N4	2.42	0.68
3:L5:4018:G:N2	3:L5:4018:G:OP2	2.27	0.68
3:L5:4787:A:H5'	3:L5:4788:G:H5''	1.74	0.68
13:LK:137:SER:HB3	13:LK:143:GLU:HB3	1.75	0.68
39:LI:50:PHE:O	39:LI:55:ARG:NH1	2.27	0.68
49:S2:1548:C:N4	49:S2:1587:U:O4	2.25	0.68
61:SP:160:ILE:HG13	61:SP:162:ILE:HD11	1.76	0.68
3:L5:2039:G:N7	8:LF:306:ARG:NH2	2.39	0.68
57:SL:34:MET:HE3	57:SL:154:LEU:HD21	1.76	0.68
3:L5:1931:U:O2'	3:L5:1941:A:OP1	2.10	0.68
2:I:56:A:N6	2:I:126:C:O2	2.26	0.68
2:I:68:U:O2'	2:I:164:C:N3	2.27	0.68
3:L5:989:G:H1	3:L5:1123:C:H42	1.40	0.68
1:B:446:LEU:CD1	52:SD:146:LEU:HD21	2.20	0.68
12:LJ:87:LEU:HD21	12:LJ:182:CYS:HB2	1.75	0.68
20:LS:128:ARG:NH1	20:LS:130:TYR:OH	2.27	0.68
55:SG:258:ILE:HD11	55:SG:268:ASP:HB2	1.76	0.68
73:Sb:97:GLN:HB2	73:Sb:105:LYS:HD3	1.74	0.68
3:L5:3416:G:OP1	6:LD:174:ARG:NH2	2.27	0.68
49:S2:1019:U:H5''	70:SY:71:ILE:HG21	1.74	0.68
49:S2:1193:U:OP2	80:Si:119:ARG:NH2	2.27	0.68
4:L7:51:G:H21	15:LM:12:MET:HE3	1.58	0.67
5:L8:82:A:H1'	38:Lk:49:VAL:HG11	1.76	0.67
27:LZ:105:ARG:NH2	63:SR:151:ASP:OD1	2.27	0.67
2:I:96:G:N1	2:I:99:U:OP2	2.27	0.67
3:L5:1391:C:H1'	32:Le:106:ARG:HH22	1.59	0.67
5:L8:81:C:O2'	38:Lk:2:ALA:N	2.28	0.67
79:Sh:80:ASP:OD1	79:Sh:124:LYS:NZ	2.26	0.67
2:I:52:A:N1	2:I:75:A:N6	2.42	0.67
49:S2:430:C:O2'	49:S2:812:A:N1	2.26	0.67
3:L5:4381:A:OP1	3:L5:4382:PSU:O2'	2.12	0.67
3:L5:4416:C:O2'	3:L5:4418:A:OP2	2.12	0.67
33:Lf:103:ASP:OD1	33:Lf:106:ARG:NH2	2.28	0.67
1:B:658:ARG:CZ	49:S2:1575:C:OP2	2.43	0.67
2:I:159:G:H2'	2:I:160:G:C8	2.30	0.67
4:L7:48:G:OP1	9:LG:94:ASN:ND2	2.28	0.67
14:LL:76:MET:HE3	14:LL:138:ILE:HG21	1.76	0.67
21:LT:61:LEU:HD22	21:LT:82:VAL:HG11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:La:100:VAL:HG21	28:La:109:ILE:HG12	1.77	0.67
49:S2:800:U:OP1	64:SS:108:SER:OG	2.13	0.67
2:I:44:G:H1	2:I:83:U:H3	1.42	0.67
8:LF:293:LEU:O	8:LF:299:GLN:NE2	2.27	0.66
49:S2:1355:G:N2	49:S2:1358:A:OP2	2.27	0.66
59:SN:108:LYS:HE3	59:SN:233:LEU:HD23	1.77	0.66
3:L5:756:G:H1	3:L5:799:C:H42	1.43	0.66
3:L5:1060:G:O4'	3:L5:1086:G:N2	2.28	0.66
3:L5:4287:G:N2	3:L5:4290:A:OP2	2.27	0.66
11:LI:148:SER:HA	11:LI:244:ARG:HH22	1.60	0.66
49:S2:381:G:N1	49:S2:384:G:OP2	2.28	0.66
49:S2:929:G:H1	49:S2:1014:U:H3	1.40	0.66
3:L5:2444:A:N6	3:L5:2587:A:OP2	2.28	0.66
63:SR:30:LYS:HD3	63:SR:36:VAL:HG11	1.77	0.66
3:L5:1918:A:H8	3:L5:1927:G:H1	1.43	0.66
3:L5:2037:G:H22	3:L5:2046:A:H5''	1.60	0.66
35:Lh:89:LEU:HD13	35:Lh:118:LEU:HG	1.76	0.66
49:S2:1417:C:H5'	76:Se:129:ARG:CZ	2.26	0.66
49:S2:1458:U:OP2	74:Sc:59:LYS:NZ	2.28	0.66
63:SR:225:GLN:O	63:SR:229:ALA:N	2.28	0.66
3:L5:1624:A:OP1	32:Le:18:ARG:NH2	2.28	0.66
3:L5:223:G:N3	8:LF:223:ASN:ND2	2.43	0.66
3:L5:2302:G:N2	3:L5:2305:C:OP2	2.29	0.66
11:LI:104:VAL:HG13	11:LI:135:VAL:HG12	1.76	0.66
11:LI:155:LYS:HG3	11:LI:156:ARG:HG2	1.78	0.66
17:LP:119:ARG:HE	19:LR:193:THR:HG22	1.60	0.66
2:I:147:C:H4'	82:Sk:78:LYS:HD2	1.76	0.66
3:L5:458:C:O2'	10:LH:113:ARG:NH2	2.28	0.66
3:L5:752:G:N2	3:L5:804:C:O2	2.29	0.66
3:L5:2538:A:OP1	41:Ln:35:LYS:NZ	2.27	0.66
13:LK:101:ILE:HG21	13:LK:179:ILE:HD11	1.78	0.66
49:S2:484:C:H5''	80:Si:48:LYS:HE2	1.75	0.66
49:S2:1087:G:OP2	54:SF:12:LYS:NZ	2.28	0.66
15:LM:63:ARG:HH22	44:Lq:105:GLN:HA	1.61	0.65
23:LV:118:ARG:O	23:LV:120:ARG:NH1	2.29	0.65
28:La:107:HIS:O	28:La:111:GLN:NE2	2.28	0.65
72:Sa:18:ARG:HD2	75:Sd:88:LYS:HG2	1.77	0.65
3:L5:2688:A:H61	3:L5:3575:C:H42	1.43	0.65
36:Li:43:LEU:O	36:Li:109:ARG:NH1	2.25	0.65
3:L5:1924:G:H1'	3:L5:1942:G:H2'	1.78	0.65
3:L5:4268:G:O2'	3:L5:4271:C:OP2	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2496:C:OP1	37:Lj:54:ARG:NH2	2.29	0.65
49:S2:606:A:HO2'	49:S2:639:C:HO2'	1.43	0.65
49:S2:985:C:O2'	71:SZ:138:ASP:OD2	2.14	0.65
3:L5:346:G:OP1	29:Lb:8:THR:OG1	2.15	0.65
3:L5:1703:G:N2	3:L5:1707:C:N3	2.44	0.65
3:L5:4786:C:O2'	3:L5:4789:C:OP2	2.15	0.65
49:S2:197:U:H1'	49:S2:203:G:H22	1.59	0.65
49:S2:1390:C:O2'	60:SO:162:ASP:OD1	2.15	0.65
3:L5:1434:G:H21	16:LO:184:MET:HE1	1.62	0.65
3:L5:3449:A:OP2	3:L5:3467:G:N2	2.29	0.65
49:S2:1216:C:H42	49:S2:1221:A:H61	1.43	0.65
10:LH:212:PRO:HB2	10:LH:215:LEU:HD23	1.78	0.65
55:SG:249:CYS:HB3	55:SG:258:ILE:HG22	1.78	0.65
3:L5:3351:G:O2'	22:LU:82:LYS:NZ	2.25	0.65
6:LD:27:ALA:O	6:LD:128:ARG:NH1	2.30	0.65
6:LD:116:LEU:HB3	6:LD:126:LEU:HB2	1.78	0.65
15:LM:158:SER:OG	15:LM:161:GLU:OE1	2.15	0.65
29:Lb:43:ASN:ND2	29:Lb:127:GLN:OE1	2.27	0.65
49:S2:231:A:H2	49:S2:898:U:H3	1.45	0.65
49:S2:1417:C:N4	49:S2:1425:G:O6	2.19	0.65
1:B:445:GLN:OE1	52:SD:147:THR:HB	1.97	0.65
3:L5:2105:G:OP2	46:Ls:107:ARG:NH2	2.30	0.65
3:L5:4203:PSU:OP1	26:LY:50:ASN:ND2	2.30	0.65
3:L5:4790:C:O2'	7:LE:325:GLU:OE2	2.15	0.65
28:La:86:ALA:HB1	28:La:97:VAL:HG21	1.79	0.65
49:S2:1567:G:N7	76:Se:101:ARG:NH2	2.45	0.65
60:SO:10:LYS:HZ2	77:Sf:111:GLU:HG2	1.62	0.65
21:LT:18:PRO:HG3	21:LT:29:VAL:HG21	1.79	0.65
45:Lr:56:HIS:HD2	45:Lr:63:THR:HG22	1.60	0.65
57:SL:17:LYS:HB3	57:SL:173:LEU:HD11	1.78	0.65
48:S:1114:A:H5'	48:S:1155:A:C6	2.32	0.64
3:L5:2007:C:OP1	36:Li:15:LYS:NZ	2.29	0.64
3:L5:2400:G:H1	3:L5:2413:U:H3	1.45	0.64
25:LX:96:LEU:HG	25:LX:100:LEU:HD23	1.77	0.64
8:LF:266:THR:HG23	8:LF:269:LYS:H	1.61	0.64
22:LU:140:GLU:OE1	22:LU:144:LYS:NZ	2.30	0.64
49:S2:380:C:O2	65:ST:5:ARG:NH1	2.29	0.64
55:SG:40:ILE:HB	55:SG:59:LEU:HB2	1.79	0.64
69:SX:49:LEU:HB3	69:SX:111:VAL:HB	1.78	0.64
21:LT:79:THR:HB	21:LT:136:THR:HG23	1.78	0.64
48:S:1118:U:OP1	72:Sa:61:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:642:A:OP1	66:SU:40:LYS:NZ	2.29	0.64
55:SG:11:LEU:HB2	55:SG:307:VAL:HB	1.79	0.64
73:Sb:11:GLN:OE1	73:Sb:24:HIS:ND1	2.29	0.64
3:L5:4218:G:O2'	43:Lp:100:TYR:O	2.14	0.64
21:LT:85:THR:HG22	21:LT:104:ARG:HB3	1.78	0.64
2:I:132:U:H3	2:I:154:A:H2	1.46	0.64
3:L5:279:A:N7	18:LQ:12:ARG:NH1	2.46	0.64
3:L5:1746:C:O3'	24:LW:110:LYS:NZ	2.31	0.64
3:L5:3831:C:N3	3:L5:3835:G:N2	2.45	0.64
11:LI:46:ARG:HE	11:LI:49:ILE:HD11	1.61	0.64
21:LT:63:LEU:HB2	21:LT:88:ASP:HA	1.80	0.64
3:L5:1871:A:OP1	19:LR:49:ARG:NH2	2.30	0.64
49:S2:1131:G:OP2	49:S2:1131:G:N2	2.30	0.64
71:SZ:62:VAL:HG12	71:SZ:64:ALA:H	1.63	0.64
3:L5:2510:C:OP1	22:LU:100:ARG:NH1	2.30	0.64
49:S2:1240:U:H5''	72:Sa:124:LYS:HE3	1.79	0.64
66:SU:81:LEU:HD12	66:SU:97:ILE:HD12	1.79	0.64
3:L5:3555:G:N2	3:L5:3555:G:OP2	2.31	0.64
82:Sk:60:LYS:O	82:Sk:64:ASN:ND2	2.31	0.64
2:I:46:U:H3	2:I:81:A:HO2'	1.44	0.64
3:L5:364:G:O6	40:Lm:52:LYS:NZ	2.31	0.64
49:S2:49:C:H2'	49:S2:473:C:H41	1.62	0.64
2:I:63:A:N6	2:I:169:U:O2	2.28	0.63
3:L5:2250:G:O6	42:Lo:2:SER:N	2.31	0.63
3:L5:3852:G:N2	12:LJ:43:GLN:O	2.30	0.63
3:L5:3862:G:N7	3:L5:3897:G:N2	2.45	0.63
24:LW:84:ILE:HD11	32:Le:23:LYS:HA	1.79	0.63
3:L5:1297:G:N7	21:LT:104:ARG:NH2	2.44	0.63
3:L5:4764:C:O2'	3:L5:4767:G:N3	2.30	0.63
19:LR:61:ARG:HA	19:LR:70:PRO:HD2	1.81	0.63
35:Lh:47:ARG:HE	35:Lh:49:PHE:HE2	1.46	0.63
76:Se:53:PHE:HE1	76:Se:103:VAL:HG22	1.62	0.63
3:L5:4744:G:N2	3:L5:4780:G:O2'	2.31	0.63
15:LM:63:ARG:NH2	44:Lq:104:ILE:O	2.31	0.63
49:S2:142:C:N4	49:S2:330:G:OP1	2.31	0.63
49:S2:313:G:O2'	63:SR:191:ARG:NH1	2.32	0.63
73:Sb:37:ARG:HG2	76:Se:7:LYS:HB3	1.79	0.63
3:L5:2399:G:O3'	30:Lc:109:LYS:NZ	2.32	0.63
67:SV:85:LEU:HD12	67:SV:89:ILE:HG13	1.79	0.63
74:Sc:31:ASN:HD22	74:Sc:55:THR:HG22	1.64	0.63
3:L5:1334:G:N2	3:L5:1337:G:OP2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:421:G:O2'	49:S2:661:C:N3	2.31	0.63
49:S2:1084:A:N7	49:S2:1842:C:O2'	2.32	0.63
55:SG:245:ARG:NH2	55:SG:295:GLY:O	2.32	0.63
3:L5:3986:G:OP1	15:LM:145:LYS:NZ	2.32	0.63
3:L5:4666:G:N2	3:L5:4666:G:OP2	2.31	0.63
77:Sf:51:LYS:HB3	77:Sf:90:ASP:HB2	1.79	0.63
3:L5:512:U:OP2	31:Ld:85:GLN:NE2	2.32	0.63
3:L5:1900:G:N2	3:L5:1963:G:O2'	2.31	0.63
13:LK:44:GLU:OE1	17:LP:2:VAL:N	2.32	0.63
55:SG:54:ILE:HG12	55:SG:55:PRO:HD2	1.80	0.63
81:Sj:13:MET:SD	81:Sj:22:GLN:NE2	2.71	0.63
45:Lr:38:THR:HA	45:Lr:45:THR:HA	1.81	0.63
49:S2:153:G:N3	63:SR:13:GLN:NE2	2.46	0.63
61:SP:64:ILE:HD11	81:Sj:18:LEU:HD22	1.80	0.63
3:L5:3491:A:O2'	49:S2:1827:G:O2'	2.15	0.62
7:LE:56:ILE:HD12	7:LE:365:LEU:HD22	1.81	0.62
10:LH:181:PRO:HD2	10:LH:184:LEU:HD12	1.79	0.62
49:S2:1553:G:OP1	49:S2:1579:U:N3	2.30	0.62
49:S2:1867:A:N6	54:SF:85:ARG:O	2.32	0.62
3:L5:308:G:N2	3:L5:308:G:OP2	2.32	0.62
49:S2:295:U:N3	68:SW:65:ASN:OD1	2.32	0.62
21:LT:79:THR:OG1	21:LT:99:LYS:NZ	2.27	0.62
29:Lb:67:ILE:O	29:Lb:84:ARG:NH2	2.32	0.62
33:Lf:8:LYS:O	33:Lf:12:GLU:N	2.27	0.62
35:Lh:67:LYS:O	35:Lh:75:ARG:NH2	2.31	0.62
49:S2:104:A:OP1	65:ST:12:ARG:NH1	2.32	0.62
3:L5:3602:C:O3'	7:LE:261:ARG:NH2	2.32	0.62
56:SH:3:HIS:HB3	56:SH:6:LEU:HB3	1.81	0.62
54:SF:11:ALA:HB3	54:SF:33:ASP:HB2	1.82	0.62
7:LE:19:ARG:HB2	7:LE:234:ARG:HH21	1.64	0.62
49:S2:162:C:O3'	63:SR:95:LYS:NZ	2.33	0.62
49:S2:869:G:OP2	49:S2:869:G:N2	2.27	0.62
54:SF:58:VAL:HG11	71:SZ:28:PHE:HZ	1.64	0.62
3:L5:1059:G:N2	3:L5:1086:G:O6	2.32	0.62
3:L5:1237:G:OP2	3:L5:1237:G:N2	2.26	0.62
5:L8:71:A:N1	5:L8:84:A:O2'	2.30	0.62
82:Sk:102:LYS:HA	82:Sk:107:VAL:HG12	1.82	0.62
3:L5:1601:A:O2'	40:Lm:49:TRP:O	2.15	0.62
4:L7:99:G:N7	23:LV:55:LYS:NZ	2.39	0.62
9:LG:155:THR:HG22	9:LG:179:ARG:HD3	1.82	0.62
61:SP:44:LEU:HD21	61:SP:72:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sg:3:ASN:OD1	78:Sg:7:GLU:N	2.33	0.62
3:L5:2601:G:O2'	3:L5:2608:A:N3	2.30	0.62
6:LD:36:GLU:OE1	6:LD:163:ARG:NH1	2.33	0.62
54:SF:85:ARG:NH2	54:SF:86:ASN:OD1	2.33	0.62
68:SW:150:GLY:HA3	70:SY:133:ARG:HH22	1.65	0.62
1:B:446:LEU:HD21	52:SD:146:LEU:HD22	1.75	0.61
3:L5:152:U:OP2	18:LQ:49:ARG:NH2	2.29	0.61
3:L5:1011:C:N3	3:L5:1012:C:N4	2.47	0.61
3:L5:1260:OMG:HM22	3:L5:1261:U:H5'	1.82	0.61
3:L5:2146:C:OP1	35:Lh:107:ASN:ND2	2.32	0.61
49:S2:1869:U:O2'	54:SF:100:ARG:NH2	2.33	0.61
56:SH:19:ARG:HD2	56:SH:32:ARG:HH12	1.64	0.61
3:L5:996:C:O2	3:L5:1109:G:N2	2.29	0.61
21:LT:6:ARG:HH21	32:Le:18:ARG:HD2	1.64	0.61
49:S2:1288:A:OP2	52:SD:97:LYS:NZ	2.33	0.61
2:I:113:U:O5'	62:SQ:198:ARG:NH2	2.33	0.61
3:L5:2052:G:H2'	3:L5:2053:A:H8	1.64	0.61
3:L5:4440:G:OP1	3:L5:4440:G:N2	2.31	0.61
49:S2:1076:C:OP1	70:SY:107:LYS:NZ	2.32	0.61
57:SL:69:GLU:HG3	59:SN:270:THR:HG21	1.82	0.61
61:SP:11:ARG:HA	61:SP:28:ALA:HB2	1.82	0.61
77:Sf:54:VAL:HG13	77:Sf:88:LEU:HB2	1.81	0.61
25:LX:28:PRO:HB2	25:LX:34:MET:HG2	1.82	0.61
77:Sf:61:LEU:HB2	77:Sf:82:MET:HB3	1.81	0.61
23:LV:11:LYS:HD2	23:LV:29:ARG:HD2	1.82	0.61
49:S2:1390:C:OP1	74:Sc:43:SER:OG	2.15	0.61
76:Se:9:VAL:HG21	76:Se:138:VAL:HG13	1.81	0.61
16:LO:64:VAL:HA	16:LO:67:HIS:HD2	1.66	0.61
20:LS:42:ARG:HH21	20:LS:159:LYS:HG3	1.64	0.61
3:L5:843:A:N7	11:LI:150:ASN:ND2	2.49	0.61
51:SC:14:VAL:HG12	51:SC:32:VAL:HG12	1.83	0.61
55:SG:14:HIS:O	55:SG:305:ASN:ND2	2.28	0.61
64:SS:133:LEU:HD11	64:SS:176:VAL:HG23	1.83	0.61
7:LE:286:LYS:HB3	7:LE:332:MET:HG3	1.82	0.61
9:LG:64:ILE:HG12	9:LG:105:LEU:HD21	1.83	0.61
49:S2:1674:U:O2'	62:SQ:84:GLY:O	2.16	0.61
3:L5:419:A:N3	3:L5:1276:C:O2'	2.33	0.60
12:LJ:134:PRO:HB3	12:LJ:206:GLN:HG3	1.82	0.60
14:LL:38:ARG:HB3	14:LL:41:ALA:HB2	1.82	0.60
44:Lq:36:GLN:OE1	44:Lq:39:ARG:NH2	2.34	0.60
3:L5:393:U:O3'	20:LS:96:LYS:NZ	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3848:U:C4	37:Lj:97:ILE:HG22	2.36	0.60
6:LD:111:THR:HG23	45:Lr:83:ILE:HD11	1.82	0.60
49:S2:1455:A:OP1	74:Sc:49:LYS:NZ	2.35	0.60
62:SQ:80:GLY:HA2	62:SQ:83:ASN:HB2	1.83	0.60
3:L5:374:G:OP2	40:Lm:56:ARG:NH2	2.26	0.60
3:L5:382:G:N1	3:L5:385:A:OP2	2.31	0.60
24:LW:143:THR:OG1	24:LW:146:LYS:O	2.20	0.60
49:S2:1143:G:N2	49:S2:1146:A:OP2	2.35	0.60
60:SO:31:GLU:HA	60:SO:107:TYR:HE2	1.66	0.60
3:L5:4636:G:N2	3:L5:4663:C:O2	2.34	0.60
49:S2:825:C:H1'	66:SU:144:ILE:HG21	1.83	0.60
64:SS:58:LYS:HB2	64:SS:90:LYS:HG2	1.84	0.60
3:L5:2718:C:OP2	45:Lr:7:LYS:NZ	2.34	0.60
3:L5:4026:A:N6	9:LG:28:THR:O	2.33	0.60
12:LJ:257:LYS:O	12:LJ:261:LEU:N	2.30	0.60
24:LW:79:GLN:HA	24:LW:84:ILE:HG22	1.83	0.60
31:Ld:39:HIS:O	31:Ld:42:ARG:N	2.33	0.60
49:S2:98:C:OP2	49:S2:427:A:O2'	2.20	0.60
57:SL:77:ILE:HB	57:SL:124:VAL:HG12	1.84	0.60
59:SN:106:VAL:HG12	59:SN:128:VAL:HG12	1.84	0.60
1:B:448:VAL:HG11	52:SD:119:ARG:HH12	1.67	0.60
3:L5:266:C:O3'	38:Lk:109:ARG:NH2	2.34	0.60
3:L5:3415:C:OP1	6:LD:132:ASN:ND2	2.35	0.60
10:LH:179:THR:HG22	10:LH:181:PRO:HA	1.84	0.60
33:Lf:6:LYS:HA	33:Lf:9:LYS:HB2	1.84	0.60
3:L5:1293:G:H5'	21:LT:19:LYS:HD2	1.82	0.60
3:L5:4335:A:N1	3:L5:4367:C:O2'	2.32	0.60
16:LO:56:ARG:NH1	16:LO:74:ARG:O	2.35	0.60
29:Lb:34:LEU:HD23	29:Lb:38:LEU:HB3	1.84	0.60
49:S2:53:C:O2'	49:S2:508:G:N7	2.34	0.60
58:SM:122:GLU:HG2	58:SM:140:VAL:HG22	1.84	0.60
3:L5:4516:G:P	19:LR:176:ARG:HH21	2.24	0.60
6:LD:20:VAL:HG23	6:LD:23:ARG:HD2	1.83	0.60
10:LH:200:THR:HG22	10:LH:202:THR:H	1.66	0.60
49:S2:346:U:O2	61:SP:33:THR:OG1	2.18	0.60
49:S2:923:A:OP2	79:Sh:3:ARG:NH1	2.22	0.60
75:Sd:60:THR:OG1	75:Sd:62:ASP:OD1	2.20	0.60
1:B:448:VAL:HG22	52:SD:148:TYR:HB3	0.71	0.60
1:B:726:VAL:HG22	1:B:766:THR:HG21	1.84	0.60
3:L5:24:G:OP2	40:Lm:46:LYS:NZ	2.33	0.60
17:LP:30:VAL:HG11	23:LV:150:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:497:C:OP1	61:SP:49:ARG:NH2	2.31	0.60
64:SS:140:VAL:HG12	70:SY:19:ARG:HD3	1.83	0.60
3:L5:1741:A:O2'	3:L5:1776:A:OP1	2.20	0.60
3:L5:4036:U:OP2	44:Lq:8:ARG:NH2	2.35	0.60
3:L5:4645:C:O2	3:L5:4655:G:N2	2.34	0.60
21:LT:66:MET:HE1	21:LT:100:VAL:HG13	1.84	0.60
49:S2:521:A:O2'	49:S2:826:A:N3	2.31	0.60
55:SG:249:CYS:SG	55:SG:291:TRP:NE1	2.75	0.60
57:SL:63:ARG:HH21	78:Sg:38:GLU:HA	1.66	0.60
58:SM:137:LEU:HD11	58:SM:176:VAL:HG21	1.84	0.60
3:L5:1078:G:O2'	9:LG:272:SER:OG	2.19	0.59
3:L5:1741:A:H5''	3:L5:1742:G:H5'	1.84	0.59
3:L5:4068:G:N2	3:L5:4071:A:OP2	2.34	0.59
17:LP:40:GLY:HA3	17:LP:45:VAL:HB	1.84	0.59
30:Lc:59:LYS:HZ3	30:Lc:60:LYS:HE3	1.67	0.59
59:SN:199:PRO:HG3	66:SU:58:ARG:HE	1.67	0.59
60:SO:177:LEU:HD23	60:SO:182:LEU:HD13	1.84	0.59
60:SO:213:PRO:HG3	74:Sc:19:LYS:HD3	1.83	0.59
62:SQ:24:SER:O	62:SQ:107:ASN:ND2	2.30	0.59
62:SQ:35:LEU:HD12	62:SQ:117:ILE:HG22	1.83	0.59
73:Sb:31:LEU:HD21	73:Sb:33:LYS:HE2	1.83	0.59
3:L5:1955:C:H2'	3:L5:1956:A:H8	1.66	0.59
8:LF:140:LYS:HE3	8:LF:245:HIS:HB2	1.84	0.59
21:LT:50:ARG:HB3	21:LT:83:VAL:HG21	1.83	0.59
49:S2:1675:G:H4'	62:SQ:77:MET:HE1	1.84	0.59
13:LK:50:LYS:O	13:LK:53:LYS:NZ	2.35	0.59
29:Lb:123:ALA:O	29:Lb:127:GLN:NE2	2.36	0.59
65:ST:80:ASP:OD1	65:ST:81:VAL:N	2.35	0.59
65:ST:199:LEU:HD13	65:ST:202:ILE:HD11	1.84	0.59
3:L5:239:C:OP1	29:Lb:46:SER:OG	2.20	0.59
3:L5:1131:G:N2	3:L5:1210:C:N3	2.50	0.59
3:L5:2032:G:O2'	3:L5:2100:C:N4	2.35	0.59
22:LU:44:LEU:HD22	22:LU:49:LEU:HD12	1.84	0.59
49:S2:1257:G:O5'	56:SH:40:ARG:NH1	2.35	0.59
49:S2:1379:A:H61	57:SL:109:THR:HG21	1.65	0.59
49:S2:1551:G:H3'	49:S2:1580:A:H61	1.68	0.59
49:S2:1663:U:O4	49:S2:1664:A:N6	2.35	0.59
3:L5:85:G:O2'	3:L5:97:G:O6	2.18	0.59
3:L5:1829:G:OP2	3:L5:1829:G:N2	2.35	0.59
3:L5:4442:C:O2'	43:Lp:106:ARG:NH1	2.35	0.59
8:LF:187:GLN:NE2	8:LF:203:GLN:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SQ:38:TYR:HD2	62:SQ:143:PRO:HB2	1.67	0.59
2:I:106:U:O2'	2:I:107:A:OP1	2.20	0.59
2:I:144:G:H1'	2:I:145:C:H4'	1.83	0.59
3:L5:2161:G:N2	3:L5:2164:G:OP2	2.31	0.59
3:L5:3352:G:OP1	3:L5:3354:C:N4	2.34	0.59
8:LF:14:LYS:HA	8:LF:173:LYS:HD3	1.84	0.59
8:LF:159:GLU:OE2	8:LF:215:ASN:N	2.28	0.59
15:LM:144:LYS:O	15:LM:148:THR:OG1	2.20	0.59
49:S2:1446:PSU:O2	49:S2:1447:A:N6	2.36	0.59
68:SW:119:ASP:O	68:SW:147:LYS:NZ	2.27	0.59
77:Sf:35:VAL:HG21	77:Sf:110:VAL:HG11	1.84	0.59
3:L5:1479:A2M:HM'1	3:L5:4134:A:H1'	1.85	0.59
3:L5:2149:G:OP1	35:Lh:128:ARG:NH2	2.36	0.59
3:L5:3455:A:H2'	3:L5:3456:A2M:H8	1.84	0.59
55:SG:214:GLY:HA2	55:SG:236:ILE:HG12	1.83	0.59
3:L5:3789:U:H2'	3:L5:3790:A:H8	1.68	0.59
16:LO:25:TRP:HE1	18:LQ:199:GLN:HG3	1.68	0.59
80:Si:3:LYS:HG3	80:Si:5:ARG:HE	1.68	0.59
3:L5:2039:G:OP1	8:LF:306:ARG:NH1	2.36	0.59
3:L5:3374:A:O2'	40:Lm:2:THR:N	2.33	0.59
3:L5:4416:C:H2'	26:LY:15:ARG:HH22	1.67	0.59
18:LQ:8:GLN:OE1	18:LQ:12:ARG:NH2	2.35	0.59
69:SX:20:GLU:HA	69:SX:23:LYS:HD2	1.84	0.59
2:I:44:G:H1'	2:I:84:A:H61	1.68	0.59
2:I:161:A:H2'	2:I:162:A:C8	2.38	0.59
3:L5:1458:A:H4'	3:L5:1459:G:H5'	1.85	0.59
3:L5:2499:U:H5''	30:Lc:38:TYR:HB3	1.85	0.59
3:L5:3479:A:C8	6:LD:245:ARG:HD2	2.38	0.59
3:L5:3707:C:H42	3:L5:3764:G:H1	1.49	0.59
49:S2:1345:A:N1	49:S2:1386:G:O2'	2.36	0.59
55:SG:120:ILE:HB	55:SG:132:TRP:HB2	1.84	0.59
72:Sa:123:TYR:OH	75:Sd:124:ARG:NH1	2.35	0.59
1:B:691:CYS:HB3	1:B:749:ILE:HD11	1.84	0.58
2:I:43:U:H3	2:I:86:U:H1'	1.66	0.58
2:I:104:G:N2	2:I:135:C:O2	2.36	0.58
3:L5:4327:G:OP2	7:LE:28:LYS:NZ	2.36	0.58
7:LE:41:VAL:HA	7:LE:187:GLY:HA3	1.85	0.58
49:S2:1465:C:H5'	74:Sc:60:ARG:NH2	2.18	0.58
68:SW:68:ILE:HG21	68:SW:143:LEU:HD11	1.85	0.58
3:L5:757:A:N6	3:L5:795:A:N1	2.50	0.58
3:L5:1892:U:OP2	23:LV:139:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2139:G:OP2	8:LF:190:ARG:NH2	2.36	0.58
17:LP:101:LYS:HA	17:LP:104:MET:HE3	1.84	0.58
30:Lc:89:ILE:HD12	30:Lc:90:PRO:HD2	1.85	0.58
49:S2:1550:U:OP1	56:SH:34:TYR:OH	2.17	0.58
54:SF:74:CYS:SG	54:SF:76:SER:OG	2.60	0.58
69:SX:36:ARG:HG3	69:SX:40:LYS:HE3	1.85	0.58
2:I:53:U:O2'	2:I:129:G:O2'	2.12	0.58
3:L5:1860:C:O2'	23:LV:160:ARG:NH1	2.36	0.58
3:L5:2471:U:OP1	25:LX:93:LYS:NZ	2.36	0.58
3:L5:3669:C:H1'	18:LQ:125:SER:HB3	1.84	0.58
5:L8:134:G:H5''	28:La:63:LYS:HD2	1.86	0.58
13:LK:56:ARG:NH2	13:LK:58:ASP:OD2	2.36	0.58
20:LS:39:MET:HE2	20:LS:43:LYS:HE2	1.84	0.58
49:S2:360:U:OP2	80:Si:18:ARG:NH1	2.35	0.58
49:S2:1851:MA6:N6	49:S2:1852:MA6:H103	2.18	0.58
58:SM:92:GLN:NE2	58:SM:229:MET:SD	2.76	0.58
71:SZ:53:ILE:HD13	71:SZ:90:ILE:HD11	1.85	0.58
3:L5:303:C:OP2	18:LQ:68:ARG:NH2	2.36	0.58
3:L5:1067:C:O2	3:L5:1076:G:N2	2.32	0.58
18:LQ:146:PRO:HB2	38:Lk:104:THR:HG23	1.85	0.58
35:Lh:38:PRO:HG2	35:Lh:46:ARG:HB3	1.85	0.58
49:S2:74:G:H2'	49:S2:75:G:H8	1.68	0.58
49:S2:126:G:OP2	63:SR:195:LYS:NZ	2.36	0.58
65:ST:141:ARG:HB2	65:ST:146:GLN:HG2	1.84	0.58
1:B:443:LYS:CB	52:SD:144:CYS:O	2.52	0.58
3:L5:2038:C:H3'	8:LF:308:LYS:HZ3	1.68	0.58
5:L8:141:C:OP1	18:LQ:38:ARG:NH1	2.36	0.58
13:LK:114:ILE:HB	13:LK:124:ARG:HB2	1.86	0.58
46:Ls:65:LYS:NZ	46:Ls:70:GLN:OE1	2.36	0.58
49:S2:1392:OMC:HM22	49:S2:1393:U:H5'	1.84	0.58
57:SL:50:ASN:HD22	57:SL:53:ARG:HH11	1.50	0.58
64:SS:39:GLN:HG3	64:SS:75:ILE:HD13	1.84	0.58
69:SX:52:LEU:HB2	69:SX:76:LEU:HD11	1.85	0.58
77:Sf:98:VAL:HG13	77:Sf:101:ILE:HD12	1.84	0.58
3:L5:43:U:H5''	18:LQ:85:VAL:HG13	1.85	0.58
3:L5:1093:C:H2'	3:L5:1094:A:C8	2.38	0.58
23:LV:82:LEU:HG	23:LV:93:MET:HB3	1.86	0.58
58:SM:72:ALA:HB3	71:SZ:128:ARG:HH12	1.68	0.58
70:SY:5:HIS:HB3	70:SY:117:LEU:HD23	1.86	0.58
3:L5:716:G:OP1	3:L5:835:G:N1	2.35	0.58
1:B:446:LEU:HD23	52:SD:147:THR:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:115:A:H1'	62:SQ:198:ARG:NH2	2.19	0.58
3:L5:513:C:OP2	16:LO:163:LYS:NZ	2.37	0.58
3:L5:1449:U:H2'	3:L5:1450:G:H8	1.68	0.58
3:L5:3830:C:N3	3:L5:3837:G:N2	2.52	0.58
18:LQ:165:THR:HG23	18:LQ:168:GLY:H	1.69	0.58
22:LU:173:ARG:NH2	49:S2:911:G:OP2	2.35	0.58
49:S2:1398:U:OP2	49:S2:1398:U:H6	1.86	0.58
69:SX:91:LEU:HG	69:SX:106:CYS:HB2	1.85	0.58
3:L5:279:A:C5	18:LQ:12:ARG:HD2	2.39	0.58
3:L5:1388:A:N6	3:L5:1406:G:O2'	2.36	0.58
55:SG:152:SER:H	55:SG:169:GLY:HA2	1.68	0.58
81:Sj:34:THR:HG22	81:Sj:62:THR:HG21	1.84	0.58
3:L5:734:G:OP2	17:LP:71:LYS:NZ	2.29	0.58
3:L5:3347:G:H1'	27:LZ:44:ARG:HE	1.68	0.58
3:L5:4061:A:OP1	24:LW:69:GLN:NE2	2.37	0.58
3:L5:4682:A:OP1	10:LH:157:THR:OG1	2.21	0.58
70:SY:47:PRO:HD2	70:SY:86:GLU:OE1	2.04	0.58
75:Sd:36:VAL:HG23	75:Sd:40:TYR:HB3	1.86	0.58
3:L5:856:A:H1'	3:L5:2015:G:H5''	1.85	0.57
49:S2:1260:A:N6	49:S2:1520:U:OP1	2.37	0.57
49:S2:1662:A:OP1	56:SH:19:ARG:NH2	2.36	0.57
59:SN:90:GLU:HB2	59:SN:93:ILE:HG13	1.85	0.57
61:SP:211:LYS:HE3	61:SP:215:GLY:HA2	1.86	0.57
3:L5:400:A2M:OP1	20:LS:4:TYR:OH	2.19	0.57
3:L5:460:C:H42	3:L5:689:G:H1	1.52	0.57
3:L5:1757:G:N2	3:L5:1757:G:OP2	2.34	0.57
3:L5:1810:A2M:HM'2	3:L5:1811:G:H5'	1.87	0.57
3:L5:2738:A:H5''	22:LU:136:ARG:HH22	1.69	0.57
32:Le:65:MET:O	32:Le:68:ARG:NH1	2.37	0.57
58:SM:62:LEU:O	58:SM:88:THR:OG1	2.20	0.57
58:SM:138:PHE:O	58:SM:213:ARG:N	2.37	0.57
60:SO:74:GLN:NE2	60:SO:79:PHE:O	2.36	0.57
3:L5:2652:G:O2'	3:L5:4390:G:OP1	2.21	0.57
7:LE:213:GLN:NE2	7:LE:285:TYR:O	2.33	0.57
72:Sa:37:TYR:HB3	72:Sa:41:GLN:HB2	1.85	0.57
77:Sf:23:THR:HB	77:Sf:113:GLU:HB3	1.86	0.57
1:B:686:LEU:HD21	72:Sa:32:GLN:OE1	2.04	0.57
3:L5:1215:G:H5''	32:Le:110:ALA:HB1	1.86	0.57
7:LE:283:LYS:HE3	7:LE:363:ILE:HD11	1.85	0.57
13:LK:4:ILE:HB	23:LV:144:GLN:HE22	1.69	0.57
46:Ls:98:ARG:HH12	46:Ls:107:ARG:HH21	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:629:A:N6	49:S2:1501:G:O2'	2.38	0.57
49:S2:963:A:N1	49:S2:1056:A:O2'	2.36	0.57
49:S2:1180:G:N2	49:S2:1183:A:OP2	2.36	0.57
57:SL:74:VAL:HG12	57:SL:121:LEU:HB3	1.86	0.57
59:SN:187:ARG:HE	59:SN:192:LEU:HD12	1.67	0.57
59:SN:191:VAL:HG11	59:SN:236:PHE:HA	1.86	0.57
3:L5:2653:U:H5''	22:LU:70:ARG:HH22	1.68	0.57
48:S:1147:C:H2'	48:S:1148:A:C8	2.40	0.57
3:L5:2301:C:H5''	18:LQ:67:ARG:HD2	1.86	0.57
5:L8:153:C:OP1	12:LJ:185:LYS:NZ	2.37	0.57
61:SP:112:HIS:NE2	61:SP:237:SER:O	2.37	0.57
3:L5:1085:G:H2'	3:L5:1086:G:N7	2.19	0.57
49:S2:571:C:O2	81:Sj:34:THR:OG1	2.20	0.57
49:S2:1453:A:O2'	49:S2:1476:G:N2	2.38	0.57
72:Sa:49:LEU:HD22	72:Sa:53:GLN:HG3	1.85	0.57
2:I:44:G:H1'	2:I:84:A:N6	2.19	0.57
3:L5:327:U:O2'	39:Ll:30:ARG:NH1	2.38	0.57
3:L5:1085:G:H2'	3:L5:1086:G:C8	2.40	0.57
3:L5:3640:A:N7	3:L5:4195:A:N6	2.53	0.57
16:LO:16:LYS:NZ	18:LQ:196:ASN:OD1	2.30	0.57
31:Ld:126:ALA:HB3	31:Ld:129:PHE:CE1	2.40	0.57
3:L5:198:A:OP1	29:Lb:126:ARG:NH2	2.37	0.57
55:SG:80:SER:OG	55:SG:90:TRP:NE1	2.36	0.57
3:L5:48:G:OP1	18:LQ:192:TRP:NE1	2.34	0.57
3:L5:2251:U:OP2	42:Lo:42:ARG:NH2	2.37	0.57
3:L5:2699:C:O2	7:LE:242:ARG:NH2	2.38	0.57
3:L5:4636:G:N1	3:L5:4637:G:N3	2.53	0.57
18:LQ:116:LEU:HD22	18:LQ:135:ILE:HD11	1.85	0.57
24:LW:46:GLY:O	24:LW:49:GLN:NE2	2.37	0.57
37:Lj:5:LEU:HD21	37:Lj:30:ILE:HG13	1.86	0.57
38:Lk:73:TYR:HB3	38:Lk:79:LYS:HG3	1.87	0.57
42:Lo:42:ARG:HH11	42:Lo:49:LEU:HD11	1.70	0.57
46:Ls:28:GLU:OE2	46:Ls:31:ASN:ND2	2.35	0.57
49:S2:467:G:H1'	63:SR:59:GLN:HE21	1.70	0.57
49:S2:1551:G:O2'	49:S2:1559:C:O2	2.22	0.57
51:SC:44:ARG:HH12	51:SC:63:ARG:HE	1.51	0.57
51:SC:59:LEU:HD21	62:SQ:122:ARG:HE	1.70	0.57
3:L5:1060:G:O6	3:L5:1085:G:N2	2.31	0.56
3:L5:2318:G:N2	28:La:51:THR:O	2.36	0.56
3:L5:4735:C:H4'	34:Lg:26:THR:HG23	1.86	0.56
9:LG:83:LEU:HB3	9:LG:88:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LZ:94:ARG:NE	63:SR:144:LEU:O	2.37	0.56
51:SC:57:THR:HB	62:SQ:146:ARG:HH22	1.70	0.56
62:SQ:50:PRO:HB3	62:SQ:69:VAL:HG12	1.87	0.56
65:ST:130:THR:OG1	65:ST:132:GLU:OE1	2.18	0.56
66:SU:78:LEU:HD23	66:SU:97:ILE:HD11	1.85	0.56
3:L5:1127:G:O2'	32:Le:120:ARG:O	2.23	0.56
3:L5:1452:A:N6	21:LT:175:GLU:O	2.37	0.56
3:L5:3812:G:O6	6:LD:72:ARG:NH2	2.38	0.56
3:L5:4350:G:N2	3:L5:4353:A:OP2	2.38	0.56
5:L8:78:G:O2'	38:Lk:45:SER:OG	2.22	0.56
48:S:1128:A:H62	48:S:1144:G:H22	1.51	0.56
49:S2:319:A:N1	63:SR:186:GLN:NE2	2.45	0.56
1:B:460:GLU:HG3	1:B:464:HIS:HE1	1.69	0.56
2:I:38:G:O6	2:I:87:G:N2	2.38	0.56
4:L7:55:A:O2'	15:LM:151:ILE:O	2.19	0.56
8:LF:94:ASN:HD22	8:LF:102:PHE:HB2	1.70	0.56
9:LG:40:ASP:HB3	9:LG:43:LYS:HG3	1.87	0.56
11:LI:189:LEU:HD21	11:LI:207:LEU:HD21	1.88	0.56
19:LR:81:TRP:HB2	19:LR:104:VAL:HG21	1.88	0.56
27:LZ:90:ILE:O	27:LZ:94:ARG:N	2.38	0.56
35:Lh:78:LEU:O	46:Ls:20:ARG:NH1	2.39	0.56
49:S2:115:U:O2'	49:S2:382:C:O2	2.20	0.56
49:S2:1311:U:OP1	69:SX:36:ARG:NH2	2.39	0.56
49:S2:1399:G:O3'	55:SG:88:ARG:NH2	2.39	0.56
49:S2:1766:C:H1'	49:S2:1769:A:H61	1.70	0.56
61:SP:124:CYS:HB3	61:SP:141:THR:HB	1.86	0.56
75:Sd:27:ALA:HB2	75:Sd:52:LEU:HD12	1.88	0.56
77:Sf:55:ARG:CZ	77:Sf:87:ARG:HH12	2.19	0.56
80:Si:67:ARG:NH2	80:Si:114:ASP:OD2	2.38	0.56
3:L5:1822:G:O2'	35:Lh:48:ARG:O	2.21	0.56
3:L5:3591:G:OP2	20:LS:25:HIS:NE2	2.33	0.56
3:L5:3820:G:H2'	3:L5:3821:G:C8	2.40	0.56
3:L5:4679:C:OP1	10:LH:159:ARG:NH2	2.39	0.56
8:LF:67:TRP:HB3	8:LF:71:ARG:HD3	1.87	0.56
49:S2:468:G:O5'	63:SR:72:ARG:NH2	2.38	0.56
49:S2:1398:U:H5''	49:S2:1399:G:H5'	1.88	0.56
58:SM:71:LEU:HD11	58:SM:189:ILE:HG23	1.87	0.56
3:L5:175:C:H2'	3:L5:176:G:H8	1.70	0.56
3:L5:308:G:H5'	39:Ll:85:ARG:HH12	1.70	0.56
3:L5:440:U:O2'	36:Li:91:ASN:O	2.23	0.56
3:L5:2363:C:H1'	3:L5:2483:G:H21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L8:85:U:O4	29:Lb:50:ARG:NH2	2.37	0.56
6:LD:206:PRO:HG3	6:LD:213:GLY:HA3	1.88	0.56
16:LO:150:LEU:HD23	16:LO:154:VAL:HG12	1.86	0.56
17:LP:104:MET:HE2	19:LR:199:HIS:HB3	1.86	0.56
49:S2:237:C:O2	49:S2:893:U:N3	2.38	0.56
49:S2:397:U:H1'	65:ST:14:THR:HG23	1.87	0.56
49:S2:1014:U:OP1	49:S2:1130:G:O2'	2.24	0.56
63:SR:227:GLN:HA	63:SR:230:LYS:HE2	1.87	0.56
65:ST:116:HIS:O	65:ST:152:ARG:NH2	2.39	0.56
73:Sb:34:VAL:HB	73:Sb:70:VAL:HG23	1.87	0.56
3:L5:484:G:H3'	3:L5:485:U:H2'	1.88	0.56
3:L5:3432:C:O2'	3:L5:3506:A:N3	2.34	0.56
9:LG:280:VAL:HG13	14:LL:206:LEU:HD21	1.88	0.56
35:Lh:99:ILE:HG22	35:Lh:103:VAL:HG11	1.85	0.56
49:S2:125:C:O5'	63:SR:198:ARG:NH2	2.38	0.56
58:SM:144:LYS:HD3	58:SM:208:HIS:HB3	1.87	0.56
80:Si:46:HIS:HB3	80:Si:101:LEU:HD11	1.87	0.56
2:I:134:C:H2'	2:I:135:C:H4'	1.86	0.56
3:L5:1065:G:H2'	3:L5:1066:A:C8	2.41	0.56
3:L5:1065:G:H2'	3:L5:1066:A:H8	1.71	0.56
3:L5:1942:G:N2	3:L5:1943:U:O4	2.36	0.56
7:LE:14:LEU:HA	7:LE:17:LEU:HD13	1.88	0.56
13:LK:59:LYS:HE2	13:LK:66:GLU:HB3	1.88	0.56
55:SG:11:LEU:N	55:SG:307:VAL:O	2.35	0.56
60:SO:126:ILE:HG21	60:SO:188:ILE:HD12	1.86	0.56
3:L5:4636:G:O2'	3:L5:4666:G:N7	2.38	0.56
22:LU:42:ARG:HA	22:LU:45:ILE:HD12	1.88	0.56
49:S2:152:U:O4'	63:SR:132:ARG:NH1	2.39	0.56
49:S2:528:C:O3'	66:SU:121:LYS:NZ	2.39	0.56
49:S2:660:G:H21	80:Si:17:ARG:HH22	1.52	0.56
49:S2:1338:4AC:H2'	49:S2:1339:G:C8	2.41	0.56
49:S2:1396:C:O2'	49:S2:1397:A:H5'	2.06	0.56
49:S2:1598:C:OP2	82:Sk:85:ARG:NH2	2.39	0.56
65:ST:90:LEU:HD12	65:ST:95:THR:HG21	1.88	0.56
3:L5:338:A:OP1	16:LO:31:ARG:NH2	2.39	0.56
3:L5:2651:G:O3'	22:LU:60:ARG:NH1	2.39	0.56
3:L5:4611:G:OP2	17:LP:94:LYS:NZ	2.35	0.56
8:LF:159:GLU:HG3	8:LF:215:ASN:HB2	1.88	0.56
11:LI:154:TYR:OH	11:LI:187:GLU:OE2	2.24	0.56
59:SN:196:ILE:HB	59:SN:223:TYR:HB2	1.87	0.56
71:SZ:74:ALA:HB1	71:SZ:115:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:HG22	52:SD:148:TYR:CA	2.34	0.56
3:L5:1011:C:H2'	3:L5:1012:C:C6	2.41	0.56
13:LK:20:LEU:HD13	13:LK:47:LEU:HD23	1.88	0.56
25:LX:40:GLU:HB2	25:LX:65:ARG:HD3	1.87	0.56
28:La:91:GLU:HA	28:La:147:LEU:HD21	1.87	0.56
34:Lg:19:GLU:OE1	34:Lg:92:ARG:NH1	2.39	0.56
49:S2:231:A:H2'	49:S2:232:A:C8	2.41	0.56
49:S2:374:G:OP1	68:SW:135:SER:OG	2.20	0.56
49:S2:926:G:OP1	70:SY:121:ARG:NH1	2.39	0.56
77:Sf:22:ILE:HB	77:Sf:89:ILE:HB	1.87	0.56
82:Sk:79:ILE:HB	82:Sk:83:LEU:HD23	1.88	0.56
3:L5:1004:G:H1'	11:LI:73:MET:HE2	1.88	0.55
9:LG:272:SER:OG	9:LG:275:GLN:OE1	2.21	0.55
58:SM:152:LYS:HD3	74:Sc:133:GLY:HA3	1.87	0.55
58:SM:189:ILE:HB	58:SM:190:PRO:HD3	1.88	0.55
62:SQ:70:GLU:O	62:SQ:74:ASN:ND2	2.39	0.55
82:Sk:111:ARG:HD2	82:Sk:114:LYS:HE3	1.87	0.55
3:L5:3819:G:N2	3:L5:3905:C:N3	2.54	0.55
3:L5:4213:A:O2'	3:L5:4256:A:N3	2.37	0.55
7:LE:285:TYR:CD1	7:LE:363:ILE:HD13	2.42	0.55
49:S2:847:G:H1	61:SP:51:ARG:HH22	1.55	0.55
61:SP:247:THR:N	61:SP:250:GLU:OE1	2.39	0.55
62:SQ:38:TYR:CD2	62:SQ:143:PRO:HB2	2.41	0.55
3:L5:2233:G:H22	3:L5:2668:A:H2	1.55	0.55
7:LE:312:LYS:HD2	7:LE:370:THR:HG21	1.87	0.55
13:LK:173:ARG:NH1	43:Lp:125:LYS:O	2.35	0.55
31:Ld:37:GLY:HA3	31:Ld:53:PHE:HZ	1.71	0.55
55:SG:29:ASP:OD1	55:SG:47:ARG:NH1	2.38	0.55
1:B:637:LEU:HD21	1:B:696:PRO:HG3	1.88	0.55
3:L5:1392:C:OP2	32:Le:106:ARG:NH1	2.38	0.55
3:L5:1697:G:H2'	3:L5:1698:G:H8	1.70	0.55
3:L5:2148:U:O2'	35:Lh:104:SER:OG	2.18	0.55
3:L5:3422:U:O2'	3:L5:3549:A:N3	2.35	0.55
49:S2:1383:A:H2'	49:S2:1384:A2M:H8	1.88	0.55
55:SG:39:THR:HG22	55:SG:60:ARG:HG2	1.87	0.55
55:SG:167:SER:OG	55:SG:177:TRP:NE1	2.25	0.55
74:Sc:106:LEU:HA	74:Sc:109:LEU:HB2	1.88	0.55
75:Sd:22:GLY:HA2	75:Sd:56:ALA:HB3	1.88	0.55
3:L5:109:G:OP2	16:LO:74:ARG:NH2	2.40	0.55
23:LV:161:ARG:HD2	23:LV:164:LYS:HG3	1.89	0.55
30:Lc:11:VAL:HG12	30:Lc:82:PRO:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S:1110:C:O2'	48:S:1155:A:N6	2.40	0.55
49:S2:822:G:H22	66:SU:148:ILE:HG23	1.71	0.55
49:S2:1329:OMG:HM22	49:S2:1330:U:H5'	1.88	0.55
49:S2:1547:G:H21	49:S2:1671:C:H1'	1.72	0.55
3:L5:1353:G:H2'	3:L5:1354:G:C8	2.41	0.55
3:L5:4745:U:H4'	3:L5:4746:A:H5'	1.89	0.55
9:LG:63:GLN:HB3	9:LG:74:ILE:HD13	1.89	0.55
10:LH:193:HIS:HB3	10:LH:196:PHE:HD2	1.70	0.55
11:LI:154:TYR:HA	11:LI:186:MET:HE1	1.88	0.55
18:LQ:113:LEU:HD22	18:LQ:136:ASP:HA	1.87	0.55
21:LT:176:ARG:O	21:LT:181:ARG:NH1	2.40	0.55
33:Lf:11:LEU:HD13	33:Lf:75:SER:HB2	1.88	0.55
49:S2:318:C:OP2	63:SR:183:ARG:NH2	2.39	0.55
55:SG:175:LYS:HG3	55:SG:187:ASN:HA	1.89	0.55
62:SQ:25:THR:OG1	62:SQ:41:VAL:O	2.25	0.55
3:L5:1351:G:N1	3:L5:1366:C:O2	2.39	0.55
3:L5:1580:OMG:HM23	18:LQ:81:TYR:HE1	1.70	0.55
3:L5:2459:C:OP1	22:LU:64:ARG:NH1	2.40	0.55
3:L5:3347:G:OP2	27:LZ:48:GLN:NE2	2.40	0.55
16:LO:203:ALA:O	16:LO:207:VAL:N	2.34	0.55
44:Lq:34:TYR:O	44:Lq:39:ARG:NH1	2.37	0.55
49:S2:381:G:OP1	65:ST:56:ARG:NH2	2.39	0.55
49:S2:746:C:H42	49:S2:798:C:H42	1.54	0.55
52:SD:102:VAL:HA	52:SD:105:TYR:HD1	1.72	0.55
58:SM:164:ILE:O	58:SM:168:MET:N	2.40	0.55
59:SN:264:SER:H	59:SN:267:GLN:HE21	1.54	0.55
64:SS:134:VAL:O	64:SS:137:SER:OG	2.23	0.55
82:Sk:69:THR:HG23	82:Sk:71:ALA:H	1.71	0.55
1:B:463:GLN:HA	1:B:701:ILE:HG12	1.88	0.55
3:L5:2190:A:N3	35:Lh:30:LYS:NZ	2.55	0.55
15:LM:13:ARG:O	15:LM:136:ARG:NH1	2.40	0.55
20:LS:61:ARG:O	20:LS:64:ASN:ND2	2.40	0.55
49:S2:1513:C:H5''	56:SH:8:TRP:HZ3	1.71	0.55
57:SL:82:THR:HG22	57:SL:171:VAL:HG21	1.89	0.55
61:SP:15:PRO:HG3	61:SP:39:ARG:HD3	1.88	0.55
62:SQ:124:ASP:OD1	62:SQ:125:SER:N	2.34	0.55
65:ST:101:ILE:HD12	65:ST:190:LEU:HD21	1.87	0.55
77:Sf:40:ILE:HG13	77:Sf:50:VAL:HG21	1.88	0.55
3:L5:66:A:O2'	3:L5:326:C:O2	2.24	0.55
3:L5:2330:G:H1'	5:L8:125:C:H1'	1.89	0.55
3:L5:3351:G:H22	3:L5:3356:A:H1'	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4269:A2M:O2'	7:LE:246:ARG:NH1	2.39	0.55
3:L5:4278:PSU:OP2	3:L5:4300:G:N1	2.39	0.55
27:LZ:52:THR:HG23	27:LZ:55:TYR:H	1.72	0.55
48:S:1136:C:N4	48:S:1139:U:O4'	2.39	0.55
49:S2:1399:G:C5'	55:SG:61:GLY:HA2	2.37	0.55
49:S2:1832:A:H2'	49:S2:1833:6MZ:H8	1.89	0.55
52:SD:126:CYS:HB2	52:SD:130:VAL:HG21	1.89	0.55
61:SP:85:GLY:N	61:SP:88:ASP:OD2	2.32	0.55
71:SZ:31:CYS:HA	71:SZ:44:VAL:HA	1.87	0.55
3:L5:172:C:O2	38:Lk:112:ARG:NH1	2.40	0.55
3:L5:1866:U:OP1	3:L5:1888:U:O2'	2.19	0.55
6:LD:5:ILE:HG12	6:LD:8:GLN:HG2	1.88	0.55
40:Lm:48:ASN:HA	40:Lm:54:LYS:HZ3	1.72	0.55
51:SC:49:PRO:HG2	62:SQ:144:LEU:HD23	1.89	0.55
63:SR:57:ASP:OD1	63:SR:61:PHE:N	2.39	0.55
65:ST:12:ARG:NH1	65:ST:18:ARG:HH11	2.05	0.55
3:L5:1485:G:O6	3:L5:1598:A:N6	2.40	0.54
3:L5:2358:G:OP2	37:Lj:17:SER:OG	2.24	0.54
3:L5:2602:G:H1'	3:L5:2607:A:H2	1.71	0.54
4:L7:54:A:O3'	15:LM:154:LYS:NZ	2.40	0.54
6:LD:4:VAL:HG13	6:LD:8:GLN:HB2	1.88	0.54
48:S:1123:C:N3	48:S:1146:G:N1	2.55	0.54
57:SL:181:GLU:OE2	57:SL:191:ARG:NH2	2.38	0.54
70:SY:101:HIS:NE2	70:SY:108:ASP:OD2	2.29	0.54
76:Se:83:GLN:HB2	76:Se:93:SER:HB2	1.88	0.54
77:Sf:68:THR:OG1	77:Sf:70:CYS:O	2.18	0.54
3:L5:1091:G:H2'	3:L5:1092:U:C6	2.43	0.54
3:L5:4707:A:P	7:LE:120:LYS:HG2	2.47	0.54
10:LH:227:LYS:HZ2	10:LH:240:LYS:HD3	1.72	0.54
49:S2:861:G:N2	79:Sh:107:SER:HG	2.05	0.54
49:S2:1162:U:O4	80:Si:2:GLY:N	2.40	0.54
49:S2:1411:C:H2'	49:S2:1412:G:C8	2.42	0.54
3:L5:3403:G:OP1	18:LQ:72:LYS:NZ	2.40	0.54
3:L5:3811:U:OP1	6:LD:123:ARG:NH1	2.40	0.54
6:LD:133:TYR:HB3	6:LD:168:VAL:HG23	1.90	0.54
7:LE:94:GLU:HG2	19:LR:152:VAL:HG13	1.89	0.54
51:SC:49:PRO:HB2	62:SQ:61:PHE:CE2	2.43	0.54
52:SD:133:ALA:HB3	52:SD:140:TYR:HB3	1.87	0.54
3:L5:394:G:N2	3:L5:397:G:OP2	2.35	0.54
3:L5:1528:G:OP1	22:LU:92:LYS:NZ	2.41	0.54
3:L5:1827:A:N6	3:L5:3605:G:O2'	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1913:U:H3	3:L5:1941:A:H2	1.53	0.54
7:LE:35:ASP:OD2	7:LE:193:LYS:NZ	2.29	0.54
34:Lg:24:GLU:OE2	34:Lg:87:ARG:NH2	2.38	0.54
49:S2:694:A:H2'	49:S2:695:G:H8	1.72	0.54
3:L5:194:C:O2'	29:Lb:121:ARG:NH2	2.41	0.54
3:L5:424:U:OP1	20:LS:34:GLN:NE2	2.41	0.54
35:Lh:126:ASN:O	35:Lh:126:ASN:ND2	2.36	0.54
49:S2:282:C:N4	49:S2:892:G:O5'	2.41	0.54
49:S2:1666:G:H22	76:Se:87:VAL:HB	1.72	0.54
55:SG:238:ALA:H	55:SG:251:ALA:HB3	1.73	0.54
73:Sb:37:ARG:NH2	76:Se:11:GLN:OE1	2.41	0.54
74:Sc:28:PHE:HA	74:Sc:55:THR:HG21	1.90	0.54
3:L5:2653:U:OP1	22:LU:70:ARG:NH1	2.40	0.54
3:L5:4600:G:OP1	19:LR:169:ARG:NH2	2.41	0.54
3:L5:4632:A:OP1	19:LR:188:LYS:NZ	2.36	0.54
8:LF:262:ASP:OD1	8:LF:272:SER:OG	2.25	0.54
30:Lc:33:THR:OG1	30:Lc:35:ASP:OD1	2.25	0.54
68:SW:74:SER:HB2	68:SW:125:ILE:HD11	1.88	0.54
3:L5:3680:C:H2'	3:L5:3681:A:C8	2.43	0.54
16:LO:88:LYS:HG3	16:LO:89:LYS:HG3	1.90	0.54
23:LV:93:MET:SD	23:LV:95:ARG:NH2	2.81	0.54
37:Lj:105:LYS:O	37:Lj:109:ALA:N	2.38	0.54
49:S2:527:A:OP1	53:SE:109:ARG:NH2	2.30	0.54
71:SZ:101:GLY:HA3	71:SZ:134:PRO:HG2	1.90	0.54
3:L5:1308:U:OP2	16:LO:36:ARG:NH2	2.34	0.54
4:L7:26:C:O2'	15:LM:147:ARG:NH1	2.40	0.54
12:LJ:172:ALA:HB3	39:Ll:43:MET:HE1	1.89	0.54
55:SG:244:ASN:ND2	55:SG:294:ASP:O	2.41	0.54
55:SG:287:THR:N	55:SG:301:GLY:O	2.30	0.54
67:SV:21:MET:HG2	67:SV:49:MET:HE3	1.90	0.54
3:L5:459:C:H4'	10:LH:113:ARG:HH12	1.72	0.54
3:L5:835:G:OP1	17:LP:23:LYS:NZ	2.35	0.54
7:LE:95:THR:OG1	7:LE:98:GLY:O	2.22	0.54
21:LT:67:ILE:HG22	21:LT:98:LEU:HD11	1.90	0.54
40:Lm:22:CYS:HB3	40:Lm:37:CYS:HB3	1.90	0.54
49:S2:64:A:H2	49:S2:83:A:H62	1.56	0.54
49:S2:1571:G:N7	76:Se:97:LYS:NZ	2.48	0.54
49:S2:1598:C:N4	49:S2:1599:G:O6	2.40	0.54
62:SQ:32:ASP:OD2	62:SQ:34:SER:OG	2.21	0.54
69:SX:58:GLU:OE1	69:SX:61:TYR:N	2.37	0.54
3:L5:1217:G:OP2	32:Le:117:ARG:NE	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LI:86:PRO:HG2	11:LI:143:TYR:CG	2.43	0.54
31:Ld:137:ILE:HD11	31:Ld:144:CYS:HB2	1.89	0.54
49:S2:1017:U:H5''	70:SY:14:SER:HB2	1.89	0.54
58:SM:133:TYR:HD2	58:SM:217:MET:HE1	1.73	0.54
70:SY:93:LYS:HA	70:SY:150:VAL:HG21	1.90	0.54
11:LI:89:ALA:HB2	11:LI:124:LEU:HD21	1.90	0.53
23:LV:69:GLU:HG3	23:LV:101:THR:HG22	1.90	0.53
25:LX:100:LEU:HD12	25:LX:112:LEU:HB3	1.88	0.53
49:S2:283:G:O6	49:S2:892:G:O2'	2.26	0.53
49:S2:1284:C:H42	69:SX:102:LYS:HD3	1.73	0.53
49:S2:1513:C:O2'	56:SH:7:TYR:O	2.20	0.53
60:SO:106:ARG:HG3	60:SO:175:VAL:HB	1.90	0.53
66:SU:63:LEU:HD11	66:SU:69:ARG:HH21	1.73	0.53
73:Sb:19:ALA:HB2	73:Sb:75:GLY:HA3	1.90	0.53
75:Sd:34:LYS:HB3	75:Sd:103:LEU:HD23	1.89	0.53
3:L5:859:G:C8	10:LH:126:ARG:HG2	2.43	0.53
3:L5:1753:C:O2'	32:Le:42:ASN:OD1	2.23	0.53
3:L5:4270:G:OP1	3:L5:4305:A:N6	2.40	0.53
16:LO:130:LYS:HD2	16:LO:131:PRO:HD2	1.89	0.53
16:LO:189:ALA:HB2	39:Ll:10:GLY:HA2	1.90	0.53
21:LT:22:ASP:OD2	21:LT:25:LEU:N	2.33	0.53
23:LV:147:ASP:HB3	23:LV:150:ILE:HB	1.90	0.53
51:SC:54:ASP:OD1	51:SC:55:VAL:N	2.41	0.53
55:SG:216:ALA:N	55:SG:230:LEU:O	2.36	0.53
66:SU:170:PRO:O	66:SU:175:ARG:NH1	2.36	0.53
68:SW:125:ILE:HG23	68:SW:146:THR:HB	1.90	0.53
70:SY:86:GLU:HA	70:SY:89:TYR:HB3	1.90	0.53
3:L5:69:A:N1	3:L5:324:A:O2'	2.39	0.53
3:L5:1811:G:O2'	3:L5:3965:A:N3	2.40	0.53
3:L5:3513:C:OP1	83:Sl:19:LYS:NZ	2.41	0.53
35:Lh:37:LYS:HD3	35:Lh:38:PRO:HD2	1.90	0.53
47:Lx:86:ASP:H	47:Lx:89:ALA:HB3	1.74	0.53
49:S2:75:G:O2'	49:S2:77:A:OP1	2.26	0.53
49:S2:351:C:HO2'	49:S2:384:G:H1	1.56	0.53
49:S2:604:C:N4	49:S2:621:G:O6	2.42	0.53
57:SL:207:PRO:HA	57:SL:210:ILE:HB	1.90	0.53
59:SN:252:THR:OG1	59:SN:254:ASP:OD1	2.25	0.53
70:SY:50:ILE:HB	70:SY:71:ILE:HD11	1.89	0.53
3:L5:4219:A:OP1	43:Lp:124:LYS:NZ	2.41	0.53
33:Lf:87:LYS:NZ	33:Lf:89:TYR:OH	2.37	0.53
49:S2:1623:U:OP1	75:Sd:120:HIS:ND1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SO:132:LYS:NZ	60:SO:190:LEU:O	2.41	0.53
61:SP:80:ILE:HG13	61:SP:81:THR:HG23	1.90	0.53
80:Si:70:VAL:HG11	80:Si:94:ILE:HG21	1.90	0.53
2:I:99:U:OP1	2:I:100:U:O2'	2.12	0.53
3:L5:3353:A:O2'	3:L5:4404:G:O2'	2.23	0.53
3:L5:4004:C:H5'	15:LM:68:ILE:HD11	1.90	0.53
3:L5:4011:U:N3	9:LG:17:GLN:O	2.39	0.53
38:Lk:58:LEU:O	38:Lk:62:ASN:ND2	2.40	0.53
46:Ls:51:VAL:HG12	46:Ls:117:ILE:HD12	1.89	0.53
49:S2:230:A:H2	49:S2:899:U:H3	1.55	0.53
58:SM:129:THR:OG1	58:SM:131:ASP:OD1	2.25	0.53
79:Sh:26:LEU:HD21	79:Sh:60:LYS:HE3	1.91	0.53
2:I:57:A:H62	2:I:162:A:H1'	1.72	0.53
2:I:172:G:O2'	2:I:173:C:OP1	2.24	0.53
3:L5:12:A:H4'	28:La:53:ARG:HE	1.74	0.53
3:L5:1546:U:OP2	3:L5:2699:C:O2'	2.22	0.53
3:L5:3825:G:H2'	3:L5:3841:U:C4	2.44	0.53
7:LE:229:LYS:HG3	7:LE:272:LYS:HD3	1.89	0.53
11:LI:121:PHE:O	11:LI:204:ASN:ND2	2.31	0.53
15:LM:146:ARG:HG2	15:LM:147:ARG:HG3	1.91	0.53
16:LO:64:VAL:HA	16:LO:67:HIS:CD2	2.44	0.53
27:LZ:107:GLN:O	27:LZ:111:ALA:N	2.42	0.53
46:Ls:39:ARG:O	46:Ls:103:ARG:NH2	2.42	0.53
47:Lx:39:LYS:N	47:Lx:200:ASN:O	2.37	0.53
64:SS:135:PHE:CG	64:SS:136:PRO:HA	2.43	0.53
65:ST:103:LEU:HD12	65:ST:170:LYS:HB3	1.91	0.53
1:B:446:LEU:CD2	52:SD:147:THR:H	2.22	0.53
2:I:75:A:O2'	2:I:76:U:O5'	2.27	0.53
3:L5:17:A:OP1	38:Lk:84:ARG:NH2	2.35	0.53
3:L5:2161:G:O6	35:Lh:19:LYS:NZ	2.41	0.53
3:L5:4381:A:H3'	3:L5:4382:PSU:H4'	1.90	0.53
49:S2:917:A:C5	70:SY:73:ARG:HD3	2.43	0.53
49:S2:1684:C:H5'	62:SQ:130:ARG:HD2	1.90	0.53
58:SM:115:LYS:HB3	58:SM:118:GLN:HE21	1.74	0.53
65:ST:72:CYS:HG	65:ST:112:TRP:CG	2.26	0.53
3:L5:3804:G:OP1	12:LJ:73:ARG:NH2	2.35	0.53
3:L5:4340:U:H2'	3:L5:4341:G:H8	1.73	0.53
6:LD:147:ARG:HG2	6:LD:157:VAL:HG12	1.89	0.53
7:LE:78:ILE:HD13	7:LE:332:MET:HE1	1.90	0.53
21:LT:86:VAL:HB	21:LT:105:VAL:HG12	1.91	0.53
21:LT:105:VAL:O	21:LT:110:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1147:C:O2'	49:S2:1151:A:N1	2.42	0.53
49:S2:1299:G:H4'	72:Sa:78:THR:HA	1.91	0.53
57:SL:156:TYR:HE1	78:Sg:61:ARG:HD2	1.73	0.53
2:I:37:U:O2'	2:I:39:A:OP2	2.23	0.53
3:L5:251:C:H5'	40:Lm:85:LYS:HZ1	1.73	0.53
3:L5:423:G:N3	20:LS:118:GLN:NE2	2.57	0.53
3:L5:1584:G:OP2	6:LD:9:ARG:NH2	2.42	0.53
3:L5:2022:C:OP2	21:LT:14:ARG:NH2	2.41	0.53
6:LD:53:GLY:O	6:LD:192:LYS:NZ	2.37	0.53
48:S:1121:G:N2	48:S:1149:G:O6	2.41	0.53
49:S2:795:A:N1	49:S2:796:A:N6	2.57	0.53
55:SG:77:PHE:HB3	55:SG:89:LEU:HD11	1.91	0.53
59:SN:136:HIS:HB3	59:SN:162:ILE:HD11	1.91	0.53
62:SQ:39:ILE:HG23	62:SQ:68:ILE:HG13	1.89	0.53
75:Sd:65:GLU:HA	75:Sd:68:ILE:HD12	1.91	0.53
80:Si:67:ARG:HG3	80:Si:115:ILE:HG12	1.91	0.53
3:L5:231:U:H4'	29:Lb:100:HIS:CD2	2.43	0.53
3:L5:2177:C:OP2	8:LF:195:LYS:NZ	2.43	0.53
8:LF:13:GLU:HG3	8:LF:14:LYS:HD3	1.90	0.53
9:LG:264:LYS:NZ	9:LG:265:ARG:O	2.41	0.53
19:LR:125:LYS:HG3	19:LR:129:LEU:HD12	1.91	0.53
49:S2:1666:G:N2	76:Se:87:VAL:HB	2.24	0.53
49:S2:1842:C:H2'	49:S2:1843:4AC:H6	1.89	0.53
3:L5:51:A:N3	3:L5:1483:U:O2'	2.42	0.52
3:L5:184:U:H3	3:L5:253:G:H22	1.57	0.52
24:LW:115:LYS:HG2	24:LW:126:VAL:HG11	1.90	0.52
40:Lm:48:ASN:HA	40:Lm:54:LYS:NZ	2.24	0.52
45:Lr:51:ALA:H	45:Lr:54:ILE:HB	1.75	0.52
49:S2:1338:4AC:H2'	49:S2:1339:G:H8	1.74	0.52
58:SM:222:LYS:H	58:SM:222:LYS:HD2	1.74	0.52
61:SP:180:LEU:N	61:SP:231:GLY:O	2.42	0.52
3:L5:1013:G:N2	3:L5:1091:G:O5'	2.42	0.52
3:L5:1110:G:N1	3:L5:1111:G:O6	2.42	0.52
3:L5:1699:G:H2'	3:L5:1700:G:H8	1.75	0.52
11:LI:85:GLU:OE2	24:LW:136:ARG:N	2.39	0.52
49:S2:104:A:H4'	65:ST:18:ARG:HH12	1.74	0.52
49:S2:845:U:H2'	49:S2:846:G:H8	1.75	0.52
56:SH:23:VAL:HG21	56:SH:38:MET:HE3	1.90	0.52
61:SP:123:LEU:HD13	61:SP:236:ILE:HD11	1.90	0.52
65:ST:3:ILE:O	65:ST:30:GLY:N	2.41	0.52
3:L5:114:G:N2	3:L5:158:A:H61	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3386:G:O2'	3:L5:3425:U:OP1	2.21	0.52
15:LM:57:VAL:HG12	15:LM:60:PHE:H	1.74	0.52
18:LQ:97:SER:O	18:LQ:100:SER:OG	2.23	0.52
49:S2:1080:C:O2'	49:S2:1183:A:N1	2.41	0.52
49:S2:1651:A:H5''	73:Sb:139:ALA:HB2	1.91	0.52
52:SD:138:ARG:HA	52:SD:149:CYS:HA	1.91	0.52
3:L5:2712:U:O2'	3:L5:2724:A:N7	2.37	0.52
8:LF:221:PHE:HB3	8:LF:227:ILE:HG21	1.91	0.52
11:LI:66:THR:O	11:LI:70:MET:HG2	2.09	0.52
34:Lg:23:ARG:NH2	34:Lg:25:TYR:OH	2.40	0.52
55:SG:201:SER:OG	55:SG:203:ASP:OD1	2.22	0.52
59:SN:169:TYR:OH	59:SN:175:GLY:O	2.28	0.52
3:L5:877:C:O3'	11:LI:46:ARG:NH1	2.42	0.52
3:L5:1879:G:H22	3:L5:4180:C:H5''	1.75	0.52
3:L5:1924:G:OP1	3:L5:1924:G:N2	2.42	0.52
3:L5:2622:C:O2'	5:L8:112:G:OP1	2.18	0.52
3:L5:2736:U:O3'	65:ST:205:ARG:NH1	2.42	0.52
5:L8:102:G:OP2	5:L8:104:A:O2'	2.28	0.52
7:LE:285:TYR:HD1	7:LE:363:ILE:HD13	1.74	0.52
8:LF:39:PHE:O	8:LF:43:ASN:ND2	2.39	0.52
13:LK:44:GLU:HB2	13:LK:58:ASP:HB2	1.90	0.52
49:S2:355:OMU:OP1	68:SW:90:ARG:NH2	2.43	0.52
58:SM:224:GLU:OE1	58:SM:227:LYS:N	2.28	0.52
66:SU:46:VAL:HG11	66:SU:106:LEU:HD22	1.92	0.52
3:L5:1298:A:N6	3:L5:1458:A:O4'	2.42	0.52
3:L5:1299:G:OP1	21:LT:108:ARG:NH1	2.43	0.52
9:LG:33:ARG:HE	9:LG:37:VAL:HG11	1.74	0.52
41:Ln:8:ILE:HD11	41:Ln:56:LEU:HD13	1.92	0.52
49:S2:1153:U:O2	79:Sh:16:ASN:ND2	2.35	0.52
54:SF:52:ASP:OD2	71:SZ:117:ARG:NH1	2.43	0.52
81:Sj:80:ASP:OD1	81:Sj:81:TYR:N	2.42	0.52
1:B:448:VAL:HG22	52:SD:148:TYR:CG	2.39	0.52
1:B:448:VAL:HG13	52:SD:119:ARG:NH1	2.21	0.52
3:L5:27:C:OP1	18:LQ:193:ARG:NH1	2.43	0.52
3:L5:1494:G:H4'	6:LD:194:ASN:HB2	1.92	0.52
3:L5:1609:G:H5''	31:Ld:26:ARG:HG2	1.91	0.52
3:L5:2388:U:OP2	5:L8:125:C:N4	2.42	0.52
3:L5:3952:C:O2'	3:L5:4081:C:O2'	2.27	0.52
7:LE:160:ILE:HG21	7:LE:193:LYS:HB3	1.91	0.52
7:LE:305:THR:HG23	7:LE:308:ASP:H	1.75	0.52
7:LE:330:PHE:CD1	7:LE:332:MET:HE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LH:115:MET:O	46:Ls:87:ARG:NH1	2.42	0.52
10:LH:287:HIS:CE1	10:LH:288:LYS:HG2	2.45	0.52
17:LP:28:VAL:HG11	17:LP:47:ARG:HH12	1.74	0.52
19:LR:30:GLY:HA2	19:LR:101:ARG:NH1	2.25	0.52
33:Lf:20:LEU:HB3	33:Lf:102:SER:HB2	1.90	0.52
49:S2:1031:A:H2'	49:S2:1032:A2M:H8	1.92	0.52
55:SG:85:GLY:HA2	55:SG:108:VAL:HG23	1.90	0.52
55:SG:170:TRP:HA	55:SG:194:TYR:HB2	1.90	0.52
1:B:671:ARG:NH2	1:B:753:ASP:O	2.35	0.52
2:I:172:G:N2	2:I:175:G:O6	2.42	0.52
3:L5:1397:C:H2'	3:L5:1398:A:H8	1.74	0.52
3:L5:3516:A:O2'	3:L5:3517:A2M:H3'	2.09	0.52
3:L5:3599:A2M:HM'3	3:L5:3612:G:H21	1.74	0.52
3:L5:3632:G:OP1	3:L5:3633:A:O2'	2.23	0.52
10:LH:81:ARG:HA	10:LH:84:ARG:HD2	1.91	0.52
10:LH:164:ARG:O	10:LH:185:ASN:ND2	2.42	0.52
26:LY:61:VAL:O	26:LY:79:ALA:N	2.34	0.52
49:S2:1099:C:H2'	49:S2:1100:G:C8	2.44	0.52
58:SM:28:LYS:HE3	58:SM:48:LEU:HG	1.91	0.52
63:SR:124:LEU:HD23	63:SR:125:THR:HG23	1.91	0.52
1:B:444:SER:O	52:SD:145:CYS:O	2.28	0.52
3:L5:109:G:O3'	16:LO:92:ARG:NH1	2.43	0.52
3:L5:3393:G:N7	6:LD:152:SER:OG	2.41	0.52
3:L5:3838:C:H2'	3:L5:3839:U:C5	2.45	0.52
8:LF:169:LEU:HD11	8:LF:173:LYS:HE2	1.92	0.52
13:LK:23:ARG:HA	13:LK:45:LEU:HD12	1.92	0.52
16:LO:108:GLU:OE1	16:LO:108:GLU:N	2.40	0.52
27:LZ:101:ARG:NH1	63:SR:146:ASN:OD1	2.41	0.52
40:Lm:69:ILE:HD12	40:Lm:72:ARG:HH21	1.75	0.52
61:SP:171:ASP:OD1	61:SP:172:PHE:N	2.43	0.52
66:SU:37:LEU:HD11	66:SU:106:LEU:HD11	1.92	0.52
3:L5:242:U:H4'	29:Lb:2:LYS:NZ	2.25	0.52
3:L5:1331:A:N6	3:L5:1341:A:OP2	2.39	0.52
3:L5:1859:C:H3'	3:L5:1860:C:H5''	1.92	0.52
3:L5:2539:A:C4	41:Ln:69:LEU:HD21	2.45	0.52
3:L5:3625:C:O2'	3:L5:4718:A:N1	2.43	0.52
8:LF:326:LEU:O	11:LI:46:ARG:NH2	2.42	0.52
13:LK:169:ASN:O	13:LK:169:ASN:ND2	2.41	0.52
16:LO:99:ASP:OD2	16:LO:102:ARG:N	2.43	0.52
49:S2:17:C:O2'	49:S2:1195:A:N1	2.43	0.52
55:SG:219:TRP:CD1	55:SG:226:HIS:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SR:39:ASP:OD1	63:SR:47:GLY:N	2.44	0.52
66:SU:3:VAL:HG21	66:SU:5:ARG:HE	1.75	0.52
67:SV:27:VAL:HB	67:SV:43:LEU:HD13	1.91	0.52
76:Se:129:ARG:HB3	76:Se:133:ARG:NH1	2.25	0.52
3:L5:519:C:H2'	3:L5:520:G:C8	2.45	0.51
3:L5:1095:C:H2'	3:L5:1096:G:C8	2.44	0.51
12:LJ:234:ARG:NH1	39:Ll:46:GLU:O	2.43	0.51
14:LL:61:SER:HA	14:LL:126:VAL:HG23	1.92	0.51
40:Lm:47:TYR:O	40:Lm:54:LYS:NZ	2.33	0.51
49:S2:21:U:O2'	66:SU:17:ARG:O	2.27	0.51
49:S2:1462:G:O2'	49:S2:1465:C:N4	2.40	0.51
49:S2:1569:C:OP1	76:Se:96:SER:OG	2.26	0.51
55:SG:143:GLN:NE2	55:SG:144:ASP:OD1	2.43	0.51
2:I:157:C:H2'	2:I:158:A:H4'	1.92	0.51
36:Li:4:ARG:NH1	36:Li:6:TRP:O	2.44	0.51
49:S2:754:C:N3	49:S2:793:C:H1'	2.26	0.51
49:S2:831:A:OP2	49:S2:847:G:N2	2.44	0.51
49:S2:1763:C:H2'	49:S2:1764:G:C8	2.45	0.51
49:S2:1809:U:H2'	49:S2:1810:A:C8	2.45	0.51
55:SG:72:SER:OG	55:SG:74:ASP:OD1	2.20	0.51
55:SG:236:ILE:HD13	55:SG:252:THR:HG22	1.92	0.51
57:SL:34:MET:HG2	57:SL:154:LEU:HD11	1.92	0.51
3:L5:1095:C:H2'	3:L5:1096:G:H8	1.76	0.51
3:L5:1340:G:HO2'	3:L5:1423:C:HO2'	1.52	0.51
3:L5:1391:C:O2	32:Le:106:ARG:NH2	2.44	0.51
5:L8:36:G:OP2	38:Lk:88:THR:OG1	2.22	0.51
8:LF:133:LEU:HD13	46:Ls:6:GLN:HE21	1.75	0.51
49:S2:1565:C:OP1	76:Se:121:ARG:NH2	2.34	0.51
49:S2:1655:G:OP1	76:Se:82:ARG:NH2	2.34	0.51
61:SP:18:TRP:HB3	61:SP:20:LEU:HD13	1.93	0.51
61:SP:64:ILE:HD12	81:Sj:17:LEU:HB3	1.92	0.51
3:L5:62:A:N3	3:L5:77:U:O2'	2.39	0.51
3:L5:4138:OMG:N3	3:L5:4193:5MC:HM52	2.25	0.51
8:LF:7:LEU:HB3	8:LF:21:ASN:HB3	1.93	0.51
13:LK:20:LEU:HD21	13:LK:55:LEU:HD21	1.93	0.51
14:LL:54:SER:HA	14:LL:163:GLN:HG3	1.92	0.51
22:LU:92:LYS:O	22:LU:96:MET:HG2	2.11	0.51
31:Ld:71:PRO:HG2	31:Ld:108:TYR:HA	1.92	0.51
39:Ll:99:LYS:HG3	39:Ll:103:LYS:HE2	1.92	0.51
42:Lo:43:HIS:HD1	42:Lo:45:ARG:H	1.57	0.51
49:S2:522:A:H5'	49:S2:826:A:H1'	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:83:VAL:HG22	80:Si:68:LYS:HE2	1.93	0.51
55:SG:44:LYS:HB2	55:SG:56:GLN:HG2	1.93	0.51
64:SS:66:VAL:N	64:SS:67:PRO:HD2	2.25	0.51
68:SW:24:LEU:HD12	68:SW:25:LEU:HG	1.93	0.51
2:I:128:A:H61	2:I:159:G:N2	2.07	0.51
3:L5:156:G:N2	3:L5:157:U:O4	2.43	0.51
3:L5:4269:A2M:H5''	3:L5:4270:G:H5'	1.92	0.51
3:L5:4476:C:O2'	3:L5:4479:C:N3	2.43	0.51
8:LF:337:ARG:NH1	10:LH:60:SER:HA	2.26	0.51
9:LG:256:LYS:HD2	9:LG:257:PRO:HD2	1.92	0.51
35:Lh:90:MET:N	35:Lh:90:MET:SD	2.84	0.51
49:S2:220:U:H2'	49:S2:221:A:C8	2.45	0.51
49:S2:1581:A:H8	77:Sf:56:MET:HE3	1.74	0.51
56:SH:5:GLN:OE1	56:SH:5:GLN:N	2.43	0.51
63:SR:58:LYS:HA	63:SR:107:SER:HB2	1.93	0.51
63:SR:230:LYS:HA	63:SR:233:ARG:HB3	1.92	0.51
74:Sc:76:GLU:OE2	74:Sc:80:ARG:NH1	2.43	0.51
3:L5:67:C:N4	3:L5:325:U:O3'	2.43	0.51
3:L5:150:U:OP2	12:LJ:200:THR:OG1	2.23	0.51
3:L5:3585:PSU:O2'	3:L5:4718:A:N3	2.43	0.51
3:L5:3704:A:N6	3:L5:3777:U:OP2	2.44	0.51
3:L5:3897:G:H2'	3:L5:3898:G:H8	1.74	0.51
5:L8:90:C:H2'	5:L8:91:A:C8	2.46	0.51
11:LI:100:VAL:HG12	11:LI:138:TYR:HE2	1.75	0.51
49:S2:120:U:H1'	61:SP:33:THR:HG23	1.92	0.51
49:S2:1098:G:H4'	57:SL:32:PHE:CD1	2.46	0.51
49:S2:1374:C:OP1	74:Sc:7:LYS:HD3	2.10	0.51
49:S2:1649:G:O2'	49:S2:1675:G:O6	2.29	0.51
55:SG:40:ILE:HD11	55:SG:66:VAL:HG11	1.93	0.51
63:SR:10:THR:HB	63:SR:128:THR:HA	1.93	0.51
75:Sd:28:PHE:O	75:Sd:31:THR:OG1	2.28	0.51
81:Sj:51:THR:OG1	81:Sj:53:ASP:OD1	2.27	0.51
1:B:721:GLN:HB3	1:B:723:ILE:HG12	1.93	0.51
3:L5:70:A:OP2	31:Ld:64:LYS:NZ	2.44	0.51
3:L5:2005:C:H5''	36:Li:36:ARG:NH1	2.25	0.51
3:L5:3792:C:H2'	3:L5:3793:G:C8	2.46	0.51
3:L5:4051:G:N7	24:LW:87:LYS:NZ	2.47	0.51
3:L5:4122:A:O2'	31:Ld:42:ARG:NH1	2.43	0.51
3:L5:4166:PSU:O2	3:L5:4221:G:N2	2.43	0.51
20:LS:84:PRO:HB2	20:LS:87:SER:HB3	1.93	0.51
22:LU:17:CYS:SG	22:LU:18:GLY:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ls:63:VAL:HG22	46:Ls:79:ARG:HG2	1.92	0.51
46:Ls:108:MET:HA	46:Ls:111:ILE:HG12	1.91	0.51
48:S:1133:G:O6	48:S:1139:U:N3	2.44	0.51
49:S2:1599:G:N7	82:Sk:85:ARG:NH1	2.51	0.51
55:SG:32:LEU:HD12	55:SG:40:ILE:HG22	1.92	0.51
55:SG:87:LEU:HD21	55:SG:108:VAL:HG11	1.92	0.51
64:SS:57:ARG:NH1	64:SS:171:GLU:OE2	2.44	0.51
71:SZ:65:ASP:HA	71:SZ:68:GLU:HG3	1.92	0.51
3:L5:1621:C:O2'	3:L5:1643:G:OP1	2.25	0.51
10:LH:189:LEU:HD21	10:LH:256:VAL:HG11	1.93	0.51
16:LO:180:ALA:O	16:LO:184:MET:HG2	2.11	0.51
19:LR:98:ALA:HA	19:LR:101:ARG:HE	1.75	0.51
30:Lc:26:VAL:O	30:Lc:93:LYS:NZ	2.44	0.51
55:SG:99:ARG:NH2	55:SG:135:LEU:O	2.41	0.51
81:Sj:35:VAL:HG23	81:Sj:40:ILE:HD11	1.93	0.51
2:I:42:U:H3	2:I:88:C:H5'	1.76	0.51
2:I:51:A:H2'	2:I:52:A:C8	2.46	0.51
3:L5:4714:G:O2'	3:L5:4716:A:N6	2.40	0.51
11:LI:88:LEU:HD11	11:LI:121:PHE:HB3	1.92	0.51
15:LM:46:GLN:NE2	15:LM:72:CYS:SG	2.84	0.51
49:S2:528:C:H2'	49:S2:529:A:C8	2.45	0.51
49:S2:1118:C:O2'	49:S2:1119:C:O4'	2.27	0.51
63:SR:121:ILE:N	63:SR:125:THR:OG1	2.43	0.51
3:L5:1078:G:OP2	3:L5:1078:G:N2	2.36	0.51
3:L5:2146:C:O2'	3:L5:2175:A:N1	2.38	0.51
3:L5:2207:OMG:N1	3:L5:3590:C:N3	2.51	0.51
3:L5:2675:A:OP1	34:Lg:47:LYS:NZ	2.39	0.51
6:LD:47:ASP:OD1	6:LD:48:ILE:N	2.44	0.51
17:LP:126:GLU:OE2	19:LR:181:ALA:HB1	2.11	0.51
21:LT:105:VAL:HG23	21:LT:110:ARG:CZ	2.41	0.51
49:S2:454:C:O2'	63:SR:92:ARG:O	2.18	0.51
72:Sa:83:MET:HB3	72:Sa:116:LEU:HD12	1.93	0.51
75:Sd:5:ILE:HG12	82:Sk:49:LEU:HB2	1.91	0.51
2:I:56:A:H2'	2:I:57:A:C4	2.46	0.50
3:L5:397:G:H22	20:LS:90:PHE:HE1	1.57	0.50
3:L5:1743:A:H5'	3:L5:1745:G:O4'	2.10	0.50
3:L5:1941:A:H5''	3:L5:1942:G:H8	1.75	0.50
3:L5:4612:G:H22	19:LR:176:ARG:NH2	2.06	0.50
11:LI:85:GLU:HG2	24:LW:135:PRO:HB3	1.94	0.50
49:S2:615:C:O2'	49:S2:627:G:N2	2.44	0.50
50:SB:67:THR:OG1	50:SB:70:LYS:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SM:134:LEU:HG	58:SM:218:LEU:HD13	1.92	0.50
65:ST:81:VAL:HG22	65:ST:102:VAL:HG12	1.94	0.50
74:Sc:29:HIS:HA	74:Sc:32:LYS:HE2	1.93	0.50
2:I:129:G:H1	2:I:157:C:H42	1.58	0.50
3:L5:988:G:H1	3:L5:1125:C:H42	1.60	0.50
3:L5:1510:G:N7	45:Lr:4:ARG:NH2	2.58	0.50
3:L5:1955:C:H2'	3:L5:1956:A:C8	2.44	0.50
3:L5:2328:U:H3	3:L5:2336:G:H1	1.60	0.50
3:L5:2495:G:N1	45:Lr:58:GLY:O	2.26	0.50
3:L5:4314:A:O3'	7:LE:21:ARG:NH2	2.44	0.50
3:L5:4627:C:H2'	3:L5:4628:G:H8	1.77	0.50
7:LE:78:ILE:HG13	7:LE:320:PHE:CE1	2.47	0.50
23:LV:154:LEU:HB3	23:LV:157:ARG:HD3	1.92	0.50
58:SM:150:ILE:HG23	74:Sc:132:ARG:HH12	1.75	0.50
65:ST:56:ARG:NH1	65:ST:180:GLY:O	2.45	0.50
73:Sb:16:LYS:HG3	73:Sb:17:LYS:H	1.76	0.50
3:L5:1631:C:H41	3:L5:4124:A:H5''	1.76	0.50
3:L5:3789:U:H2'	3:L5:3790:A:C8	2.46	0.50
8:LF:40:VAL:HG11	8:LF:123:ALA:HB2	1.92	0.50
10:LH:137:SER:OG	10:LH:138:GLN:OE1	2.23	0.50
49:S2:212:C:H2'	49:S2:213:G:C8	2.46	0.50
55:SG:5:MET:HE1	55:SG:312:VAL:HG13	1.94	0.50
57:SL:42:LYS:HD3	57:SL:46:ILE:HB	1.92	0.50
64:SS:143:ARG:HB2	64:SS:155:LYS:HB2	1.93	0.50
65:ST:43:ILE:HG22	65:ST:57:ALA:HA	1.93	0.50
2:I:125:U:H1'	2:I:162:A:H2	1.77	0.50
3:L5:837:U:OP2	17:LP:48:GLN:NE2	2.45	0.50
3:L5:2004:G:O2'	36:Li:80:ASN:OD1	2.26	0.50
3:L5:3831:C:H2'	3:L5:3832:G:H4'	1.94	0.50
3:L5:4644:C:H42	3:L5:4655:G:H1	1.58	0.50
5:L8:9:A:H2'	5:L8:10:G:H8	1.77	0.50
7:LE:283:LYS:NZ	7:LE:359:ALA:O	2.43	0.50
14:LL:53:VAL:HA	14:LL:134:VAL:HA	1.93	0.50
23:LV:112:ASP:OD1	23:LV:116:ARG:NH1	2.34	0.50
46:Ls:108:MET:HE2	46:Ls:111:ILE:HD11	1.93	0.50
49:S2:861:G:N2	79:Sh:107:SER:OG	2.44	0.50
49:S2:1399:G:H1'	55:SG:63:SER:HB3	1.93	0.50
63:SR:159:ARG:HB3	63:SR:171:THR:HB	1.92	0.50
75:Sd:101:ASN:O	75:Sd:105:ASN:ND2	2.45	0.50
1:B:460:GLU:O	1:B:464:HIS:ND1	2.41	0.50
2:I:115:A:H1'	62:SQ:198:ARG:HH21	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:127:C:O2	2:I:160:G:N1	2.45	0.50
3:L5:1138:G:H2'	3:L5:1202:C:O2	2.12	0.50
3:L5:1391:C:O2'	32:Le:103:LYS:NZ	2.44	0.50
3:L5:2300:G:OP1	18:LQ:65:ARG:NH2	2.39	0.50
3:L5:4083:C:N3	44:Lq:61:LYS:NZ	2.59	0.50
7:LE:107:ALA:HB2	7:LE:201:LEU:HD22	1.92	0.50
12:LJ:260:GLU:O	12:LJ:264:LYS:N	2.44	0.50
49:S2:172:OMU:H6	49:S2:315:U:H1'	1.94	0.50
61:SP:175:PHE:HZ	61:SP:208:VAL:HG11	1.75	0.50
71:SZ:83:GLN:NE2	71:SZ:87:GLU:OE2	2.45	0.50
3:L5:1345:C:OP1	32:Le:51:LYS:NZ	2.31	0.50
3:L5:3588:A:H5''	20:LS:83:TRP:O	2.12	0.50
3:L5:3849:G:N7	45:Lr:62:LYS:NZ	2.55	0.50
3:L5:3897:G:H2'	3:L5:3898:G:C8	2.46	0.50
3:L5:4099:PSU:H5'	3:L5:4100:U:H5'	1.93	0.50
6:LD:177:LYS:HG3	45:Lr:26:VAL:HG23	1.92	0.50
8:LF:332:ALA:O	8:LF:336:ARG:HG2	2.12	0.50
13:LK:95:VAL:HG22	43:Lp:82:LEU:HB3	1.93	0.50
27:LZ:63:GLN:OE1	27:LZ:63:GLN:N	2.41	0.50
30:Lc:92:ASP:HB3	30:Lc:95:VAL:HG12	1.94	0.50
48:S:1139:U:H2'	48:S:1140:G:C8	2.46	0.50
49:S2:964:A:OP1	71:SZ:66:ARG:NH1	2.45	0.50
49:S2:1011:G:H2'	49:S2:1012:A:C8	2.46	0.50
55:SG:291:TRP:CE2	55:SG:298:LEU:HD13	2.47	0.50
73:Sb:93:VAL:HG13	73:Sb:105:LYS:HG3	1.94	0.50
82:Sk:71:ALA:O	82:Sk:74:SER:OG	2.26	0.50
3:L5:1381:G:N1	3:L5:1413:C:OP2	2.40	0.50
3:L5:1980:A:N7	3:L5:4180:C:O2'	2.43	0.50
3:L5:2245:G:O2'	37:Lj:10:ARG:O	2.30	0.50
3:L5:3973:OMU:HM21	3:L5:4082:A:H1'	1.94	0.50
3:L5:4610:C:N4	23:LV:171:ARG:O	2.44	0.50
7:LE:217:ILE:HD13	7:LE:284:ILE:HD11	1.94	0.50
3:L5:483:G:O2'	3:L5:486:C:OP2	2.29	0.50
3:L5:699:G:OP1	35:Lh:5:ARG:NH2	2.45	0.50
3:L5:1509:A:OP2	45:Lr:4:ARG:NE	2.37	0.50
3:L5:3952:C:HO2'	3:L5:4081:C:HO2'	1.56	0.50
16:LO:50:PRO:HG3	38:Lk:121:VAL:HG12	1.94	0.50
26:LY:21:PRO:HA	26:LY:54:ALA:HA	1.94	0.50
37:Lj:111:ALA:O	37:Lj:115:LYS:N	2.31	0.50
68:SW:103:GLU:OE2	68:SW:105:ARG:NH1	2.44	0.50
80:Si:50:ILE:HG13	80:Si:75:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:267:G:H4'	38:Lk:113:LEU:HD11	1.94	0.50
3:L5:2420:C:H2'	3:L5:2421:G:H8	1.75	0.50
3:L5:4333:G:O2'	7:LE:14:LEU:O	2.30	0.50
3:L5:4698:U:H2'	3:L5:4699:G:C8	2.46	0.50
9:LG:33:ARG:NH2	9:LG:72:ASP:OD1	2.45	0.50
15:LM:56:THR:HG22	15:LM:64:ARG:H	1.77	0.50
19:LR:23:VAL:HG23	19:LR:33:VAL:HG11	1.93	0.50
49:S2:682:PSU:H4'	80:Si:9:THR:HG22	1.93	0.50
55:SG:130:LYS:HD2	55:SG:138:CYS:SG	2.52	0.50
74:Sc:32:LYS:HD2	74:Sc:47:ARG:HH12	1.77	0.50
3:L5:629:G:H2'	3:L5:630:G:C8	2.47	0.49
3:L5:2225:A:N1	3:L5:2672:U:O2'	2.38	0.49
3:L5:3701:G:O2'	47:Lx:166:ALA:O	2.30	0.49
3:L5:3872:G:H22	3:L5:3885:C:H2'	1.76	0.49
7:LE:89:ILE:HG12	7:LE:197:ALA:HB1	1.94	0.49
29:Lb:86:GLN:HG3	29:Lb:94:THR:HG23	1.93	0.49
30:Lc:25:ILE:HA	30:Lc:43:VAL:HG12	1.94	0.49
49:S2:659:U:O2	80:Si:17:ARG:NH1	2.44	0.49
49:S2:665:A:O2'	49:S2:671:A:N1	2.40	0.49
49:S2:1396:C:C2'	49:S2:1397:A:H5'	2.42	0.49
58:SM:115:LYS:HD3	58:SM:116:LYS:H	1.77	0.49
58:SM:136:ARG:HB2	58:SM:218:LEU:HD11	1.94	0.49
82:Sk:43:LYS:NZ	82:Sk:44:LEU:O	2.43	0.49
3:L5:18:C:H4'	18:LQ:138:PHE:CD2	2.47	0.49
3:L5:279:A:OP2	18:LQ:12:ARG:NH2	2.45	0.49
3:L5:3872:G:N2	3:L5:3885:C:H2'	2.28	0.49
16:LO:91:ALA:HB1	16:LO:96:ILE:HB	1.94	0.49
17:LP:11:ARG:NH1	17:LP:58:THR:O	2.45	0.49
35:Lh:28:TYR:HB3	35:Lh:30:LYS:HG2	1.93	0.49
49:S2:1231:C:OP1	75:Sd:130:ARG:NH2	2.45	0.49
59:SN:121:ARG:NH1	59:SN:123:ARG:HD3	2.27	0.49
62:SQ:50:PRO:HG2	62:SQ:90:VAL:HG23	1.94	0.49
63:SR:148:SER:N	63:SR:151:ASP:OD2	2.41	0.49
80:Si:140:ARG:HB3	80:Si:142:ARG:HG2	1.93	0.49
81:Sj:27:VAL:HB	81:Sj:69:THR:HB	1.95	0.49
3:L5:1784:U:H2'	3:L5:1785:G:H8	1.77	0.49
3:L5:1926:C:H2'	3:L5:1927:G:C8	2.47	0.49
3:L5:3708:C:N3	3:L5:3764:G:N2	2.61	0.49
3:L5:3826:A:O4'	3:L5:3841:U:N3	2.45	0.49
6:LD:108:PRO:HG2	45:Lr:86:LEU:HD23	1.95	0.49
31:Ld:72:THR:HB	31:Ld:112:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Ld:127:LYS:HZ1	39:Ll:7:MET:HA	1.78	0.49
36:Li:14:TYR:OH	36:Li:92:LEU:O	2.20	0.49
49:S2:1139:C:N3	78:Sg:61:ARG:NH2	2.61	0.49
49:S2:1402:A:N6	49:S2:1442:U:O2'	2.46	0.49
65:ST:97:VAL:HG12	65:ST:100:CYS:HB3	1.93	0.49
67:SV:21:MET:HB3	67:SV:69:TRP:HB2	1.94	0.49
67:SV:55:ARG:HE	67:SV:57:TYR:HE2	1.60	0.49
73:Sb:53:GLU:HG3	73:Sb:54:PRO:HD3	1.95	0.49
3:L5:278:G:H5''	18:LQ:8:GLN:OE1	2.12	0.49
3:L5:1673:G:N2	3:L5:1674:U:O4	2.33	0.49
3:L5:1844:U:OP2	36:Li:76:ARG:NH2	2.38	0.49
3:L5:2557:G:H2'	3:L5:2558:G:H8	1.77	0.49
3:L5:3989:C:OP2	3:L5:4010:G:N1	2.40	0.49
3:L5:4802:G:O6	7:LE:124:LYS:NZ	2.38	0.49
18:LQ:119:TYR:HE1	18:LQ:133:ILE:HD11	1.78	0.49
19:LR:27:VAL:HG11	19:LR:102:LEU:HB2	1.94	0.49
20:LS:42:ARG:HH11	20:LS:42:ARG:HA	1.77	0.49
21:LT:98:LEU:HB2	21:LT:113:ILE:HD11	1.94	0.49
39:Ll:38:LYS:NZ	39:Ll:42:ASP:OD2	2.40	0.49
39:Ll:72:PHE:O	39:Ll:76:ARG:HG2	2.12	0.49
49:S2:1758:G:H2'	49:S2:1759:G:H8	1.77	0.49
3:L5:18:C:H4'	18:LQ:138:PHE:HD2	1.76	0.49
3:L5:459:C:H5'	10:LH:113:ARG:HH22	1.77	0.49
3:L5:2118:G:H2'	3:L5:2119:A:C8	2.47	0.49
18:LQ:143:ARG:NH2	38:Lk:93:ARG:O	2.46	0.49
21:LT:113:ILE:HG21	21:LT:120:ILE:HD11	1.93	0.49
24:LW:117:LYS:HG2	24:LW:120:LYS:HZ2	1.78	0.49
36:Li:33:VAL:HG13	36:Li:38:GLU:HB3	1.94	0.49
49:S2:5:U:H2'	49:S2:6:G:H8	1.77	0.49
57:SL:184:ARG:HD3	57:SL:191:ARG:HG2	1.94	0.49
63:SR:138:ALA:HA	63:SR:176:ILE:HD11	1.93	0.49
65:ST:22:HIS:ND1	65:ST:23:LYS:O	2.45	0.49
1:B:444:SER:HA	49:S2:1293:C:H4'	1.95	0.49
3:L5:721:C:OP1	11:LI:72:ARG:NH2	2.43	0.49
3:L5:1394:U:O2'	11:LI:33:ARG:HD2	2.12	0.49
3:L5:2119:A:H2'	3:L5:2120:C:O4'	2.12	0.49
3:L5:2496:C:O4'	37:Lj:54:ARG:NH1	2.46	0.49
3:L5:3693:G:H2'	3:L5:3695:A:N7	2.28	0.49
3:L5:4373:U:H4'	7:LE:373:LYS:HE3	1.93	0.49
20:LS:138:PRO:HB3	20:LS:140:MET:HE2	1.94	0.49
22:LU:2:SER:OG	22:LU:3:MET:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:590:G:N2	53:SE:97:GLU:OE2	2.46	0.49
55:SG:154:VAL:O	55:SG:155:ARG:NH1	2.40	0.49
3:L5:186:G:N2	3:L5:186:G:OP2	2.45	0.49
3:L5:266:C:O2	38:Lk:109:ARG:NH1	2.45	0.49
3:L5:1208:C:H2'	3:L5:1209:G:C8	2.47	0.49
3:L5:3400:C:OP1	6:LD:8:GLN:NE2	2.46	0.49
28:La:64:SER:HB2	38:Lk:69:LEU:HD13	1.95	0.49
48:S:1126:A:HO2'	48:S:1142:U:H3	1.59	0.49
48:S:1129:A:H61	48:S:1143:G:H1'	1.77	0.49
49:S2:1590:A:N3	49:S2:1654:U:O2'	2.41	0.49
56:SH:34:TYR:HB3	60:SO:12:VAL:HG21	1.95	0.49
3:L5:1712:U:H2'	3:L5:1713:C:C6	2.47	0.49
3:L5:1757:G:OP1	9:LG:43:LYS:NZ	2.44	0.49
4:L7:48:G:OP1	9:LG:226:TYR:OH	2.24	0.49
5:L8:47:C:H1'	5:L8:61:A:H2'	1.94	0.49
8:LF:284:MET:HE3	8:LF:287:THR:HA	1.95	0.49
32:Le:43:MET:HE3	32:Le:43:MET:O	2.13	0.49
39:Ll:63:VAL:HG23	39:Ll:65:LYS:HD3	1.94	0.49
49:S2:417:U:HO2'	49:S2:653:U:HO2'	1.61	0.49
57:SL:76:VAL:HG23	57:SL:98:PRO:HA	1.95	0.49
58:SM:45:GLY:HA3	71:SZ:47:LEU:HD11	1.95	0.49
58:SM:150:ILE:HG23	74:Sc:132:ARG:NH1	2.28	0.49
3:L5:1517:G:N2	3:L5:1520:A:OP2	2.44	0.49
3:L5:1804:G:N2	3:L5:1807:A:OP2	2.39	0.49
3:L5:3820:G:C6	3:L5:3821:G:C6	3.01	0.49
3:L5:4512:G:OP1	13:LK:23:ARG:NH1	2.46	0.49
4:L7:119:U:OP2	9:LG:259:ARG:NH2	2.43	0.49
20:LS:31:GLU:HG2	20:LS:60:PHE:HA	1.93	0.49
33:Lf:45:LEU:HB3	33:Lf:96:ILE:HD11	1.93	0.49
49:S2:1289:OMU:C5	52:SD:95:ARG:HH22	2.26	0.49
55:SG:51:ASN:ND2	55:SG:53:GLY:O	2.45	0.49
68:SW:22:ARG:HG2	68:SW:28:THR:HB	1.95	0.49
69:SX:25:ALA:O	69:SX:30:GLY:N	2.40	0.49
3:L5:1016:C:H2'	3:L5:1059:G:H1'	1.95	0.49
3:L5:1348:G:N2	3:L5:1369:C:H1'	2.28	0.49
3:L5:3662:U:H3	3:L5:3926:G:H1	1.59	0.49
10:LH:193:HIS:HE1	10:LH:195:LYS:HG3	1.77	0.49
31:Ld:34:ASN:HB2	31:Ld:45:PHE:HZ	1.77	0.49
49:S2:30:C:O3'	80:Si:137:LYS:NZ	2.33	0.49
55:SG:159:ASN:ND2	55:SG:204:GLY:O	2.46	0.49
57:SL:16:LEU:HD11	74:Sc:116:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2110:U:OP1	46:Ls:37:SER:OG	2.23	0.48
3:L5:2375:C:O2'	28:La:93:ASN:ND2	2.43	0.48
3:L5:2399:G:H2'	3:L5:2400:G:H8	1.78	0.48
3:L5:3850:G:C5	37:Lj:97:ILE:HD11	2.48	0.48
3:L5:4333:G:N2	7:LE:15:GLY:O	2.35	0.48
3:L5:4511:A:N6	13:LK:60:TRP:O	2.39	0.48
37:Lj:25:THR:HG22	37:Lj:29:ARG:O	2.13	0.48
46:Ls:119:ARG:O	46:Ls:122:LYS:HG2	2.13	0.48
49:S2:197:U:H2'	49:S2:198:U:C6	2.47	0.48
49:S2:1588:G:N1	76:Se:74:SER:OG	2.46	0.48
55:SG:101:PHE:CE2	55:SG:136:GLY:HA2	2.48	0.48
55:SG:212:LYS:HA	55:SG:235:ILE:HG13	1.95	0.48
61:SP:95:THR:HA	81:Sj:16:ARG:HD2	1.95	0.48
74:Sc:103:LYS:HB3	74:Sc:107:LYS:HZ1	1.78	0.48
81:Sj:78:SER:OG	81:Sj:80:ASP:OD1	2.26	0.48
3:L5:2232:A:H4'	34:Lg:70:LYS:HG3	1.95	0.48
3:L5:2250:G:N2	3:L5:2250:G:OP2	2.45	0.48
3:L5:4437:A:O2'	13:LK:68:ALA:O	2.22	0.48
21:LT:39:THR:HG22	21:LT:41:SER:H	1.78	0.48
49:S2:229:A:H2	49:S2:900:U:H3	1.61	0.48
49:S2:378:G:H5'	65:ST:98:LYS:HB3	1.96	0.48
49:S2:1320:U:H2'	49:S2:1321:G:C8	2.48	0.48
55:SG:29:ASP:HA	55:SG:45:LEU:HB2	1.95	0.48
55:SG:134:THR:HG23	55:SG:135:LEU:HD22	1.94	0.48
74:Sc:14:ARG:HG2	74:Sc:69:ILE:HD11	1.94	0.48
79:Sh:111:MET:HE3	79:Sh:116:ALA:HA	1.94	0.48
80:Si:107:ARG:HB3	80:Si:110:HIS:HB3	1.95	0.48
3:L5:859:G:O2'	3:L5:2106:A:N6	2.46	0.48
3:L5:1572:G:H1'	3:L5:2356:A:N6	2.28	0.48
3:L5:3700:U:H2'	3:L5:3701:G:C8	2.48	0.48
3:L5:4609:G:H5''	17:LP:91:TRP:CE2	2.48	0.48
8:LF:40:VAL:HG23	8:LF:115:VAL:HG11	1.94	0.48
10:LH:45:HIS:ND1	10:LH:46:CYS:O	2.41	0.48
20:LS:116:HIS:CE1	20:LS:118:GLN:HB2	2.48	0.48
25:LX:63:ILE:HG22	25:LX:72:VAL:HG22	1.96	0.48
29:Lb:8:THR:HG21	29:Lb:13:LYS:HB2	1.96	0.48
49:S2:1233:PSU:H2'	49:S2:1234:G:H8	1.78	0.48
49:S2:1865:U:OP2	54:SF:4:LYS:NZ	2.38	0.48
54:SF:41:ILE:HG22	54:SF:66:LYS:HE2	1.94	0.48
62:SQ:39:ILE:HA	62:SQ:68:ILE:HD11	1.95	0.48
73:Sb:53:GLU:OE2	73:Sb:85:ARG:NH2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sg:17:CYS:HB2	78:Sg:56:CYS:HB3	1.96	0.48
3:L5:113:A:O2'	18:LQ:50:ARG:HG2	2.13	0.48
3:L5:375:G:OP1	8:LF:62:THR:HG23	2.13	0.48
3:L5:843:A:H1'	11:LI:57:HIS:HD2	1.77	0.48
3:L5:2501:G:O6	33:Lf:32:LYS:NZ	2.44	0.48
6:LD:24:LYS:HG3	6:LD:49:ILE:HD12	1.95	0.48
9:LG:204:VAL:O	9:LG:208:MET:N	2.41	0.48
11:LI:153:ILE:HD12	11:LI:190:ILE:HG12	1.95	0.48
17:LP:104:MET:O	17:LP:109:ARG:NH2	2.47	0.48
50:SB:28:PRO:HG3	70:SY:17:PRO:HG3	1.95	0.48
55:SG:304:ASP:OD1	55:SG:308:ARG:NH1	2.45	0.48
59:SN:80:GLU:HA	59:SN:83:LEU:HB2	1.95	0.48
1:B:446:LEU:HD22	52:SD:146:LEU:HD23	1.87	0.48
3:L5:1678:G:N3	3:L5:1681:A:N6	2.61	0.48
3:L5:1968:A:H2'	3:L5:1969:A:C8	2.48	0.48
3:L5:2536:G:OP2	41:Ln:33:LYS:NZ	2.47	0.48
3:L5:2691:G:O2'	3:L5:3570:U:O4	2.25	0.48
15:LM:56:THR:HG22	15:LM:64:ARG:N	2.29	0.48
49:S2:1609:U:H4'	75:Sd:130:ARG:NH1	2.29	0.48
53:SE:109:ARG:HD3	66:SU:124:HIS:CE1	2.49	0.48
64:SS:80:VAL:HG13	64:SS:92:VAL:HB	1.95	0.48
69:SX:52:LEU:HD13	69:SX:76:LEU:HD21	1.96	0.48
3:L5:2146:C:H5''	35:Lh:104:SER:HB2	1.95	0.48
3:L5:2507:G:H4'	3:L5:2520:G:H4'	1.94	0.48
3:L5:3698:A:H2'	3:L5:3699:G:C8	2.48	0.48
3:L5:3834:G:H1'	3:L5:3835:G:C8	2.49	0.48
3:L5:3930:G:H5'	6:LD:233:ARG:HB2	1.96	0.48
3:L5:4020:A:H2'	3:L5:4021:G:C8	2.49	0.48
3:L5:4705:A:H5'	7:LE:128:LYS:HG3	1.95	0.48
3:L5:4780:G:N1	7:LE:389:MET:O	2.42	0.48
4:L7:74:A:N1	4:L7:100:A:H5''	2.28	0.48
8:LF:108:TRP:O	18:LQ:204:ARG:NH2	2.47	0.48
38:Lk:4:ILE:HG22	38:Lk:56:ARG:HD2	1.95	0.48
49:S2:1715:U:H2'	49:S2:1716:A:C8	2.48	0.48
69:SX:27:ILE:HG23	69:SX:28:HIS:ND1	2.29	0.48
70:SY:130:LYS:NZ	70:SY:139:TRP:O	2.32	0.48
3:L5:1102:G:O2'	11:LI:69:ARG:NH1	2.46	0.48
3:L5:1140:C:H42	3:L5:1200:G:H2'	1.79	0.48
3:L5:1353:G:H2'	3:L5:1354:G:H8	1.78	0.48
3:L5:1703:G:N2	3:L5:1706:A:OP2	2.47	0.48
3:L5:2364:G:O3'	37:Lj:25:THR:OG1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4104:U:H4'	16:LO:197:LYS:HD2	1.95	0.48
3:L5:4638:G:H1	3:L5:4660:C:H42	1.62	0.48
3:L5:4699:G:H2'	3:L5:4700:G:C8	2.48	0.48
7:LE:19:ARG:HB2	7:LE:234:ARG:NH2	2.27	0.48
23:LV:86:SER:N	23:LV:89:GLY:O	2.43	0.48
49:S2:65:C:N4	63:SR:133:LEU:HB3	2.28	0.48
55:SG:19:THR:H	55:SG:35:SER:HA	1.79	0.48
62:SQ:78:MET:HB2	62:SQ:159:ARG:NH2	2.29	0.48
63:SR:7:PHE:HB2	63:SR:124:LEU:HD21	1.96	0.48
3:L5:308:G:H5'	39:Ll:85:ARG:HH22	1.78	0.48
3:L5:837:U:H5'	17:LP:48:GLN:HG2	1.95	0.48
3:L5:1532:G:OP1	45:Lr:17:ARG:NH2	2.47	0.48
3:L5:1939:G:N2	3:L5:1939:G:OP2	2.46	0.48
3:L5:4403:U:O2'	3:L5:4405:G:OP2	2.32	0.48
3:L5:4708:C:OP2	7:LE:120:LYS:HD2	2.13	0.48
10:LH:49:ASN:HB2	10:LH:64:MET:SD	2.54	0.48
10:LH:182:LEU:HD12	10:LH:186:ARG:HA	1.96	0.48
12:LJ:39:PHE:CD1	12:LJ:47:PRO:HD3	2.49	0.48
12:LJ:96:LEU:O	12:LJ:100:HIS:N	2.45	0.48
14:LL:149:VAL:HG23	14:LL:165:ILE:HG21	1.96	0.48
16:LO:135:LYS:N	16:LO:138:ASP:OD2	2.41	0.48
16:LO:169:ILE:HG12	31:Ld:123:ILE:HD11	1.96	0.48
17:LP:28:VAL:HG11	17:LP:47:ARG:NH1	2.28	0.48
21:LT:178:ARG:N	31:Ld:51:GLY:HA2	2.29	0.48
22:LU:172:ARG:HH12	49:S2:909:A:H5''	1.77	0.48
34:Lg:37:GLY:O	34:Lg:41:ARG:HG3	2.12	0.48
34:Lg:87:ARG:HB3	34:Lg:107:THR:HG23	1.95	0.48
49:S2:1100:G:H22	49:S2:1134:A:H2	1.60	0.48
60:SO:105:LEU:HD12	60:SO:122:VAL:HG11	1.95	0.48
65:ST:39:GLY:O	65:ST:61:ASP:HB2	2.14	0.48
3:L5:475:G:H2'	3:L5:476:G:H8	1.79	0.48
3:L5:1871:A:H8	19:LR:49:ARG:HH22	1.60	0.48
3:L5:4198:U:OP2	3:L5:4268:G:N1	2.30	0.48
3:L5:4508:G:H5''	19:LR:12:ARG:CZ	2.43	0.48
10:LH:78:PRO:O	10:LH:84:ARG:NE	2.46	0.48
49:S2:28:U:H2'	49:S2:29:G:H8	1.78	0.48
63:SR:217:MET:O	63:SR:221:LYS:N	2.38	0.48
72:Sa:94:VAL:HG22	72:Sa:107:ILE:HD11	1.96	0.48
75:Sd:71:MET:HE2	75:Sd:99:LEU:HD13	1.96	0.48
81:Sj:86:GLU:HG2	81:Sj:90:ARG:HD2	1.95	0.48
3:L5:858:G:H1'	10:LH:128:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1212:C:O2	32:Le:120:ARG:NH2	2.46	0.48
3:L5:1617:C:OP2	35:Lh:39:ARG:NH2	2.47	0.48
3:L5:2592:C:H2'	3:L5:2593:G:H8	1.78	0.48
3:L5:3610:C:OP1	3:L5:4146:G:O2'	2.29	0.48
3:L5:4060:C:OP1	24:LW:70:HIS:N	2.39	0.48
3:L5:4171:G:OP1	43:Lp:100:TYR:OH	2.28	0.48
7:LE:226:LYS:HG2	7:LE:273:GLY:HA3	1.95	0.48
49:S2:809:A:H3'	49:S2:810:A:H8	1.79	0.48
49:S2:1157:U:OP1	79:Sh:71:LYS:NZ	2.37	0.48
49:S2:1514:C:H2'	49:S2:1515:G:C8	2.48	0.48
57:SL:37:TYR:HA	57:SL:53:ARG:HD3	1.94	0.48
57:SL:89:LYS:HZ2	74:Sc:82:ASP:HB3	1.79	0.48
57:SL:205:ARG:HH22	74:Sc:84:TYR:HD2	1.62	0.48
63:SR:220:ALA:O	63:SR:224:ARG:N	2.37	0.48
75:Sd:82:TRP:CD1	75:Sd:82:TRP:H	2.32	0.48
3:L5:1860:C:C5	17:LP:17:PHE:HB3	2.49	0.47
7:LE:161:ARG:HG2	7:LE:184:GLN:HA	1.96	0.47
42:Lo:42:ARG:NH1	42:Lo:49:LEU:HD21	2.28	0.47
49:S2:25:A:HO2'	49:S2:26:U:H6	1.62	0.47
49:S2:496:U:OP1	61:SP:49:ARG:NH1	2.46	0.47
69:SX:91:LEU:HD12	69:SX:104:VAL:HG23	1.95	0.47
74:Sc:95:ILE:HD11	74:Sc:118:GLN:HB2	1.96	0.47
3:L5:369:G:N2	3:L5:372:A:OP2	2.45	0.47
3:L5:2546:G:OP1	25:LX:113:ARG:NH1	2.46	0.47
3:L5:4486:G:H2'	3:L5:4489:G:H5'	1.95	0.47
4:L7:87:G:N2	4:L7:90:A:OP2	2.44	0.47
4:L7:92:C:H2'	4:L7:93:G:H8	1.79	0.47
5:L8:21:C:N4	5:L8:22:U:O4	2.47	0.47
7:LE:120:LYS:HG3	7:LE:121:ASN:N	2.29	0.47
7:LE:315:ASN:N	7:LE:315:ASN:OD1	2.48	0.47
16:LO:130:LYS:HE3	16:LO:132:SER:HB2	1.96	0.47
16:LO:204:GLU:HA	16:LO:207:VAL:HB	1.95	0.47
17:LP:118:MET:O	17:LP:122:ILE:HG12	2.14	0.47
21:LT:75:ARG:HA	21:LT:78:LYS:HD2	1.96	0.47
21:LT:177:ALA:O	21:LT:184:ARG:HB2	2.14	0.47
49:S2:605:A:H4'	66:SU:22:LYS:HE2	1.96	0.47
49:S2:1846:A:H2'	49:S2:1847:G:C8	2.50	0.47
49:S2:1860:A:P	54:SF:10:ARG:HH12	2.38	0.47
75:Sd:35:GLY:O	75:Sd:97:GLN:NE2	2.48	0.47
3:L5:228:C:H2'	3:L5:229:G:H8	1.79	0.47
3:L5:1463:A:OP1	8:LF:110:ARG:NH1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2036:A:H3'	3:L5:2037:G:H5'	1.95	0.47
3:L5:2204:G:O2'	3:L5:3591:G:O6	2.24	0.47
3:L5:2654:G:N2	3:L5:2657:C:OP2	2.46	0.47
9:LG:40:ASP:OD1	24:LW:69:GLN:HA	2.14	0.47
9:LG:223:PHE:HB3	9:LG:226:TYR:HB2	1.95	0.47
16:LO:120:TYR:HB2	16:LO:155:MET:HE1	1.96	0.47
23:LV:71:SER:HB2	23:LV:74:ARG:HD3	1.96	0.47
49:S2:914:A:N6	64:SS:119:SER:O	2.42	0.47
50:SB:54:VAL:HG23	50:SB:63:LEU:HB2	1.96	0.47
55:SG:298:LEU:HB3	55:SG:310:TRP:HB2	1.96	0.47
66:SU:74:GLY:HA2	66:SU:94:LEU:HD21	1.97	0.47
81:Sj:68:LYS:NZ	81:Sj:69:THR:O	2.48	0.47
2:I:67:G:OP1	2:I:67:G:H4'	2.09	0.47
3:L5:1416:C:P	21:LT:144:LYS:HD3	2.54	0.47
3:L5:2509:U:OP2	22:LU:124:TYR:OH	2.28	0.47
3:L5:3660:A:N1	6:LD:230:PRO:HB3	2.29	0.47
7:LE:90:VAL:HG13	7:LE:161:ARG:HB2	1.96	0.47
31:Ld:125:LYS:HD3	31:Ld:147:VAL:HG21	1.96	0.47
35:Lh:104:SER:O	35:Lh:108:ARG:HG3	2.14	0.47
49:S2:384:G:O3'	68:SW:132:ARG:NH1	2.47	0.47
49:S2:669:A2M:HM'1	49:S2:1198:G:H1'	1.96	0.47
49:S2:1403:A:N6	49:S2:1442:U:O2'	2.46	0.47
54:SF:51:ARG:O	54:SF:55:GLU:HG2	2.14	0.47
55:SG:83:TRP:HD1	55:SG:107:ASP:HB3	1.78	0.47
66:SU:134:HIS:O	66:SU:160:SER:N	2.41	0.47
67:SV:14:LEU:HD22	67:SV:21:MET:HE1	1.97	0.47
68:SW:18:GLN:O	68:SW:22:ARG:NH1	2.43	0.47
75:Sd:25:LYS:O	75:Sd:29:ALA:N	2.47	0.47
2:I:75:A:H5'	2:I:157:C:H5''	1.95	0.47
3:L5:764:G:N2	3:L5:789:G:N7	2.61	0.47
3:L5:1755:C:O3'	32:Le:38:LYS:NZ	2.48	0.47
3:L5:2272:A:H5''	42:Lo:43:HIS:NE2	2.29	0.47
3:L5:2518:G:N1	33:Lf:33:GLN:OE1	2.46	0.47
3:L5:3464:A:H2'	3:L5:3465:A:C8	2.50	0.47
3:L5:4050:A:OP2	3:L5:4051:G:N2	2.45	0.47
3:L5:4639:C:O2'	3:L5:4641:C:OP2	2.30	0.47
18:LQ:113:LEU:HB2	18:LQ:134:LEU:HD12	1.96	0.47
22:LU:10:LEU:HD12	22:LU:38:ARG:HG2	1.97	0.47
48:S:1129:A:H2	49:S2:1296:A:H1'	1.78	0.47
49:S2:970:U:OP1	49:S2:971:G:O2'	2.26	0.47
49:S2:1184:A:OP1	83:Sl:15:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1516:G:H2'	49:S2:1517:G:H8	1.79	0.47
55:SG:7:LEU:HD11	55:SG:308:ARG:HB3	1.97	0.47
55:SG:23:THR:HG22	55:SG:31:ILE:HD12	1.97	0.47
60:SO:48:ILE:HG13	60:SO:86:LEU:HD23	1.96	0.47
72:Sa:103:ASN:OD1	72:Sa:120:SER:OG	2.25	0.47
75:Sd:84:LEU:O	75:Sd:87:GLN:NE2	2.40	0.47
3:L5:88:A:N7	21:LT:173:LYS:NZ	2.61	0.47
3:L5:1927:G:H2'	3:L5:1928:G:H8	1.80	0.47
3:L5:3817:G:H2'	3:L5:3818:G:C8	2.49	0.47
3:L5:4006:U:H2'	3:L5:4007:C:C6	2.50	0.47
3:L5:4443:U:H4'	43:Lp:104:HIS:CE1	2.50	0.47
3:L5:4627:C:H2'	3:L5:4628:G:C8	2.50	0.47
15:LM:84:GLU:O	15:LM:88:LYS:HG2	2.15	0.47
16:LO:179:PHE:N	31:Ld:134:GLU:OE1	2.36	0.47
19:LR:196:LEU:HD12	19:LR:201:LEU:HB3	1.97	0.47
24:LW:18:PRO:HG2	24:LW:21:LYS:HB2	1.96	0.47
24:LW:40:VAL:HG21	24:LW:96:ILE:HD12	1.96	0.47
31:Ld:127:LYS:O	31:Ld:127:LYS:HE3	2.15	0.47
33:Lf:47:ILE:HD12	33:Lf:94:LEU:HD12	1.96	0.47
49:S2:563:U:H2'	49:S2:564:G:C8	2.50	0.47
49:S2:1395:G:H21	49:S2:1476:G:H1'	1.80	0.47
59:SN:78:LEU:HA	59:SN:81:ILE:HD13	1.95	0.47
59:SN:200:ARG:O	66:SU:54:ARG:NH2	2.39	0.47
63:SR:52:ILE:HG23	63:SR:109:LEU:HD21	1.97	0.47
75:Sd:46:ARG:HH21	76:Se:50:GLU:HG2	1.80	0.47
1:B:432:GLN:HG2	49:S2:1291:G:C1'	2.37	0.47
2:I:158:A:H2'	2:I:159:G:C4	2.50	0.47
3:L5:475:G:H2'	3:L5:476:G:C8	2.50	0.47
3:L5:865:G:C8	11:LI:28:LYS:HE2	2.49	0.47
3:L5:1013:G:C8	3:L5:1089:G:C2	3.03	0.47
3:L5:1572:G:O3'	40:Lm:12:ARG:NH2	2.48	0.47
3:L5:1699:G:N2	3:L5:1711:C:O2	2.43	0.47
3:L5:1809:C:H2'	3:L5:1810:A2M:H8	1.97	0.47
3:L5:2247:A:OP2	42:Lo:2:SER:OG	2.19	0.47
3:L5:3480:A:O5'	6:LD:243:THR:OG1	2.33	0.47
3:L5:3998:C:H42	15:LM:25:CYS:HB3	1.80	0.47
3:L5:4445:U:H1'	3:L5:4446:A:H5''	1.96	0.47
3:L5:4599:G:H5''	19:LR:169:ARG:NH1	2.29	0.47
4:L7:1:GTP:H8	4:L7:1:GTP:O5'	1.98	0.47
4:L7:92:C:H2'	4:L7:93:G:C8	2.50	0.47
6:LD:80:GLU:HB2	6:LD:170:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LD:201:GLY:HA3	6:LD:209:HIS:CE1	2.50	0.47
7:LE:63:PRO:HA	7:LE:68:ASN:ND2	2.27	0.47
7:LE:378:ARG:HG2	27:LZ:32:LEU:HD21	1.97	0.47
9:LG:152:ARG:O	9:LG:157:ASN:ND2	2.48	0.47
12:LJ:88:ASP:OD1	12:LJ:88:ASP:N	2.40	0.47
14:LL:53:VAL:HG13	14:LL:164:LYS:HB2	1.96	0.47
15:LM:24:ILE:HG21	15:LM:36:ALA:HB1	1.97	0.47
21:LT:124:ASP:N	21:LT:124:ASP:OD1	2.47	0.47
25:LX:69:LYS:NZ	25:LX:71:THR:OG1	2.47	0.47
29:Lb:74:TYR:CE2	29:Lb:76:LYS:HB3	2.50	0.47
32:Le:65:MET:HG2	32:Le:68:ARG:CZ	2.45	0.47
49:S2:496:U:H4'	61:SP:24:THR:HG22	1.97	0.47
49:S2:684:OMG:N1	49:S2:1023:U:OP2	2.33	0.47
49:S2:1411:C:H2'	49:S2:1412:G:H8	1.78	0.47
49:S2:1546:A:H4'	73:Sb:74:GLY:HA2	1.96	0.47
49:S2:1652:A:H61	49:S2:1674:U:H3	1.63	0.47
54:SF:12:LYS:N	54:SF:33:ASP:OD2	2.48	0.47
55:SG:133:ASN:HD21	55:SG:137:VAL:HB	1.80	0.47
59:SN:206:SER:HB2	59:SN:210:PRO:HG2	1.95	0.47
61:SP:100:ARG:HB2	61:SP:114:ILE:HD13	1.97	0.47
66:SU:63:LEU:O	66:SU:70:ARG:NH1	2.48	0.47
73:Sb:82:TYR:HA	73:Sb:85:ARG:HD3	1.95	0.47
74:Sc:17:ILE:HD11	74:Sc:21:TYR:HD1	1.80	0.47
74:Sc:57:LEU:HA	74:Sc:60:ARG:HG3	1.96	0.47
3:L5:4201:G:OP1	7:LE:5:LYS:HD3	2.15	0.47
3:L5:4283:C:H2'	3:L5:4284:G:C8	2.50	0.47
11:LI:53:ALA:HB2	11:LI:187:GLU:HG3	1.97	0.47
58:SM:88:THR:HG22	58:SM:98:THR:HG22	1.95	0.47
64:SS:21:SER:O	64:SS:24:SER:OG	2.27	0.47
64:SS:34:SER:HA	64:SS:37:LYS:HG3	1.96	0.47
78:Sg:67:ASP:OD2	78:Sg:71:ARG:NH1	2.44	0.47
1:B:431:GLN:HG3	49:S2:1292:A:H5'	1.96	0.47
3:L5:1868:A:C8	3:L5:1871:A:H1'	2.50	0.47
3:L5:2243:G:H21	37:Lj:6:THR:HG22	1.80	0.47
3:L5:2583:U:O2'	3:L5:2585:G:N2	2.47	0.47
3:L5:2688:A:H61	3:L5:3575:C:N4	2.12	0.47
3:L5:4640:G:N2	3:L5:4660:C:N3	2.63	0.47
3:L5:4699:G:H2'	3:L5:4700:G:H8	1.80	0.47
8:LF:190:ARG:N	8:LF:200:ARG:O	2.41	0.47
8:LF:266:THR:OG1	8:LF:267:TRP:N	2.47	0.47
9:LG:265:ARG:NE	9:LG:269:PRO:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LH:64:MET:O	10:LH:68:LYS:HG2	2.14	0.47
11:LI:133:ARG:HA	11:LI:136:GLU:HG3	1.96	0.47
19:LR:12:ARG:HB2	19:LR:37:ARG:HD2	1.97	0.47
31:Ld:131:ARG:HH21	31:Ld:132:ARG:CZ	2.28	0.47
49:S2:892:G:H2'	49:S2:893:U:C6	2.50	0.47
49:S2:1366:G:H2'	49:S2:1367:G:C8	2.50	0.47
49:S2:1399:G:H4'	55:SG:61:GLY:O	2.14	0.47
50:SB:33:MET:HE2	50:SB:48:SER:HA	1.97	0.47
62:SQ:133:THR:OG1	62:SQ:135:ARG:NH1	2.39	0.47
71:SZ:61:LYS:NZ	71:SZ:76:LEU:O	2.48	0.47
1:B:460:GLU:HG3	1:B:464:HIS:CE1	2.50	0.47
3:L5:723:G:OP1	23:LV:63:TYR:OH	2.23	0.47
3:L5:3819:G:C6	3:L5:3820:G:C6	3.03	0.47
3:L5:4515:G:OP1	19:LR:168:TYR:OH	2.32	0.47
9:LG:52:ILE:HB	9:LG:63:GLN:HB2	1.97	0.47
11:LI:66:THR:OG1	11:LI:69:ARG:NH2	2.48	0.47
19:LR:65:ASN:OD1	19:LR:67:SER:OG	2.23	0.47
19:LR:119:VAL:HG11	23:LV:171:ARG:HD3	1.96	0.47
20:LS:78:TRP:CD1	20:LS:80:GLN:H	2.33	0.47
39:Ll:33:LEU:HD21	39:Ll:38:LYS:HD3	1.96	0.47
46:Ls:82:ILE:HG22	46:Ls:89:THR:HG22	1.97	0.47
49:S2:193:C:H42	49:S2:208:G:N2	2.13	0.47
49:S2:602:OMG:HM22	49:S2:603:G:H5'	1.96	0.47
49:S2:1737:G:H2'	49:S2:1738:G:C8	2.50	0.47
49:S2:1809:U:H2'	49:S2:1810:A:H8	1.79	0.47
55:SG:150:TRP:HB2	55:SG:170:TRP:CD1	2.50	0.47
59:SN:205:VAL:O	59:SN:224:THR:OG1	2.28	0.47
65:ST:69:SER:HB2	65:ST:191:GLU:OE1	2.15	0.47
73:Sb:101:ASP:OD1	73:Sb:104:SER:OG	2.28	0.47
77:Sf:24:LEU:HB2	77:Sf:87:ARG:HB2	1.96	0.47
80:Si:107:ARG:HG3	80:Si:112:VAL:HG22	1.97	0.47
2:I:34:A:H2'	2:I:35:U:C6	2.51	0.46
3:L5:75:G:O2'	16:LO:99:ASP:OD1	2.28	0.46
3:L5:882:U:OP2	10:LH:48:ARG:NH2	2.48	0.46
3:L5:1016:C:O2'	3:L5:1086:G:H2'	2.16	0.46
3:L5:1210:C:OP2	32:Le:111:ARG:NH1	2.37	0.46
3:L5:2329:G:H5''	3:L5:2332:C:H42	1.80	0.46
8:LF:330:PRO:HD3	11:LI:46:ARG:HH21	1.80	0.46
31:Ld:14:HIS:O	31:Ld:16:SER:N	2.48	0.46
47:Lx:66:CYS:N	47:Lx:109:ALA:O	2.47	0.46
48:S:1144:G:H4'	48:S:1145:G:OP1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:528:C:H2'	49:S2:529:A:H8	1.80	0.46
49:S2:630:A:O2'	49:S2:632:U:OP1	2.33	0.46
49:S2:1455:A:H2	49:S2:1477:A:H1'	1.80	0.46
62:SQ:133:THR:H	62:SQ:135:ARG:NH1	2.13	0.46
65:ST:114:GLU:HG3	65:ST:136:ILE:HG22	1.97	0.46
3:L5:1724:C:OP1	14:LL:133:GLN:NE2	2.44	0.46
8:LF:66:SER:HA	8:LF:77:PRO:HA	1.97	0.46
11:LI:227:VAL:HA	23:LV:39:VAL:HG22	1.97	0.46
13:LK:117:PHE:O	13:LK:120:GLU:HB2	2.14	0.46
37:Lj:60:ARG:HB2	37:Lj:63:VAL:HG23	1.97	0.46
49:S2:944:U:OP1	58:SM:214:LYS:NZ	2.43	0.46
3:L5:1804:G:OP2	14:LL:98:ARG:NH2	2.40	0.46
3:L5:2338:U:H2'	3:L5:2339:G:H8	1.79	0.46
3:L5:4361:C:P	7:LE:357:ARG:HH22	2.37	0.46
7:LE:206:PRO:HG2	7:LE:209:GLN:HG3	1.96	0.46
7:LE:286:LYS:N	7:LE:332:MET:HB2	2.30	0.46
9:LG:115:MET:HA	9:LG:118:ILE:HD13	1.98	0.46
49:S2:746:C:H2'	49:S2:747:C:C2	2.50	0.46
49:S2:1325:G:O2'	49:S2:1511:G:O2'	2.30	0.46
49:S2:1366:G:H2'	49:S2:1367:G:H8	1.80	0.46
49:S2:1519:C:OP1	49:S2:1520:U:O2'	2.31	0.46
55:SG:234:ASP:HB2	55:SG:252:THR:HB	1.96	0.46
71:SZ:140:THR:OG1	71:SZ:141:ARG:N	2.48	0.46
79:Sh:77:PRO:HB2	80:Si:7:LEU:HD22	1.98	0.46
1:B:446:LEU:HD21	52:SD:146:LEU:HA	1.97	0.46
3:L5:62:A:OP1	18:LQ:172:ARG:NH1	2.47	0.46
3:L5:670:C:H2'	3:L5:671:G:C8	2.51	0.46
3:L5:1001:C:H2'	3:L5:1002:A:C8	2.51	0.46
3:L5:3694:A:N7	3:L5:3777:U:N3	2.63	0.46
3:L5:4447:A:H1'	13:LK:41:ILE:HD11	1.98	0.46
12:LJ:63:LEU:HD12	18:LQ:32:GLN:HB2	1.97	0.46
17:LP:24:LEU:HB2	17:LP:43:THR:HG21	1.98	0.46
19:LR:162:GLU:HG2	19:LR:163:LYS:N	2.29	0.46
32:Le:61:ASN:O	32:Le:65:MET:N	2.35	0.46
49:S2:400:C:N3	68:SW:89:ARG:NH2	2.63	0.46
49:S2:473:C:O2	49:S2:476:C:N4	2.46	0.46
49:S2:1172:G:O2'	49:S2:1188:G:O6	2.34	0.46
51:SC:29:GLN:NE2	51:SC:66:ARG:O	2.44	0.46
55:SG:73:SER:OG	55:SG:117:ASN:ND2	2.32	0.46
59:SN:120:GLN:OE1	59:SN:120:GLN:N	2.48	0.46
66:SU:26:ASP:OD1	66:SU:27:GLN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Sa:121:ILE:HD12	75:Sd:120:HIS:HD2	1.80	0.46
3:L5:1276:C:H2'	3:L5:1277:A:C8	2.49	0.46
3:L5:1548:A:H5''	3:L5:2682:U:H5''	1.98	0.46
3:L5:1672:G:N3	3:L5:3960:A:H2'	2.31	0.46
3:L5:4135:C:H2'	3:L5:4136:A:C8	2.51	0.46
14:LL:162:ARG:HH21	14:LL:164:LYS:NZ	2.14	0.46
19:LR:177:LEU:O	19:LR:181:ALA:N	2.46	0.46
47:Lx:99:LEU:O	47:Lx:103:LEU:N	2.39	0.46
49:S2:17:C:H2'	49:S2:18:C:C6	2.51	0.46
49:S2:116:OMU:O5'	49:S2:116:OMU:H6	2.14	0.46
49:S2:1008:C:H2'	49:S2:1009:A:C8	2.50	0.46
49:S2:1375:C:H2'	49:S2:1376:G:O4'	2.16	0.46
49:S2:1452:G:OP1	74:Sc:33:ARG:NH2	2.49	0.46
3:L5:92:C:C2	31:Ld:55:LYS:HD3	2.51	0.46
3:L5:2032:G:H5''	3:L5:2034:A:O4'	2.15	0.46
6:LD:57:PRO:HG2	6:LD:78:ALA:HB3	1.97	0.46
6:LD:83:HIS:CE1	6:LD:86:GLN:HB2	2.51	0.46
11:LI:237:ASP:O	11:LI:240:ASN:ND2	2.37	0.46
13:LK:103:VAL:HG11	13:LK:144:LEU:HD21	1.96	0.46
17:LP:24:LEU:HD11	17:LP:86:TRP:CG	2.51	0.46
17:LP:91:TRP:O	17:LP:95:ILE:HG13	2.16	0.46
44:Lq:59:LYS:H	44:Lq:59:LYS:HD2	1.80	0.46
49:S2:220:U:H2'	49:S2:221:A:H8	1.80	0.46
49:S2:1453:A:OP2	74:Sc:32:LYS:NZ	2.48	0.46
55:SG:57:ARG:HH22	73:Sb:99:TYR:C	2.24	0.46
65:ST:173:ALA:HA	65:ST:189:VAL:HA	1.98	0.46
69:SX:72:HIS:HD1	69:SX:74:ILE:HD11	1.78	0.46
3:L5:85:G:N2	3:L5:98:A:OP2	2.30	0.46
3:L5:318:A:H2'	3:L5:319:A:C8	2.51	0.46
3:L5:827:C:H2'	3:L5:828:A:C8	2.50	0.46
3:L5:2106:A:H5''	46:Ls:108:MET:SD	2.55	0.46
3:L5:2362:U:H1'	3:L5:2363:C:C6	2.51	0.46
3:L5:2372:A:O2'	3:L5:2374:C:OP2	2.33	0.46
3:L5:3422:U:H5	6:LD:200:ARG:HD3	1.81	0.46
3:L5:3776:A:H4'	3:L5:3777:U:H5'	1.97	0.46
3:L5:3850:G:O2'	30:Lc:136:PHE:OXT	2.29	0.46
3:L5:4346:G:O2'	3:L5:4355:G:O6	2.28	0.46
8:LF:221:PHE:HB2	8:LF:229:LEU:HD21	1.98	0.46
9:LG:122:GLN:O	9:LG:248:ARG:NH2	2.48	0.46
12:LJ:255:LYS:HA	12:LJ:258:ALA:HB3	1.97	0.46
18:LQ:94:PHE:CE2	18:LQ:96:ARG:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LQ:157:LYS:O	18:LQ:162:ARG:NH1	2.49	0.46
49:S2:65:C:C6	63:SR:174:PRO:HB3	2.49	0.46
49:S2:1102:U:H2'	49:S2:1103:G:C8	2.51	0.46
57:SL:56:GLU:OE2	78:Sg:80:SER:OG	2.33	0.46
58:SM:48:LEU:O	71:SZ:51:GLU:HG3	2.15	0.46
62:SQ:35:LEU:HD23	62:SQ:143:PRO:HB3	1.97	0.46
76:Se:99:VAL:O	76:Se:103:VAL:HG23	2.16	0.46
82:Sk:50:PHE:HE1	82:Sk:79:ILE:HG21	1.80	0.46
2:I:56:A:N1	2:I:126:C:O2'	2.49	0.46
2:I:134:C:N4	2:I:135:C:C2	2.84	0.46
2:I:146:C:H1'	82:Sk:76:ARG:NH1	2.31	0.46
3:L5:67:C:OP2	3:L5:312:G:N2	2.46	0.46
3:L5:2423:U:H4'	30:Lc:74:VAL:O	2.16	0.46
6:LD:30:ARG:HG2	6:LD:74:GLU:HG3	1.97	0.46
8:LF:209:VAL:HB	8:LF:229:LEU:HD13	1.98	0.46
49:S2:1123:A:N3	58:SM:146:ARG:NH1	2.64	0.46
68:SW:38:LYS:N	68:SW:62:PHE:O	2.49	0.46
2:I:32:A:H2'	2:I:94:U:C2	2.51	0.46
2:I:40:U:O2	2:I:87:G:H5'	2.16	0.46
2:I:105:U:O2'	2:I:154:A:N6	2.49	0.46
3:L5:1001:C:H2'	3:L5:1002:A:H8	1.79	0.46
3:L5:1972:A:OP1	14:LL:162:ARG:NH2	2.49	0.46
3:L5:3819:G:H2'	3:L5:3820:G:C8	2.51	0.46
3:L5:4621:U:H1'	36:Li:1:MET:H2	1.80	0.46
6:LD:136:VAL:HG12	6:LD:148:VAL:HG12	1.96	0.46
11:LI:126:LYS:HB2	24:LW:133:ALA:HB3	1.98	0.46
12:LJ:31:LEU:HD21	30:Lc:123:LYS:HA	1.96	0.46
13:LK:40:HIS:ND1	13:LK:41:ILE:HG12	2.30	0.46
20:LS:19:GLY:N	20:LS:146:ILE:O	2.45	0.46
26:LY:85:ARG:N	26:LY:101:ASN:OD1	2.46	0.46
29:Lb:73:VAL:HG12	29:Lb:80:ILE:HG22	1.98	0.46
49:S2:294:C:O2'	49:S2:295:U:H3'	2.16	0.46
49:S2:503:C:O4'	61:SP:66:MET:HG3	2.15	0.46
49:S2:1309:U:O2'	49:S2:1310:C:O4'	2.31	0.46
49:S2:1514:C:P	56:SH:12:ARG:HH22	2.39	0.46
64:SS:135:PHE:CD1	64:SS:136:PRO:HA	2.51	0.46
71:SZ:118:ALA:HA	71:SZ:121:ARG:HB2	1.97	0.46
75:Sd:15:VAL:O	75:Sd:18:THR:OG1	2.28	0.46
1:B:448:VAL:CG2	52:SD:148:TYR:CB	2.52	0.46
3:L5:1013:G:C8	3:L5:1091:G:C2	3.04	0.46
3:L5:1016:C:C4	3:L5:1086:G:N7	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2664:U:OP1	22:LU:21:LYS:NZ	2.38	0.46
6:LD:36:GLU:O	6:LD:92:LYS:N	2.45	0.46
17:LP:118:MET:HE2	17:LP:122:ILE:HD11	1.98	0.46
49:S2:61:A:HO2'	49:S2:316:C:HO2'	1.59	0.46
49:S2:450:A:O3'	61:SP:3:ARG:NH1	2.49	0.46
49:S2:523:A:H5''	66:SU:145:PRO:HD2	1.98	0.46
49:S2:1076:C:H2'	49:S2:1077:G:C8	2.51	0.46
49:S2:1846:A:H2'	49:S2:1847:G:H8	1.81	0.46
53:SE:122:THR:HG22	53:SE:124:GLY:H	1.81	0.46
55:SG:60:ARG:NH1	73:Sb:97:GLN:OE1	2.49	0.46
58:SM:99:ASN:OD1	58:SM:100:PHE:N	2.48	0.46
60:SO:72:VAL:HG11	67:SV:70:TYR:HE1	1.81	0.46
63:SR:22:ARG:HG2	63:SR:25:ARG:HH12	1.79	0.46
66:SU:134:HIS:ND1	66:SU:163:SER:OG	2.36	0.46
74:Sc:35:CYS:HA	74:Sc:38:ILE:HG12	1.97	0.46
74:Sc:54:VAL:O	74:Sc:58:MET:N	2.49	0.46
76:Se:129:ARG:CZ	76:Se:129:ARG:HA	2.46	0.46
3:L5:1259:C:OP2	35:Lh:44:ARG:NH1	2.48	0.45
3:L5:2742:C:P	22:LU:108:ARG:HH22	2.40	0.45
3:L5:4614:G:H5''	23:LV:170:LYS:NZ	2.31	0.45
10:LH:215:LEU:HD12	10:LH:220:PHE:CZ	2.50	0.45
13:LK:91:LYS:HB2	13:LK:183:GLU:HB2	1.97	0.45
23:LV:7:LEU:HD23	23:LV:107:THR:HA	1.98	0.45
25:LX:46:ARG:HB3	25:LX:86:LEU:HD11	1.98	0.45
27:LZ:105:ARG:O	27:LZ:109:ILE:N	2.34	0.45
48:S:1142:U:H2'	48:S:1143:G:C5	2.51	0.45
51:SC:45:ASN:O	62:SQ:139:VAL:HG13	2.16	0.45
57:SL:125:THR:HG22	57:SL:175:TRP:HE1	1.81	0.45
61:SP:222:LEU:O	61:SP:225:ILE:HG22	2.16	0.45
3:L5:1680:G:O6	4:L7:103:A:O2'	2.24	0.45
3:L5:2200:G:OP1	20:LS:121:LYS:NZ	2.41	0.45
3:L5:2678:A:O2'	7:LE:228:TYR:O	2.32	0.45
3:L5:3816:C:O2	12:LJ:53:ARG:NH2	2.49	0.45
3:L5:4204:C:H2'	3:L5:4205:U:C6	2.51	0.45
5:L8:58:G:N7	40:Lm:63:ARG:NH2	2.59	0.45
5:L8:74:U:H3	29:Lb:72:GLN:NE2	2.14	0.45
6:LD:104:VAL:HA	6:LD:107:MET:HE2	1.98	0.45
7:LE:286:LYS:H	7:LE:332:MET:HB2	1.80	0.45
10:LH:68:LYS:HG3	10:LH:70:LEU:HG	1.98	0.45
24:LW:2:THR:OG1	24:LW:3:ASN:N	2.49	0.45
24:LW:84:ILE:HG13	32:Le:24:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1764:G:H2'	49:S2:1765:G:C8	2.50	0.45
55:SG:61:GLY:O	55:SG:88:ARG:NE	2.49	0.45
55:SG:258:ILE:HG13	55:SG:268:ASP:H	1.81	0.45
55:SG:272:GLN:OE1	55:SG:308:ARG:NH2	2.49	0.45
57:SL:189:ILE:HG22	57:SL:191:ARG:H	1.81	0.45
59:SN:91:SER:HB3	59:SN:156:ILE:HG23	1.98	0.45
2:I:32:A:H2	2:I:94:U:H3'	1.82	0.45
3:L5:708:G:O2'	8:LF:316:LYS:NZ	2.49	0.45
3:L5:801:C:H2'	3:L5:802:C:C6	2.52	0.45
3:L5:1524:U:H2'	3:L5:1525:G:C8	2.51	0.45
3:L5:1909:A:O2'	3:L5:1956:A:N6	2.50	0.45
3:L5:2422:G:N2	3:L5:2425:A:OP2	2.41	0.45
3:L5:3432:C:H2'	3:L5:3478:A:H61	1.81	0.45
3:L5:3488:A:H2'	3:L5:3489:G:H8	1.82	0.45
5:L8:67:U:H2'	5:L8:68:G:C8	2.51	0.45
7:LE:131:THR:O	7:LE:135:LYS:NZ	2.49	0.45
7:LE:150:PHE:HD1	7:LE:194:LEU:HD21	1.80	0.45
13:LK:4:ILE:HG12	13:LK:61:TRP:CH2	2.51	0.45
20:LS:95:LEU:HD11	20:LS:114:ILE:HD11	1.97	0.45
49:S2:417:U:H2'	49:S2:418:C:O4'	2.16	0.45
49:S2:1373:U:OP1	49:S2:1386:G:N2	2.36	0.45
58:SM:75:GLN:HB3	58:SM:78:GLU:HG3	1.98	0.45
61:SP:127:ARG:NE	61:SP:142:HIS:HA	2.31	0.45
3:L5:1399:G:N2	3:L5:1399:G:OP2	2.49	0.45
3:L5:3478:A:H5'	6:LD:243:THR:HG23	1.99	0.45
3:L5:3479:A:H8	6:LD:245:ARG:HD2	1.78	0.45
3:L5:3827:G:C2	3:L5:3840:C:C2	3.05	0.45
3:L5:4043:G:H2'	3:L5:4044:A:H8	1.81	0.45
7:LE:66:LYS:HE2	26:LY:11:GLY:HA3	1.98	0.45
16:LO:40:GLN:O	16:LO:44:ARG:HG3	2.16	0.45
25:LX:33:ILE:HD12	25:LX:100:LEU:HD21	1.97	0.45
28:La:39:LYS:HG3	28:La:40:ILE:HG23	1.98	0.45
32:Le:107:ARG:NH1	32:Le:107:ARG:HA	2.31	0.45
48:S:1115:C:O2'	48:S:1116:G:O5'	2.33	0.45
49:S2:417:U:O2'	49:S2:653:U:O2'	2.34	0.45
49:S2:649:A:N3	80:Si:45:SER:OG	2.40	0.45
49:S2:875:G:H2'	49:S2:876:A:H8	1.81	0.45
60:SO:133:GLY:HA3	60:SO:156:LEU:O	2.15	0.45
65:ST:57:ALA:HB2	65:ST:183:GLY:HA2	1.97	0.45
73:Sb:116:ASP:OD2	73:Sb:118:THR:OG1	2.28	0.45
3:L5:800:U:H2'	3:L5:801:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1784:U:H2'	3:L5:1785:G:C8	2.51	0.45
3:L5:2595:G:H4'	37:Lj:78:TYR:HE1	1.82	0.45
11:LI:141:TRP:CZ2	11:LI:234:ASN:HB2	2.52	0.45
18:LQ:3:ALA:O	18:LQ:7:ILE:HG12	2.16	0.45
40:Lm:22:CYS:SG	40:Lm:24:SER:OG	2.65	0.45
43:Lp:110:CYS:SG	43:Lp:111:ARG:N	2.89	0.45
48:S:1126:A:H4'	48:S:1127:A:OP2	2.17	0.45
49:S2:165:G:H2'	49:S2:166:A2M:H8	1.97	0.45
49:S2:234:C:H2'	49:S2:235:A:C8	2.52	0.45
49:S2:531:U:H2'	49:S2:532:A:H8	1.81	0.45
49:S2:827:A:O2'	66:SU:9:CYS:SG	2.56	0.45
49:S2:1205:A:N6	49:S2:1694:G:O6	2.50	0.45
49:S2:1485:A:H2'	49:S2:1486:U:C6	2.51	0.45
49:S2:1758:G:H2'	49:S2:1759:G:C8	2.51	0.45
51:SC:63:ARG:HH12	62:SQ:138:ALA:HB3	1.82	0.45
53:SE:102:ARG:HH21	53:SE:110:MET:HG3	1.81	0.45
57:SL:108:PHE:HB2	57:SL:136:GLU:HG2	1.99	0.45
59:SN:110:MET:HE2	59:SN:127:PHE:HE2	1.82	0.45
60:SO:132:LYS:HE2	60:SO:189:MET:HE2	1.99	0.45
71:SZ:149:ARG:HH12	71:SZ:151:LEU:HD13	1.82	0.45
73:Sb:132:PHE:O	73:Sb:140:ARG:NH2	2.44	0.45
3:L5:685:C:P	10:LH:117:ARG:HH21	2.40	0.45
3:L5:2573:U:H2'	3:L5:2574:C:C6	2.52	0.45
3:L5:2687:A:O2'	3:L5:4377:G:H4'	2.16	0.45
3:L5:4269:A2M:O3'	7:LE:246:ARG:NH1	2.49	0.45
6:LD:114:CYS:SG	6:LD:115:CYS:N	2.89	0.45
13:LK:44:GLU:O	13:LK:57:VAL:HA	2.17	0.45
19:LR:165:LYS:O	19:LR:169:ARG:HG3	2.17	0.45
30:Lc:47:ASP:N	30:Lc:69:LYS:O	2.47	0.45
32:Le:101:HIS:CE1	32:Le:103:LYS:HB3	2.52	0.45
49:S2:1278:C:H2'	49:S2:1279:A:H8	1.82	0.45
49:S2:1581:A:O2'	49:S2:1582:C:H5'	2.17	0.45
60:SO:66:ILE:HD11	60:SO:86:LEU:HB3	1.99	0.45
66:SU:34:GLU:HG3	66:SU:35:TYR:CD1	2.52	0.45
67:SV:27:VAL:HG23	67:SV:28:HIS:CD2	2.51	0.45
70:SY:66:VAL:HG13	70:SY:67:THR:HG23	1.99	0.45
2:I:172:G:HO2'	2:I:173:C:P	2.38	0.45
3:L5:29:G:H5''	18:LQ:172:ARG:HG2	1.99	0.45
3:L5:882:U:H2'	3:L5:883:C:C6	2.51	0.45
3:L5:1292:U:H2'	3:L5:1293:G:C8	2.50	0.45
3:L5:1815:U:H2'	3:L5:1816:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2271:A:H8	42:Lo:45:ARG:HH21	1.64	0.45
12:LJ:48:LYS:HB3	28:La:42:THR:HG23	1.98	0.45
18:LQ:120:TRP:HZ2	18:LQ:123:GLU:HG2	1.82	0.45
32:Le:101:HIS:C	32:Le:109:ARG:HH22	2.24	0.45
35:Lh:46:ARG:HA	35:Lh:55:MET:SD	2.56	0.45
49:S2:371:G:O2'	65:ST:10:LYS:NZ	2.50	0.45
49:S2:668:U:O4	49:S2:1144:A:N6	2.50	0.45
49:S2:1061:A:O2'	49:S2:1063:A:N7	2.42	0.45
49:S2:1693:PSU:O3'	54:SF:92:ARG:NH2	2.50	0.45
49:S2:1864:A:OP2	54:SF:4:LYS:NZ	2.49	0.45
52:SD:132:MET:HB3	52:SD:139:HIS:HB3	1.99	0.45
59:SN:179:THR:HG21	59:SN:198:ALA:O	2.16	0.45
61:SP:175:PHE:HE1	61:SP:198:ARG:HD2	1.82	0.45
71:SZ:33:ILE:HG13	71:SZ:97:LEU:HA	1.99	0.45
78:Sg:73:ALA:HB1	78:Sg:78:ILE:HB	1.99	0.45
82:Sk:65:TYR:HB2	82:Sk:68:ILE:HD11	1.97	0.45
1:B:431:GLN:CB	49:S2:1291:G:O2'	2.61	0.45
2:I:53:U:H3'	2:I:54:A:H5'	1.99	0.45
3:L5:2216:C:H5'	34:Lg:46:LEU:HD22	1.99	0.45
3:L5:2243:G:N2	37:Lj:6:THR:HG22	2.31	0.45
3:L5:2281:A:O2'	3:L5:2283:U:OP2	2.25	0.45
3:L5:2364:G:H2'	3:L5:2365:G:C8	2.51	0.45
3:L5:3934:U:H2'	3:L5:3935:U:C6	2.52	0.45
3:L5:4634:U:O2	17:LP:132:ARG:NH1	2.48	0.45
7:LE:43:LEU:HB2	7:LE:210:VAL:HG12	1.98	0.45
9:LG:60:ILE:HB	9:LG:80:ALA:HB2	1.99	0.45
15:LM:141:ILE:HA	15:LM:144:LYS:HG2	1.99	0.45
28:La:72:ASP:O	28:La:76:ILE:HG12	2.17	0.45
35:Lh:107:ASN:O	35:Lh:111:ILE:HG12	2.17	0.45
49:S2:1708:U:O2	49:S2:1850:G:N2	2.46	0.45
55:SG:261:LEU:O	55:SG:264:LYS:NZ	2.34	0.45
79:Sh:90:GLN:HA	79:Sh:94:LEU:HD23	1.98	0.45
1:B:697:ASN:OD1	1:B:730:ASN:HB2	2.16	0.45
3:L5:257:C:H2'	3:L5:258:G:H8	1.82	0.45
3:L5:345:C:H2'	3:L5:346:G:C8	2.51	0.45
3:L5:3923:C:H2'	3:L5:3924:A:H8	1.82	0.45
3:L5:4383:OMG:HM23	3:L5:4383:OMG:H1'	1.73	0.45
12:LJ:85:GLN:HE22	12:LJ:229:ARG:NH1	2.14	0.45
14:LL:87:ILE:HD13	14:LL:138:ILE:HG23	1.99	0.45
14:LL:91:LEU:HD12	14:LL:135:ILE:HG23	1.98	0.45
40:Lm:73:ARG:NH2	40:Lm:80:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S:1134:C:H2'	48:S:1135:C:H2'	1.99	0.45
57:SL:33:GLN:OE1	57:SL:154:LEU:HB2	2.17	0.45
63:SR:85:ARG:O	63:SR:87:ARG:NH1	2.50	0.45
69:SX:31:LEU:HD13	69:SX:111:VAL:HG22	1.98	0.45
72:Sa:100:LYS:HG2	72:Sa:101:THR:HG23	1.99	0.45
81:Sj:108:LYS:HA	81:Sj:111:LYS:HG2	1.98	0.45
3:L5:1415:C:H5''	21:LT:144:LYS:HG3	1.97	0.45
3:L5:1701:C:H2'	3:L5:1702:C:C6	2.52	0.45
3:L5:3601:OMC:HM23	3:L5:3601:OMC:H1'	1.76	0.45
3:L5:3792:C:H2'	3:L5:3793:G:H8	1.81	0.45
3:L5:4394:A:OP1	22:LU:62:ARG:NH2	2.50	0.45
6:LD:70:LYS:HE3	6:LD:70:LYS:HB3	1.88	0.45
6:LD:209:HIS:CE1	6:LD:235:VAL:HG11	2.52	0.45
9:LG:211:LEU:HD23	9:LG:219:TYR:HA	1.99	0.45
10:LH:227:LYS:NZ	10:LH:241:GLU:H	2.15	0.45
27:LZ:49:ILE:O	27:LZ:52:THR:HG22	2.17	0.45
37:Lj:8:ARG:HB2	37:Lj:34:TYR:HE1	1.82	0.45
43:Lp:96:CYS:HA	43:Lp:121:LEU:HD13	1.98	0.45
46:Ls:18:ILE:O	46:Ls:25:TYR:N	2.41	0.45
49:S2:987:G:O4'	71:SZ:138:ASP:HB2	2.17	0.45
57:SL:176:TRP:CD2	57:SL:199:PRO:HG3	2.52	0.45
57:SL:198:MET:HE3	57:SL:200:ASP:HB2	1.98	0.45
76:Se:128:GLN:NE2	76:Se:132:ASP:OD2	2.50	0.45
3:L5:474:C:H2'	3:L5:475:G:C8	2.52	0.44
3:L5:707:C:H2'	3:L5:708:G:C8	2.53	0.44
3:L5:1869:U:OP2	19:LR:49:ARG:HD2	2.17	0.44
3:L5:2104:G:P	46:Ls:94:ARG:HD2	2.58	0.44
3:L5:2706:G:O2'	22:LU:82:LYS:O	2.26	0.44
3:L5:4176:G:O5'	14:LL:63:GLU:HG3	2.17	0.44
3:L5:4203:PSU:H1'	7:LE:252:ALA:HB3	1.99	0.44
3:L5:4371:C:P	7:LE:223:THR:HG1	2.39	0.44
3:L5:4766:C:H5'	3:L5:4767:G:C8	2.51	0.44
7:LE:165:HIS:HB3	7:LE:180:LEU:HD23	1.99	0.44
7:LE:234:ARG:HA	7:LE:272:LYS:HD2	1.99	0.44
8:LF:37:VAL:HG11	8:LF:246:VAL:HG13	1.99	0.44
8:LF:218:VAL:HA	8:LF:229:LEU:HG	1.98	0.44
9:LG:51:MET:HE2	9:LG:64:ILE:HD11	1.98	0.44
49:S2:914:A:N3	64:SS:66:VAL:HG11	2.32	0.44
61:SP:103:TYR:HE1	61:SP:109:PHE:HE1	1.64	0.44
68:SW:40:ILE:HG21	68:SW:61:PRO:HB2	1.98	0.44
3:L5:242:U:H4'	29:Lb:2:LYS:HZ1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:420:A:H61	5:L8:15:G:H1'	1.82	0.44
3:L5:1457:G:H1	21:LT:89:ASP:HA	1.82	0.44
3:L5:2167:C:O2'	35:Lh:98:GLU:OE1	2.35	0.44
3:L5:2257:G:H2'	3:L5:2258:OMU:H6	1.99	0.44
6:LD:247:ARG:HG3	49:S2:1070:U:H4'	1.99	0.44
7:LE:83:PRO:O	7:LE:167:GLN:NE2	2.50	0.44
7:LE:231:VAL:HG21	7:LE:251:VAL:HG23	1.98	0.44
17:LP:10:GLY:HA2	17:LP:64:PHE:CE1	2.52	0.44
19:LR:42:ASN:HD22	19:LR:125:LYS:HD3	1.80	0.44
20:LS:120:ASN:O	20:LS:145:HIS:N	2.42	0.44
40:Lm:25:LYS:HD3	42:Lo:51:LEU:HB2	1.99	0.44
49:S2:163:U:OP2	63:SR:87:ARG:NH2	2.50	0.44
49:S2:564:G:N7	66:SU:172:ARG:NH2	2.66	0.44
49:S2:1845:U:H2'	49:S2:1846:A:C8	2.52	0.44
57:SL:149:ASN:OD1	57:SL:150:THR:N	2.38	0.44
65:ST:192:GLY:HA3	68:SW:19:ASN:OD1	2.17	0.44
70:SY:75:LEU:HD12	70:SY:80:LEU:HB2	1.98	0.44
80:Si:49:GLY:HA2	80:Si:75:ILE:HG12	1.98	0.44
1:B:432:GLN:OE1	49:S2:1312:C:H1'	2.17	0.44
3:L5:491:C:H2'	3:L5:492:G:C8	2.52	0.44
3:L5:1296:C:H2'	3:L5:1297:G:O4'	2.17	0.44
3:L5:1351:G:H22	3:L5:1366:C:H1'	1.82	0.44
3:L5:3794:U:H4'	39:Ll:59:GLU:OE2	2.17	0.44
3:L5:4381:A:O2'	3:L5:4383:OMG:H5'	2.17	0.44
10:LH:79:LYS:HE3	10:LH:79:LYS:HB2	1.82	0.44
31:Ld:71:PRO:HB2	31:Ld:108:TYR:HD1	1.83	0.44
49:S2:845:U:H2'	49:S2:846:G:C8	2.51	0.44
49:S2:1857:C:H2'	49:S2:1858:G:C8	2.52	0.44
50:SB:8:LEU:HD21	79:Sh:51:GLU:HG2	1.99	0.44
57:SL:110:ASN:OD1	57:SL:113:GLN:HG3	2.18	0.44
65:ST:76:THR:HG21	65:ST:104:ILE:HD12	1.99	0.44
80:Si:140:ARG:HH21	80:Si:142:ARG:HD2	1.83	0.44
3:L5:121:A:OP1	12:LJ:110:LYS:NZ	2.34	0.44
3:L5:413:G:H5'	42:Lo:36:ARG:HH12	1.81	0.44
3:L5:522:U:H2'	3:L5:523:C:C6	2.52	0.44
3:L5:994:C:C4	3:L5:1112:G:H2'	2.52	0.44
3:L5:1322:C:C2	16:LO:158:ARG:HD2	2.52	0.44
3:L5:1460:C:H2'	3:L5:1461:G:C8	2.53	0.44
3:L5:1489:A2M:H2'	3:L5:1489:A2M:H5'	1.79	0.44
3:L5:2323:G:H2'	3:L5:2324:G:C8	2.52	0.44
3:L5:3892:G:H2'	3:L5:3893:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4270:G:C2	7:LE:252:ALA:HB1	2.51	0.44
3:L5:4328:C:O2'	7:LE:99:LEU:O	2.22	0.44
3:L5:4635:G:H2'	3:L5:4636:G:C8	2.52	0.44
5:L8:151:G:O2'	12:LJ:64:GLN:NE2	2.51	0.44
16:LO:170:THR:HG23	16:LO:172:GLU:H	1.82	0.44
17:LP:88:ALA:O	17:LP:93:LYS:NZ	2.50	0.44
21:LT:122:THR:OG1	21:LT:124:ASP:OD1	2.31	0.44
23:LV:82:LEU:HA	23:LV:127:MET:HG3	1.99	0.44
38:Lk:13:LYS:HD3	38:Lk:15:GLU:H	1.82	0.44
47:Lx:86:ASP:N	47:Lx:89:ALA:HB3	2.32	0.44
49:S2:589:G:OP2	49:S2:589:G:N2	2.36	0.44
49:S2:1483:C:OP1	56:SH:54:LYS:NZ	2.41	0.44
58:SM:160:GLN:O	58:SM:164:ILE:HG22	2.17	0.44
78:Sg:53:TYR:OH	78:Sg:76:ASP:OD2	2.27	0.44
1:B:438:LYS:C	1:B:440:ASN:H	2.26	0.44
3:L5:151:G:O6	12:LJ:142:THR:OG1	2.31	0.44
3:L5:995:C:H2'	3:L5:996:C:C6	2.52	0.44
3:L5:1009:G:H2'	3:L5:1010:A:C8	2.53	0.44
3:L5:1294:C:H4'	8:LF:36:ILE:HD11	1.99	0.44
3:L5:1674:U:H1'	3:L5:3960:A:H5'	2.00	0.44
3:L5:1697:G:H2'	3:L5:1698:G:C8	2.52	0.44
3:L5:2321:C:H2'	3:L5:2322:G:O4'	2.17	0.44
3:L5:3983:C:H2'	3:L5:3984:G:C8	2.53	0.44
3:L5:4124:A:O2'	3:L5:4125:A:H2'	2.17	0.44
3:L5:4612:G:H1	19:LR:176:ARG:CZ	2.29	0.44
3:L5:4792:U:O2'	3:L5:4793:C:O4'	2.32	0.44
4:L7:75:G:H5''	23:LV:49:SER:O	2.17	0.44
7:LE:288:GLY:HA3	7:LE:330:PHE:CZ	2.53	0.44
10:LH:121:THR:HG21	35:Lh:92:ASN:OD1	2.17	0.44
22:LU:7:GLN:HG3	22:LU:32:ILE:HG22	1.99	0.44
32:Le:117:ARG:HG3	32:Le:118:LEU:HD22	1.99	0.44
35:Lh:124:ASN:N	35:Lh:124:ASN:OD1	2.50	0.44
49:S2:69:C:H42	49:S2:80:G:H1	1.66	0.44
49:S2:115:U:H2'	49:S2:116:OMU:C6	2.47	0.44
49:S2:201:C:H3'	49:S2:202:G:H8	1.82	0.44
49:S2:1397:A:H8	49:S2:1450:G:H22	1.66	0.44
49:S2:1399:G:H22	49:S2:1449:A:H2	1.65	0.44
55:SG:44:LYS:HB3	55:SG:54:ILE:HG22	2.00	0.44
71:SZ:92:ALA:HA	71:SZ:125:LYS:HB2	1.99	0.44
72:Sa:28:MET:HG2	72:Sa:33:LEU:HG	1.99	0.44
3:L5:1412:G:O2'	21:LT:75:ARG:NH2	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1939:G:O2'	3:L5:1956:A:N1	2.32	0.44
3:L5:2252:U:H4'	3:L5:2271:A:H4'	1.99	0.44
3:L5:3649:A:H2'	3:L5:3650:G:H8	1.83	0.44
3:L5:3703:G:H1'	3:L5:3778:A:H61	1.81	0.44
3:L5:3882:G:H2'	3:L5:3883:G:C8	2.52	0.44
3:L5:4005:C:O4'	15:LM:23:ASN:ND2	2.50	0.44
7:LE:325:GLU:OE1	7:LE:325:GLU:N	2.51	0.44
11:LI:84:ALA:HB2	24:LW:138:ALA:N	2.32	0.44
17:LP:126:GLU:HG2	19:LR:185:VAL:HG11	2.00	0.44
29:Lb:80:ILE:HG12	29:Lb:99:ILE:O	2.18	0.44
34:Lg:64:ILE:HG23	34:Lg:68:LEU:HD23	1.99	0.44
37:Lj:69:LYS:O	37:Lj:73:HIS:ND1	2.45	0.44
49:S2:30:C:O2'	49:S2:597:U:OP1	2.34	0.44
49:S2:1276:G:N2	49:S2:1507:A:OP2	2.46	0.44
49:S2:1743:C:H2'	49:S2:1744:G:O4'	2.18	0.44
49:S2:1757:C:H2'	49:S2:1758:G:C8	2.53	0.44
54:SF:44:ILE:HD12	54:SF:65:PRO:HG2	1.98	0.44
58:SM:128:LYS:HA	58:SM:134:LEU:HA	1.99	0.44
66:SU:93:LYS:HB2	66:SU:96:TYR:CD2	2.53	0.44
72:Sa:85:ILE:HG22	72:Sa:112:ILE:HD13	1.99	0.44
75:Sd:70:ILE:HG12	75:Sd:77:TYR:CD2	2.53	0.44
2:I:53:U:N3	2:I:159:G:O2'	2.49	0.44
3:L5:1524:U:H2'	3:L5:1525:G:H8	1.83	0.44
3:L5:1933:C:H2'	3:L5:1934:G:C8	2.52	0.44
3:L5:3515:A:O5'	3:L5:3516:A:H5'	2.18	0.44
3:L5:4506:C:OP2	19:LR:171:LYS:NZ	2.38	0.44
5:L8:94:G:C5	40:Lm:84:PRO:HD3	2.53	0.44
7:LE:300:LYS:HE2	7:LE:313:SER:HB3	2.00	0.44
16:LO:124:LEU:HD11	38:Lk:119:TYR:HB2	1.99	0.44
19:LR:98:ALA:HA	19:LR:101:ARG:NE	2.33	0.44
49:S2:892:G:P	49:S2:892:G:H8	2.41	0.44
49:S2:983:G:H2'	49:S2:984:A:C8	2.53	0.44
56:SH:23:VAL:HG22	67:SV:64:TRP:CZ3	2.53	0.44
75:Sd:46:ARG:NH2	76:Se:50:GLU:HG2	2.32	0.44
3:L5:1007:G:H2'	3:L5:1008:C:C6	2.53	0.44
3:L5:1351:G:H2'	3:L5:1352:C:O4'	2.18	0.44
3:L5:1688:A:H2'	3:L5:1689:G:C8	2.52	0.44
3:L5:4640:G:H22	3:L5:4659:C:H42	1.65	0.44
3:L5:4757:C:H2'	3:L5:4758:A:C8	2.53	0.44
15:LM:90:ARG:NH2	15:LM:108:GLY:O	2.50	0.44
15:LM:94:LEU:HD23	15:LM:99:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LR:178:ARG:O	19:LR:182:GLU:HG2	2.17	0.44
25:LX:65:ARG:HG3	25:LX:70:ILE:HG12	2.00	0.44
31:Ld:146:LEU:HD23	39:Ll:5:TYR:HD2	1.83	0.44
33:Lf:6:LYS:O	33:Lf:10:SER:N	2.47	0.44
48:S:1126:A:N6	48:S:1141:G:OP1	2.51	0.44
49:S2:601:G:H2'	49:S2:602:OMG:H8	1.83	0.44
49:S2:1402:A:O2'	77:Sf:53:PRO:O	2.36	0.44
65:ST:149:TYR:O	65:ST:153:LYS:HG3	2.17	0.44
81:Sj:29:HIS:HE2	81:Sj:69:THR:HG1	1.62	0.44
82:Sk:58:LEU:O	82:Sk:62:VAL:HB	2.18	0.44
3:L5:115:C:OP1	18:LQ:2:GLY:N	2.51	0.44
3:L5:684:C:H2'	3:L5:685:C:C6	2.53	0.44
3:L5:1339:U:H2'	3:L5:1340:G:O4'	2.18	0.44
3:L5:1533:U:OP2	3:L5:3369:PSU:O2'	2.32	0.44
3:L5:1643:G:H2'	3:L5:1644:G:C8	2.52	0.44
3:L5:2515:C:P	45:Lr:44:LYS:HZ1	2.41	0.44
3:L5:4621:U:O2	36:Li:1:MET:N	2.50	0.44
7:LE:47:LEU:HD23	7:LE:84:MET:HE1	2.00	0.44
11:LI:94:ILE:HD13	11:LI:140:ALA:HB2	2.00	0.44
23:LV:11:LYS:HE2	23:LV:67:VAL:HG21	1.99	0.44
49:S2:235:A:H2'	49:S2:236:A:C8	2.53	0.44
49:S2:447:G:OP2	65:ST:47:ARG:NH2	2.51	0.44
49:S2:1278:C:H2'	49:S2:1279:A:C8	2.52	0.44
54:SF:46:GLU:N	71:SZ:113:GLN:OE1	2.49	0.44
57:SL:78:SER:O	57:SL:84:GLN:NE2	2.50	0.44
58:SM:108:ASP:OD1	58:SM:108:ASP:N	2.50	0.44
69:SX:43:ASP:O	69:SX:45:ARG:NH2	2.51	0.44
1:B:687:ARG:HG2	1:B:721:GLN:CG	2.47	0.43
2:I:174:G:H1'	2:I:175:G:N7	2.33	0.43
3:L5:279:A:N1	3:L5:306:A:H5''	2.33	0.43
3:L5:994:C:N3	3:L5:1112:G:H2'	2.33	0.43
3:L5:1261:U:H2'	3:L5:1262:C:C6	2.53	0.43
3:L5:1815:U:H2'	3:L5:1816:G:H8	1.83	0.43
3:L5:2221:G:N2	3:L5:2224:A:OP2	2.51	0.43
3:L5:2426:C:H5''	37:Lj:74:VAL:HG21	1.99	0.43
3:L5:2505:G:H2'	3:L5:2506:G:C8	2.53	0.43
3:L5:3347:G:H1'	27:LZ:44:ARG:NE	2.33	0.43
3:L5:3622:A:N6	3:L5:4316:G:O2'	2.50	0.43
3:L5:3997:A:H5''	15:LM:108:GLY:HA3	2.00	0.43
3:L5:4782:A:OP1	7:LE:393:LYS:NZ	2.37	0.43
3:L5:4787:A:OP1	34:Lg:31:LYS:NZ	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LD:101:VAL:HG22	6:LD:165:VAL:HG22	2.00	0.43
22:LU:17:CYS:HB2	22:LU:52:ARG:HH11	1.83	0.43
22:LU:90:PRO:HG2	22:LU:93:VAL:HB	2.00	0.43
37:Lj:41:ALA:O	37:Lj:52:ARG:NH1	2.48	0.43
49:S2:77:A:N3	63:SR:176:ILE:HG22	2.33	0.43
49:S2:694:A:H2'	49:S2:695:G:C8	2.52	0.43
49:S2:750:U:H2'	49:S2:751:C:C6	2.52	0.43
49:S2:1449:A:H2'	49:S2:1450:G:O4'	2.18	0.43
49:S2:1513:C:H5''	56:SH:8:TRP:CZ3	2.51	0.43
49:S2:1551:G:N2	49:S2:1560:C:O2	2.49	0.43
55:SG:30:MET:HG3	55:SG:42:MET:HE3	2.00	0.43
58:SM:29:ASP:OD1	58:SM:51:ARG:NH2	2.51	0.43
63:SR:49:VAL:HG23	63:SR:114:VAL:HB	1.99	0.43
68:SW:111:VAL:HG12	68:SW:140:PHE:HB2	1.99	0.43
3:L5:318:A:H2'	3:L5:319:A:H8	1.83	0.43
3:L5:2207:OMG:HM23	3:L5:2207:OMG:H1'	1.85	0.43
3:L5:2286:G:OP2	3:L5:2359:G:N2	2.48	0.43
3:L5:2315:A:N3	28:La:48:ARG:NH1	2.65	0.43
3:L5:3474:G:H2'	3:L5:3475:G:H8	1.82	0.43
3:L5:4159:C:O2	14:LL:158:LYS:NZ	2.41	0.43
3:L5:4361:C:OP1	7:LE:357:ARG:NH1	2.48	0.43
3:L5:4708:C:H2'	3:L5:4709:C:C6	2.53	0.43
7:LE:46:PHE:CZ	7:LE:84:MET:HG3	2.53	0.43
8:LF:30:ALA:HB2	8:LF:279:LEU:HD12	1.99	0.43
16:LO:62:PRO:O	16:LO:63:THR:OG1	2.31	0.43
18:LQ:143:ARG:HH12	38:Lk:95:LEU:HA	1.83	0.43
19:LR:98:ALA:O	19:LR:101:ARG:HG2	2.19	0.43
19:LR:130:LYS:HB2	19:LR:133:ARG:HG2	2.01	0.43
34:Lg:29:ILE:HG13	34:Lg:84:ILE:HD13	2.00	0.43
39:Ll:66:ASP:OD1	39:Ll:66:ASP:N	2.51	0.43
48:S:1114:A:C8	48:S:1154:G:H8	2.35	0.43
49:S2:526:A:H2'	49:S2:527:A:H8	1.84	0.43
49:S2:815:PSU:OP1	61:SP:22:LYS:NZ	2.51	0.43
49:S2:1076:C:H2'	49:S2:1077:G:H8	1.82	0.43
49:S2:1232:C:O2'	49:S2:1254:A:N6	2.51	0.43
49:S2:1260:A:H1'	49:S2:1265:C:N4	2.34	0.43
49:S2:1734:U:H2'	49:S2:1735:G:O4'	2.18	0.43
54:SF:46:GLU:OE1	54:SF:48:ALA:N	2.45	0.43
55:SG:199:THR:HG23	55:SG:241:PHE:CE2	2.53	0.43
58:SM:67:PHE:CE1	71:SZ:48:SER:HB3	2.53	0.43
59:SN:133:TYR:CZ	59:SN:216:MET:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SP:137:PRO:HG2	61:SP:149:TYR:HA	2.00	0.43
63:SR:5:ILE:HD13	63:SR:16:ILE:HD12	2.00	0.43
64:SS:8:ILE:HD13	64:SS:24:SER:HB3	2.00	0.43
78:Sg:3:ASN:ND2	78:Sg:7:GLU:HB3	2.33	0.43
1:B:466:GLN:HB2	1:B:701:ILE:HG13	2.01	0.43
2:I:104:G:N1	2:I:135:C:N3	2.66	0.43
3:L5:667:C:H2'	3:L5:668:G:C8	2.53	0.43
3:L5:1009:G:N2	3:L5:1095:C:N3	2.66	0.43
3:L5:1699:G:H2'	3:L5:1700:G:C8	2.52	0.43
3:L5:2741:G:OP1	22:LU:101:ILE:HD11	2.18	0.43
3:L5:3334:C:H2'	3:L5:3335:G:H8	1.83	0.43
3:L5:3509:G:O2'	3:L5:3547:G:O6	2.27	0.43
3:L5:4516:G:H5''	19:LR:176:ARG:HE	1.82	0.43
3:L5:4805:U:H2'	3:L5:4806:U:C6	2.53	0.43
8:LF:37:VAL:HG23	8:LF:237:ILE:HD11	2.01	0.43
14:LL:68:ALA:HB1	14:LL:155:ALA:HB1	2.01	0.43
15:LM:18:ARG:HG3	15:LM:135:GLY:HA3	2.00	0.43
22:LU:10:LEU:HD13	22:LU:10:LEU:HA	1.84	0.43
49:S2:1038:G:H4'	49:S2:1846:A:H4'	2.00	0.43
49:S2:1256:G:OP1	49:S2:1257:G:O2'	2.21	0.43
49:S2:1387:A:OP2	60:SO:160:SER:OG	2.31	0.43
49:S2:1398:U:OP2	49:S2:1398:U:C6	2.70	0.43
57:SL:187:GLY:N	78:Sg:45:ARG:HH22	2.16	0.43
58:SM:32:ASP:OD1	58:SM:33:VAL:N	2.52	0.43
63:SR:4:ASN:O	63:SR:111:LEU:N	2.48	0.43
3:L5:305:A:P	18:LQ:15:GLN:HE22	2.41	0.43
3:L5:1348:G:H22	3:L5:1369:C:H1'	1.83	0.43
3:L5:1365:U:H2'	3:L5:1366:C:O4'	2.17	0.43
3:L5:1768:G:H4'	32:Le:61:ASN:ND2	2.34	0.43
3:L5:1860:C:O3'	23:LV:160:ARG:NH1	2.51	0.43
3:L5:2548:G:H2'	3:L5:2549:G:H8	1.83	0.43
3:L5:2612:U:C2	37:Lj:69:LYS:HG3	2.53	0.43
3:L5:2665:G:H5''	22:LU:18:GLY:HA3	2.01	0.43
3:L5:3392:C:H2'	3:L5:3414:A:H61	1.82	0.43
3:L5:4151:G:OP2	14:LL:7:ARG:NH2	2.50	0.43
3:L5:4450:C:H2'	3:L5:4451:A:C8	2.53	0.43
3:L5:4796:C:O2'	34:Lg:23:ARG:NH2	2.51	0.43
6:LD:226:ARG:NH2	6:LD:230:PRO:HD3	2.34	0.43
7:LE:181:MET:HE3	7:LE:181:MET:HB2	1.91	0.43
11:LI:108:LEU:HG	11:LI:135:VAL:HG11	2.01	0.43
12:LJ:157:ILE:HB	12:LJ:183:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LJ:165:GLU:OE2	18:LQ:26:ARG:NH2	2.33	0.43
17:LP:122:ILE:O	17:LP:126:GLU:HG3	2.18	0.43
21:LT:50:ARG:CB	21:LT:83:VAL:HG21	2.48	0.43
22:LU:84:THR:HG23	22:LU:87:ALA:H	1.83	0.43
22:LU:119:MET:HE3	22:LU:119:MET:HB3	1.92	0.43
26:LY:83:ARG:NH1	26:LY:120:PRO:O	2.43	0.43
49:S2:190:G:OP1	65:ST:149:TYR:OH	2.27	0.43
49:S2:561:A:H5'	66:SU:174:LYS:HB2	2.00	0.43
55:SG:245:ARG:HH12	55:SG:312:VAL:HG11	1.84	0.43
61:SP:87:MET:HE2	61:SP:87:MET:HB3	1.94	0.43
70:SY:46:THR:O	70:SY:50:ILE:HG12	2.18	0.43
78:Sg:3:ASN:HD21	78:Sg:7:GLU:HB3	1.84	0.43
3:L5:197:A:N1	3:L5:225:G:O2'	2.40	0.43
3:L5:223:G:H4'	3:L5:225:G:N7	2.33	0.43
3:L5:262:G:H2'	3:L5:263:G:H8	1.83	0.43
3:L5:424:U:H2'	3:L5:425:U:C6	2.54	0.43
3:L5:1858:G:N2	23:LV:163:HIS:O	2.38	0.43
3:L5:4426:G:H2'	3:L5:4427:A:C8	2.54	0.43
3:L5:4727:U:OP2	7:LE:123:HIS:ND1	2.45	0.43
3:L5:4791:C:H5'	7:LE:325:GLU:CD	2.44	0.43
6:LD:30:ARG:NH1	6:LD:36:GLU:OE2	2.52	0.43
6:LD:181:LYS:HD3	6:LD:184:ARG:HH21	1.82	0.43
9:LG:2:AAC:O3	9:LG:4:VAL:HG22	2.19	0.43
11:LI:105:ARG:NH1	21:LT:4:ASP:OD1	2.51	0.43
14:LL:40:LYS:HE3	14:LL:40:LYS:HB3	1.81	0.43
15:LM:91:GLU:HG2	15:LM:93:GLU:HG2	2.01	0.43
17:LP:128:LYS:HA	17:LP:131:GLN:HG2	1.99	0.43
20:LS:60:PHE:CE1	20:LS:82:ARG:HB2	2.54	0.43
49:S2:202:G:H2'	49:S2:203:G:C8	2.53	0.43
49:S2:830:C:OP1	61:SP:21:ASP:HB2	2.18	0.43
49:S2:1017:U:OP1	50:SB:30:SER:OG	2.32	0.43
58:SM:25:PHE:HZ	71:SZ:53:ILE:HA	1.83	0.43
60:SO:163:PRO:HA	60:SO:166:TYR:CE2	2.54	0.43
61:SP:122:LYS:HD2	61:SP:164:LEU:HD11	2.00	0.43
63:SR:64:LYS:HB2	63:SR:97:VAL:HG21	1.99	0.43
73:Sb:58:LEU:HD11	73:Sb:108:ILE:HG23	2.00	0.43
3:L5:230:G:H2'	3:L5:231:U:O4'	2.19	0.43
3:L5:1072:C:H1'	3:L5:1074:C:C2	2.53	0.43
3:L5:1785:G:P	32:Le:25:ARG:HH22	2.42	0.43
5:L8:132:G:P	28:La:108:GLN:HE22	2.41	0.43
8:LF:171:LEU:HD12	8:LF:176:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LF:212:ASN:HA	8:LF:232:VAL:HG12	2.01	0.43
17:LP:86:TRP:O	17:LP:89:THR:HG22	2.19	0.43
26:LY:68:GLY:O	26:LY:73:ARG:NH1	2.51	0.43
49:S2:294:C:H4'	68:SW:38:LYS:HZ2	1.83	0.43
49:S2:753:G:N2	49:S2:793:C:N3	2.67	0.43
49:S2:1629:C:H2'	49:S2:1630:C:C6	2.53	0.43
60:SO:107:TYR:HD1	60:SO:110:LEU:HD12	1.83	0.43
61:SP:122:LYS:O	61:SP:161:GLN:NE2	2.52	0.43
70:SY:4:MET:SD	70:SY:124:ARG:NH2	2.91	0.43
3:L5:315:G:C8	31:Ld:62:HIS:HB2	2.54	0.43
3:L5:1303:G:H4'	18:LQ:203:TYR:HB2	2.01	0.43
3:L5:1352:C:H2'	3:L5:1353:G:O4'	2.18	0.43
3:L5:1666:U:H5'	11:LI:130:ASN:HD21	1.83	0.43
3:L5:3763:G:H2'	3:L5:3764:G:C8	2.53	0.43
4:L7:63:C:H5'	4:L7:64:G:H5''	2.00	0.43
16:LO:42:ARG:HG2	16:LO:45:ARG:HH21	1.83	0.43
21:LT:85:THR:HA	21:LT:104:ARG:O	2.19	0.43
29:Lb:28:LYS:O	29:Lb:31:SER:OG	2.30	0.43
31:Ld:85:GLN:HA	31:Ld:88:VAL:HG22	2.01	0.43
32:Le:118:LEU:HB3	32:Le:120:ARG:NE	2.33	0.43
33:Lf:22:MET:HA	33:Lf:27:TYR:CE1	2.54	0.43
49:S2:1416:C:H2'	49:S2:1417:C:C6	2.54	0.43
49:S2:1746:A:O3'	63:SR:31:ARG:NH1	2.51	0.43
55:SG:258:ILE:HG13	55:SG:267:VAL:HB	2.01	0.43
56:SH:19:ARG:HE	56:SH:32:ARG:HH22	1.65	0.43
67:SV:26:ASP:O	67:SV:42:ASN:ND2	2.52	0.43
71:SZ:103:ASN:HD21	71:SZ:140:THR:HG23	1.84	0.43
75:Sd:42:HIS:O	75:Sd:46:ARG:HG2	2.19	0.43
80:Si:71:ARG:NH1	80:Si:82:THR:OG1	2.51	0.43
82:Sk:90:GLU:O	82:Sk:93:SER:OG	2.29	0.43
3:L5:52:G:H4'	3:L5:1484:G:H4'	2.01	0.43
3:L5:308:G:H2'	39:Ll:41:ARG:HH12	1.84	0.43
3:L5:522:U:O2	3:L5:636:G:N2	2.48	0.43
3:L5:2149:G:O2'	3:L5:2174:G:N1	2.41	0.43
3:L5:4614:G:H5''	23:LV:170:LYS:HZ3	1.83	0.43
4:L7:3:C:OP1	4:L7:58:A:O2'	2.22	0.43
9:LG:39:GLN:OE1	9:LG:40:ASP:N	2.50	0.43
22:LU:105:LEU:HD12	22:LU:135:LYS:HE3	2.01	0.43
26:LY:112:MET:SD	26:LY:117:ILE:HD11	2.58	0.43
44:Lq:26:TYR:HB3	44:Lq:67:VAL:HB	2.00	0.43
49:S2:434:A:H5''	65:ST:22:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1221:A:N3	49:S2:1678:U:O2'	2.49	0.43
49:S2:1524:C:OP1	75:Sd:141:ARG:HB3	2.19	0.43
57:SL:69:GLU:CD	57:SL:69:GLU:H	2.26	0.43
58:SM:107:ARG:HH12	71:SZ:133:THR:C	2.24	0.43
59:SN:121:ARG:NH1	59:SN:123:ARG:HH11	2.16	0.43
60:SO:34:TYR:HE1	60:SO:37:VAL:HG13	1.83	0.43
73:Sb:63:PHE:CE1	73:Sb:92:LEU:HD22	2.54	0.43
80:Si:101:LEU:HB3	80:Si:124:LYS:HB2	2.00	0.43
1:B:649:LEU:HD21	1:B:738:LEU:HD23	2.00	0.43
3:L5:1105:C:N3	32:Le:91:ARG:NH2	2.60	0.43
3:L5:1416:C:H2'	3:L5:1417:A:C8	2.53	0.43
3:L5:1452:A:H1'	21:LT:164:LYS:HD3	2.01	0.43
3:L5:2142:G:OP1	8:LF:182:LYS:NZ	2.43	0.43
3:L5:2310:U:H4'	3:L5:2311:U:H5'	2.00	0.43
3:L5:4035:U:H2'	3:L5:4036:U:C6	2.54	0.43
8:LF:133:LEU:O	8:LF:137:VAL:HG12	2.19	0.43
9:LG:20:PHE:HE2	24:LW:24:VAL:HB	1.83	0.43
10:LH:197:VAL:O	36:Li:108:SER:OG	2.34	0.43
11:LI:161:ILE:HB	11:LI:166:ILE:HD12	2.01	0.43
15:LM:19:LYS:HE3	15:LM:75:ARG:HH12	1.83	0.43
16:LO:90:VAL:O	16:LO:93:THR:OG1	2.25	0.43
21:LT:50:ARG:HD3	21:LT:83:VAL:HG21	2.01	0.43
24:LW:17:ARG:NH1	24:LW:18:PRO:HD2	2.33	0.43
26:LY:60:MET:HA	26:LY:80:VAL:HG12	2.00	0.43
30:Lc:121:ARG:O	30:Lc:124:THR:OG1	2.36	0.43
46:Ls:61:VAL:HA	46:Ls:81:THR:HA	2.01	0.43
48:S:1141:G:H3'	48:S:1142:U:C6	2.53	0.43
49:S2:71:G:O6	63:SR:170:ARG:NH1	2.51	0.43
49:S2:990:C:O3'	54:SF:32:LYS:NZ	2.52	0.43
49:S2:1414:G:H2'	49:S2:1415:A:H8	1.83	0.43
62:SQ:40:ALA:HB1	62:SQ:45:TYR:CG	2.53	0.43
67:SV:86:PRO:HG2	67:SV:89:ILE:HG12	2.00	0.43
75:Sd:7:GLU:H	75:Sd:7:GLU:CD	2.27	0.43
1:B:444:SER:H	52:SD:145:CYS:CB	2.32	0.43
1:B:675:LEU:HB3	1:B:747:VAL:HG13	1.99	0.43
2:I:146:C:O3'	82:Sk:76:ARG:NH2	2.52	0.43
3:L5:250:C:O3'	40:Lm:85:LYS:NZ	2.38	0.43
3:L5:422:C:H2'	3:L5:423:G:C8	2.54	0.43
3:L5:1006:C:H2'	3:L5:1007:G:C8	2.54	0.43
3:L5:1694:C:H2'	3:L5:1695:U:O4'	2.18	0.43
3:L5:1911:G:H2'	3:L5:1912:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2156:A:H5'	3:L5:2157:G:OP2	2.18	0.43
3:L5:2592:C:H2'	3:L5:2593:G:C8	2.53	0.43
3:L5:3767:G:H2'	3:L5:3768:C:C6	2.54	0.43
3:L5:3850:G:O3'	37:Lj:90:ARG:NH2	2.52	0.43
3:L5:4345:A:N1	3:L5:4356:A:H5''	2.33	0.43
3:L5:4741:U:H2'	3:L5:4742:U:C6	2.54	0.43
4:L7:11:A:N1	4:L7:66:G:O2'	2.51	0.43
21:LT:146:ARG:HB3	21:LT:148:VAL:HG12	2.01	0.43
37:Lj:25:THR:HG23	37:Lj:27:GLY:H	1.84	0.43
49:S2:125:C:P	63:SR:198:ARG:HH21	2.42	0.43
49:S2:196:C:H2'	49:S2:204:G:H21	1.83	0.43
49:S2:449:A:H5''	65:ST:25:ARG:HA	2.00	0.43
49:S2:1241:A:N3	49:S2:1268:C:O2'	2.49	0.43
49:S2:1266:A:O2'	49:S2:1328:G:OP2	2.24	0.43
55:SG:107:ASP:OD2	74:Sc:33:ARG:NH1	2.52	0.43
57:SL:33:GLN:HB2	57:SL:154:LEU:HD13	2.01	0.43
59:SN:94:ILE:H	59:SN:94:ILE:HD12	1.84	0.43
61:SP:86:PHE:CE2	61:SP:87:MET:HG3	2.53	0.43
64:SS:142:LYS:HB3	79:Sh:54:ASP:HB3	1.99	0.43
71:SZ:42:VAL:HG11	71:SZ:81:VAL:HG11	2.01	0.43
72:Sa:50:ARG:H	72:Sa:53:GLN:CD	2.26	0.43
75:Sd:3:LEU:O	82:Sk:49:LEU:HB3	2.19	0.43
1:B:731:ARG:CZ	48:S:1112:U:O4	2.67	0.42
2:I:122:C:H4'	2:I:123:G:O5'	2.19	0.42
3:L5:1290:C:H2'	3:L5:1291:G:C8	2.53	0.42
3:L5:1474:C:H2'	3:L5:1475:C:C6	2.54	0.42
3:L5:1772:G:N2	3:L5:1774:G:O4'	2.52	0.42
3:L5:2248:G:N7	42:Lo:2:SER:HB2	2.34	0.42
3:L5:3703:G:H1'	3:L5:3778:A:N6	2.34	0.42
3:L5:3825:G:H2'	3:L5:3841:U:O4	2.19	0.42
8:LF:289:LEU:HG	8:LF:293:LEU:HD23	2.00	0.42
13:LK:20:LEU:HD23	13:LK:45:LEU:HB3	2.00	0.42
13:LK:141:LYS:H	13:LK:141:LYS:HG2	1.69	0.42
18:LQ:113:LEU:HA	18:LQ:137:PRO:HD3	2.01	0.42
31:Ld:103:VAL:HB	31:Ld:108:TYR:HB2	2.01	0.42
38:Lk:68:ASN:HA	38:Lk:71:LYS:NZ	2.34	0.42
49:S2:26:U:H2'	49:S2:27:A2M:O4'	2.19	0.42
49:S2:1788:G:H2'	49:S2:1789:A:C8	2.54	0.42
58:SM:87:ILE:HG22	58:SM:101:HIS:HB2	2.01	0.42
67:SV:3:MET:SD	67:SV:8:ARG:NH2	2.92	0.42
69:SX:24:THR:O	69:SX:27:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Se:30:VAL:HA	76:Se:53:PHE:HE2	1.83	0.42
2:I:84:A:N6	2:I:85:G:N3	2.67	0.42
3:L5:4:G:H2'	3:L5:5:A:C8	2.54	0.42
3:L5:229:G:H5''	29:Lb:11:ARG:HG3	2.02	0.42
3:L5:837:U:OP1	17:LP:46:ARG:NH1	2.52	0.42
3:L5:2277:G:O3'	28:La:83:THR:HG21	2.19	0.42
3:L5:2332:C:H4'	3:L5:2333:U:H5	1.83	0.42
3:L5:3862:G:OP2	3:L5:3862:G:N2	2.34	0.42
3:L5:4161:A:H2'	3:L5:4162:G:O4'	2.20	0.42
3:L5:4164:G:H2'	3:L5:4167:C:H42	1.83	0.42
3:L5:4672:C:H42	3:L5:4673:A:H62	1.66	0.42
4:L7:23:A:N3	4:L7:118:C:O2'	2.45	0.42
5:L8:30:U:H2'	5:L8:31:G:C8	2.54	0.42
7:LE:181:MET:HG3	7:LE:182:GLU:N	2.34	0.42
9:LG:51:MET:HE3	9:LG:51:MET:HB2	1.90	0.42
9:LG:216:GLU:O	9:LG:220:LYS:HG2	2.20	0.42
11:LI:135:VAL:O	11:LI:139:ILE:HG12	2.19	0.42
21:LT:106:THR:HG23	21:LT:109:ALA:H	1.84	0.42
22:LU:67:THR:O	22:LU:71:ARG:HG2	2.18	0.42
35:Lh:35:TRP:CZ2	35:Lh:56:PRO:HD2	2.55	0.42
46:Ls:64:MET:HE2	46:Ls:64:MET:HB2	1.98	0.42
49:S2:107:A:H2'	49:S2:108:G:C8	2.54	0.42
49:S2:196:C:C2	49:S2:204:G:C2	3.07	0.42
49:S2:562:A:N7	66:SU:173:VAL:HG21	2.34	0.42
49:S2:1439:A:H2'	49:S2:1440:A:C8	2.54	0.42
49:S2:1590:A:O3'	76:Se:82:ARG:HD2	2.19	0.42
52:SD:94:LYS:NZ	52:SD:95:ARG:O	2.52	0.42
59:SN:183:LYS:HA	59:SN:195:LEU:O	2.19	0.42
63:SR:42:GLY:HA3	63:SR:45:TRP:HD1	1.84	0.42
65:ST:79:ILE:HD12	65:ST:170:LYS:HG2	2.01	0.42
71:SZ:78:ALA:HB3	71:SZ:118:ALA:HB3	2.01	0.42
1:B:442:LYS:NZ	49:S2:1292:A:O3'	2.41	0.42
3:L5:1813:A:OP1	32:Le:9:THR:HG22	2.20	0.42
3:L5:2022:C:P	21:LT:14:ARG:HH22	2.42	0.42
6:LD:80:GLU:HG3	45:Lr:66:GLY:HA2	2.01	0.42
6:LD:83:HIS:HB3	45:Lr:64:VAL:HG22	2.02	0.42
11:LI:93:ARG:NH1	11:LI:108:LEU:HD13	2.34	0.42
12:LJ:93:THR:HG22	12:LJ:97:LYS:NZ	2.35	0.42
21:LT:9:LYS:HD3	21:LT:9:LYS:HA	1.84	0.42
28:La:62:ARG:HA	28:La:62:ARG:HD3	1.81	0.42
30:Lc:81:MET:HE2	37:Lj:96:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:298:A:H2'	49:S2:299:G:H8	1.84	0.42
49:S2:1321:G:H2'	49:S2:1322:G:O4'	2.20	0.42
49:S2:1529:G:O2'	49:S2:1667:C:OP1	2.31	0.42
49:S2:1788:G:H2'	49:S2:1789:A:H8	1.84	0.42
75:Sd:124:ARG:NE	75:Sd:130:ARG:O	2.26	0.42
1:B:446:LEU:CG	52:SD:146:LEU:CD2	2.97	0.42
1:B:670:LYS:HE3	1:B:670:LYS:HB2	1.93	0.42
2:I:78:A:H2'	2:I:79:C:C2	2.54	0.42
3:L5:461:G:H2'	3:L5:462:G:H8	1.84	0.42
3:L5:670:C:H2'	3:L5:671:G:H8	1.84	0.42
3:L5:1206:C:N4	3:L5:1207:G:O6	2.52	0.42
3:L5:1341:A:N7	31:Ld:114:LYS:HD2	2.35	0.42
3:L5:1397:C:H2'	3:L5:1398:A:C8	2.55	0.42
3:L5:3786:U:H2'	3:L5:3787:C:C6	2.54	0.42
3:L5:3923:C:H2'	3:L5:3924:A:C8	2.55	0.42
14:LL:12:CYS:HA	14:LL:59:GLN:HE21	1.85	0.42
21:LT:101:CYS:HA	21:LT:121:LEU:O	2.19	0.42
29:Lb:74:TYR:HD2	29:Lb:77:LYS:H	1.67	0.42
46:Ls:101:LYS:HD3	46:Ls:101:LYS:HA	1.74	0.42
49:S2:689:U:C5	64:SS:102:PRO:HA	2.55	0.42
49:S2:1567:G:N2	49:S2:1570:A:OP2	2.49	0.42
51:SC:56:LEU:HD23	62:SQ:143:PRO:HD3	2.00	0.42
55:SG:35:SER:OG	55:SG:36:ARG:N	2.52	0.42
59:SN:169:TYR:CD1	59:SN:173:LYS:HG3	2.54	0.42
75:Sd:78:LYS:HA	75:Sd:78:LYS:HD3	1.88	0.42
1:B:687:ARG:HG2	1:B:721:GLN:HG3	2.01	0.42
2:I:115:A:H2'	2:I:116:G:H8	1.84	0.42
3:L5:113:A:H2'	3:L5:114:G:O4'	2.20	0.42
3:L5:1138:G:N2	3:L5:1202:C:H2'	2.35	0.42
3:L5:1235:G:OP1	10:LH:222:LYS:NZ	2.48	0.42
3:L5:1296:C:O2'	3:L5:1300:U:OP1	2.35	0.42
3:L5:1793:G:N2	3:L5:4140:A:O4'	2.53	0.42
3:L5:2457:C:O2'	3:L5:2651:G:OP1	2.35	0.42
3:L5:3639:G:H2'	3:L5:4193:5MC:O2'	2.20	0.42
3:L5:4035:U:HO2'	3:L5:4066:G:HO2'	1.55	0.42
3:L5:4331:U:H2'	3:L5:4332:G:H8	1.85	0.42
7:LE:77:THR:HG21	7:LE:337:VAL:HG22	2.02	0.42
8:LF:154:VAL:HG11	8:LF:174:LEU:HD21	2.01	0.42
8:LF:211:TYR:HE1	8:LF:229:LEU:HB3	1.84	0.42
14:LL:146:GLU:CD	14:LL:146:GLU:H	2.27	0.42
16:LO:81:LEU:HD13	16:LO:86:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LS:30:ARG:CZ	20:LS:62:ARG:HE	2.33	0.42
23:LV:77:ASN:OD1	23:LV:98:ARG:NH1	2.53	0.42
34:Lg:81:PRO:HB2	34:Lg:84:ILE:HD11	2.01	0.42
49:S2:1026:U:H2'	49:S2:1027:C:O4'	2.19	0.42
49:S2:1116:U:H1'	49:S2:1117:C:H2'	2.02	0.42
49:S2:1126:C:OP1	74:Sc:129:LYS:HD2	2.20	0.42
49:S2:1822:U:H2'	49:S2:1823:A:C8	2.54	0.42
55:SG:60:ARG:HH22	73:Sb:97:GLN:HE22	1.67	0.42
62:SQ:25:THR:O	62:SQ:28:VAL:HG12	2.20	0.42
62:SQ:71:ARG:NH2	62:SQ:148:ASN:OD1	2.53	0.42
62:SQ:179:ASN:HB3	62:SQ:187:SER:HB2	2.01	0.42
63:SR:164:LYS:HG2	63:SR:165:GLU:H	1.84	0.42
64:SS:47:ALA:HB3	64:SS:63:PHE:HD2	1.85	0.42
72:Sa:64:LYS:NZ	72:Sa:73:PRO:HG3	2.34	0.42
72:Sa:68:PRO:HD2	72:Sa:71:GLU:HB2	2.02	0.42
73:Sb:76:GLY:H	73:Sb:79:ALA:HB3	1.83	0.42
76:Se:98:SER:O	76:Se:102:ARG:HG2	2.19	0.42
78:Sg:3:ASN:OD1	78:Sg:6:GLY:N	2.52	0.42
2:I:125:U:H1'	2:I:162:A:C2	2.54	0.42
3:L5:175:C:H2'	3:L5:176:G:C8	2.52	0.42
3:L5:2112:C:O2'	46:Ls:11:ARG:NH2	2.52	0.42
3:L5:2262:C:OP2	20:LS:23:ARG:NH1	2.53	0.42
3:L5:2323:G:H2'	3:L5:2324:G:H8	1.85	0.42
3:L5:2719:OMG:C8	45:Lr:16:THR:HG22	2.54	0.42
3:L5:3600:G:H22	3:L5:3632:G:H1'	1.85	0.42
3:L5:4060:C:O2'	32:Le:36:ASP:OD1	2.35	0.42
3:L5:4265:C:OP1	3:L5:4266:G:H5''	2.20	0.42
7:LE:307:TYR:CZ	7:LE:366:LYS:HE3	2.54	0.42
10:LH:121:THR:O	46:Ls:112:ARG:HD3	2.19	0.42
20:LS:42:ARG:NH2	20:LS:160:PRO:HD2	2.34	0.42
21:LT:100:VAL:HB	21:LT:120:ILE:HD13	2.01	0.42
31:Ld:58:MET:HE2	31:Ld:58:MET:HB3	1.84	0.42
36:Li:93:PRO:HB2	36:Li:95:LYS:HG2	2.00	0.42
40:Lm:27:TYR:HA	40:Lm:34:CYS:HA	2.00	0.42
46:Ls:33:LYS:HD3	46:Ls:40:TYR:CE2	2.54	0.42
49:S2:13:C:O2'	49:S2:1144:A:O2'	2.29	0.42
49:S2:1301:U:H4'	49:S2:1302:A:H5'	2.00	0.42
68:SW:135:SER:O	68:SW:139:ARG:NH1	2.51	0.42
79:Sh:106:THR:HG21	79:Sh:111:MET:HE2	2.01	0.42
3:L5:218:A:O2'	3:L5:219:G:H5'	2.20	0.42
3:L5:243:A:H5''	29:Lb:3:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:323:C:H2'	3:L5:324:A:C8	2.55	0.42
3:L5:435:A:O2'	35:Lh:26:ASP:OD2	2.24	0.42
3:L5:459:C:H2'	3:L5:460:C:C6	2.55	0.42
3:L5:1015:U:C2	3:L5:1088:C:C2	3.07	0.42
3:L5:1467:G:OP1	31:Ld:7:LYS:NZ	2.33	0.42
3:L5:1713:C:H2'	3:L5:1714:A:C8	2.55	0.42
3:L5:2104:G:H4'	10:LH:115:MET:HE3	2.00	0.42
3:L5:3707:C:N4	3:L5:3764:G:H1	2.17	0.42
3:L5:4156:G:H1	3:L5:4178:C:H42	1.66	0.42
6:LD:114:CYS:N	6:LD:165:VAL:O	2.48	0.42
9:LG:155:THR:HG22	9:LG:179:ARG:HA	2.02	0.42
37:Lj:8:ARG:N	37:Lj:34:TYR:OH	2.51	0.42
38:Lk:80:PRO:HD2	38:Lk:83:LEU:HD12	2.00	0.42
49:S2:1508:G:O5'	52:SD:89:LYS:NZ	2.53	0.42
49:S2:1867:A:N6	54:SF:84:VAL:HG22	2.34	0.42
55:SG:15:ASN:H	55:SG:37:ASP:HB3	1.85	0.42
58:SM:191:ASP:O	58:SM:195:LYS:HG2	2.18	0.42
61:SP:192:ILE:HB	61:SP:243:GLY:HA3	2.00	0.42
65:ST:38:ILE:HD11	65:ST:81:VAL:HG23	2.02	0.42
66:SU:22:LYS:HD3	66:SU:22:LYS:HA	1.95	0.42
69:SX:13:ASP:HB3	69:SX:16:THR:HG22	2.02	0.42
74:Sc:28:PHE:CE2	74:Sc:32:LYS:HD3	2.54	0.42
1:B:630:ARG:HG2	1:B:632:TYR:CZ	2.55	0.42
2:I:160:G:H2'	2:I:161:A:O4'	2.20	0.42
3:L5:251:C:H5'	40:Lm:85:LYS:NZ	2.33	0.42
3:L5:385:A:H4'	3:L5:386:A:H5'	2.01	0.42
3:L5:708:G:H2'	3:L5:709:G:H8	1.84	0.42
3:L5:1453:G:OP2	21:LT:150:ARG:NH2	2.53	0.42
3:L5:1666:U:H5'	11:LI:130:ASN:ND2	2.35	0.42
3:L5:3359:OMG:HM23	3:L5:3359:OMG:H1'	1.87	0.42
3:L5:4323:U:H2'	3:L5:4324:G:C8	2.55	0.42
6:LD:29:LEU:O	6:LD:123:ARG:NE	2.40	0.42
6:LD:34:PHE:HE1	12:LJ:41:ILE:HD11	1.85	0.42
6:LD:180:LEU:HD21	45:Lr:22:LEU:HB3	2.02	0.42
7:LE:66:LYS:HA	7:LE:66:LYS:HD3	1.77	0.42
10:LH:281:THR:OG1	10:LH:282:ASN:N	2.53	0.42
12:LJ:166:LEU:HA	18:LQ:7:ILE:HD11	2.01	0.42
15:LM:72:CYS:SG	15:LM:73:THR:N	2.92	0.42
16:LO:196:ALA:O	16:LO:200:LYS:HG2	2.20	0.42
16:LO:201:GLU:O	16:LO:205:GLN:N	2.41	0.42
18:LQ:201:HIS:O	18:LQ:204:ARG:NH1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LR:16:LEU:HD12	19:LR:80:PHE:HD1	1.85	0.42
19:LR:172:LYS:O	19:LR:176:ARG:NH1	2.53	0.42
28:La:72:ASP:OD1	28:La:73:HIS:N	2.50	0.42
41:Ln:18:LYS:HE3	41:Ln:18:LYS:HB3	1.88	0.42
49:S2:1204:G:H4'	59:SN:116:THR:HA	2.02	0.42
49:S2:1673:U:OP1	73:Sb:18:THR:HG22	2.20	0.42
49:S2:1870:A:C5	58:SM:115:LYS:HE3	2.54	0.42
50:SB:42:LYS:NZ	50:SB:57:VAL:HB	2.34	0.42
55:SG:91:ASP:OD2	55:SG:93:THR:OG1	2.27	0.42
60:SO:39:VAL:HG22	60:SO:48:ILE:HG22	2.02	0.42
65:ST:107:THR:O	65:ST:111:GLN:HG2	2.19	0.42
78:Sg:67:ASP:O	78:Sg:71:ARG:HG3	2.20	0.42
79:Sh:2:VAL:HG23	79:Sh:4:MET:SD	2.60	0.42
2:I:69:U:OP1	2:I:71:A:N6	2.52	0.42
3:L5:401:G:OP1	20:LS:16:LYS:NZ	2.48	0.42
3:L5:2142:G:H5'	46:Ls:15:SER:HB2	2.02	0.42
3:L5:2161:G:H5''	35:Lh:67:LYS:HG3	2.01	0.42
3:L5:4646:G:C2	3:L5:4654:G:C2	3.08	0.42
7:LE:266:VAL:HG13	7:LE:268:ARG:HD3	2.02	0.42
11:LI:226:PHE:N	11:LI:232:ALA:O	2.52	0.42
16:LO:127:PHE:CE1	16:LO:144:LEU:HG	2.55	0.42
19:LR:7:LEU:HD23	19:LR:33:VAL:HG13	2.01	0.42
25:LX:111:GLU:CD	25:LX:113:ARG:HE	2.28	0.42
29:Lb:134:LYS:HE3	29:Lb:134:LYS:HB3	1.94	0.42
35:Lh:77:PHE:O	35:Lh:98:GLU:N	2.51	0.42
49:S2:196:C:C2	49:S2:205:G:C2	3.08	0.42
49:S2:567:U:H2'	49:S2:568:C:O4'	2.20	0.42
65:ST:66:SER:HA	65:ST:73:THR:HB	2.02	0.42
65:ST:107:THR:OG1	65:ST:108:PRO:HD3	2.20	0.42
76:Se:75:MET:HE3	76:Se:79:TYR:HE2	1.84	0.42
2:I:33:A:OP2	2:I:94:U:N3	2.52	0.42
3:L5:74:G:H5'	16:LO:60:ARG:O	2.19	0.42
3:L5:422:C:H2'	3:L5:423:G:H8	1.85	0.42
3:L5:707:C:O2	10:LH:133:LYS:NZ	2.53	0.42
3:L5:795:A:H3'	3:L5:796:C:C6	2.55	0.42
3:L5:1105:C:O2	32:Le:91:ARG:NE	2.53	0.42
3:L5:1805:U:H2'	3:L5:1806:A:O4'	2.20	0.42
3:L5:2284:C:H2'	3:L5:2285:G:C8	2.55	0.42
3:L5:2705:G:N3	3:L5:3356:A:H2'	2.35	0.42
3:L5:4116:OMG:H5''	44:Lq:64:LYS:HE2	2.00	0.42
5:L8:8:U:H2'	5:L8:9:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L8:134:G:OP2	28:La:67:ARG:NH2	2.35	0.42
8:LF:316:LYS:HB2	8:LF:324:ILE:HG13	2.01	0.42
15:LM:62:ILE:HG23	15:LM:68:ILE:HG21	2.01	0.42
17:LP:128:LYS:HE3	17:LP:128:LYS:HB3	1.82	0.42
21:LT:27:LEU:HD23	21:LT:30:LYS:HD3	2.01	0.42
21:LT:54:SER:OG	21:LT:55:ARG:N	2.52	0.42
35:Lh:124:ASN:HB2	35:Lh:127:ALA:HB2	2.01	0.42
37:Lj:105:LYS:HA	37:Lj:108:LYS:HB3	2.00	0.42
49:S2:687:PSU:O4	64:SS:118:ARG:NH2	2.40	0.42
49:S2:756:C:N4	49:S2:790:G:O6	2.53	0.42
49:S2:956:A:N1	49:S2:969:U:O2'	2.48	0.42
49:S2:992:G:C6	49:S2:1135:G:H4'	2.55	0.42
51:SC:29:GLN:HG2	51:SC:45:ASN:OD1	2.20	0.42
55:SG:42:MET:HG2	55:SG:56:GLN:HB2	2.02	0.42
59:SN:179:THR:HG22	59:SN:221:ASP:HB2	2.01	0.42
81:Sj:56:PHE:O	81:Sj:74:MET:N	2.37	0.42
2:I:66:G:H3'	2:I:67:G:C5'	2.50	0.41
3:L5:448:G:OP2	3:L5:449:C:O2'	2.28	0.41
3:L5:751:G:C2	3:L5:805:G:C2	3.07	0.41
3:L5:1138:G:C6	3:L5:1202:C:C4	3.07	0.41
3:L5:1387:G:C6	3:L5:1406:G:C6	3.09	0.41
3:L5:1586:A:C8	6:LD:199:VAL:HG21	2.55	0.41
3:L5:1651:C:H2'	3:L5:1652:G:O4'	2.20	0.41
3:L5:2034:A:N6	3:L5:2035:G:O6	2.53	0.41
3:L5:2322:G:H2'	3:L5:2323:G:H8	1.85	0.41
3:L5:2338:U:H2'	3:L5:2339:G:C8	2.55	0.41
3:L5:2401:C:H2'	3:L5:2402:G:C8	2.54	0.41
3:L5:3422:U:H2'	3:L5:3423:G:O4'	2.20	0.41
3:L5:3831:C:N4	3:L5:3832:G:N3	2.68	0.41
3:L5:4047:U:H4'	24:LW:54:HIS:CD2	2.55	0.41
4:L7:74:A:O3'	23:LV:53:LYS:NZ	2.53	0.41
11:LI:100:VAL:HG12	11:LI:138:TYR:CE2	2.54	0.41
13:LK:48:LEU:HD11	13:LK:56:ARG:NH1	2.35	0.41
21:LT:43:PHE:CD1	21:LT:133:GLY:HA3	2.55	0.41
22:LU:78:ILE:HD13	22:LU:81:ARG:NH1	2.35	0.41
35:Lh:40:GLY:O	35:Lh:46:ARG:HD3	2.20	0.41
37:Lj:48:VAL:O	45:Lr:61:MET:HG2	2.20	0.41
48:S:1111:A:H4'	48:S:1112:U:OP2	2.21	0.41
49:S2:92:A:C6	49:S2:447:G:C6	3.08	0.41
49:S2:617:A:H4'	53:SE:82:ARG:O	2.19	0.41
49:S2:619:C:H41	80:Si:67:ARG:NH2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:1434:C:O2'	49:S2:1435:C:O4'	2.38	0.41
49:S2:1543:C:P	76:Se:62:ARG:HH21	2.43	0.41
49:S2:1714:C:H2'	49:S2:1715:U:C6	2.55	0.41
49:S2:1833:6MZ:H8	49:S2:1833:6MZ:O5'	2.20	0.41
49:S2:1837:G:OP1	49:S2:1840:U:H4'	2.20	0.41
55:SG:107:ASP:C	55:SG:124:SER:HG	2.26	0.41
57:SL:4:ALA:H	78:Sg:80:SER:HB3	1.85	0.41
57:SL:52:LYS:HB2	74:Sc:109:LEU:HD11	2.02	0.41
57:SL:173:LEU:HD12	74:Sc:91:LEU:HD13	2.01	0.41
62:SQ:118:ASN:O	62:SQ:193:LYS:HE2	2.20	0.41
78:Sg:1:AME:HT23	78:Sg:1:AME:HA	1.49	0.41
79:Sh:101:PHE:HA	79:Sh:113:HIS:CE1	2.55	0.41
2:I:43:U:H2'	2:I:85:G:H21	1.84	0.41
3:L5:1307:C:OP2	16:LO:39:ARG:NH2	2.52	0.41
3:L5:2473:U:OP1	25:LX:48:LYS:NZ	2.49	0.41
3:L5:3515:A:OP2	3:L5:3540:OMC:N4	2.52	0.41
3:L5:3816:C:H2'	3:L5:3817:G:C8	2.55	0.41
3:L5:3818:G:H2'	3:L5:3819:G:C8	2.55	0.41
3:L5:4514:C:H2'	3:L5:4515:G:H8	1.85	0.41
3:L5:4634:U:C2	17:LP:129:LYS:HE3	2.55	0.41
6:LD:28:ARG:HH11	6:LD:123:ARG:HD3	1.85	0.41
6:LD:137:ILE:HD11	6:LD:149:LYS:HB2	2.02	0.41
7:LE:245:HIC:ND1	7:LE:246:ARG:N	2.67	0.41
22:LU:168:GLU:OE1	22:LU:172:ARG:NE	2.52	0.41
26:LY:75:LYS:HE2	26:LY:77:HIS:NE2	2.35	0.41
28:La:83:THR:HG22	28:La:85:SER:H	1.83	0.41
31:Ld:136:LYS:HE2	31:Ld:136:LYS:HB2	1.90	0.41
49:S2:380:C:H5'	65:ST:33:ALA:HA	2.02	0.41
49:S2:749:C:H2'	49:S2:750:U:H5''	2.02	0.41
49:S2:899:U:H2'	49:S2:900:U:C6	2.55	0.41
49:S2:935:G:H22	49:S2:1009:A:H2	1.67	0.41
49:S2:1276:G:O4'	49:S2:1507:A:N6	2.53	0.41
49:S2:1798:U:H2'	49:S2:1799:C:C6	2.55	0.41
49:S2:1861:A:N7	54:SF:34:LYS:NZ	2.68	0.41
55:SG:92:LEU:HD13	55:SG:92:LEU:HA	1.93	0.41
62:SQ:156:THR:HA	62:SQ:159:ARG:NH1	2.35	0.41
63:SR:71:GLY:H	63:SR:98:ARG:NH1	2.18	0.41
66:SU:138:ARG:NH1	66:SU:153:SER:OG	2.52	0.41
79:Sh:24:GLN:NE2	79:Sh:64:ASN:OD1	2.49	0.41
81:Sj:13:MET:HB3	81:Sj:22:GLN:HG3	2.01	0.41
3:L5:746:G:H2'	3:L5:747:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1726:A:N3	3:L5:3956:U:O2'	2.49	0.41
3:L5:1760:G:H4'	3:L5:1761:U:H5''	2.01	0.41
3:L5:1768:G:H2'	3:L5:1769:G:C8	2.54	0.41
3:L5:2356:A:H1'	37:Lj:15:THR:HG21	2.01	0.41
3:L5:2399:G:H2'	3:L5:2400:G:C8	2.56	0.41
3:L5:2451:G:H2'	3:L5:2452:G:H8	1.85	0.41
3:L5:2470:C:OP1	25:LX:92:LYS:NZ	2.37	0.41
8:LF:27:VAL:HA	8:LF:279:LEU:HD11	2.02	0.41
9:LG:37:VAL:HG12	9:LG:50:ARG:HD3	2.01	0.41
10:LH:153:LEU:HD13	10:LH:199:ALA:HA	2.02	0.41
21:LT:178:ARG:H	31:Ld:51:GLY:HA2	1.85	0.41
26:LY:89:ARG:HB2	26:LY:95:PHE:CE1	2.56	0.41
48:S:1126:A:H1'	48:S:1144:G:O6	2.20	0.41
49:S2:697:G:N1	49:S2:731:C:O2	2.34	0.41
49:S2:1491:OMG:HM23	49:S2:1491:OMG:H1'	1.76	0.41
49:S2:1588:G:N7	76:Se:67:NMM:HD2	2.35	0.41
49:S2:1654:U:H3	49:S2:1672:G:H1	1.67	0.41
49:S2:1771:G:H2'	49:S2:1772:G:H8	1.84	0.41
70:SY:99:ARG:NH2	70:SY:119:GLU:OE2	2.48	0.41
71:SZ:16:SER:OG	71:SZ:17:LEU:N	2.51	0.41
78:Sg:19:ALA:HB2	78:Sg:68:SER:OG	2.21	0.41
79:Sh:104:LEU:HD13	79:Sh:125:ILE:HA	2.02	0.41
81:Sj:100:LYS:HE2	81:Sj:100:LYS:HB3	1.90	0.41
3:L5:456:C:H2'	3:L5:457:G:C8	2.54	0.41
3:L5:1315:A:N1	5:L8:28:C:O2'	2.52	0.41
3:L5:1466:U:OP1	31:Ld:7:LYS:N	2.52	0.41
3:L5:1532:G:O2'	3:L5:1567:G:H4'	2.20	0.41
3:L5:1926:C:N4	3:L5:1927:G:O6	2.53	0.41
3:L5:2364:G:H2'	3:L5:2365:G:H8	1.85	0.41
3:L5:3524:OMG:HM23	3:L5:3524:OMG:H1'	1.89	0.41
3:L5:3664:U:H2'	3:L5:3665:G:C8	2.55	0.41
3:L5:3665:G:H2'	3:L5:3666:G:H8	1.85	0.41
3:L5:3674:A:H2'	3:L5:3675:A:C8	2.55	0.41
3:L5:4012:G:H2'	3:L5:4012:G:N3	2.34	0.41
3:L5:4032:C:H2'	3:L5:4033:G:H8	1.85	0.41
3:L5:4331:U:H2'	3:L5:4332:G:C8	2.55	0.41
4:L7:24:C:H2'	4:L7:25:G:O4'	2.20	0.41
25:LX:41:GLN:O	25:LX:44:GLN:HG2	2.20	0.41
27:LZ:57:ARG:HA	27:LZ:63:GLN:HE22	1.84	0.41
37:Lj:87:VAL:O	37:Lj:91:ILE:HG12	2.20	0.41
49:S2:354:C:H2'	49:S2:355:OMU:H6	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:852:C:H5''	49:S2:853:G:H5'	2.01	0.41
49:S2:1469:C:H2'	49:S2:1470:A:C8	2.55	0.41
49:S2:1605:G:C6	49:S2:1606:G:C4	3.08	0.41
49:S2:1851:MA6:H93	49:S2:1852:MA6:H92	2.02	0.41
49:S2:1865:U:H3'	54:SF:5:ARG:HH21	1.85	0.41
51:SC:17:VAL:HA	51:SC:30:VAL:HG12	2.02	0.41
60:SO:137:VAL:HB	60:SO:185:LYS:HB2	2.01	0.41
70:SY:5:HIS:CD2	70:SY:121:ARG:HG3	2.56	0.41
76:Se:129:ARG:HH22	76:Se:132:ASP:HB2	1.85	0.41
79:Sh:15:ASN:ND2	79:Sh:71:LYS:HG3	2.35	0.41
1:B:435:ASP:CB	49:S2:1312:C:O2'	2.68	0.41
1:B:444:SER:C	49:S2:1293:C:O2'	2.64	0.41
1:B:691:CYS:SG	1:B:692:ILE:N	2.94	0.41
3:L5:226:G:OP2	29:Lb:1:MET:N	2.51	0.41
3:L5:511:A:C4	31:Ld:82:VAL:HG12	2.55	0.41
3:L5:1413:C:H2'	3:L5:1414:A:O4'	2.20	0.41
3:L5:1984:G:O6	3:L5:3602:C:O2'	2.38	0.41
3:L5:2265:OMC:HM23	3:L5:2265:OMC:H1'	1.89	0.41
3:L5:3866:C:O2	3:L5:3893:G:N1	2.52	0.41
3:L5:4071:A:H1'	9:LG:36:LEU:HD23	2.01	0.41
3:L5:4324:G:H2'	3:L5:4325:PSU:C6	2.56	0.41
4:L7:35:U:O2	4:L7:45:U:O2'	2.32	0.41
5:L8:65:A:OP1	38:Lk:56:ARG:NH1	2.48	0.41
7:LE:305:THR:OG1	7:LE:306:ASP:N	2.54	0.41
12:LJ:159:HIS:ND1	12:LJ:185:LYS:HA	2.35	0.41
14:LL:19:LYS:HB2	14:LL:19:LYS:HE3	1.85	0.41
18:LQ:99:GLN:HB3	18:LQ:130:PHE:CE2	2.55	0.41
23:LV:32:ILE:HG21	23:LV:40:ALA:HA	2.01	0.41
31:Ld:76:ASP:HB3	31:Ld:115:GLY:HA3	2.03	0.41
34:Lg:24:GLU:HG2	34:Lg:87:ARG:HB2	2.03	0.41
46:Ls:12:ASN:OD1	46:Ls:19:LYS:HE2	2.20	0.41
49:S2:234:C:H2'	49:S2:235:A:H8	1.85	0.41
49:S2:374:G:OP1	68:SW:137:THR:HG22	2.19	0.41
49:S2:672:A:OP1	49:S2:1164:C:O2'	2.37	0.41
49:S2:868:OMG:H1'	49:S2:868:OMG:HM23	1.79	0.41
49:S2:1376:G:H2'	49:S2:1377:A:C8	2.55	0.41
49:S2:1417:C:H5'	76:Se:129:ARG:NH1	2.35	0.41
55:SG:60:ARG:HH12	73:Sb:97:GLN:HE22	1.68	0.41
58:SM:47:THR:OG1	58:SM:48:LEU:N	2.54	0.41
59:SN:192:LEU:HB3	59:SN:227:ARG:HG2	2.01	0.41
61:SP:14:ALA:HB1	61:SP:18:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SQ:50:PRO:HA	62:SQ:70:GLU:HG2	2.02	0.41
70:SY:38:TYR:O	70:SY:42:LYS:HG2	2.20	0.41
73:Sb:8:GLN:O	73:Sb:26:LYS:HA	2.19	0.41
3:L5:266:C:H1'	38:Lk:109:ARG:NH1	2.28	0.41
3:L5:2537:G:H5'	3:L5:2538:A:C2	2.55	0.41
3:L5:3465:A:H2'	3:L5:3466:PSU:O4'	2.20	0.41
3:L5:3599:A2M:HM'3	3:L5:3612:G:N2	2.35	0.41
3:L5:3888:C:H2'	3:L5:3889:G:C8	2.55	0.41
3:L5:4052:OMU:HM23	3:L5:4052:OMU:H1'	1.86	0.41
3:L5:4515:G:O3'	19:LR:176:ARG:NH2	2.53	0.41
3:L5:4739:G:OP2	7:LE:394:LYS:NZ	2.38	0.41
5:L8:91:A:H2'	5:L8:92:U:O4'	2.20	0.41
7:LE:223:THR:CG2	7:LE:275:HIS:H	2.33	0.41
11:LI:145:ASN:N	11:LI:240:ASN:OD1	2.49	0.41
15:LM:85:LYS:HG3	15:LM:115:LEU:HD12	2.01	0.41
18:LQ:50:ARG:HE	18:LQ:50:ARG:HB2	1.65	0.41
21:LT:70:MET:SD	21:LT:80:ALA:HB2	2.61	0.41
23:LV:45:TRP:HA	23:LV:48:VAL:HG22	2.02	0.41
24:LW:128:LEU:H	24:LW:128:LEU:HD23	1.85	0.41
26:LY:99:GLU:HB3	27:LZ:24:THR:HG23	2.01	0.41
30:Lc:95:VAL:HG13	30:Lc:96:VAL:HG23	2.01	0.41
46:Ls:105:ASP:OD1	46:Ls:105:ASP:N	2.52	0.41
48:S:1140:G:H2'	48:S:1141:G:H8	1.85	0.41
49:S2:875:G:H2'	49:S2:876:A:C8	2.54	0.41
49:S2:1514:C:H2'	49:S2:1515:G:H8	1.85	0.41
52:SD:100:LEU:HB3	52:SD:103:LEU:HG	2.02	0.41
55:SG:10:THR:HA	55:SG:308:ARG:HA	2.01	0.41
55:SG:192:THR:HG23	60:SO:218:LEU:HD22	2.03	0.41
57:SL:89:LYS:HG2	57:SL:201:LEU:HG	2.02	0.41
59:SN:139:LEU:HD12	59:SN:213:LEU:HD21	2.02	0.41
59:SN:200:ARG:O	66:SU:98:LEU:HB3	2.21	0.41
61:SP:36:HIS:CG	61:SP:85:GLY:HA3	2.55	0.41
61:SP:86:PHE:CD2	61:SP:87:MET:HG3	2.55	0.41
67:SV:1:MET:HB3	67:SV:2:LEU:H	1.66	0.41
76:Se:83:GLN:N	76:Se:91:HIS:O	2.46	0.41
79:Sh:111:MET:HB2	79:Sh:115:GLU:CD	2.46	0.41
2:I:40:U:C4	2:I:41:C:C4	3.09	0.41
2:I:101:U:H2'	2:I:102:A:C8	2.56	0.41
3:L5:43:U:H1'	44:Lq:44:LYS:NZ	2.36	0.41
3:L5:323:C:H2'	3:L5:324:A:H8	1.85	0.41
3:L5:722:U:OP1	11:LI:75:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2348:C:H5''	3:L5:2349:G:O4'	2.20	0.41
3:L5:2544:U:H2'	3:L5:2545:C:C6	2.56	0.41
3:L5:3688:G:O2'	3:L5:3698:A:OP2	2.38	0.41
3:L5:3881:G:H2'	3:L5:3882:G:C8	2.56	0.41
3:L5:4088:C:O3'	44:Lq:37:GLY:HA3	2.21	0.41
3:L5:4339:C:H2'	3:L5:4340:U:C6	2.56	0.41
3:L5:4340:U:H2'	3:L5:4341:G:C8	2.53	0.41
3:L5:4351:A:H2'	3:L5:4352:G:O4'	2.19	0.41
3:L5:4364:OMG:HM23	3:L5:4364:OMG:H1'	1.84	0.41
3:L5:4792:U:H3'	3:L5:4793:C:C6	2.56	0.41
7:LE:258:HIS:HA	7:LE:259:PRO:C	2.45	0.41
8:LF:308:LYS:HE2	8:LF:308:LYS:HB2	1.91	0.41
9:LG:94:ASN:N	9:LG:94:ASN:OD1	2.53	0.41
10:LH:287:HIS:ND1	36:Li:38:GLU:OE2	2.47	0.41
14:LL:48:LEU:HB2	14:LL:142:LEU:HD13	2.03	0.41
27:LZ:99:GLU:O	27:LZ:103:ALA:N	2.54	0.41
49:S2:792:C:H2'	49:S2:793:C:C6	2.55	0.41
49:S2:894:U:H2'	49:S2:895:G:C8	2.55	0.41
49:S2:929:G:H2'	49:S2:930:G:C8	2.56	0.41
49:S2:982:A:H2'	49:S2:983:G:C8	2.56	0.41
49:S2:991:A:OP2	54:SF:37:LYS:HE3	2.21	0.41
49:S2:1040:C:H2'	49:S2:1041:G:C8	2.55	0.41
57:SL:158:ASP:O	78:Sg:66:ASP:HA	2.21	0.41
61:SP:176:ASP:OD1	61:SP:177:THR:N	2.54	0.41
63:SR:2:LYS:HB3	63:SR:15:LEU:HD11	2.02	0.41
66:SU:103:GLU:HA	66:SU:106:LEU:HB2	2.02	0.41
71:SZ:19:PRO:O	71:SZ:21:VAL:HG23	2.21	0.41
74:Sc:114:LEU:HD12	74:Sc:117:LEU:HD11	2.02	0.41
79:Sh:11:LEU:HD12	79:Sh:74:VAL:HB	2.03	0.41
2:I:133:G:H2'	2:I:134:C:C5	2.56	0.41
2:I:144:G:H4'	2:I:145:C:OP1	2.20	0.41
3:L5:58:G:H4'	3:L5:59:A:H4'	2.03	0.41
3:L5:850:G:H2'	3:L5:851:G:H8	1.86	0.41
3:L5:1013:G:C2	3:L5:1089:G:H2'	2.56	0.41
3:L5:1265:G:H2'	3:L5:3608:A:N7	2.35	0.41
3:L5:1302:G:O2'	3:L5:1304:G:O6	2.34	0.41
3:L5:1573:G:OP1	40:Lm:13:ASN:ND2	2.38	0.41
3:L5:2131:G:O2'	3:L5:2133:C:O5'	2.38	0.41
3:L5:2232:A:H5'	34:Lg:70:LYS:HE2	2.03	0.41
3:L5:2386:A:O2'	3:L5:2387:G:O4'	2.37	0.41
3:L5:2432:C:H2'	3:L5:2433:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2648:C:H1'	37:Lj:5:LEU:O	2.21	0.41
3:L5:3783:U:H2'	3:L5:3784:A:O4'	2.21	0.41
3:L5:3796:U:O2'	3:L5:3797:U:H5''	2.20	0.41
3:L5:4501:G:OP2	36:Li:4:ARG:HG3	2.20	0.41
3:L5:4636:G:H21	3:L5:4665:C:N4	2.19	0.41
5:L8:87:G:OP1	38:Lk:5:LYS:NZ	2.46	0.41
6:LD:97:ASN:HB2	6:LD:100:ASN:ND2	2.35	0.41
7:LE:248:LEU:HD12	7:LE:249:ARG:HG3	2.02	0.41
8:LF:336:ARG:HA	8:LF:336:ARG:HD2	1.95	0.41
9:LG:22:ARG:HB3	9:LG:28:THR:HG23	2.02	0.41
16:LO:198:ARG:HA	16:LO:201:GLU:HG3	2.03	0.41
21:LT:82:VAL:HG12	21:LT:139:LEU:HB2	2.01	0.41
26:LY:62:MET:HE3	26:LY:62:MET:HB2	1.66	0.41
33:Lf:35:LEU:HD23	33:Lf:35:LEU:HA	1.85	0.41
38:Lk:13:LYS:HD3	38:Lk:14:LYS:N	2.35	0.41
40:Lm:39:TYR:CG	40:Lm:40:PRO:HA	2.56	0.41
48:S:1123:C:O5'	48:S:1123:C:H6	2.04	0.41
49:S2:28:U:H2'	49:S2:29:G:C8	2.56	0.41
49:S2:759:C:H42	49:S2:788:G:H1'	1.86	0.41
49:S2:1289:OMU:C5	52:SD:95:ARG:HH12	2.34	0.41
52:SD:104:LYS:HE2	52:SD:104:LYS:HB3	1.95	0.41
61:SP:105:THR:O	61:SP:245:ARG:NE	2.53	0.41
71:SZ:97:LEU:HD21	71:SZ:108:PRO:HB3	2.03	0.41
82:Sk:51:ASP:N	82:Sk:54:THR:OG1	2.54	0.41
1:B:628:ARG:C	1:B:630:ARG:H	2.28	0.41
2:I:65:A:H2'	2:I:66:G:C8	2.56	0.41
2:I:112:U:N3	62:SQ:195:GLU:OE2	2.33	0.41
3:L5:228:C:H2'	3:L5:229:G:C8	2.56	0.41
3:L5:1224:C:O2'	8:LF:321:ASN:OD1	2.30	0.41
3:L5:1608:A:OP2	31:Ld:27:LYS:HG2	2.20	0.41
3:L5:1624:A:P	32:Le:18:ARG:HH22	2.44	0.41
3:L5:1676:A:H2'	3:L5:1677:A:O4'	2.21	0.41
3:L5:1727:A:H2'	14:LL:22:PHE:CE2	2.56	0.41
3:L5:2295:G:H21	3:L5:2350:A:H62	1.69	0.41
3:L5:3421:G:OP1	6:LD:202:VAL:HG23	2.21	0.41
3:L5:3488:A:H2'	3:L5:3489:G:C8	2.54	0.41
3:L5:3899:C:H2'	3:L5:3900:G:H8	1.85	0.41
3:L5:4314:A:O2'	3:L5:4720:G:N7	2.52	0.41
3:L5:4436:G:O6	3:L5:4444:C:H5''	2.21	0.41
5:L8:60:G:O6	5:L8:96:C:O2'	2.37	0.41
5:L8:75:OMG:HM23	5:L8:75:OMG:H1'	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LF:152:LEU:HD23	8:LF:251:ILE:HD12	2.03	0.41
8:LF:341:LEU:HG	10:LH:52:LEU:HD11	2.01	0.41
13:LK:26:ILE:HD12	13:LK:35:ARG:HG2	2.02	0.41
17:LP:9:VAL:HG21	17:LP:66:HIS:HB3	2.03	0.41
17:LP:38:VAL:HG11	17:LP:55:MET:SD	2.61	0.41
18:LQ:28:TRP:HA	18:LQ:31:ARG:NH1	2.36	0.41
18:LQ:178:HIS:HA	18:LQ:181:HIS:NE2	2.36	0.41
19:LR:15:LEU:HA	19:LR:42:ASN:O	2.20	0.41
19:LR:18:ARG:CZ	19:LR:128:ARG:HH21	2.33	0.41
19:LR:176:ARG:HA	19:LR:176:ARG:HD3	1.88	0.41
20:LS:153:LYS:HD3	20:LS:153:LYS:HA	1.94	0.41
21:LT:169:SER:HB3	21:LT:174:PHE:CE2	2.56	0.41
29:Lb:39:ARG:NH1	29:Lb:45:ARG:HD2	2.35	0.41
29:Lb:103:LYS:HA	29:Lb:103:LYS:HD3	1.87	0.41
31:Ld:125:LYS:HA	31:Ld:145:VAL:O	2.20	0.41
33:Lf:12:GLU:O	33:Lf:16:SER:N	2.48	0.41
38:Lk:91:MET:HA	38:Lk:94:ARG:HG3	2.01	0.41
39:Li:73:ILE:O	39:Li:77:VAL:HG12	2.21	0.41
40:Lm:54:LYS:HZ2	40:Lm:54:LYS:HG3	1.64	0.41
49:S2:1324:U:H2'	49:S2:1325:G:C8	2.56	0.41
49:S2:1416:C:O3'	76:Se:129:ARG:NH1	2.54	0.41
49:S2:1525:G:OP2	75:Sd:141:ARG:NH1	2.51	0.41
49:S2:1588:G:OP1	49:S2:1588:G:N2	2.53	0.41
49:S2:1680:A:H2'	62:SQ:60:ARG:HD2	2.02	0.41
49:S2:1767:C:H4'	49:S2:1768:C:H5	1.85	0.41
54:SF:39:PHE:HD1	54:SF:70:LYS:HB2	1.85	0.41
55:SG:291:TRP:CD2	55:SG:298:LEU:HD13	2.56	0.41
57:SL:140:VAL:HG23	57:SL:142:LEU:HB2	2.02	0.41
58:SM:190:PRO:O	58:SM:192:SER:N	2.52	0.41
59:SN:104:ASP:HB3	59:SN:130:ILE:HG22	2.01	0.41
60:SO:74:GLN:HG2	60:SO:79:PHE:HB2	2.02	0.41
61:SP:102:ILE:HD13	61:SP:239:PRO:HD3	2.03	0.41
61:SP:152:PRO:HD2	63:SR:216:ARG:HG3	2.03	0.41
64:SS:130:LEU:HD21	64:SS:156:VAL:HG21	2.02	0.41
65:ST:130:THR:HG23	65:ST:133:GLU:HG2	2.02	0.41
67:SV:53:LYS:HE3	67:SV:60:GLU:HB3	2.02	0.41
67:SV:86:PRO:HB2	67:SV:88:GLU:OE1	2.20	0.41
72:Sa:28:MET:HE3	72:Sa:28:MET:HB2	1.99	0.41
74:Sc:13:ALA:O	74:Sc:17:ILE:HG22	2.21	0.41
74:Sc:54:VAL:O	74:Sc:58:MET:HG2	2.20	0.41
77:Sf:107:GLU:HB2	77:Sf:110:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sk:92:LEU:HD22	82:Sk:109:TYR:HE1	1.85	0.41
3:L5:417:G:H1'	5:L8:16:G:N2	2.35	0.41
3:L5:1768:G:H2'	3:L5:1769:G:H8	1.86	0.41
3:L5:1941:A:H5''	3:L5:1942:G:C8	2.55	0.41
3:L5:1972:A:O2'	3:L5:1973:G:H5''	2.21	0.41
3:L5:2254:C:H2'	3:L5:2255:A:C8	2.56	0.41
3:L5:2653:U:H5''	22:LU:70:ARG:HH12	1.86	0.41
3:L5:3942:OMG:H1'	3:L5:3942:OMG:HM23	1.87	0.41
3:L5:4312:U:O2'	7:LE:234:ARG:NH1	2.49	0.41
3:L5:4605:C:H2'	3:L5:4606:G:C8	2.56	0.41
3:L5:4621:U:H1'	36:Li:1:MET:N	2.35	0.41
9:LG:59:ASP:OD1	9:LG:60:ILE:N	2.54	0.41
14:LL:54:SER:HB2	14:LL:135:ILE:HD11	2.02	0.41
24:LW:19:PHE:CE2	24:LW:20:ARG:HG3	2.56	0.41
37:Lj:23:SER:HB3	37:Lj:33:LEU:HD23	2.02	0.41
48:S:1136:C:N3	48:S:1138:C:H4'	2.36	0.41
49:S2:27:A2M:HM'3	49:S2:27:A2M:H1'	1.80	0.41
49:S2:1610:C:OP2	75:Sd:134:GLN:NE2	2.49	0.41
64:SS:147:LYS:NZ	64:SS:153:LEU:HB2	2.36	0.41
66:SU:38:ARG:NH1	66:SU:42:GLU:OE2	2.53	0.41
66:SU:160:SER:HB3	66:SU:163:SER:HB2	2.02	0.41
82:Sk:61:GLU:HG2	82:Sk:62:VAL:N	2.35	0.41
2:I:221:G:N2	49:S2:1699:C:OP2	2.54	0.40
3:L5:98:A:H4'	18:LQ:195:ARG:NH1	2.36	0.40
3:L5:299:C:H2'	3:L5:300:A:C8	2.56	0.40
3:L5:2176:G:H5'	8:LF:195:LYS:HE3	2.02	0.40
3:L5:3630:G:N3	7:LE:261:ARG:HA	2.36	0.40
3:L5:3657:OMU:H1'	3:L5:3657:OMU:HM23	1.89	0.40
3:L5:3863:G:C2	3:L5:3896:G:N2	2.89	0.40
5:L8:93:C:O2'	5:L8:94:G:H8	2.04	0.40
8:LF:279:LEU:HD13	8:LF:279:LEU:HA	1.98	0.40
13:LK:12:ILE:HD12	13:LK:53:LYS:HB3	2.01	0.40
13:LK:36:ARG:HH21	13:LK:76:HIS:CD2	2.39	0.40
14:LL:76:MET:HB3	14:LL:85:PHE:CD1	2.56	0.40
15:LM:95:ARG:HD3	15:LM:175:LEU:HB3	2.03	0.40
22:LU:101:ILE:HD12	22:LU:101:ILE:HA	1.81	0.40
26:LY:31:ASN:ND2	26:LY:115:SER:OG	2.42	0.40
27:LZ:23:ARG:HB3	27:LZ:25:ASP:OD1	2.21	0.40
36:Li:47:CYS:SG	36:Li:74:VAL:HG23	2.61	0.40
37:Lj:108:LYS:O	37:Lj:112:GLN:N	2.51	0.40
48:S:1114:A:H4'	48:S:1155:A:C4	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:S2:656:A:H4'	49:S2:657:G:H3'	2.03	0.40
49:S2:1278:C:OP1	67:SV:51:SER:OG	2.22	0.40
49:S2:1579:U:O3'	60:SO:6:SER:HA	2.21	0.40
49:S2:1758:G:H1	49:S2:1776:U:H3	1.69	0.40
59:SN:82:TYR:CZ	59:SN:164:PRO:HD3	2.56	0.40
59:SN:254:ASP:HB2	78:Sg:1:AME:HT22	2.03	0.40
62:SQ:91:ARG:HD2	82:Sk:103:HIS:CE1	2.56	0.40
65:ST:77:ARG:NH1	65:ST:79:ILE:HG12	2.36	0.40
76:Se:42:HIS:HB2	76:Se:83:GLN:HA	2.03	0.40
1:B:686:LEU:HD12	1:B:688:LYS:NZ	2.37	0.40
2:I:44:G:H22	2:I:83:U:H3	1.69	0.40
3:L5:253:G:H2'	3:L5:254:G:C8	2.56	0.40
3:L5:672:C:H2'	3:L5:673:C:C6	2.57	0.40
3:L5:1068:U:H2'	3:L5:1069:G:C8	2.56	0.40
3:L5:1076:G:H2'	3:L5:1077:U:C6	2.56	0.40
3:L5:1514:G:OP1	22:LU:126:LYS:NZ	2.53	0.40
3:L5:2382:C:H2'	3:L5:2383:C:C6	2.56	0.40
3:L5:2494:C:O2'	37:Lj:54:ARG:NH2	2.54	0.40
5:L8:92:U:H2'	5:L8:93:C:O4'	2.21	0.40
8:LF:141:GLY:C	8:LF:204:ARG:HH12	2.28	0.40
13:LK:93:ARG:HD2	13:LK:143:GLU:HG2	2.02	0.40
22:LU:13:SER:OG	22:LU:38:ARG:NH1	2.52	0.40
24:LW:106:LEU:O	24:LW:110:LYS:HG2	2.21	0.40
28:La:109:ILE:O	28:La:113:VAL:HG12	2.21	0.40
38:Lk:103:LYS:HE2	38:Lk:107:GLN:HG2	2.03	0.40
49:S2:568:C:H2'	49:S2:569:C:H5''	2.03	0.40
49:S2:828:A:OP1	66:SU:10:ARG:NH1	2.53	0.40
49:S2:879:G:H22	49:S2:909:A:H2	1.68	0.40
49:S2:1164:C:H2'	49:S2:1165:G:H8	1.85	0.40
55:SG:223:GLU:HG3	55:SG:225:LYS:HG2	2.04	0.40
60:SO:28:GLU:HG2	67:SV:61:GLN:HE21	1.87	0.40
60:SO:43:PRO:O	60:SO:45:ARG:NH1	2.53	0.40
66:SU:37:LEU:HD12	66:SU:43:VAL:HG22	2.03	0.40
68:SW:77:VAL:HA	68:SW:88:ILE:HG22	2.02	0.40
72:Sa:86:LEU:HB3	72:Sa:88:GLU:OE1	2.21	0.40
72:Sa:86:LEU:O	72:Sa:89:MET:HG2	2.21	0.40
74:Sc:61:ILE:O	74:Sc:74:GLN:NE2	2.55	0.40
75:Sd:14:ARG:NH2	75:Sd:17:ASN:HA	2.35	0.40
76:Se:129:ARG:HB3	76:Se:133:ARG:HH12	1.86	0.40
80:Si:115:ILE:HA	80:Si:116:PRO:HD3	1.94	0.40
81:Sj:29:HIS:NE2	81:Sj:69:THR:OG1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:GLN:O	1:B:775:THR:OG1	2.36	0.40
3:L5:848:C:H2'	3:L5:849:G:C8	2.57	0.40
3:L5:857:G:C2	3:L5:1227:G:H2'	2.56	0.40
3:L5:1292:U:H2'	3:L5:1293:G:H8	1.87	0.40
3:L5:1499:G:H5''	37:Lj:14:ASN:O	2.21	0.40
3:L5:2026:C:OP2	21:LT:37:ARG:NH1	2.46	0.40
3:L5:2499:U:OP1	30:Lc:78:ASN:ND2	2.54	0.40
3:L5:4482:C:H2'	3:L5:4483:G:H8	1.85	0.40
3:L5:4757:C:H2'	3:L5:4758:A:H8	1.85	0.40
4:L7:89:G:N2	14:LL:10:ARG:HH22	2.19	0.40
5:L8:15:G:C6	5:L8:16:G:N1	2.90	0.40
5:L8:36:G:C5	38:Lk:89:ARG:HD3	2.56	0.40
19:LR:54:TYR:O	19:LR:58:LEU:N	2.54	0.40
22:LU:126:LYS:HB3	22:LU:131:VAL:HG11	2.03	0.40
30:Lc:17:ARG:NH2	30:Lc:18:TYR:OH	2.54	0.40
31:Ld:39:HIS:O	31:Ld:41:HIS:N	2.55	0.40
37:Lj:18:ASN:HD21	37:Lj:34:TYR:HE2	1.68	0.40
44:Lq:74:GLU:HB3	44:Lq:77:CYS:HB3	2.03	0.40
49:S2:27:A2M:H2'	49:S2:28:U:O4'	2.21	0.40
49:S2:836:C:H2'	49:S2:838:A:N3	2.37	0.40
49:S2:949:C:H2'	49:S2:950:G:H8	1.87	0.40
49:S2:1229:A:H2'	49:S2:1230:G:C8	2.56	0.40
49:S2:1469:C:H2'	49:S2:1470:A:H8	1.86	0.40
49:S2:1758:G:N2	49:S2:1776:U:O2	2.48	0.40
55:SG:59:LEU:HD23	55:SG:90:TRP:CD2	2.56	0.40
55:SG:145:GLU:HB3	55:SG:184:LEU:HD23	2.03	0.40
55:SG:216:ALA:HB3	55:SG:230:LEU:HB2	2.02	0.40
57:SL:123:VAL:HA	57:SL:145:ILE:O	2.22	0.40
58:SM:150:ILE:HD12	58:SM:150:ILE:HA	1.94	0.40
59:SN:208:PRO:O	59:SN:212:LYS:HG2	2.21	0.40
73:Sb:28:GLY:HA3	73:Sb:67:ASP:HB2	2.02	0.40
73:Sb:40:GLU:HG2	73:Sb:41:MET:SD	2.61	0.40
74:Sc:111:PHE:O	74:Sc:114:LEU:HG	2.21	0.40
82:Sk:57:LYS:HA	82:Sk:60:LYS:NZ	2.36	0.40
3:L5:92:C:OP2	3:L5:4087:C:O2'	2.32	0.40
3:L5:208:A:H2	3:L5:233:U:H5''	1.86	0.40
3:L5:728:G:O3'	17:LP:70:GLN:NE2	2.53	0.40
3:L5:845:U:O2'	3:L5:846:C:H5''	2.22	0.40
3:L5:1250:C:H2'	3:L5:1251:A:C8	2.56	0.40
3:L5:1907:G:N2	3:L5:1959:U:H1'	2.37	0.40
3:L5:2102:G:O3'	10:LH:111:LYS:NZ	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2225:A:N6	3:L5:2265:OMC:O2	2.54	0.40
3:L5:2621:G:H22	5:L8:113:C:P	2.44	0.40
3:L5:4270:G:N3	7:LE:252:ALA:HB1	2.36	0.40
3:L5:4675:G:N7	10:LH:186:ARG:HD3	2.37	0.40
3:L5:4678:C:H3'	10:LH:159:ARG:HH22	1.86	0.40
5:L8:84:A:C5	5:L8:88:A:H4'	2.56	0.40
8:LF:56:GLU:HG3	8:LF:57:LEU:HD12	2.02	0.40
9:LG:41:LYS:HB2	24:LW:68:THR:O	2.21	0.40
9:LG:108:ARG:CZ	9:LG:253:TYR:HB2	2.52	0.40
10:LH:286:PRO:HB2	36:Li:41:PHE:CE2	2.57	0.40
11:LI:181:TYR:CZ	11:LI:202:GLU:HG2	2.56	0.40
20:LS:30:ARG:NH2	20:LS:34:GLN:HE21	2.20	0.40
20:LS:52:THR:HG23	20:LS:85:LYS:HG3	2.03	0.40
26:LY:60:MET:HE3	26:LY:129:TRP:CH2	2.57	0.40
29:Lb:47:MET:HG2	29:Lb:115:ARG:HH21	1.87	0.40
41:Ln:34:PHE:HZ	41:Ln:53:ALA:HB1	1.86	0.40
49:S2:79:A:H3'	49:S2:80:G:H8	1.87	0.40
49:S2:195:C:H2'	49:S2:205:G:N2	2.36	0.40
49:S2:544:C:H2'	49:S2:545:G:C8	2.57	0.40
49:S2:1789:A:H2'	49:S2:1790:G:O4'	2.22	0.40
55:SG:20:GLN:HG2	55:SG:69:VAL:H	1.85	0.40
72:Sa:20:VAL:HG11	72:Sa:28:MET:HE1	2.03	0.40
76:Se:114:GLU:HB2	76:Se:124:THR:HG22	2.03	0.40
79:Sh:30:CYS:SG	79:Sh:31:SER:N	2.93	0.40
81:Sj:60:PHE:CD1	81:Sj:71:GLY:HA3	2.56	0.40
3:L5:4:G:H2'	3:L5:5:A:H8	1.86	0.40
3:L5:190:G:H2'	3:L5:191:G:C8	2.56	0.40
3:L5:693:C:H2'	3:L5:694:G:C8	2.56	0.40
3:L5:1060:G:O5'	3:L5:1086:G:N2	2.55	0.40
3:L5:2667:OMC:H1'	3:L5:2667:OMC:HM23	1.87	0.40
3:L5:3869:G:H1'	3:L5:3890:G:H22	1.85	0.40
3:L5:3935:U:H2'	3:L5:3936:U:O4'	2.22	0.40
3:L5:4014:A:H2'	3:L5:4015:G:O4'	2.22	0.40
8:LF:25:PRO:HB2	8:LF:27:VAL:HG12	2.03	0.40
8:LF:62:THR:HG22	8:LF:64:ALA:H	1.85	0.40
9:LG:21:ARG:O	9:LG:25:GLU:HG2	2.20	0.40
12:LJ:171:PRO:HB3	12:LJ:181:TYR:CE2	2.56	0.40
12:LJ:173:LEU:HB2	39:Ll:43:MET:HE2	2.03	0.40
13:LK:67:LEU:O	13:LK:70:VAL:HG12	2.21	0.40
13:LK:113:GLU:OE1	13:LK:115:ARG:NH2	2.49	0.40
14:LL:30:LYS:HG2	14:LL:63:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LM:152:GLY:O	15:LM:156:ARG:HG3	2.21	0.40
17:LP:7:VAL:HG22	23:LV:152:PHE:O	2.22	0.40
20:LS:15:CYS:SG	20:LS:102:ALA:HB2	2.61	0.40
21:LT:68:ARG:HG2	21:LT:71:LYS:HZ2	1.86	0.40
24:LW:112:ASN:O	24:LW:116:LYS:N	2.55	0.40
35:Lh:75:ARG:HD3	35:Lh:95:TYR:CE1	2.57	0.40
38:Lk:79:LYS:HE2	38:Lk:79:LYS:HB2	1.82	0.40
49:S2:556:A:N3	53:SE:99:LYS:NZ	2.68	0.40
49:S2:689:U:H5	64:SS:102:PRO:HA	1.86	0.40
49:S2:945:A:H1'	71:SZ:136:PRO:HB3	2.02	0.40
49:S2:1093:G:H2'	49:S2:1094:A:C8	2.57	0.40
49:S2:1125:C:OP1	58:SM:150:ILE:HG22	2.21	0.40
50:SB:25:VAL:HG23	79:Sh:53:ILE:HD11	2.03	0.40
55:SG:68:ASP:OD1	55:SG:69:VAL:N	2.54	0.40
55:SG:259:TRP:HD1	55:SG:266:ILE:HA	1.85	0.40
61:SP:18:TRP:HH2	61:SP:31:PRO:HD3	1.86	0.40
61:SP:112:HIS:CE1	61:SP:237:SER:HG	2.34	0.40
72:Sa:92:SER:OG	72:Sa:93:MET:N	2.54	0.40
81:Sj:23:MET:SD	81:Sj:23:MET:N	2.95	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	B	200/854 (23%)	171 (86%)	28 (14%)	1 (0%)	24	57
6	LD	251/257 (98%)	238 (95%)	13 (5%)	0	100	100
7	LE	395/403 (98%)	386 (98%)	9 (2%)	0	100	100
8	LF	360/413 (87%)	354 (98%)	6 (2%)	0	100	100
9	LG	291/297 (98%)	286 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	LH	239/291 (82%)	231 (97%)	8 (3%)	0	100	100
11	LI	224/247 (91%)	218 (97%)	6 (3%)	0	100	100
12	LJ	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
13	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
14	LL	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
15	LM	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
16	LO	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
17	LP	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
18	LQ	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	LR	197/203 (97%)	197 (100%)	0	0	100	100
20	LS	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
21	LT	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
22	LU	178/196 (91%)	178 (100%)	0	0	100	100
23	LV	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
24	LW	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
25	LX	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
26	LY	137/140 (98%)	137 (100%)	0	0	100	100
27	LZ	89/157 (57%)	89 (100%)	0	0	100	100
28	La	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
29	Lb	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
30	Lc	133/136 (98%)	133 (100%)	0	0	100	100
31	Ld	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	18	49
32	Le	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
33	Lf	106/115 (92%)	106 (100%)	0	0	100	100
34	Lg	105/125 (84%)	105 (100%)	0	0	100	100
35	Lh	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
36	Li	108/110 (98%)	108 (100%)	0	0	100	100
37	Lj	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
38	Lk	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
39	Ll	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
40	Lm	84/97 (87%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Ln	67/70 (96%)	67 (100%)	0	0	100	100
42	Lo	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	Lp	49/128 (38%)	49 (100%)	0	0	100	100
44	Lq	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
45	Lr	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
46	Ls	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
47	Lx	161/217 (74%)	143 (89%)	18 (11%)	0	100	100
50	SB	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
51	SC	61/69 (88%)	61 (100%)	0	0	100	100
52	SD	65/156 (42%)	64 (98%)	1 (2%)	0	100	100
53	SE	55/133 (41%)	55 (100%)	0	0	100	100
54	SF	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
55	SG	311/317 (98%)	300 (96%)	11 (4%)	0	100	100
56	SH	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
57	SL	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
58	SM	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
59	SN	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
60	SO	223/281 (79%)	220 (99%)	3 (1%)	0	100	100
61	SP	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
62	SQ	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
63	SR	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
64	SS	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
65	ST	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
66	SU	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
67	SV	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
68	SW	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
69	SX	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
70	SY	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
71	SZ	134/151 (89%)	128 (96%)	6 (4%)	0	100	100
72	Sa	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
73	Sb	139/172 (81%)	132 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Sc	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
75	Sd	139/152 (91%)	136 (98%)	3 (2%)	0	100	100
76	Se	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
77	Sf	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
78	Sg	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
79	Sh	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
80	Si	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
81	Sj	123/130 (95%)	123 (100%)	0	0	100	100
82	Sk	73/124 (59%)	71 (97%)	2 (3%)	0	100	100
83	Sl	23/25 (92%)	23 (100%)	0	0	100	100
All	All	11653/14208 (82%)	11397 (98%)	254 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	703	SER
31	Ld	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	102/761 (13%)	99 (97%)	3 (3%)	37	66
6	LD	195/199 (98%)	192 (98%)	3 (2%)	57	75
7	LE	344/347 (99%)	334 (97%)	10 (3%)	37	66
8	LF	302/337 (90%)	297 (98%)	5 (2%)	53	74
9	LG	247/250 (99%)	242 (98%)	5 (2%)	48	72
10	LH	216/251 (86%)	212 (98%)	4 (2%)	50	73
11	LI	197/215 (92%)	193 (98%)	4 (2%)	48	72
12	LJ	199/223 (89%)	196 (98%)	3 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	LK	169/171 (99%)	166 (98%)	3 (2%)	51	73
14	LL	180/181 (99%)	176 (98%)	4 (2%)	45	71
15	LM	143/149 (96%)	142 (99%)	1 (1%)	76	82
16	LO	175/176 (99%)	171 (98%)	4 (2%)	44	70
17	LP	117/161 (73%)	115 (98%)	2 (2%)	53	74
18	LQ	171/172 (99%)	168 (98%)	3 (2%)	51	73
19	LR	171/173 (99%)	167 (98%)	4 (2%)	44	70
20	LS	139/163 (85%)	138 (99%)	1 (1%)	76	82
21	LT	164/165 (99%)	155 (94%)	9 (6%)	19	50
22	LU	159/175 (91%)	158 (99%)	1 (1%)	78	83
23	LV	154/154 (100%)	149 (97%)	5 (3%)	34	64
24	LW	139/140 (99%)	139 (100%)	0	100	100
25	LX	88/113 (78%)	87 (99%)	1 (1%)	65	78
26	LY	106/107 (99%)	105 (99%)	1 (1%)	70	80
27	LZ	79/126 (63%)	79 (100%)	0	100	100
28	La	106/134 (79%)	104 (98%)	2 (2%)	50	73
29	Lb	124/135 (92%)	122 (98%)	2 (2%)	55	75
30	Lc	117/118 (99%)	115 (98%)	2 (2%)	53	74
31	Ld	118/120 (98%)	113 (96%)	5 (4%)	26	58
32	Le	87/183 (48%)	84 (97%)	3 (3%)	32	63
33	Lf	92/98 (94%)	89 (97%)	3 (3%)	33	63
34	Lg	98/110 (89%)	93 (95%)	5 (5%)	21	52
35	Lh	116/121 (96%)	112 (97%)	4 (3%)	32	63
36	Li	89/89 (100%)	89 (100%)	0	100	100
37	Lj	98/100 (98%)	97 (99%)	1 (1%)	68	79
38	Lk	109/110 (99%)	106 (97%)	3 (3%)	38	66
39	Ll	86/89 (97%)	83 (96%)	3 (4%)	32	62
40	Lm	73/80 (91%)	73 (100%)	0	100	100
41	Ln	64/65 (98%)	62 (97%)	2 (3%)	35	64
42	Lo	47/48 (98%)	44 (94%)	3 (6%)	16	44
43	Lp	47/115 (41%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	Lq	92/93 (99%)	91 (99%)	1 (1%)	65	78
45	Lr	74/75 (99%)	72 (97%)	2 (3%)	39	67
46	Ls	109/120 (91%)	106 (97%)	3 (3%)	38	66
50	SB	75/76 (99%)	72 (96%)	3 (4%)	28	60
51	SC	56/62 (90%)	56 (100%)	0	100	100
52	SD	60/140 (43%)	60 (100%)	0	100	100
53	SE	47/106 (44%)	46 (98%)	1 (2%)	47	71
54	SF	88/98 (90%)	87 (99%)	1 (1%)	65	78
55	SG	272/275 (99%)	267 (98%)	5 (2%)	51	73
56	SH	48/49 (98%)	48 (100%)	0	100	100
57	SL	182/243 (75%)	179 (98%)	3 (2%)	55	75
58	SM	203/231 (88%)	199 (98%)	4 (2%)	48	72
59	SN	185/223 (83%)	182 (98%)	3 (2%)	55	75
60	SO	189/232 (82%)	186 (98%)	3 (2%)	55	75
61	SP	224/225 (100%)	222 (99%)	2 (1%)	70	80
62	SQ	161/170 (95%)	159 (99%)	2 (1%)	63	78
63	SR	207/218 (95%)	206 (100%)	1 (0%)	81	85
64	SS	170/360 (47%)	167 (98%)	3 (2%)	51	73
65	ST	178/180 (99%)	174 (98%)	4 (2%)	45	71
66	SU	161/168 (96%)	160 (99%)	1 (1%)	78	83
67	SV	87/136 (64%)	86 (99%)	1 (1%)	65	78
68	SW	139/142 (98%)	137 (99%)	2 (1%)	59	76
69	SX	103/108 (95%)	101 (98%)	2 (2%)	50	73
70	SY	130/131 (99%)	125 (96%)	5 (4%)	29	60
71	SZ	106/119 (89%)	101 (95%)	5 (5%)	23	55
72	Sa	113/130 (87%)	110 (97%)	3 (3%)	39	67
73	Sb	117/140 (84%)	115 (98%)	2 (2%)	53	74
74	Sc	120/121 (99%)	116 (97%)	4 (3%)	33	63
75	Sd	122/131 (93%)	119 (98%)	3 (2%)	42	69
76	Se	112/114 (98%)	111 (99%)	1 (1%)	70	80
77	Sf	92/107 (86%)	89 (97%)	3 (3%)	33	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	Sg	67/67 (100%)	63 (94%)	4 (6%)	17	47
79	Sh	112/113 (99%)	109 (97%)	3 (3%)	39	67
80	Si	112/114 (98%)	109 (97%)	3 (3%)	39	67
81	Sj	107/112 (96%)	105 (98%)	2 (2%)	50	73
82	Sk	66/102 (65%)	63 (96%)	3 (4%)	24	56
83	Sl	24/24 (100%)	24 (100%)	0	100	100
All	All	9937/11879 (84%)	9735 (98%)	202 (2%)	48	72

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	674	VAL
1	B	729	LEU
1	B	738	LEU
6	LD	114	CYS
6	LD	118	GLU
6	LD	224	THR
7	LE	5	LYS
7	LE	78	ILE
7	LE	181	MET
7	LE	182	GLU
7	LE	262	VAL
7	LE	315	ASN
7	LE	340	THR
7	LE	344	VAL
7	LE	346	THR
7	LE	355	THR
8	LF	137	VAL
8	LF	150	LEU
8	LF	187	GLN
8	LF	202	ILE
8	LF	281	MET
9	LG	4	VAL
9	LG	55	VAL
9	LG	74	ILE
9	LG	94	ASN
9	LG	214	GLU
10	LH	51	VAL
10	LH	52	LEU
10	LH	94	THR

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Mol	Chain	Res	Type
10	LH	290	VAL
11	LI	41	LEU
11	LI	124	LEU
11	LI	155	LYS
11	LI	222	LYS
12	LJ	82	GLN
12	LJ	106	THR
12	LJ	253	LEU
13	LK	10	VAL
13	LK	55	LEU
13	LK	169	ASN
14	LL	53	VAL
14	LL	126	VAL
14	LL	134	VAL
14	LL	206	LEU
15	LM	168	GLN
16	LO	59	VAL
16	LO	64	VAL
16	LO	125	VAL
16	LO	154	VAL
17	LP	30	VAL
17	LP	43	THR
18	LQ	8	GLN
18	LQ	50	ARG
18	LQ	183	THR
19	LR	7	LEU
19	LR	49	ARG
19	LR	138	LEU
19	LR	162	GLU
20	LS	95	LEU
21	LT	6	ARG
21	LT	19	LYS
21	LT	28	LEU
21	LT	83	VAL
21	LT	87	THR
21	LT	105	VAL
21	LT	121	LEU
21	LT	128	LEU
21	LT	136	THR
22	LU	10	LEU
23	LV	6	THR
23	LV	13	VAL

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Mol	Chain	Res	Type
23	LV	17	LEU
23	LV	129	VAL
23	LV	132	MET
25	LX	61	VAL
26	LY	76	VAL
28	La	124	VAL
28	La	138	VAL
29	Lb	2	LYS
29	Lb	73	VAL
30	Lc	54	THR
30	Lc	72	VAL
31	Ld	26	ARG
31	Ld	67	GLN
31	Ld	111	VAL
31	Ld	124	VAL
31	Ld	127	LYS
32	Le	54	LEU
32	Le	58	GLN
32	Le	92	LYS
33	Lf	20	LEU
33	Lf	39	ARG
33	Lf	92	CYS
34	Lg	20	VAL
34	Lg	26	THR
34	Lg	59	THR
34	Lg	77	ILE
34	Lg	80	VAL
35	Lh	13	VAL
35	Lh	15	LYS
35	Lh	122	VAL
35	Lh	126	ASN
37	Lj	18	ASN
38	Lk	30	GLN
38	Lk	58	LEU
38	Lk	105	LYS
39	Ll	7	MET
39	Ll	40	VAL
39	Ll	48	CYS
41	Ln	32	VAL
41	Ln	66	VAL
42	Lo	6	THR
42	Lo	30	LYS

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Mol	Chain	Res	Type
42	Lo	51	LEU
44	Lq	64	LYS
45	Lr	52	VAL
45	Lr	63	THR
46	Ls	19	LYS
46	Ls	61	VAL
46	Ls	113	ARG
50	SB	8	LEU
50	SB	53	VAL
50	SB	74	THR
53	SE	132	ASN
54	SF	75	VAL
55	SG	54	ILE
55	SG	138	CYS
55	SG	141	THR
55	SG	174	VAL
55	SG	235	ILE
57	SL	84	GLN
57	SL	109	THR
57	SL	197	VAL
58	SM	91	VAL
58	SM	113	MET
58	SM	114	VAL
58	SM	212	VAL
59	SN	70	VAL
59	SN	83	LEU
59	SN	230	THR
60	SO	46	THR
60	SO	48	ILE
60	SO	162	ASP
61	SP	33	THR
61	SP	246	LEU
62	SQ	103	LEU
62	SQ	169	ILE
63	SR	124	LEU
64	SS	66	VAL
64	SS	69	LEU
64	SS	84	GLU
65	ST	48	VAL
65	ST	90	LEU
65	ST	130	THR
65	ST	190	LEU

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Mol	Chain	Res	Type
66	SU	17	ARG
67	SV	15	LEU
68	SW	87	VAL
68	SW	125	ILE
69	SX	42	LEU
69	SX	65	VAL
70	SY	11	LEU
70	SY	46	THR
70	SY	66	VAL
70	SY	75	LEU
70	SY	118	ILE
71	SZ	52	THR
71	SZ	57	THR
71	SZ	91	THR
71	SZ	132	VAL
71	SZ	140	THR
72	Sa	16	THR
72	Sa	76	VAL
72	Sa	126	VAL
73	Sb	34	VAL
73	Sb	70	VAL
74	Sc	40	ILE
74	Sc	60	ARG
74	Sc	119	VAL
74	Sc	126	MET
75	Sd	36	VAL
75	Sd	38	ARG
75	Sd	139	THR
76	Se	88	MET
77	Sf	54	VAL
77	Sf	98	VAL
77	Sf	100	GLN
78	Sg	9	VAL
78	Sg	13	VAL
78	Sg	36	VAL
78	Sg	42	VAL
79	Sh	52	ILE
79	Sh	97	ARG
79	Sh	126	LEU
80	Si	7	LEU
80	Si	72	VAL
80	Si	125	VAL

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Mol	Chain	Res	Type
81	Sj	5	VAL
81	Sj	18	LEU
82	Sk	61	GLU
82	Sk	67	LEU
82	Sk	69	THR

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

Mol	Chain	Res	Type
1	B	431	GLN
1	B	656	GLN
1	B	683	HIS
1	B	739	ASN
6	LD	215	ASN
7	LE	68	ASN
7	LE	354	GLN
8	LF	21	ASN
8	LF	89	GLN
8	LF	347	HIS
11	LI	57	HIS
11	LI	118	ASN
11	LI	130	ASN
12	LJ	66	GLN
14	LL	59	GLN
16	LO	67	HIS
16	LO	104	ASN
17	LP	34	ASN
17	LP	48	GLN
18	LQ	37	HIS
18	LQ	117	ASN
19	LR	63	ASN
19	LR	173	GLN
21	LT	125	GLN
24	LW	79	GLN
24	LW	90	ASN
26	LY	135	ASN
27	LZ	95	ASN
29	Lb	56	GLN
29	Lb	72	GLN
31	Ld	66	ASN
32	Le	6	ASN
32	Le	60	ASN

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Mol	Chain	Res	Type
35	Lh	80	HIS
37	Lj	18	ASN
43	Lp	90	ASN
44	Lq	102	GLN
46	Ls	4	HIS
46	Ls	6	GLN
46	Ls	36	ASN
52	SD	139	HIS
55	SG	26	GLN
55	SG	159	ASN
56	SH	37	ASN
57	SL	50	ASN
57	SL	113	GLN
58	SM	40	ASN
58	SM	160	GLN
58	SM	163	GLN
58	SM	208	HIS
59	SN	267	GLN
60	SO	165	ASN
61	SP	142	HIS
61	SP	161	GLN
61	SP	188	ASN
61	SP	216	ASN
62	SQ	79	HIS
62	SQ	118	ASN
62	SQ	149	GLN
63	SR	65	GLN
64	SS	157	HIS
64	SS	163	GLN
65	ST	165	GLN
65	ST	167	GLN
67	SV	44	HIS
68	SW	11	GLN
69	SX	55	ASN
70	SY	49	GLN
74	Sc	26	ASN
74	Sc	48	ASN
74	Sc	118	GLN
75	Sd	42	HIS
78	Sg	35	ASN
78	Sg	81	GLN
79	Sh	5	ASN

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Mol	Chain	Res	Type
79	Sh	15	ASN
79	Sh	44	HIS
80	Si	92	ASN
81	Sj	106	GLN
82	Sk	112	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	160/163 (98%)	90 (56%)	6 (3%)
3	L5	3719/4808 (77%)	532 (14%)	3 (0%)
4	L7	118/120 (98%)	8 (6%)	0
48	S	45/855 (5%)	19 (42%)	4 (8%)
49	S2	1764/1870 (94%)	244 (13%)	2 (0%)
5	L8	155/158 (98%)	18 (11%)	0
All	All	5961/7974 (74%)	911 (15%)	15 (0%)

All (911) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	33	A
2	I	37	U
2	I	39	A
2	I	44	G
2	I	46	U
2	I	47	U
2	I	49	U
2	I	52	A
2	I	54	A
2	I	56	A
2	I	60	U
2	I	61	U
2	I	62	G
2	I	67	G
2	I	68	U
2	I	74	A
2	I	75	A
2	I	76	U
2	I	80	A
2	I	81	A
2	I	82	G

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Mol	Chain	Res	Type
2	I	84	A
2	I	86	U
2	I	87	G
2	I	88	C
2	I	89	U
2	I	90	A
2	I	93	U
2	I	95	U
2	I	96	G
2	I	99	U
2	I	100	U
2	I	101	U
2	I	105	U
2	I	106	U
2	I	107	A
2	I	112	U
2	I	113	U
2	I	114	U
2	I	115	A
2	I	118	U
2	I	120	U
2	I	122	C
2	I	123	G
2	I	124	U
2	I	127	C
2	I	128	A
2	I	129	G
2	I	130	G
2	I	131	A
2	I	133	G
2	I	135	C
2	I	136	U
2	I	138	G
2	I	142	C
2	I	143	A
2	I	145	C
2	I	146	C
2	I	147	C
2	I	149	A
2	I	153	U
2	I	154	A
2	I	155	U

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Mol	Chain	Res	Type
2	I	157	C
2	I	158	A
2	I	163	G
2	I	165	C
2	I	166	C
2	I	167	U
2	I	168	C
2	I	169	U
2	I	170	C
2	I	171	U
2	I	172	G
2	I	173	C
2	I	174	G
2	I	175	G
2	I	177	U
2	I	178	U
2	I	179	U
2	I	180	U
2	I	181	C
2	I	200	A
2	I	201	C
2	I	202	C
2	I	217	U
2	I	218	G
2	I	219	A
2	I	220	G
2	I	221	G
3	L5	39	A
3	L5	42	A
3	L5	58	G
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	85	G
3	L5	91	G
3	L5	98	A
3	L5	109	G
3	L5	119	G
3	L5	122	U
3	L5	127	G
3	L5	135	G
3	L5	136	U

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Mol	Chain	Res	Type
3	L5	142	G
3	L5	144	G
3	L5	159	C
3	L5	187	U
3	L5	188	G
3	L5	200	U
3	L5	201	C
3	L5	209	U
3	L5	210	C
3	L5	218	A
3	L5	219	G
3	L5	220	C
3	L5	233	U
3	L5	234	G
3	L5	266	C
3	L5	297	U
3	L5	308	G
3	L5	309	C
3	L5	315	G
3	L5	316	U
3	L5	326	C
3	L5	334	A
3	L5	340	C
3	L5	363	A
3	L5	386	A
3	L5	387	G
3	L5	409	G
3	L5	410	A
3	L5	412	G
3	L5	440	U
3	L5	446	C
3	L5	449	C
3	L5	450	G
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	455	C
3	L5	463	A
3	L5	467	U
3	L5	468	U
3	L5	482	U
3	L5	483	G

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Mol	Chain	Res	Type
3	L5	485	U
3	L5	486	C
3	L5	488	G
3	L5	493	U
3	L5	497	G
3	L5	499	C
3	L5	502	U
3	L5	503	C
3	L5	504	U
3	L5	505	C
3	L5	506	G
3	L5	512	U
3	L5	515	U
3	L5	516	U
3	L5	517	C
3	L5	633	U
3	L5	634	C
3	L5	635	G
3	L5	636	G
3	L5	660	G
3	L5	661	A
3	L5	682	U
3	L5	691	G
3	L5	698	C
3	L5	699	G
3	L5	724	G
3	L5	725	G
3	L5	732	C
3	L5	734	G
3	L5	739	G
3	L5	748	C
3	L5	751	G
3	L5	757	A
3	L5	758	C
3	L5	759	G
3	L5	763	C
3	L5	790	G
3	L5	791	C
3	L5	792	G
3	L5	793	C
3	L5	795	A
3	L5	797	C

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Mol	Chain	Res	Type
3	L5	798	C
3	L5	810	U
3	L5	812	A
3	L5	814	A
3	L5	815	G
3	L5	824	C
3	L5	825	G
3	L5	831	A
3	L5	832	G
3	L5	834	A
3	L5	835	G
3	L5	841	C
3	L5	843	A
3	L5	844	A
3	L5	845	U
3	L5	846	C
3	L5	856	A
3	L5	859	G
3	L5	860	A
3	L5	861	G
3	L5	866	A
3	L5	867	C
3	L5	868	C
3	L5	869	U
3	L5	870	G
3	L5	879	C
3	L5	884	U
3	L5	983	G
3	L5	985	G
3	L5	987	C
3	L5	988	G
3	L5	989	G
3	L5	995	C
3	L5	1004	G
3	L5	1012	C
3	L5	1014	C
3	L5	1060	G
3	L5	1072	C
3	L5	1073	C
3	L5	1074	C
3	L5	1078	G
3	L5	1083	C

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Mol	Chain	Res	Type
3	L5	1084	C
3	L5	1085	G
3	L5	1086	G
3	L5	1087	G
3	L5	1090	U
3	L5	1102	G
3	L5	1105	C
3	L5	1106	U
3	L5	1124	A
3	L5	1130	C
3	L5	1131	G
3	L5	1133	C
3	L5	1136	G
3	L5	1137	C
3	L5	1138	G
3	L5	1139	C
3	L5	1202	C
3	L5	1214	A
3	L5	1215	G
3	L5	1216	C
3	L5	1217	G
3	L5	1219	G
3	L5	1221	G
3	L5	1228	G
3	L5	1231	G
3	L5	1239	U
3	L5	1240	G
3	L5	1246	U
3	L5	1247	A
3	L5	1270	A2M
3	L5	1298	A
3	L5	1299	G
3	L5	1303	G
3	L5	1309	C
3	L5	1310	G
3	L5	1323	C
3	L5	1325	U
3	L5	1331	A
3	L5	1341	A
3	L5	1342	A
3	L5	1351	G
3	L5	1362	C

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Mol	Chain	Res	Type
3	L5	1367	G
3	L5	1375	A
3	L5	1391	C
3	L5	1393	C
3	L5	1398	A
3	L5	1401	C
3	L5	1452	A
3	L5	1453	G
3	L5	1457	G
3	L5	1489	A2M
3	L5	1490	C
3	L5	1502	A
3	L5	1521	C
3	L5	1533	U
3	L5	1546	U
3	L5	1551	U
3	L5	1579	G
3	L5	1580	OMG
3	L5	1586	A
3	L5	1588	G
3	L5	1589	A
3	L5	1593	A
3	L5	1596	G
3	L5	1609	G
3	L5	1616	C
3	L5	1631	C
3	L5	1632	PSU
3	L5	1646	G
3	L5	1653	C
3	L5	1657	C
3	L5	1658	C
3	L5	1673	G
3	L5	1694	C
3	L5	1704	A
3	L5	1705	A
3	L5	1726	A
3	L5	1743	A
3	L5	1745	G
3	L5	1767	C
3	L5	1774	G
3	L5	1775	G
3	L5	1776	A

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Mol	Chain	Res	Type
3	L5	1781	G
3	L5	1782	A
3	L5	1794	G
3	L5	1808	G
3	L5	1836	A
3	L5	1857	U
3	L5	1859	C
3	L5	1860	C
3	L5	1861	G
3	L5	1870	C
3	L5	1871	A
3	L5	1879	G
3	L5	1887	G
3	L5	1891	G
3	L5	1898	U
3	L5	1899	A
3	L5	1900	G
3	L5	1910	C
3	L5	1911	G
3	L5	1914	G
3	L5	1915	G
3	L5	1922	A
3	L5	1923	A
3	L5	1924	G
3	L5	1926	C
3	L5	1934	G
3	L5	1936	U
3	L5	1940	G
3	L5	1942	G
3	L5	1943	U
3	L5	1959	U
3	L5	1963	G
3	L5	1964	A
3	L5	1965	A
3	L5	1984	G
3	L5	1985	G
3	L5	1987	U
3	L5	1994	G
3	L5	1995	G
3	L5	2008	A
3	L5	2023	U
3	L5	2032	G

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Mol	Chain	Res	Type
3	L5	2034	A
3	L5	2036	A
3	L5	2037	G
3	L5	2041	G
3	L5	2044	A
3	L5	2045	G
3	L5	2046	A
3	L5	2050	U
3	L5	2051	G
3	L5	2101	C
3	L5	2132	C
3	L5	2143	A
3	L5	2144	G
3	L5	2156	A
3	L5	2157	G
3	L5	2159	G
3	L5	2174	G
3	L5	2191	G
3	L5	2194	OMC
3	L5	2203	A
3	L5	2238	A
3	L5	2253	C
3	L5	2264	G
3	L5	2268	U
3	L5	2269	U
3	L5	2329	G
3	L5	2332	C
3	L5	2333	U
3	L5	2334	C
3	L5	2349	G
3	L5	2354	A
3	L5	2356	A
3	L5	2363	C
3	L5	2372	A
3	L5	2380	A
3	L5	2386	A
3	L5	2387	G
3	L5	2388	U
3	L5	2390	G
3	L5	2397	U
3	L5	2409	G
3	L5	2429	G

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Mol	Chain	Res	Type
3	L5	2430	A
3	L5	2444	A
3	L5	2461	G
3	L5	2470	C
3	L5	2496	C
3	L5	2503	A
3	L5	2504	U
3	L5	2512	C
3	L5	2530	U
3	L5	2537	G
3	L5	2538	A
3	L5	2539	A
3	L5	2551	U
3	L5	2552	C
3	L5	2553	C
3	L5	2554	G
3	L5	2586	A
3	L5	2606	U
3	L5	2612	U
3	L5	2631	U
3	L5	2633	U
3	L5	2657	C
3	L5	2658	A2M
3	L5	2669	U
3	L5	2670	G
3	L5	2672	U
3	L5	2698	G
3	L5	2745	G
3	L5	3329	G
3	L5	3350	C
3	L5	3358	G
3	L5	3367	A
3	L5	3378	A
3	L5	3385	A
3	L5	3394	A
3	L5	3405	C
3	L5	3424	A
3	L5	3428	C
3	L5	3443	A
3	L5	3444	A
3	L5	3485	G
3	L5	3492	A2M

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Mol	Chain	Res	Type
3	L5	3493	C
3	L5	3498	A
3	L5	3508	G
3	L5	3509	G
3	L5	3515	A
3	L5	3516	A
3	L5	3543	G
3	L5	3546	U
3	L5	3549	A
3	L5	3550	U
3	L5	3551	G
3	L5	3570	U
3	L5	3572	U
3	L5	3609	A
3	L5	3610	C
3	L5	3611	G
3	L5	3629	G
3	L5	3630	G
3	L5	3633	A
3	L5	3638	A
3	L5	3639	G
3	L5	3640	A
3	L5	3647	U
3	L5	3648	G
3	L5	3670	G
3	L5	3671	G
3	L5	3677	A
3	L5	3678	G
3	L5	3683	G
3	L5	3688	G
3	L5	3695	A
3	L5	3697	A
3	L5	3698	A
3	L5	3700	U
3	L5	3701	G
3	L5	3703	G
3	L5	3704	A
3	L5	3765	C
3	L5	3770	G
3	L5	3778	A
3	L5	3783	U
3	L5	3785	C

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Mol	Chain	Res	Type
3	L5	3804	G
3	L5	3812	G
3	L5	3823	G
3	L5	3824	C
3	L5	3825	G
3	L5	3826	A
3	L5	3828	C
3	L5	3832	G
3	L5	3833	A
3	L5	3834	G
3	L5	3839	U
3	L5	3840	C
3	L5	3847	C
3	L5	3849	G
3	L5	3850	G
3	L5	3855	A
3	L5	3869	G
3	L5	3875	C
3	L5	3886	G
3	L5	3891	C
3	L5	3892	G
3	L5	3896	G
3	L5	3904	C
3	L5	3909	U
3	L5	3916	A
3	L5	3929	G
3	L5	3930	G
3	L5	3937	G
3	L5	3949	A
3	L5	3971	G
3	L5	3975	U
3	L5	3979	A
3	L5	3997	A
3	L5	4000	G
3	L5	4004	C
3	L5	4012	G
3	L5	4014	A
3	L5	4017	A
3	L5	4019	A
3	L5	4027	A
3	L5	4037	G
3	L5	4051	G

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Mol	Chain	Res	Type
3	L5	4052	OMU
3	L5	4060	C
3	L5	4072	G
3	L5	4075	G
3	L5	4076	G
3	L5	4078	C
3	L5	4096	C
3	L5	4100	U
3	L5	4119	G
3	L5	4123	G
3	L5	4124	A
3	L5	4126	A
3	L5	4133	C
3	L5	4137	G
3	L5	4140	A
3	L5	4161	A
3	L5	4168	A
3	L5	4183	U
3	L5	4194	G
3	L5	4210	A
3	L5	4212	C
3	L5	4258	U
3	L5	4259	A
3	L5	4261	G
3	L5	4268	G
3	L5	4270	G
3	L5	4294	A
3	L5	4306	C
3	L5	4313	G
3	L5	4321	G
3	L5	4336	A2M
3	L5	4382	PSU
3	L5	4383	OMG
3	L5	4402	A
3	L5	4416	C
3	L5	4418	A
3	L5	4437	A
3	L5	4446	A
3	L5	4454	A
3	L5	4455	U
3	L5	4465	G
3	L5	4475	A

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Mol	Chain	Res	Type
3	L5	4476	C
3	L5	4477	G
3	L5	4478	G
3	L5	4479	C
3	L5	4484	C
3	L5	4486	G
3	L5	4487	A
3	L5	4488	A
3	L5	4489	G
3	L5	4490	G
3	L5	4492	G
3	L5	4498	G
3	L5	4501	G
3	L5	4504	C
3	L5	4506	C
3	L5	4508	G
3	L5	4512	G
3	L5	4518	C
3	L5	4609	G
3	L5	4610	C
3	L5	4614	G
3	L5	4621	U
3	L5	4622	C
3	L5	4634	U
3	L5	4637	G
3	L5	4638	G
3	L5	4639	C
3	L5	4640	G
3	L5	4641	C
3	L5	4644	C
3	L5	4645	C
3	L5	4646	G
3	L5	4649	A
3	L5	4651	G
3	L5	4665	C
3	L5	4705	A
3	L5	4706	A
3	L5	4715	U
3	L5	4724	U
3	L5	4727	U
3	L5	4728	U
3	L5	4729	C

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Mol	Chain	Res	Type
3	L5	4753	A
3	L5	4756	G
3	L5	4761	U
3	L5	4762	C
3	L5	4763	C
3	L5	4765	U
3	L5	4766	C
3	L5	4780	G
3	L5	4786	C
3	L5	4789	C
3	L5	4793	C
3	L5	4801	G
3	L5	4808	U
4	L7	7	G
4	L7	50	A
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	110	G
4	L7	120	U
5	L8	34	U
5	L8	35	C
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	75	OMG
5	L8	81	C
5	L8	84	A
5	L8	87	G
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	110	U
5	L8	114	G
5	L8	123	U
5	L8	127	U
5	L8	153	C
5	L8	156	U
48	S	1112	U
48	S	1113	G
48	S	1114	A

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Mol	Chain	Res	Type
48	S	1116	G
48	S	1122	C
48	S	1124	U
48	S	1126	A
48	S	1127	A
48	S	1132	A
48	S	1134	C
48	S	1135	C
48	S	1136	C
48	S	1137	G
48	S	1138	C
48	S	1143	G
48	S	1144	G
48	S	1145	G
48	S	1154	G
48	S	1155	A
49	S2	3	C
49	S2	4	C
49	S2	33	G
49	S2	41	G
49	S2	44	U
49	S2	46	A
49	S2	56	G
49	S2	58	C
49	S2	67	C
49	S2	68	A
49	S2	73	C
49	S2	74	G
49	S2	76	U
49	S2	77	A
49	S2	79	A
49	S2	99	A2M
49	S2	103	A
49	S2	113	G
49	S2	115	U
49	S2	124	U
49	S2	126	G
49	S2	130	G
49	S2	143	U
49	S2	147	A
49	S2	155	G
49	S2	162	C

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Mol	Chain	Res	Type
49	S2	168	C
49	S2	178	C
49	S2	184	G
49	S2	187	G
49	S2	188	C
49	S2	192	C
49	S2	195	C
49	S2	196	C
49	S2	205	G
49	S2	210	PSU
49	S2	226	A
49	S2	228	C
49	S2	239	C
49	S2	282	C
49	S2	306	U
49	S2	307	C
49	S2	308	G
49	S2	310	G
49	S2	313	G
49	S2	320	C
49	S2	324	C
49	S2	325	U
49	S2	327	C
49	S2	328	G
49	S2	329	U
49	S2	336	G
49	S2	348	G
49	S2	363	C
49	S2	365	A
49	S2	370	C
49	S2	386	G
49	S2	387	C
49	S2	401	C
49	S2	410	C
49	S2	422	G
49	S2	439	G
49	S2	449	A
49	S2	450	A
49	S2	451	C
49	S2	465	A
49	S2	466	A
49	S2	472	G

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Mol	Chain	Res	Type
49	S2	473	C
49	S2	474	A
49	S2	475	G
49	S2	483	G
49	S2	488	U
49	S2	493	C
49	S2	497	C
49	S2	502	C
49	S2	518	OMC
49	S2	526	A
49	S2	549	C
49	S2	565	A
49	S2	569	C
49	S2	577	A2M
49	S2	584	A
49	S2	590	G
49	S2	592	U
49	S2	607	G
49	S2	608	U
49	S2	609	C
49	S2	615	C
49	S2	632	U
49	S2	633	C
49	S2	644	A
49	S2	645	OMG
49	S2	656	A
49	S2	661	C
49	S2	669	A2M
49	S2	670	A
49	S2	671	A
49	S2	672	A
49	S2	673	A
49	S2	730	C
49	S2	731	C
49	S2	733	U
49	S2	734	C
49	S2	735	C
49	S2	746	C
49	S2	747	C
49	S2	748	U
49	S2	750	U
49	S2	752	G

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Mol	Chain	Res	Type
49	S2	754	C
49	S2	755	G
49	S2	756	C
49	S2	757	C
49	S2	789	G
49	S2	790	G
49	S2	798	C
49	S2	799	G
49	S2	802	PSU
49	S2	812	A
49	S2	822	G
49	S2	823	PSU
49	S2	831	A
49	S2	832	G
49	S2	837	G
49	S2	838	A
49	S2	839	G
49	S2	840	C
49	S2	841	C
49	S2	842	G
49	S2	848	A
49	S2	871	A
49	S2	873	A
49	S2	879	G
49	S2	886	U
49	S2	892	G
49	S2	910	G
49	S2	914	A
49	S2	915	U
49	S2	921	A
49	S2	923	A
49	S2	934	G
49	S2	944	U
49	S2	956	A
49	S2	964	A
49	S2	972	G
49	S2	991	A
49	S2	993	A
49	S2	1000	G
49	S2	1024	A
49	S2	1062	U
49	S2	1063	A

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Mol	Chain	Res	Type
49	S2	1084	A
49	S2	1086	C
49	S2	1116	U
49	S2	1117	C
49	S2	1118	C
49	S2	1119	C
49	S2	1122	G
49	S2	1124	C
49	S2	1134	A
49	S2	1145	A
49	S2	1154	C
49	S2	1155	U
49	S2	1196	A
49	S2	1216	C
49	S2	1225	G
49	S2	1243	U
49	S2	1252	A
49	S2	1254	A
49	S2	1257	G
49	S2	1258	G
49	S2	1260	A
49	S2	1272	C
49	S2	1275	G
49	S2	1276	G
49	S2	1283	A
49	S2	1296	A
49	S2	1303	G
49	S2	1304	C
49	S2	1316	U
49	S2	1343	U
49	S2	1359	U
49	S2	1372	U
49	S2	1379	A
49	S2	1392	OMC
49	S2	1397	A
49	S2	1399	G
49	S2	1403	A
49	S2	1406	A
49	S2	1407	G
49	S2	1419	C
49	S2	1420	C
49	S2	1422	A

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Mol	Chain	Res	Type
49	S2	1424	C
49	S2	1436	C
49	S2	1450	G
49	S2	1455	A
49	S2	1463	U
49	S2	1464	U
49	S2	1486	U
49	S2	1490	A
49	S2	1491	OMG
49	S2	1498	G
49	S2	1510	U
49	S2	1522	C
49	S2	1523	A
49	S2	1534	A
49	S2	1553	G
49	S2	1571	G
49	S2	1581	A
49	S2	1586	U
49	S2	1589	A
49	S2	1602	A
49	S2	1607	G
49	S2	1622	U
49	S2	1624	A
49	S2	1655	G
49	S2	1662	A
49	S2	1666	G
49	S2	1681	G
49	S2	1699	C
49	S2	1700	A
49	S2	1722	U
49	S2	1723	G
49	S2	1749	G
49	S2	1782	A
49	S2	1783	G
49	S2	1784	C
49	S2	1785	G
49	S2	1826	A
49	S2	1827	G
49	S2	1830	G
49	S2	1832	A
49	S2	1836	A
49	S2	1837	G

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Mol	Chain	Res	Type
49	S2	1839	U
49	S2	1850	G
49	S2	1852	MA6
49	S2	1862	G
49	S2	1863	G
49	S2	1864	A
49	S2	1865	U
49	S2	1866	C

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	I	106	U
2	I	122	C
2	I	127	C
2	I	137	A
2	I	144	G
2	I	172	G
3	L5	1588	G
3	L5	3549	A
3	L5	4445	U
48	S	1111	A
48	S	1112	U
48	S	1113	G
48	S	1144	G
49	S2	191	A
49	S2	1485	A

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

219 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	$\# Z > 2$
49	PSU	S2	36	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	A2M	S2	1679	49	22,25,26	1.73	6 (27%)	31,36,39	2.43	15 (48%)
3	PSU	L5	3583	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	4 (18%)
3	A2M	L5	4269	3	22,25,26	1.72	7 (31%)	31,36,39	2.48	15 (48%)
3	PSU	L5	3494	3	18,21,22	1.42	3 (16%)	22,30,33	1.80	5 (22%)
3	PSU	L5	3616	3	18,21,22	1.38	3 (16%)	22,30,33	1.90	5 (22%)
3	PSU	L5	4169	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	3447	3	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
3	A2M	L5	1270	3	22,25,26	1.73	7 (31%)	31,36,39	2.48	15 (48%)
3	PSU	L5	4058	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)
49	PSU	S2	1245	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
49	A2M	S2	159	49	22,25,26	1.69	6 (27%)	31,36,39	2.42	14 (45%)
49	A2M	S2	577	49	22,25,26	1.71	7 (31%)	31,36,39	2.42	14 (45%)
3	OMG	L5	3476	3	23,26,27	1.18	2 (8%)	33,38,41	1.90	9 (27%)
3	PSU	L5	4322	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
49	PSU	S2	407	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	4383	3	23,26,27	1.19	3 (13%)	33,38,41	1.90	9 (27%)
3	OMU	L5	3973	3	19,22,23	1.00	2 (10%)	26,31,34	1.83	6 (23%)
3	OMG	L5	3942	3	23,26,27	1.17	2 (8%)	33,38,41	1.89	9 (27%)
49	A2M	S2	1384	49	22,25,26	1.72	6 (27%)	31,36,39	2.45	13 (41%)
3	OMC	L5	2667	3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
3	OMU	L5	4244	3	19,22,23	1.02	2 (10%)	26,31,34	1.79	5 (19%)
49	A2M	S2	166	49	22,25,26	1.72	6 (27%)	31,36,39	2.46	14 (45%)
49	PSU	S2	1626	49	18,21,22	1.42	3 (16%)	22,30,33	1.77	4 (18%)
49	PSU	S2	210	49	18,21,22	1.45	3 (16%)	22,30,33	1.80	5 (22%)
49	PSU	S2	1178	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
3	PSU	L5	4278	3	18,21,22	1.48	2 (11%)	22,30,33	1.65	3 (13%)
49	4AC	S2	1843	49	21,24,25	1.12	2 (9%)	29,34,37	1.30	3 (10%)
49	PSU	S2	1175	49	18,21,22	1.41	3 (16%)	22,30,33	1.80	4 (18%)
3	OMC	L5	2208	3	19,22,23	1.16	2 (10%)	26,31,34	0.95	1 (3%)
49	PSU	S2	687	49	18,21,22	1.41	3 (16%)	22,30,33	1.81	5 (22%)
3	1MA	L5	1266	3	21,25,26	1.82	4 (19%)	31,37,40	1.94	5 (16%)
3	PSU	L5	4325	3	18,21,22	1.37	3 (16%)	22,30,33	1.85	5 (22%)
49	OMG	S2	1491	49	23,26,27	1.16	2 (8%)	33,38,41	1.87	9 (27%)
49	PSU	S2	218	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
49	OMU	S2	1805	49	19,22,23	0.99	2 (10%)	26,31,34	1.76	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5MC	L5	3514	3	18,22,23	1.34	3 (16%)	26,32,35	1.24	3 (11%)
3	5MC	L5	4193	3	18,22,23	1.29	3 (16%)	26,32,35	1.48	4 (15%)
3	OMC	L5	2647	3	19,22,23	1.15	2 (10%)	26,31,34	1.01	1 (3%)
3	OMC	L5	4202	3	19,22,23	1.16	2 (10%)	26,31,34	0.91	1 (3%)
80	HY3	Si	62	80	6,8,9	1.30	1 (16%)	5,10,12	1.40	1 (20%)
3	OMG	L5	2207	3	23,26,27	1.18	3 (13%)	33,38,41	1.86	9 (27%)
46	SAC	Ls	2	46	7,8,9	0.52	0	8,9,11	0.84	1 (12%)
78	AME	Sg	1	78	9,10,11	0.67	0	9,11,13	1.07	1 (11%)
3	PSU	L5	3554	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
3	OMC	L5	3573	3	19,22,23	1.14	2 (10%)	26,31,34	0.90	0
32	MLZ	Le	5	32	8,9,10	0.49	0	4,9,11	0.19	0
3	OMC	L5	2265	3	19,22,23	1.15	2 (10%)	26,31,34	0.89	0
49	OMC	S2	1392	49	19,22,23	1.17	2 (10%)	26,31,34	0.96	1 (3%)
3	PSU	L5	3652	3	18,21,22	1.37	3 (16%)	22,30,33	1.88	5 (22%)
49	OMG	S2	602	49	23,26,27	1.17	3 (13%)	33,38,41	1.89	9 (27%)
3	PSU	L5	4382	3	18,21,22	1.38	3 (16%)	22,30,33	1.76	4 (18%)
49	PSU	S2	1046	49	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
3	OMC	L5	1284	3	19,22,23	1.18	2 (10%)	26,31,34	0.89	0
3	PSU	L5	4217	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	4 (18%)
3	PSU	L5	4099	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	4 (18%)
49	PSU	S2	1005	49	18,21,22	1.43	3 (16%)	22,30,33	1.82	4 (18%)
3	OMC	L5	2704	3	19,22,23	1.15	2 (10%)	26,31,34	0.87	1 (3%)
5	PSU	L8	55	5	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	A2M	L5	4317	3	22,25,26	1.73	6 (27%)	31,36,39	2.43	13 (41%)
3	OMU	L5	4052	3	19,22,23	0.99	2 (10%)	26,31,34	1.78	4 (15%)
3	PSU	L5	4149	3	18,21,22	1.36	3 (16%)	22,30,33	1.90	4 (18%)
3	PSU	L5	4203	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
3	A2M	L5	3456	3	22,25,26	1.72	6 (27%)	31,36,39	2.45	13 (41%)
3	OMG	L5	3631	3	23,26,27	1.19	2 (8%)	33,38,41	1.88	9 (27%)
3	PSU	L5	4045	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
49	PSU	S2	1348	49	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
3	A2M	L5	2244	3	22,25,26	1.73	6 (27%)	31,36,39	2.47	15 (48%)
3	PSU	L5	4188	3	18,21,22	1.37	3 (16%)	22,30,33	1.90	4 (18%)
3	A2M	L5	2630	3	22,25,26	1.72	6 (27%)	31,36,39	2.54	17 (54%)
3	PSU	L5	3585	3	18,21,22	1.39	3 (16%)	22,30,33	1.81	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	M3L	Lp	98	43	10,11,12	0.51	0	9,14,16	0.47	0
49	PSU	S2	1233	49	18,21,22	1.42	3 (16%)	22,30,33	1.82	5 (22%)
3	PSU	L5	1731	3	18,21,22	1.37	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	682	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)
3	PSU	L5	4042	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	5 (22%)
49	OMU	S2	628	49	19,22,23	1.01	1 (5%)	26,31,34	1.84	5 (19%)
3	A2M	L5	3557	3	22,25,26	1.72	7 (31%)	31,36,39	2.45	13 (41%)
49	MA6	S2	1852	49	23,26,27	1.46	4 (17%)	34,38,41	2.37	11 (32%)
3	UR3	L5	4276	3	19,22,23	1.29	3 (15%)	26,32,35	1.24	2 (7%)
49	OMU	S2	1443	49	19,22,23	0.99	2 (10%)	26,31,34	1.74	4 (15%)
3	PSU	L5	4749	3	18,21,22	1.42	3 (16%)	22,30,33	1.82	4 (18%)
49	OMG	S2	437	49	23,26,27	1.16	2 (8%)	33,38,41	1.91	9 (27%)
49	A2M	S2	591	49	22,25,26	1.71	6 (27%)	31,36,39	2.60	15 (48%)
3	PSU	L5	2475	3	18,21,22	1.41	3 (16%)	22,30,33	1.87	4 (18%)
3	A2M	L5	400	3	22,25,26	1.72	6 (27%)	31,36,39	2.45	13 (41%)
49	PSU	S2	816	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	1260	3	23,26,27	1.19	3 (13%)	33,38,41	1.92	9 (27%)
3	PSU	L5	4177	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
49	OMU	S2	355	49	19,22,23	0.99	2 (10%)	26,31,34	1.78	5 (19%)
3	PSU	L5	4246	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	5 (22%)
76	NMM	Se	67	76	9,11,12	1.57	1 (11%)	6,12,14	3.46	2 (33%)
3	A2M	L5	1810	3	22,25,26	1.72	7 (31%)	31,36,39	2.47	15 (48%)
3	PSU	L5	1718	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3462	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
3	OMG	L5	4240	3	23,26,27	1.18	2 (8%)	33,38,41	1.88	10 (30%)
3	PSU	L5	4711	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	4740	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
49	PSU	S2	864	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
49	PSU	S2	573	49	18,21,22	1.42	3 (16%)	22,30,33	1.81	4 (18%)
3	OMG	L5	2267	3	23,26,27	1.16	2 (8%)	33,38,41	1.88	9 (27%)
3	PSU	L5	4298	3	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
3	OMC	L5	3601	3	19,22,23	1.14	2 (10%)	26,31,34	0.96	2 (7%)
49	PSU	S2	93	49	18,21,22	1.41	3 (16%)	22,30,33	1.79	4 (18%)
49	OMU	S2	1289	49	19,22,23	0.98	2 (10%)	26,31,34	1.74	5 (19%)
3	PSU	L5	4435	3	18,21,22	1.39	3 (16%)	22,30,33	1.89	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	OMC	S2	174	49	19,22,23	1.17	2 (10%)	26,31,34	0.90	0
8	AYA	LF	2	8	6,7,8	0.73	0	5,8,10	0.33	0
3	PSU	L5	1721	3	18,21,22	1.41	3 (16%)	22,30,33	1.84	4 (18%)
3	OMC	L5	1820	3	19,22,23	1.16	2 (10%)	26,31,34	0.93	0
49	PSU	S2	119	49	18,21,22	1.43	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	1644	49	18,21,22	1.43	3 (16%)	22,30,33	1.83	4 (18%)
49	A2M	S2	99	49	22,25,26	1.72	6 (27%)	31,36,39	2.47	14 (45%)
3	PSU	L5	1683	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	5 (22%)
3	OMC	L5	3619	3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
49	PSU	S2	1057	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
3	OMC	L5	3433	3	19,22,23	1.17	2 (10%)	26,31,34	0.98	1 (3%)
49	A2M	S2	1032	49	22,25,26	1.73	7 (31%)	31,36,39	2.47	13 (41%)
3	OMU	L5	3657	3	19,22,23	0.99	2 (10%)	26,31,34	1.85	5 (19%)
3	A2M	L5	3492	3,49	22,25,26	1.70	6 (27%)	31,36,39	2.68	16 (51%)
49	PSU	S2	815	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	OMU	S2	429	49	19,22,23	1.01	2 (10%)	26,31,34	1.82	6 (23%)
3	OMG	L5	4138	3	23,26,27	1.17	3 (13%)	33,38,41	1.93	10 (30%)
49	OMG	S2	645	49	23,26,27	1.16	3 (13%)	33,38,41	1.91	10 (30%)
75	SAC	Sd	2	75	7,8,9	0.54	0	8,9,11	0.85	1 (12%)
3	PSU	L5	3371	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
3	A2M	L5	3517	3	22,25,26	1.73	7 (31%)	31,36,39	2.59	17 (54%)
49	A2M	S2	485	49	22,25,26	1.70	7 (31%)	31,36,39	2.44	14 (45%)
3	OMC	L5	3540	3	19,22,23	1.14	2 (10%)	26,31,34	0.88	1 (3%)
3	6MZ	L5	3966	3	22,25,26	1.42	4 (18%)	30,36,39	2.22	9 (30%)
3	PSU	L5	1491	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
3	PSU	L5	4419	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
3	A2M	L5	2206	3	22,25,26	1.72	6 (27%)	31,36,39	2.43	14 (45%)
49	OMC	S2	1704	49	19,22,23	1.17	2 (10%)	26,31,34	0.88	1 (3%)
49	4AC	S2	1338	49	21,24,25	1.10	2 (9%)	29,34,37	1.19	3 (10%)
49	OMG	S2	684	49	23,26,27	1.17	2 (8%)	33,38,41	1.87	10 (30%)
3	PSU	L5	4374	3	18,21,22	1.40	3 (16%)	22,30,33	1.88	5 (22%)
3	A2M	L5	3450	3	22,25,26	1.71	6 (27%)	31,36,39	2.41	13 (41%)
3	OMG	L5	3676	3	23,26,27	1.16	2 (8%)	33,38,41	1.92	10 (30%)
49	OMG	S2	1448	49	23,26,27	1.15	2 (8%)	33,38,41	1.88	9 (27%)
49	PSU	S2	650	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PSU	S2	1693	49	18,21,22	1.41	3 (16%)	22,30,33	1.84	5 (22%)
49	MA6	S2	1851	49	23,26,27	1.44	4 (17%)	34,38,41	2.37	13 (38%)
3	OMU	L5	2258	3	19,22,23	1.01	2 (10%)	26,31,34	1.75	5 (19%)
49	PSU	S2	610	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
49	PSU	S2	802	49	18,21,22	1.43	3 (16%)	22,30,33	1.80	5 (22%)
49	A2M	S2	513	49	22,25,26	1.71	6 (27%)	31,36,39	2.46	14 (45%)
3	PSU	L5	3576	3	18,21,22	1.39	3 (16%)	22,30,33	1.71	4 (18%)
3	A2M	L5	3599	3	22,25,26	1.73	7 (31%)	31,36,39	2.51	15 (48%)
3	PSU	L5	3427	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
49	PSU	S2	652	49	18,21,22	1.42	3 (16%)	22,30,33	1.85	5 (22%)
3	A2M	L5	4336	3	22,25,26	1.72	6 (27%)	31,36,39	2.48	15 (48%)
3	A2M	L5	2658	3	22,25,26	1.72	6 (27%)	31,36,39	2.49	13 (41%)
49	OMG	S2	1329	49	23,26,27	1.15	2 (8%)	33,38,41	1.90	9 (27%)
5	PSU	L8	69	5	18,21,22	1.38	3 (16%)	22,30,33	1.85	4 (18%)
49	OMU	S2	116	49	19,22,23	1.00	2 (10%)	26,31,34	1.73	6 (23%)
49	OMG	S2	510	49	23,26,27	1.16	2 (8%)	33,38,41	1.92	10 (30%)
49	OMU	S2	1327	49	19,22,23	1.00	2 (10%)	26,31,34	1.81	5 (19%)
3	PSU	L5	1801	3	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
49	OMU	S2	172	49	19,22,23	0.99	2 (10%)	26,31,34	1.82	4 (15%)
49	PSU	S2	1239	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
3	A2M	L5	1489	3	22,25,26	1.72	6 (27%)	31,36,39	2.49	13 (41%)
3	OMC	L5	2194	3	19,22,23	1.15	2 (10%)	26,31,34	0.94	1 (3%)
49	PSU	S2	105	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)
3	OMG	L5	3974	3	23,26,27	1.16	3 (13%)	33,38,41	1.89	11 (33%)
3	OMG	L5	4116	3	23,26,27	1.18	3 (13%)	33,38,41	1.89	9 (27%)
49	7MG	S2	1640	49	22,26,27	1.18	2 (9%)	29,39,42	2.13	9 (31%)
5	OMG	L8	75	5	23,26,27	1.20	3 (13%)	33,38,41	1.85	9 (27%)
49	PSU	S2	34	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)
3	A2M	L5	3562	3	22,25,26	1.72	7 (31%)	31,36,39	2.44	14 (45%)
44	MLZ	Lq	53	44	8,9,10	0.48	0	4,9,11	0.16	0
49	PSU	S2	109	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	4166	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	OMC	S2	463	49	19,22,23	1.18	2 (10%)	26,31,34	0.88	0
49	PSU	S2	967	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	4 (18%)
3	OMC	L5	4282	3	19,22,23	1.16	2 (10%)	26,31,34	0.94	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1638	3	18,21,22	1.38	3 (16%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3466	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
49	PSU	S2	1368	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3490	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4107	3	18,21,22	1.38	3 (16%)	22,30,33	1.80	4 (18%)
49	A2M	S2	469	49	22,25,26	1.71	6 (27%)	31,36,39	2.48	14 (45%)
3	OMU	L5	4366	3	19,22,23	0.99	2 (10%)	26,31,34	1.80	5 (19%)
49	A2M	S2	27	49	22,25,26	1.70	7 (31%)	31,36,39	2.47	13 (41%)
3	PSU	L5	1632	3	18,21,22	1.44	4 (22%)	22,30,33	1.70	4 (18%)
3	PSU	L5	4267	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
49	OMG	S2	868	49	23,26,27	1.16	2 (8%)	33,38,41	1.86	9 (27%)
3	PSU	L5	3496	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
3	OMG	L5	2719	3	23,26,27	1.16	2 (8%)	33,38,41	2.08	11 (33%)
49	OMU	S2	121	49	19,22,23	1.01	2 (10%)	26,31,34	1.77	6 (23%)
3	A2M	L5	1479	3	22,25,26	1.73	7 (31%)	31,36,39	2.48	14 (45%)
49	PSU	S2	1082	49	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	1799	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
3	PSU	L5	3369	3	18,21,22	1.35	3 (16%)	22,30,33	1.85	4 (18%)
3	PSU	L5	3500	3	18,21,22	1.42	3 (16%)	22,30,33	1.84	5 (22%)
4	GTP	L7	1	4	30,34,34	1.21	3 (10%)	46,54,54	1.39	4 (8%)
3	OMG	L5	1580	3	23,26,27	1.17	2 (8%)	33,38,41	1.94	10 (30%)
49	PSU	S2	1446	49	18,21,22	1.44	3 (16%)	22,30,33	1.81	4 (18%)
57	SAC	SL	2	57	7,8,9	0.52	0	8,9,11	0.89	1 (12%)
3	A2M	L5	398	3	22,25,26	1.72	6 (27%)	31,36,39	2.43	13 (41%)
3	PSU	L5	1720	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
49	PSU	S2	823	49	18,21,22	1.39	3 (16%)	22,30,33	1.80	5 (22%)
3	PSU	L5	1537	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	OMG	L5	4364	3	23,26,27	1.17	2 (8%)	33,38,41	1.90	9 (27%)
7	HIC	LE	245	7	10,11,12	0.63	0	8,14,16	0.35	0
3	OMG	L5	3359	3	23,26,27	1.17	2 (8%)	33,38,41	1.92	10 (30%)
3	OMG	L5	4245	3	23,26,27	1.17	3 (13%)	33,38,41	1.87	9 (27%)
49	PSU	S2	867	49	18,21,22	1.42	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	1047	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	3524	3	23,26,27	1.18	2 (8%)	33,38,41	1.89	9 (27%)
3	PSU	L5	3502	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	2351	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	OMU	L5	2680	3	19,22,23	1.01	2 (10%)	26,31,34	1.81	6 (23%)
3	OMG	L5	1477	3	23,26,27	1.18	3 (13%)	33,38,41	1.91	10 (30%)
3	OMG	L5	4369	3	23,26,27	1.18	3 (13%)	33,38,41	1.89	9 (27%)
49	OMC	S2	518	49	19,22,23	1.15	2 (10%)	26,31,34	0.92	1 (3%)
3	PSU	L5	4039	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	5 (22%)
49	6MZ	S2	1833	49	22,25,26	1.41	4 (18%)	30,36,39	2.16	9 (30%)
49	A2M	S2	669	49	22,25,26	1.73	7 (31%)	31,36,39	2.64	17 (54%)

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
49	PSU	S2	36	49	-	0/7/25/26	0/2/2/2
49	A2M	S2	1679	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	3583	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4269	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3494	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3616	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4169	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3447	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1270	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4058	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1245	49	-	0/7/25/26	0/2/2/2
49	A2M	S2	159	49	-	0/9/27/28	0/3/3/3
49	A2M	S2	577	49	-	2/9/27/28	0/3/3/3
3	OMG	L5	3476	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4322	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	407	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	4383	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	3973	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3942	3	-	0/9/27/28	0/3/3/3
49	A2M	S2	1384	49	-	0/9/27/28	0/3/3/3
3	OMC	L5	2667	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4244	3	-	0/9/27/28	0/2/2/2
49	A2M	S2	166	49	-	0/9/27/28	0/3/3/3
49	PSU	S2	1626	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	210	49	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PSU	S2	1178	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4278	3	-	0/7/25/26	0/2/2/2
49	4AC	S2	1843	49	-	2/11/29/30	0/2/2/2
49	PSU	S2	1175	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	2208	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	687	49	-	0/7/25/26	0/2/2/2
3	1MA	L5	1266	3	-	0/7/25/26	0/3/3/3
3	PSU	L5	4325	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	1491	49	-	1/9/27/28	0/3/3/3
49	PSU	S2	218	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	1805	49	-	0/9/27/28	0/2/2/2
3	5MC	L5	3514	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4193	3	-	4/7/25/26	0/2/2/2
3	OMC	L5	2647	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	4202	3	-	0/9/27/28	0/2/2/2
80	HY3	Si	62	80	-	0/1/12/14	0/1/1/1
3	OMG	L5	2207	3	-	0/9/27/28	0/3/3/3
46	SAC	Ls	2	46	-	0/7/8/10	-
78	AME	Sg	1	78	-	2/9/10/12	-
3	PSU	L5	3554	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3573	3	-	0/9/27/28	0/2/2/2
32	MLZ	Le	5	32	-	1/7/8/10	-
3	OMC	L5	2265	3	-	2/9/27/28	0/2/2/2
49	OMC	S2	1392	49	-	1/9/27/28	0/2/2/2
3	PSU	L5	3652	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	602	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	4382	3	-	4/7/25/26	0/2/2/2
49	PSU	S2	1046	49	-	2/7/25/26	0/2/2/2
3	OMC	L5	1284	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4217	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4099	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1005	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	2704	3	-	0/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	A2M	L5	4317	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4052	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4149	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4203	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3456	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3631	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4045	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PSU	S2	1348	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	2244	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4188	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2630	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3585	3	-	0/7/25/26	0/2/2/2
43	M3L	Lp	98	43	-	0/9/10/12	-
49	PSU	S2	1233	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1731	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	682	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4042	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	628	49	-	2/9/27/28	0/2/2/2
3	A2M	L5	3557	3	-	0/9/27/28	0/3/3/3
49	MA6	S2	1852	49	-	2/11/29/30	0/3/3/3
3	UR3	L5	4276	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	1443	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4749	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	437	49	-	0/9/27/28	0/3/3/3
49	A2M	S2	591	49	-	1/9/27/28	0/3/3/3
3	PSU	L5	2475	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
49	PSU	S2	816	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	1260	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4177	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	355	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4246	3	-	2/7/25/26	0/2/2/2
76	NMM	Se	67	76	-	2/9/11/13	-
3	A2M	L5	1810	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1718	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3462	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4240	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4711	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4740	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	864	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	573	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	2267	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4298	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3601	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	93	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	1289	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4435	3	-	0/7/25/26	0/2/2/2
49	OMC	S2	174	49	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	AYA	LF	2	8	-	2/4/6/8	-
3	PSU	L5	1721	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	1820	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	119	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1644	49	-	0/7/25/26	0/2/2/2
49	A2M	S2	99	49	-	1/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3619	3	-	1/9/27/28	0/2/2/2
49	PSU	S2	1057	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	3433	3	-	4/9/27/28	0/2/2/2
49	A2M	S2	1032	49	-	0/9/27/28	0/3/3/3
3	OMU	L5	3657	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3492	3,49	-	0/9/27/28	0/3/3/3
49	PSU	S2	815	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	429	49	-	4/9/27/28	0/2/2/2
3	OMG	L5	4138	3	-	0/9/27/28	0/3/3/3
49	OMG	S2	645	49	-	3/9/27/28	0/3/3/3
75	SAC	Sd	2	75	-	0/7/8/10	-
3	PSU	L5	3371	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3517	3	-	5/9/27/28	0/3/3/3
49	A2M	S2	485	49	-	0/9/27/28	0/3/3/3
3	OMC	L5	3540	3	-	0/9/27/28	0/2/2/2
3	6MZ	L5	3966	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1491	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4419	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2206	3	-	0/9/27/28	0/3/3/3
49	OMC	S2	1704	49	-	0/9/27/28	0/2/2/2
49	4AC	S2	1338	49	-	4/11/29/30	0/2/2/2
49	OMG	S2	684	49	-	2/9/27/28	0/3/3/3
3	PSU	L5	4374	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3450	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3676	3	-	0/9/27/28	0/3/3/3
49	OMG	S2	1448	49	-	1/9/27/28	0/3/3/3
49	PSU	S2	650	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1693	49	-	0/7/25/26	0/2/2/2
49	MA6	S2	1851	49	-	1/11/29/30	0/3/3/3
3	OMU	L5	2258	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	610	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	802	49	-	2/7/25/26	0/2/2/2
49	A2M	S2	513	49	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3576	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	3599	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3427	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	652	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	4336	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	2658	3	-	1/9/27/28	0/3/3/3
49	OMG	S2	1329	49	-	0/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
49	OMU	S2	116	49	-	0/9/27/28	0/2/2/2
49	OMG	S2	510	49	-	0/9/27/28	0/3/3/3
49	OMU	S2	1327	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	1801	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	172	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	1239	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	1489	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	2194	3	-	2/9/27/28	0/2/2/2
49	PSU	S2	105	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3974	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4116	3	-	0/9/27/28	0/3/3/3
49	7MG	S2	1640	49	-	0/7/37/38	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
49	PSU	S2	34	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	3562	3	-	0/9/27/28	0/3/3/3
44	MLZ	Lq	53	44	-	0/7/8/10	-
49	PSU	S2	109	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4166	3	-	0/7/25/26	0/2/2/2
49	OMC	S2	463	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	967	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	4282	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1638	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3466	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1368	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	3490	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4107	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	469	49	-	0/9/27/28	0/3/3/3
3	OMU	L5	4366	3	-	0/9/27/28	0/2/2/2
49	A2M	S2	27	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	1632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4267	3	-	2/7/25/26	0/2/2/2
49	OMG	S2	868	49	-	0/9/27/28	0/3/3/3
3	PSU	L5	3496	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2719	3	-	0/9/27/28	0/3/3/3
49	OMU	S2	121	49	-	0/9/27/28	0/2/2/2
3	A2M	L5	1479	3	-	1/9/27/28	0/3/3/3
49	PSU	S2	1082	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1799	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3369	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3500	3	-	0/7/25/26	0/2/2/2
4	GTP	L7	1	4	-	0/22/38/38	0/3/3/3
3	OMG	L5	1580	3	-	2/9/27/28	0/3/3/3
49	PSU	S2	1446	49	-	0/7/25/26	0/2/2/2
57	SAC	SL	2	57	-	1/7/8/10	-
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1720	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	823	49	-	2/7/25/26	0/2/2/2
3	PSU	L5	1537	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4364	3	-	0/9/27/28	0/3/3/3
7	HIC	LE	245	7	-	2/5/6/8	0/1/1/1
3	OMG	L5	3359	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4245	3	-	0/9/27/28	0/3/3/3
49	PSU	S2	867	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1047	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3502	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2351	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2680	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1477	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4369	3	-	0/9/27/28	0/3/3/3
49	OMC	S2	518	49	-	2/9/27/28	0/2/2/2
3	PSU	L5	4039	3	-	0/7/25/26	0/2/2/2
49	6MZ	S2	1833	49	-	0/9/27/28	0/3/3/3
49	A2M	S2	669	49	-	4/9/27/28	0/3/3/3

All (684) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1266	1MA	C2-N3	4.92	1.39	1.30
49	S2	1852	MA6	C5-C4	4.50	1.47	1.39
49	S2	1851	MA6	C5-C4	4.39	1.47	1.39
49	S2	1833	6MZ	C5-C4	4.38	1.47	1.39
3	L5	3966	6MZ	C5-C4	4.35	1.47	1.39
76	Se	67	NMM	CZ-NH2	4.26	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1266	1MA	C5-C6	-3.91	1.33	1.43
3	L5	4278	PSU	C6-C5	3.75	1.39	1.35
3	L5	3502	PSU	C6-C5	3.74	1.39	1.35
49	S2	210	PSU	C6-C5	3.73	1.39	1.35
49	S2	802	PSU	C6-C5	3.73	1.39	1.35
3	L5	3494	PSU	C6-C5	3.71	1.39	1.35
49	S2	1005	PSU	C6-C5	3.71	1.39	1.35
49	S2	864	PSU	C6-C5	3.71	1.39	1.35
4	L7	1	GTP	C5-C4	3.70	1.49	1.38
49	S2	1178	PSU	C6-C5	3.70	1.39	1.35
3	L5	1632	PSU	C6-C5	3.69	1.39	1.35
49	S2	1626	PSU	C6-C5	3.69	1.39	1.35
49	S2	967	PSU	C6-C5	3.68	1.39	1.35
49	S2	1239	PSU	C6-C5	3.67	1.39	1.35
49	S2	1245	PSU	C6-C5	3.67	1.39	1.35
49	S2	652	PSU	C6-C5	3.66	1.39	1.35
49	S2	1446	PSU	C6-C5	3.66	1.39	1.35
3	L5	4749	PSU	C6-C5	3.66	1.39	1.35
49	S2	1175	PSU	C6-C5	3.65	1.39	1.35
3	L5	1799	PSU	C6-C5	3.65	1.39	1.35
49	S2	867	PSU	C6-C5	3.65	1.39	1.35
49	S2	1644	PSU	C6-C5	3.64	1.39	1.35
49	S2	105	PSU	C6-C5	3.64	1.39	1.35
49	S2	1693	PSU	C6-C5	3.63	1.39	1.35
49	S2	1233	PSU	C6-C5	3.63	1.39	1.35
3	L5	3496	PSU	C6-C5	3.63	1.39	1.35
49	S2	119	PSU	C6-C5	3.63	1.39	1.35
49	S2	687	PSU	C6-C5	3.62	1.39	1.35
3	L5	3447	PSU	C6-C5	3.62	1.39	1.35
3	L5	2475	PSU	C6-C5	3.61	1.39	1.35
3	L5	2351	PSU	C6-C5	3.61	1.39	1.35
3	L5	3500	PSU	C6-C5	3.61	1.39	1.35
49	S2	816	PSU	C6-C5	3.61	1.39	1.35
3	L5	3576	PSU	C6-C5	3.61	1.39	1.35
3	L5	4058	PSU	C6-C5	3.61	1.39	1.35
49	S2	815	PSU	C6-C5	3.60	1.39	1.35
3	L5	3554	PSU	C6-C5	3.60	1.39	1.35
3	L5	4177	PSU	C6-C5	3.60	1.39	1.35
49	S2	1348	PSU	C6-C5	3.60	1.39	1.35
49	S2	34	PSU	C6-C5	3.59	1.39	1.35
49	S2	682	PSU	C6-C5	3.59	1.39	1.35
3	L5	4435	PSU	C6-C5	3.59	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	109	PSU	C6-C5	3.58	1.39	1.35
3	L5	1721	PSU	C6-C5	3.58	1.39	1.35
3	L5	3490	PSU	C6-C5	3.58	1.39	1.35
3	L5	4711	PSU	C6-C5	3.58	1.39	1.35
49	S2	650	PSU	C6-C5	3.58	1.39	1.35
3	L5	4166	PSU	C6-C5	3.58	1.39	1.35
3	L5	4217	PSU	C6-C5	3.58	1.39	1.35
49	S2	218	PSU	C6-C5	3.58	1.39	1.35
49	S2	1368	PSU	C6-C5	3.57	1.39	1.35
3	L5	4740	PSU	C6-C5	3.57	1.39	1.35
49	S2	36	PSU	C6-C5	3.57	1.39	1.35
3	L5	1491	PSU	C6-C5	3.57	1.39	1.35
49	S2	610	PSU	C6-C5	3.57	1.39	1.35
49	S2	573	PSU	C6-C5	3.56	1.39	1.35
3	L5	1683	PSU	C6-C5	3.56	1.39	1.35
3	L5	3462	PSU	C6-C5	3.56	1.39	1.35
49	S2	1640	7MG	C4-N9	-3.56	1.33	1.37
49	S2	407	PSU	C6-C5	3.55	1.39	1.35
3	L5	4099	PSU	C6-C5	3.55	1.39	1.35
5	L8	55	PSU	C6-C5	3.55	1.39	1.35
3	L5	4322	PSU	C6-C5	3.54	1.39	1.35
3	L5	4419	PSU	C6-C5	3.54	1.39	1.35
49	S2	1047	PSU	C6-C5	3.54	1.39	1.35
3	L5	3583	PSU	C6-C5	3.54	1.39	1.35
49	S2	1046	PSU	C6-C5	3.54	1.39	1.35
49	S2	93	PSU	C6-C5	3.54	1.39	1.35
3	L5	4045	PSU	C6-C5	3.53	1.39	1.35
3	L5	4374	PSU	C6-C5	3.53	1.39	1.35
3	L5	3466	PSU	C6-C5	3.52	1.39	1.35
3	L5	4039	PSU	C6-C5	3.52	1.39	1.35
3	L5	4042	PSU	C6-C5	3.52	1.39	1.35
3	L5	1537	PSU	C6-C5	3.51	1.39	1.35
49	S2	1640	7MG	C5-C6	-3.51	1.34	1.43
3	L5	4246	PSU	C6-C5	3.51	1.39	1.35
3	L5	3427	PSU	C6-C5	3.51	1.39	1.35
3	L5	3616	PSU	C6-C5	3.51	1.39	1.35
49	S2	1057	PSU	C6-C5	3.51	1.39	1.35
3	L5	4107	PSU	C6-C5	3.50	1.39	1.35
3	L5	4382	PSU	C6-C5	3.50	1.39	1.35
3	L5	4169	PSU	C6-C5	3.50	1.39	1.35
3	L5	4267	PSU	C6-C5	3.49	1.39	1.35
3	L5	1720	PSU	C6-C5	3.48	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3585	PSU	C6-C5	3.47	1.39	1.35
3	L5	1801	PSU	C6-C5	3.47	1.39	1.35
3	L5	4203	PSU	C6-C5	3.47	1.39	1.35
3	L5	1718	PSU	C6-C5	3.47	1.39	1.35
3	L5	1731	PSU	C6-C5	3.47	1.39	1.35
49	S2	823	PSU	C6-C5	3.46	1.39	1.35
3	L5	1638	PSU	C6-C5	3.45	1.39	1.35
3	L5	4188	PSU	C6-C5	3.45	1.39	1.35
3	L5	3492	A2M	C2-N1	3.42	1.40	1.33
3	L5	4298	PSU	C6-C5	3.42	1.39	1.35
3	L5	4325	PSU	C6-C5	3.41	1.39	1.35
3	L5	3371	PSU	C6-C5	3.41	1.39	1.35
5	L8	69	PSU	C6-C5	3.40	1.39	1.35
49	S2	166	A2M	C2-N3	3.39	1.40	1.33
3	L5	4149	PSU	C6-C5	3.38	1.39	1.35
3	L5	3652	PSU	C6-C5	3.38	1.39	1.35
49	S2	1384	A2M	C2-N3	3.37	1.40	1.33
49	S2	1082	PSU	C6-C5	3.37	1.39	1.35
49	S2	1679	A2M	C2-N3	3.35	1.40	1.33
49	S2	469	A2M	C2-N3	3.34	1.40	1.33
3	L5	3456	A2M	C2-N3	3.34	1.40	1.33
3	L5	3599	A2M	C2-N3	3.34	1.40	1.33
49	S2	577	A2M	C2-N3	3.33	1.40	1.33
3	L5	3369	PSU	C6-C5	3.33	1.39	1.35
49	S2	99	A2M	C2-N3	3.32	1.40	1.33
49	S2	591	A2M	C2-N3	3.32	1.40	1.33
3	L5	398	A2M	C2-N3	3.31	1.40	1.33
3	L5	3492	A2M	C2-N3	3.31	1.40	1.33
3	L5	400	A2M	C2-N3	3.30	1.40	1.33
3	L5	2244	A2M	C2-N3	3.30	1.40	1.33
3	L5	3557	A2M	C2-N3	3.30	1.40	1.33
49	S2	485	A2M	C2-N3	3.29	1.40	1.33
3	L5	4336	A2M	C2-N3	3.29	1.40	1.33
3	L5	4317	A2M	C2-N3	3.29	1.40	1.33
3	L5	2658	A2M	C2-N3	3.27	1.40	1.33
3	L5	3517	A2M	C2-N3	3.27	1.40	1.33
3	L5	2630	A2M	C2-N3	3.26	1.40	1.33
49	S2	1032	A2M	C2-N3	3.26	1.40	1.33
49	S2	577	A2M	C2-N1	3.24	1.39	1.33
49	S2	159	A2M	C2-N3	3.24	1.39	1.33
3	L5	3562	A2M	C2-N3	3.24	1.39	1.33
49	S2	513	A2M	C2-N3	3.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1489	A2M	C2-N3	3.23	1.39	1.33
3	L5	1479	A2M	C2-N3	3.23	1.39	1.33
49	S2	27	A2M	C2-N3	3.22	1.39	1.33
3	L5	3514	5MC	C4-N3	3.22	1.39	1.34
3	L5	4269	A2M	C2-N3	3.22	1.39	1.33
3	L5	2206	A2M	C2-N3	3.21	1.39	1.33
49	S2	1679	A2M	C2-N1	3.21	1.39	1.33
3	L5	1810	A2M	C2-N3	3.20	1.39	1.33
3	L5	1489	A2M	C5-N7	-3.19	1.33	1.39
49	S2	1384	A2M	C2-N1	3.19	1.39	1.33
3	L5	3450	A2M	C2-N3	3.18	1.39	1.33
49	S2	166	A2M	C2-N1	3.18	1.39	1.33
3	L5	1270	A2M	C2-N3	3.17	1.39	1.33
3	L5	4317	A2M	C2-N1	3.17	1.39	1.33
3	L5	398	A2M	C5-N7	-3.17	1.33	1.39
3	L5	2244	A2M	C2-N1	3.17	1.39	1.33
3	L5	1270	A2M	C2-N1	3.16	1.39	1.33
3	L5	3562	A2M	C2-N1	3.16	1.39	1.33
3	L5	4269	A2M	C2-N1	3.16	1.39	1.33
3	L5	3450	A2M	C2-N1	3.16	1.39	1.33
49	S2	669	A2M	C5-C4	-3.16	1.33	1.39
3	L5	1810	A2M	C2-N1	3.16	1.39	1.33
3	L5	4278	PSU	C2-N1	3.15	1.41	1.36
3	L5	2719	OMG	C5-N7	-3.15	1.33	1.39
3	L5	3517	A2M	C5-N7	-3.15	1.33	1.39
49	S2	669	A2M	C2-N1	3.15	1.39	1.33
49	S2	469	A2M	C2-N1	3.15	1.39	1.33
3	L5	1479	A2M	C5-N7	-3.14	1.33	1.39
49	S2	485	A2M	C2-N1	3.14	1.39	1.33
49	S2	159	A2M	C2-N1	3.14	1.39	1.33
3	L5	4317	A2M	C5-N7	-3.14	1.33	1.39
49	S2	27	A2M	C2-N1	3.14	1.39	1.33
3	L5	2206	A2M	C5-N7	-3.13	1.33	1.39
4	L7	1	GTP	C5-N7	-3.13	1.33	1.39
3	L5	1810	A2M	C5-N7	-3.13	1.33	1.39
3	L5	1479	A2M	C2-N1	3.13	1.39	1.33
3	L5	2207	OMG	C5-C6	-3.13	1.33	1.44
3	L5	2658	A2M	C5-N7	-3.13	1.33	1.39
49	S2	591	A2M	C5-N7	-3.13	1.33	1.39
49	S2	591	A2M	C2-N1	3.12	1.39	1.33
49	S2	513	A2M	C2-N1	3.12	1.39	1.33
3	L5	3562	A2M	C5-N7	-3.12	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3456	A2M	C2-N1	3.12	1.39	1.33
3	L5	3557	A2M	C2-N1	3.12	1.39	1.33
3	L5	2244	A2M	C5-N7	-3.12	1.33	1.39
3	L5	400	A2M	C5-N7	-3.11	1.33	1.39
49	S2	1032	A2M	C2-N1	3.11	1.39	1.33
49	S2	99	A2M	C5-N7	-3.11	1.33	1.39
3	L5	3631	OMG	C5-C6	-3.11	1.33	1.44
49	S2	99	A2M	C2-N1	3.11	1.39	1.33
3	L5	400	A2M	C2-N1	3.11	1.39	1.33
3	L5	3599	A2M	C2-N1	3.10	1.39	1.33
3	L5	3524	OMG	C5-C6	-3.10	1.33	1.44
3	L5	4116	OMG	C5-C6	-3.10	1.33	1.44
3	L5	3557	A2M	C5-N7	-3.10	1.33	1.39
3	L5	398	A2M	C2-N1	3.10	1.39	1.33
3	L5	4369	OMG	C5-C6	-3.10	1.33	1.44
5	L8	75	OMG	C5-C6	-3.10	1.33	1.44
49	S2	1384	A2M	C5-N7	-3.09	1.33	1.39
3	L5	4240	OMG	C5-C6	-3.09	1.33	1.44
3	L5	2207	OMG	C5-N7	-3.09	1.33	1.39
3	L5	3450	A2M	C5-N7	-3.09	1.33	1.39
3	L5	1270	A2M	C5-N7	-3.09	1.33	1.39
49	S2	1843	4AC	C4-N4	-3.08	1.35	1.39
3	L5	3517	A2M	C2-N1	3.08	1.39	1.33
3	L5	1580	OMG	C5-N7	-3.08	1.33	1.39
3	L5	3476	OMG	C5-C6	-3.08	1.33	1.44
49	S2	1032	A2M	C5-N7	-3.08	1.33	1.39
3	L5	1260	OMG	C5-C6	-3.07	1.33	1.44
3	L5	3942	OMG	C5-C6	-3.07	1.33	1.44
3	L5	2630	A2M	C2-N1	3.07	1.39	1.33
3	L5	3524	OMG	C5-N7	-3.07	1.33	1.39
49	S2	602	OMG	C5-C6	-3.07	1.33	1.44
3	L5	3599	A2M	C5-N7	-3.07	1.33	1.39
3	L5	2630	A2M	C5-N7	-3.07	1.33	1.39
3	L5	4269	A2M	C5-N7	-3.07	1.33	1.39
3	L5	3974	OMG	C5-C6	-3.06	1.33	1.44
3	L5	3359	OMG	C5-C6	-3.06	1.33	1.44
3	L5	4383	OMG	C5-C6	-3.06	1.33	1.44
49	S2	1679	A2M	C5-N7	-3.06	1.33	1.39
3	L5	4336	A2M	C5-N7	-3.06	1.33	1.39
3	L5	2658	A2M	C2-N1	3.06	1.39	1.33
3	L5	4336	A2M	C2-N1	3.06	1.39	1.33
49	S2	469	A2M	C5-N7	-3.05	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	684	OMG	C5-C6	-3.05	1.33	1.44
49	S2	485	A2M	C5-N7	-3.05	1.33	1.39
49	S2	1491	OMG	C5-C6	-3.05	1.33	1.44
3	L5	3456	A2M	C5-N7	-3.05	1.33	1.39
3	L5	1477	OMG	C5-N7	-3.05	1.33	1.39
3	L5	2206	A2M	C2-N1	3.05	1.39	1.33
3	L5	1477	OMG	C5-C6	-3.05	1.33	1.44
49	S2	513	A2M	C5-N7	-3.05	1.33	1.39
3	L5	2267	OMG	C5-C6	-3.05	1.33	1.44
3	L5	2719	OMG	C5-C6	-3.04	1.33	1.44
3	L5	4138	OMG	C5-C6	-3.04	1.33	1.44
3	L5	1580	OMG	C5-C6	-3.04	1.33	1.44
3	L5	1489	A2M	C5-C4	-3.04	1.33	1.39
3	L5	4240	OMG	C5-N7	-3.04	1.33	1.39
49	S2	1448	OMG	C5-N7	-3.04	1.33	1.39
3	L5	4369	OMG	C5-N7	-3.04	1.33	1.39
3	L5	1489	A2M	C2-N1	3.04	1.39	1.33
3	L5	1270	A2M	C5-C4	-3.03	1.33	1.39
49	S2	645	OMG	C5-C6	-3.03	1.33	1.44
3	L5	4364	OMG	C5-C6	-3.03	1.33	1.44
3	L5	4193	5MC	C6-C5	3.03	1.39	1.34
3	L5	4245	OMG	C5-C6	-3.03	1.33	1.44
49	S2	1338	4AC	C4-N4	-3.03	1.35	1.39
49	S2	868	OMG	C5-C6	-3.02	1.33	1.44
3	L5	3676	OMG	C5-C6	-3.02	1.33	1.44
3	L5	3631	OMG	C5-N7	-3.02	1.33	1.39
49	S2	159	A2M	C5-N7	-3.02	1.33	1.39
3	L5	4138	OMG	C5-N7	-3.02	1.33	1.39
49	S2	669	A2M	C2-N3	3.02	1.39	1.33
3	L5	3476	OMG	C5-N7	-3.01	1.33	1.39
3	L5	3942	OMG	C5-N7	-3.01	1.33	1.39
49	S2	166	A2M	C5-N7	-3.01	1.33	1.39
49	S2	577	A2M	C5-N7	-3.01	1.33	1.39
49	S2	437	OMG	C5-C6	-3.01	1.33	1.44
3	L5	2630	A2M	C5-C4	-3.01	1.33	1.39
3	L5	2267	OMG	C5-N7	-3.01	1.33	1.39
49	S2	510	OMG	C5-C6	-3.01	1.33	1.44
49	S2	27	A2M	C5-N7	-3.01	1.33	1.39
5	L8	75	OMG	C5-N7	-3.01	1.33	1.39
49	S2	684	OMG	C5-N7	-3.00	1.33	1.39
49	S2	1448	OMG	C5-C6	-3.00	1.33	1.44
3	L5	1266	1MA	C5-N7	-3.00	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4116	OMG	C5-N7	-3.00	1.33	1.39
3	L5	1260	OMG	C5-N7	-3.00	1.33	1.39
3	L5	3517	A2M	C5-C4	-2.99	1.33	1.39
49	S2	1329	OMG	C5-C6	-2.99	1.33	1.44
49	S2	513	A2M	C5-C4	-2.99	1.33	1.39
3	L5	2206	A2M	C5-C4	-2.99	1.33	1.39
3	L5	4269	A2M	C5-C4	-2.99	1.33	1.39
49	S2	868	OMG	C5-N7	-2.99	1.33	1.39
49	S2	1491	OMG	C5-N7	-2.99	1.33	1.39
3	L5	3359	OMG	C5-N7	-2.98	1.33	1.39
3	L5	4383	OMG	C5-N7	-2.97	1.33	1.39
3	L5	3676	OMG	C5-N7	-2.97	1.33	1.39
49	S2	510	OMG	C5-N7	-2.97	1.33	1.39
49	S2	669	A2M	C5-N7	-2.97	1.33	1.39
3	L5	3562	A2M	C5-C4	-2.97	1.33	1.39
49	S2	602	OMG	C5-N7	-2.97	1.33	1.39
3	L5	4336	A2M	C5-C4	-2.96	1.33	1.39
3	L5	400	A2M	C5-C4	-2.96	1.33	1.39
3	L5	4245	OMG	C5-N7	-2.96	1.33	1.39
3	L5	3517	A2M	C5-C6	-2.96	1.33	1.41
3	L5	3557	A2M	C5-C4	-2.96	1.33	1.39
3	L5	4364	OMG	C5-N7	-2.96	1.33	1.39
49	S2	27	A2M	C5-C4	-2.96	1.33	1.39
49	S2	485	A2M	C5-C4	-2.95	1.33	1.39
3	L5	1810	A2M	C5-C4	-2.95	1.33	1.39
3	L5	2244	A2M	C5-C4	-2.95	1.33	1.39
49	S2	645	OMG	C5-N7	-2.95	1.33	1.39
49	S2	99	A2M	C5-C4	-2.94	1.33	1.39
3	L5	398	A2M	C5-C4	-2.94	1.33	1.39
3	L5	3599	A2M	C5-C4	-2.94	1.33	1.39
49	S2	437	OMG	C5-N7	-2.94	1.33	1.39
3	L5	3974	OMG	C5-N7	-2.94	1.33	1.39
49	S2	1032	A2M	C5-C4	-2.94	1.33	1.39
3	L5	3456	A2M	C5-C4	-2.93	1.33	1.39
3	L5	3450	A2M	C5-C4	-2.92	1.33	1.39
3	L5	2658	A2M	C5-C4	-2.91	1.33	1.39
3	L5	4317	A2M	C5-C4	-2.91	1.33	1.39
49	S2	469	A2M	C5-C4	-2.89	1.33	1.39
49	S2	159	A2M	C5-C4	-2.89	1.33	1.39
49	S2	577	A2M	C5-C4	-2.89	1.33	1.39
49	S2	1384	A2M	C5-C4	-2.89	1.33	1.39
3	L5	1270	A2M	C5-C6	-2.88	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	1329	OMG	C5-N7	-2.88	1.33	1.39
49	S2	1679	A2M	C5-C4	-2.87	1.33	1.39
3	L5	3492	A2M	C5-N7	-2.87	1.33	1.39
49	S2	1032	A2M	C5-C6	-2.87	1.33	1.41
3	L5	1479	A2M	C5-C4	-2.87	1.33	1.39
3	L5	1489	A2M	C5-C6	-2.86	1.33	1.41
3	L5	3599	A2M	C5-C6	-2.86	1.33	1.41
49	S2	166	A2M	C5-C4	-2.86	1.33	1.39
49	S2	669	A2M	C5-C6	-2.85	1.33	1.41
49	S2	27	A2M	C5-C6	-2.85	1.33	1.41
3	L5	3456	A2M	C5-C6	-2.85	1.33	1.41
3	L5	4276	UR3	C4-N3	-2.85	1.34	1.40
3	L5	2630	A2M	C5-C6	-2.85	1.33	1.41
49	S2	1679	A2M	C5-C6	-2.85	1.33	1.41
3	L5	1479	A2M	C5-C6	-2.85	1.33	1.41
3	L5	2244	A2M	C5-C6	-2.84	1.33	1.41
3	L5	1810	A2M	C5-C6	-2.84	1.33	1.41
3	L5	3562	A2M	C5-C6	-2.84	1.33	1.41
3	L5	4269	A2M	C5-C6	-2.83	1.33	1.41
3	L5	2658	A2M	C5-C6	-2.83	1.33	1.41
3	L5	4336	A2M	C5-C6	-2.83	1.33	1.41
49	S2	591	A2M	C5-C6	-2.83	1.33	1.41
3	L5	2206	A2M	C5-C6	-2.83	1.33	1.41
49	S2	1384	A2M	C5-C6	-2.82	1.33	1.41
49	S2	485	A2M	C5-C6	-2.82	1.33	1.41
49	S2	99	A2M	C5-C6	-2.82	1.33	1.41
3	L5	398	A2M	C5-C6	-2.82	1.33	1.41
49	S2	513	A2M	C5-C6	-2.81	1.33	1.41
3	L5	4317	A2M	C5-C6	-2.81	1.33	1.41
3	L5	3450	A2M	C5-C6	-2.81	1.33	1.41
3	L5	3557	A2M	C5-C6	-2.81	1.33	1.41
3	L5	4276	UR3	C2-N1	-2.81	1.34	1.38
49	S2	577	A2M	C5-C6	-2.80	1.33	1.41
49	S2	469	A2M	C5-C6	-2.79	1.33	1.41
3	L5	400	A2M	C5-C6	-2.79	1.33	1.41
49	S2	591	A2M	C5-C4	-2.78	1.33	1.39
49	S2	159	A2M	C5-C6	-2.75	1.33	1.41
3	L5	3492	A2M	C5-C4	-2.75	1.33	1.39
49	S2	34	PSU	C2-N1	2.74	1.40	1.36
49	S2	166	A2M	C5-C6	-2.74	1.33	1.41
49	S2	1446	PSU	C2-N1	2.73	1.40	1.36
3	L5	4193	5MC	C4-N3	2.73	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	119	PSU	C2-N1	2.72	1.40	1.36
49	S2	1245	PSU	C2-N1	2.72	1.40	1.36
3	L5	3514	5MC	C6-C5	2.72	1.39	1.34
49	S2	1851	MA6	C5-C6	2.72	1.48	1.41
49	S2	1392	OMC	C4-N3	2.71	1.40	1.34
49	S2	815	PSU	C2-N1	2.71	1.40	1.36
49	S2	867	PSU	C2-N1	2.71	1.40	1.36
49	S2	1644	PSU	C2-N1	2.70	1.40	1.36
49	S2	1852	MA6	C5-C6	2.69	1.48	1.41
49	S2	573	PSU	C2-N1	2.68	1.40	1.36
3	L5	3466	PSU	C2-N1	2.68	1.40	1.36
49	S2	1082	PSU	C2-N1	2.67	1.40	1.36
3	L5	3619	OMC	C2-N1	-2.66	1.34	1.40
49	S2	210	PSU	C2-N1	2.66	1.40	1.36
3	L5	4749	PSU	C2-N1	2.66	1.40	1.36
49	S2	1057	PSU	C2-N1	2.65	1.40	1.36
5	L8	69	PSU	C2-N1	2.65	1.40	1.36
3	L5	3500	PSU	C2-N1	2.65	1.40	1.36
3	L5	1820	OMC	C2-N1	-2.65	1.34	1.40
80	Si	62	HY3	C3-CA	-2.65	1.52	1.55
3	L5	2667	OMC	C2-N1	-2.65	1.34	1.40
3	L5	4202	OMC	C2-N1	-2.65	1.34	1.40
49	S2	816	PSU	C2-N1	2.64	1.40	1.36
3	L5	2351	PSU	C2-N1	2.64	1.40	1.36
3	L5	4166	PSU	C2-N1	2.64	1.40	1.36
3	L5	1284	OMC	C2-N1	-2.64	1.34	1.40
3	L5	2208	OMC	C2-N1	-2.64	1.34	1.40
3	L5	3433	OMC	C2-N1	-2.64	1.34	1.40
49	S2	687	PSU	C2-N1	2.63	1.40	1.36
3	L5	3433	OMC	C4-N3	2.63	1.39	1.34
3	L5	3502	PSU	C2-N1	2.63	1.40	1.36
49	S2	407	PSU	C2-N1	2.63	1.40	1.36
3	L5	3583	PSU	C2-N1	2.63	1.40	1.36
49	S2	218	PSU	C2-N1	2.63	1.40	1.36
49	S2	1047	PSU	C2-N1	2.62	1.40	1.36
3	L5	4282	OMC	C2-N1	-2.62	1.34	1.40
49	S2	610	PSU	C2-N1	2.62	1.40	1.36
49	S2	36	PSU	C2-N1	2.61	1.40	1.36
49	S2	1178	PSU	C2-N1	2.61	1.40	1.36
49	S2	1239	PSU	C2-N1	2.61	1.40	1.36
49	S2	1046	PSU	C2-N1	2.61	1.40	1.36
49	S2	1704	OMC	C2-N1	-2.61	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1721	PSU	C2-N1	2.61	1.40	1.36
49	S2	682	PSU	C2-N1	2.61	1.40	1.36
49	S2	1368	PSU	C2-N1	2.60	1.40	1.36
3	L5	4244	OMU	C2-N1	-2.60	1.34	1.38
3	L5	3490	PSU	C2-N1	2.60	1.40	1.36
49	S2	967	PSU	C2-N1	2.59	1.40	1.36
3	L5	4188	PSU	C2-N1	2.59	1.40	1.36
49	S2	1327	OMU	C2-N1	-2.59	1.34	1.38
49	S2	463	OMC	C2-N1	-2.59	1.34	1.40
49	S2	429	OMU	C2-N1	-2.59	1.34	1.38
49	S2	628	OMU	C2-N1	-2.58	1.34	1.38
49	S2	463	OMC	C4-N3	2.58	1.39	1.34
49	S2	652	PSU	C2-N1	2.58	1.40	1.36
5	L8	55	PSU	C2-N1	2.58	1.40	1.36
3	L5	2475	PSU	C2-N1	2.58	1.40	1.36
3	L5	3494	PSU	C2-N1	2.57	1.40	1.36
3	L5	2680	OMU	C2-N1	-2.57	1.34	1.38
49	S2	1693	PSU	C2-N1	2.57	1.40	1.36
3	L5	1284	OMC	C4-N3	2.57	1.39	1.34
49	S2	650	PSU	C2-N1	2.57	1.40	1.36
3	L5	4107	PSU	C2-N1	2.57	1.40	1.36
3	L5	2704	OMC	C2-N1	-2.57	1.34	1.40
3	L5	3496	PSU	C2-N1	2.57	1.40	1.36
49	S2	1704	OMC	C4-N3	2.57	1.39	1.34
3	L5	2647	OMC	C4-N3	2.57	1.39	1.34
3	L5	4099	PSU	C2-N1	2.56	1.40	1.36
3	L5	4282	OMC	C4-N3	2.56	1.39	1.34
49	S2	109	PSU	C2-N1	2.56	1.40	1.36
3	L5	4217	PSU	C2-N1	2.56	1.40	1.36
49	S2	518	OMC	C4-N3	2.56	1.39	1.34
3	L5	1731	PSU	C2-N1	2.56	1.40	1.36
3	L5	2647	OMC	C2-N1	-2.56	1.34	1.40
49	S2	174	OMC	C4-N3	2.56	1.39	1.34
49	S2	1348	PSU	C2-N1	2.55	1.40	1.36
3	L5	3427	PSU	C2-N1	2.55	1.40	1.36
3	L5	1801	PSU	C2-N1	2.55	1.40	1.36
3	L5	4149	PSU	C2-N1	2.55	1.40	1.36
3	L5	2265	OMC	C4-N3	2.55	1.39	1.34
3	L5	3371	PSU	C2-N1	2.55	1.40	1.36
3	L5	3573	OMC	C2-N1	-2.55	1.34	1.40
49	S2	864	PSU	C2-N1	2.55	1.40	1.36
3	L5	3462	PSU	C2-N1	2.55	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3554	PSU	C2-N1	2.54	1.40	1.36
3	L5	1537	PSU	C2-N1	2.54	1.40	1.36
3	L5	4193	5MC	C2-N1	-2.54	1.34	1.40
49	S2	1233	PSU	C2-N1	2.54	1.40	1.36
3	L5	2208	OMC	C4-N3	2.53	1.39	1.34
3	L5	2667	OMC	C4-N3	2.53	1.39	1.34
49	S2	669	A2M	C8-N9	-2.53	1.33	1.37
3	L5	3369	PSU	C2-N1	2.53	1.40	1.36
3	L5	3540	OMC	C2-N1	-2.53	1.34	1.40
3	L5	3601	OMC	C2-N1	-2.53	1.34	1.40
3	L5	2704	OMC	C4-N3	2.53	1.39	1.34
3	L5	1799	PSU	C2-N1	2.53	1.40	1.36
3	L5	4045	PSU	C2-N1	2.53	1.40	1.36
49	S2	1005	PSU	C2-N1	2.53	1.40	1.36
3	L5	3652	PSU	C2-N1	2.52	1.40	1.36
3	L5	4203	PSU	C2-N1	2.52	1.40	1.36
3	L5	2258	OMU	C2-N1	-2.52	1.34	1.38
3	L5	4042	PSU	C2-N1	2.52	1.40	1.36
3	L5	4711	PSU	C2-N1	2.52	1.40	1.36
3	L5	3447	PSU	C2-N1	2.51	1.40	1.36
3	L5	4039	PSU	C2-N1	2.51	1.40	1.36
3	L5	2194	OMC	C4-N3	2.51	1.39	1.34
3	L5	3973	OMU	C2-N1	-2.51	1.34	1.38
3	L5	4202	OMC	C4-N3	2.51	1.39	1.34
3	L5	3540	OMC	C4-N3	2.51	1.39	1.34
3	L5	3619	OMC	C4-N3	2.50	1.39	1.34
49	S2	121	OMU	C2-N1	-2.50	1.34	1.38
3	L5	2194	OMC	C2-N1	-2.50	1.34	1.40
3	L5	1718	PSU	C2-N1	2.50	1.40	1.36
49	S2	518	OMC	C2-N1	-2.50	1.34	1.40
49	S2	174	OMC	C2-N1	-2.49	1.34	1.40
3	L5	4419	PSU	C2-N1	2.49	1.40	1.36
3	L5	3601	OMC	C4-N3	2.49	1.39	1.34
49	S2	802	PSU	C2-N1	2.49	1.40	1.36
49	S2	1626	PSU	C2-N1	2.49	1.40	1.36
3	L5	2265	OMC	C2-N1	-2.49	1.34	1.40
49	S2	93	PSU	C2-N1	2.49	1.40	1.36
3	L5	1720	PSU	C2-N1	2.49	1.40	1.36
3	L5	1638	PSU	C2-N1	2.49	1.40	1.36
49	S2	1175	PSU	C2-N1	2.49	1.40	1.36
3	L5	4366	OMU	C2-N1	-2.48	1.34	1.38
3	L5	4322	PSU	C2-N1	2.48	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3657	OMU	C2-N1	-2.48	1.34	1.38
3	L5	4169	PSU	C2-N1	2.48	1.40	1.36
3	L5	3517	A2M	C8-N9	-2.47	1.33	1.37
3	L5	4740	PSU	C2-N1	2.47	1.40	1.36
3	L5	4267	PSU	C2-N1	2.47	1.40	1.36
3	L5	1491	PSU	C2-N1	2.47	1.40	1.36
49	S2	172	OMU	C2-N1	-2.47	1.34	1.38
3	L5	1489	A2M	C8-N9	-2.47	1.33	1.37
3	L5	3492	A2M	C5-C6	-2.47	1.34	1.41
3	L5	1683	PSU	C2-N1	2.47	1.40	1.36
3	L5	4177	PSU	C2-N1	2.46	1.40	1.36
49	S2	116	OMU	C2-N1	-2.46	1.34	1.38
3	L5	4246	PSU	C2-N1	2.46	1.40	1.36
49	S2	355	OMU	C2-N1	-2.46	1.34	1.38
3	L5	4325	PSU	C2-N1	2.45	1.40	1.36
3	L5	4374	PSU	C2-N1	2.44	1.40	1.36
3	L5	1820	OMC	C4-N3	2.44	1.39	1.34
3	L5	3573	OMC	C4-N3	2.44	1.39	1.34
3	L5	3585	PSU	C2-N1	2.44	1.40	1.36
3	L5	1270	A2M	C8-N9	-2.43	1.33	1.37
3	L5	1632	PSU	C2-N1	2.43	1.40	1.36
3	L5	4336	A2M	C8-N9	-2.43	1.33	1.37
49	S2	105	PSU	C2-N1	2.43	1.40	1.36
3	L5	4052	OMU	C2-N1	-2.43	1.34	1.38
3	L5	3514	5MC	C2-N1	-2.43	1.34	1.40
3	L5	2658	A2M	C8-N9	-2.42	1.33	1.37
3	L5	1479	A2M	C8-N9	-2.41	1.33	1.37
49	S2	1032	A2M	C8-N9	-2.41	1.33	1.37
3	L5	2206	A2M	C8-N9	-2.40	1.33	1.37
3	L5	4276	UR3	C2-N3	-2.40	1.34	1.39
49	S2	1833	6MZ	C5-N7	-2.40	1.34	1.39
3	L5	2244	A2M	C8-N9	-2.40	1.33	1.37
3	L5	3599	A2M	C8-N9	-2.40	1.33	1.37
3	L5	3966	6MZ	C5-C6	2.40	1.48	1.41
49	S2	823	PSU	C2-N1	2.40	1.40	1.36
49	S2	823	PSU	C6-N1	-2.39	1.32	1.36
49	S2	469	A2M	C8-N9	-2.39	1.33	1.37
3	L5	4382	PSU	C6-N1	-2.39	1.32	1.36
49	S2	1392	OMC	C2-N1	-2.39	1.34	1.40
3	L5	3616	PSU	C2-N1	2.38	1.40	1.36
3	L5	4374	PSU	C6-N1	-2.38	1.32	1.36
3	L5	4435	PSU	C2-N1	2.38	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	1851	MA6	C8-N7	2.38	1.36	1.31
3	L5	1810	A2M	C8-N9	-2.37	1.33	1.37
3	L5	3652	PSU	C6-N1	-2.37	1.32	1.36
3	L5	4203	PSU	C6-N1	-2.37	1.32	1.36
3	L5	4058	PSU	C2-N1	2.37	1.39	1.36
49	S2	513	A2M	C8-N9	-2.37	1.33	1.37
49	S2	591	A2M	C8-N9	-2.37	1.33	1.37
3	L5	3562	A2M	C8-N9	-2.36	1.33	1.37
3	L5	1537	PSU	C6-N1	-2.36	1.32	1.36
3	L5	4177	PSU	C6-N1	-2.36	1.32	1.36
49	S2	27	A2M	C8-N9	-2.35	1.33	1.37
3	L5	1491	PSU	C6-N1	-2.35	1.32	1.36
49	S2	1805	OMU	C2-N1	-2.35	1.34	1.38
3	L5	400	A2M	C8-N9	-2.35	1.33	1.37
3	L5	4435	PSU	C6-N1	-2.35	1.32	1.36
3	L5	2630	A2M	C8-N9	-2.35	1.33	1.37
3	L5	3616	PSU	C6-N1	-2.35	1.32	1.36
49	S2	1679	A2M	C8-N9	-2.35	1.33	1.37
3	L5	4169	PSU	C6-N1	-2.34	1.32	1.36
3	L5	3369	PSU	C6-N1	-2.34	1.32	1.36
3	L5	4269	A2M	C8-N9	-2.34	1.33	1.37
3	L5	4317	A2M	C8-N9	-2.34	1.33	1.37
3	L5	4419	PSU	C6-N1	-2.33	1.32	1.36
3	L5	1801	PSU	C6-N1	-2.33	1.32	1.36
3	L5	4267	PSU	C6-N1	-2.33	1.32	1.36
3	L5	3456	A2M	C8-N9	-2.33	1.33	1.37
3	L5	4246	PSU	C6-N1	-2.32	1.32	1.36
3	L5	2475	PSU	C6-N1	-2.32	1.32	1.36
3	L5	1718	PSU	C6-N1	-2.32	1.32	1.36
49	S2	93	PSU	C6-N1	-2.32	1.32	1.36
3	L5	1632	PSU	C6-N1	-2.32	1.32	1.36
3	L5	3371	PSU	C6-N1	-2.32	1.32	1.36
3	L5	4042	PSU	C6-N1	-2.32	1.32	1.36
49	S2	105	PSU	C6-N1	-2.32	1.32	1.36
3	L5	1720	PSU	C6-N1	-2.32	1.32	1.36
3	L5	4298	PSU	C2-N1	2.31	1.39	1.36
3	L5	3427	PSU	C6-N1	-2.31	1.32	1.36
3	L5	3492	A2M	C8-N9	-2.31	1.33	1.37
49	S2	166	A2M	C8-N9	-2.31	1.33	1.37
3	L5	4149	PSU	C6-N1	-2.31	1.32	1.36
3	L5	4298	PSU	C6-N1	-2.31	1.32	1.36
3	L5	3966	6MZ	C8-N7	2.30	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1638	PSU	C6-N1	-2.30	1.32	1.36
3	L5	3576	PSU	C6-N1	-2.30	1.32	1.36
49	S2	485	A2M	C8-N9	-2.30	1.33	1.37
49	S2	99	A2M	C8-N9	-2.30	1.33	1.37
3	L5	4217	PSU	C6-N1	-2.30	1.32	1.36
49	S2	682	PSU	C6-N1	-2.30	1.32	1.36
3	L5	3966	6MZ	C5-N7	-2.30	1.34	1.39
49	S2	1057	PSU	C6-N1	-2.30	1.32	1.36
49	S2	1175	PSU	C6-N1	-2.30	1.32	1.36
49	S2	1368	PSU	C6-N1	-2.29	1.32	1.36
3	L5	4711	PSU	C6-N1	-2.29	1.32	1.36
3	L5	1721	PSU	C6-N1	-2.29	1.32	1.36
49	S2	610	PSU	C6-N1	-2.29	1.32	1.36
3	L5	3585	PSU	C6-N1	-2.29	1.32	1.36
3	L5	3557	A2M	C8-N9	-2.29	1.33	1.37
3	L5	4045	PSU	C6-N1	-2.29	1.32	1.36
3	L5	1683	PSU	C6-N1	-2.28	1.32	1.36
3	L5	1799	PSU	C6-N1	-2.28	1.32	1.36
3	L5	3496	PSU	C6-N1	-2.28	1.32	1.36
49	S2	1446	PSU	C6-N1	-2.28	1.32	1.36
3	L5	3576	PSU	C2-N1	2.28	1.39	1.36
3	L5	4058	PSU	C6-N1	-2.28	1.32	1.36
3	L5	4188	PSU	C6-N1	-2.28	1.32	1.36
49	S2	1384	A2M	C8-N9	-2.28	1.33	1.37
49	S2	1693	PSU	C6-N1	-2.28	1.32	1.36
3	L5	4166	PSU	C6-N1	-2.28	1.32	1.36
3	L5	3447	PSU	C6-N1	-2.28	1.32	1.36
3	L5	4322	PSU	C6-N1	-2.27	1.32	1.36
49	S2	1233	PSU	C6-N1	-2.27	1.32	1.36
49	S2	1046	PSU	C6-N1	-2.27	1.32	1.36
3	L5	4740	PSU	C6-N1	-2.27	1.32	1.36
3	L5	4099	PSU	C6-N1	-2.27	1.32	1.36
3	L5	4039	PSU	C6-N1	-2.27	1.32	1.36
3	L5	4382	PSU	C2-N1	2.27	1.39	1.36
49	S2	1644	PSU	C6-N1	-2.27	1.32	1.36
3	L5	3583	PSU	C6-N1	-2.27	1.32	1.36
49	S2	1843	4AC	C7-N4	-2.27	1.32	1.37
3	L5	398	A2M	C8-N9	-2.27	1.33	1.37
3	L5	4107	PSU	C6-N1	-2.27	1.32	1.36
3	L5	3500	PSU	C6-N1	-2.26	1.32	1.36
3	L5	1731	PSU	C6-N1	-2.26	1.32	1.36
3	L5	3554	PSU	C6-N1	-2.26	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4325	PSU	C6-N1	-2.26	1.32	1.36
49	S2	109	PSU	C6-N1	-2.26	1.32	1.36
49	S2	1852	MA6	C5-N7	-2.26	1.34	1.39
49	S2	407	PSU	C6-N1	-2.26	1.32	1.36
49	S2	159	A2M	C8-N9	-2.26	1.33	1.37
49	S2	652	PSU	C6-N1	-2.26	1.32	1.36
3	L5	3450	A2M	C8-N9	-2.26	1.33	1.37
49	S2	573	PSU	C6-N1	-2.25	1.32	1.36
3	L5	3462	PSU	C6-N1	-2.25	1.32	1.36
3	L5	4749	PSU	C6-N1	-2.25	1.32	1.36
49	S2	1833	6MZ	C5-C6	2.25	1.47	1.41
49	S2	577	A2M	C8-N9	-2.25	1.33	1.37
49	S2	802	PSU	C6-N1	-2.25	1.32	1.36
3	L5	3490	PSU	C6-N1	-2.25	1.32	1.36
3	L5	3494	PSU	C6-N1	-2.25	1.32	1.36
49	S2	1005	PSU	C6-N1	-2.25	1.32	1.36
49	S2	1047	PSU	C6-N1	-2.25	1.32	1.36
49	S2	36	PSU	C6-N1	-2.25	1.32	1.36
3	L5	3502	PSU	C6-N1	-2.24	1.32	1.36
5	L8	69	PSU	C6-N1	-2.24	1.32	1.36
49	S2	1178	PSU	C6-N1	-2.24	1.32	1.36
49	S2	1239	PSU	C6-N1	-2.24	1.32	1.36
49	S2	864	PSU	C6-N1	-2.23	1.32	1.36
49	S2	1852	MA6	C8-N7	2.23	1.35	1.31
49	S2	1348	PSU	C6-N1	-2.23	1.32	1.36
49	S2	210	PSU	C6-N1	-2.22	1.32	1.36
49	S2	1245	PSU	C6-N1	-2.21	1.32	1.36
49	S2	816	PSU	C6-N1	-2.21	1.32	1.36
5	L8	55	PSU	C6-N1	-2.21	1.32	1.36
49	S2	815	PSU	C6-N1	-2.21	1.32	1.36
49	S2	867	PSU	C6-N1	-2.21	1.32	1.36
3	L5	2351	PSU	C6-N1	-2.21	1.32	1.36
49	S2	687	PSU	C6-N1	-2.21	1.32	1.36
49	S2	669	A2M	C4-N9	-2.20	1.32	1.37
49	S2	119	PSU	C6-N1	-2.20	1.32	1.36
49	S2	1626	PSU	C6-N1	-2.20	1.32	1.36
49	S2	34	PSU	C6-N1	-2.19	1.32	1.36
49	S2	1443	OMU	C2-N1	-2.19	1.34	1.38
49	S2	1082	PSU	C6-N1	-2.19	1.32	1.36
49	S2	650	PSU	C6-N1	-2.19	1.32	1.36
49	S2	967	PSU	C6-N1	-2.18	1.32	1.36
3	L5	3466	PSU	C6-N1	-2.18	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	218	PSU	C6-N1	-2.17	1.32	1.36
49	S2	1289	OMU	C2-N1	-2.16	1.35	1.38
49	S2	116	OMU	C5-C4	-2.15	1.38	1.43
3	L5	1266	1MA	C6-N6	2.14	1.33	1.28
3	L5	2680	OMU	C5-C4	-2.13	1.38	1.43
49	S2	1851	MA6	C5-N7	-2.13	1.35	1.39
3	L5	1632	PSU	C1'-C5	2.12	1.55	1.50
3	L5	2258	OMU	C5-C4	-2.12	1.38	1.43
3	L5	1479	A2M	C4-N9	-2.12	1.33	1.37
49	S2	1833	6MZ	C8-N7	2.12	1.35	1.31
3	L5	4244	OMU	C5-C4	-2.11	1.39	1.43
3	L5	4052	OMU	C5-C4	-2.10	1.39	1.43
3	L5	4366	OMU	C5-C4	-2.10	1.39	1.43
3	L5	4383	OMG	C8-N9	-2.09	1.32	1.37
49	S2	355	OMU	C5-C4	-2.09	1.39	1.43
49	S2	172	OMU	C5-C4	-2.07	1.39	1.43
49	S2	121	OMU	C5-C4	-2.07	1.39	1.43
49	S2	1805	OMU	C5-C4	-2.06	1.39	1.43
3	L5	1270	A2M	C4-N9	-2.06	1.33	1.37
49	S2	429	OMU	C5-C4	-2.05	1.39	1.43
3	L5	3973	OMU	C5-C4	-2.05	1.39	1.43
3	L5	3557	A2M	C4-N9	-2.04	1.33	1.37
49	S2	1443	OMU	C5-C4	-2.04	1.39	1.43
5	L8	75	OMG	C4-N9	-2.04	1.32	1.38
49	S2	1032	A2M	C4-N9	-2.03	1.33	1.37
3	L5	4269	A2M	C4-N9	-2.03	1.33	1.37
3	L5	4245	OMG	C8-N9	-2.03	1.33	1.37
49	S2	27	A2M	C4-N9	-2.03	1.33	1.37
49	S2	1289	OMU	C5-C4	-2.02	1.39	1.43
3	L5	2207	OMG	C8-N9	-2.02	1.33	1.37
3	L5	3657	OMU	C5-C4	-2.02	1.39	1.43
3	L5	1260	OMG	C8-N9	-2.02	1.33	1.37
49	S2	1327	OMU	C5-C4	-2.02	1.39	1.43
4	L7	1	GTP	C4-N9	-2.02	1.32	1.38
49	S2	1338	4AC	C7-N4	-2.01	1.33	1.37
49	S2	645	OMG	C8-N9	-2.01	1.33	1.37
3	L5	4138	OMG	C8-N9	-2.01	1.33	1.37
49	S2	485	A2M	C4-N9	-2.01	1.33	1.37
3	L5	3599	A2M	C4-N9	-2.01	1.33	1.37
49	S2	577	A2M	C4-N9	-2.01	1.33	1.37
3	L5	3517	A2M	C4-N9	-2.01	1.33	1.37
3	L5	1810	A2M	C4-N9	-2.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3562	A2M	C4-N9	-2.01	1.33	1.37
3	L5	4116	OMG	C8-N9	-2.01	1.33	1.37
3	L5	1477	OMG	C8-N9	-2.00	1.33	1.37
49	S2	602	OMG	C8-N9	-2.00	1.33	1.37
3	L5	3974	OMG	C8-N9	-2.00	1.33	1.37
3	L5	4369	OMG	C8-N9	-2.00	1.33	1.37

All (1361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	Se	67	NMM	NE-CZ-NH2	-7.43	112.67	119.48
3	L5	1266	1MA	N1-C2-N3	-7.03	117.65	126.00
3	L5	4269	A2M	N3-C2-N1	-6.83	117.91	128.60
3	L5	1270	A2M	N3-C2-N1	-6.80	117.97	128.60
3	L5	2630	A2M	N3-C2-N1	-6.80	117.97	128.60
3	L5	1489	A2M	N3-C2-N1	-6.76	118.02	128.60
49	S2	669	A2M	N3-C2-N1	-6.74	118.05	128.60
49	S2	27	A2M	N3-C2-N1	-6.73	118.07	128.60
49	S2	1032	A2M	N3-C2-N1	-6.72	118.09	128.60
49	S2	485	A2M	N3-C2-N1	-6.71	118.10	128.60
3	L5	3562	A2M	N3-C2-N1	-6.71	118.10	128.60
3	L5	3599	A2M	N3-C2-N1	-6.70	118.13	128.60
49	S2	1679	A2M	N3-C2-N1	-6.69	118.14	128.60
3	L5	3557	A2M	N3-C2-N1	-6.68	118.15	128.60
3	L5	2244	A2M	N3-C2-N1	-6.68	118.15	128.60
3	L5	3456	A2M	N3-C2-N1	-6.68	118.16	128.60
49	S2	99	A2M	N3-C2-N1	-6.67	118.16	128.60
49	S2	577	A2M	N3-C2-N1	-6.67	118.16	128.60
3	L5	4317	A2M	N3-C2-N1	-6.66	118.18	128.60
49	S2	513	A2M	N3-C2-N1	-6.66	118.19	128.60
49	S2	591	A2M	N3-C2-N1	-6.65	118.21	128.60
3	L5	4336	A2M	N3-C2-N1	-6.64	118.21	128.60
49	S2	469	A2M	N3-C2-N1	-6.64	118.21	128.60
3	L5	400	A2M	N3-C2-N1	-6.62	118.24	128.60
3	L5	1479	A2M	N3-C2-N1	-6.62	118.25	128.60
3	L5	398	A2M	N3-C2-N1	-6.62	118.25	128.60
49	S2	166	A2M	N3-C2-N1	-6.60	118.28	128.60
3	L5	1810	A2M	N3-C2-N1	-6.59	118.29	128.60
49	S2	159	A2M	N3-C2-N1	-6.59	118.30	128.60
49	S2	1384	A2M	N3-C2-N1	-6.57	118.32	128.60
3	L5	3450	A2M	N3-C2-N1	-6.56	118.34	128.60
3	L5	2206	A2M	N3-C2-N1	-6.55	118.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1833	6MZ	C5-C4-N3	-6.54	118.22	126.75
3	L5	2658	A2M	N3-C2-N1	-6.52	118.40	128.60
3	L5	3492	A2M	N3-C2-N1	-6.52	118.40	128.60
3	L5	3517	A2M	N3-C2-N1	-6.47	118.48	128.60
3	L5	3966	6MZ	C5-C4-N3	-6.19	118.67	126.75
49	S2	1852	MA6	C5-C4-N3	-6.12	118.77	126.75
49	S2	1851	MA6	C5-C4-N3	-6.05	118.86	126.75
49	S2	1833	6MZ	N3-C4-N9	5.38	135.94	127.08
49	S2	1640	7MG	C5-C6-N1	5.33	120.39	110.99
3	L5	4149	PSU	C4-N3-C2	-5.29	118.71	126.34
49	S2	34	PSU	C4-N3-C2	-5.27	118.75	126.34
3	L5	4188	PSU	C4-N3-C2	-5.27	118.75	126.34
3	L5	3652	PSU	C4-N3-C2	-5.25	118.77	126.34
5	L8	69	PSU	C4-N3-C2	-5.25	118.78	126.34
49	S2	1046	PSU	C4-N3-C2	-5.25	118.78	126.34
3	L5	4374	PSU	C4-N3-C2	-5.25	118.78	126.34
3	L5	4099	PSU	C4-N3-C2	-5.24	118.78	126.34
3	L5	2475	PSU	C4-N3-C2	-5.24	118.79	126.34
49	S2	218	PSU	C4-N3-C2	-5.24	118.79	126.34
49	S2	1644	PSU	C4-N3-C2	-5.24	118.79	126.34
49	S2	628	OMU	C4-N3-C2	-5.24	119.67	126.58
3	L5	3616	PSU	C4-N3-C2	-5.24	118.79	126.34
49	S2	1057	PSU	C4-N3-C2	-5.24	118.80	126.34
3	L5	1801	PSU	C4-N3-C2	-5.24	118.80	126.34
3	L5	4325	PSU	C4-N3-C2	-5.23	118.80	126.34
49	S2	119	PSU	C4-N3-C2	-5.23	118.80	126.34
3	L5	1491	PSU	C4-N3-C2	-5.23	118.81	126.34
49	S2	1082	PSU	C4-N3-C2	-5.22	118.81	126.34
49	S2	682	PSU	C4-N3-C2	-5.22	118.83	126.34
3	L5	3657	OMU	C4-N3-C2	-5.21	119.70	126.58
3	L5	4267	PSU	C4-N3-C2	-5.21	118.83	126.34
3	L5	4042	PSU	C4-N3-C2	-5.21	118.83	126.34
3	L5	4322	PSU	C4-N3-C2	-5.21	118.84	126.34
3	L5	1731	PSU	C4-N3-C2	-5.20	118.84	126.34
49	S2	650	PSU	C4-N3-C2	-5.20	118.85	126.34
3	L5	4203	PSU	C4-N3-C2	-5.20	118.85	126.34
3	L5	4435	PSU	C4-N3-C2	-5.20	118.85	126.34
3	L5	3369	PSU	C4-N3-C2	-5.20	118.85	126.34
49	S2	867	PSU	C4-N3-C2	-5.20	118.85	126.34
3	L5	4298	PSU	C4-N3-C2	-5.20	118.85	126.34
49	S2	109	PSU	C4-N3-C2	-5.19	118.86	126.34
49	S2	815	PSU	C4-N3-C2	-5.19	118.86	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	407	PSU	C4-N3-C2	-5.19	118.86	126.34
3	L5	4246	PSU	C4-N3-C2	-5.19	118.86	126.34
3	L5	4711	PSU	C4-N3-C2	-5.19	118.86	126.34
3	L5	1638	PSU	C4-N3-C2	-5.19	118.86	126.34
3	L5	2351	PSU	C4-N3-C2	-5.19	118.86	126.34
49	S2	1693	PSU	C4-N3-C2	-5.19	118.86	126.34
3	L5	3427	PSU	C4-N3-C2	-5.19	118.86	126.34
49	S2	1047	PSU	C4-N3-C2	-5.18	118.87	126.34
3	L5	1721	PSU	C4-N3-C2	-5.18	118.88	126.34
49	S2	652	PSU	C4-N3-C2	-5.17	118.88	126.34
3	L5	4166	PSU	C4-N3-C2	-5.17	118.89	126.34
5	L8	55	PSU	C4-N3-C2	-5.17	118.89	126.34
3	L5	4740	PSU	C4-N3-C2	-5.17	118.89	126.34
3	L5	1537	PSU	C4-N3-C2	-5.17	118.89	126.34
3	L5	3500	PSU	C4-N3-C2	-5.17	118.89	126.34
3	L5	4045	PSU	C4-N3-C2	-5.17	118.89	126.34
49	S2	816	PSU	C4-N3-C2	-5.16	118.90	126.34
3	L5	3490	PSU	C4-N3-C2	-5.16	118.90	126.34
3	L5	4749	PSU	C4-N3-C2	-5.16	118.91	126.34
3	L5	3973	OMU	C4-N3-C2	-5.16	119.78	126.58
3	L5	1720	PSU	C4-N3-C2	-5.16	118.91	126.34
49	S2	591	A2M	C5-C4-N3	-5.16	120.02	126.75
49	S2	1005	PSU	C4-N3-C2	-5.15	118.92	126.34
49	S2	1640	7MG	C2-N3-C4	5.15	121.48	112.30
3	L5	3466	PSU	C4-N3-C2	-5.15	118.92	126.34
49	S2	687	PSU	C4-N3-C2	-5.15	118.92	126.34
49	S2	967	PSU	C4-N3-C2	-5.15	118.92	126.34
49	S2	1368	PSU	C4-N3-C2	-5.15	118.92	126.34
3	L5	3583	PSU	C4-N3-C2	-5.15	118.92	126.34
49	S2	1327	OMU	C4-N3-C2	-5.15	119.79	126.58
49	S2	864	PSU	C4-N3-C2	-5.15	118.93	126.34
3	L5	4177	PSU	C4-N3-C2	-5.14	118.93	126.34
49	S2	1233	PSU	C4-N3-C2	-5.14	118.93	126.34
3	L5	3371	PSU	C4-N3-C2	-5.14	118.94	126.34
3	L5	1718	PSU	C4-N3-C2	-5.14	118.94	126.34
3	L5	3496	PSU	C4-N3-C2	-5.14	118.94	126.34
49	S2	36	PSU	C4-N3-C2	-5.14	118.94	126.34
3	L5	3462	PSU	C4-N3-C2	-5.14	118.94	126.34
49	S2	1446	PSU	C4-N3-C2	-5.13	118.95	126.34
3	L5	3502	PSU	C4-N3-C2	-5.13	118.95	126.34
49	S2	573	PSU	C4-N3-C2	-5.13	118.95	126.34
49	S2	1348	PSU	C4-N3-C2	-5.12	118.96	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2719	OMG	C5-C4-N3	-5.12	120.16	128.46
49	S2	429	OMU	C4-N3-C2	-5.11	119.83	126.58
3	L5	3447	PSU	C4-N3-C2	-5.11	118.97	126.34
49	S2	610	PSU	C4-N3-C2	-5.11	118.98	126.34
49	S2	1245	PSU	C4-N3-C2	-5.11	118.98	126.34
3	L5	3554	PSU	C4-N3-C2	-5.11	118.98	126.34
3	L5	4039	PSU	C4-N3-C2	-5.10	118.98	126.34
3	L5	4217	PSU	C4-N3-C2	-5.10	118.99	126.34
3	L5	4419	PSU	C4-N3-C2	-5.10	118.99	126.34
49	S2	1178	PSU	C4-N3-C2	-5.10	118.99	126.34
3	L5	1799	PSU	C4-N3-C2	-5.10	118.99	126.34
49	S2	1175	PSU	C4-N3-C2	-5.10	119.00	126.34
3	L5	4058	PSU	C4-N3-C2	-5.10	119.00	126.34
3	L5	4107	PSU	C4-N3-C2	-5.10	119.00	126.34
49	S2	1239	PSU	C4-N3-C2	-5.09	119.00	126.34
49	S2	93	PSU	C4-N3-C2	-5.09	119.00	126.34
3	L5	4169	PSU	C4-N3-C2	-5.08	119.02	126.34
49	S2	210	PSU	C4-N3-C2	-5.08	119.02	126.34
49	S2	105	PSU	C4-N3-C2	-5.07	119.03	126.34
3	L5	1683	PSU	C4-N3-C2	-5.06	119.05	126.34
49	S2	823	PSU	C4-N3-C2	-5.06	119.05	126.34
3	L5	3585	PSU	C4-N3-C2	-5.06	119.05	126.34
3	L5	4244	OMU	C4-N3-C2	-5.06	119.91	126.58
3	L5	3494	PSU	C4-N3-C2	-5.04	119.08	126.34
3	L5	2680	OMU	C4-N3-C2	-5.04	119.94	126.58
49	S2	802	PSU	C4-N3-C2	-5.03	119.09	126.34
49	S2	1626	PSU	C4-N3-C2	-5.03	119.09	126.34
3	L5	2719	OMG	C2-N3-C4	5.02	121.25	112.30
49	S2	172	OMU	C4-N3-C2	-5.02	119.96	126.58
49	S2	1805	OMU	C4-N3-C2	-4.99	120.00	126.58
3	L5	2258	OMU	C4-N3-C2	-4.99	120.00	126.58
3	L5	4052	OMU	C4-N3-C2	-4.98	120.01	126.58
49	S2	355	OMU	C4-N3-C2	-4.98	120.02	126.58
3	L5	4366	OMU	C4-N3-C2	-4.97	120.02	126.58
3	L5	1489	A2M	C5-C4-N3	-4.96	120.28	126.75
3	L5	398	A2M	C5-C4-N3	-4.92	120.34	126.75
49	S2	121	OMU	C4-N3-C2	-4.92	120.10	126.58
3	L5	3517	A2M	C5-C4-N3	-4.89	120.36	126.75
49	S2	1289	OMU	C4-N3-C2	-4.87	120.15	126.58
3	L5	2658	A2M	C5-C4-N3	-4.86	120.41	126.75
3	L5	1580	OMG	C2-N3-C4	4.84	120.93	112.30
3	L5	3966	6MZ	N3-C4-N9	4.83	135.04	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	99	A2M	C5-C4-N3	-4.83	120.45	126.75
49	S2	166	A2M	C5-C4-N3	-4.82	120.46	126.75
3	L5	2206	A2M	C5-C4-N3	-4.82	120.46	126.75
3	L5	4138	OMG	C2-N3-C4	4.82	120.89	112.30
49	S2	1443	OMU	C4-N3-C2	-4.82	120.23	126.58
3	L5	400	A2M	C5-C4-N3	-4.81	120.47	126.75
49	S2	669	A2M	N9-C8-N7	-4.81	107.33	113.91
3	L5	4382	PSU	C4-N3-C2	-4.80	119.42	126.34
49	S2	1384	A2M	C5-C4-N3	-4.79	120.50	126.75
3	L5	3557	A2M	C5-C4-N3	-4.79	120.50	126.75
3	L5	3456	A2M	C5-C4-N3	-4.79	120.50	126.75
3	L5	2267	OMG	C2-N3-C4	4.79	120.83	112.30
3	L5	4278	PSU	C4-N3-C2	-4.78	119.44	126.34
3	L5	2630	A2M	C5-C4-N3	-4.78	120.51	126.75
3	L5	3492	A2M	C5-C4-N3	-4.78	120.51	126.75
3	L5	4336	A2M	C5-C4-N3	-4.77	120.53	126.75
49	S2	437	OMG	C2-N3-C4	4.77	120.79	112.30
3	L5	1477	OMG	C2-N3-C4	4.77	120.79	112.30
3	L5	3576	PSU	C4-N3-C2	-4.76	119.47	126.34
3	L5	3450	A2M	C5-C4-N3	-4.76	120.54	126.75
3	L5	3676	OMG	C2-N3-C4	4.75	120.77	112.30
49	S2	602	OMG	C2-N3-C4	4.75	120.77	112.30
49	S2	1032	A2M	C5-C4-N3	-4.75	120.55	126.75
3	L5	4116	OMG	C2-N3-C4	4.75	120.76	112.30
3	L5	2244	A2M	C5-C4-N3	-4.75	120.56	126.75
3	L5	4364	OMG	C2-N3-C4	4.75	120.75	112.30
49	S2	1448	OMG	C2-N3-C4	4.74	120.75	112.30
49	S2	1852	MA6	N3-C4-N9	4.74	134.89	127.08
3	L5	3476	OMG	C2-N3-C4	4.73	120.74	112.30
3	L5	4383	OMG	C2-N3-C4	4.73	120.73	112.30
3	L5	3359	OMG	C2-N3-C4	4.73	120.73	112.30
3	L5	3942	OMG	C2-N3-C4	4.73	120.73	112.30
3	L5	4317	A2M	C5-C4-N3	-4.73	120.58	126.75
49	S2	116	OMU	C4-N3-C2	-4.73	120.34	126.58
3	L5	3524	OMG	C2-N3-C4	4.73	120.73	112.30
3	L5	1580	OMG	C5-C4-N3	-4.73	120.79	128.46
3	L5	1810	A2M	C5-C4-N3	-4.73	120.58	126.75
49	S2	1329	OMG	C2-N3-C4	4.72	120.72	112.30
3	L5	3657	OMU	N3-C2-N1	4.72	121.16	114.89
49	S2	868	OMG	C2-N3-C4	4.72	120.71	112.30
3	L5	3599	A2M	C5-C4-N3	-4.72	120.59	126.75
49	S2	645	OMG	C2-N3-C4	4.72	120.71	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1679	A2M	C5-C4-N3	-4.72	120.60	126.75
3	L5	1260	OMG	C2-N3-C4	4.72	120.70	112.30
3	L5	4138	OMG	C5-C4-N3	-4.71	120.82	128.46
3	L5	4369	OMG	C2-N3-C4	4.71	120.69	112.30
49	S2	469	A2M	C5-C4-N3	-4.71	120.61	126.75
3	L5	1479	A2M	C5-C4-N3	-4.71	120.61	126.75
3	L5	2207	OMG	C5-C4-N3	-4.70	120.83	128.46
3	L5	3942	OMG	C5-C4-N3	-4.70	120.83	128.46
49	S2	1448	OMG	C5-C4-N3	-4.70	120.83	128.46
49	S2	510	OMG	C2-N3-C4	4.70	120.67	112.30
3	L5	2207	OMG	C2-N3-C4	4.70	120.67	112.30
49	S2	1491	OMG	C2-N3-C4	4.69	120.66	112.30
3	L5	4240	OMG	C2-N3-C4	4.69	120.66	112.30
3	L5	4269	A2M	C5-C4-N3	-4.69	120.63	126.75
3	L5	3974	OMG	C2-N3-C4	4.69	120.65	112.30
3	L5	3631	OMG	C2-N3-C4	4.69	120.65	112.30
3	L5	1632	PSU	C4-N3-C2	-4.68	119.59	126.34
49	S2	27	A2M	C5-C4-N3	-4.68	120.64	126.75
5	L8	75	OMG	C2-N3-C4	4.68	120.64	112.30
3	L5	3524	OMG	C5-C4-N3	-4.68	120.87	128.46
49	S2	159	A2M	C5-C4-N3	-4.67	120.66	126.75
49	S2	513	A2M	C5-C4-N3	-4.67	120.66	126.75
3	L5	4245	OMG	C2-N3-C4	4.65	120.59	112.30
49	S2	684	OMG	C2-N3-C4	4.65	120.58	112.30
49	S2	485	A2M	C5-C4-N3	-4.64	120.70	126.75
3	L5	1477	OMG	C5-C4-N3	-4.64	120.94	128.46
3	L5	3476	OMG	C5-C4-N3	-4.64	120.94	128.46
49	S2	602	OMG	C5-C4-N3	-4.63	120.95	128.46
3	L5	3492	A2M	C5-C6-N6	-4.62	113.37	123.43
49	S2	1843	4AC	N4-C4-N3	4.62	121.61	113.85
49	S2	1491	OMG	C5-C4-N3	-4.61	120.98	128.46
3	L5	2267	OMG	C5-C4-N3	-4.61	120.98	128.46
3	L5	1270	A2M	C5-C4-N3	-4.61	120.73	126.75
3	L5	2680	OMU	N3-C2-N1	4.61	121.00	114.89
3	L5	4193	5MC	C5-C6-N1	-4.60	118.60	123.34
3	L5	4369	OMG	C5-C4-N3	-4.60	120.99	128.46
49	S2	577	A2M	C5-C4-N3	-4.60	120.75	126.75
3	L5	3562	A2M	C5-C4-N3	-4.59	120.76	126.75
3	L5	4240	OMG	C5-C4-N3	-4.59	121.01	128.46
49	S2	645	OMG	C5-C4-N3	-4.59	121.02	128.46
3	L5	1266	1MA	C5-C4-N3	-4.58	120.43	127.26
3	L5	3973	OMU	N3-C2-N1	4.58	120.96	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3359	OMG	C5-C4-N3	-4.57	121.04	128.46
3	L5	4116	OMG	C5-C4-N3	-4.57	121.05	128.46
49	S2	437	OMG	C5-C4-N3	-4.56	121.06	128.46
3	L5	1270	A2M	N9-C8-N7	-4.56	107.68	113.91
49	S2	469	A2M	N9-C8-N7	-4.55	107.69	113.91
49	S2	27	A2M	N9-C8-N7	-4.55	107.69	113.91
3	L5	3599	A2M	N9-C8-N7	-4.54	107.70	113.91
3	L5	4244	OMU	N3-C2-N1	4.54	120.91	114.89
3	L5	3974	OMG	C5-C4-N3	-4.54	121.10	128.46
3	L5	4364	OMG	C5-C4-N3	-4.52	121.12	128.46
49	S2	1851	MA6	N3-C4-N9	4.52	134.53	127.08
49	S2	513	A2M	N9-C8-N7	-4.52	107.73	113.91
3	L5	4336	A2M	N9-C8-N7	-4.52	107.73	113.91
3	L5	3676	OMG	C5-C4-N3	-4.51	121.14	128.46
3	L5	4269	A2M	N9-C8-N7	-4.51	107.74	113.91
49	S2	1329	OMG	C5-C4-N3	-4.51	121.14	128.46
3	L5	4435	PSU	N1-C2-N3	4.51	120.24	115.13
49	S2	1032	A2M	N9-C8-N7	-4.50	107.75	113.91
49	S2	868	OMG	C5-C4-N3	-4.50	121.16	128.46
3	L5	4366	OMU	N3-C2-N1	4.48	120.84	114.89
49	S2	510	OMG	C5-C4-N3	-4.48	121.19	128.46
3	L5	1260	OMG	C5-C4-N3	-4.48	121.19	128.46
49	S2	684	OMG	C5-C4-N3	-4.48	121.20	128.46
3	L5	2658	A2M	N9-C8-N7	-4.47	107.80	113.91
3	L5	2244	A2M	N9-C8-N7	-4.47	107.80	113.91
3	L5	1810	A2M	N9-C8-N7	-4.46	107.81	113.91
49	S2	355	OMU	N3-C2-N1	4.45	120.80	114.89
3	L5	4383	OMG	C5-C4-N3	-4.45	121.24	128.46
3	L5	3492	A2M	N9-C8-N7	-4.45	107.83	113.91
3	L5	3616	PSU	N1-C2-N3	4.45	120.17	115.13
3	L5	4374	PSU	N1-C2-N3	4.44	120.16	115.13
3	L5	2206	A2M	N9-C8-N7	-4.44	107.84	113.91
3	L5	3631	OMG	C5-C4-N3	-4.43	121.27	128.46
3	L5	3562	A2M	N9-C8-N7	-4.43	107.85	113.91
3	L5	2258	OMU	N3-C2-N1	4.43	120.77	114.89
3	L5	3456	A2M	N9-C8-N7	-4.43	107.86	113.91
3	L5	4052	OMU	N3-C2-N1	4.43	120.77	114.89
3	L5	4245	OMG	C5-C4-N3	-4.42	121.29	128.46
49	S2	166	A2M	N9-C8-N7	-4.42	107.87	113.91
3	L5	1489	A2M	N9-C8-N7	-4.42	107.87	113.91
3	L5	3652	PSU	N1-C2-N3	4.41	120.13	115.13
49	S2	99	A2M	N9-C8-N7	-4.41	107.88	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3557	A2M	N9-C8-N7	-4.40	107.90	113.91
49	S2	1805	OMU	N3-C2-N1	4.39	120.71	114.89
3	L5	4188	PSU	N1-C2-N3	4.38	120.09	115.13
3	L5	2630	A2M	N9-C8-N7	-4.38	107.92	113.91
49	S2	1851	MA6	C2-N1-C6	4.38	122.10	111.75
5	L8	75	OMG	C5-C4-N3	-4.37	121.37	128.46
3	L5	4177	PSU	N1-C2-N3	4.37	120.08	115.13
49	S2	121	OMU	N3-C2-N1	4.37	120.69	114.89
3	L5	4149	PSU	N1-C2-N3	4.37	120.08	115.13
49	S2	159	A2M	N9-C8-N7	-4.36	107.94	113.91
49	S2	1384	A2M	N9-C8-N7	-4.36	107.95	113.91
49	S2	1852	MA6	C2-N1-C6	4.36	122.05	111.75
3	L5	4317	A2M	N9-C8-N7	-4.35	107.96	113.91
49	S2	669	A2M	C5-C4-N3	-4.35	121.07	126.75
49	S2	1338	4AC	N4-C4-N3	4.35	121.15	113.85
49	S2	577	A2M	N9-C8-N7	-4.35	107.97	113.91
3	L5	3517	A2M	N9-C8-N7	-4.35	107.97	113.91
3	L5	400	A2M	N9-C8-N7	-4.35	107.97	113.91
49	S2	485	A2M	N9-C8-N7	-4.34	107.98	113.91
3	L5	4246	PSU	N1-C2-N3	4.34	120.04	115.13
3	L5	2475	PSU	N1-C2-N3	4.33	120.04	115.13
49	S2	652	PSU	N1-C2-N3	4.32	120.02	115.13
3	L5	4099	PSU	N1-C2-N3	4.31	120.02	115.13
49	S2	1046	PSU	N1-C2-N3	4.31	120.01	115.13
3	L5	1479	A2M	N9-C8-N7	-4.31	108.02	113.91
5	L8	69	PSU	N1-C2-N3	4.31	120.01	115.13
3	L5	4166	PSU	N1-C2-N3	4.30	120.00	115.13
3	L5	4298	PSU	N1-C2-N3	4.29	120.00	115.13
3	L5	3369	PSU	N1-C2-N3	4.29	120.00	115.13
3	L5	4325	PSU	N1-C2-N3	4.29	119.99	115.13
49	S2	105	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	1731	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	4267	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	3554	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	4042	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	4322	PSU	N1-C2-N3	4.29	119.99	115.13
3	L5	3490	PSU	N1-C2-N3	4.28	119.98	115.13
3	L5	1537	PSU	N1-C2-N3	4.28	119.98	115.13
3	L5	4203	PSU	N1-C2-N3	4.28	119.98	115.13
49	S2	116	OMU	N3-C2-N1	4.28	120.57	114.89
3	L5	1720	PSU	N1-C2-N3	4.28	119.97	115.13
3	L5	1638	PSU	N1-C2-N3	4.27	119.97	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4058	PSU	N1-C2-N3	4.27	119.97	115.13
49	S2	429	OMU	N3-C2-N1	4.27	120.56	114.89
49	S2	1693	PSU	N1-C2-N3	4.27	119.97	115.13
3	L5	4740	PSU	N1-C2-N3	4.27	119.97	115.13
49	S2	1047	PSU	N1-C2-N3	4.27	119.96	115.13
3	L5	3427	PSU	N1-C2-N3	4.27	119.96	115.13
49	S2	628	OMU	N3-C2-N1	4.26	120.55	114.89
3	L5	1491	PSU	N1-C2-N3	4.26	119.96	115.13
49	S2	218	PSU	N1-C2-N3	4.26	119.95	115.13
3	L5	3496	PSU	N1-C2-N3	4.26	119.95	115.13
3	L5	4039	PSU	N1-C2-N3	4.26	119.95	115.13
49	S2	682	PSU	N1-C2-N3	4.26	119.95	115.13
49	S2	1368	PSU	N1-C2-N3	4.26	119.95	115.13
3	L5	1801	PSU	N1-C2-N3	4.25	119.95	115.13
3	L5	3502	PSU	N1-C2-N3	4.25	119.95	115.13
49	S2	1082	PSU	N1-C2-N3	4.25	119.95	115.13
3	L5	3583	PSU	N1-C2-N3	4.25	119.95	115.13
3	L5	4169	PSU	N1-C2-N3	4.25	119.95	115.13
49	S2	1057	PSU	N1-C2-N3	4.25	119.94	115.13
49	S2	815	PSU	N1-C2-N3	4.25	119.94	115.13
49	S2	34	PSU	N1-C2-N3	4.24	119.94	115.13
49	S2	823	PSU	N1-C2-N3	4.24	119.93	115.13
49	S2	650	PSU	N1-C2-N3	4.23	119.92	115.13
49	S2	687	PSU	N1-C2-N3	4.23	119.92	115.13
49	S2	610	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	4045	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	3371	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	4419	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	1721	PSU	N1-C2-N3	4.23	119.92	115.13
3	L5	3500	PSU	N1-C2-N3	4.23	119.92	115.13
49	S2	109	PSU	N1-C2-N3	4.22	119.92	115.13
3	L5	398	A2M	N9-C8-N7	-4.22	108.14	113.91
3	L5	4711	PSU	N1-C2-N3	4.22	119.92	115.13
49	S2	1233	PSU	N1-C2-N3	4.22	119.91	115.13
3	L5	3494	PSU	N1-C2-N3	4.22	119.91	115.13
49	S2	1289	OMU	N3-C2-N1	4.22	120.49	114.89
3	L5	2351	PSU	N1-C2-N3	4.22	119.91	115.13
3	L5	3585	PSU	N1-C2-N3	4.22	119.91	115.13
49	S2	1005	PSU	N1-C2-N3	4.21	119.90	115.13
49	S2	816	PSU	N1-C2-N3	4.21	119.90	115.13
49	S2	1175	PSU	N1-C2-N3	4.21	119.90	115.13
49	S2	407	PSU	N1-C2-N3	4.21	119.90	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L8	55	PSU	N1-C2-N3	4.21	119.90	115.13
3	L5	1718	PSU	N1-C2-N3	4.21	119.90	115.13
3	L5	1799	PSU	N1-C2-N3	4.21	119.90	115.13
49	S2	802	PSU	N1-C2-N3	4.21	119.89	115.13
49	S2	1644	PSU	N1-C2-N3	4.21	119.89	115.13
49	S2	36	PSU	N1-C2-N3	4.20	119.89	115.13
49	S2	1679	A2M	N9-C8-N7	-4.20	108.17	113.91
49	S2	967	PSU	N1-C2-N3	4.20	119.89	115.13
49	S2	573	PSU	N1-C2-N3	4.19	119.88	115.13
3	L5	3466	PSU	N1-C2-N3	4.19	119.88	115.13
3	L5	4749	PSU	N1-C2-N3	4.19	119.88	115.13
49	S2	864	PSU	N1-C2-N3	4.18	119.87	115.13
3	L5	3447	PSU	N1-C2-N3	4.18	119.87	115.13
49	S2	1852	MA6	C9-N6-C6	-4.18	109.57	120.40
49	S2	172	OMU	N3-C2-N1	4.18	120.43	114.89
3	L5	3450	A2M	N9-C8-N7	-4.17	108.21	113.91
49	S2	1178	PSU	N1-C2-N3	4.17	119.86	115.13
49	S2	119	PSU	N1-C2-N3	4.17	119.85	115.13
49	S2	867	PSU	N1-C2-N3	4.17	119.85	115.13
3	L5	3462	PSU	N1-C2-N3	4.16	119.85	115.13
3	L5	1683	PSU	N1-C2-N3	4.16	119.85	115.13
3	L5	4217	PSU	N1-C2-N3	4.16	119.85	115.13
49	S2	1239	PSU	N1-C2-N3	4.16	119.84	115.13
49	S2	1851	MA6	C9-N6-C6	-4.16	109.62	120.40
3	L5	4107	PSU	N1-C2-N3	4.15	119.84	115.13
49	S2	1348	PSU	N1-C2-N3	4.15	119.83	115.13
49	S2	1443	OMU	N3-C2-N1	4.15	120.40	114.89
49	S2	93	PSU	N1-C2-N3	4.15	119.83	115.13
49	S2	1446	PSU	N1-C2-N3	4.15	119.83	115.13
49	S2	1327	OMU	N3-C2-N1	4.13	120.38	114.89
49	S2	210	PSU	N1-C2-N3	4.11	119.79	115.13
49	S2	1626	PSU	N1-C2-N3	4.11	119.79	115.13
49	S2	1245	PSU	N1-C2-N3	4.11	119.78	115.13
49	S2	591	A2M	N9-C8-N7	-4.09	108.31	113.91
3	L5	4382	PSU	N1-C2-N3	4.09	119.76	115.13
3	L5	1632	PSU	N1-C2-N3	4.01	119.67	115.13
3	L5	1266	1MA	C2-N3-C4	4.01	120.29	112.41
4	L7	1	GTP	N9-C4-N3	4.01	133.98	125.94
3	L5	3576	PSU	N1-C2-N3	3.98	119.64	115.13
4	L7	1	GTP	C5-C4-N3	-3.95	122.05	128.46
3	L5	3966	6MZ	C9-N6-C6	-3.95	119.47	122.87
3	L5	2719	OMG	C2-N1-C6	-3.94	117.92	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4138	OMG	C2-N1-C6	-3.87	118.04	125.10
3	L5	3966	6MZ	C2-N3-C4	3.87	120.90	111.75
3	L5	3476	OMG	C2-N1-C6	-3.87	118.04	125.10
3	L5	1580	OMG	C2-N1-C6	-3.86	118.06	125.10
49	S2	1833	6MZ	C2-N3-C4	3.86	120.86	111.75
49	S2	1851	MA6	C2-N3-C4	3.86	120.86	111.75
3	L5	3942	OMG	C2-N1-C6	-3.85	118.08	125.10
49	S2	645	OMG	C2-N1-C6	-3.84	118.10	125.10
3	L5	4369	OMG	C2-N1-C6	-3.83	118.11	125.10
49	S2	1491	OMG	C2-N1-C6	-3.83	118.12	125.10
49	S2	1448	OMG	C2-N1-C6	-3.83	118.12	125.10
76	Se	67	NMM	NE-CZ-NH1	3.83	127.43	120.26
3	L5	3524	OMG	C2-N1-C6	-3.83	118.12	125.10
49	S2	602	OMG	C2-N1-C6	-3.83	118.12	125.10
3	L5	2267	OMG	C2-N1-C6	-3.83	118.12	125.10
49	S2	437	OMG	C2-N1-C6	-3.82	118.13	125.10
3	L5	3359	OMG	C2-N1-C6	-3.82	118.14	125.10
49	S2	1329	OMG	C2-N1-C6	-3.82	118.14	125.10
3	L5	1477	OMG	C2-N1-C6	-3.82	118.14	125.10
49	S2	1640	7MG	C5-C4-N3	-3.81	120.86	128.13
3	L5	4364	OMG	C2-N1-C6	-3.81	118.15	125.10
3	L5	4116	OMG	C2-N1-C6	-3.80	118.16	125.10
5	L8	75	OMG	C2-N1-C6	-3.80	118.17	125.10
3	L5	4383	OMG	C2-N1-C6	-3.79	118.18	125.10
49	S2	510	OMG	C2-N1-C6	-3.79	118.19	125.10
3	L5	1260	OMG	C2-N1-C6	-3.79	118.19	125.10
49	S2	868	OMG	C2-N1-C6	-3.79	118.20	125.10
3	L5	4240	OMG	C2-N1-C6	-3.78	118.21	125.10
49	S2	1852	MA6	C2-N3-C4	3.78	120.68	111.75
3	L5	3631	OMG	C2-N1-C6	-3.77	118.22	125.10
3	L5	4245	OMG	C2-N1-C6	-3.75	118.26	125.10
3	L5	3676	OMG	C2-N1-C6	-3.74	118.28	125.10
3	L5	3974	OMG	C2-N1-C6	-3.73	118.29	125.10
49	S2	684	OMG	C2-N1-C6	-3.72	118.31	125.10
49	S2	1640	7MG	C2-N1-C6	-3.70	118.36	125.10
3	L5	4276	UR3	C4-N3-C2	-3.67	121.11	124.56
49	S2	1851	MA6	C10-N6-C6	-3.63	111.00	120.40
4	L7	1	GTP	PA-O3A-PB	-3.61	120.42	132.83
4	L7	1	GTP	PB-O3B-PG	-3.60	120.47	132.83
3	L5	2207	OMG	C2-N1-C6	-3.59	118.54	125.10
49	S2	1851	MA6	C4-C5-N7	-3.59	106.25	110.62
3	L5	3492	A2M	C5-N7-C8	3.57	108.58	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3492	A2M	N6-C6-N1	3.57	126.17	118.35
3	L5	1489	A2M	C2-N3-C4	3.53	120.09	111.75
49	S2	591	A2M	C2-N3-C4	3.52	120.07	111.75
3	L5	1479	A2M	O4'-C4'-C3'	-3.52	98.15	105.11
3	L5	2630	A2M	C2-N3-C4	3.49	120.00	111.75
3	L5	3492	A2M	C6-C5-C4	3.47	121.85	117.18
3	L5	4269	A2M	C2-N3-C4	3.47	119.95	111.75
3	L5	4278	PSU	N1-C2-N3	3.46	119.05	115.13
49	S2	669	A2M	O4'-C4'-C3'	-3.45	98.30	105.11
3	L5	3557	A2M	C2-N3-C4	3.44	119.87	111.75
49	S2	99	A2M	C2-N3-C4	3.44	119.87	111.75
49	S2	1852	MA6	N1-C6-N6	3.43	120.84	117.08
49	S2	669	A2M	C5-N7-C8	3.43	108.39	103.51
3	L5	398	A2M	C2-N3-C4	3.43	119.86	111.75
3	L5	3517	A2M	C5-C6-N6	-3.43	115.97	123.43
49	S2	27	A2M	C2-N3-C4	3.42	119.83	111.75
49	S2	1852	MA6	C4-C5-N7	-3.42	106.46	110.62
3	L5	400	A2M	C2-N3-C4	3.42	119.82	111.75
3	L5	1270	A2M	C2-N3-C4	3.41	119.81	111.75
49	S2	166	A2M	C2-N3-C4	3.41	119.81	111.75
3	L5	3456	A2M	C2-N3-C4	3.41	119.80	111.75
3	L5	4336	A2M	C2-N3-C4	3.40	119.79	111.75
49	S2	1032	A2M	C2-N3-C4	3.40	119.78	111.75
3	L5	3599	A2M	C2-N3-C4	3.40	119.78	111.75
3	L5	2206	A2M	C5-N7-C8	3.39	108.33	103.51
49	S2	1679	A2M	C2-N3-C4	3.39	119.76	111.75
3	L5	4317	A2M	C2-N3-C4	3.39	119.76	111.75
49	S2	485	A2M	C2-N3-C4	3.39	119.76	111.75
49	S2	1852	MA6	C10-N6-C6	-3.39	111.61	120.40
3	L5	2206	A2M	C2-N3-C4	3.39	119.76	111.75
3	L5	3517	A2M	O4'-C1'-C2'	-3.39	100.62	106.57
3	L5	2244	A2M	C2-N3-C4	3.39	119.76	111.75
49	S2	469	A2M	C2-N3-C4	3.38	119.75	111.75
49	S2	513	A2M	C2-N3-C4	3.38	119.74	111.75
3	L5	2658	A2M	C2-N3-C4	3.38	119.74	111.75
3	L5	3450	A2M	C2-N3-C4	3.38	119.73	111.75
49	S2	1384	A2M	C2-N3-C4	3.38	119.72	111.75
3	L5	4336	A2M	C5-N7-C8	3.37	108.30	103.51
3	L5	1479	A2M	C2-N3-C4	3.37	119.72	111.75
49	S2	1679	A2M	C5-C6-N6	-3.37	116.09	123.43
3	L5	1810	A2M	C2-N3-C4	3.37	119.72	111.75
3	L5	3562	A2M	C2-N3-C4	3.37	119.72	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	159	A2M	C2-N3-C4	3.37	119.71	111.75
3	L5	4269	A2M	C5-N7-C8	3.37	108.30	103.51
49	S2	469	A2M	C5-N7-C8	3.36	108.29	103.51
3	L5	2658	A2M	C5-N7-C8	3.36	108.29	103.51
49	S2	669	A2M	C2-N3-C4	3.36	119.69	111.75
3	L5	3599	A2M	C5-C6-N6	-3.36	116.12	123.43
3	L5	1270	A2M	C5-N7-C8	3.36	108.28	103.51
3	L5	1489	A2M	C5-N7-C8	3.36	108.28	103.51
3	L5	2244	A2M	C5-N7-C8	3.35	108.28	103.51
3	L5	3966	6MZ	C6-C5-N7	3.35	136.02	132.39
3	L5	3562	A2M	C5-C6-N6	-3.35	116.13	123.43
3	L5	3599	A2M	C5-N7-C8	3.35	108.27	103.51
49	S2	513	A2M	C5-N7-C8	3.35	108.27	103.51
49	S2	27	A2M	C5-N7-C8	3.35	108.26	103.51
49	S2	99	A2M	C5-N7-C8	3.34	108.26	103.51
49	S2	1032	A2M	C5-N7-C8	3.34	108.26	103.51
3	L5	2630	A2M	C5-N7-C8	3.34	108.25	103.51
49	S2	591	A2M	C5-C6-N6	-3.34	116.16	123.43
3	L5	3456	A2M	C5-C6-N6	-3.34	116.17	123.43
3	L5	3517	A2M	C2-N3-C4	3.33	119.62	111.75
3	L5	400	A2M	C5-N7-C8	3.33	108.24	103.51
3	L5	1270	A2M	C2'-C3'-C4'	-3.33	94.77	101.99
49	S2	577	A2M	C2-N3-C4	3.33	119.61	111.75
3	L5	1810	A2M	C5-N7-C8	3.32	108.23	103.51
49	S2	577	A2M	C5-C6-N6	-3.32	116.21	123.43
49	S2	27	A2M	C5-C6-N6	-3.32	116.21	123.43
49	S2	166	A2M	C5-N7-C8	3.32	108.22	103.51
49	S2	166	A2M	C5-C6-N6	-3.31	116.22	123.43
3	L5	2244	A2M	C5-C6-N6	-3.31	116.22	123.43
49	S2	469	A2M	C2'-C3'-C4'	-3.31	94.80	101.99
3	L5	1489	A2M	C5-C6-N6	-3.31	116.22	123.43
3	L5	398	A2M	C5-C6-N6	-3.31	116.22	123.43
3	L5	3557	A2M	C5-N7-C8	3.30	108.20	103.51
49	S2	485	A2M	C5-C6-N6	-3.30	116.24	123.43
49	S2	469	A2M	C5-C6-N6	-3.30	116.25	123.43
49	S2	1032	A2M	C5-C6-N6	-3.30	116.25	123.43
49	S2	1384	A2M	C5-C6-N6	-3.30	116.25	123.43
3	L5	1810	A2M	C5-C6-N6	-3.30	116.25	123.43
3	L5	4336	A2M	C5-C6-N6	-3.30	116.25	123.43
3	L5	2719	OMG	C1'-N9-C8	-3.29	117.32	126.70
3	L5	4317	A2M	C5-C6-N6	-3.29	116.27	123.43
49	S2	159	A2M	C5-N7-C8	3.29	108.19	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1384	A2M	C5-N7-C8	3.29	108.18	103.51
3	L5	2658	A2M	C5-C6-N6	-3.29	116.28	123.43
49	S2	513	A2M	C5-C6-N6	-3.28	116.28	123.43
49	S2	99	A2M	C5-C6-N6	-3.28	116.28	123.43
3	L5	2630	A2M	C5-C6-N6	-3.28	116.29	123.43
3	L5	400	A2M	C5-C6-N6	-3.27	116.31	123.43
3	L5	1479	A2M	C5-C6-N6	-3.27	116.31	123.43
3	L5	3557	A2M	C5-C6-N6	-3.27	116.31	123.43
49	S2	99	A2M	C2'-C3'-C4'	-3.27	94.89	101.99
49	S2	669	A2M	C5-C6-N6	-3.27	116.32	123.43
3	L5	4269	A2M	C5-C6-N6	-3.26	116.33	123.43
3	L5	398	A2M	C5-N7-C8	3.26	108.14	103.51
3	L5	3456	A2M	C5-N7-C8	3.26	108.14	103.51
3	L5	1270	A2M	C5-C6-N6	-3.26	116.34	123.43
3	L5	3450	A2M	C5-C6-N6	-3.26	116.34	123.43
3	L5	4317	A2M	C5-N7-C8	3.25	108.13	103.51
3	L5	2206	A2M	C5-C6-N6	-3.25	116.35	123.43
49	S2	159	A2M	C5-C6-N6	-3.25	116.35	123.43
3	L5	2647	OMC	CM2-O2'-C2'	-3.25	106.00	114.52
49	S2	513	A2M	C2'-C3'-C4'	-3.25	94.94	101.99
3	L5	3562	A2M	C5-N7-C8	3.25	108.12	103.51
49	S2	1327	OMU	C5-C4-N3	3.24	119.69	114.84
49	S2	485	A2M	C5-N7-C8	3.23	108.10	103.51
3	L5	1810	A2M	C2'-C3'-C4'	-3.23	94.98	101.99
3	L5	4052	OMU	C5-C4-N3	3.22	119.66	114.84
49	S2	1851	MA6	N1-C2-N3	-3.22	123.57	128.60
3	L5	3450	A2M	C5-N7-C8	3.21	108.08	103.51
3	L5	3599	A2M	C2'-C3'-C4'	-3.21	95.03	101.99
49	S2	628	OMU	C5-C4-N3	3.21	119.64	114.84
3	L5	3492	A2M	O4'-C4'-C3'	-3.20	98.78	105.11
3	L5	3966	6MZ	C4-C5-N7	-3.19	106.73	110.62
49	S2	1640	7MG	C5-C4-N9	3.19	110.49	106.35
3	L5	2244	A2M	C2'-C3'-C4'	-3.19	95.06	101.99
49	S2	577	A2M	C5-N7-C8	3.19	108.04	103.51
3	L5	4193	5MC	C5-C4-N4	-3.19	116.71	121.48
49	S2	591	A2M	C1'-N9-C8	-3.18	119.94	127.14
3	L5	3492	A2M	C2-N3-C4	3.18	119.27	111.75
49	S2	429	OMU	C5-C4-N3	3.18	119.60	114.84
3	L5	1479	A2M	C5-N7-C8	3.18	108.03	103.51
3	L5	3966	6MZ	N1-C2-N3	-3.18	123.62	128.60
3	L5	3517	A2M	C5-N7-C8	3.18	108.02	103.51
49	S2	1679	A2M	C2'-C3'-C4'	-3.18	95.09	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3514	5MC	C5-C4-N4	-3.18	116.73	121.48
49	S2	591	A2M	C5-N7-C8	3.17	108.01	103.51
3	L5	3973	OMU	C5-C4-N3	3.16	119.57	114.84
49	S2	591	A2M	O4'-C4'-C3'	-3.16	98.86	105.11
3	L5	3517	A2M	C3'-C2'-C1'	-3.15	96.96	102.89
3	L5	3657	OMU	C5-C4-N3	3.15	119.56	114.84
3	L5	4269	A2M	C2'-C3'-C4'	-3.15	95.15	101.99
49	S2	669	A2M	O4'-C1'-N9	-3.15	101.85	108.06
3	L5	4244	OMU	C5-C4-N3	3.14	119.53	114.84
3	L5	2258	OMU	C5-C4-N3	3.13	119.52	114.84
49	S2	1443	OMU	C5-C4-N3	3.13	119.52	114.84
49	S2	591	A2M	N3-C4-N9	3.12	132.23	127.08
49	S2	172	OMU	C5-C4-N3	3.12	119.50	114.84
49	S2	1679	A2M	C5-N7-C8	3.12	107.94	103.51
49	S2	437	OMG	N9-C8-N7	-3.11	107.54	113.39
3	L5	4245	OMG	N9-C8-N7	-3.11	107.54	113.39
49	S2	1384	A2M	C2'-C3'-C4'	-3.10	95.26	101.99
3	L5	3514	5MC	C5-C6-N1	-3.10	120.15	123.34
3	L5	3676	OMG	N9-C8-N7	-3.10	107.56	113.39
3	L5	2719	OMG	N9-C4-N3	3.10	132.15	125.94
49	S2	1852	MA6	N1-C2-N3	-3.09	123.77	128.60
49	S2	355	OMU	C5-C4-N3	3.09	119.46	114.84
49	S2	1805	OMU	C5-C4-N3	3.09	119.46	114.84
3	L5	4383	OMG	N9-C8-N7	-3.09	107.58	113.39
49	S2	1329	OMG	N9-C8-N7	-3.07	107.60	113.39
3	L5	2680	OMU	C5-C4-N3	3.06	119.42	114.84
49	S2	1851	MA6	N1-C6-N6	3.06	120.43	117.08
49	S2	510	OMG	N9-C8-N7	-3.05	107.64	113.39
49	S2	121	OMU	C5-C4-N3	3.05	119.41	114.84
49	S2	1032	A2M	C2'-C3'-C4'	-3.05	95.37	101.99
3	L5	1260	OMG	N9-C8-N7	-3.04	107.67	113.39
3	L5	3359	OMG	N9-C8-N7	-3.04	107.67	113.39
3	L5	4366	OMU	C5-C4-N3	3.03	119.38	114.84
49	S2	669	A2M	C4'-O4'-C1'	-3.03	102.78	109.47
49	S2	116	OMU	C5-C4-N3	3.03	119.38	114.84
3	L5	4138	OMG	N9-C8-N7	-3.02	107.71	113.39
49	S2	645	OMG	N9-C8-N7	-3.02	107.71	113.39
3	L5	1477	OMG	N9-C8-N7	-3.01	107.73	113.39
49	S2	1289	OMU	C5-C4-N3	3.00	119.32	114.84
3	L5	3974	OMG	N9-C8-N7	-3.00	107.75	113.39
3	L5	3557	A2M	C2'-C3'-C4'	-2.99	95.49	101.99
3	L5	3517	A2M	N3-C4-N9	2.99	132.02	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4364	OMG	N9-C8-N7	-2.99	107.75	113.39
3	L5	2658	A2M	C2'-C3'-C4'	-2.99	95.49	101.99
3	L5	3631	OMG	N9-C8-N7	-2.99	107.76	113.39
49	S2	166	A2M	C2'-C3'-C4'	-2.99	95.51	101.99
3	L5	4116	OMG	N9-C8-N7	-2.98	107.77	113.39
3	L5	4336	A2M	C2'-C3'-C4'	-2.98	95.51	101.99
49	S2	1833	6MZ	N1-C2-N3	-2.98	123.94	128.60
3	L5	3476	OMG	N9-C8-N7	-2.98	107.78	113.39
49	S2	577	A2M	C2'-C3'-C4'	-2.97	95.54	101.99
49	S2	591	A2M	C6-C5-C4	2.97	121.17	117.18
3	L5	3562	A2M	C2'-C3'-C4'	-2.94	95.60	101.99
5	L8	75	OMG	N9-C8-N7	-2.94	107.85	113.39
49	S2	602	OMG	N9-C8-N7	-2.94	107.86	113.39
49	S2	868	OMG	N9-C8-N7	-2.94	107.86	113.39
3	L5	3517	A2M	C6-C5-C4	2.94	121.13	117.18
3	L5	3492	A2M	C2'-C3'-C4'	-2.93	95.62	101.99
49	S2	684	OMG	N9-C8-N7	-2.93	107.87	113.39
3	L5	4188	PSU	C6-C5-C4	2.93	120.25	118.20
3	L5	4369	OMG	N9-C8-N7	-2.93	107.88	113.39
3	L5	2267	OMG	N9-C8-N7	-2.92	107.89	113.39
3	L5	3524	OMG	N9-C8-N7	-2.91	107.91	113.39
49	S2	1851	MA6	C5-N7-C8	2.91	107.64	103.51
3	L5	4240	OMG	N9-C8-N7	-2.90	107.92	113.39
49	S2	591	A2M	C2'-C3'-C4'	-2.90	95.69	101.99
49	S2	669	A2M	C4-N9-C1'	-2.89	119.70	126.59
3	L5	4149	PSU	C6-C5-C4	2.89	120.22	118.20
3	L5	2658	A2M	N3-C4-N9	2.89	131.84	127.08
49	S2	1327	OMU	O4-C4-C5	-2.88	120.09	125.16
3	L5	1580	OMG	N9-C8-N7	-2.88	107.96	113.39
3	L5	3942	OMG	N9-C8-N7	-2.88	107.97	113.39
49	S2	159	A2M	C2'-C3'-C4'	-2.87	95.76	101.99
49	S2	1491	OMG	N9-C8-N7	-2.87	107.99	113.39
3	L5	2206	A2M	C2'-C3'-C4'	-2.86	95.78	101.99
3	L5	2719	OMG	C1'-N9-C4	2.86	134.99	126.50
49	S2	1833	6MZ	C4-C5-N7	-2.85	107.14	110.62
3	L5	2207	OMG	N9-C4-N3	2.85	131.66	125.94
49	S2	172	OMU	O4-C4-C5	-2.85	120.15	125.16
3	L5	2658	A2M	C6-C5-C4	2.85	121.01	117.18
3	L5	3456	A2M	C2'-C3'-C4'	-2.85	95.81	101.99
3	L5	398	A2M	C6-C5-C4	2.84	121.01	117.18
49	S2	429	OMU	O4-C4-C5	-2.82	120.20	125.16
49	S2	485	A2M	CM'-O2'-C2'	-2.82	107.12	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2207	OMG	N9-C8-N7	-2.82	108.08	113.39
3	L5	4366	OMU	O4-C4-C5	-2.82	120.21	125.16
49	S2	1443	OMU	O4-C4-C5	-2.81	120.21	125.16
3	L5	1489	A2M	N3-C4-N9	2.81	131.72	127.08
49	S2	628	OMU	O4-C4-C5	-2.81	120.21	125.16
49	S2	27	A2M	CM'-O2'-C2'	-2.81	107.15	114.52
49	S2	1852	MA6	C5-N7-C8	2.81	107.50	103.51
49	S2	1384	A2M	C6-C5-C4	2.81	120.96	117.18
3	L5	4244	OMU	O4-C4-C5	-2.81	120.22	125.16
49	S2	1448	OMG	N9-C8-N7	-2.80	108.11	113.39
3	L5	2206	A2M	C6-C5-C4	2.80	120.95	117.18
3	L5	1266	1MA	N9-C8-N7	-2.80	108.11	113.39
3	L5	398	A2M	C2'-C3'-C4'	-2.80	95.91	101.99
49	S2	116	OMU	O4-C4-C5	-2.80	120.23	125.16
3	L5	1489	A2M	C6-C5-C4	2.80	120.95	117.18
3	L5	400	A2M	C6-C5-C4	2.80	120.94	117.18
3	L5	3450	A2M	C6-C5-C4	2.80	120.94	117.18
49	S2	166	A2M	N3-C4-N9	2.79	131.69	127.08
3	L5	2630	A2M	C2'-C3'-C4'	-2.79	95.93	101.99
3	L5	3456	A2M	C6-C5-C4	2.77	120.91	117.18
49	S2	1289	OMU	O4-C4-C5	-2.77	120.29	125.16
3	L5	3456	A2M	N3-C4-N9	2.77	131.65	127.08
3	L5	2258	OMU	O4-C4-C5	-2.77	120.29	125.16
49	S2	1384	A2M	C3'-C2'-C1'	-2.77	97.69	102.89
3	L5	3492	A2M	C4'-O4'-C1'	-2.77	103.37	109.47
3	L5	2244	A2M	C6-C5-C4	2.76	120.90	117.18
49	S2	166	A2M	C6-C5-C4	2.76	120.90	117.18
49	S2	1032	A2M	C6-C5-C4	2.76	120.90	117.18
49	S2	1448	OMG	N9-C4-N3	2.76	131.49	125.94
3	L5	4317	A2M	C6-C5-C4	2.76	120.90	117.18
3	L5	3557	A2M	C6-C5-C4	2.76	120.89	117.18
3	L5	1810	A2M	C6-C5-C4	2.75	120.89	117.18
49	S2	355	OMU	O4-C4-C5	-2.75	120.32	125.16
49	S2	99	A2M	C6-C5-C4	2.75	120.89	117.18
3	L5	3599	A2M	N3-C4-N9	2.75	131.61	127.08
3	L5	1479	A2M	C6-C5-C4	2.75	120.88	117.18
3	L5	4052	OMU	O4-C4-C5	-2.75	120.33	125.16
49	S2	1805	OMU	O4-C4-C5	-2.74	120.34	125.16
3	L5	3973	OMU	O4-C4-C5	-2.74	120.34	125.16
49	S2	1679	A2M	N3-C4-N9	2.74	131.60	127.08
49	S2	121	OMU	O4-C4-C5	-2.74	120.34	125.16
3	L5	4336	A2M	N3-C4-N9	2.74	131.59	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	27	A2M	C2'-C3'-C4'	-2.73	96.07	101.99
3	L5	398	A2M	N3-C4-N9	2.73	131.58	127.08
49	S2	1679	A2M	C6-C5-C4	2.72	120.84	117.18
3	L5	3524	OMG	N9-C4-N3	2.72	131.40	125.94
49	S2	469	A2M	C6-C5-C4	2.72	120.84	117.18
3	L5	4336	A2M	C6-C5-C4	2.72	120.84	117.18
49	S2	469	A2M	N3-C4-N9	2.72	131.56	127.08
3	L5	2680	OMU	O4-C4-C5	-2.72	120.39	125.16
3	L5	4382	PSU	O2-C2-N1	-2.71	119.81	122.79
3	L5	1479	A2M	CM'-O2'-C2'	-2.70	107.43	114.52
3	L5	3492	A2M	C4-C5-N7	-2.70	107.33	110.62
3	L5	400	A2M	N3-C4-N9	2.70	131.53	127.08
3	L5	2244	A2M	N3-C4-N9	2.70	131.53	127.08
49	S2	577	A2M	C6-C5-C4	2.70	120.81	117.18
3	L5	1580	OMG	N9-C4-N3	2.70	131.35	125.94
3	L5	3942	OMG	N9-C4-N3	2.70	131.35	125.94
3	L5	1479	A2M	C4'-O4'-C1'	-2.69	103.53	109.47
49	S2	513	A2M	C6-C5-C4	2.69	120.80	117.18
49	S2	1384	A2M	N3-C4-N9	2.69	131.51	127.08
49	S2	602	OMG	N9-C4-N3	2.69	131.34	125.94
3	L5	2206	A2M	N3-C4-N9	2.69	131.51	127.08
49	S2	1032	A2M	N3-C4-N9	2.68	131.51	127.08
3	L5	1270	A2M	C6-C5-C4	2.68	120.78	117.18
49	S2	159	A2M	C6-C5-C4	2.68	120.78	117.18
3	L5	1479	A2M	N3-C4-N9	2.67	131.48	127.08
3	L5	4269	A2M	C6-C5-C4	2.67	120.77	117.18
3	L5	1810	A2M	N3-C4-N9	2.67	131.48	127.08
3	L5	3599	A2M	O4'-C4'-C3'	-2.67	99.84	105.11
3	L5	4317	A2M	N3-C4-N9	2.66	131.47	127.08
49	S2	591	A2M	C4'-O4'-C1'	-2.66	103.59	109.47
3	L5	2630	A2M	C6-C5-C4	2.66	120.76	117.18
3	L5	3599	A2M	C6-C5-C4	2.66	120.76	117.18
3	L5	4317	A2M	C2'-C3'-C4'	-2.66	96.22	101.99
49	S2	823	PSU	O2-C2-N1	-2.66	119.86	122.79
49	S2	27	A2M	C6-C5-C4	2.66	120.76	117.18
3	L5	3562	A2M	C6-C5-C4	2.66	120.75	117.18
49	S2	99	A2M	N3-C4-N9	2.66	131.46	127.08
3	L5	3966	6MZ	C5-N7-C8	2.66	107.28	103.51
49	S2	669	A2M	C4-N9-C8	2.65	108.60	105.73
3	L5	3557	A2M	N3-C4-N9	2.65	131.45	127.08
49	S2	1640	7MG	C4-C5-N7	2.65	109.21	105.53
49	S2	513	A2M	N3-C4-N9	2.65	131.45	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1032	A2M	CM'-O2'-C2'	-2.65	107.58	114.52
3	L5	4138	OMG	C5-C6-N1	2.65	119.91	113.19
49	S2	485	A2M	C6-C5-C4	2.65	120.74	117.18
49	S2	27	A2M	N3-C4-N9	2.64	131.44	127.08
3	L5	3450	A2M	C2'-C3'-C4'	-2.64	96.25	101.99
3	L5	3562	A2M	N3-C4-N9	2.63	131.42	127.08
3	L5	2267	OMG	C5-C6-N1	2.63	119.87	113.19
3	L5	2719	OMG	C5-C6-N1	2.63	119.87	113.19
3	L5	3942	OMG	C5-C6-N1	2.63	119.86	113.19
3	L5	3657	OMU	O4-C4-C5	-2.62	120.54	125.16
5	L8	69	PSU	C6-C5-C4	2.62	120.03	118.20
49	S2	645	OMG	N9-C4-N3	2.62	131.20	125.94
3	L5	4240	OMG	N9-C4-N3	2.62	131.19	125.94
3	L5	1270	A2M	N3-C4-N9	2.62	131.39	127.08
49	S2	577	A2M	N3-C4-N9	2.61	131.39	127.08
49	S2	437	OMG	N9-C4-N3	2.61	131.19	125.94
49	S2	1329	OMG	C5-C6-N1	2.61	119.82	113.19
49	S2	510	OMG	C5-C6-N1	2.61	119.81	113.19
49	S2	437	OMG	C5-C6-N1	2.61	119.81	113.19
3	L5	1477	OMG	C5-C6-N1	2.60	119.80	113.19
49	S2	645	OMG	C5-C6-N1	2.60	119.80	113.19
3	L5	3524	OMG	C5-C6-N1	2.60	119.79	113.19
3	L5	3496	PSU	O2-C2-N1	-2.60	119.93	122.79
3	L5	3359	OMG	C5-C6-N1	2.60	119.79	113.19
3	L5	2630	A2M	C4-N9-C1'	-2.59	120.41	126.59
3	L5	4116	OMG	C5-C6-N1	2.59	119.78	113.19
3	L5	3476	OMG	N9-C4-N3	2.59	131.14	125.94
3	L5	1580	OMG	C5-C6-N1	2.59	119.77	113.19
3	L5	3476	OMG	C5-C6-N1	2.59	119.77	113.19
3	L5	2630	A2M	N3-C4-N9	2.59	131.35	127.08
3	L5	3599	A2M	C4'-O4'-C1'	-2.59	103.76	109.47
49	S2	1843	4AC	C6-C5-C4	2.59	120.13	116.96
3	L5	4364	OMG	C5-C6-N1	2.59	119.76	113.19
3	L5	2719	OMG	N9-C8-N7	-2.58	108.52	113.39
49	S2	602	OMG	C5-C6-N1	2.58	119.75	113.19
3	L5	4383	OMG	C5-C6-N1	2.58	119.75	113.19
3	L5	3676	OMG	C5-C6-N1	2.58	119.74	113.19
3	L5	4369	OMG	C5-C6-N1	2.58	119.74	113.19
49	S2	1448	OMG	C5-C6-N1	2.58	119.73	113.19
3	L5	1260	OMG	C5-C6-N1	2.58	119.73	113.19
3	L5	2208	OMC	CM2-O2'-C2'	-2.57	107.77	114.52
49	S2	1491	OMG	C5-C6-N1	2.57	119.72	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1491	OMG	N9-C4-N3	2.56	131.09	125.94
3	L5	4269	A2M	N3-C4-N9	2.56	131.30	127.08
49	S2	1057	PSU	C6-C5-C4	2.56	119.99	118.20
49	S2	868	OMG	C5-C6-N1	2.56	119.69	113.19
3	L5	3631	OMG	C5-C6-N1	2.56	119.68	113.19
3	L5	3466	PSU	C6-C5-C4	2.56	119.98	118.20
3	L5	4240	OMG	C5-C6-N1	2.55	119.66	113.19
3	L5	3676	OMG	N9-C4-N3	2.55	131.06	125.94
3	L5	4138	OMG	N9-C4-N3	2.55	131.06	125.94
78	Sg	1	AME	O-C-CA	-2.55	118.10	124.78
3	L5	4298	PSU	O2-C2-N1	-2.55	119.99	122.79
3	L5	4116	OMG	N9-C4-N3	2.54	131.05	125.94
3	L5	3517	A2M	O4'-C1'-N9	2.54	113.07	108.06
3	L5	3450	A2M	CM'-O2'-C2'	-2.54	107.85	114.52
49	S2	159	A2M	N3-C4-N9	2.54	131.27	127.08
49	S2	119	PSU	C6-C5-C4	2.54	119.97	118.20
3	L5	3616	PSU	O2-C2-N1	-2.54	119.99	122.79
49	S2	684	OMG	N9-C4-N3	2.54	131.03	125.94
5	L8	75	OMG	C5-C6-N1	2.54	119.63	113.19
3	L5	4245	OMG	C5-C6-N1	2.54	119.63	113.19
49	S2	1047	PSU	C6-C5-C4	2.53	119.97	118.20
49	S2	1233	PSU	O2-C2-N1	-2.53	120.00	122.79
3	L5	3974	OMG	N9-C4-N3	2.53	131.02	125.94
3	L5	4058	PSU	O2-C2-N1	-2.53	120.00	122.79
3	L5	3974	OMG	C5-C6-N1	2.53	119.61	113.19
49	S2	868	OMG	N9-C4-N3	2.53	131.02	125.94
3	L5	2267	OMG	N9-C4-N3	2.53	131.02	125.94
49	S2	1082	PSU	C6-C5-C4	2.53	119.97	118.20
3	L5	3616	PSU	C6-C5-C4	2.53	119.97	118.20
3	L5	3652	PSU	C6-C5-C4	2.53	119.96	118.20
49	S2	105	PSU	O2-C2-N1	-2.52	120.01	122.79
49	S2	485	A2M	N3-C4-N9	2.52	131.24	127.08
3	L5	4383	OMG	N9-C4-N3	2.52	131.01	125.94
3	L5	3359	OMG	N9-C4-N3	2.52	131.00	125.94
49	S2	684	OMG	C5-C6-N1	2.52	119.59	113.19
49	S2	1833	6MZ	C4-N9-C8	2.52	108.46	105.73
3	L5	4276	UR3	C6-N1-C2	-2.52	119.53	121.79
3	L5	4246	PSU	O2-C2-N1	-2.51	120.02	122.79
3	L5	3966	6MZ	C4-N9-C8	2.51	108.45	105.73
3	L5	1477	OMG	N9-C4-N3	2.51	130.98	125.94
3	L5	2207	OMG	C5-C6-N1	2.51	119.55	113.19
49	S2	1329	OMG	N9-C4-N3	2.50	130.97	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3562	A2M	CM'-O2'-C2'	-2.50	107.95	114.52
3	L5	3492	A2M	N3-C4-N9	2.50	131.21	127.08
49	S2	1851	MA6	C4-N9-C8	2.50	108.44	105.73
3	L5	4045	PSU	O2-C2-N1	-2.50	120.04	122.79
3	L5	4369	OMG	N9-C4-N3	2.50	130.95	125.94
3	L5	4149	PSU	O2-C2-N1	-2.49	120.05	122.79
3	L5	3450	A2M	N3-C4-N9	2.49	131.19	127.08
3	L5	3585	PSU	O2-C2-N1	-2.49	120.05	122.79
3	L5	1489	A2M	C2'-C3'-C4'	-2.49	96.59	101.99
49	S2	1833	6MZ	C5-N7-C8	2.49	107.04	103.51
80	Si	62	HY3	O-C-CA	-2.49	117.90	124.83
3	L5	3652	PSU	O2-C2-N1	-2.49	120.05	122.79
3	L5	4169	PSU	O2-C2-N1	-2.48	120.06	122.79
3	L5	4374	PSU	O2-C2-N1	-2.48	120.06	122.79
49	S2	669	A2M	C6-C5-C4	2.48	120.52	117.18
3	L5	4245	OMG	N9-C4-N3	2.48	130.92	125.94
3	L5	4322	PSU	O2-C2-N1	-2.48	120.06	122.79
3	L5	3631	OMG	N9-C4-N3	2.48	130.91	125.94
3	L5	2475	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	4099	PSU	C6-C5-C4	2.47	119.93	118.20
3	L5	3494	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	3500	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	4177	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	4166	PSU	C6-C5-C4	2.47	119.92	118.20
49	S2	1626	PSU	O2-C2-N1	-2.47	120.08	122.79
3	L5	1801	PSU	C6-C5-C4	2.47	119.92	118.20
3	L5	4364	OMG	N9-C4-N3	2.46	130.88	125.94
49	S2	1046	PSU	C6-C5-C4	2.46	119.92	118.20
3	L5	1537	PSU	C6-C5-C4	2.46	119.92	118.20
3	L5	4244	OMU	O2-C2-N1	-2.46	119.52	122.79
3	L5	3973	OMU	O2-C2-N1	-2.46	119.52	122.79
49	S2	669	A2M	C4-C5-N7	-2.46	107.63	110.62
49	S2	34	PSU	C6-C5-C4	2.45	119.91	118.20
49	S2	1239	PSU	O2-C2-N1	-2.45	120.09	122.79
3	L5	1638	PSU	O2-C2-N1	-2.45	120.09	122.79
3	L5	2475	PSU	C6-C5-C4	2.45	119.91	118.20
3	L5	1489	A2M	C3'-C2'-C1'	-2.45	98.28	102.89
49	S2	1852	MA6	C4-N9-C8	2.45	108.38	105.73
49	S2	1368	PSU	O2-C2-N1	-2.44	120.10	122.79
3	L5	1720	PSU	O2-C2-N1	-2.44	120.10	122.79
3	L5	1683	PSU	O2-C2-N1	-2.44	120.10	122.79
3	L5	1632	PSU	C6-N1-C2	-2.44	120.19	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1843	4AC	C5-C4-N4	-2.44	118.69	122.92
3	L5	3369	PSU	C6-C5-C4	2.43	119.90	118.20
49	S2	210	PSU	O2-C2-N1	-2.43	120.11	122.79
3	L5	1799	PSU	O2-C2-N1	-2.43	120.11	122.79
49	S2	573	PSU	C6-C5-C4	2.43	119.89	118.20
3	L5	2351	PSU	O2-C2-N1	-2.43	120.12	122.79
3	L5	400	A2M	C2'-C3'-C4'	-2.43	96.72	101.99
49	S2	573	PSU	O2-C2-N1	-2.43	120.12	122.79
49	S2	218	PSU	O2-C2-N1	-2.42	120.12	122.79
3	L5	4169	PSU	C6-C5-C4	2.42	119.89	118.20
49	S2	36	PSU	O2-C2-N1	-2.42	120.13	122.79
3	L5	1260	OMG	N9-C4-N3	2.42	130.80	125.94
49	S2	1005	PSU	O2-C2-N1	-2.42	120.13	122.79
3	L5	1731	PSU	O2-C2-N1	-2.42	120.13	122.79
3	L5	3427	PSU	O2-C2-N1	-2.42	120.13	122.79
3	L5	4166	PSU	O2-C2-N1	-2.42	120.13	122.79
3	L5	4435	PSU	O2-C2-N1	-2.42	120.13	122.79
49	S2	682	PSU	C6-C5-C4	2.41	119.89	118.20
3	L5	3599	A2M	C4-N9-C8	2.41	108.34	105.73
49	S2	650	PSU	O2-C2-N1	-2.41	120.14	122.79
49	S2	610	PSU	O2-C2-N1	-2.41	120.14	122.79
3	L5	1537	PSU	O2-C2-N1	-2.41	120.14	122.79
49	S2	1833	6MZ	C6-C5-N7	2.41	135.00	132.39
3	L5	1718	PSU	O2-C2-N1	-2.41	120.14	122.79
49	S2	510	OMG	N9-C4-N3	2.41	130.78	125.94
3	L5	4374	PSU	C6-C5-C4	2.41	119.88	118.20
3	L5	3554	PSU	O2-C2-N1	-2.40	120.14	122.79
3	L5	1491	PSU	O2-C2-N1	-2.40	120.15	122.79
3	L5	3502	PSU	O2-C2-N1	-2.40	120.15	122.79
49	S2	469	A2M	C4-N9-C8	2.40	108.33	105.73
49	S2	1175	PSU	O2-C2-N1	-2.40	120.15	122.79
3	L5	4419	PSU	O2-C2-N1	-2.40	120.15	122.79
5	L8	55	PSU	O2-C2-N1	-2.40	120.15	122.79
49	S2	652	PSU	O2-C2-N1	-2.40	120.15	122.79
49	S2	1046	PSU	O2-C2-N1	-2.40	120.15	122.79
49	S2	816	PSU	O2-C2-N1	-2.40	120.15	122.79
3	L5	4711	PSU	O2-C2-N1	-2.39	120.16	122.79
3	L5	4042	PSU	O2-C2-N1	-2.39	120.16	122.79
3	L5	1270	A2M	C4-N9-C8	2.39	108.32	105.73
3	L5	4740	PSU	O2-C2-N1	-2.39	120.16	122.79
3	L5	3583	PSU	C6-C5-C4	2.38	119.86	118.20
49	S2	218	PSU	C6-C5-C4	2.38	119.86	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1057	PSU	O2-C2-N1	-2.38	120.17	122.79
49	S2	1644	PSU	C6-C5-C4	2.38	119.86	118.20
57	SL	2	SAC	O-C-CA	-2.38	118.55	124.78
3	L5	400	A2M	CM'-O2'-C2'	-2.38	108.29	114.52
49	S2	27	A2M	C4-N9-C8	2.38	108.30	105.73
3	L5	3462	PSU	O2-C2-N1	-2.38	120.18	122.79
3	L5	4382	PSU	C6-N1-C2	-2.37	120.25	122.68
3	L5	4740	PSU	C6-C5-C4	2.37	119.86	118.20
49	S2	429	OMU	O2-C2-N1	-2.37	119.63	122.79
49	S2	1348	PSU	O2-C2-N1	-2.37	120.18	122.79
3	L5	3447	PSU	O2-C2-N1	-2.37	120.18	122.79
3	L5	4203	PSU	O2-C2-N1	-2.37	120.18	122.79
49	S2	628	OMU	O2-C2-N1	-2.37	119.64	122.79
49	S2	1644	PSU	O2-C2-N1	-2.37	120.18	122.79
3	L5	3371	PSU	C6-C5-C4	2.37	119.85	118.20
3	L5	3369	PSU	O2-C2-N1	-2.37	120.18	122.79
3	L5	4107	PSU	O2-C2-N1	-2.37	120.19	122.79
49	S2	510	OMG	CM2-O2'-C2'	-2.37	108.32	114.52
49	S2	867	PSU	O2-C2-N1	-2.36	120.19	122.79
49	S2	1047	PSU	O2-C2-N1	-2.36	120.19	122.79
3	L5	4138	OMG	CM2-O2'-C2'	-2.36	108.32	114.52
3	L5	2630	A2M	O4'-C1'-N9	-2.36	103.41	108.06
49	S2	591	A2M	C4-N9-C1'	2.36	132.22	126.59
3	L5	2206	A2M	C4-C5-N7	-2.36	107.75	110.62
3	L5	2630	A2M	C4-C5-N7	-2.36	107.75	110.62
3	L5	4267	PSU	O2-C2-N1	-2.35	120.20	122.79
49	S2	93	PSU	O2-C2-N1	-2.35	120.20	122.79
3	L5	3490	PSU	O2-C2-N1	-2.35	120.20	122.79
49	S2	1446	PSU	C6-C5-C4	2.35	119.84	118.20
3	L5	4042	PSU	C6-C5-C4	2.35	119.84	118.20
5	L8	55	PSU	C6-C5-C4	2.35	119.84	118.20
3	L5	4269	A2M	C4-C5-N7	-2.35	107.76	110.62
3	L5	1731	PSU	C6-C5-C4	2.35	119.84	118.20
3	L5	4099	PSU	O2-C2-N1	-2.35	120.21	122.79
49	S2	577	A2M	C3'-C2'-C1'	-2.35	98.48	102.89
3	L5	4298	PSU	C6-C5-C4	2.35	119.84	118.20
49	S2	864	PSU	O2-C2-N1	-2.35	120.21	122.79
3	L5	2351	PSU	C6-C5-C4	2.34	119.84	118.20
49	S2	1640	7MG	O6-C6-C5	-2.34	121.79	127.54
3	L5	1810	A2M	CM'-O2'-C2'	-2.34	108.38	114.52
3	L5	4317	A2M	CM'-O2'-C2'	-2.34	108.38	114.52
3	L5	1801	PSU	O2-C2-N1	-2.34	120.21	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	802	PSU	O2-C2-N1	-2.34	120.22	122.79
49	S2	1327	OMU	O2-C2-N1	-2.34	119.68	122.79
3	L5	4188	PSU	O2-C2-N1	-2.34	120.22	122.79
3	L5	4336	A2M	C4-N9-C8	2.33	108.26	105.73
3	L5	4202	OMC	CM2-O2'-C2'	-2.33	108.40	114.52
49	S2	1338	4AC	C6-C5-C4	2.33	119.82	116.96
49	S2	109	PSU	O2-C2-N1	-2.33	120.22	122.79
3	L5	4322	PSU	C6-C5-C4	2.33	119.83	118.20
3	L5	3450	A2M	C4-C5-N7	-2.33	107.78	110.62
3	L5	1721	PSU	O2-C2-N1	-2.33	120.22	122.79
49	S2	1368	PSU	C6-C5-C4	2.33	119.83	118.20
49	S2	1178	PSU	O2-C2-N1	-2.33	120.23	122.79
3	L5	3466	PSU	O2-C2-N1	-2.33	120.23	122.79
3	L5	2658	A2M	C4-N9-C8	2.32	108.25	105.73
3	L5	1718	PSU	C6-C5-C4	2.32	119.82	118.20
3	L5	3433	OMC	CM2-O2'-C2'	-2.32	108.43	114.52
3	L5	3517	A2M	C4-N9-C8	2.32	108.24	105.73
5	L8	75	OMG	N9-C4-N3	2.32	130.60	125.94
49	S2	407	PSU	O2-C2-N1	-2.32	120.24	122.79
49	S2	1032	A2M	C4-N9-C8	2.32	108.24	105.73
75	Sd	2	SAC	O-C-CA	-2.32	118.71	124.78
3	L5	1270	A2M	CM'-O2'-C2'	-2.31	108.45	114.52
3	L5	3557	A2M	CM'-O2'-C2'	-2.31	108.45	114.52
49	S2	1851	MA6	C10-N6-C9	-2.31	108.67	116.12
49	S2	867	PSU	C6-C5-C4	2.31	119.82	118.20
49	S2	669	A2M	CM'-O2'-C2'	-2.31	108.45	114.52
49	S2	1245	PSU	O2-C2-N1	-2.31	120.25	122.79
49	S2	99	A2M	C4-C5-N7	-2.31	107.80	110.62
49	S2	1032	A2M	C4-C5-N7	-2.31	107.80	110.62
49	S2	513	A2M	C4-N9-C8	2.31	108.23	105.73
3	L5	4435	PSU	C6-N1-C2	-2.31	120.32	122.68
49	S2	159	A2M	C4-C5-N7	-2.31	107.81	110.62
49	S2	669	A2M	N3-C4-N9	2.31	130.88	127.08
49	S2	99	A2M	C3'-C2'-C1'	-2.31	98.55	102.89
3	L5	4336	A2M	CM'-O2'-C2'	-2.30	108.48	114.52
3	L5	2719	OMG	O6-C6-C5	-2.30	120.49	126.60
49	S2	1446	PSU	O2-C2-N1	-2.30	120.26	122.79
3	L5	3500	PSU	C6-C5-C4	2.30	119.81	118.20
49	S2	682	PSU	O2-C2-N1	-2.30	120.26	122.79
49	S2	407	PSU	C6-C5-C4	2.30	119.81	118.20
3	L5	4039	PSU	O2-C2-N1	-2.30	120.26	122.79
3	L5	1489	A2M	C4-C5-N7	-2.30	107.82	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1693	PSU	O2-C2-N1	-2.29	120.27	122.79
49	S2	27	A2M	C4-C5-N7	-2.29	107.82	110.62
3	L5	4336	A2M	C4-C5-N7	-2.29	107.83	110.62
3	L5	3973	OMU	CM2-O2'-C2'	-2.29	108.51	114.52
49	S2	109	PSU	C6-C5-C4	2.29	119.80	118.20
3	L5	4138	OMG	C8-N7-C5	2.29	108.39	104.24
49	S2	815	PSU	C6-C5-C4	2.29	119.80	118.20
49	S2	967	PSU	C6-C5-C4	2.29	119.80	118.20
3	L5	4435	PSU	C6-C5-C4	2.29	119.80	118.20
49	S2	34	PSU	O2-C2-N1	-2.29	120.28	122.79
3	L5	1477	OMG	C8-N7-C5	2.29	108.38	104.24
3	L5	2244	A2M	C4-C5-N7	-2.28	107.84	110.62
3	L5	3557	A2M	C4-C5-N7	-2.28	107.84	110.62
49	S2	36	PSU	C6-C5-C4	2.28	119.79	118.20
3	L5	4246	PSU	C6-C5-C4	2.28	119.79	118.20
3	L5	3599	A2M	CM'-O2'-C2'	-2.28	108.54	114.52
3	L5	3583	PSU	O2-C2-N1	-2.28	120.28	122.79
3	L5	1721	PSU	C6-C5-C4	2.28	119.79	118.20
3	L5	400	A2M	C4-C5-N7	-2.28	107.84	110.62
49	S2	650	PSU	C6-C5-C4	2.28	119.79	118.20
3	L5	4217	PSU	O2-C2-N1	-2.28	120.28	122.79
49	S2	1329	OMG	C8-N7-C5	2.27	108.36	104.24
3	L5	1270	A2M	C4-C5-N7	-2.27	107.85	110.62
5	L8	69	PSU	O2-C2-N1	-2.27	120.29	122.79
3	L5	3494	PSU	C6-C5-C4	2.27	119.79	118.20
3	L5	3676	OMG	C8-N7-C5	2.27	108.35	104.24
3	L5	4245	OMG	C8-N7-C5	2.27	108.35	104.24
3	L5	398	A2M	C3'-C2'-C1'	-2.27	98.62	102.89
3	L5	3562	A2M	C4-N9-C8	2.27	108.19	105.73
3	L5	3502	PSU	C6-C5-C4	2.27	119.78	118.20
49	S2	1348	PSU	C6-C5-C4	2.27	119.78	118.20
49	S2	437	OMG	C8-N7-C5	2.27	108.34	104.24
49	S2	469	A2M	C4-C5-N7	-2.27	107.86	110.62
3	L5	4240	OMG	CM2-O2'-C2'	-2.27	108.58	114.52
49	S2	816	PSU	C6-C5-C4	2.27	119.78	118.20
3	L5	4711	PSU	C6-C5-C4	2.27	119.78	118.20
49	S2	119	PSU	O2-C2-N1	-2.26	120.30	122.79
49	S2	1338	4AC	C5-C4-N4	-2.26	118.99	122.92
49	S2	602	OMG	O6-C6-C5	-2.26	120.60	126.60
3	L5	3427	PSU	C6-C5-C4	2.26	119.78	118.20
3	L5	4193	5MC	N4-C4-N3	2.26	122.60	118.48
3	L5	3371	PSU	O2-C2-N1	-2.26	120.30	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3456	A2M	C4-N9-C8	2.26	108.18	105.73
49	S2	1245	PSU	C6-C5-C4	2.26	119.78	118.20
49	S2	510	OMG	C8-N7-C5	2.26	108.33	104.24
3	L5	2244	A2M	C4-N9-C8	2.26	108.17	105.73
3	L5	1810	A2M	C4-C5-N7	-2.26	107.87	110.62
3	L5	3490	PSU	C6-C5-C4	2.26	119.78	118.20
49	S2	1833	6MZ	C9-N6-C6	-2.25	120.93	122.87
49	S2	1640	7MG	N1-C2-N3	-2.25	119.12	123.32
49	S2	967	PSU	O2-C2-N1	-2.25	120.31	122.79
49	S2	166	A2M	C4-N9-C8	2.25	108.17	105.73
3	L5	2207	OMG	N1-C2-N3	-2.25	119.12	123.32
3	L5	3631	OMG	O6-C6-C5	-2.25	120.63	126.60
49	S2	485	A2M	C4-C5-N7	-2.25	107.88	110.62
49	S2	815	PSU	O2-C2-N1	-2.25	120.31	122.79
49	S2	513	A2M	C4-C5-N7	-2.25	107.88	110.62
3	L5	4325	PSU	O2-C2-N1	-2.25	120.31	122.79
46	Ls	2	SAC	O-C-CA	-2.25	118.88	124.78
3	L5	4749	PSU	O2-C2-N1	-2.25	120.31	122.79
49	S2	1289	OMU	CM2-O2'-C2'	-2.25	108.63	114.52
49	S2	1384	A2M	C4-C5-N7	-2.25	107.88	110.62
49	S2	687	PSU	O2-C2-N1	-2.25	120.32	122.79
49	S2	652	PSU	C6-C5-C4	2.25	119.77	118.20
3	L5	3562	A2M	C3'-C2'-C1'	-2.25	98.67	102.89
49	S2	166	A2M	C4-C5-N7	-2.24	107.89	110.62
3	L5	3657	OMU	O2-C2-N1	-2.24	119.80	122.79
3	L5	4045	PSU	C6-C5-C4	2.24	119.77	118.20
3	L5	3676	OMG	O6-C6-C5	-2.24	120.65	126.60
3	L5	1720	PSU	C6-C5-C4	2.24	119.77	118.20
3	L5	4116	OMG	O6-C6-C5	-2.24	120.65	126.60
3	L5	3514	5MC	N4-C4-N3	2.24	122.56	118.48
3	L5	3517	A2M	C2'-C1'-N9	-2.24	109.76	113.53
49	S2	645	OMG	C8-N7-C5	2.24	108.29	104.24
3	L5	2680	OMU	O2-C2-N1	-2.24	119.81	122.79
3	L5	3599	A2M	C4-C5-N7	-2.24	107.89	110.62
49	S2	823	PSU	C6-C5-C4	2.24	119.76	118.20
3	L5	4177	PSU	C6-C5-C4	2.24	119.76	118.20
3	L5	3359	OMG	C8-N7-C5	2.24	108.29	104.24
3	L5	2194	OMC	O2-C2-N3	-2.23	118.70	122.33
49	S2	1178	PSU	C6-C5-C4	2.23	119.76	118.20
49	S2	1448	OMG	O6-C6-C5	-2.23	120.67	126.60
49	S2	1239	PSU	C6-C5-C4	2.23	119.76	118.20
3	L5	3496	PSU	C6-C5-C4	2.23	119.76	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1580	OMG	O6-C6-C5	-2.23	120.69	126.60
3	L5	4269	A2M	C4-N9-C8	2.23	108.14	105.73
3	L5	1810	A2M	C4-N9-C8	2.23	108.14	105.73
49	S2	645	OMG	CM2-O2'-C2'	-2.23	108.69	114.52
3	L5	2658	A2M	C4-C5-N7	-2.22	107.91	110.62
3	L5	3974	OMG	C8-N7-C5	2.22	108.27	104.24
3	L5	2244	A2M	O4'-C4'-C3'	-2.22	100.72	105.11
3	L5	4039	PSU	C6-N1-C2	-2.22	120.41	122.68
3	L5	398	A2M	C4-C5-N7	-2.22	107.91	110.62
3	L5	3585	PSU	C6-C5-C4	2.22	119.75	118.20
3	L5	1799	PSU	C6-C5-C4	2.22	119.75	118.20
3	L5	1632	PSU	O2-C2-N1	-2.22	120.35	122.79
5	L8	75	OMG	O6-C6-C5	-2.22	120.72	126.60
3	L5	4383	OMG	C8-N7-C5	2.21	108.25	104.24
3	L5	3524	OMG	O6-C6-C5	-2.21	120.73	126.60
3	L5	3476	OMG	C8-N7-C5	2.21	108.25	104.24
3	L5	4240	OMG	O6-C6-C5	-2.21	120.73	126.60
49	S2	429	OMU	CM2-O2'-C2'	-2.21	108.73	114.52
49	S2	868	OMG	O6-C6-C5	-2.21	120.75	126.60
3	L5	4217	PSU	C6-C5-C4	2.21	119.74	118.20
49	S2	684	OMG	O6-C6-C5	-2.21	120.75	126.60
49	S2	437	OMG	O6-C6-C5	-2.20	120.75	126.60
3	L5	4203	PSU	C6-C5-C4	2.20	119.74	118.20
49	S2	577	A2M	C4-N9-C8	2.20	108.12	105.73
3	L5	4317	A2M	C4-C5-N7	-2.20	107.94	110.62
3	L5	3476	OMG	O6-C6-C5	-2.20	120.76	126.60
3	L5	2207	OMG	O6-C6-C5	-2.20	120.76	126.60
49	S2	105	PSU	C6-N1-C2	-2.20	120.43	122.68
3	L5	3942	OMG	O6-C6-C5	-2.20	120.76	126.60
3	L5	1479	A2M	C4-C5-N7	-2.20	107.94	110.62
49	S2	210	PSU	C6-C5-C4	2.20	119.74	118.20
49	S2	645	OMG	O6-C6-C5	-2.20	120.77	126.60
3	L5	4364	OMG	C8-N7-C5	2.20	108.22	104.24
3	L5	3576	PSU	O2-C2-N1	-2.20	120.37	122.79
3	L5	4383	OMG	O6-C6-C5	-2.20	120.77	126.60
3	L5	3599	A2M	C5-C6-N1	2.20	122.11	117.39
3	L5	398	A2M	CM'-O2'-C2'	-2.20	108.76	114.52
3	L5	1491	PSU	C6-C5-C4	2.20	119.73	118.20
3	L5	1270	A2M	C4'-O4'-C1'	-2.19	104.63	109.47
3	L5	3601	OMC	CM2-O2'-C2'	-2.19	108.77	114.52
3	L5	4325	PSU	C6-C5-C4	2.19	119.73	118.20
3	L5	4116	OMG	C8-N7-C5	2.19	108.21	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1260	OMG	C8-N7-C5	2.19	108.20	104.24
49	S2	1491	OMG	O6-C6-C5	-2.19	120.79	126.60
3	L5	1479	A2M	C4-N9-C8	2.19	108.10	105.73
49	S2	684	OMG	CM2-O2'-C2'	-2.19	108.79	114.52
3	L5	2267	OMG	C8-N7-C5	2.19	108.20	104.24
49	S2	1329	OMG	O6-C6-C5	-2.18	120.80	126.60
3	L5	1260	OMG	O6-C6-C5	-2.18	120.81	126.60
3	L5	4138	OMG	O6-C6-C5	-2.18	120.82	126.60
3	L5	2630	A2M	C5-C6-N1	2.18	122.07	117.39
3	L5	3676	OMG	N1-C2-N3	-2.18	119.26	123.32
49	S2	864	PSU	C6-C5-C4	2.18	119.72	118.20
3	L5	4369	OMG	O6-C6-C5	-2.18	120.82	126.60
3	L5	1580	OMG	C8-N7-C5	2.18	108.18	104.24
3	L5	4245	OMG	O6-C6-C5	-2.18	120.83	126.60
3	L5	3517	A2M	C5-C6-N1	2.18	122.06	117.39
3	L5	4369	OMG	C8-N7-C5	2.18	108.18	104.24
49	S2	1693	PSU	C6-C5-C4	2.18	119.72	118.20
3	L5	3456	A2M	C4-C5-N7	-2.18	107.97	110.62
3	L5	3585	PSU	C6-N1-C2	-2.17	120.46	122.68
3	L5	4177	PSU	C6-N1-C2	-2.17	120.46	122.68
3	L5	1683	PSU	C6-C5-C4	2.17	119.72	118.20
3	L5	1810	A2M	C3'-C2'-C1'	-2.17	98.81	102.89
3	L5	1489	A2M	C5-C6-N1	2.17	122.05	117.39
3	L5	3616	PSU	C6-N1-C2	-2.17	120.46	122.68
3	L5	4282	OMC	CM2-O2'-C2'	-2.17	108.83	114.52
3	L5	1477	OMG	O6-C6-C5	-2.17	120.84	126.60
3	L5	4749	PSU	C6-C5-C4	2.17	119.72	118.20
3	L5	3359	OMG	O6-C6-C5	-2.17	120.85	126.60
3	L5	4116	OMG	N1-C2-N3	-2.17	119.28	123.32
49	S2	610	PSU	C6-C5-C4	2.17	119.71	118.20
49	S2	518	OMC	CM2-O2'-C2'	-2.17	108.84	114.52
3	L5	3496	PSU	C6-N1-C2	-2.16	120.47	122.68
49	S2	166	A2M	C5-C6-N1	2.16	122.03	117.39
3	L5	4364	OMG	O6-C6-C5	-2.16	120.86	126.60
49	S2	99	A2M	C5-C6-N1	2.16	122.03	117.39
3	L5	2267	OMG	O6-C6-C5	-2.16	120.86	126.60
3	L5	4336	A2M	C5-C6-N1	2.16	122.03	117.39
3	L5	4058	PSU	C6-N1-C2	-2.16	120.48	122.68
3	L5	3942	OMG	C8-N7-C5	2.16	108.14	104.24
3	L5	1477	OMG	CM2-O2'-C2'	-2.16	108.86	114.52
3	L5	4278	PSU	C6-C5-C4	2.16	119.71	118.20
49	S2	1384	A2M	C5-C6-N1	2.16	122.02	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	802	PSU	C6-N1-C2	-2.15	120.48	122.68
49	S2	1491	OMG	C8-N7-C5	2.15	108.14	104.24
49	S2	1005	PSU	C6-C5-C4	2.15	119.70	118.20
3	L5	3554	PSU	C6-C5-C4	2.15	119.70	118.20
3	L5	4383	OMG	N1-C2-N3	-2.15	119.31	123.32
3	L5	398	A2M	C5-C6-N1	2.15	122.01	117.39
49	S2	1679	A2M	C5-C6-N1	2.15	122.00	117.39
3	L5	3492	A2M	C5-C4-N9	2.15	108.28	105.78
49	S2	469	A2M	O4'-C4'-C3'	-2.15	100.86	105.11
3	L5	4240	OMG	C8-N7-C5	2.15	108.13	104.24
3	L5	3450	A2M	C5-C4-N9	2.15	108.28	105.78
3	L5	3462	PSU	C6-C5-C4	2.15	119.70	118.20
3	L5	3974	OMG	O6-C6-C5	-2.15	120.91	126.60
49	S2	868	OMG	C8-N7-C5	2.15	108.12	104.24
49	S2	510	OMG	O6-C6-C5	-2.14	120.91	126.60
49	S2	610	PSU	C6-N1-C2	-2.14	120.49	122.68
49	S2	166	A2M	C3'-C2'-C1'	-2.14	98.86	102.89
3	L5	4374	PSU	C6-N1-C2	-2.14	120.49	122.68
49	S2	1082	PSU	O2-C2-N1	-2.14	120.43	122.79
49	S2	27	A2M	C5-C6-N1	2.14	121.99	117.39
3	L5	1638	PSU	C6-C5-C4	2.14	119.69	118.20
3	L5	3576	PSU	C6-N1-C2	-2.14	120.50	122.68
49	S2	577	A2M	C4-C5-N7	-2.14	108.01	110.62
49	S2	485	A2M	C5-C6-N1	2.14	121.98	117.39
3	L5	3456	A2M	C5-C6-N1	2.14	121.98	117.39
3	L5	3631	OMG	N1-C2-N3	-2.14	119.34	123.32
3	L5	3562	A2M	C4-C5-N7	-2.13	108.02	110.62
49	S2	591	A2M	C5-C6-N1	2.13	121.97	117.39
3	L5	1260	OMG	N1-C2-N3	-2.13	119.34	123.32
3	L5	2206	A2M	C4-N9-C8	2.13	108.04	105.73
49	S2	1448	OMG	C8-N7-C5	2.13	108.10	104.24
3	L5	2244	A2M	C5-C6-N1	2.13	121.97	117.39
49	S2	577	A2M	CM'-O2'-C2'	-2.13	108.93	114.52
3	L5	2658	A2M	O4'-C1'-N9	-2.13	103.86	108.06
49	S2	684	OMG	C8-N7-C5	2.13	108.10	104.24
3	L5	3557	A2M	C5-C6-N1	2.13	121.96	117.39
3	L5	2267	OMG	N1-C2-N3	-2.13	119.35	123.32
3	L5	3652	PSU	C6-N1-C2	-2.13	120.51	122.68
3	L5	2206	A2M	C5-C6-N1	2.13	121.95	117.39
5	L8	75	OMG	N1-C2-N3	-2.13	119.36	123.32
3	L5	4169	PSU	C6-N1-C2	-2.13	120.51	122.68
49	S2	469	A2M	C5-C6-N1	2.12	121.95	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4246	PSU	C6-N1-C2	-2.12	120.51	122.68
3	L5	1810	A2M	C5-C6-N1	2.12	121.95	117.39
3	L5	2258	OMU	O2-C2-N1	-2.12	119.96	122.79
3	L5	2658	A2M	C5-C6-N1	2.12	121.94	117.39
49	S2	513	A2M	C5-C6-N1	2.12	121.94	117.39
3	L5	1489	A2M	C4-N9-C8	2.12	108.03	105.73
3	L5	3524	OMG	C8-N7-C5	2.12	108.08	104.24
3	L5	4366	OMU	O2-C2-N1	-2.12	119.97	122.79
3	L5	3554	PSU	C6-N1-C2	-2.12	120.52	122.68
5	L8	75	OMG	C8-N7-C5	2.12	108.08	104.24
3	L5	400	A2M	C5-C6-N1	2.12	121.94	117.39
3	L5	1270	A2M	O4'-C4'-C3'	-2.12	100.92	105.11
49	S2	868	OMG	N1-C2-N3	-2.12	119.37	123.32
49	S2	1679	A2M	C3'-C2'-C1'	-2.12	98.91	102.89
49	S2	1392	OMC	O2-C2-N3	-2.12	118.89	122.33
49	S2	1329	OMG	N1-C2-N3	-2.12	119.37	123.32
49	S2	1640	7MG	N9-C4-N3	2.12	128.63	125.47
49	S2	159	A2M	CM'-O2'-C2'	-2.12	108.97	114.52
3	L5	4317	A2M	C4-N9-C8	2.12	108.02	105.73
3	L5	1266	1MA	C8-N7-C5	2.12	108.07	104.24
49	S2	602	OMG	C8-N7-C5	2.11	108.07	104.24
3	L5	2206	A2M	CM'-O2'-C2'	-2.11	108.98	114.52
3	L5	3447	PSU	C6-C5-C4	2.11	119.68	118.20
3	L5	2704	OMC	CM2-O2'-C2'	-2.11	108.98	114.52
3	L5	4364	OMG	N1-C2-N3	-2.11	119.38	123.32
49	S2	159	A2M	C5-C6-N1	2.11	121.92	117.39
3	L5	3974	OMG	N1-C2-N3	-2.11	119.38	123.32
3	L5	4245	OMG	N1-C2-N3	-2.11	119.38	123.32
49	S2	684	OMG	N1-C2-N3	-2.11	119.39	123.32
49	S2	105	PSU	C6-C5-C4	2.11	119.67	118.20
3	L5	4267	PSU	C6-C5-C4	2.11	119.67	118.20
3	L5	4419	PSU	C6-N1-C2	-2.11	120.53	122.68
3	L5	3557	A2M	C4-N9-C8	2.11	108.01	105.73
49	S2	437	OMG	N1-C2-N3	-2.11	119.39	123.32
49	S2	602	OMG	N1-C2-N3	-2.11	119.39	123.32
3	L5	4419	PSU	C6-C5-C4	2.11	119.67	118.20
49	S2	513	A2M	CM'-O2'-C2'	-2.11	109.00	114.52
49	S2	669	A2M	C5-C6-N1	2.11	121.91	117.39
3	L5	3492	A2M	CM'-O2'-C2'	-2.10	109.00	114.52
49	S2	510	OMG	N1-C2-N3	-2.10	119.40	123.32
3	L5	3631	OMG	C8-N7-C5	2.10	108.05	104.24
3	L5	4269	A2M	C5-C6-N1	2.10	121.91	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2207	OMG	C8-N7-C5	2.10	108.05	104.24
3	L5	3562	A2M	C5-C6-N1	2.10	121.90	117.39
49	S2	823	PSU	C6-N1-C2	-2.10	120.54	122.68
49	S2	577	A2M	C5-C6-N1	2.10	121.90	117.39
3	L5	3359	OMG	CM2-O2'-C2'	-2.10	109.02	114.52
49	S2	1032	A2M	C5-C6-N1	2.10	121.89	117.39
3	L5	4317	A2M	C5-C6-N1	2.10	121.89	117.39
49	S2	159	A2M	C3'-C2'-C1'	-2.10	98.94	102.89
3	L5	4138	OMG	N1-C2-N3	-2.10	119.41	123.32
3	L5	1477	OMG	N1-C2-N3	-2.10	119.41	123.32
49	S2	485	A2M	C2'-C3'-C4'	-2.10	97.44	101.99
49	S2	166	A2M	CM'-O2'-C2'	-2.09	109.03	114.52
49	S2	99	A2M	CM'-O2'-C2'	-2.09	109.03	114.52
49	S2	1679	A2M	C4-N9-C8	2.09	108.00	105.73
3	L5	1638	PSU	C6-N1-C2	-2.09	120.54	122.68
49	S2	1384	A2M	C4-N9-C8	2.09	108.00	105.73
49	S2	645	OMG	N1-C2-N3	-2.09	119.42	123.32
3	L5	1580	OMG	N1-C2-N3	-2.09	119.42	123.32
49	S2	1233	PSU	C6-C5-C4	2.09	119.66	118.20
3	L5	3601	OMC	O2-C2-N3	-2.09	118.93	122.33
3	L5	3450	A2M	C5-C6-N1	2.09	121.88	117.39
3	L5	2719	OMG	N1-C2-N3	-2.09	119.42	123.32
3	L5	1270	A2M	C5-C6-N1	2.09	121.87	117.39
3	L5	3359	OMG	N1-C2-N3	-2.09	119.43	123.32
49	S2	93	PSU	C6-N1-C2	-2.09	120.55	122.68
49	S2	159	A2M	C4-N9-C8	2.09	107.99	105.73
3	L5	3524	OMG	N1-C2-N3	-2.09	119.43	123.32
3	L5	1479	A2M	C5-C6-N1	2.09	121.87	117.39
3	L5	4336	A2M	O4'-C4'-C3'	-2.08	100.99	105.11
49	S2	1851	MA6	N9-C8-N7	-2.08	111.06	113.91
3	L5	2244	A2M	C4'-O4'-C1'	-2.08	104.88	109.47
3	L5	4269	A2M	O4'-C4'-C3'	-2.08	101.00	105.11
3	L5	2206	A2M	C3'-C2'-C1'	-2.08	98.98	102.89
49	S2	591	A2M	C4-C5-N7	-2.08	108.09	110.62
49	S2	485	A2M	O4'-C1'-N9	-2.08	103.97	108.06
49	S2	687	PSU	C6-C5-C4	2.08	119.65	118.20
49	S2	1679	A2M	C4-C5-N7	-2.08	108.09	110.62
3	L5	3492	A2M	C4-N9-C8	2.08	107.98	105.73
49	S2	121	OMU	O2-C2-N1	-2.07	120.03	122.79
49	S2	469	A2M	CM'-O2'-C2'	-2.07	109.08	114.52
49	S2	485	A2M	C4-N9-C8	2.07	107.97	105.73
49	S2	652	PSU	C6-N1-C2	-2.07	120.56	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	36	PSU	C6-N1-C2	-2.07	120.57	122.68
3	L5	2630	A2M	CM'-O2'-C2'	-2.07	109.09	114.52
3	L5	3476	OMG	N1-C2-N3	-2.07	119.46	123.32
3	L5	4240	OMG	N1-C2-N3	-2.07	119.46	123.32
49	S2	1175	PSU	C6-N1-C2	-2.07	120.57	122.68
49	S2	802	PSU	C6-C5-C4	2.07	119.64	118.20
49	S2	99	A2M	C4-N9-C8	2.07	107.97	105.73
3	L5	4740	PSU	C6-N1-C2	-2.07	120.57	122.68
3	L5	4269	A2M	CM'-O2'-C2'	-2.07	109.10	114.52
3	L5	4369	OMG	N1-C2-N3	-2.07	119.47	123.32
3	L5	3494	PSU	C6-N1-C2	-2.07	120.57	122.68
3	L5	3942	OMG	N1-C2-N3	-2.06	119.48	123.32
3	L5	4267	PSU	C6-N1-C2	-2.06	120.58	122.68
3	L5	3371	PSU	C6-N1-C2	-2.06	120.58	122.68
49	S2	1491	OMG	N1-C2-N3	-2.06	119.48	123.32
3	L5	2680	OMU	CM2-O2'-C2'	-2.06	109.13	114.52
3	L5	4193	5MC	O2-C2-N3	-2.06	118.99	122.33
3	L5	400	A2M	C4-N9-C8	2.05	107.95	105.73
49	S2	1448	OMG	N1-C2-N3	-2.05	119.49	123.32
3	L5	3500	PSU	C6-N1-C2	-2.05	120.58	122.68
3	L5	3456	A2M	CM'-O2'-C2'	-2.05	109.14	114.52
3	L5	3676	OMG	O2'-C2'-C1'	2.05	113.08	109.08
3	L5	4336	A2M	C4'-O4'-C1'	-2.05	104.95	109.47
3	L5	3517	A2M	CM'-O2'-C2'	-2.05	109.15	114.52
3	L5	1537	PSU	C6-N1-C2	-2.05	120.59	122.68
49	S2	1233	PSU	C6-N1-C2	-2.05	120.59	122.68
3	L5	4269	A2M	C4'-O4'-C1'	-2.05	104.96	109.47
49	S2	116	OMU	O2-C2-N1	-2.04	120.07	122.79
49	S2	1704	OMC	CM2-O2'-C2'	-2.04	109.17	114.52
3	L5	3490	PSU	C6-N1-C2	-2.04	120.60	122.68
3	L5	4107	PSU	C6-C5-C4	2.04	119.62	118.20
3	L5	2630	A2M	C4-N9-C8	2.04	107.94	105.73
49	S2	121	OMU	CM2-O2'-C2'	-2.04	109.18	114.52
3	L5	1718	PSU	C6-N1-C2	-2.04	120.60	122.68
3	L5	4039	PSU	C6-C5-C4	2.03	119.62	118.20
3	L5	4058	PSU	C6-C5-C4	2.03	119.62	118.20
3	L5	1720	PSU	C6-N1-C2	-2.03	120.60	122.68
3	L5	4203	PSU	C6-N1-C2	-2.03	120.61	122.68
3	L5	4325	PSU	C6-N1-C2	-2.03	120.61	122.68
3	L5	3974	OMG	O2'-C2'-C1'	2.03	113.04	109.08
3	L5	3517	A2M	C4-C5-N7	-2.03	108.14	110.62
49	S2	210	PSU	C6-N1-C2	-2.03	120.61	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3462	PSU	C6-N1-C2	-2.03	120.61	122.68
3	L5	1683	PSU	C6-N1-C2	-2.03	120.61	122.68
49	S2	687	PSU	C6-N1-C2	-2.03	120.61	122.68
3	L5	3540	OMC	CM2-O2'-C2'	-2.03	109.21	114.52
3	L5	2630	A2M	C5-C4-N9	2.02	108.14	105.78
3	L5	4045	PSU	C6-N1-C2	-2.02	120.61	122.68
49	S2	355	OMU	O2-C2-N1	-2.02	120.10	122.79
3	L5	4298	PSU	C6-N1-C2	-2.02	120.61	122.68
49	S2	1679	A2M	C4'-O4'-C1'	-2.02	105.01	109.47
3	L5	1799	PSU	C6-N1-C2	-2.02	120.62	122.68
3	L5	3974	OMG	CM2-O2'-C2'	-2.02	109.22	114.52
49	S2	513	A2M	C3'-C2'-C1'	-2.02	99.09	102.89
49	S2	116	OMU	CM2-O2'-C2'	-2.02	109.23	114.52
3	L5	1580	OMG	CM2-O2'-C2'	-2.02	109.23	114.52
3	L5	3427	PSU	C6-N1-C2	-2.02	120.62	122.68
3	L5	2244	A2M	CM'-O2'-C2'	-2.02	109.24	114.52
3	L5	2630	A2M	O4'-C4'-C3'	-2.01	101.13	105.11
49	S2	1626	PSU	C6-N1-C2	-2.01	120.63	122.68
3	L5	1810	A2M	O4'-C4'-C3'	-2.01	101.14	105.11
49	S2	1693	PSU	C6-N1-C2	-2.01	120.63	122.68
49	S2	669	A2M	C1'-N9-C8	2.01	131.67	127.14
3	L5	3502	PSU	C6-N1-C2	-2.01	120.63	122.68
3	L5	4042	PSU	C6-N1-C2	-2.00	120.63	122.68
3	L5	3517	A2M	C4'-O4'-C1'	-2.00	105.05	109.47
49	S2	1368	PSU	C6-N1-C2	-2.00	120.64	122.68
3	L5	2719	OMG	C8-N7-C5	2.00	107.86	104.24
49	S2	1679	A2M	CM'-O2'-C2'	-2.00	109.27	114.52

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	S2	429	OMU	C2'-C1'-N1-C2
49	S2	429	OMU	C2'-C1'-N1-C6
49	S2	577	A2M	C3'-C4'-C5'-O5'
49	S2	645	OMG	O4'-C4'-C5'-O5'
49	S2	645	OMG	C3'-C4'-C5'-O5'
49	S2	684	OMG	C3'-C4'-C5'-O5'
49	S2	802	PSU	C3'-C4'-C5'-O5'
3	L5	2194	OMC	C1'-C2'-O2'-CM2
3	L5	3494	PSU	C3'-C4'-C5'-O5'
3	L5	4336	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
3	L5	4382	PSU	O4'-C1'-C5-C4
3	L5	4382	PSU	O4'-C1'-C5-C6
3	L5	4382	PSU	C3'-C4'-C5'-O5'
49	S2	1338	4AC	N3-C4-N4-C7
49	S2	1338	4AC	C5-C4-N4-C7
49	S2	1338	4AC	O7-C7-N4-C4
49	S2	1338	4AC	CM7-C7-N4-C4
49	S2	1843	4AC	N3-C4-N4-C7
49	S2	1843	4AC	C5-C4-N4-C7
3	L5	3433	OMC	C2'-C1'-N1-C6
49	S2	684	OMG	O4'-C4'-C5'-O5'
49	S2	823	PSU	C3'-C4'-C5'-O5'
3	L5	3494	PSU	O4'-C4'-C5'-O5'
78	Sg	1	AME	CT2-CT1-N-CA
78	Sg	1	AME	OT-CT1-N-CA
49	S2	210	PSU	C3'-C4'-C5'-O5'
49	S2	210	PSU	O4'-C4'-C5'-O5'
49	S2	577	A2M	O4'-C4'-C5'-O5'
49	S2	669	A2M	C3'-C4'-C5'-O5'
49	S2	802	PSU	O4'-C4'-C5'-O5'
49	S2	823	PSU	O4'-C4'-C5'-O5'
3	L5	4382	PSU	O4'-C4'-C5'-O5'
3	L5	4383	OMG	O4'-C4'-C5'-O5'
3	L5	4383	OMG	C3'-C4'-C5'-O5'
3	L5	1580	OMG	C3'-C2'-O2'-CM2
3	L5	3433	OMC	C2'-C1'-N1-C2
3	L5	4193	5MC	C2'-C1'-N1-C6
3	L5	1489	A2M	C4'-C5'-O5'-P
3	L5	2265	OMC	C3'-C4'-C5'-O5'
49	S2	628	OMU	O4'-C4'-C5'-O5'
49	S2	1046	PSU	O4'-C4'-C5'-O5'
49	S2	628	OMU	C3'-C4'-C5'-O5'
3	L5	2265	OMC	O4'-C4'-C5'-O5'
3	L5	3517	A2M	C2'-C1'-N9-C8
7	LE	245	HIC	CA-CB-CG-ND1
49	S2	99	A2M	O4'-C4'-C5'-O5'
49	S2	518	OMC	O4'-C4'-C5'-O5'
49	S2	1448	OMG	C3'-C4'-C5'-O5'
3	L5	2630	A2M	C2'-C1'-N9-C8
49	S2	1046	PSU	C3'-C4'-C5'-O5'
3	L5	4193	5MC	O4'-C1'-N1-C6
3	L5	3433	OMC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
49	S2	1491	OMG	C4'-C5'-O5'-P
49	S2	1852	MA6	C4'-C5'-O5'-P
3	L5	3576	PSU	C4'-C5'-O5'-P
3	L5	3619	OMC	C4'-C5'-O5'-P
49	S2	518	OMC	C3'-C4'-C5'-O5'
3	L5	1260	OMG	C3'-C2'-O2'-CM2
3	L5	1489	A2M	C3'-C2'-O2'-CM'
32	Le	5	MLZ	N-CA-CB-CG
76	Se	67	NMM	N-CA-CB-CG
3	L5	2475	PSU	O4'-C4'-C5'-O5'
3	L5	4193	5MC	O4'-C1'-N1-C2
3	L5	4193	5MC	C2'-C1'-N1-C2
49	S2	645	OMG	C4'-C5'-O5'-P
49	S2	1392	OMC	C4'-C5'-O5'-P
3	L5	1270	A2M	C4'-C5'-O5'-P
3	L5	3599	A2M	C4'-C5'-O5'-P
3	L5	4246	PSU	C4'-C5'-O5'-P
49	S2	429	OMU	O4'-C1'-N1-C6
49	S2	1851	MA6	C5-C6-N6-C10
49	S2	1852	MA6	C5-C6-N6-C10
3	L5	3433	OMC	O4'-C1'-N1-C2
49	S2	669	A2M	C3'-C2'-O2'-CM'
3	L5	3517	A2M	O4'-C4'-C5'-O5'
3	L5	2630	A2M	C2'-C1'-N9-C4
3	L5	3517	A2M	C2'-C1'-N9-C4
49	S2	669	A2M	O4'-C4'-C5'-O5'
3	L5	2475	PSU	C3'-C4'-C5'-O5'
49	S2	429	OMU	O4'-C1'-N1-C2
7	LE	245	HIC	CA-CB-CG-CD2
3	L5	4267	PSU	O4'-C1'-C5-C4
3	L5	2658	A2M	C4'-C5'-O5'-P
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	1489	A2M	O4'-C4'-C5'-O5'
3	L5	3517	A2M	C3'-C4'-C5'-O5'
3	L5	4269	A2M	O4'-C4'-C5'-O5'
76	Se	67	NMM	C-CA-CB-CG
3	L5	2630	A2M	O4'-C1'-N9-C8
3	L5	1580	OMG	C4'-C5'-O5'-P
3	L5	1479	A2M	O4'-C1'-N9-C8
3	L5	3517	A2M	O4'-C1'-N9-C8
3	L5	3576	PSU	C3'-C4'-C5'-O5'
8	LF	2	AYA	C-CA-N-CT

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Mol	Chain	Res	Type	Atoms
3	L5	4267	PSU	O4'-C1'-C5-C6
3	L5	2194	OMC	O4'-C4'-C5'-O5'
3	L5	4246	PSU	C3'-C4'-C5'-O5'
57	SL	2	SAC	C-CA-N-C1A
8	LF	2	AYA	CB-CA-N-CT
49	S2	669	A2M	C2'-C1'-N9-C8
49	S2	591	A2M	O4'-C1'-N9-C8

There are no ring outliers.

70 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	S2	1679	A2M	1	0
3	L5	4269	A2M	3	0
3	L5	4383	OMG	2	0
3	L5	3973	OMU	1	0
3	L5	3942	OMG	1	0
49	S2	1384	A2M	1	0
3	L5	2667	OMC	1	0
49	S2	166	A2M	1	0
3	L5	4278	PSU	1	0
49	S2	1843	4AC	2	0
49	S2	687	PSU	1	0
3	L5	4325	PSU	1	0
49	S2	1491	OMG	1	0
3	L5	4193	5MC	2	0
3	L5	2207	OMG	2	0
78	Sg	1	AME	2	0
3	L5	2265	OMC	2	0
49	S2	1392	OMC	1	0
49	S2	602	OMG	2	0
3	L5	4382	PSU	2	0
3	L5	4099	PSU	1	0
3	L5	4052	OMU	1	0
3	L5	4203	PSU	2	0
3	L5	3456	A2M	1	0
3	L5	3585	PSU	1	0
49	S2	1233	PSU	1	0
49	S2	682	PSU	1	0
49	S2	1852	MA6	2	0
3	L5	400	A2M	1	0
3	L5	1260	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	S2	355	OMU	2	0
76	Se	67	NMM	1	0
3	L5	1810	A2M	2	0
3	L5	3601	OMC	1	0
49	S2	1289	OMU	2	0
49	S2	1032	A2M	1	0
3	L5	3657	OMU	1	0
49	S2	815	PSU	1	0
3	L5	4138	OMG	1	0
3	L5	3517	A2M	1	0
3	L5	3540	OMC	1	0
49	S2	1338	4AC	2	0
49	S2	684	OMG	1	0
49	S2	1693	PSU	1	0
49	S2	1851	MA6	2	0
3	L5	2258	OMU	1	0
3	L5	3599	A2M	2	0
49	S2	1329	OMG	1	0
49	S2	116	OMU	2	0
49	S2	172	OMU	1	0
3	L5	1489	A2M	1	0
3	L5	4116	OMG	1	0
5	L8	75	OMG	2	0
3	L5	4166	PSU	1	0
3	L5	3466	PSU	1	0
3	L5	4366	OMU	1	0
49	S2	27	A2M	3	0
49	S2	868	OMG	1	0
3	L5	2719	OMG	1	0
3	L5	1479	A2M	1	0
3	L5	3369	PSU	1	0
4	L7	1	GTP	1	0
3	L5	1580	OMG	1	0
49	S2	1446	PSU	1	0
3	L5	4364	OMG	1	0
7	LE	245	HIC	1	0
3	L5	3359	OMG	1	0
3	L5	3524	OMG	1	0
49	S2	1833	6MZ	2	0
49	S2	669	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
2	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	181:C	O3'	199:A	P	24.04
1	I	202:C	O3'	216:U	P	23.09

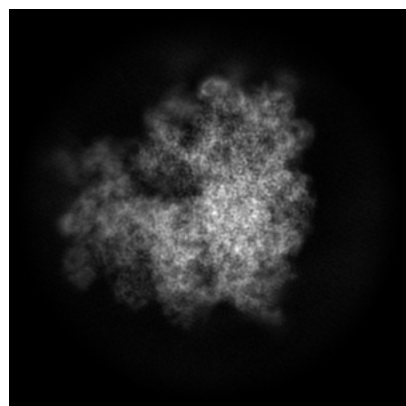
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14752. These allow visual inspection of the internal detail of the map and identification of artifacts.

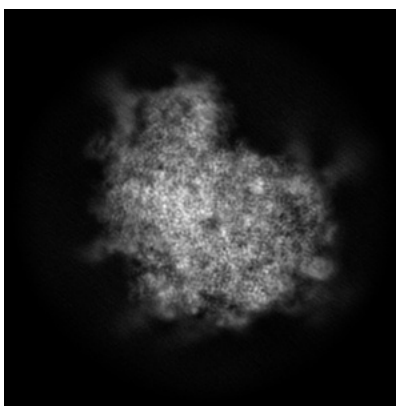
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

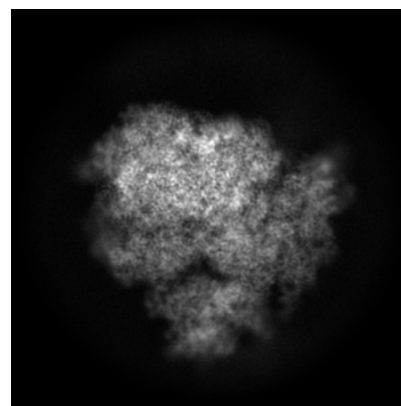
6.1.1 Primary map



X

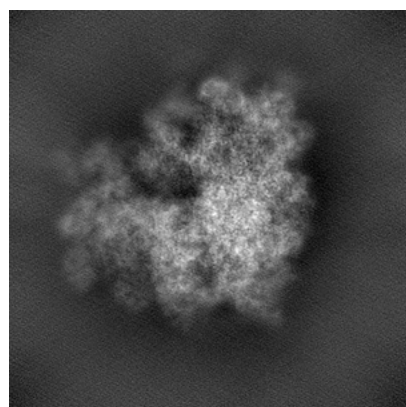


Y

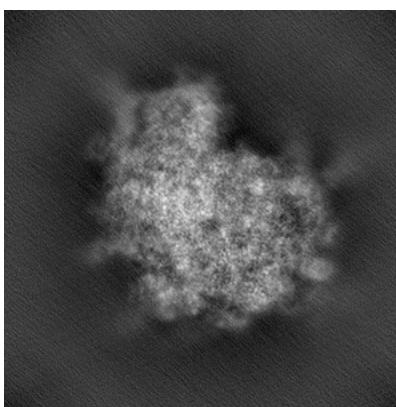


Z

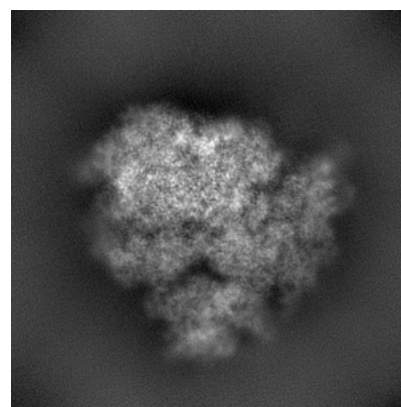
6.1.2 Raw map



X



Y

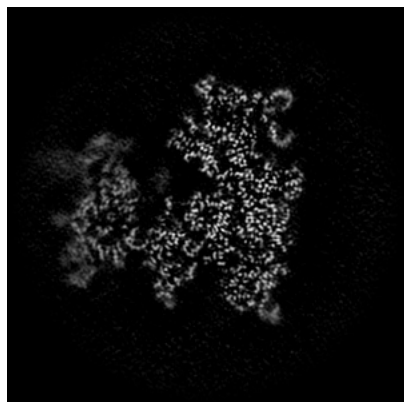


Z

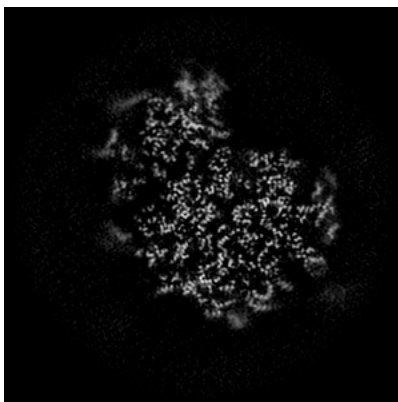
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

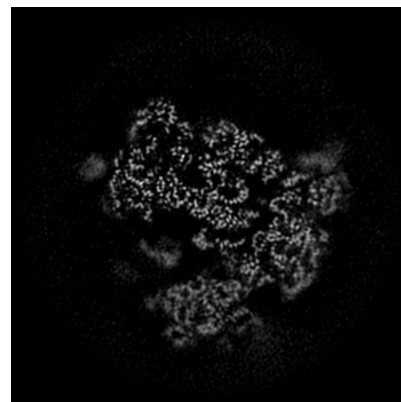
6.2.1 Primary map



X Index: 165

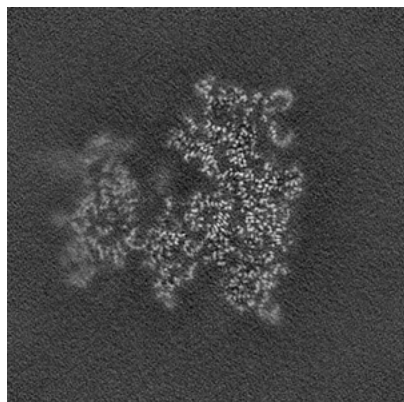


Y Index: 165

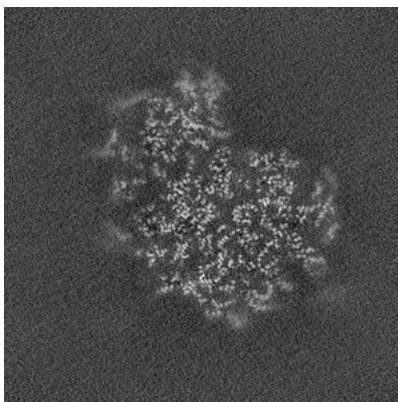


Z Index: 165

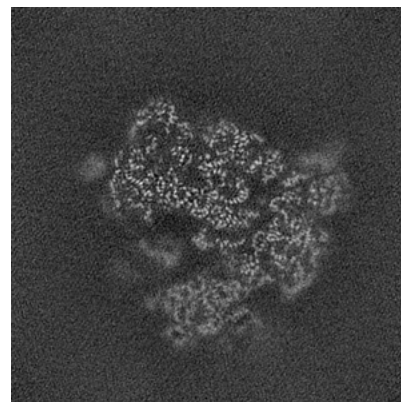
6.2.2 Raw map



X Index: 165



Y Index: 165

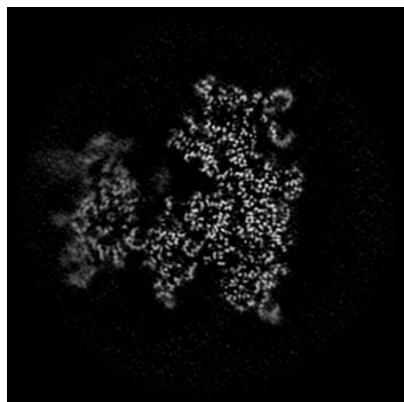


Z Index: 165

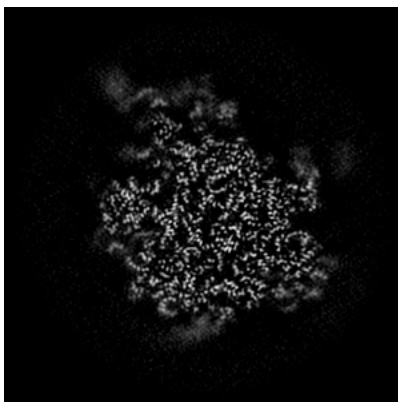
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

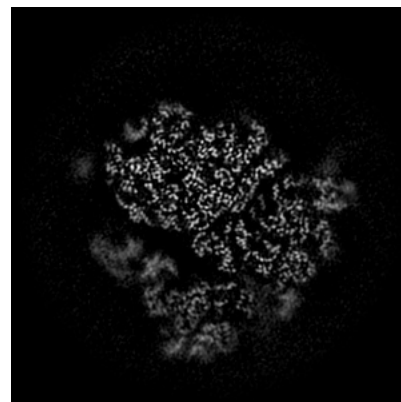
6.3.1 Primary map



X Index: 165

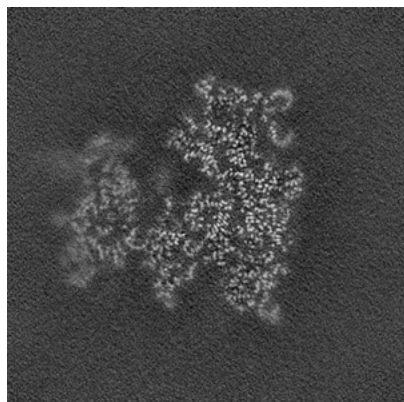


Y Index: 194

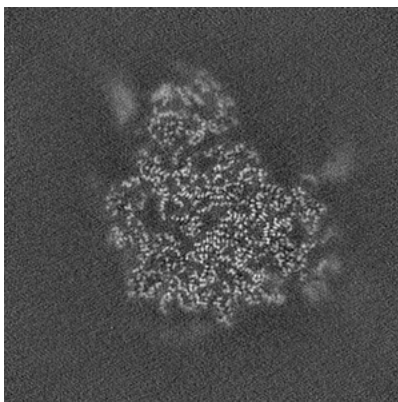


Z Index: 150

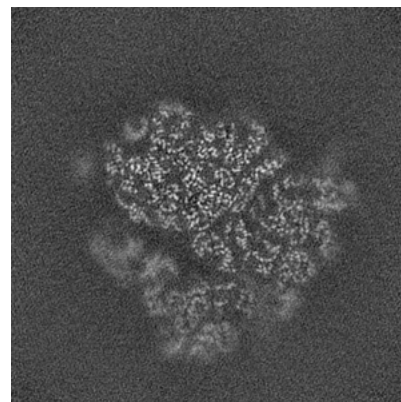
6.3.2 Raw map



X Index: 165



Y Index: 186

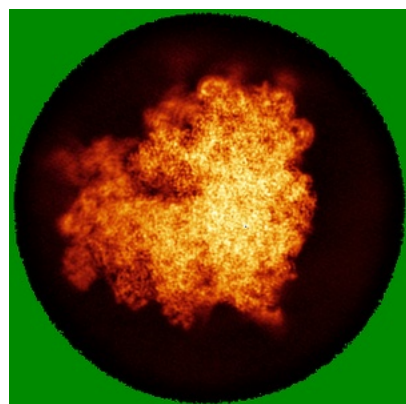


Z Index: 150

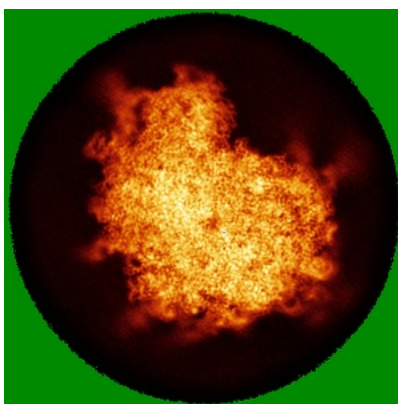
The images above show the largest variance slices of the map in three orthogonal directions.

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

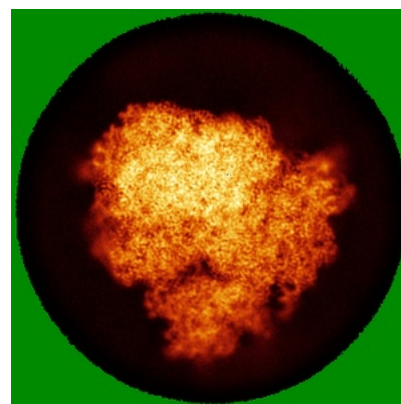
6.4.1 Primary map



X

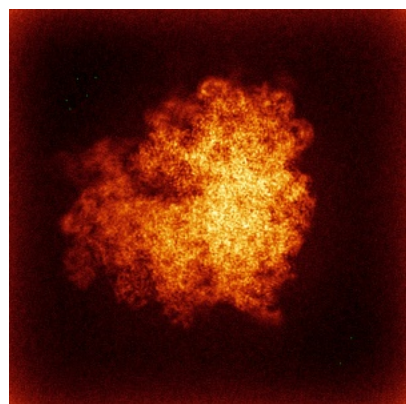


Y

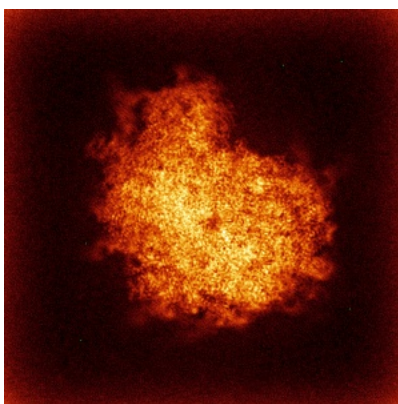


Z

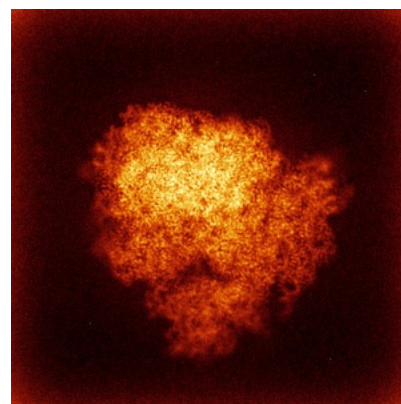
6.4.2 Raw map



X



Y

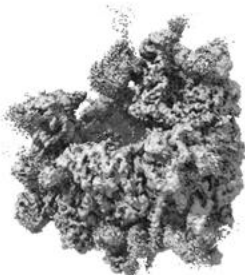


Z

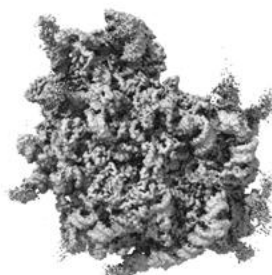
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



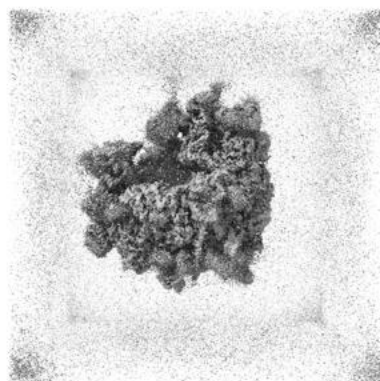
Y



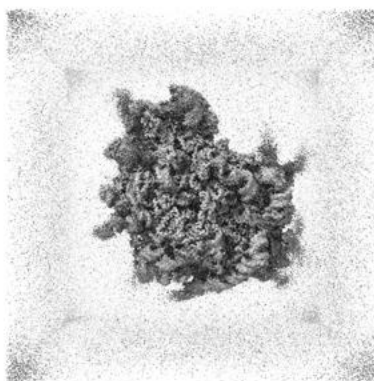
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

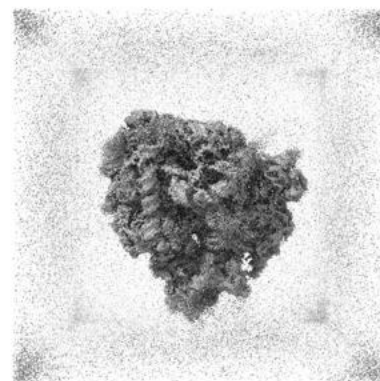
6.5.2 Raw map



X



Y



Z

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.

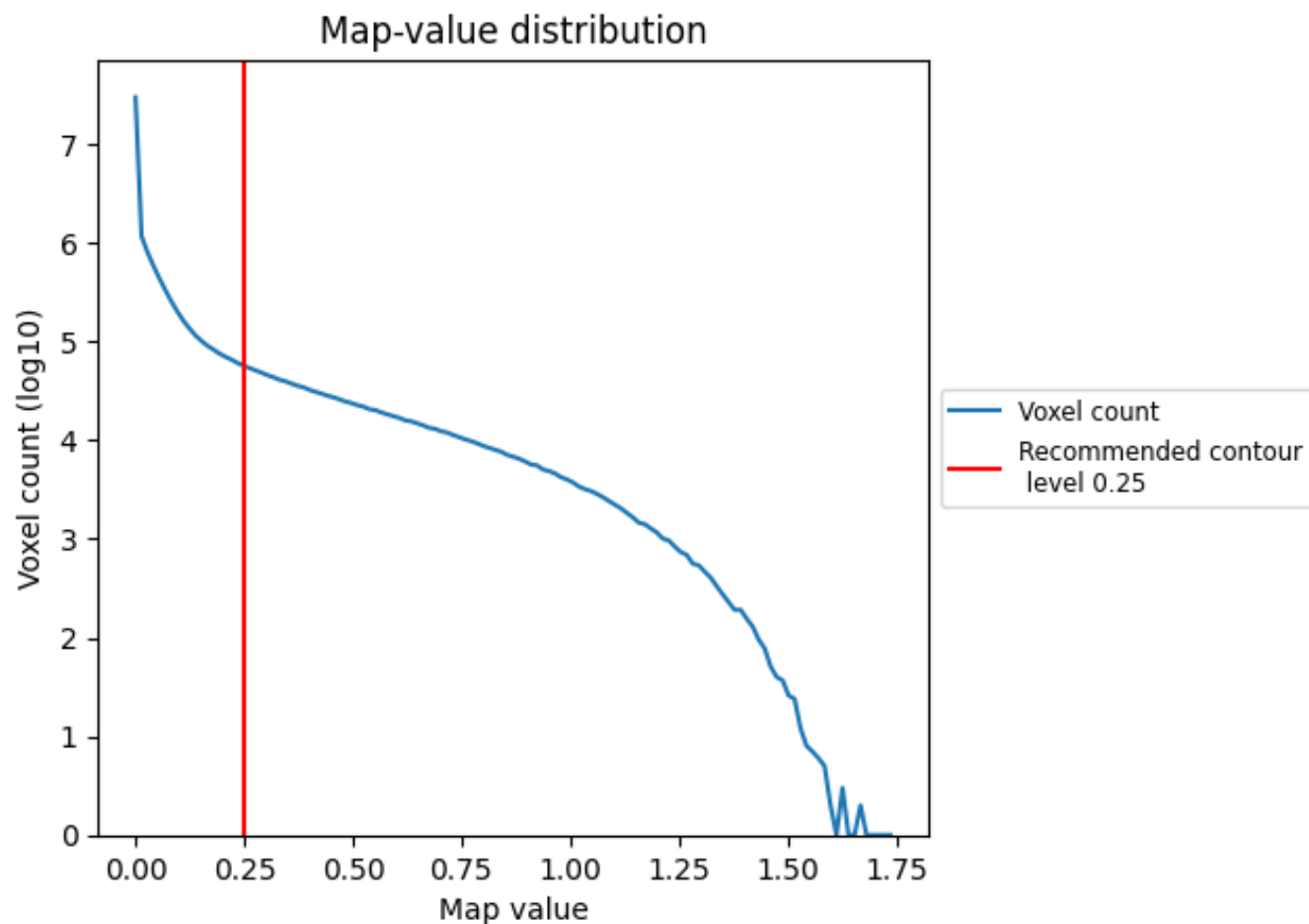
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

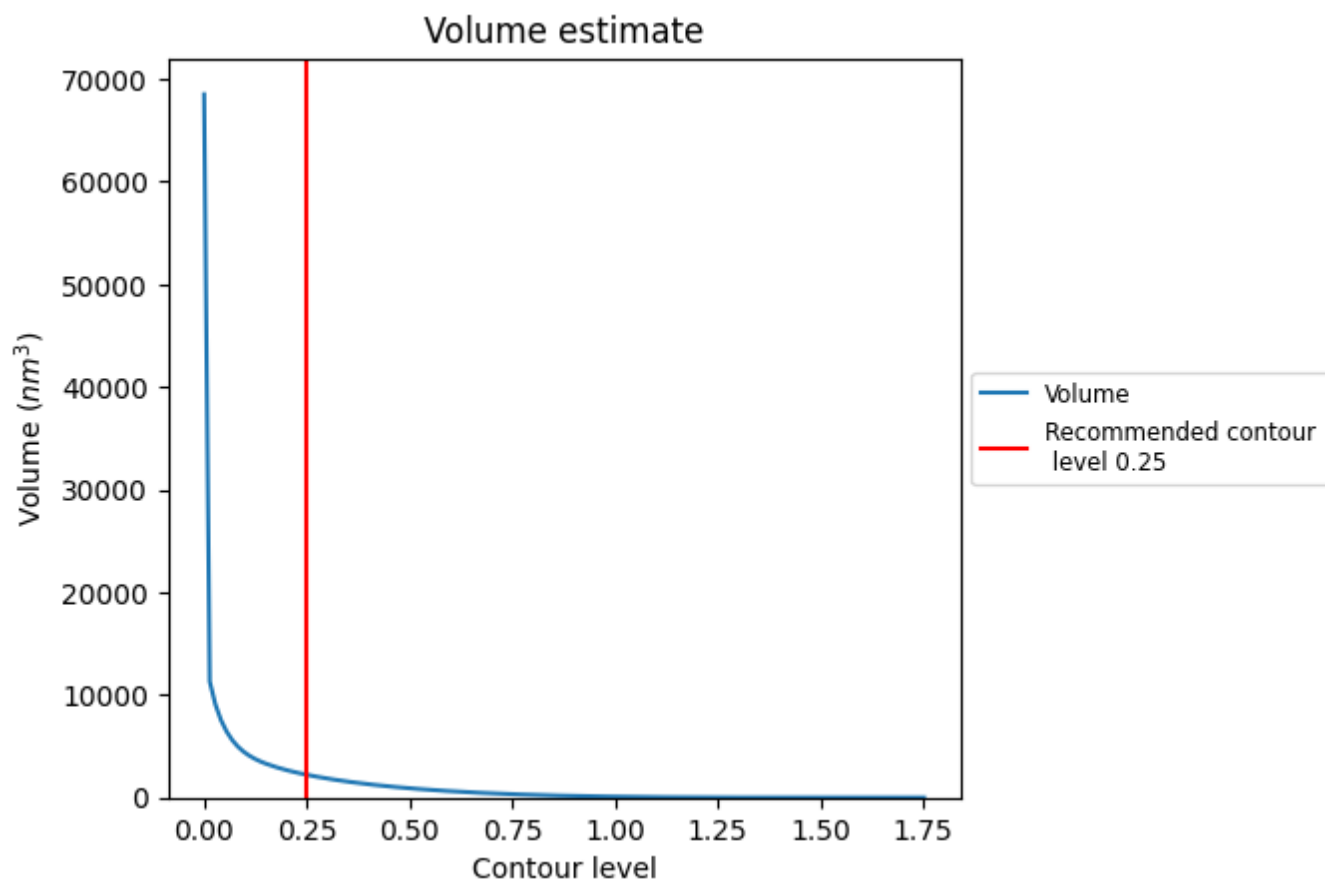
This section contains the results of statistical analysis of the map.

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.

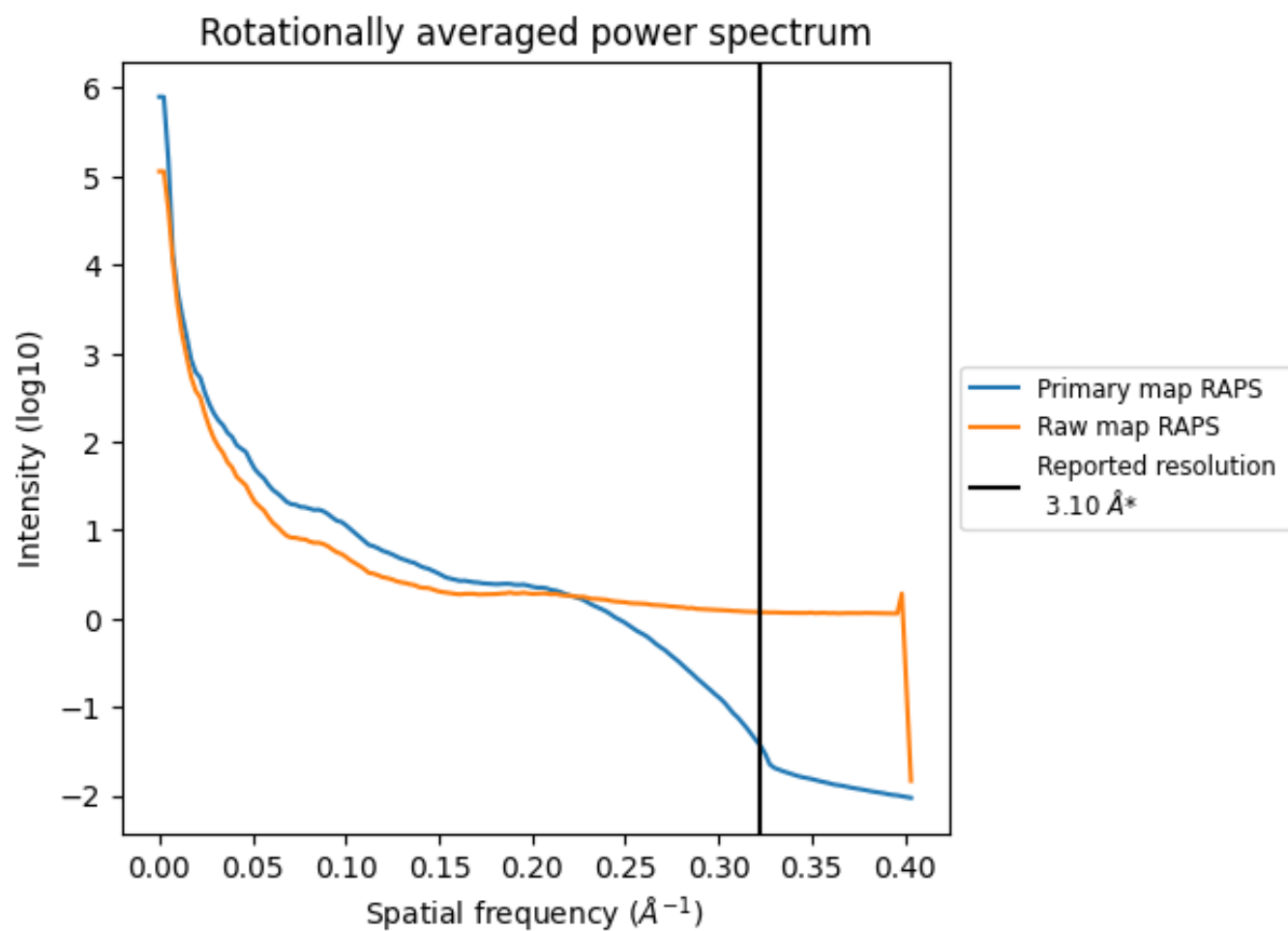
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2219 nm³; this corresponds to an approximate mass of 2005 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

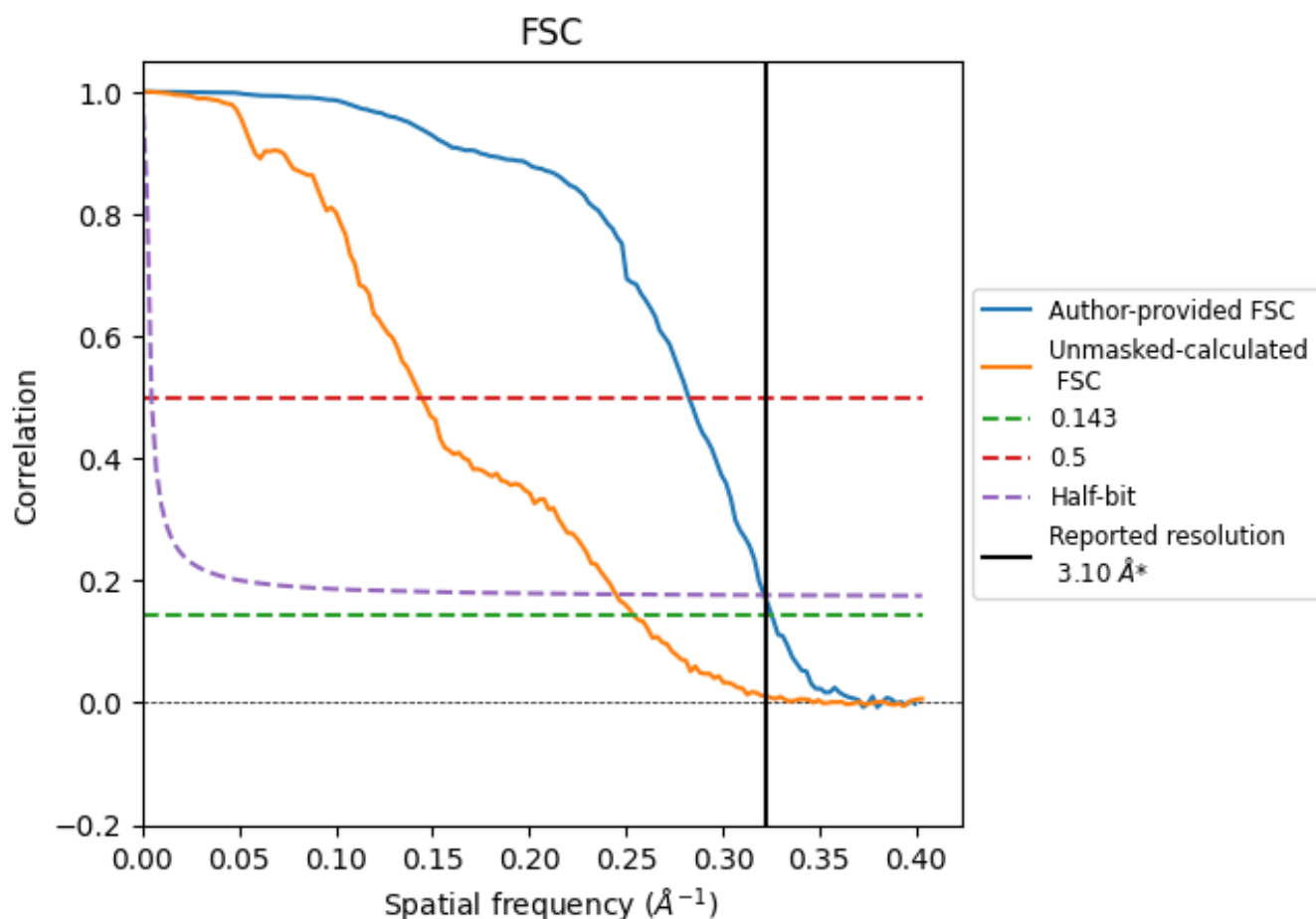


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

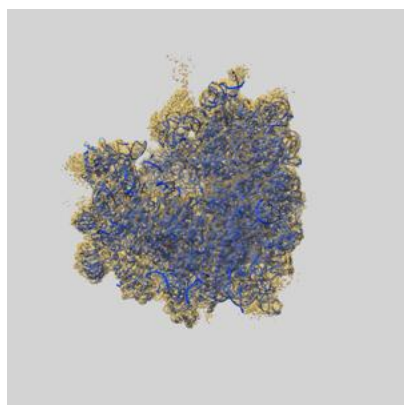
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.54	3.11
Unmasked-calculated*	3.94	6.93	4.08

*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 3.94 differs from the reported value 3.1 by more than 10 %

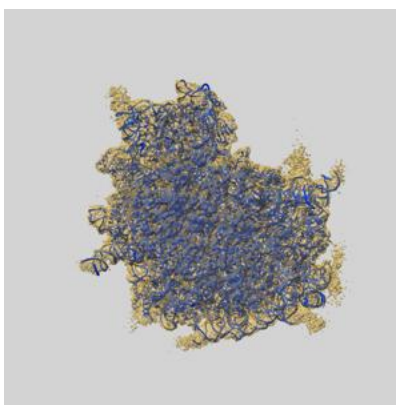
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14752 and PDB model 7ZJX. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

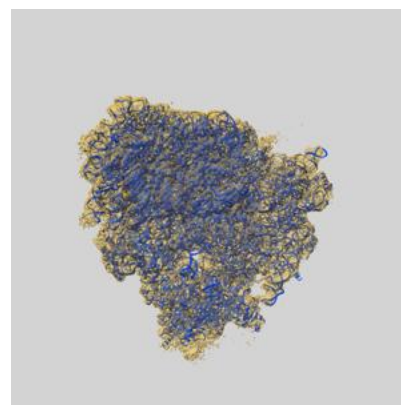
9.1 Map-model overlay [i](#)



X



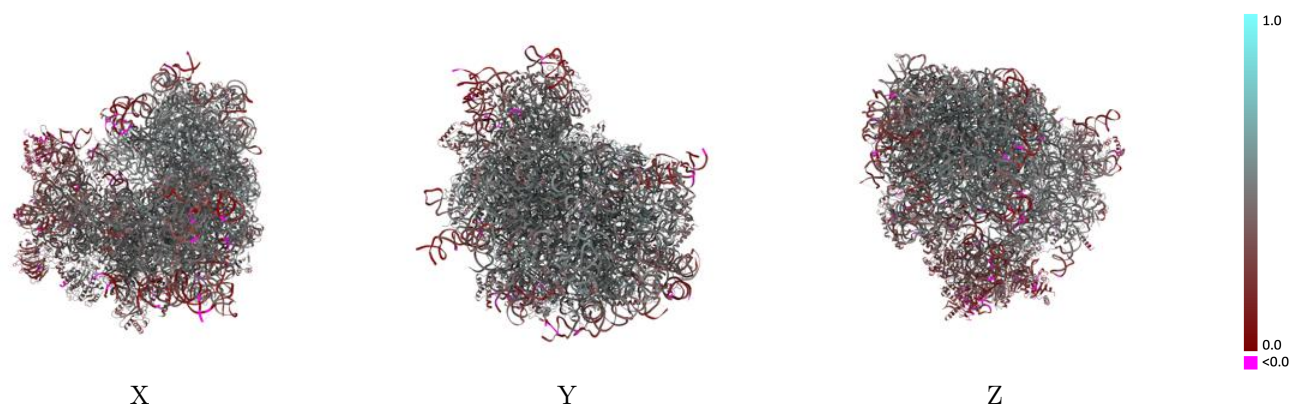
Y



Z

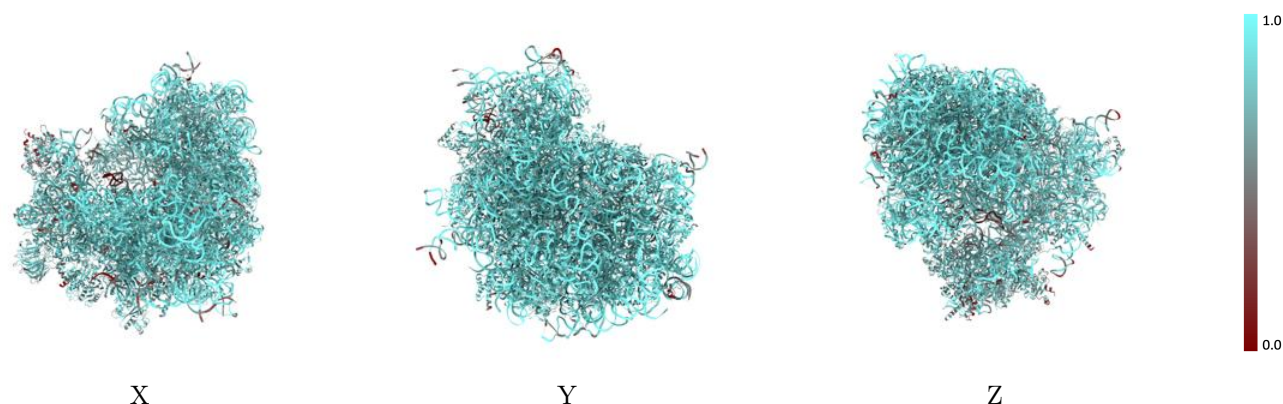
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



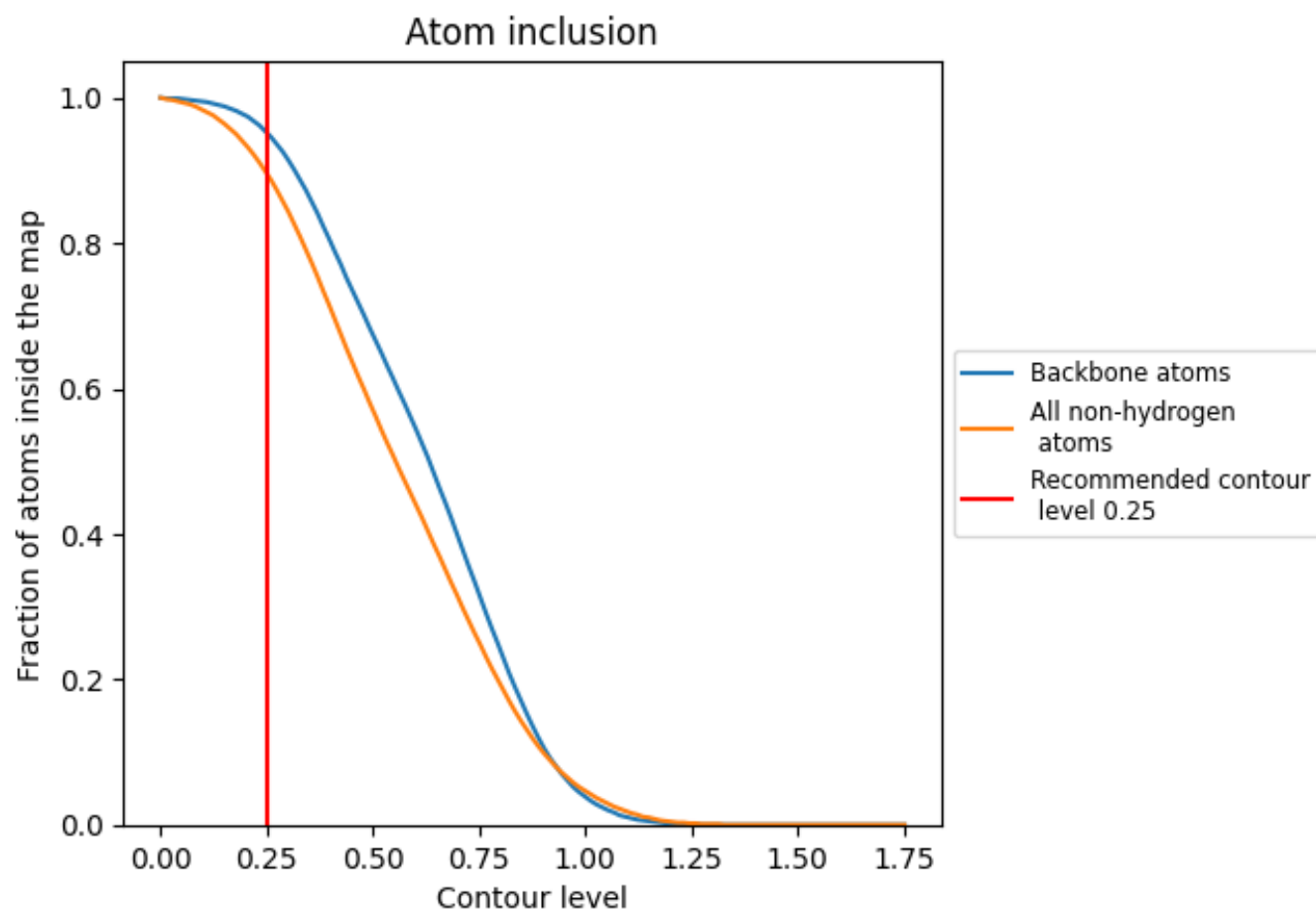
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.4280
B	 0.5320	 0.1750
I	 0.6960	 0.1580
L5	 0.9580	 0.4480
L7	 0.9920	 0.4880
L8	 0.9680	 0.4730
LD	 0.8600	 0.5080
LE	 0.8940	 0.4970
LF	 0.8860	 0.4920
LG	 0.8860	 0.4490
LH	 0.8290	 0.4210
LI	 0.8610	 0.4830
LJ	 0.8620	 0.4420
LK	 0.8690	 0.4790
LL	 0.8030	 0.4740
LM	 0.8070	 0.4090
LO	 0.8570	 0.4520
LP	 0.8970	 0.4600
LQ	 0.9190	 0.5190
LR	 0.8740	 0.4890
LS	 0.8720	 0.4930
LT	 0.8770	 0.4920
LU	 0.8710	 0.4630
LV	 0.8880	 0.5030
LW	 0.8370	 0.4790
LX	 0.8900	 0.4380
LY	 0.8280	 0.4910
LZ	 0.7810	 0.3950
La	 0.8560	 0.4730
Lb	 0.8720	 0.4800
Lc	 0.9230	 0.4830
Ld	 0.9300	 0.5100
Le	 0.7920	 0.3950
Lf	 0.7950	 0.4400
Lg	 0.8910	 0.4910



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Chain	Atom inclusion	Q-score
Lh	 0.8630	 0.4970
Li	 0.8920	 0.5140
Lj	 0.8630	 0.4790
Lk	 0.8660	 0.4640
Ll	 0.8440	 0.4370
Lm	 0.9050	 0.5140
Ln	 0.8420	 0.4420
Lo	 0.8530	 0.4670
Lp	 0.8740	 0.4850
Lq	 0.7960	 0.4680
Lr	 0.8240	 0.4830
Ls	 0.8960	 0.4910
Lx	 0.8010	 0.1730
S	 0.7810	 0.1380
S2	 0.9450	 0.4130
SB	 0.8330	 0.4410
SC	 0.6650	 0.3490
SD	 0.6800	 0.2290
SE	 0.7000	 0.3620
SF	 0.8240	 0.4520
SG	 0.7540	 0.2530
SH	 0.8170	 0.3830
SL	 0.8010	 0.4180
SM	 0.8140	 0.4400
SN	 0.8200	 0.4540
SO	 0.7080	 0.3550
SP	 0.8460	 0.4500
SQ	 0.7410	 0.3230
SR	 0.8400	 0.3770
SS	 0.7700	 0.3820
ST	 0.8460	 0.4560
SU	 0.8380	 0.4240
SV	 0.7630	 0.3430
SW	 0.7640	 0.4440
SX	 0.5510	 0.1750
SY	 0.8290	 0.4600
SZ	 0.8410	 0.4580
Sa	 0.6580	 0.3070
Sb	 0.7780	 0.3230
Sc	 0.7350	 0.3580
Sd	 0.6990	 0.2790
Se	 0.8020	 0.3240

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Chain	Atom inclusion	Q-score
Sf	 0.7700	 0.3470
Sg	 0.8360	 0.4270
Sh	 0.8330	 0.4650
Si	 0.8390	 0.4840
Sj	 0.8450	 0.3800
Sk	 0.7560	 0.2420
Sl	 0.8490	 0.4840