



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 06:04 am BST

PDB ID : 8QOI / pdb_00008qoi
EMDB ID : EMD-18539
Title : Structure of the human 80S ribosome at 1.9 Å resolution - the molecular role of chemical modifications and ions in RNA
Authors : Holvec, S.; Barchet, C.; Frechin, L.; Hazemann, I.; von Loeffelholz, O.; Klaholz, B.P.
Deposited on : 2023-09-29
Resolution : 1.90 Å (reported)
Based on initial model : 6QZP

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:

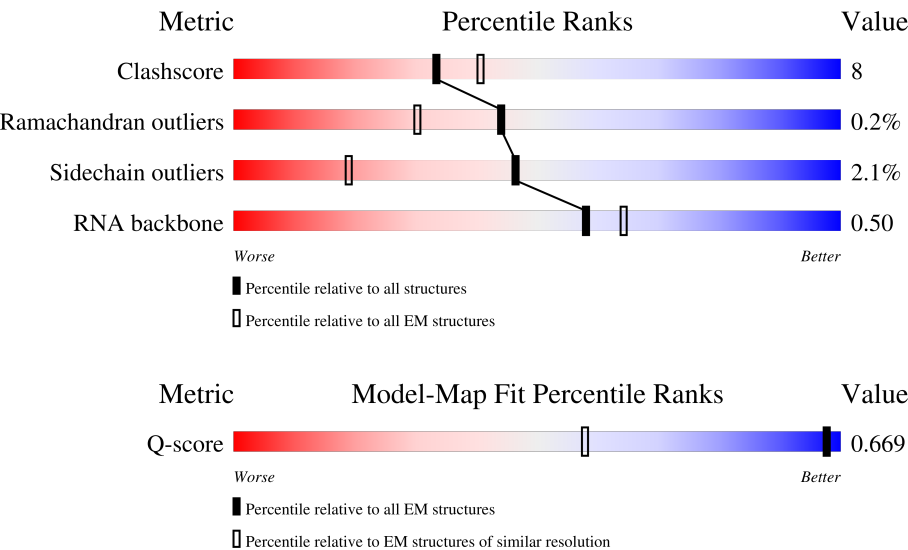
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 1.90 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	1185 (1.40 - 2.40)

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	L5	5069	17% 37% 29% 8% 26%
2	L7	120	62% 32% . .
3	L8	157	11% 48% 41% 10% ..

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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	402	
6	LC	368	
7	LD	293	
8	LE	247	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	

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Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	S2	1869	
47	SE	263	
48	SA	295	
49	SB	264	
50	SD	243	
51	SF	204	
52	SH	194	
53	SI	208	

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Mol	Chain	Length	Quality of chain
54	SK	165	
55	SL	158	
56	SP	145	
57	SQ	146	
58	SS	152	
59	ST	145	
60	SU	119	
61	SV	83	
62	SX	143	
63	Sa	115	
64	Sc	69	
65	Sd	56	
66	Sg	317	
67	SC	293	
68	SG	249	
69	SJ	194	
70	SM	132	
71	SN	151	
72	SO	151	
73	SW	130	
74	SY	133	
75	SZ	125	
76	Sb	84	
77	Se	133	
78	Sf	156	

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Mol	Chain	Length	Quality of chain
79	SR	135	22% 67% 30%

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 233370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA (3773-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3773	Total	C	N	O	P	0	0
			80205	35722	14588	26123	3772		

- Molecule 2 is a RNA chain called 5S rRNA (120-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA (156-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1713	1083	329	285	16		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	122	Total	C	N	O	S	0	0
			997	622	203	168	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	99	Total	C	N	O	S	0	0
			808	502	177	125	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	99	Total	C	N	O	S	0	0
			813	509	173	126	5		

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

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

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

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

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	51	Total	C	N	O	S	0	0
			419	260	88	65	6		

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

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	102	Total	C	N	O	S	1	0
			842	527	174	135	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lp	88	Total	C	N	O	S	0	0
			681	430	131	113	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	123	Total	C	N	O	S	0	0
			987	612	205	166	4		

- Molecule 46 is a RNA chain called 18S rRNA (1740-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S2	1740	Total	C	N	O	P	0	0
			36955	16511	6600	12105	1739		

- Molecule 47 is a protein called 40S ribosomal protein S4, X isoform.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SA	219	Total	C	N	O	S	0	0
			1727	1096	302	320	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	215	Total	C	N	O	S	0	0
			1747	1109	312	312	14		

- Molecule 50 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 53 is a protein called 40S ribosomal protein S8.

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

- Molecule 54 is a protein called 40S ribosomal protein S10.

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

- Molecule 55 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	154	Total	C	N	O	S	0	0
			1258	802	235	215	6		

- Molecule 56 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SP	125	Total	C	N	O	S	0	0
			1027	653	193	174	7		

- Molecule 57 is a protein called 40S ribosomal protein S16.

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

- Molecule 58 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 59 is a protein called Small ribosomal subunit protein eS19.

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

- Molecule 60 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SU	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 61 is a protein called 40S ribosomal protein S21.

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

- Molecule 62 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 63 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sa	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 64 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 65 is a protein called 40S ribosomal protein S29.

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

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SC	221	Total	C	N	O	S	1	0
			1724	1115	298	301	10		

- Molecule 68 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SG	234	Total	C	N	O	S	0	0
			1903	1188	384	324	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SJ	182	Total	C	N	O	S	1	0
			1520	967	306	245	2		

- Molecule 70 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SM	118	Total	C	N	O	S	0	0
			906	568	158	172	8		

- Molecule 71 is a protein called 40S ribosomal protein S13.

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

- Molecule 72 is a protein called 40S ribosomal protein S14.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SO	138	IAS	ASP	conflict	UNP P62263

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

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SY	128	Total	C	N	O	S	1	0
			1048	661	207	175	5		

- Molecule 75 is a protein called 40S ribosomal protein S25.

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

- Molecule 76 is a protein called 40S ribosomal protein S27.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 79 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SR	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	L5	198	Total	Mg	0
			198	198	
80	L7	2	Total	Mg	0
			2	2	
80	L8	4	Total	Mg	0
			4	4	
80	LI	1	Total	Mg	0
			1	1	
80	LN	1	Total	Mg	0
			1	1	
80	LP	1	Total	Mg	0
			1	1	

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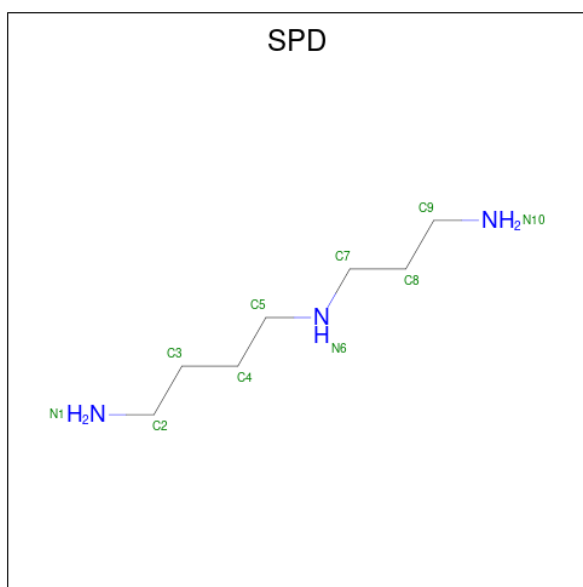
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Mol	Chain	Residues	Atoms		AltConf
80	LV	1	Total 1	Mg 1	0
80	S2	84	Total 84	Mg 84	0

- Molecule 81 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
81	L5	78	Total 78	K 78	0
81	L7	1	Total 1	K 1	0
81	LA	1	Total 1	K 1	0
81	LB	1	Total 1	K 1	0
81	LI	1	Total 1	K 1	0
81	Le	1	Total 1	K 1	0
81	Lf	1	Total 1	K 1	0
81	Lo	1	Total 1	K 1	0
81	S2	21	Total 21	K 21	0
81	Sd	1	Total 1	K 1	0
81	SO	1	Total 1	K 1	0

- Molecule 82 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



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

- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 84 is water.

Mol	Chain	Residues	Atoms		AltConf
84	L5	9116	Total 9116	O 9116	0
84	L7	175	Total 175	O 175	0
84	L8	376	Total 376	O 376	0
84	LA	176	Total 176	O 176	0
84	LB	135	Total 135	O 135	0
84	LC	149	Total 149	O 149	0
84	LD	29	Total 29	O 29	0
84	LE	32	Total 32	O 32	0
84	LF	83	Total 83	O 83	0
84	LG	40	Total 40	O 40	0
84	LH	27	Total 27	O 27	0
84	LI	36	Total 36	O 36	0
84	LJ	5	Total 5	O 5	0
84	LL	71	Total 71	O 71	0
84	LM	16	Total 16	O 16	0
84	LN	131	Total 131	O 131	0
84	LO	59	Total 59	O 59	0
84	LP	61	Total 61	O 61	0
84	LQ	99	Total 99	O 99	0
84	LR	103	Total 103	O 103	0
84	LS	55	Total 55	O 55	0
84	LT	59	Total 59	O 59	0

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Mol	Chain	Residues	Atoms		AltConf
84	LU	6	Total 6	O 6	0
84	LV	61	Total 61	O 61	0
84	LW	49	Total 49	O 49	0
84	LX	32	Total 32	O 32	0
84	LY	36	Total 36	O 36	0
84	LZ	13	Total 13	O 13	0
84	La	70	Total 70	O 70	0
84	Lb	34	Total 34	O 34	0
84	Lc	55	Total 55	O 55	0
84	Ld	29	Total 29	O 29	0
84	Le	81	Total 81	O 81	0
84	Lf	47	Total 47	O 47	0
84	Lg	52	Total 52	O 52	0
84	Lh	34	Total 34	O 34	0
84	Li	24	Total 24	O 24	0
84	Lj	55	Total 55	O 55	0
84	Lk	6	Total 6	O 6	0
84	Ll	22	Total 22	O 22	0
84	Lm	17	Total 17	O 17	0
84	Ln	39	Total 39	O 39	0
84	Lo	22	Total 22	O 22	0

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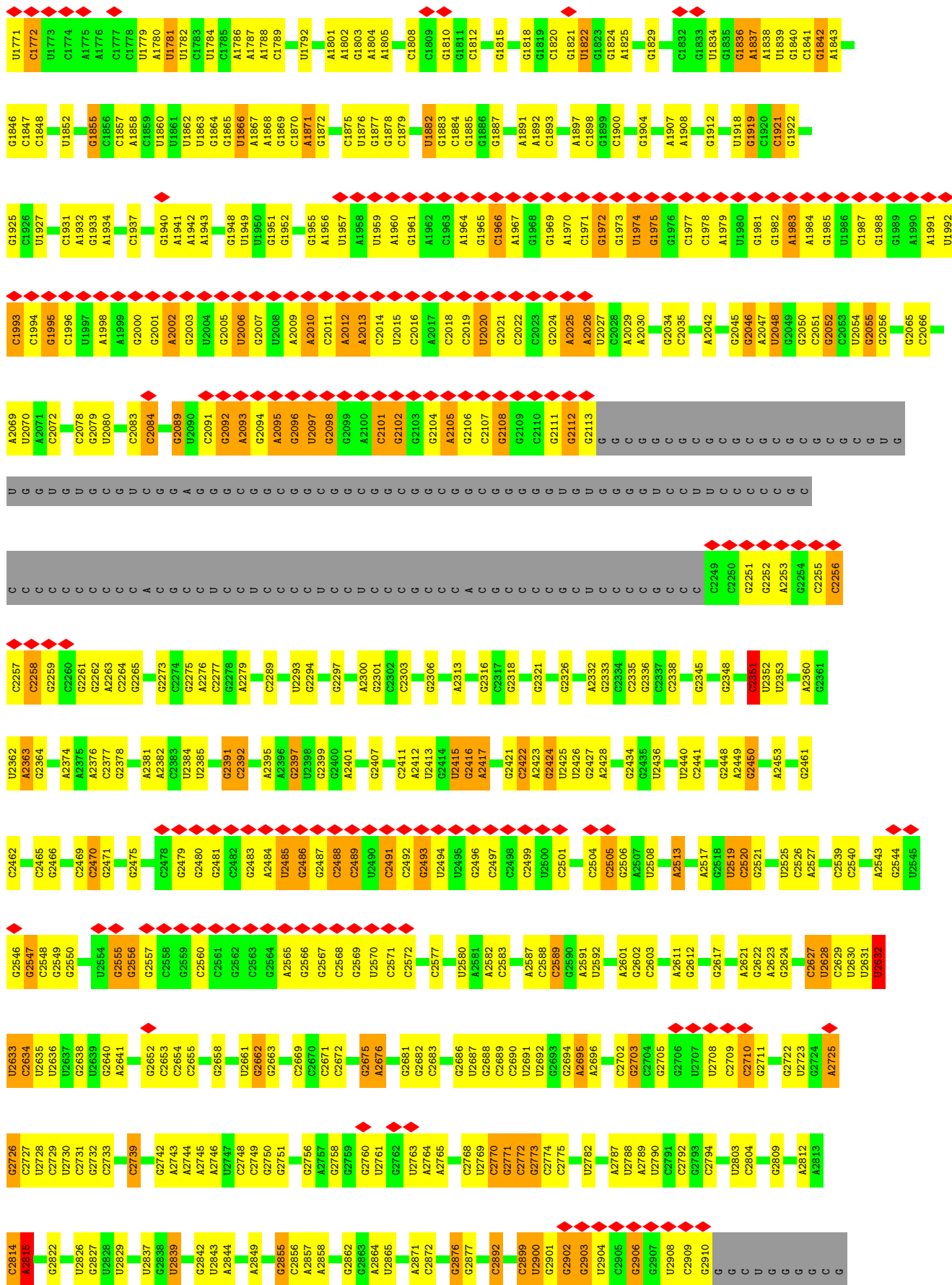
Mol	Chain	Residues	Atoms		AltConf
84	Lp	82	Total 82	O 82	0
84	Lr	41	Total 41	O 41	0
84	S2	4529	Total 4529	O 4529	0
84	SE	85	Total 85	O 85	0
84	SA	26	Total 26	O 26	0
84	SB	71	Total 71	O 71	0
84	SD	53	Total 53	O 53	0
84	SF	39	Total 39	O 39	0
84	SH	18	Total 18	O 18	0
84	SI	96	Total 96	O 96	0
84	SK	1	Total 1	O 1	0
84	SL	98	Total 98	O 98	0
84	SP	8	Total 8	O 8	0
84	SQ	29	Total 29	O 29	0
84	SS	10	Total 10	O 10	0
84	ST	15	Total 15	O 15	0
84	SU	8	Total 8	O 8	0
84	SV	27	Total 27	O 27	0
84	SX	95	Total 95	O 95	0
84	Sa	62	Total 62	O 62	0
84	Sc	21	Total 21	O 21	0

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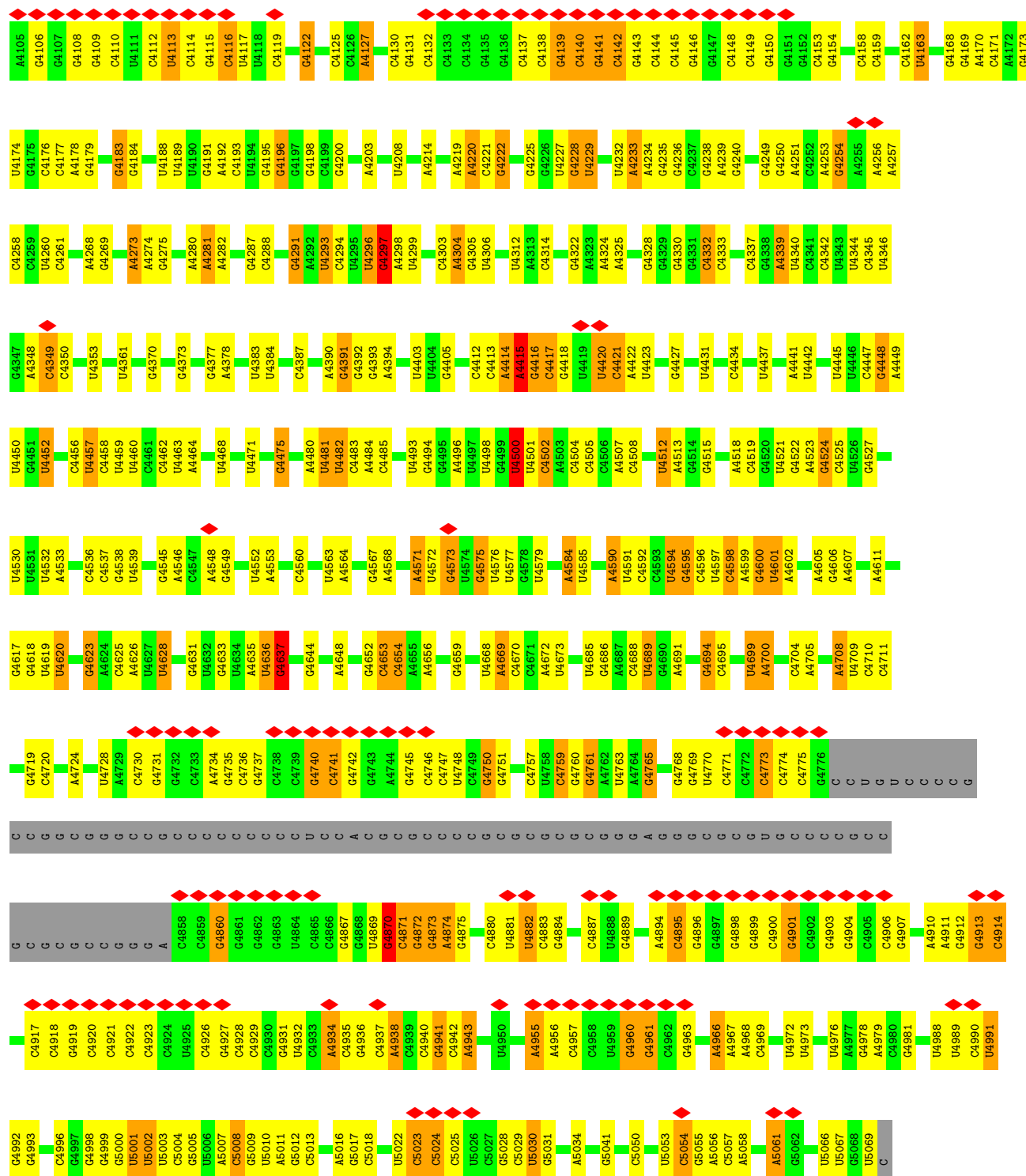
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Mol	Chain	Residues	Atoms		AltConf
84	Sd	8	Total 8	O 8	0
84	Sg	3	Total 3	O 3	0
84	SC	79	Total 79	O 79	0
84	SG	28	Total 28	O 28	0
84	SJ	76	Total 76	O 76	0
84	SN	87	Total 87	O 87	0
84	SO	52	Total 52	O 52	0
84	SW	64	Total 64	O 64	0
84	SY	32	Total 32	O 32	0
84	SZ	1	Total 1	O 1	0
84	Sb	27	Total 27	O 27	0
84	Se	21	Total 21	O 21	0
84	SR	29	Total 29	O 29	0



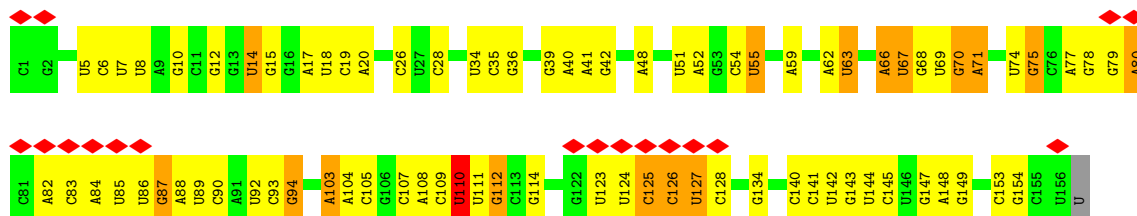




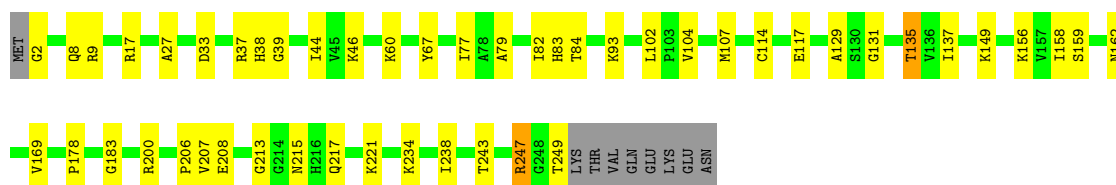
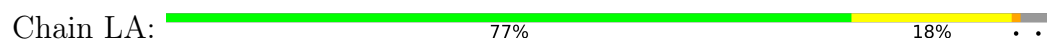




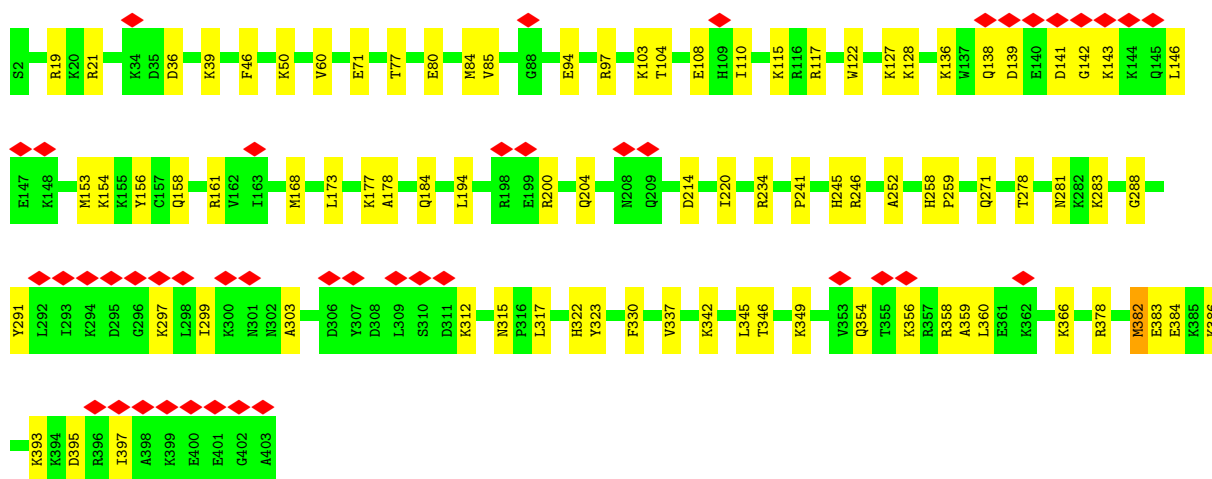
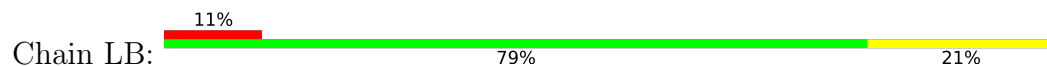
- Molecule 3: 5.8S rRNA (156-MER)



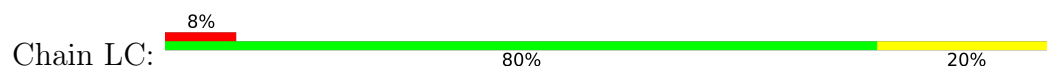
- Molecule 4: 60S ribosomal protein L8

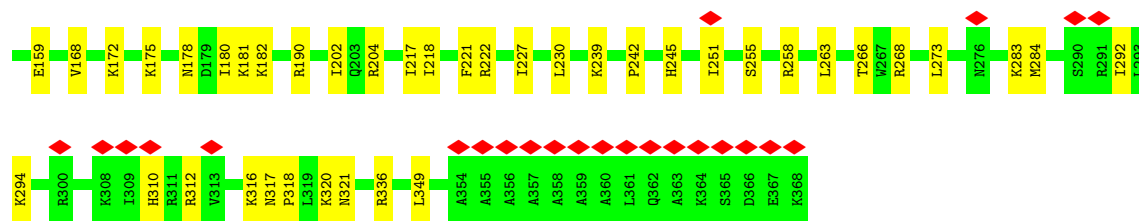


- Molecule 5: Large ribosomal subunit protein uL3

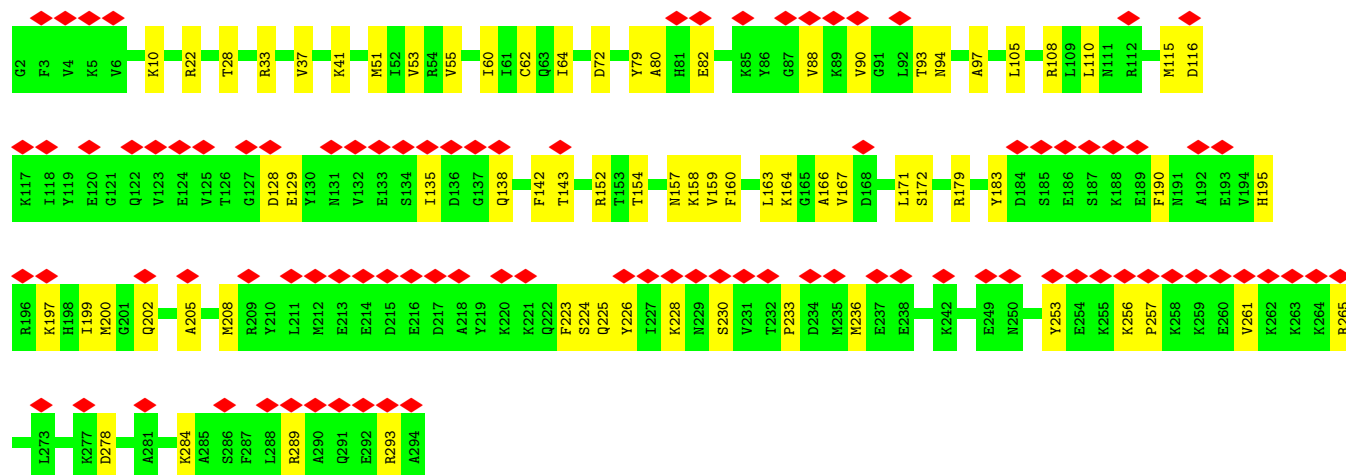
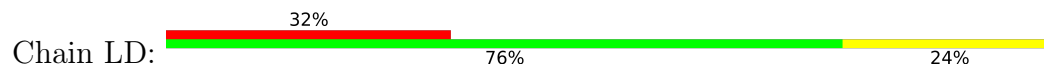


- Molecule 6: Large ribosomal subunit protein uL4

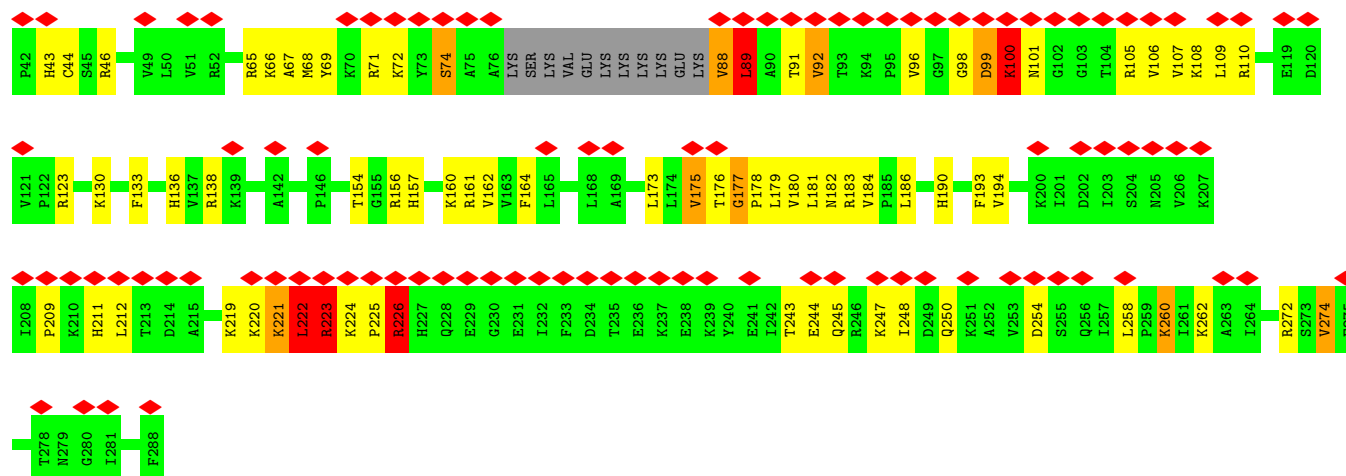
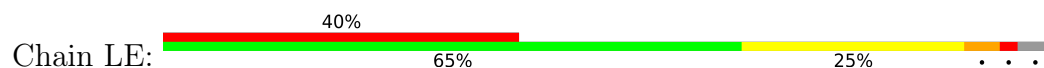




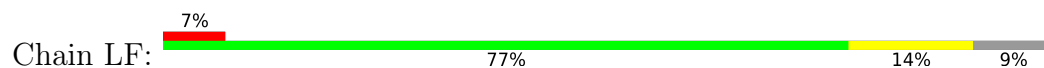
• Molecule 7: Large ribosomal subunit protein uL18

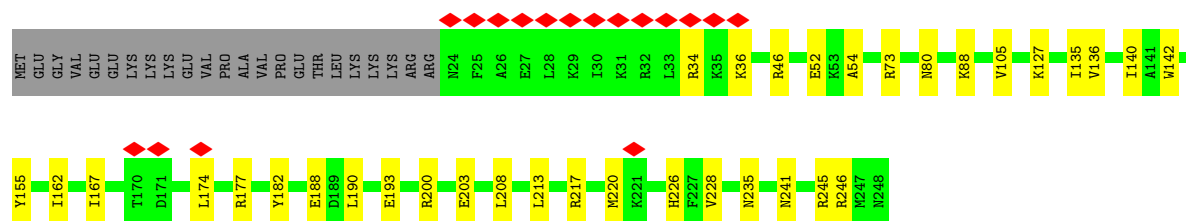


• Molecule 8: Large ribosomal subunit protein eL6

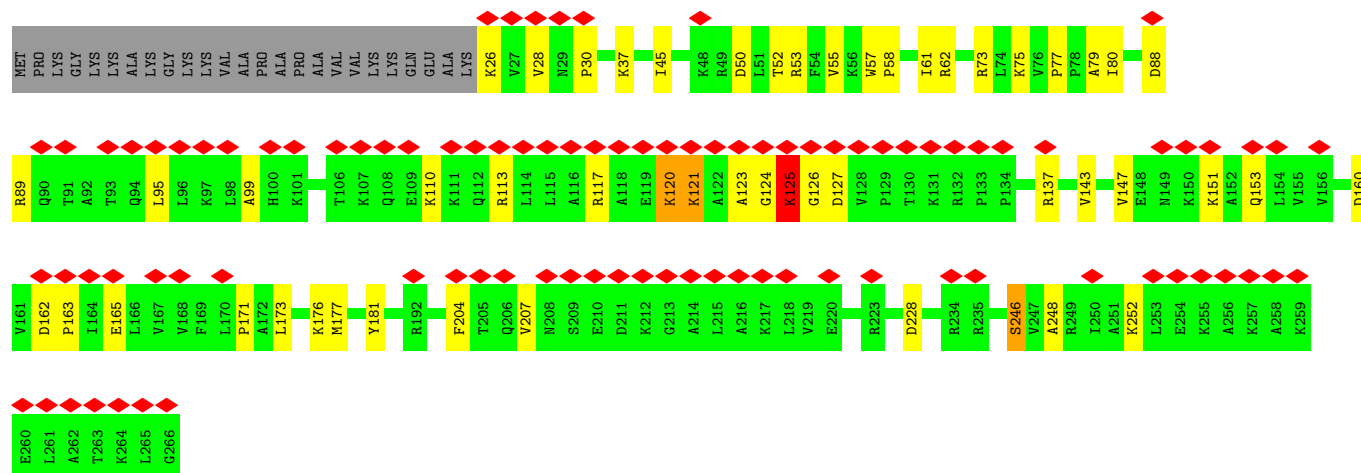
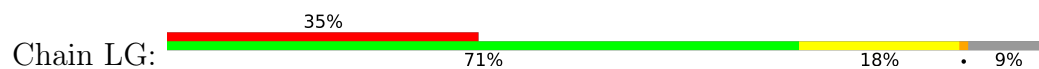


• Molecule 9: Large ribosomal subunit protein uL30

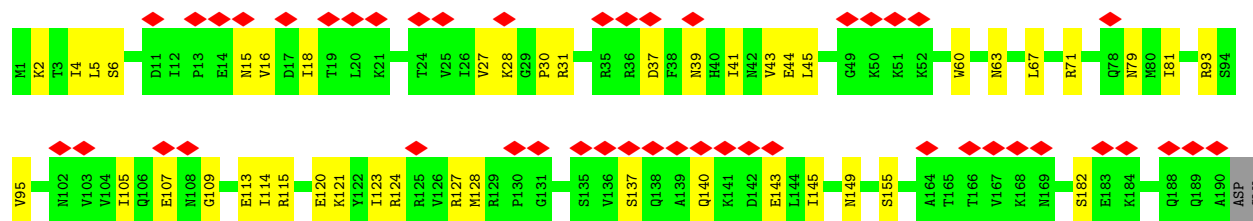
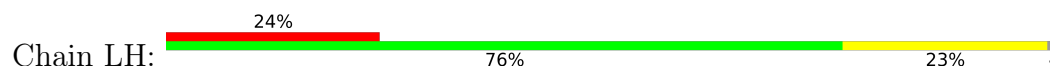




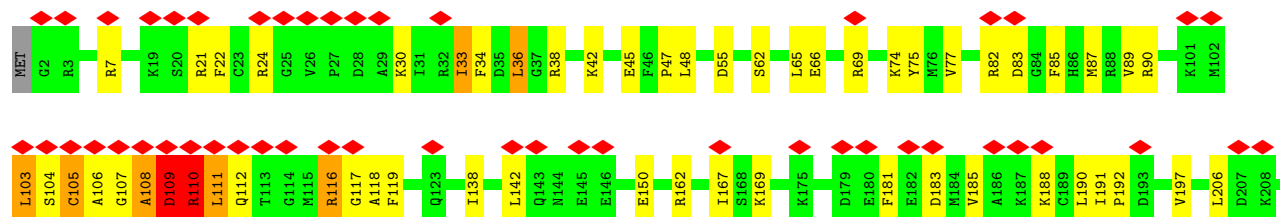
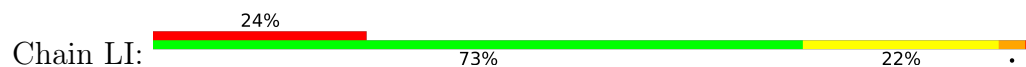
• Molecule 10: 60S ribosomal protein L7a

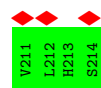


• Molecule 11: 60S ribosomal protein L9



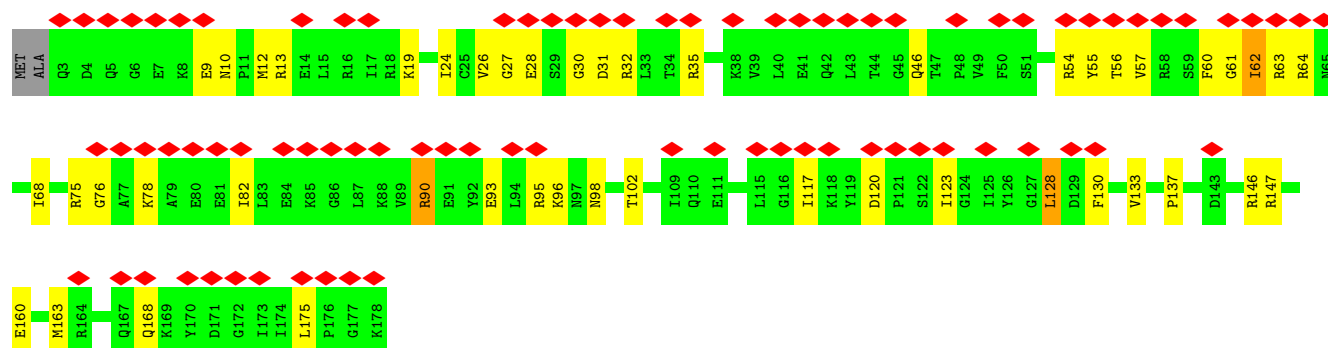
• Molecule 12: 60S ribosomal protein L10-like





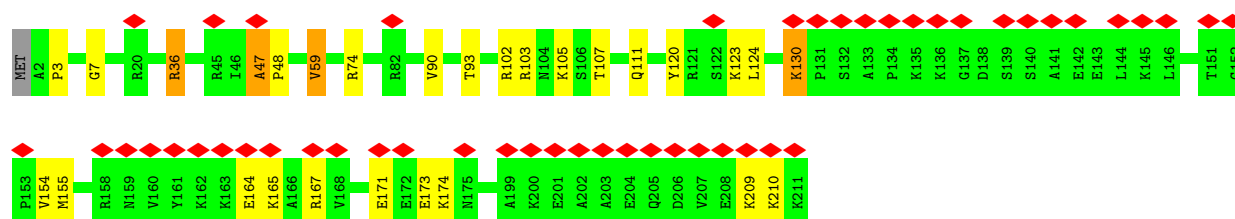
• Molecule 13: 60S ribosomal protein L11

Chain LJ: 46% 72% 25%



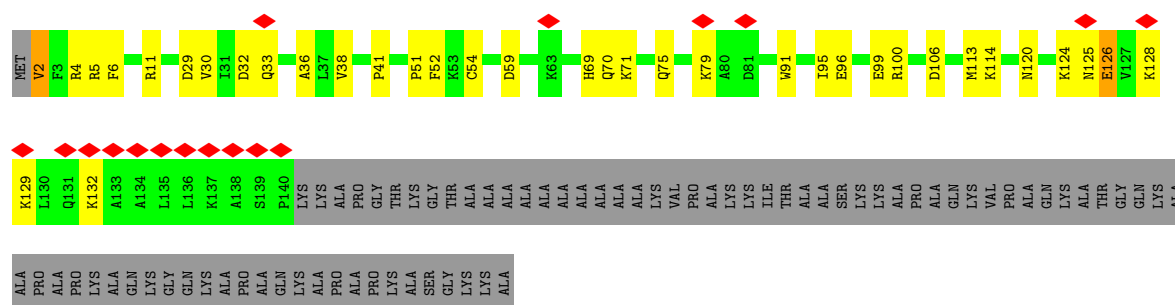
• Molecule 14: 60S ribosomal protein L13

Chain LL: 23% 86% 11%



• Molecule 15: 60S ribosomal protein L14

Chain LM: 8% 48% 16% 35%

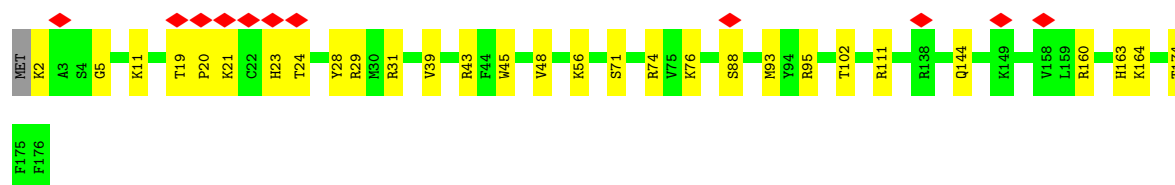


• Molecule 16: 60S ribosomal protein L15

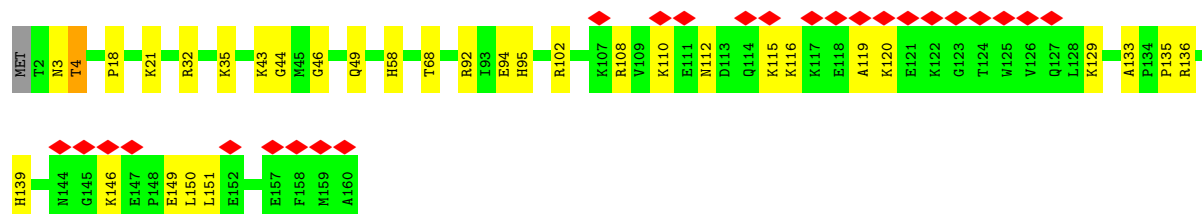
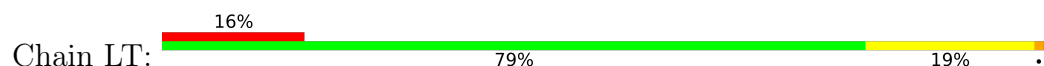
Chain LN: 84% 15%



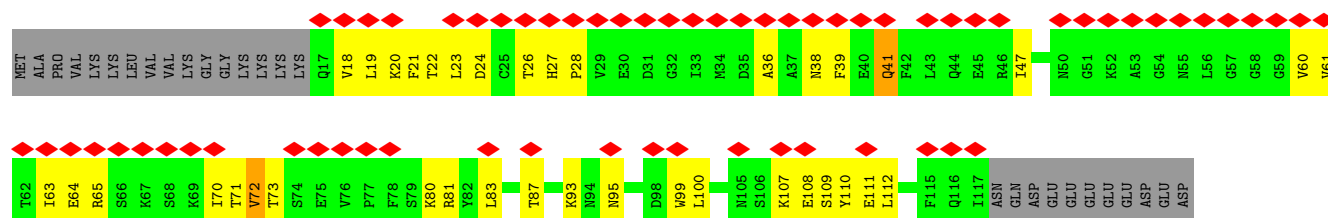
- Chain LS: 



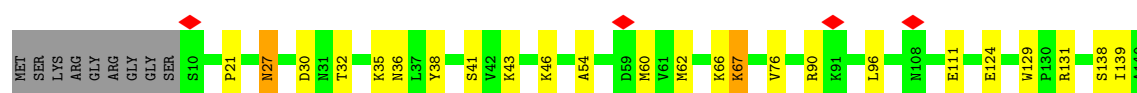
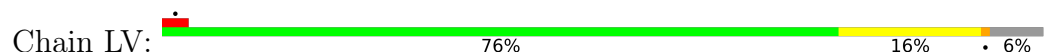
- Molecule 22: 60S ribosomal protein L21



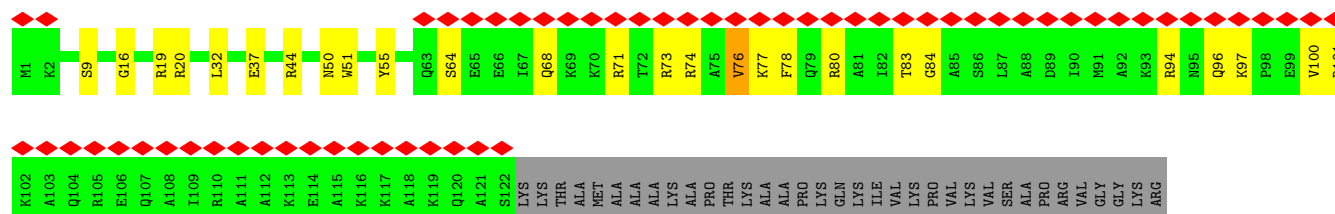
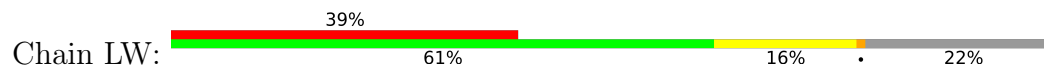
- Molecule 23: 60S ribosomal protein L22



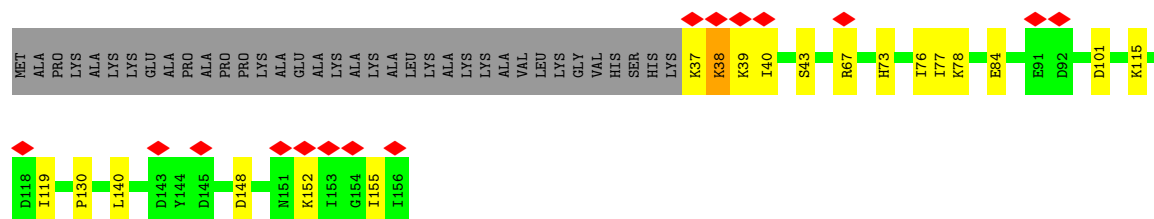
- Molecule 24: 60S ribosomal protein L23



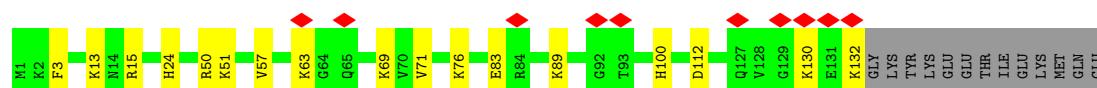
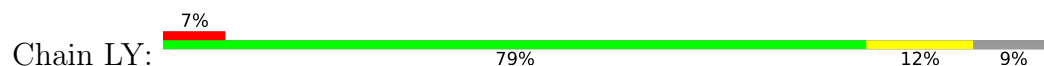
- Molecule 25: 60S ribosomal protein L24



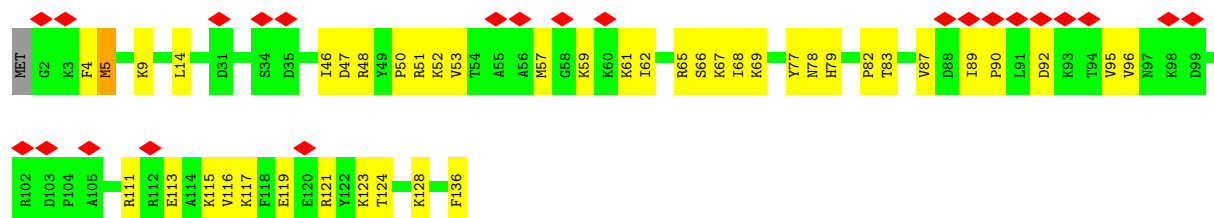
- Molecule 26: 60S ribosomal protein L23a



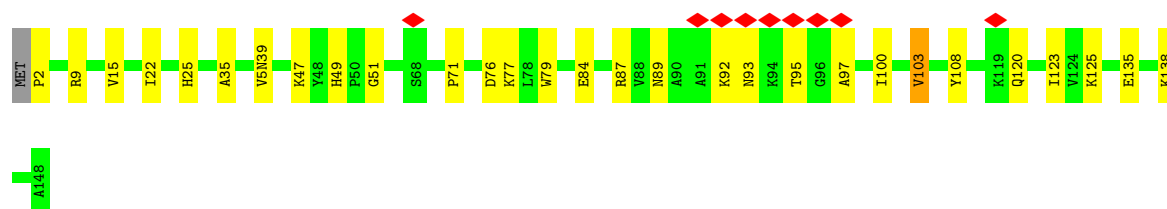
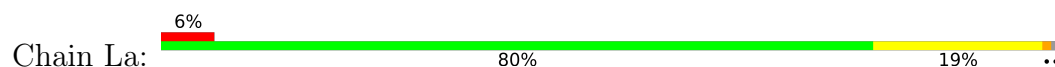
- Molecule 27: 60S ribosomal protein L26



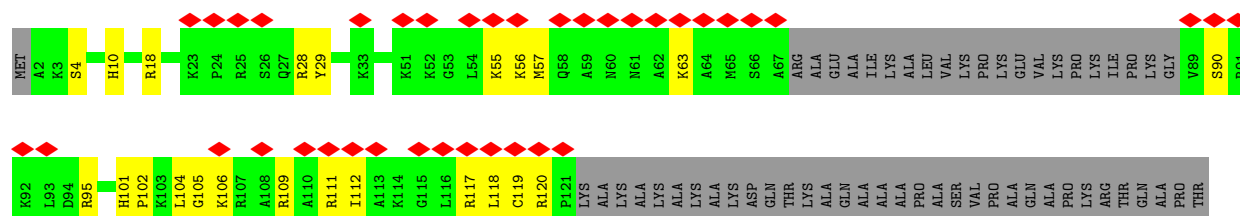
- Molecule 28: 60S ribosomal protein L27



- Molecule 29: Large ribosomal subunit protein uL15

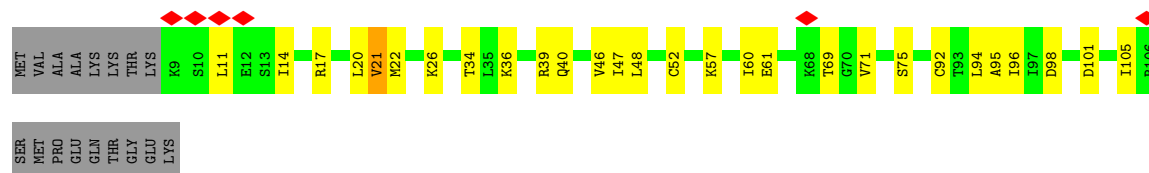


- Molecule 30: 60S ribosomal protein L29

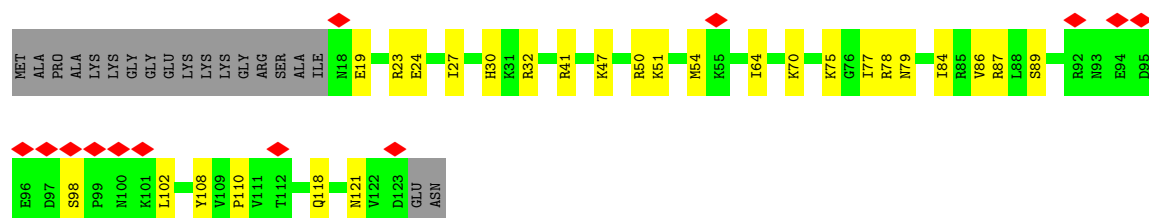


LYS
ALA
SER
GLU

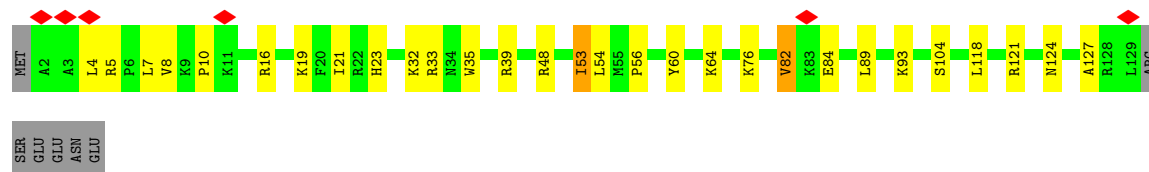
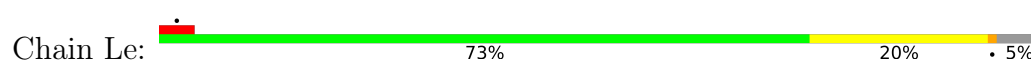
- Molecule 31: 60S ribosomal protein L30



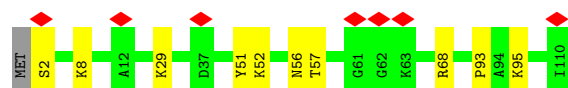
- Molecule 32: 60S ribosomal protein L31



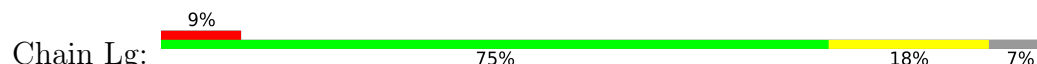
- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35

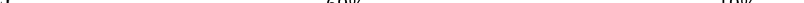
M1 R6 K7 S24 LYS

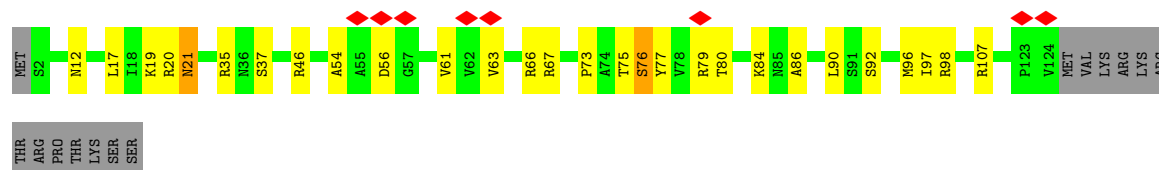
- Chain Lo: 

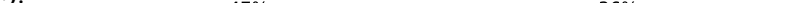


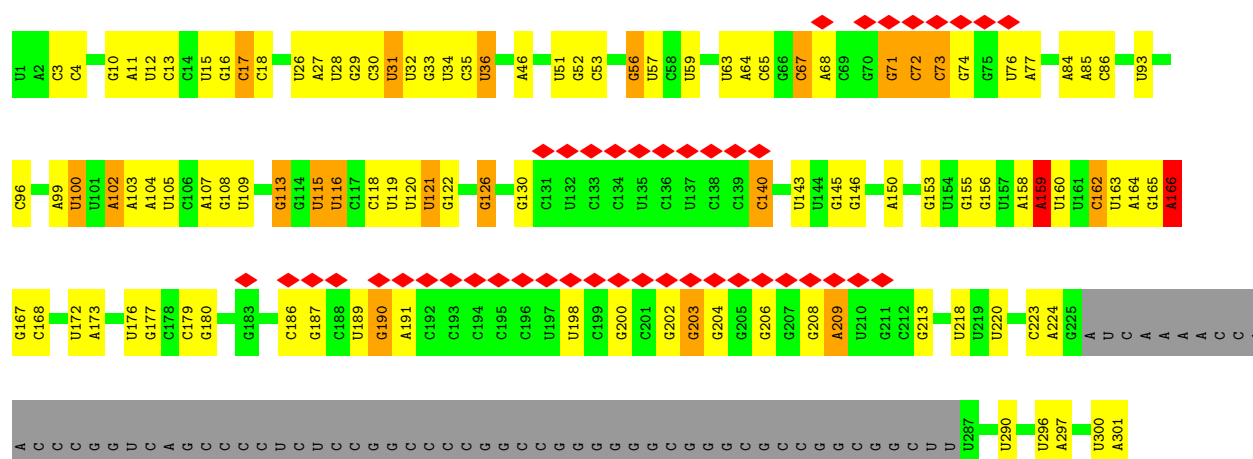
- Chain Lp: 77% 18% .

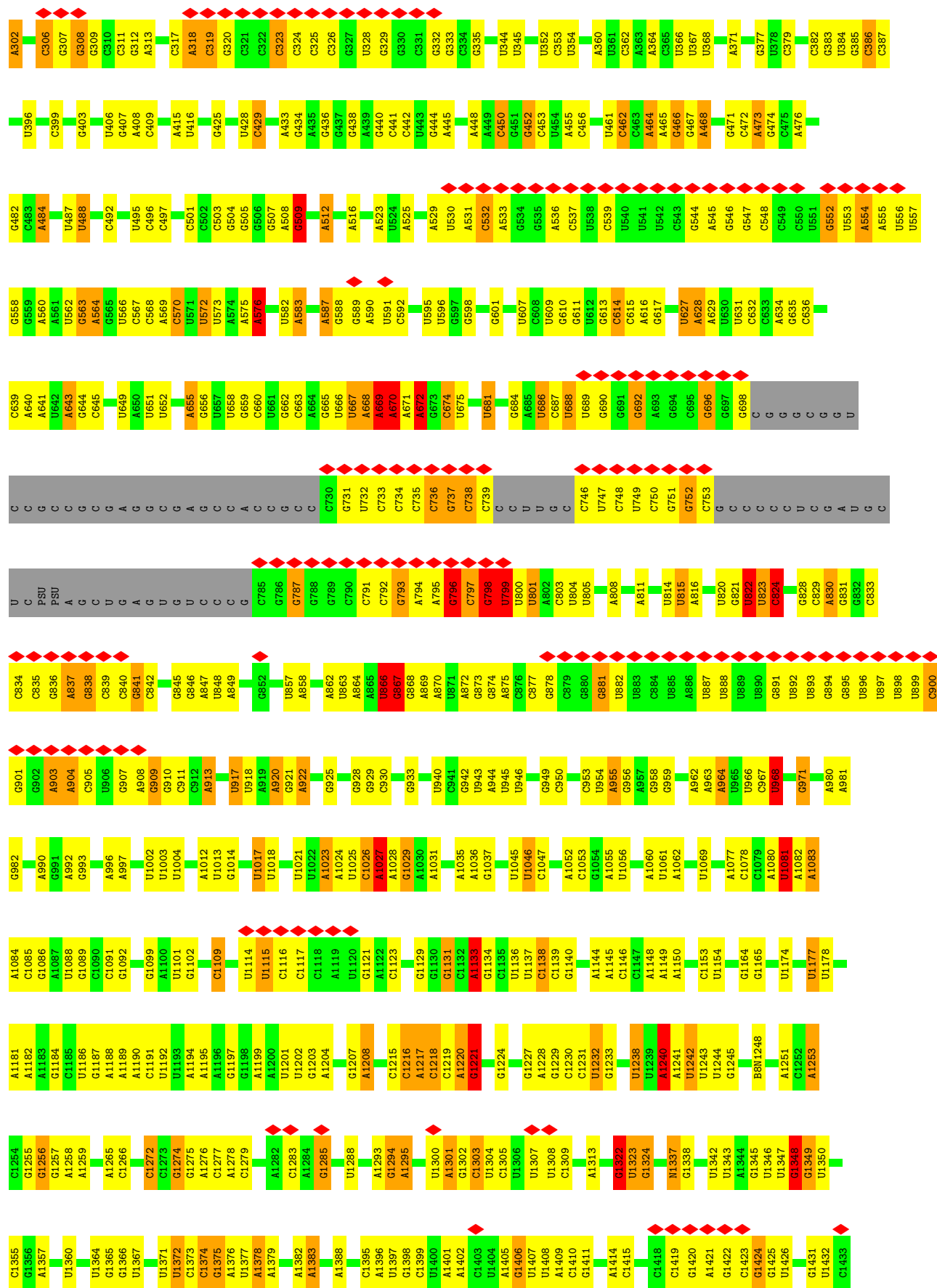


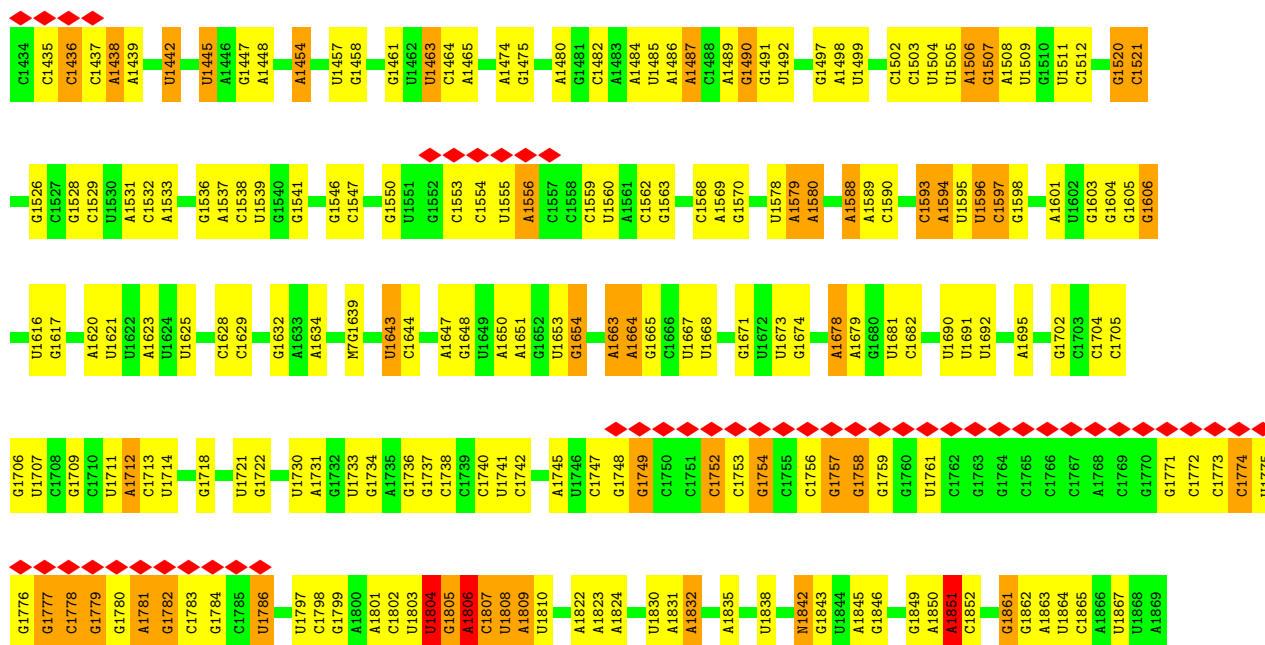
- Chain Lr: 



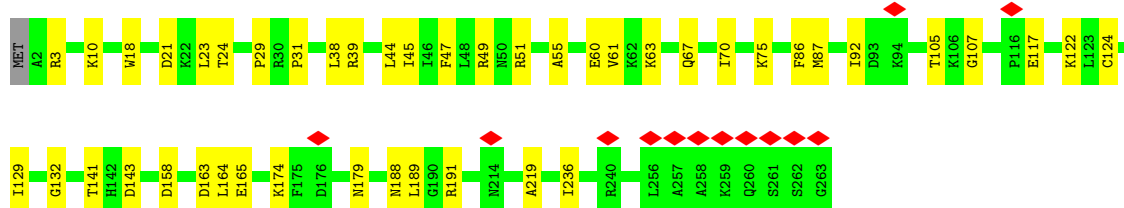
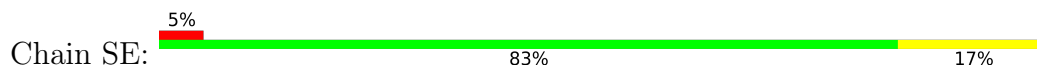
- Chain S2: 



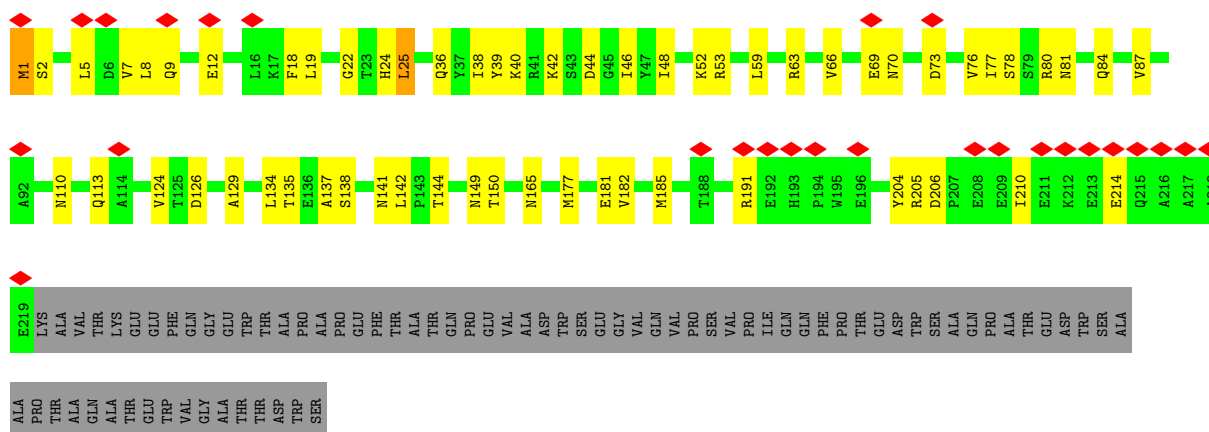




- Molecule 47: 40S ribosomal protein S4, X isoform

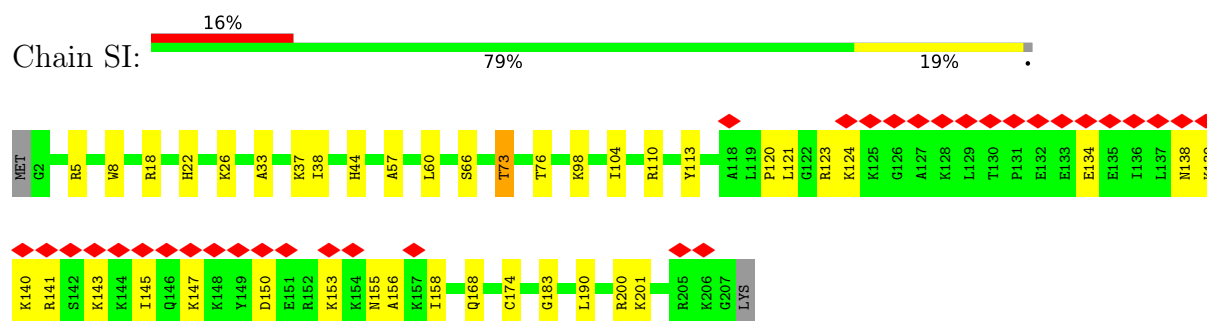


- Molecule 48: 40S ribosomal protein SA

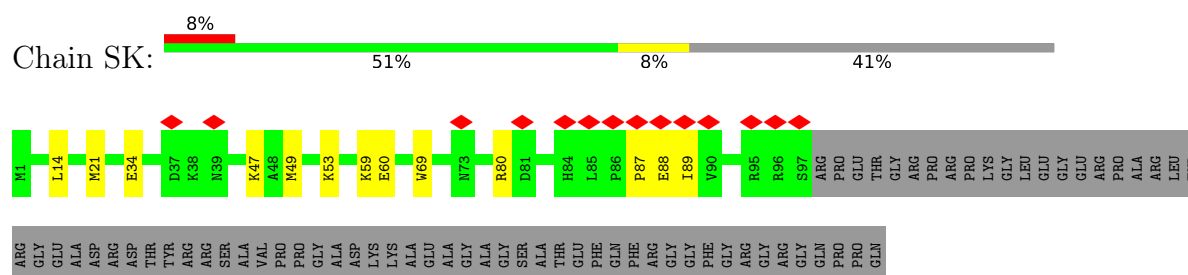


- Molecule 49: 40S ribosomal protein S3a

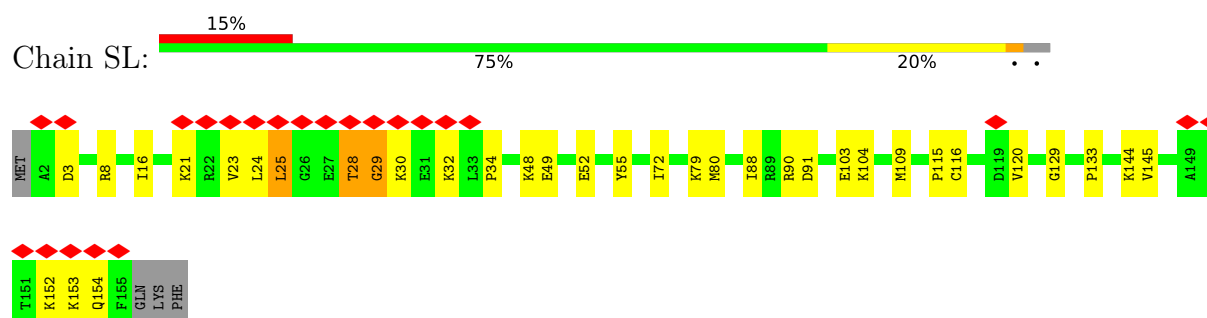
- Molecule 53: 40S ribosomal protein S8



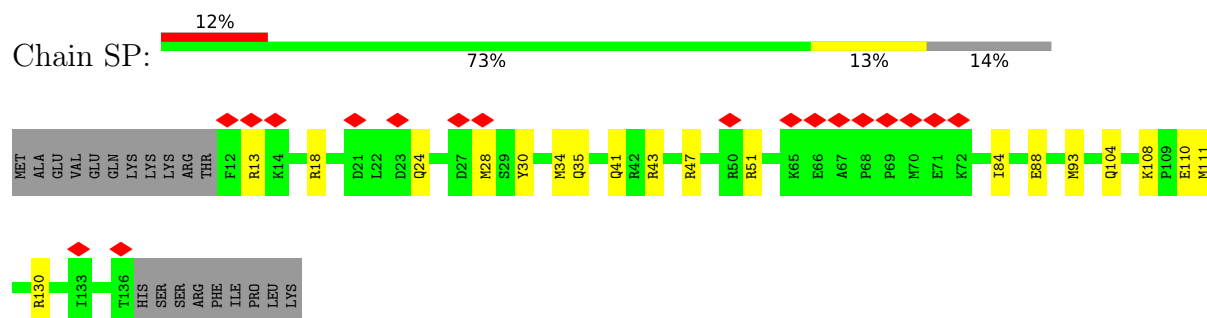
- Molecule 54: 40S ribosomal protein S10



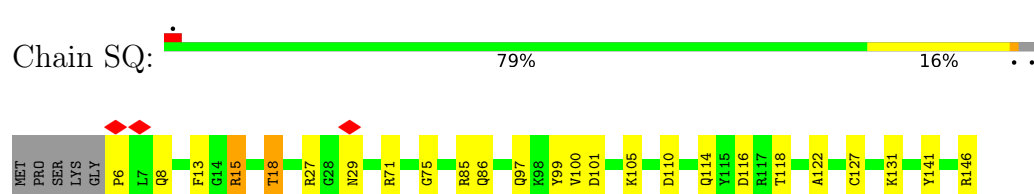
- Molecule 55: 40S ribosomal protein S11



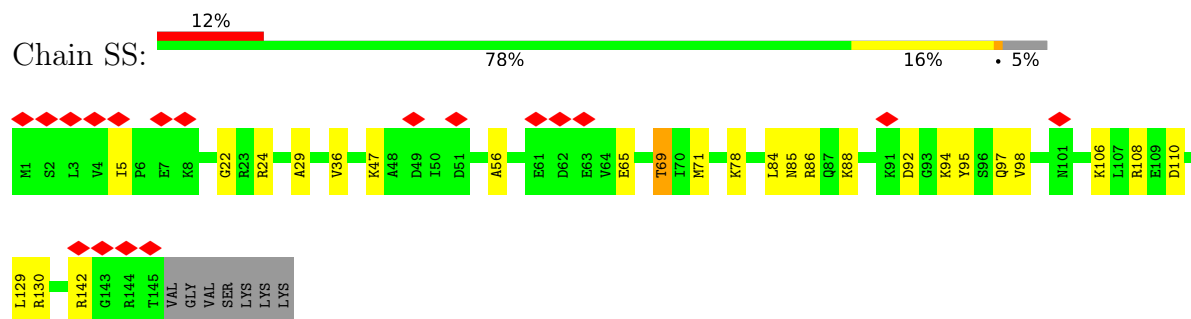
- Molecule 56: 40S ribosomal protein S15



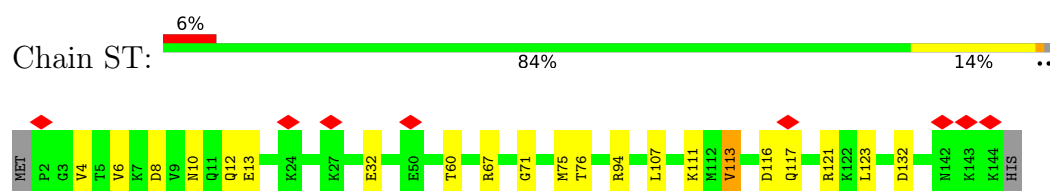
- Molecule 57: 40S ribosomal protein S16



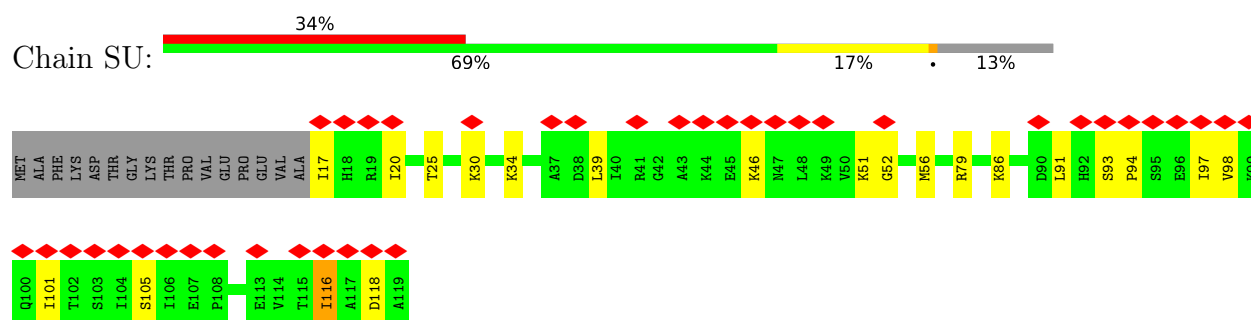
- Molecule 58: 40S ribosomal protein S18



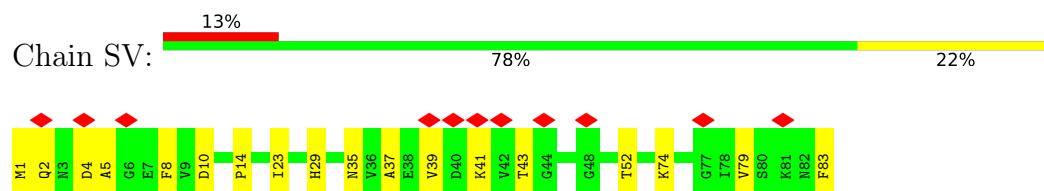
- Molecule 59: Small ribosomal subunit protein eS19



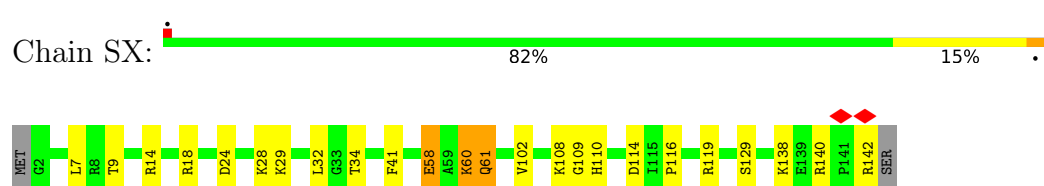
- Molecule 60: 40S ribosomal protein S20



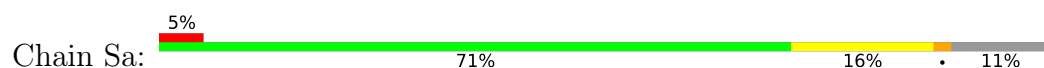
- Molecule 61: 40S ribosomal protein S21



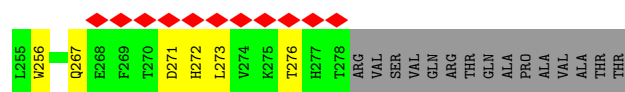
- Molecule 62: 40S ribosomal protein S23



- Molecule 63: 40S ribosomal protein S26

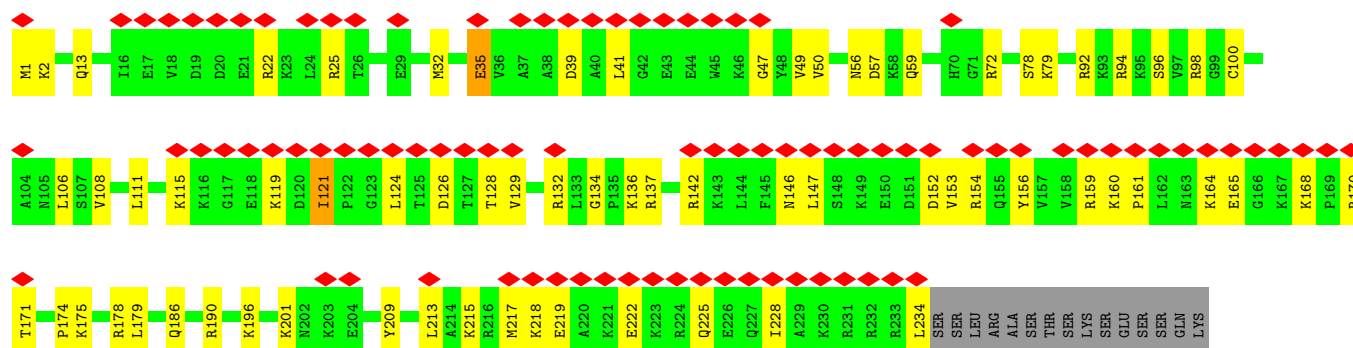






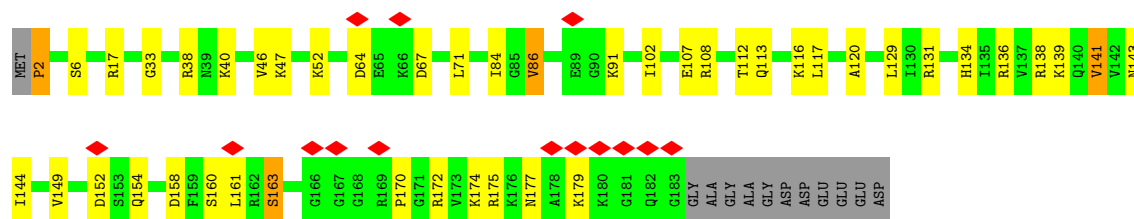
- Molecule 68: 40S ribosomal protein S6

Chain SG: 37% 66% 27% 6%



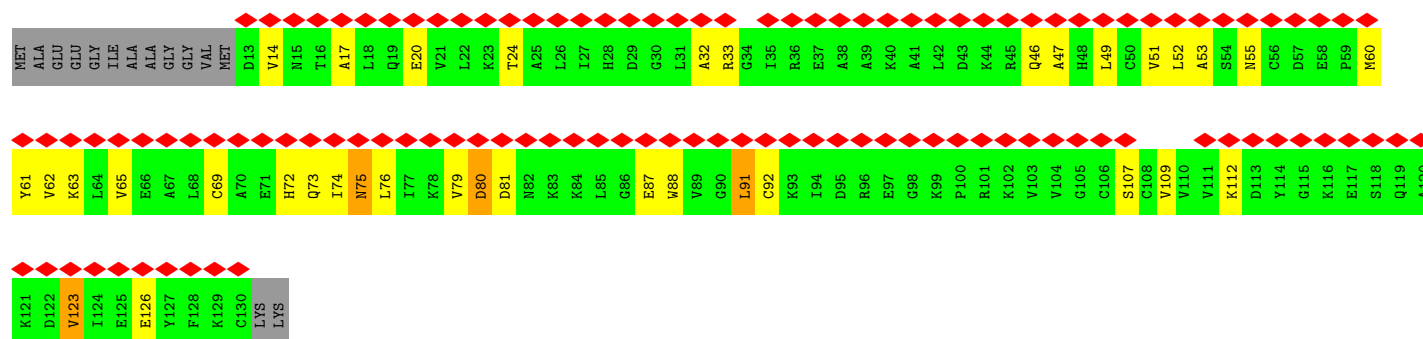
- Molecule 69: 40S ribosomal protein S9

Chain SJ: 7% 71% 21% 6%



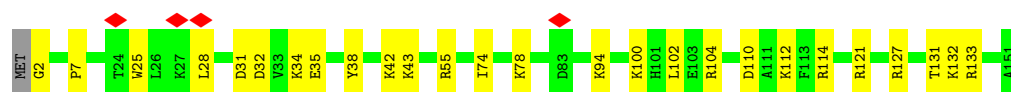
- Molecule 70: 40S ribosomal protein S12

Chain SM: 86% 62% 24% 11%

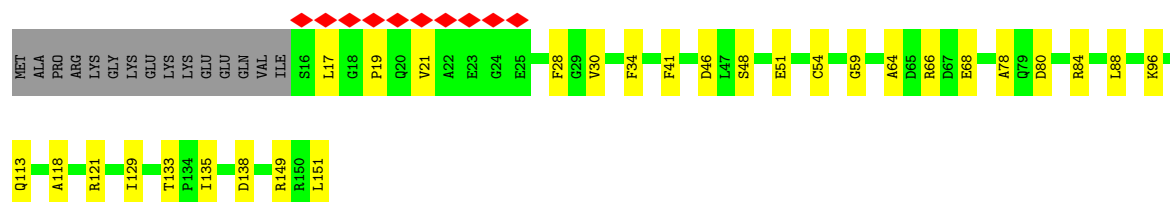
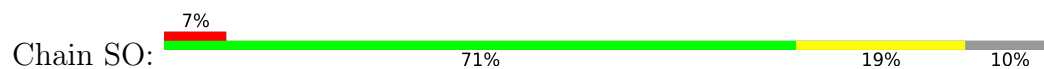


- Molecule 71: 40S ribosomal protein S13

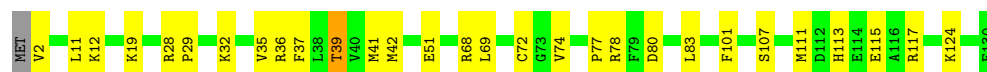
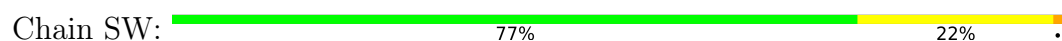
Chain SN: 82% 17%



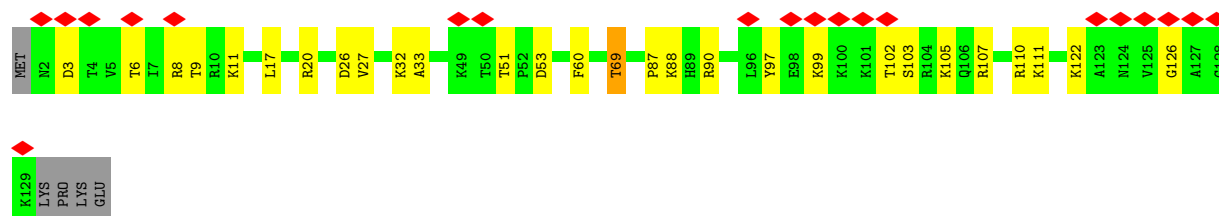
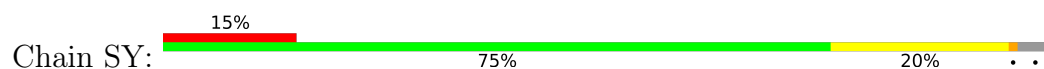
- Molecule 72: 40S ribosomal protein S14



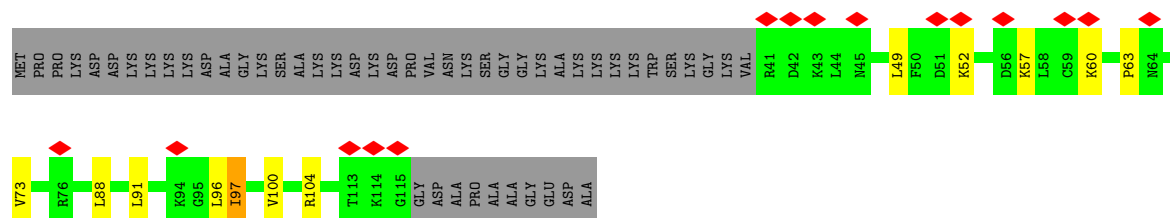
- Molecule 73: 40S ribosomal protein S15a



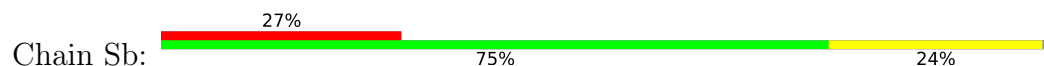
- Molecule 74: 40S ribosomal protein S24

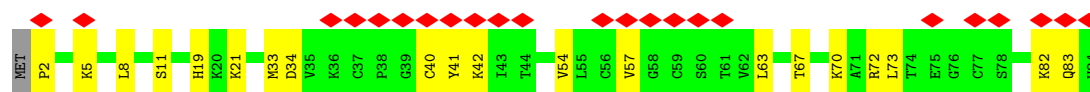


- Molecule 75: 40S ribosomal protein S25

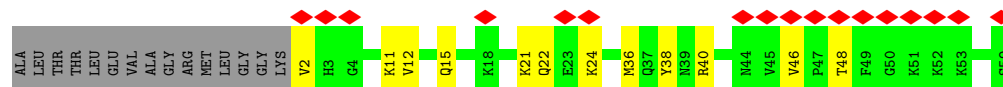
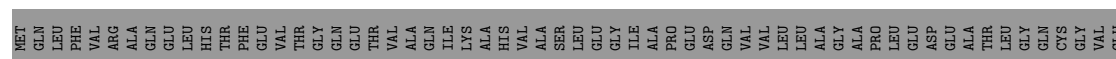
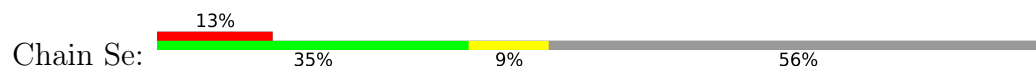


- Molecule 76: 40S ribosomal protein S27

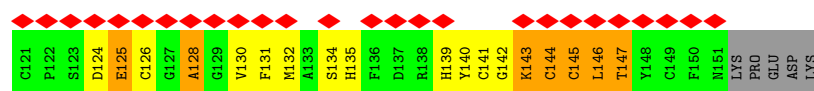
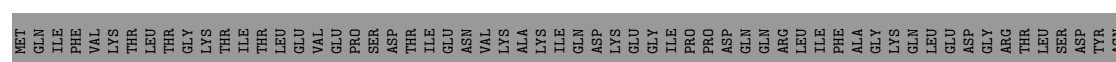
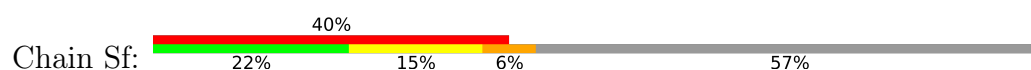




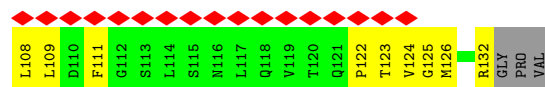
- Molecule 77: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



- Molecule 78: Ubiquitin-40S ribosomal protein S27a



- Molecule 79: 40S ribosomal protein S17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	382016	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, JEOL CRYO ARM 300	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0, 1.0	Depositor
Minimum defocus (nm)	500, 1000	Depositor
Maximum defocus (nm)	1100, 2000	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	FEI FALCON IV (4k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.426	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0266	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M7G, OMC, 6MZ, ZN, 5MC, OMU, SPD, MG, 4AC, B8N, HIC, UR3, MA6, NMM, OMG, A2M, K, IAS, UY1, V5N, 1MA, PSU

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	L5	0.28	1/86723 (0.0%)	0.47	170/135219 (0.1%)
2	L7	0.29	0/2858	0.53	12/4455 (0.3%)
3	L8	0.28	0/3609	0.48	10/5623 (0.2%)
4	LA	0.23	0/1936	0.40	0/2596
5	LB	0.21	0/3294	0.39	0/4406
6	LC	0.16	0/2981	0.34	0/4002
7	LD	0.15	0/2428	0.33	0/3252
8	LE	0.35	0/1942	0.49	0/2606
9	LF	0.16	0/1916	0.32	0/2553
10	LG	0.20	0/1971	0.39	0/2651
11	LH	0.15	0/1537	0.30	0/2066
12	LI	0.31	0/1753	0.46	0/2343
13	LJ	0.24	0/1433	0.45	0/1915
14	LL	0.17	0/1732	0.34	0/2315
15	LM	0.14	0/1161	0.31	0/1554
16	LN	0.18	0/1746	0.33	0/2338
17	LO	0.17	0/1682	0.38	0/2250
18	LP	0.17	0/1268	0.34	0/1701
19	LQ	0.16	0/1537	0.38	0/2052
20	LR	0.17	0/1582	0.34	0/2091
21	LS	0.17	0/1493	0.36	0/2003
22	LT	0.16	0/1326	0.34	0/1770
23	LU	0.14	0/839	0.34	0/1126
24	LV	0.28	0/993	0.47	0/1332
25	LW	0.19	0/1012	0.37	0/1342
26	LX	0.23	0/1002	0.35	0/1345
27	LY	0.16	0/1119	0.33	0/1488
28	LZ	0.16	0/1130	0.31	0/1507
29	La	0.17	0/1179	0.36	0/1573
30	Lb	0.14	0/821	0.33	0/1084
31	Lc	0.20	0/774	0.36	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.17	0/894	0.37	0/1204
33	Le	0.18	0/1071	0.38	0/1429
34	Lf	0.17	0/895	0.30	0/1198
35	Lg	0.16	0/878	0.32	0/1170
36	Lh	0.15	0/1023	0.32	0/1351
37	Li	0.15	0/824	0.35	0/1090
38	Lj	0.18	0/720	0.34	0/952
39	Lk	0.14	0/565	0.29	0/750
40	Ll	0.16	0/454	0.34	0/599
41	Lm	0.37	0/425	0.49	0/564
42	Ln	0.24	0/231	0.38	0/294
43	Lo	0.15	0/858	0.32	0/1131
44	Lp	0.27	0/691	0.43	0/919
45	Lr	0.27	0/1002	0.42	0/1344
46	S2	0.30	1/39125 (0.0%)	0.50	101/60957 (0.2%)
47	SE	0.15	0/2118	0.34	0/2849
48	SA	0.29	0/1764	0.45	0/2396
49	SB	0.16	0/1774	0.34	0/2373
50	SD	0.16	0/1793	0.31	0/2414
51	SF	0.14	0/1531	0.35	0/2059
52	SH	0.16	0/1519	0.39	0/2033
53	SI	0.19	0/1715	0.34	0/2287
54	SK	0.18	0/840	0.47	2/1133 (0.2%)
55	SL	0.29	0/1280	0.40	0/1712
56	SP	0.13	0/1047	0.29	0/1399
57	SQ	0.24	0/1142	0.45	0/1528
58	SS	0.13	0/1216	0.31	0/1628
59	ST	0.14	0/1119	0.30	0/1498
60	SU	0.15	0/827	0.35	0/1110
61	SV	0.16	0/643	0.33	0/860
62	SX	0.28	0/1116	0.44	0/1490
63	Sa	0.19	0/847	0.37	0/1135
64	Sc	0.21	0/508	0.45	0/680
65	Sd	0.14	0/470	0.35	0/623
66	Sg	0.13	0/2493	0.33	0/3394
67	SC	0.16	0/1764	0.31	0/2382
68	SG	0.25	0/1926	0.38	0/2563
69	SJ	0.15	0/1548	0.35	0/2066
70	SM	0.15	0/916	0.40	0/1233
71	SN	0.19	0/1232	0.30	0/1656
72	SO	0.19	0/1020	0.37	0/1366
73	SW	0.27	0/1051	0.47	0/1406
74	SY	0.14	0/1068	0.30	0/1418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SZ	0.16	0/604	0.40	0/810
76	Sb	0.15	0/665	0.35	0/891
77	Se	0.14	0/465	0.36	0/612
78	Sf	0.46	0/560	0.58	0/745
79	SR	0.15	0/1078	0.37	0/1447
All	All	0.25	2/226092 (0.0%)	0.44	295/331744 (0.1%)

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
8	LE	0	2
12	LI	0	2
14	LL	0	1
41	Lm	0	1
57	SQ	0	1
73	SW	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3785	A2M	O3'-P	5.13	1.61	1.56
46	S2	1383	A2M	O3'-P	5.13	1.61	1.56

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SK	87	PRO	CA-N-CD	-9.83	98.24	112.00
46	S2	1804	OMU	P-O3'-C3'	-9.64	108.14	119.70
46	S2	609	PSU	P-O3'-C3'	-9.49	105.97	120.20
46	S2	1081	U	P-O3'-C3'	-9.47	105.99	120.20
1	L5	5010	PSU	P-O3'-C3'	-9.13	106.51	120.20
46	S2	798	G	P-O3'-C3'	-9.09	106.56	120.20
1	L5	513	U	P-O3'-C3'	-8.78	107.03	120.20
1	L5	1366	G	P-O3'-C3'	-8.70	107.15	120.20
3	L8	111	U	P-O3'-C3'	-8.65	107.22	120.20
2	L7	36	C	P-O3'-C3'	-8.60	107.30	120.20
1	L5	3730	PSU	P-O3'-C3'	-8.57	107.34	120.20
1	L5	4998	G	P-O3'-C3'	-8.51	107.43	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1454	G	P-O3'-C3'	-8.51	107.44	120.20
1	L5	4869	U	P-O3'-C3'	-8.47	107.50	120.20
1	L5	3724	A2M	P-O3'-C3'	-8.43	109.59	119.70
1	L5	714	G	P-O3'-C3'	-8.41	107.59	120.20
46	S2	1808	U	P-O3'-C3'	-8.38	107.63	120.20
1	L5	4293	PSU	P-O3'-C3'	-8.33	107.71	120.20
1	L5	3764	PSU	P-O3'-C3'	-8.26	107.81	120.20
46	S2	968	U	P-O3'-C3'	-8.24	107.83	120.20
1	L5	4415	A	P-O3'-C3'	-8.21	107.89	120.20
3	L8	67	U	P-O3'-C3'	-8.09	108.07	120.20
46	S2	672	A	P-O3'-C3'	-8.04	108.14	120.20
1	L5	4867	G	P-O3'-C3'	-8.02	108.17	120.20
1	L5	1741	G	P-O3'-C3'	-8.00	108.20	120.20
46	S2	1345	G	P-O3'-C3'	-7.96	108.26	120.20
1	L5	979	C	P-O3'-C3'	-7.96	108.27	120.20
3	L8	70	G	P-O3'-C3'	-7.96	108.27	120.20
1	L5	1742	A	P-O3'-C3'	-7.94	108.29	120.20
1	L5	1517	G	P-O3'-C3'	-7.93	108.30	120.20
2	L7	35	U	P-O3'-C3'	-7.93	108.31	120.20
1	L5	4412	C	P-O3'-C3'	-7.90	108.36	120.20
46	S2	1216	C	P-O3'-C3'	-7.86	108.41	120.20
1	L5	730	G	P-O3'-C3'	-7.86	108.41	120.20
1	L5	4502	C	P-O3'-C3'	-7.80	108.51	120.20
1	L5	1368	A	P-O3'-C3'	-7.79	108.51	120.20
46	S2	1504	U	P-O3'-C3'	-7.78	108.52	120.20
1	L5	1456	U	P-O3'-C3'	-7.76	108.56	120.20
1	L5	1864	G	P-O3'-C3'	-7.69	108.66	120.20
46	S2	614	C	P-O3'-C3'	-7.69	108.66	120.20
1	L5	4417	C	P-O3'-C3'	-7.67	108.69	120.20
1	L5	2775	C	P-O3'-C3'	-7.66	108.71	120.20
1	L5	4532	PSU	P-O3'-C3'	-7.64	108.74	120.20
46	S2	1807	C	P-O3'-C3'	-7.63	108.75	120.20
1	L5	4597	U	P-O3'-C3'	-7.63	108.75	120.20
1	L5	4082	G	P-O3'-C3'	-7.62	108.77	120.20
1	L5	1863	U	P-O3'-C3'	-7.59	108.81	120.20
46	S2	799	U	P-O3'-C3'	-7.58	108.82	120.20
46	S2	1218	C	P-O3'-C3'	-7.58	108.83	120.20
2	L7	31	G	P-O3'-C3'	-7.58	108.84	120.20
46	S2	610	G	P-O3'-C3'	-7.57	108.84	120.20
1	L5	1453	G	P-O3'-C3'	-7.56	108.86	120.20
1	L5	4080	C	P-O3'-C3'	-7.52	108.92	120.20
1	L5	3814	U	P-O3'-C3'	-7.52	108.92	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4500	PSU	P-O3'-C3'	-7.51	108.93	120.20
1	L5	1365	C	P-O3'-C3'	-7.50	108.95	120.20
1	L5	1364	U	P-O3'-C3'	-7.48	108.97	120.20
1	L5	4414	A	P-O3'-C3'	-7.47	108.99	120.20
46	S2	820	U	P-O3'-C3'	-7.45	109.02	120.20
2	L7	32	A	P-O3'-C3'	-7.45	109.03	120.20
46	S2	867	OMG	P-O3'-C3'	-7.42	109.07	120.20
1	L5	4297	G	P-O3'-C3'	-7.41	109.09	120.20
1	L5	1739	G	P-O3'-C3'	-7.40	109.10	120.20
2	L7	33	U	P-O3'-C3'	-7.38	109.14	120.20
1	L5	3908	A	P-O3'-C3'	-7.36	109.17	120.20
46	S2	1503	C	P-O3'-C3'	-7.28	109.29	120.20
1	L5	4452	U	P-O3'-C3'	-7.25	109.32	120.20
3	L8	107	C	P-O3'-C3'	-7.25	109.33	120.20
46	S2	801	PSU	P-O3'-C3'	-7.23	109.35	120.20
46	S2	1324	G	P-O3'-C3'	-7.23	109.35	120.20
46	S2	1322	G	P-O3'-C3'	-7.22	109.37	120.20
46	S2	868	G	P-O3'-C3'	-7.21	109.38	120.20
46	S2	1711	U	P-O3'-C3'	-7.20	109.40	120.20
1	L5	3720	G	P-O3'-C3'	-7.20	109.41	120.20
46	S2	1594	A	P-O3'-C3'	-7.17	109.44	120.20
46	S2	1507	G	P-O3'-C3'	-7.14	109.49	120.20
46	S2	1485	U	P-O3'-C3'	-7.14	109.49	120.20
46	S2	1376	A	P-O3'-C3'	-7.13	109.50	120.20
1	L5	1882	U	P-O3'-C3'	-7.12	109.52	120.20
1	L5	374	G	P-O3'-C3'	-7.11	109.53	120.20
46	S2	34	PSU	P-O3'-C3'	-7.10	109.55	120.20
46	S2	1357	A	P-O3'-C3'	-7.10	109.55	120.20
1	L5	1737	A	P-O3'-C3'	-7.08	109.59	120.20
1	L5	4081	G	P-O3'-C3'	-7.06	109.61	120.20
46	S2	686	PSU	P-O3'-C3'	-7.06	109.61	120.20
46	S2	31	U	P-O3'-C3'	-7.05	109.62	120.20
46	S2	613	G	P-O3'-C3'	-7.05	109.63	120.20
1	L5	3762	PSU	P-O3'-C3'	-7.02	109.67	120.20
1	L5	2629	C	P-O3'-C3'	-6.98	109.73	120.20
1	L5	4598	C	P-O3'-C3'	-6.98	109.73	120.20
1	L5	2047	A	P-O3'-C3'	-6.97	109.74	120.20
46	S2	1806	A	P-O3'-C3'	-6.97	109.75	120.20
46	S2	1024	A	P-O3'-C3'	-6.96	109.76	120.20
46	S2	1323	U	P-O3'-C3'	-6.94	109.79	120.20
1	L5	976	G	P-O3'-C3'	-6.93	109.81	120.20
1	L5	2771	G	P-O3'-C3'	-6.93	109.81	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4416	G	P-O3'-C3'	-6.87	109.90	120.20
46	S2	669	A	P-O3'-C3'	-6.86	109.91	120.20
1	L5	2770	C	P-O3'-C3'	-6.85	109.93	120.20
46	S2	1375	G	P-O3'-C3'	-6.84	109.93	120.20
46	S2	967	C	P-O3'-C3'	-6.84	109.94	120.20
1	L5	2772	C	P-O3'-C3'	-6.84	109.94	120.20
46	S2	863	PSU	P-O3'-C3'	-6.83	109.95	120.20
1	L5	1883	G	P-O3'-C3'	-6.82	109.97	120.20
1	L5	4577	U	P-O3'-C3'	-6.80	110.00	120.20
1	L5	4501	U	P-O3'-C3'	-6.80	110.00	120.20
2	L7	34	C	P-O3'-C3'	-6.79	110.01	120.20
1	L5	512	U	P-O3'-C3'	-6.79	110.02	120.20
1	L5	4530	UR3	P-O3'-C3'	-6.76	111.58	119.70
1	L5	4594	U	P-O3'-C3'	-6.74	110.09	120.20
1	L5	514	U	P-O3'-C3'	-6.73	110.10	120.20
1	L5	4873	G	P-O3'-C3'	-6.73	110.11	120.20
46	S2	822	PSU	P-O3'-C3'	-6.71	110.13	120.20
1	L5	715	G	P-O3'-C3'	-6.69	110.16	120.20
1	L5	4448	G	P-O3'-C3'	-6.68	110.18	120.20
46	S2	1373	C	P-O3'-C3'	-6.68	110.18	120.20
1	L5	4483	C	P-O3'-C3'	-6.67	110.20	120.20
1	L5	4596	C	P-O3'-C3'	-6.66	110.20	120.20
46	S2	1709	G	P-O3'-C3'	-6.65	110.22	120.20
1	L5	4413	C	P-O3'-C3'	-6.65	110.22	120.20
46	S2	824	C	P-O3'-C3'	-6.65	110.23	120.20
46	S2	1502	C	P-O3'-C3'	-6.62	110.28	120.20
1	L5	510	U	P-O3'-C3'	-6.61	110.28	120.20
46	S2	1245	G	P-O3'-C3'	-6.61	110.28	120.20
1	L5	3722	G	P-O3'-C3'	-6.61	110.28	120.20
1	L5	4595	G	P-O3'-C3'	-6.60	110.30	120.20
1	L5	3731	C	P-O3'-C3'	-6.59	110.32	120.20
1	L5	5007	A	P-O3'-C3'	-6.59	110.32	120.20
1	L5	1839	U	P-O3'-C3'	-6.57	110.35	120.20
46	S2	1593	C	P-O3'-C3'	-6.54	110.39	120.20
46	S2	1372	U	P-O3'-C3'	-6.52	110.42	120.20
1	L5	4669	A	P-O3'-C3'	-6.51	110.44	120.20
1	L5	4870	G	P-O3'-C3'	-6.51	110.44	120.20
3	L8	69	PSU	P-O3'-C3'	-6.50	110.45	120.20
1	L5	4576	PSU	P-O3'-C3'	-6.50	110.45	120.20
3	L8	112	G	P-O3'-C3'	-6.50	110.45	120.20
1	L5	2774	C	P-O3'-C3'	-6.50	110.45	120.20
1	L5	980	U	P-O3'-C3'	-6.49	110.46	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3765	G	P-O3'-C3'	-6.49	110.47	120.20
46	S2	1134	G	P-O3'-C3'	-6.48	110.47	120.20
1	L5	35	U	P-O3'-C3'	-6.48	110.48	120.20
46	S2	1244	PSU	P-O3'-C3'	-6.47	110.49	120.20
1	L5	3721	U	P-O3'-C3'	-6.46	110.50	120.20
46	S2	1184	G	P-O3'-C3'	-6.44	110.53	120.20
1	L5	4083	U	P-O3'-C3'	-6.43	110.56	120.20
1	L5	1738	A	P-O3'-C3'	-6.43	110.56	120.20
1	L5	4480	A	P-O3'-C3'	-6.42	110.56	120.20
1	L5	977	C	P-O3'-C3'	-6.42	110.57	120.20
1	L5	1519	C	P-O3'-C3'	-6.42	110.57	120.20
2	L7	105	C	P-O3'-C3'	-6.40	110.61	120.20
1	L5	3766	A	P-O3'-C3'	-6.39	110.61	120.20
46	S2	1188	A	P-O3'-C3'	-6.39	110.61	120.20
1	L5	1455	G	P-O3'-C3'	-6.39	110.61	120.20
3	L8	66	A	P-O3'-C3'	-6.38	110.62	120.20
46	S2	611	G	P-O3'-C3'	-6.38	110.63	120.20
46	S2	1506	A	P-O3'-C3'	-6.37	110.65	120.20
1	L5	4482	U	P-O3'-C3'	-6.36	110.66	120.20
46	S2	1482	C	P-O3'-C3'	-6.36	110.66	120.20
46	S2	1598	G	P-O3'-C3'	-6.35	110.68	120.20
1	L5	2632	PSU	P-O3'-C3'	-6.35	110.68	120.20
1	L5	1866	U	P-O3'-C3'	-6.34	110.68	120.20
1	L5	4484	A	P-O3'-C3'	-6.34	110.68	120.20
46	S2	32	U	P-O3'-C3'	-6.34	110.69	120.20
46	S2	1486	A	P-O3'-C3'	-6.33	110.70	120.20
2	L7	101	A	P-O3'-C3'	-6.33	110.71	120.20
46	S2	797	C	P-O3'-C3'	-6.32	110.72	120.20
1	L5	728	U	P-O3'-C3'	-6.31	110.73	120.20
1	L5	1841	C	P-O3'-C3'	-6.31	110.74	120.20
1	L5	2051	C	P-O3'-C3'	-6.30	110.74	120.20
1	L5	31	U	P-O3'-C3'	-6.29	110.76	120.20
46	S2	1712	A	P-O3'-C3'	-6.29	110.76	120.20
1	L5	4296	PSU	P-O3'-C3'	-6.28	110.78	120.20
1	L5	727	C	P-O3'-C3'	-6.25	110.83	120.20
46	S2	1186	PSU	P-O3'-C3'	-6.25	110.82	120.20
46	S2	1136	PSU	P-O3'-C3'	-6.25	110.83	120.20
46	S2	1133	A	P-O3'-C3'	-6.24	110.84	120.20
1	L5	3909	C	P-O3'-C3'	-6.22	110.87	120.20
1	L5	3637	PSU	P-O3'-C3'	-6.20	110.90	120.20
1	L5	713	C	P-O3'-C3'	-6.20	110.91	120.20
1	L5	4485	C	P-O3'-C3'	-6.20	110.91	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4999	G	P-O3'-C3'	-6.20	110.91	120.20
46	S2	36	PSU	P-O3'-C3'	-6.19	110.91	120.20
1	L5	1514	U	P-O3'-C3'	-6.19	110.92	120.20
1	L5	975	C	P-O3'-C3'	-6.18	110.93	120.20
1	L5	4673	PSU	P-O3'-C3'	-6.17	110.95	120.20
1	L5	5002	U	P-O3'-C3'	-6.17	110.95	120.20
1	L5	716	C	P-O3'-C3'	-6.16	110.96	120.20
46	S2	966	PSU	P-O3'-C3'	-6.16	110.96	120.20
46	S2	1240	A	P-O3'-C3'	-6.14	110.99	120.20
2	L7	104	C	P-O3'-C3'	-6.13	111.01	120.20
46	S2	796	G	P-O3'-C3'	-6.11	111.04	120.20
1	L5	978	G	P-O3'-C3'	-6.10	111.04	120.20
46	S2	684	G	P-O3'-C3'	-6.09	111.07	120.20
46	S2	1487	A	P-O3'-C3'	-6.09	111.07	120.20
1	L5	4668	U	P-O3'-C3'	-6.09	111.07	120.20
1	L5	1515	A	P-O3'-C3'	-6.08	111.07	120.20
46	S2	674	C	P-O3'-C3'	-6.08	111.08	120.20
1	L5	1885	G	P-O3'-C3'	-6.07	111.09	120.20
3	L8	71	A	P-O3'-C3'	-6.06	111.11	120.20
46	S2	1349	G	P-O3'-C3'	-6.06	111.11	120.20
1	L5	32	G	P-O3'-C3'	-6.05	111.13	120.20
1	L5	4084	G	P-O3'-C3'	-6.05	111.13	120.20
1	L5	4333	C	P-O3'-C3'	-6.04	111.14	120.20
46	S2	1027	A	P-O3'-C3'	-6.04	111.15	120.20
2	L7	100	A	P-O3'-C3'	-6.03	111.15	120.20
1	L5	511	C	P-O3'-C3'	-6.01	111.18	120.20
1	L5	712	C	P-O3'-C3'	-6.01	111.19	120.20
46	S2	1137	U	P-O3'-C3'	-6.00	111.19	120.20
46	S2	1596	PSU	P-O3'-C3'	-5.99	111.22	120.20
46	S2	1083	A	P-O3'-C3'	-5.96	111.26	120.20
46	S2	1505	U	P-O3'-C3'	-5.94	111.29	120.20
1	L5	731	G	P-O3'-C3'	-5.94	111.29	120.20
1	L5	2773	G	P-O3'-C3'	-5.94	111.29	120.20
1	L5	3647	A	P-O3'-C3'	-5.91	111.33	120.20
1	L5	1840	G	P-O3'-C3'	-5.90	111.35	120.20
1	L5	3772	U	P-O3'-C3'	-5.89	111.37	120.20
46	S2	1484	A	P-O3'-C3'	-5.88	111.38	120.20
1	L5	2630	U	P-O3'-C3'	-5.85	111.43	120.20
1	L5	3725	G	P-O3'-C3'	-5.84	111.43	120.20
1	L5	3688	U	P-O3'-C3'	-5.83	111.46	120.20
54	SK	87	PRO	N-CD-CG	-5.82	94.47	103.20
1	L5	373	G	P-O3'-C3'	-5.80	111.50	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1361	G	P-O3'-C3'	-5.80	111.50	120.20
1	L5	4599	A	P-O3'-C3'	-5.79	111.52	120.20
1	L5	2633	U	P-O3'-C3'	-5.78	111.53	120.20
1	L5	5008	C	P-O3'-C3'	-5.77	111.55	120.20
1	L5	4874	A	P-O3'-C3'	-5.77	111.55	120.20
1	L5	3639	PSU	P-O3'-C3'	-5.72	111.61	120.20
46	S2	864	A	P-O3'-C3'	-5.72	111.62	120.20
46	S2	687	C	P-O3'-C3'	-5.70	111.66	120.20
46	S2	1219	C	P-O3'-C3'	-5.67	111.69	120.20
1	L5	4573	G	P-O3'-C3'	-5.67	111.70	120.20
1	L5	4533	A	P-O3'-C3'	-5.66	111.71	120.20
1	L5	5001	PSU	P-O3'-C3'	-5.64	111.73	120.20
46	S2	1348	G	P-O3'-C3'	-5.64	111.73	120.20
1	L5	33	A	P-O3'-C3'	-5.64	111.74	120.20
1	L5	2634	C	P-O3'-C3'	-5.63	111.75	120.20
1	L5	3727	A	P-O3'-C3'	-5.63	111.75	120.20
46	S2	102	A	P-O3'-C3'	-5.62	111.78	120.20
46	S2	1805	G	C4'-C3'-C2'	-5.60	97.00	102.60
1	L5	4872	G	P-O3'-C3'	-5.59	111.81	120.20
46	S2	670	A	P-O3'-C3'	-5.58	111.83	120.20
1	L5	1740	C	P-O3'-C3'	-5.55	111.87	120.20
1	L5	3911	C	P-O3'-C3'	-5.53	111.91	120.20
1	L5	4871	C	P-O3'-C3'	-5.51	111.94	120.20
2	L7	103	A	P-O3'-C3'	-5.50	111.94	120.20
1	L5	375	G	P-O3'-C3'	-5.49	111.97	120.20
46	S2	1220	A	P-O3'-C3'	-5.49	111.97	120.20
46	S2	1029	G	P-O3'-C3'	-5.48	111.97	120.20
1	L5	3783	A	P-O3'-C3'	-5.47	111.99	120.20
46	S2	1187	G	P-O3'-C3'	-5.47	111.99	120.20
46	S2	964	A	P-O3'-C3'	-5.46	112.02	120.20
1	L5	1838	A	P-O3'-C3'	-5.45	112.03	120.20
1	L5	3820	G	P-O3'-C3'	-5.44	112.04	120.20
1	L5	509	A	P-O3'-C3'	-5.43	112.05	120.20
46	S2	100	PSU	P-O3'-C3'	-5.43	112.05	120.20
1	L5	1837	A	P-O3'-C3'	-5.43	112.06	120.20
1	L5	3687	A	P-O3'-C3'	-5.43	112.06	120.20
1	L5	2050	G	P-O3'-C3'	-5.43	112.06	120.20
1	L5	1865	G	P-O3'-C3'	-5.42	112.07	120.20
1	L5	4294	C	P-O3'-C3'	-5.40	112.10	120.20
1	L5	3816	A	P-O3'-C3'	-5.39	112.11	120.20
46	S2	1138	C	P-O3'-C3'	-5.39	112.11	120.20
1	L5	369	G	P-O3'-C3'	-5.37	112.15	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	5003	U	P-O3'-C3'	-5.36	112.15	120.20
1	L5	5012	G	P-O3'-C3'	-5.36	112.16	120.20
1	L5	4337	C	P-O3'-C3'	-5.35	112.17	120.20
46	S2	1221	G	P-O3'-C3'	-5.35	112.17	120.20
1	L5	2048	U	P-O3'-C3'	-5.35	112.18	120.20
46	S2	1078	C	P-O3'-C3'	-5.30	112.25	120.20
1	L5	5011	A	P-O3'-C3'	-5.29	112.27	120.20
1	L5	4450	U	P-O3'-C3'	-5.28	112.28	120.20
1	L5	4332	C	P-O3'-C3'	-5.27	112.29	120.20
1	L5	3690	U	P-O3'-C3'	-5.27	112.30	120.20
3	L8	110	U	P-O3'-C3'	-5.27	112.30	120.20
1	L5	3773	U	P-O3'-C3'	-5.21	112.38	120.20
1	L5	3815	G	P-O3'-C3'	-5.20	112.40	120.20
46	S2	1805	G	C2'-C3'-O3'	5.19	121.48	113.70
1	L5	4496	A	P-O3'-C3'	-5.19	112.42	120.20
2	L7	102	U	P-O3'-C3'	-5.18	112.42	120.20
46	S2	1028	A	P-O3'-C3'	-5.17	112.44	120.20
46	S2	1080	A	P-O3'-C3'	-5.16	112.46	120.20
1	L5	1369	C	P-O3'-C3'	-5.13	112.51	120.20
46	S2	1026	C	P-O3'-C3'	-5.12	112.52	120.20
46	S2	1597	C	P-O3'-C3'	-5.11	112.53	120.20
3	L8	108	A	P-O3'-C3'	-5.10	112.56	120.20
1	L5	717	U	P-O3'-C3'	-5.07	112.59	120.20
1	L5	4481	U	P-O3'-C3'	-5.04	112.64	120.20
1	L5	3906	A	P-O3'-C3'	-5.04	112.64	120.20
46	S2	1374	C	P-O3'-C3'	-5.03	112.65	120.20
46	S2	665	G	P-O3'-C3'	-5.03	112.66	120.20
46	S2	1707	U	P-O3'-C3'	-5.03	112.66	120.20
46	S2	668	A2M	P-O3'-C3'	-5.02	113.67	119.70
1	L5	2628	U	P-O3'-C3'	-5.01	112.68	120.20
46	S2	1082	A	P-O3'-C3'	-5.00	112.69	120.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	LE	223	ARG	Sidechain
8	LE	226	ARG	Sidechain
12	LI	110	ARG	Sidechain
12	LI	116	ARG	Sidechain
14	LL	36	ARG	Sidechain
41	Lm	97	ARG	Sidechain

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Mol	Chain	Res	Type	Group
57	SQ	15	ARG	Sidechain
73	SW	78	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	80205	0	40474	1122	0
2	L7	2558	0	1295	27	0
3	L8	3316	0	1687	55	0
4	LA	1898	0	1993	36	0
5	LB	3239	0	3376	59	0
6	LC	2927	0	3104	56	0
7	LD	2382	0	2410	51	0
8	LE	1904	0	2055	68	0
9	LF	1878	0	2009	29	0
10	LG	1935	0	2087	47	0
11	LH	1518	0	1601	34	0
12	LI	1713	0	1751	61	0
13	LJ	1410	0	1441	34	0
14	LL	1701	0	1818	27	0
15	LM	1138	0	1204	28	0
16	LN	1701	0	1749	26	0
17	LO	1650	0	1794	36	0
18	LP	1242	0	1269	25	0
19	LQ	1513	0	1628	23	0
20	LR	1566	0	1729	30	0
21	LS	1453	0	1490	19	0
22	LT	1298	0	1366	26	0
23	LU	825	0	850	21	0
24	LV	979	0	1039	15	0
25	LW	997	0	1053	25	0
26	LX	985	0	1066	11	0
27	LY	1102	0	1189	17	0
28	LZ	1107	0	1182	30	0
29	La	1163	0	1206	20	0
30	Lb	808	0	875	20	0
31	Lc	764	0	804	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Ld	879	0	924	17	0
33	Le	1053	0	1147	26	0
34	Lf	876	0	911	7	0
35	Lg	868	0	959	15	0
36	Lh	1015	0	1148	28	0
37	Li	813	0	894	21	0
38	Lj	705	0	737	12	0
39	Lk	559	0	624	11	0
40	Ll	444	0	483	7	0
41	Lm	419	0	452	6	0
42	Ln	230	0	276	3	0
43	Lo	842	0	914	15	0
44	Lp	681	0	731	16	0
45	Lr	987	0	1050	22	0
46	S2	36955	0	18665	513	0
47	SE	2076	0	2177	34	0
48	SA	1727	0	1729	60	0
49	SB	1747	0	1822	32	0
50	SD	1765	0	1865	33	0
51	SF	1509	0	1563	24	0
52	SH	1497	0	1590	27	0
53	SI	1686	0	1772	34	0
54	SK	816	0	841	7	0
55	SL	1258	0	1332	25	0
56	SP	1027	0	1075	13	0
57	SQ	1124	0	1193	17	0
58	SS	1198	0	1261	20	0
59	ST	1113	0	1145	13	0
60	SU	817	0	882	16	0
61	SV	636	0	637	18	0
62	SX	1098	0	1167	20	0
63	Sa	829	0	883	20	0
64	Sc	506	0	536	18	0
65	Sd	459	0	448	11	0
66	Sg	2436	0	2393	42	0
67	SC	1724	0	1817	28	0
68	SG	1903	0	2068	48	0
69	SJ	1520	0	1642	37	0
70	SM	906	0	921	21	0
71	SN	1208	0	1294	22	0
72	SO	1016	0	1038	23	0
73	SW	1034	0	1080	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	SY	1048	0	1122	26	0
75	SZ	598	0	656	12	0
76	Sb	651	0	672	14	0
77	Se	459	0	503	10	0
78	Sf	548	0	553	30	0
79	SR	1064	0	1118	26	0
80	L5	198	0	0	0	0
80	L7	2	0	0	0	0
80	L8	4	0	0	0	0
80	LI	1	0	0	0	0
80	LN	1	0	0	0	0
80	LP	1	0	0	0	0
80	LV	1	0	0	0	0
80	S2	84	0	0	0	0
81	L5	78	0	0	0	0
81	L7	1	0	0	0	0
81	LA	1	0	0	0	0
81	LB	1	0	0	0	0
81	LI	1	0	0	0	0
81	Le	1	0	0	0	0
81	Lf	1	0	0	0	0
81	Lo	1	0	0	0	0
81	S2	21	0	0	0	0
81	SO	1	0	0	0	0
81	Sd	1	0	0	0	0
82	L5	20	0	38	5	0
83	Lg	1	0	0	0	0
83	Lj	1	0	0	0	0
83	Lm	1	0	0	0	0
83	Lo	1	0	0	0	0
83	Lp	1	0	0	0	0
83	Sa	1	0	0	0	0
83	Sd	1	0	0	0	0
83	Sf	1	0	0	0	0
84	L5	9116	0	0	72	0
84	L7	175	0	0	1	0
84	L8	376	0	0	5	0
84	LA	176	0	0	1	0
84	LB	135	0	0	1	0
84	LC	149	0	0	1	0
84	LD	29	0	0	1	0
84	LE	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	LF	83	0	0	1	0
84	LG	40	0	0	0	0
84	LH	27	0	0	2	0
84	LI	36	0	0	1	0
84	LJ	5	0	0	0	0
84	LL	71	0	0	0	0
84	LM	16	0	0	0	0
84	LN	131	0	0	0	0
84	LO	59	0	0	0	0
84	LP	61	0	0	1	0
84	LQ	99	0	0	2	0
84	LR	103	0	0	3	0
84	LS	55	0	0	0	0
84	LT	59	0	0	2	0
84	LU	6	0	0	1	0
84	LV	61	0	0	1	0
84	LW	49	0	0	1	0
84	LX	32	0	0	1	0
84	LY	36	0	0	1	0
84	LZ	13	0	0	0	0
84	La	70	0	0	1	0
84	Lb	34	0	0	0	0
84	Lc	55	0	0	3	0
84	Ld	29	0	0	0	0
84	Le	81	0	0	3	0
84	Lf	47	0	0	0	0
84	Lg	52	0	0	0	0
84	Lh	34	0	0	1	0
84	Li	24	0	0	0	0
84	Lj	55	0	0	1	0
84	Lk	6	0	0	1	0
84	Ll	22	0	0	0	0
84	Lm	17	0	0	0	0
84	Ln	39	0	0	1	0
84	Lo	22	0	0	1	0
84	Lp	82	0	0	2	0
84	Lr	41	0	0	0	0
84	S2	4529	0	0	34	0
84	SA	26	0	0	0	0
84	SB	71	0	0	1	0
84	SC	79	0	0	5	0
84	SD	53	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	SE	85	0	0	1	0
84	SF	39	0	0	1	0
84	SG	28	0	0	1	0
84	SH	18	0	0	0	0
84	SI	96	0	0	4	0
84	SJ	76	0	0	1	0
84	SK	1	0	0	0	0
84	SL	98	0	0	1	0
84	SN	87	0	0	4	0
84	SO	52	0	0	1	0
84	SP	8	0	0	0	0
84	SQ	29	0	0	2	0
84	SR	29	0	0	0	0
84	SS	10	0	0	0	0
84	ST	15	0	0	0	0
84	SU	8	0	0	0	0
84	SV	27	0	0	0	0
84	SW	64	0	0	2	0
84	SX	95	0	0	2	0
84	SY	32	0	0	0	0
84	SZ	1	0	0	0	0
84	Sa	62	0	0	2	0
84	Sb	27	0	0	1	0
84	Sc	21	0	0	0	0
84	Sd	8	0	0	0	0
84	Se	21	0	0	0	0
84	Sg	3	0	0	0	0
All	All	233370	0	159342	3083	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 8.

All (3083) 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)
10:LG:121:LYS:HE2	10:LG:126:GLY:O	1.26	1.31
10:LG:121:LYS:CE	10:LG:126:GLY:O	1.98	1.10
10:LG:117:ARG:HG3	10:LG:121:LYS:HZ2	0.94	1.07
10:LG:117:ARG:HG3	10:LG:121:LYS:NZ	1.71	1.04
1:L5:2557:G:H1	1:L5:2570:U:H3	1.02	1.01
48:SA:1:MET:HE2	61:SV:79:VAL:HA	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sf:126:CYS:HB2	78:Sf:130:VAL:HG21	1.47	0.97
48:SA:1:MET:H2	48:SA:59:LEU:HB3	1.28	0.96
1:L5:1095:A:H61	1:L5:1200:G:H1	1.15	0.93
46:S2:1748:G:H1	46:S2:1786:U:H3	1.15	0.90
10:LG:117:ARG:CG	10:LG:121:LYS:HZ2	1.84	0.90
1:L5:3710:G:H21	1:L5:3711:A:H61	1.16	0.88
1:L5:3944:G:H1	1:L5:4069:U:H3	1.17	0.88
24:LV:35:LYS:HB2	24:LV:67:LYS:HG3	1.56	0.88
46:S2:925:G:H1	46:S2:1017:U:H3	1.15	0.88
1:L5:1092:G:N2	1:L5:1204:C:O2	2.05	0.88
20:LR:105:LEU:HD12	20:LR:135:LYS:HG3	1.57	0.87
46:S2:928:G:H1	46:S2:1013:U:H3	1.24	0.86
46:S2:795:A:H2'	46:S2:796:G:C8	2.11	0.85
48:SA:25:LEU:HD13	48:SA:46:ILE:HG21	1.58	0.85
46:S2:531:A:N1	46:S2:554:A:N6	2.25	0.84
1:L5:1974:U:H3	1:L5:1994:C:H42	1.22	0.84
1:L5:2708:U:H1'	20:LR:43:LYS:HE3	1.58	0.84
5:LB:317:LEU:HD11	5:LB:382:MET:HG2	1.58	0.83
51:SF:134:VAL:HB	51:SF:199:VAL:HG11	1.62	0.82
10:LG:176:LYS:HD2	37:Li:43:MET:HE1	1.61	0.82
28:LZ:90:PRO:HD2	28:LZ:117:LYS:HE2	1.62	0.82
37:Li:35:LYS:H	37:Li:35:LYS:HE2	1.45	0.82
46:S2:1220:A:H2'	46:S2:1221:G:O4'	1.80	0.82
20:LR:172:ARG:HH22	46:S2:908:A:H5''	1.45	0.81
1:L5:2611:A:H5'	1:L5:2688:G:H4'	1.60	0.81
56:SP:108:LYS:HG2	56:SP:111:MET:HE3	1.62	0.81
10:LG:121:LYS:CD	10:LG:126:GLY:O	2.27	0.81
7:LD:93:THR:HG22	7:LD:94:ASN:H	1.44	0.80
1:L5:1072:C:O2	1:L5:1240:G:N2	2.12	0.80
1:L5:684:G:H5''	8:LE:100:LYS:HG3	1.62	0.80
1:L5:2486:G:O6	1:L5:2494:U:C2	2.34	0.80
8:LE:219:LYS:HB3	8:LE:221:LYS:HZ1	1.46	0.80
1:L5:1095:A:N6	1:L5:1200:G:H1	1.79	0.79
1:L5:698:G:H21	1:L5:968:C:H42	1.29	0.79
78:Sf:107:LYS:HB3	78:Sf:117:LEU:HD21	1.63	0.79
1:L5:478:G:OP1	45:Lr:66:ARG:NH2	2.16	0.79
64:Sc:59:LEU:O	64:Sc:63:ARG:NH2	2.15	0.79
46:S2:77:A:C8	68:SG:154:ARG:HD3	2.18	0.79
1:L5:654:C:H4'	6:LC:268:ARG:HB3	1.65	0.79
1:L5:2739:C:H5''	44:Lp:69:TRP:HH2	1.47	0.79
31:Lc:11:LEU:HA	31:Lc:14:ILE:HD12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LN:123:GLU:HG2	16:LN:128:LYS:HG2	1.64	0.78
3:L8:83:C:H41	27:LY:50:ARG:HH21	1.29	0.78
1:L5:3726:A:H2'	1:L5:3727:A:C8	2.18	0.78
55:SL:103:GLU:OE1	62:SX:14:ARG:NH2	2.17	0.78
21:LS:28:TYR:HB3	22:LT:151:LEU:HD11	1.66	0.78
78:Sf:140:TYR:HE1	78:Sf:145:CYS:HA	1.49	0.78
5:LB:156:TYR:O	5:LB:158:GLN:NE2	2.16	0.78
64:Sc:60:GLU:HB2	64:Sc:63:ARG:HH22	1.47	0.77
14:LL:47:ALA:HB1	14:LL:48:PRO:HD2	1.65	0.77
48:SA:1:MET:H3	48:SA:63:ARG:HE	1.32	0.77
78:Sf:126:CYS:HB3	78:Sf:143:LYS:NZ	1.99	0.77
1:L5:728:U:H2'	1:L5:730:G:H5'	1.65	0.77
46:S2:159:A2M:H5''	46:S2:159:A2M:H8	1.67	0.77
1:L5:988:C:H42	1:L5:1065:G:H1	1.30	0.77
17:LO:197:LYS:NZ	17:LO:203:VAL:OXT	2.18	0.77
25:LW:73:ARG:NH2	68:SG:35:GLU:OE2	2.18	0.77
1:L5:1972:G:OP1	1:L5:2013:A:N6	2.17	0.76
21:LS:11:LYS:HG3	21:LS:29:ARG:HH21	1.50	0.76
48:SA:1:MET:N	48:SA:59:LEU:HB3	2.00	0.76
1:L5:4996:C:OP1	32:Ld:32:ARG:NH1	2.19	0.76
33:Le:8:VAL:HG23	33:Le:10:PRO:HD3	1.67	0.76
46:S2:1757:G:H21	46:S2:1758:G:H1'	1.50	0.76
48:SA:205:ARG:NH2	48:SA:214:GLU:OE2	2.19	0.76
1:L5:1974:U:H3	1:L5:1994:C:N4	1.84	0.76
1:L5:1439:C:H5'	9:LF:34:ARG:HH12	1.51	0.75
17:LO:5:GLN:O	17:LO:31:ARG:NH2	2.20	0.75
57:SQ:6:PRO:O	57:SQ:27:ARG:NH2	2.17	0.75
23:LU:60:VAL:HG12	23:LU:61:VAL:HG23	1.67	0.75
48:SA:1:MET:N	48:SA:63:ARG:HE	1.84	0.75
46:S2:881:G:N1	46:S2:905:C:N3	2.26	0.75
46:S2:881:G:N2	46:S2:905:C:O2	2.15	0.75
31:Lc:21:VAL:HG11	31:Lc:96:ILE:HD12	1.69	0.75
28:LZ:57:MET:HE2	28:LZ:61:LYS:HD3	1.69	0.74
46:S2:913:A:OP2	52:SH:99:ARG:NH1	2.18	0.74
1:L5:2416:G:H4'	1:L5:2417:A:OP2	1.86	0.74
17:LO:61:ARG:HA	17:LO:70:PRO:HD2	1.69	0.74
46:S2:635:G:OP1	77:Se:21:LYS:NZ	2.19	0.74
1:L5:2565:A:H3'	1:L5:2566:G:H8	1.52	0.74
48:SA:1:MET:HE3	48:SA:2:SER:N	2.03	0.74
66:Sg:244:ASN:HD21	66:Sg:295:GLY:HA3	1.50	0.74
76:Sb:40:CYS:SG	76:Sb:41:TYR:N	2.58	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4765:G:O6	15:LM:4:ARG:NH2	2.19	0.74
1:L5:1718:C:OP2	9:LF:200:ARG:NH1	2.18	0.74
1:L5:2469:C:H5	1:L5:2471:G:H1	1.33	0.74
48:SA:1:MET:HG3	61:SV:79:VAL:HG22	1.69	0.74
48:SA:1:MET:CE	61:SV:79:VAL:HA	2.17	0.73
46:S2:696:G:N3	46:S2:737:G:N2	2.37	0.73
1:L5:1092:G:N1	1:L5:1204:C:N3	2.30	0.73
1:L5:3641:U:H5	1:L5:3646:A:N7	1.86	0.73
43:Lo:69:ARG:HG3	43:Lo:82:MET:HE1	1.68	0.73
46:S2:823:U:H6	46:S2:823:U:H5''	1.52	0.73
1:L5:1441:C:N4	84:L5:5413:HOH:O	2.21	0.73
67:SC:204:ILE:HD12	67:SC:215:MET:HG2	1.70	0.73
46:S2:636:C:H5''	77:Se:22:GLN:HG2	1.71	0.73
1:L5:493:G:O6	1:L5:660:A:N1	2.21	0.73
71:SN:100:LYS:HE2	71:SN:104:ARG:HH12	1.54	0.73
1:L5:2583:C:OP2	35:Lg:76:ARG:NH1	2.21	0.72
1:L5:4694:G:O2'	11:LH:71:ARG:NH1	2.21	0.72
52:SH:63:PHE:HB3	52:SH:97:GLN:HG2	1.70	0.72
8:LE:91:THR:HG22	8:LE:108:LYS:HB3	1.71	0.72
8:LE:250:GLN:NE2	8:LE:254:ASP:OD2	2.22	0.72
8:LE:180:VAL:HG21	8:LE:258:LEU:HD11	1.70	0.72
46:S2:1091:C:HO2'	73:SW:2:VAL:N	1.87	0.72
1:L5:705:G:OP2	33:Le:5:ARG:NH2	2.21	0.72
1:L5:2079:G:OP2	33:Le:64:LYS:NZ	2.21	0.72
1:L5:3717:A:H2'	1:L5:3718:A2M:C8	2.20	0.71
1:L5:2112:G:O2'	1:L5:2251:G:N2	2.20	0.71
1:L5:3946:G:N2	1:L5:4067:U:O4	2.23	0.71
46:S2:1228:A:H2'	46:S2:1229:G:C8	2.23	0.71
16:LN:60:VAL:HG22	16:LN:134:LEU:HB2	1.70	0.71
46:S2:1737:G:OP1	68:SG:94:ARG:NH2	2.23	0.71
49:SB:144:LYS:HD2	49:SB:208:HIS:HB3	1.71	0.71
10:LG:57:TRP:O	10:LG:62:ARG:NH2	2.23	0.71
50:SD:93:THR:HG21	50:SD:198:ILE:HG22	1.72	0.71
6:LC:5:ARG:HB3	6:LC:24:LEU:HB3	1.73	0.71
8:LE:209:PRO:HB2	8:LE:212:LEU:HD23	1.72	0.71
68:SG:136:LYS:NZ	68:SG:175:LYS:O	2.24	0.71
11:LH:93:ARG:HG2	11:LH:182:SER:HB3	1.71	0.70
55:SL:23:VAL:HG23	55:SL:25:LEU:H	1.56	0.70
68:SG:22:ARG:HH22	68:SG:25:ARG:HE	1.37	0.70
1:L5:2351:OMC:HM22	1:L5:2352:U:H5'	1.72	0.70
1:L5:2486:G:O6	1:L5:2494:U:O2	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:322:HIS:O	5:LB:342:LYS:NZ	2.23	0.70
38:Lj:2:THR:HG22	38:Lj:4:GLY:H	1.55	0.70
1:L5:2544:G:N2	3:L8:126:C:OP1	2.20	0.70
70:SM:75:ASN:OD1	70:SM:75:ASN:N	2.23	0.70
60:SU:20:ILE:HG22	60:SU:116:ILE:HG22	1.72	0.70
70:SM:55:ASN:ND2	70:SM:81:ASP:OD1	2.25	0.70
46:S2:655:A:N1	84:S2:2129:HOH:O	2.25	0.70
77:Se:36:MET:HE3	77:Se:40:ARG:HH12	1.57	0.70
11:LH:44:GLU:OE2	15:LM:2:VAL:N	2.25	0.70
33:Le:4:LEU:O	33:Le:121:ARG:NH1	2.25	0.70
1:L5:3597:G:H2'	1:L5:3598:C:H6	1.56	0.69
1:L5:4873:G:N7	17:LO:179:LYS:HE3	2.07	0.69
5:LB:153:MET:HB2	5:LB:194:LEU:HD11	1.73	0.69
8:LE:177:GLY:CA	8:LE:184:VAL:HB	2.21	0.69
1:L5:2658:G:N2	1:L5:2676:A:OP2	2.24	0.69
12:LI:38:ARG:HE	12:LI:83:ASP:HB3	1.57	0.69
66:Sg:5:MET:HB2	66:Sg:270:LEU:HD21	1.74	0.69
47:SE:31:PRO:HG2	47:SE:38:LEU:HG	1.75	0.69
55:SL:91:ASP:HB3	55:SL:104:LYS:HE2	1.72	0.69
46:S2:403:G:OP2	84:S2:2101:HOH:O	2.11	0.69
1:L5:158:A:N1	1:L5:276:C:O2'	2.25	0.69
1:L5:5054:C:H4'	1:L5:5055:G:H8	1.57	0.69
7:LD:197:LYS:HB3	7:LD:202:GLN:HB2	1.74	0.69
62:SX:7:LEU:HG	73:SW:77:PRO:HB2	1.74	0.69
46:S2:1277:C:H2'	46:S2:1278:A:H8	1.58	0.68
1:L5:511:C:H2'	1:L5:512:U:C6	2.29	0.68
1:L5:4198:G:H22	12:LI:108:ALA:CB	2.05	0.68
1:L5:1095:A:N1	1:L5:1200:G:N2	2.37	0.68
78:Sf:126:CYS:HB3	78:Sf:143:LYS:HZ3	1.58	0.68
2:L7:49:A:H5''	7:LD:224:SER:HB3	1.75	0.68
1:L5:4097:G:H21	1:L5:4113:U:H5'	1.58	0.68
48:SA:52:LYS:HB2	79:SR:109:LEU:HD13	1.74	0.68
67:SC:167:ARG:HB3	67:SC:177:PRO:HB2	1.75	0.68
13:LJ:93:GLU:HG3	13:LJ:175:LEU:HD11	1.76	0.68
46:S2:1752:C:O2'	46:S2:1782:G:N2	2.26	0.68
4:LA:129:ALA:O	4:LA:169:VAL:HG21	1.94	0.67
1:L5:1705:G:O2'	1:L5:1706:A:O4'	2.12	0.67
2:L7:33:U:H2'	2:L7:34:C:C6	2.29	0.67
1:L5:2748:C:H4'	35:Lg:65:MET:HE2	1.76	0.67
11:LH:140:GLN:HB3	11:LH:143:GLU:HG3	1.75	0.67
23:LU:20:LYS:HG2	23:LU:73:THR:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SP:41:GLN:HG3	56:SP:84:ILE:HD12	1.77	0.67
1:L5:4992:G:H2'	1:L5:4993:G:C8	2.29	0.67
13:LJ:32:ARG:HA	13:LJ:35:ARG:HE	1.57	0.67
1:L5:2261:G:N2	84:L5:5486:HOH:O	2.27	0.67
1:L5:4125:C:H5'	10:LG:45:ILE:HD12	1.75	0.67
22:LT:43:LYS:O	22:LT:58:HIS:ND1	2.27	0.67
1:L5:1952:G:H4'	21:LS:93:MET:HG2	1.74	0.67
46:S2:164:A:H3'	46:S2:165:G:H21	1.60	0.67
48:SA:63:ARG:HG2	48:SA:185:MET:HE1	1.77	0.67
1:L5:4274:A:H2'	1:L5:4275:G:C8	2.29	0.67
1:L5:1460:C:H5''	19:LQ:144:LYS:HG2	1.76	0.66
1:L5:2568:C:H2'	1:L5:2569:G:H8	1.59	0.66
1:L5:2083:C:OP2	19:LQ:14:ARG:NH2	2.25	0.66
1:L5:2705:G:H22	1:L5:2710:C:H5	1.44	0.66
14:LL:123:LYS:HD2	14:LL:155:MET:HE2	1.76	0.66
23:LU:39:PHE:HZ	23:LU:87:THR:HG22	1.60	0.66
46:S2:837:A:H61	74:SY:9:THR:H	1.43	0.66
46:S2:1396:A:O2'	46:S2:1398:G:N7	2.28	0.66
1:L5:3597:G:H2'	1:L5:3598:C:C6	2.30	0.66
8:LE:243:THR:HG22	8:LE:245:GLN:H	1.60	0.66
22:LT:146:LYS:NZ	22:LT:149:GLU:OE1	2.22	0.66
1:L5:1872:G:N7	84:L5:5490:HOH:O	2.27	0.66
46:S2:102:A:H4'	46:S2:104:A:C8	2.31	0.66
1:L5:3710:G:N2	1:L5:3711:A:H61	1.93	0.66
1:L5:3953:G:N7	84:L5:5489:HOH:O	2.27	0.66
36:Lh:5:LYS:NZ	84:Lh:201:HOH:O	2.27	0.66
6:LC:138:MET:HE1	6:LC:145:GLU:HG3	1.78	0.66
1:L5:2739:C:H5''	44:Lp:69:TRP:CH2	2.31	0.66
10:LG:117:ARG:CG	10:LG:121:LYS:NZ	2.54	0.66
46:S2:99:A2M:H8	46:S2:99:A2M:O5'	1.96	0.66
53:SI:134:GLU:OE2	53:SI:138:ASN:ND2	2.29	0.66
11:LH:115:ARG:HG2	11:LH:123:ILE:HG12	1.77	0.66
45:Lr:21:ASN:N	45:Lr:21:ASN:OD1	2.23	0.66
46:S2:955:A:N6	46:S2:971:G:H1'	2.11	0.66
1:L5:498:C:N4	84:L5:5528:HOH:O	2.29	0.66
46:S2:59:U:H5''	46:S2:503:C:N4	2.11	0.66
1:L5:982:U:C4	8:LE:71:ARG:HD3	2.30	0.65
67:SC:267:GLN:NE2	84:SC:301:HOH:O	2.27	0.65
1:L5:1094:G:H2'	1:L5:1095:A:C8	2.31	0.65
1:L5:1919:G:O6	34:Lf:29:LYS:NZ	2.30	0.65
31:Lc:48:LEU:HD21	31:Lc:60:ILE:HG21	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SA:5:LEU:HD21	61:SV:41:LYS:HD3	1.77	0.65
1:L5:3717:A:H2'	1:L5:3718:A2M:H8	1.77	0.65
18:LP:115:GLU:HG2	18:LP:151:THR:HG23	1.79	0.65
48:SA:40:LYS:HD3	79:SR:101:ASP:HB3	1.79	0.65
57:SQ:86:GLN:HE22	57:SQ:122:ALA:HA	1.60	0.65
1:L5:1549:G:N7	84:L5:5545:HOH:O	2.29	0.65
46:S2:1285:G:H5'	70:SM:61:TYR:HE2	1.60	0.65
50:SD:170:THR:HG23	50:SD:187:LYS:HG2	1.77	0.65
1:L5:280:G:H5''	16:LN:14:LYS:HE2	1.79	0.65
1:L5:3950:U:H3	1:L5:4064:C:H42	1.42	0.65
29:La:25:HIS:NE2	84:La:201:HOH:O	2.28	0.65
35:Lg:41:ALA:O	35:Lg:52:ARG:NH1	2.29	0.65
1:L5:737:C:OP2	15:LM:71:LYS:NZ	2.30	0.65
46:S2:940:U:H3	46:S2:1002:U:H3	1.44	0.65
61:SV:2:GLN:H	61:SV:8:PHE:HA	1.59	0.65
68:SG:159:ARG:NH2	68:SG:171:THR:O	2.30	0.65
1:L5:215:C:OP1	1:L5:219:G:N2	2.30	0.65
1:L5:413:G:OP2	40:Ll:36:ARG:NH1	2.29	0.65
1:L5:1973:G:O6	1:L5:1995:G:O2'	2.14	0.65
1:L5:4260:U:H2'	1:L5:4261:C:C6	2.32	0.65
1:L5:4751:G:N7	34:Lf:52:LYS:NZ	2.42	0.65
28:LZ:50:PRO:HD3	28:LZ:68:ILE:HG12	1.79	0.65
61:SV:35:ASN:HD21	67:SC:267:GLN:HE22	1.44	0.65
64:Sc:18:LEU:HD11	64:Sc:43:ILE:HD12	1.79	0.65
79:SR:18:GLU:HG2	79:SR:69:ILE:HG23	1.78	0.65
46:S2:1129:G:N7	84:S2:2155:HOH:O	2.28	0.65
1:L5:2758:G:O2'	1:L5:2765:A:N3	2.29	0.65
46:S2:1774:C:N4	84:S2:2167:HOH:O	2.30	0.65
6:LC:146:GLU:HB2	6:LC:175:LYS:HB3	1.78	0.64
46:S2:1448:A:OP1	60:SU:30:LYS:NZ	2.27	0.64
1:L5:1242:G:H1'	30:Lb:120:ARG:HD2	1.77	0.64
1:L5:2756:G:O6	28:LZ:51:ARG:NH2	2.27	0.64
12:LI:38:ARG:NH1	12:LI:45:GLU:OE1	2.23	0.64
1:L5:2378:G:N2	1:L5:2381:A:OP2	2.29	0.64
17:LO:178:ARG:NH1	17:LO:182:GLU:OE2	2.30	0.64
43:Lo:2:VAL:N	43:Lo:90:HIS:O	2.31	0.64
1:L5:399:G:N2	84:L5:5554:HOH:O	2.30	0.64
1:L5:1514:U:H2'	1:L5:1515:A:C8	2.33	0.64
13:LJ:19:LYS:HE3	13:LJ:75:ARG:HH12	1.62	0.64
3:L8:12:G:OP1	18:LP:3:ARG:NH1	2.31	0.64
8:LE:245:GLN:HA	8:LE:248:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SG:22:ARG:NH2	68:SG:25:ARG:HE	1.96	0.64
1:L5:133:C:H41	36:Lh:74:LYS:HA	1.63	0.64
1:L5:2543:A:H2	1:L5:2773:G:H1	1.44	0.64
1:L5:947:C:OP1	6:LC:336:ARG:NH1	2.31	0.64
1:L5:3746:A:N1	84:L5:5561:HOH:O	2.30	0.64
37:Li:19:LYS:HE2	37:Li:19:LYS:N	2.13	0.64
1:L5:407:A:O2'	1:L5:410:A:OP1	2.16	0.63
1:L5:2486:G:O6	1:L5:2493:G:N2	2.31	0.63
46:S2:319:C:H2'	46:S2:320:G:H8	1.63	0.63
46:S2:529:A:H61	46:S2:555:A:H61	1.47	0.63
8:LE:225:PRO:HB2	8:LE:226:ARG:HE	1.64	0.63
18:LP:42:ARG:NH1	18:LP:110:ASP:OD1	2.31	0.63
24:LV:36:ASN:ND2	24:LV:67:LYS:HG2	2.14	0.63
46:S2:306:C:C4	46:S2:308:G:N2	2.66	0.63
48:SA:66:VAL:HG21	48:SA:185:MET:HE2	1.78	0.63
1:L5:1491:A:N7	84:L5:5584:HOH:O	2.30	0.63
1:L5:5023:C:H5''	53:SI:124:LYS:HD3	1.81	0.63
47:SE:87:MET:HE1	47:SE:236:ILE:HD13	1.79	0.63
50:SD:143:ARG:NH2	84:SD:303:HOH:O	2.31	0.63
51:SF:41:VAL:HG23	51:SF:42:LYS:HG3	1.79	0.63
69:SJ:84:ILE:HG13	69:SJ:86:VAL:HG13	1.80	0.63
76:Sb:72:ARG:NH2	84:Sb:101:HOH:O	2.21	0.63
1:L5:980:U:H2'	1:L5:981:C:C6	2.33	0.63
1:L5:3940:U:H5''	10:LG:75:LYS:HE3	1.80	0.63
9:LF:182:TYR:HB3	9:LF:200:ARG:HG3	1.80	0.63
49:SB:34:LYS:NZ	49:SB:43:ASN:OD1	2.29	0.63
5:LB:154:LYS:HG3	5:LB:194:LEU:HD12	1.80	0.63
35:Lg:42:PRO:HB2	35:Lg:53:LEU:HD12	1.79	0.63
46:S2:1139:C:H5	46:S2:1149:A:H62	1.47	0.63
1:L5:1992:U:H4'	1:L5:2002:A:H2	1.63	0.63
20:LR:52:ARG:NH2	84:LR:201:HOH:O	2.32	0.63
46:S2:153:G:N3	68:SG:13:GLN:NE2	2.46	0.63
1:L5:4575:G:OP1	84:L5:5401:HOH:O	2.15	0.63
46:S2:333:G:OP2	68:SG:190:ARG:NH1	2.32	0.63
60:SU:20:ILE:HD11	60:SU:91:LEU:HD12	1.80	0.63
1:L5:2565:A:H3'	1:L5:2566:G:C8	2.33	0.62
25:LW:80:ARG:NH2	46:S2:167:G:O3'	2.32	0.62
32:Ld:19:GLU:HB3	32:Ld:102:LEU:HD11	1.80	0.62
51:SF:127:ARG:O	51:SF:129:GLY:N	2.32	0.62
70:SM:79:VAL:HG11	70:SM:88:TRP:HZ3	1.64	0.62
1:L5:1326:A2M:OP2	1:L5:4445:U:O2'	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1437:C:OP1	30:Lb:106:LYS:NZ	2.23	0.62
11:LH:71:ARG:NH2	84:LH:202:HOH:O	2.32	0.62
30:Lb:90:SER:OG	30:Lb:95:ARG:NH1	2.30	0.62
50:SD:117:ARG:NH1	84:SD:302:HOH:O	2.31	0.62
63:Sa:45:VAL:HG11	63:Sa:53:ILE:HG13	1.81	0.62
1:L5:2672:C:OP1	44:Lp:44:LYS:NZ	2.29	0.62
46:S2:823:U:H5''	46:S2:823:U:C6	2.34	0.62
10:LG:120:LYS:NZ	10:LG:123:ALA:O	2.30	0.62
12:LI:87:MET:HG2	12:LI:138:ILE:HG12	1.80	0.62
46:S2:563:G:O2'	46:S2:564:A:OP1	2.14	0.62
46:S2:981:A:H2'	46:S2:982:G:C8	2.35	0.62
66:Sg:180:ALA:O	66:Sg:181:ASN:ND2	2.32	0.62
1:L5:1754:U:O2	1:L5:1755:C:N4	2.32	0.62
1:L5:3868:G:H22	1:L5:3900:G:H1'	1.65	0.62
7:LD:225:GLN:HA	7:LD:228:LYS:HG3	1.81	0.62
8:LE:274:VAL:HG21	34:Lf:2:SER:HB3	1.80	0.62
44:Lp:85:ARG:NH2	84:Lp:202:HOH:O	2.30	0.62
46:S2:1712:A:H2'	46:S2:1713:C:C6	2.35	0.62
1:L5:1481:C:H41	37:Li:4:ARG:HG3	1.65	0.62
1:L5:3594:C:N4	84:L5:5677:HOH:O	2.33	0.62
1:L5:4260:U:H2'	1:L5:4261:C:H6	1.64	0.62
46:S2:1536:G:H2'	46:S2:1537:A:H8	1.63	0.62
1:L5:515:C:H41	1:L5:647:G:H21	1.47	0.62
1:L5:3880:G:H2'	1:L5:3881:G:C8	2.35	0.62
1:L5:4522:G:O2'	1:L5:4525:C:OP2	2.15	0.62
15:LM:33:GLN:CD	15:LM:33:GLN:H	2.06	0.62
46:S2:1861:G:H5''	63:Sa:3:LYS:HA	1.82	0.62
78:Sf:146:LEU:HG	78:Sf:147:THR:H	1.65	0.62
1:L5:4724:A:O2'	5:LB:104:THR:HG22	2.00	0.62
46:S2:367:U:H4'	46:S2:371:A:C8	2.35	0.62
46:S2:1238:PSU:O4	46:S2:1242:U:H5	1.83	0.62
1:L5:2632:PSU:H2'	1:L5:2633:U:C6	2.34	0.62
1:L5:3614:G:O2'	1:L5:3615:G:OP1	2.17	0.62
1:L5:3761:C:H2'	1:L5:3762:PSU:O4'	1.99	0.62
1:L5:4198:G:H1	12:LI:108:ALA:HA	1.64	0.62
57:SQ:146:ARG:NH1	84:SQ:201:HOH:O	2.32	0.62
1:L5:1662:C:H2'	1:L5:1663:C:C6	2.35	0.62
1:L5:1812:C:H5''	30:Lb:56:LYS:HE3	1.82	0.62
1:L5:3976:C:N4	1:L5:4035:G:OP2	2.32	0.62
46:S2:377:G:H5'	53:SI:98:LYS:HB3	1.80	0.62
3:L8:63:U:O2'	36:Lh:52:LYS:NZ	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LH:31:ARG:NH1	11:LH:149:ASN:OD1	2.33	0.61
45:Lr:63:VAL:HG22	45:Lr:79:ARG:HG2	1.81	0.61
53:SI:5:ARG:NH2	84:SI:305:HOH:O	2.32	0.61
1:L5:4239:A:H2'	1:L5:4240:G:C8	2.35	0.61
8:LE:223:ARG:H	8:LE:223:ARG:HH21	1.48	0.61
1:L5:1252:C:H41	1:L5:1259:G:H21	1.48	0.61
48:SA:1:MET:SD	61:SV:79:VAL:HG22	2.40	0.61
1:L5:142:G:O2'	1:L5:144:G:OP1	2.18	0.61
1:L5:3710:G:H21	1:L5:3711:A:N6	1.95	0.61
7:LD:116:ASP:OD1	7:LD:116:ASP:N	2.33	0.61
43:Lo:81:ARG:C	43:Lo:82:MET:HE2	2.26	0.61
47:SE:174:LYS:O	47:SE:179:ASN:ND2	2.33	0.61
1:L5:3663:A:N6	1:L5:4168:G:O2'	2.33	0.61
1:L5:3714:G:N7	84:L5:5604:HOH:O	2.31	0.61
5:LB:94:GLU:N	5:LB:158:GLN:OE1	2.25	0.61
46:S2:562:U:H2'	46:S2:563:G:C8	2.35	0.61
25:LW:71:ARG:NH2	46:S2:1781:A:OP1	2.33	0.61
46:S2:795:A:H2'	46:S2:796:G:H8	1.66	0.61
48:SA:1:MET:CG	61:SV:79:VAL:HG22	2.31	0.61
69:SJ:113:GLN:O	69:SJ:117:LEU:HG	1.99	0.61
79:SR:72:LYS:HE2	79:SR:72:LYS:HA	1.82	0.61
1:L5:4537:C:H2'	1:L5:4538:G:C8	2.34	0.61
23:LU:36:ALA:HB1	23:LU:65:ARG:HD2	1.83	0.61
77:Se:36:MET:HE3	77:Se:40:ARG:NH1	2.16	0.61
4:LA:39:GLY:HA2	4:LA:93:LYS:HG3	1.82	0.61
5:LB:110:ILE:O	5:LB:115:LYS:NZ	2.34	0.61
46:S2:1230:C:OP1	58:SS:130:ARG:NH2	2.30	0.61
1:L5:4594:U:H2'	1:L5:4595:G:H8	1.66	0.61
73:SW:37:PHE:HD1	73:SW:41:MET:HE2	1.66	0.61
1:L5:2263:A:OP1	45:Lr:107:ARG:NH2	2.30	0.60
39:Lk:50:LYS:HE2	84:Lk:101:HOH:O	1.99	0.60
1:L5:278:G:OP2	37:Li:30:ARG:NH2	2.31	0.60
1:L5:1975:G:H4'	1:L5:1983:A:C8	2.36	0.60
11:LH:37:ASP:OD1	11:LH:39:ASN:ND2	2.33	0.60
67:SC:196:ILE:HB	67:SC:223:TYR:HB2	1.83	0.60
78:Sf:124:ASP:O	78:Sf:125:GLU:C	2.44	0.60
1:L5:4093:G:OP2	1:L5:4093:G:N2	2.31	0.60
1:L5:4913:G:H4'	1:L5:4914:C:O5'	2.01	0.60
46:S2:65:C:N4	68:SG:134:GLY:O	2.34	0.60
46:S2:166:A2M:H8	46:S2:166:A2M:H5''	1.82	0.60
53:SI:155:ASN:O	55:SL:21:LYS:NZ	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sg:149:GLU:OE2	79:SR:23:ARG:NH2	2.33	0.60
1:L5:121:A:H62	1:L5:152:U:H3	1.48	0.60
1:L5:711:A:H2'	1:L5:712:C:C6	2.36	0.60
25:LW:80:ARG:NH1	68:SG:129:VAL:O	2.34	0.60
50:SD:42:THR:OG1	50:SD:44:THR:O	2.19	0.60
1:L5:4291:G:H5''	1:L5:4293:PSU:C6	2.37	0.60
1:L5:5024:C:N4	1:L5:5028:G:O2'	2.35	0.60
12:LI:36:LEU:HD11	12:LI:69:ARG:HD2	1.82	0.60
10:LG:99:ALA:HA	10:LG:204:PHE:HZ	1.67	0.60
46:S2:640:A:H2'	46:S2:641:A:C8	2.37	0.60
49:SB:182:LYS:O	49:SB:186:ASN:ND2	2.33	0.60
1:L5:134:G:N2	36:Lh:83:LEU:O	2.34	0.60
1:L5:1339:U:H2'	1:L5:1340:OMC:C6	2.37	0.60
1:L5:1818:G:O2'	1:L5:1820:C:OP2	2.19	0.60
1:L5:2539:C:H2'	1:L5:2540:C:C6	2.36	0.60
1:L5:3736:A:H2'	1:L5:3737:A:C8	2.35	0.60
6:LC:317:ASN:HB3	6:LC:320:LYS:HG2	1.84	0.60
12:LI:185:VAL:O	12:LI:188:LYS:NZ	2.34	0.60
14:LL:164:GLU:OE2	29:La:125:LYS:NZ	2.31	0.60
46:S2:1035:A:N1	84:S2:2174:HOH:O	2.30	0.60
66:Sg:18:VAL:O	66:Sg:287:THR:OG1	2.18	0.60
68:SG:146:ASN:O	84:SG:301:HOH:O	2.16	0.60
46:S2:1323:U:H2'	46:S2:1324:G:C8	2.37	0.60
1:L5:1867:A:H2'	1:L5:1868:A:C8	2.37	0.60
1:L5:3727:A:H2'	1:L5:3728:A:C8	2.37	0.60
1:L5:4600:G:H1'	1:L5:4601:U:H5	1.66	0.60
46:S2:1199:A:OP1	63:Sa:2:THR:N	2.35	0.60
1:L5:4274:A:H2'	1:L5:4275:G:H8	1.66	0.60
18:LP:54:GLN:HA	18:LP:83:TRP:CD1	2.37	0.60
46:S2:12:U:H2'	46:S2:13:C:C6	2.36	0.60
46:S2:455:A:H2'	46:S2:456:C:C6	2.37	0.60
63:Sa:52:ASP:OD2	72:SO:121:ARG:HD3	2.02	0.60
1:L5:1908:A:N7	84:L5:5589:HOH:O	2.30	0.59
1:L5:2488:C:H41	3:L8:125:C:H3'	1.67	0.59
1:L5:3717:A:OP2	1:L5:3735:G:N2	2.32	0.59
1:L5:4872:G:N2	17:LO:203:VAL:H	2.01	0.59
4:LA:117:GLU:O	4:LA:162:ASN:ND2	2.35	0.59
46:S2:1536:G:H2'	46:S2:1537:A:C8	2.36	0.59
1:L5:4222:G:OP2	12:LI:117:GLY:HA2	2.02	0.59
1:L5:4694:G:HO2'	11:LH:71:ARG:HH12	1.49	0.59
1:L5:4966:A:H5'	5:LB:128:LYS:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SK:88:GLU:HG3	54:SK:89:ILE:HD13	1.83	0.59
1:L5:2450:G:OP1	4:LA:17:ARG:NH2	2.36	0.59
46:S2:57:U:OP1	46:S2:504:G:O2'	2.20	0.59
49:SB:123:ALA:HB2	49:SB:165:ARG:HG3	1.84	0.59
73:SW:28:ARG:HB3	73:SW:29:PRO:HD3	1.84	0.59
1:L5:3597:G:O5'	20:LR:143:HIS:NE2	2.36	0.59
1:L5:3707:U:H2'	1:L5:3708:C:C6	2.38	0.59
1:L5:3923:A:H2'	1:L5:3924:C:C6	2.37	0.59
4:LA:104:VAL:HG21	4:LA:158:ILE:HD11	1.84	0.59
46:S2:943:U:O2'	72:SO:135:ILE:O	2.21	0.59
74:SY:87:PRO:HG2	74:SY:90:ARG:HG3	1.84	0.59
1:L5:1308:C:H2'	1:L5:1309:C:C6	2.37	0.59
1:L5:4763:U:HO2'	21:LS:174:THR:HG1	1.47	0.59
1:L5:5054:C:H4'	1:L5:5055:G:C8	2.36	0.59
46:S2:323:C:N3	46:S2:328:U:O4	2.34	0.59
46:S2:382:C:H2'	46:S2:383:G:H8	1.65	0.59
46:S2:1822:A:H2'	46:S2:1823:A:C8	2.37	0.59
65:Sd:53:ILE:HD12	65:Sd:55:LEU:HD21	1.85	0.59
69:SJ:113:GLN:HG3	69:SJ:149:VAL:HG21	1.84	0.59
1:L5:1355:G:OP1	19:LQ:108:ARG:NH2	2.35	0.59
1:L5:1970:A:O2'	84:L5:5403:HOH:O	2.17	0.59
5:LB:378:ARG:HD3	25:LW:32:LEU:HD21	1.85	0.59
8:LE:177:GLY:N	8:LE:184:VAL:HB	2.18	0.59
13:LJ:19:LYS:HG2	13:LJ:133:VAL:HB	1.85	0.59
68:SG:57:ASP:HB3	68:SG:98:ARG:HD2	1.85	0.59
1:L5:1049:C:N4	84:L5:5730:HOH:O	2.34	0.59
46:S2:191:A:H62	46:S2:208:G:N2	2.00	0.59
46:S2:881:G:O6	46:S2:905:C:N4	2.23	0.59
75:SZ:52:LYS:HA	75:SZ:52:LYS:HE2	1.85	0.59
78:Sf:94:LYS:O	78:Sf:96:LYS:NZ	2.30	0.59
1:L5:231:U:H4'	27:LY:100:HIS:CD2	2.38	0.59
1:L5:966:A:H5''	1:L5:2092:G:H22	1.67	0.59
1:L5:1094:G:H2'	1:L5:1095:A:H8	1.66	0.59
1:L5:3643:A:N7	38:Lj:2:THR:HG23	2.18	0.59
1:L5:4498:OMU:HM23	1:L5:4500:PSU:C6	2.38	0.59
1:L5:5008:C:H2'	1:L5:5009:G:O4'	2.02	0.59
4:LA:178:PRO:HD2	44:Lp:26:VAL:HG12	1.85	0.59
46:S2:799:U:H2'	46:S2:800:U:C6	2.38	0.59
73:SW:37:PHE:CD1	73:SW:41:MET:HE2	2.37	0.59
1:L5:252:C:O2	1:L5:253:G:N2	2.31	0.59
1:L5:493:G:H1	1:L5:660:A:H2	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2258:C:O2	8:LE:89:LEU:HA	2.03	0.59
8:LE:177:GLY:H	8:LE:184:VAL:HB	1.67	0.59
31:Lc:47:ILE:HB	31:Lc:94:LEU:HG	1.85	0.59
46:S2:1867:U:O2'	63:Sa:38:LYS:NZ	2.36	0.59
1:L5:2014:C:N4	84:L5:5750:HOH:O	2.35	0.58
1:L5:4633:G:O6	84:L5:5402:HOH:O	2.15	0.58
69:SJ:136:ARG:HG2	69:SJ:160:SER:HA	1.85	0.58
1:L5:968:C:OP2	8:LE:110:ARG:NH2	2.35	0.58
1:L5:3617:G:OP1	25:LW:44:ARG:NH2	2.24	0.58
4:LA:156:LYS:NZ	84:LA:406:HOH:O	2.36	0.58
5:LB:36:ASP:HB3	5:LB:39:LYS:HE2	1.85	0.58
5:LB:108:GLU:OE1	5:LB:138:GLN:NE2	2.22	0.58
10:LG:58:PRO:HG2	10:LG:61:ILE:HD12	1.84	0.58
39:Lk:49:ASP:N	39:Lk:49:ASP:OD1	2.34	0.58
46:S2:588:G:OP2	46:S2:588:G:N2	2.31	0.58
53:SI:98:LYS:NZ	84:SI:307:HOH:O	2.36	0.58
64:Sc:61:SER:OG	64:Sc:62:GLU:N	2.32	0.58
1:L5:4198:G:H22	12:LI:108:ALA:HA	1.67	0.58
1:L5:4198:G:H22	12:LI:108:ALA:HB2	1.69	0.58
3:L8:89:U:H2'	3:L8:90:C:C6	2.39	0.58
18:LP:50:ASP:OD2	18:LP:56:GLN:NE2	2.36	0.58
46:S2:203:G:OP1	53:SI:147:LYS:NZ	2.29	0.58
46:S2:1228:A:H2'	46:S2:1229:G:H8	1.67	0.58
46:S2:1512:C:O2'	65:Sd:7:TYR:O	2.16	0.58
1:L5:2089:G:N2	1:L5:2094:G:O2'	2.36	0.58
7:LD:51:MET:HE1	7:LD:163:LEU:HA	1.84	0.58
1:L5:1709:C:N4	84:L5:5832:HOH:O	2.36	0.58
4:LA:33:ASP:O	4:LA:37:ARG:HG3	2.03	0.58
4:LA:135:THR:HG23	4:LA:149:LYS:HB3	1.85	0.58
25:LW:83:THR:HB	68:SG:132:ARG:HA	1.86	0.58
27:LY:51:LYS:NZ	27:LY:71:VAL:O	2.37	0.58
28:LZ:89:ILE:HD11	28:LZ:117:LYS:HB3	1.86	0.58
1:L5:4991:U:H2'	1:L5:4992:G:C8	2.38	0.58
8:LE:178:PRO:HD2	8:LE:181:LEU:HD12	1.84	0.58
13:LJ:96:LYS:HD2	13:LJ:163:MET:HE1	1.85	0.58
46:S2:1092:G:N7	84:S2:2202:HOH:O	2.32	0.58
1:L5:1857:C:H2'	1:L5:1858:A:H8	1.67	0.58
1:L5:3813:A:N3	1:L5:4538:G:O2'	2.37	0.58
46:S2:587:A:H5'	46:S2:592:C:H41	1.68	0.58
46:S2:1588:A:H2'	46:S2:1589:A:C8	2.39	0.58
46:S2:1779:G:H2'	46:S2:1780:G:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SQ:116:ASP:OD1	57:SQ:118:THR:OG1	2.21	0.58
1:L5:715:G:OP1	6:LC:320:LYS:NZ	2.35	0.58
1:L5:2480:G:H2'	1:L5:2481:G:C8	2.39	0.58
1:L5:4140:C:N4	1:L5:4145:C:O2'	2.37	0.58
10:LG:77:PRO:HG2	10:LG:80:ILE:HD12	1.86	0.58
11:LH:107:GLU:OE1	11:LH:127:ARG:NH1	2.36	0.58
59:ST:111:LYS:HA	59:ST:111:LYS:HE3	1.85	0.58
1:L5:3599:A:H2'	1:L5:3600:G:C8	2.39	0.58
1:L5:4884:G:N7	8:LE:272:ARG:NH2	2.51	0.58
46:S2:746:C:H2'	46:S2:747:U:C6	2.39	0.58
1:L5:4280:A:N6	7:LD:28:THR:O	2.33	0.58
10:LG:162:ASP:HB3	10:LG:163:PRO:HD3	1.86	0.58
46:S2:122:G:OP1	47:SE:75:LYS:NZ	2.27	0.58
73:SW:117:ARG:NH1	84:SW:203:HOH:O	2.36	0.58
1:L5:1175:A:H2	1:L5:1185:G:H1	1.50	0.57
1:L5:1756:U:O2'	1:L5:1758:G:OP2	2.15	0.57
1:L5:4200:G:H21	12:LI:111:LEU:HD13	1.68	0.57
1:L5:4507:A:O2'	24:LV:41:SER:OG	2.21	0.57
1:L5:4594:U:H2'	1:L5:4595:G:C8	2.39	0.57
16:LN:120:TRP:HE1	16:LN:123:GLU:HG3	1.68	0.57
19:LQ:110:ARG:HG3	19:LQ:120:ILE:HD12	1.86	0.57
42:Ln:6:ARG:NH1	84:Ln:9502:HOH:O	2.36	0.57
46:S2:563:G:HO2'	46:S2:564:A:P	2.26	0.57
63:Sa:51:ARG:HG2	63:Sa:51:ARG:HH11	1.69	0.57
1:L5:2695:A:OP1	39:Lk:35:LYS:NZ	2.36	0.57
1:L5:4257:A:H5''	13:LJ:54:ARG:NH2	2.19	0.57
9:LF:190:LEU:HD21	9:LF:208:LEU:HD21	1.85	0.57
23:LU:39:PHE:CZ	23:LU:87:THR:HG22	2.39	0.57
29:La:100:ILE:HG13	29:La:123:ILE:HB	1.85	0.57
46:S2:509:OMG:OP1	69:SJ:2:PRO:HA	2.04	0.57
46:S2:696:G:O2'	46:S2:736:C:N4	2.37	0.57
59:ST:60:THR:HG23	59:ST:75:MET:HE2	1.85	0.57
1:L5:1754:U:H2'	1:L5:1755:C:C5	2.39	0.57
1:L5:1801:A:O3'	22:LT:102:ARG:NH1	2.37	0.57
1:L5:3845:A:N3	84:L5:5634:HOH:O	2.32	0.57
12:LI:110:ARG:HG2	84:LI:417:HOH:O	2.02	0.57
23:LU:107:LYS:HE3	23:LU:108:GLU:H	1.70	0.57
46:S2:118:C:H1'	46:S2:445:A:C5	2.40	0.57
68:SG:59:GLN:OE1	68:SG:72:ARG:NH2	2.37	0.57
72:SO:151:LEU:O	84:SO:301:HOH:O	2.17	0.57
1:L5:2262:G:OP2	45:Lr:98:ARG:NH1	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4198:G:H22	12:LI:108:ALA:CA	2.17	0.57
8:LE:258:LEU:HD22	8:LE:262:LYS:HE3	1.86	0.57
46:S2:1192:U:OP1	62:SX:119:ARG:NH2	2.35	0.57
46:S2:1550:G:H3'	46:S2:1579:A:H61	1.69	0.57
1:L5:2864:A:H2'	1:L5:2865:U:C6	2.38	0.57
25:LW:68:GLN:NE2	84:LW:201:HOH:O	2.35	0.57
32:Ld:41:ARG:HG3	32:Ld:78:ARG:HA	1.86	0.57
45:Lr:17:LEU:HD21	45:Lr:19:LYS:HD2	1.87	0.57
51:SF:135:ARG:NE	51:SF:135:ARG:HA	2.19	0.57
58:SS:86:ARG:NH1	58:SS:110:ASP:OD2	2.35	0.57
1:L5:1442:C:N4	1:L5:2105:A:O2'	2.38	0.57
1:L5:2906:G:N2	84:L5:5895:HOH:O	2.38	0.57
1:L5:4591:U:H2'	1:L5:4592:C:C6	2.38	0.57
8:LE:219:LYS:HB3	8:LE:221:LYS:NZ	2.17	0.57
15:LM:126:GLU:HB3	17:LO:181:ALA:HB1	1.87	0.57
46:S2:191:A:H62	46:S2:208:G:H21	1.51	0.57
1:L5:4075:U:OP1	10:LG:246:SER:OG	2.20	0.57
1:L5:4991:U:H2'	1:L5:4992:G:H8	1.70	0.57
13:LJ:146:ARG:HG2	13:LJ:147:ARG:HG3	1.86	0.57
25:LW:74:ARG:NH2	46:S2:1748:G:OP1	2.37	0.57
25:LW:94:ARG:O	25:LW:101:ARG:NH2	2.38	0.57
49:SB:46:LYS:HE3	72:SO:19:PRO:HB2	1.87	0.57
51:SF:128:ILE:HA	51:SF:135:ARG:NE	2.20	0.57
46:S2:1277:C:H2'	46:S2:1278:A:C8	2.40	0.57
66:Sg:272:GLN:NE2	66:Sg:284:PRO:O	2.35	0.57
1:L5:1503:A:H4'	1:L5:1504:G:H5'	1.86	0.57
1:L5:2105:A:N7	84:L5:5660:HOH:O	2.32	0.57
6:LC:2:ALA:HB3	6:LC:268:ARG:HH21	1.69	0.57
8:LE:109:LEU:HD23	8:LE:109:LEU:H	1.70	0.57
46:S2:1309:C:O2	78:Sf:142:GLY:HA3	2.04	0.57
48:SA:1:MET:SD	61:SV:79:VAL:HG13	2.45	0.57
59:ST:76:THR:HG22	59:ST:94:ARG:HG2	1.87	0.57
78:Sf:126:CYS:CB	78:Sf:130:VAL:HG21	2.29	0.57
1:L5:511:C:H2'	1:L5:512:U:H6	1.69	0.57
9:LF:127:LYS:HB2	22:LT:133:ALA:HB3	1.86	0.57
10:LG:30:PRO:O	28:LZ:128:LYS:NZ	2.38	0.57
10:LG:124:GLY:O	10:LG:125:LYS:C	2.48	0.57
20:LR:105:LEU:HD11	20:LR:139:MET:HG3	1.87	0.57
46:S2:145:G:H2'	46:S2:146:G:C8	2.40	0.57
1:L5:1646:A:N7	84:L5:5637:HOH:O	2.32	0.56
1:L5:3748:A:H5''	4:LA:243:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:3974:G:OP2	1:L5:3975:C:N4	2.38	0.56
46:S2:308:G:N2	84:S2:2247:HOH:O	2.34	0.56
46:S2:656:G:N7	84:S2:2207:HOH:O	2.32	0.56
66:Sg:220:ASP:HB2	66:Sg:227:LEU:HD11	1.87	0.56
5:LB:141:ASP:OD1	5:LB:142:GLY:N	2.37	0.56
5:LB:354:GLN:HB3	5:LB:359:ALA:HB1	1.86	0.56
11:LH:113:GLU:OE2	11:LH:115:ARG:NH2	2.38	0.56
48:SA:70:ASN:HB3	48:SA:73:ASP:OD2	2.05	0.56
1:L5:500:G:N3	1:L5:504:G:O2'	2.38	0.56
1:L5:1363:C:H3'	14:LL:36:ARG:HH22	1.69	0.56
1:L5:3599:A:H2'	1:L5:3600:G:H8	1.71	0.56
1:L5:3612:C:H1'	1:L5:5016:A:C8	2.41	0.56
1:L5:4938:A:N6	8:LE:247:LYS:HD3	2.20	0.56
1:L5:4940:C:OP1	8:LE:156:ARG:NH1	2.32	0.56
7:LD:62:CYS:HB3	7:LD:105:LEU:HD22	1.87	0.56
8:LE:176:THR:O	8:LE:177:GLY:C	2.47	0.56
15:LM:29:ASP:OD1	15:LM:30:VAL:N	2.36	0.56
25:LW:84:GLY:HA2	68:SG:161:PRO:HD2	1.86	0.56
46:S2:186:C:H2'	46:S2:187:G:C8	2.40	0.56
46:S2:627:U:O2'	46:S2:628:A:OP2	2.23	0.56
46:S2:690:G:N2	46:S2:690:G:OP2	2.39	0.56
56:SP:93:MET:HE2	56:SP:104:GLN:HE21	1.69	0.56
71:SN:100:LYS:NZ	84:SN:201:HOH:O	2.38	0.56
1:L5:1604:G:H2'	1:L5:1605:G:C8	2.41	0.56
1:L5:3707:U:H2'	1:L5:3708:C:H6	1.70	0.56
1:L5:4405:G:OP2	12:LI:7:ARG:NH2	2.36	0.56
2:L7:117:G:OP1	7:LD:253:TYR:OH	2.23	0.56
11:LH:16:VAL:HG21	11:LH:81:ILE:HG23	1.87	0.56
46:S2:190:G:O2'	46:S2:209:A:N6	2.38	0.56
50:SD:150:MET:HE3	50:SD:152:PHE:HZ	1.71	0.56
51:SF:102:LEU:HD11	75:SZ:100:VAL:HG21	1.88	0.56
64:Sc:14:VAL:HA	64:Sc:32:VAL:HG12	1.86	0.56
67:SC:81:ILE:HG23	67:SC:86:LEU:HB2	1.88	0.56
1:L5:1824:G:H2'	1:L5:1825:A:C8	2.41	0.56
1:L5:2486:G:C6	1:L5:2494:U:N3	2.73	0.56
3:L8:141:C:H2'	3:L8:142:U:C6	2.41	0.56
12:LI:109:ASP:O	12:LI:110:ARG:HB2	2.05	0.56
46:S2:17:C:O2'	46:S2:1194:A:N1	2.37	0.56
46:S2:319:C:H2'	46:S2:320:G:C8	2.40	0.56
48:SA:5:LEU:O	48:SA:9:GLN:NE2	2.28	0.56
1:L5:1306:C:H2'	1:L5:1307:A:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1348:U:H2'	1:L5:1349:G:H8	1.70	0.56
5:LB:303:ALA:HB3	5:LB:312:LYS:HG3	1.88	0.56
7:LD:208:MET:HB2	7:LD:233:PRO:HG3	1.87	0.56
32:Ld:24:GLU:OE2	32:Ld:87:ARG:NH1	2.38	0.56
64:Sc:18:LEU:HD12	64:Sc:29:GLN:HG2	1.87	0.56
1:L5:1522:OMG:N7	84:L5:5672:HOH:O	2.33	0.56
1:L5:3865:A:N6	84:L5:5743:HOH:O	2.34	0.56
1:L5:4088:C:OP1	4:LA:37:ARG:NH2	2.33	0.56
1:L5:4619:U:H2'	1:L5:4620:OMU:H6	1.88	0.56
13:LJ:12:MET:HE3	13:LJ:137:PRO:HB2	1.88	0.56
46:S2:552:G:H2'	46:S2:553:U:C6	2.41	0.56
46:S2:1681:U:H2'	46:S2:1682:C:C6	2.41	0.56
1:L5:1602:U:OP1	38:Lj:2:THR:OG1	2.22	0.56
1:L5:4415:A:H4'	12:LI:74:LYS:HE3	1.88	0.56
46:S2:1139:C:H2'	46:S2:1140:G:O4'	2.06	0.56
46:S2:1438:A:H2'	46:S2:1439:A:C8	2.41	0.56
46:S2:1807:C:H2'	46:S2:1808:U:C6	2.40	0.56
74:SY:110:ARG:HG2	74:SY:110:ARG:HH11	1.70	0.56
1:L5:488:G:H2'	1:L5:489:C:C6	2.41	0.56
1:L5:644:G:N7	84:L5:5690:HOH:O	2.33	0.56
1:L5:2294:G:N7	84:L5:5694:HOH:O	2.33	0.56
1:L5:5029:C:O2'	1:L5:5030:U:O4'	2.23	0.56
17:LO:109:PRO:HB2	17:LO:111:PRO:HD2	1.87	0.56
46:S2:582:U:H1'	74:SY:33:ALA:HB2	1.88	0.56
56:SP:24:GLN:O	56:SP:28:MET:HG3	2.06	0.56
1:L5:1322:1MA:OP1	84:L5:5404:HOH:O	2.18	0.56
1:L5:1479:G:H2'	1:L5:1480:C:C6	2.40	0.56
6:LC:182:LYS:HG2	6:LC:204:ARG:HD3	1.87	0.56
7:LD:41:LYS:NZ	22:LT:32:ARG:O	2.31	0.56
36:Lh:12:LYS:NZ	36:Lh:20:GLN:OE1	2.32	0.56
46:S2:1405:A:H2'	46:S2:1406:G:O4'	2.05	0.56
70:SM:17:ALA:HB3	70:SM:123:VAL:HG23	1.88	0.56
1:L5:699:C:H2'	1:L5:700:G:H8	1.69	0.55
1:L5:903:C:N4	84:L5:5954:HOH:O	2.39	0.55
1:L5:4736:C:H2'	1:L5:4737:G:H8	1.72	0.55
1:L5:4768:G:OP1	17:LO:168:TYR:OH	2.20	0.55
8:LE:220:LYS:C	8:LE:221:LYS:HG2	2.30	0.55
46:S2:686:PSU:OP1	73:SW:32:LYS:HG2	2.06	0.55
46:S2:874:G:H2'	46:S2:875:A:H8	1.71	0.55
69:SJ:120:ALA:HB2	69:SJ:129:LEU:HD12	1.89	0.55
1:L5:511:C:H5''	14:LL:165:LYS:HZ3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1358:G:O2'	1:L5:1360:G:O6	2.19	0.55
1:L5:1820:C:H2'	1:L5:1822:U:H5'	1.88	0.55
1:L5:4441:A:H5''	12:LI:103:LEU:HD12	1.88	0.55
46:S2:191:A:N6	46:S2:208:G:H21	2.04	0.55
46:S2:1511:U:H2'	46:S2:1512:C:C6	2.41	0.55
53:SI:139:LYS:NZ	53:SI:140:LYS:O	2.39	0.55
71:SN:94:LYS:NZ	84:SN:202:HOH:O	2.39	0.55
79:SR:77:GLU:O	79:SR:81:ARG:HG2	2.07	0.55
1:L5:172:C:O2	1:L5:173:C:N4	2.39	0.55
1:L5:1093:C:H2'	1:L5:1094:G:H8	1.72	0.55
1:L5:4699:U:H1'	1:L5:4700:A:H5''	1.89	0.55
9:LF:217:ARG:O	9:LF:246:ARG:NH1	2.38	0.55
20:LR:173:ARG:NH2	46:S2:909:G:OP1	2.39	0.55
46:S2:159:A2M:H2	46:S2:468:A2M:O4'	2.05	0.55
46:S2:1563:G:OP1	59:ST:121:ARG:NH1	2.35	0.55
12:LI:112:GLN:HG2	12:LI:116:ARG:O	2.06	0.55
46:S2:3:C:N3	84:S2:2229:HOH:O	2.33	0.55
72:SO:59:GLY:HA2	72:SO:68:GLU:HG2	1.89	0.55
1:L5:4967:A:H2'	1:L5:4968:A:C8	2.41	0.55
46:S2:560:A:OP2	69:SJ:177:ASN:ND2	2.39	0.55
1:L5:153:G:H2'	1:L5:154:G:H8	1.72	0.55
1:L5:418:A:C2	3:L8:17:A:H1'	2.41	0.55
1:L5:1307:A:H2'	1:L5:1308:C:C6	2.41	0.55
18:LP:55:LYS:O	84:LP:301:HOH:O	2.18	0.55
33:Le:32:LYS:NZ	84:Le:306:HOH:O	2.40	0.55
44:Lp:13:LYS:HE3	44:Lp:14:TYR:CZ	2.41	0.55
51:SF:19:LEU:HD21	51:SF:69:VAL:HG11	1.89	0.55
1:L5:208:A:C2	1:L5:233:U:H5''	2.42	0.55
1:L5:730:G:C5	9:LF:73:ARG:HD3	2.42	0.55
1:L5:1802:A:H5''	1:L5:1803:G:H5'	1.89	0.55
2:L7:95:C:OP2	84:L7:301:HOH:O	2.18	0.55
19:LQ:19:LYS:NZ	84:LQ:203:HOH:O	2.29	0.55
31:Lc:20:LEU:HD23	31:Lc:101:ASP:HB2	1.88	0.55
46:S2:686:PSU:O4	52:SH:118:ARG:NH2	2.35	0.55
46:S2:968:U:H6	46:S2:968:U:H5''	1.72	0.55
8:LE:222:LEU:HD21	8:LE:225:PRO:HB3	1.89	0.55
23:LU:64:GLU:OE2	23:LU:71:THR:OG1	2.20	0.55
31:Lc:36:LYS:O	31:Lc:40:GLN:HG2	2.07	0.55
46:S2:942:G:H2'	46:S2:943:U:C6	2.41	0.55
50:SD:136:VAL:HG13	50:SD:152:PHE:HB2	1.88	0.55
73:SW:35:VAL:O	73:SW:39:THR:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:180:C:H2'	1:L5:181:C:O4'	2.07	0.55
1:L5:1077:C:H4'	1:L5:1215:C:N4	2.22	0.55
31:Lc:57:LYS:NZ	84:Lc:205:HOH:O	2.39	0.55
46:S2:425:G:N7	84:S2:2238:HOH:O	2.34	0.55
1:L5:9:C:OP1	16:LN:37:HIS:NE2	2.30	0.55
1:L5:93:G:H2'	1:L5:94:A:C8	2.42	0.55
1:L5:2318:G:N2	1:L5:2321:G:OP2	2.36	0.55
1:L5:4648:A:OP1	20:LR:62:ARG:NH2	2.40	0.55
3:L8:109:C:H4'	84:L8:555:HOH:O	2.06	0.55
12:LI:107:GLY:O	12:LI:109:ASP:N	2.40	0.55
13:LJ:27:GLY:HA2	13:LJ:68:ILE:HG23	1.87	0.55
46:S2:803:C:H4'	73:SW:80:ASP:OD2	2.07	0.55
46:S2:857:U:H2'	46:S2:858:A:C8	2.42	0.55
50:SD:40:ARG:HH11	50:SD:49:ILE:HD11	1.72	0.55
59:ST:10:ASN:HB3	59:ST:13:GLU:HG3	1.87	0.55
62:SX:60:LYS:HD2	62:SX:116:PRO:HB3	1.89	0.55
74:SY:3:ASP:H	74:SY:32:LYS:HE3	1.72	0.55
1:L5:135:G:N2	36:Lh:95:LEU:O	2.35	0.54
1:L5:1174:G:H1	1:L5:1186:U:H3	1.55	0.54
1:L5:4967:A:H2'	1:L5:4968:A:H8	1.72	0.54
7:LD:223:PHE:HD1	7:LD:226:TYR:CD2	2.26	0.54
10:LG:124:GLY:O	10:LG:125:LYS:O	2.25	0.54
28:LZ:92:ASP:HB3	28:LZ:95:VAL:HG12	1.89	0.54
34:Lf:93:PRO:HB2	34:Lf:95:LYS:HG2	1.89	0.54
46:S2:1740:C:OP1	53:SI:44:HIS:ND1	2.33	0.54
52:SH:63:PHE:HA	52:SH:95:ILE:O	2.07	0.54
1:L5:2844:A:O2'	1:L5:4631:G:H4'	2.06	0.54
1:L5:3709:U:H2'	1:L5:3710:G:C8	2.43	0.54
1:L5:3732:A:H2'	1:L5:3733:A:C8	2.42	0.54
1:L5:4546:A:N7	4:LA:215:ASN:ND2	2.52	0.54
12:LI:110:ARG:NE	12:LI:111:LEU:HB2	2.23	0.54
13:LJ:9:GLU:HB2	13:LJ:13:ARG:HD3	1.89	0.54
46:S2:1512:C:H5''	65:Sd:8:TRP:HZ3	1.71	0.54
73:SW:111:MET:SD	73:SW:115:GLU:HG2	2.47	0.54
1:L5:285:G:OP1	1:L5:296:A:N6	2.40	0.54
1:L5:1613:A:H5'	4:LA:183:GLY:HA2	1.90	0.54
1:L5:3917:A:H2'	1:L5:3918:G:H8	1.72	0.54
1:L5:4269:G:N7	84:L5:5691:HOH:O	2.33	0.54
28:LZ:121:ARG:O	28:LZ:124:THR:OG1	2.24	0.54
32:Ld:47:LYS:O	32:Ld:51:LYS:HG2	2.06	0.54
46:S2:4:C:H4'	67:SC:207:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SD:143:ARG:NH1	84:SD:305:HOH:O	2.38	0.54
60:SU:34:LYS:NZ	60:SU:105:SER:OG	2.40	0.54
75:SZ:73:VAL:HG21	75:SZ:88:LEU:HD21	1.90	0.54
1:L5:1364:U:H3	1:L5:1373:A:H61	1.55	0.54
1:L5:2520:C:H2'	1:L5:2521:G:C8	2.42	0.54
46:S2:107:A:H2'	46:S2:108:G:C8	2.42	0.54
51:SF:33:ILE:HA	51:SF:36:GLN:HG3	1.90	0.54
78:Sf:126:CYS:HB3	78:Sf:143:LYS:HZ2	1.71	0.54
1:L5:272:U:H2'	1:L5:273:U:C6	2.43	0.54
1:L5:2631:U:H4'	1:L5:2632:PSU:OP2	2.07	0.54
1:L5:3786:U:O2	1:L5:3814:U:H4'	2.06	0.54
3:L8:67:U:H2'	3:L8:68:G:C8	2.42	0.54
7:LD:93:THR:HG22	7:LD:94:ASN:N	2.20	0.54
21:LS:5:GLY:O	21:LS:111:ARG:NH2	2.40	0.54
21:LS:45:TRP:NE1	21:LS:56:LYS:HG3	2.22	0.54
31:Lc:11:LEU:HD22	31:Lc:75:SER:HB2	1.90	0.54
46:S2:862:A:C8	73:SW:107:SER:HA	2.42	0.54
84:S2:2308:HOH:O	47:SE:39:ARG:NH2	2.39	0.54
49:SB:77:ASP:OD1	49:SB:77:ASP:N	2.40	0.54
55:SL:152:LYS:HG3	55:SL:153:LYS:HE2	1.90	0.54
1:L5:2580:U:O2'	28:LZ:79:HIS:ND1	2.35	0.54
1:L5:3720:G:OP1	37:Li:75:LYS:NZ	2.40	0.54
1:L5:4988:U:H3'	1:L5:5061:A:H62	1.72	0.54
13:LJ:19:LYS:HE3	13:LJ:75:ARG:NH1	2.23	0.54
18:LP:151:THR:OG1	18:LP:153:LYS:NZ	2.38	0.54
46:S2:1594:A:N7	75:SZ:104:ARG:HD3	2.22	0.54
1:L5:187:U:H4'	1:L5:189:G:OP2	2.08	0.54
1:L5:716:C:OP2	6:LC:320:LYS:HE2	2.08	0.54
1:L5:4457:PSU:H1'	5:LB:252:ALA:HB3	1.88	0.54
7:LD:60:ILE:HB	7:LD:80:ALA:HB2	1.90	0.54
46:S2:656:G:H5'	46:S2:662:G:N2	2.23	0.54
46:S2:1461:G:H3'	46:S2:1463:U:H3	1.73	0.54
1:L5:746:A:H2'	1:L5:747:A:C8	2.42	0.54
1:L5:1064:G:H2'	1:L5:1065:G:C8	2.42	0.54
1:L5:1485:C:O4'	1:L5:4349:C:N4	2.40	0.54
1:L5:1662:C:H2'	1:L5:1663:C:H6	1.72	0.54
1:L5:3720:G:H22	1:L5:3733:A:H2	1.55	0.54
13:LJ:76:GLY:O	13:LJ:78:LYS:N	2.40	0.54
1:L5:1377:G:H4'	1:L5:1378:C:H3'	1.88	0.54
3:L8:153:C:H2'	3:L8:154:G:H8	1.73	0.54
4:LA:131:GLY:H	4:LA:169:VAL:HG23	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:136:LYS:HG3	5:LB:146:LEU:HD11	1.89	0.54
63:Sa:93:LYS:NZ	84:Sa:304:HOH:O	2.40	0.54
1:L5:3612:C:H1'	1:L5:5016:A:H8	1.73	0.54
1:L5:4417:C:H2'	1:L5:4418:G:O4'	2.08	0.54
12:LI:48:LEU:HD12	12:LI:142:LEU:HA	1.90	0.54
14:LL:154:VAL:HG12	14:LL:155:MET:HE3	1.90	0.54
39:Lk:26:LYS:HG2	39:Lk:69:LEU:HD12	1.89	0.54
46:S2:450:C:OP1	47:SE:3:ARG:NH1	2.41	0.54
46:S2:1512:C:H5''	65:Sd:8:TRP:CZ3	2.43	0.54
46:S2:1801:A:H2'	46:S2:1802:C:C6	2.42	0.54
1:L5:662:C:H2'	1:L5:663:G:C8	2.43	0.53
1:L5:4459:U:H2'	1:L5:4460:U:C6	2.43	0.53
2:L7:111:C:H2'	2:L7:112:U:O4'	2.08	0.53
5:LB:173:LEU:HD22	5:LB:342:LYS:HD3	1.90	0.53
6:LC:146:GLU:OE2	6:LC:178:ASN:ND2	2.40	0.53
10:LG:79:ALA:HB3	16:LN:18:VAL:HG21	1.89	0.53
17:LO:193:THR:O	17:LO:197:LYS:HG2	2.08	0.53
18:LP:114:ILE:HA	18:LP:150:LEU:HD22	1.90	0.53
33:Le:7:LEU:HB2	33:Le:93:LYS:HB3	1.89	0.53
36:Lh:13:LYS:NZ	36:Lh:15:GLU:OE1	2.39	0.53
46:S2:828:G:OP1	69:SJ:6:SER:OG	2.22	0.53
68:SG:1:MET:HE1	68:SG:106:LEU:HD12	1.89	0.53
1:L5:25:A:H2'	1:L5:26:C:H6	1.73	0.53
1:L5:1072:C:H2'	1:L5:1073:G:H8	1.73	0.53
1:L5:1726:U:H5'	9:LF:135:ILE:HD11	1.89	0.53
7:LD:197:LYS:HA	7:LD:200:MET:HB2	1.88	0.53
17:LO:180:GLN:O	17:LO:180:GLN:NE2	2.37	0.53
22:LT:115:LYS:O	22:LT:119:ALA:N	2.32	0.53
45:Lr:63:VAL:HG13	45:Lr:77:TYR:HB3	1.88	0.53
64:Sc:64:GLU:OE1	64:Sc:66:ARG:N	2.41	0.53
1:L5:921:C:H2'	1:L5:922:C:C6	2.43	0.53
1:L5:1452:A:H2'	1:L5:1453:G:O4'	2.09	0.53
1:L5:2480:G:H2'	1:L5:2481:G:H8	1.73	0.53
18:LP:11:PRO:O	18:LP:105:LYS:NZ	2.42	0.53
46:S2:120:U:H2'	46:S2:121:OMU:H6	1.91	0.53
46:S2:1148:A:H4'	46:S2:1149:A:O4'	2.09	0.53
1:L5:1521:C:OP1	6:LC:100:ARG:NH2	2.40	0.53
1:L5:2326:G:H5''	33:Le:127:ALA:HB2	1.90	0.53
1:L5:4198:G:N2	12:LI:108:ALA:HB2	2.24	0.53
1:L5:4750:G:H2'	1:L5:4751:G:H8	1.73	0.53
2:L7:110:G:H2'	2:L7:111:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:30:C:OP1	62:SX:138:LYS:NZ	2.39	0.53
46:S2:1407:U:H2'	46:S2:1408:U:C6	2.43	0.53
1:L5:1332:C:H2'	1:L5:1333:A:H8	1.72	0.53
1:L5:1942:A:H2'	1:L5:1943:A:C8	2.44	0.53
1:L5:2492:C:H2'	1:L5:2493:G:C8	2.44	0.53
1:L5:4070:U:H2'	1:L5:4071:U:C6	2.43	0.53
1:L5:4232:U:O4	43:Lo:8:ARG:NH2	2.41	0.53
8:LE:179:LEU:HD12	8:LE:183:ARG:C	2.34	0.53
36:Lh:19:LYS:NZ	36:Lh:23:ASP:OD1	2.33	0.53
46:S2:1037:G:H4'	46:S2:1845:A:H4'	1.90	0.53
63:Sa:94:ASP:OD1	63:Sa:96:THR:HG22	2.07	0.53
74:SY:51:THR:OG1	74:SY:53:ASP:OD1	2.24	0.53
1:L5:1571:G:N7	84:L5:5715:HOH:O	2.34	0.53
1:L5:4956:A:H2'	1:L5:4957:C:C6	2.43	0.53
5:LB:161:ARG:HG2	5:LB:184:GLN:HA	1.90	0.53
11:LH:128:MET:HE2	11:LH:128:MET:HA	1.91	0.53
24:LV:30:ASP:OD1	24:LV:32:THR:OG1	2.21	0.53
1:L5:172:C:H1'	1:L5:173:C:C5	2.44	0.53
1:L5:1577:G:O2'	1:L5:1612:G:H4'	2.09	0.53
1:L5:1836:G:H4'	22:LT:129:LYS:HG2	1.89	0.53
33:Le:84:GLU:OE2	45:Lr:20:ARG:NH2	2.32	0.53
46:S2:468:A2M:OP1	68:SG:96:SER:OG	2.25	0.53
51:SF:123:GLU:HG2	51:SF:200:ALA:HB1	1.91	0.53
56:SP:30:TYR:O	56:SP:34:MET:HG3	2.09	0.53
60:SU:20:ILE:HD13	60:SU:98:VAL:HG21	1.90	0.53
1:L5:3937:C:H1'	16:LN:125:SER:HB3	1.91	0.53
1:L5:4508:C:OP1	24:LV:43:LYS:NZ	2.42	0.53
2:L7:39:C:O2'	13:LJ:46:GLN:HB3	2.09	0.53
2:L7:58:A:H2'	2:L7:59:G:C8	2.44	0.53
4:LA:114:CYS:HB2	4:LA:169:VAL:HG13	1.90	0.53
7:LD:22:ARG:HB3	7:LD:28:THR:HG22	1.91	0.53
12:LI:36:LEU:HD21	12:LI:69:ARG:HH11	1.74	0.53
28:LZ:9:LYS:HD2	28:LZ:83:THR:O	2.09	0.53
46:S2:752:G:N2	46:S2:752:G:OP2	2.41	0.53
1:L5:1064:G:H2'	1:L5:1065:G:H8	1.74	0.53
1:L5:1768:C:N3	1:L5:1772:C:N4	2.57	0.53
1:L5:4537:C:H2'	1:L5:4538:G:H8	1.74	0.53
3:L8:154:G:OP1	10:LG:89:ARG:NH1	2.38	0.53
30:Lb:105:GLY:O	30:Lb:109:ARG:HG2	2.08	0.53
47:SE:107:GLY:HA2	47:SE:189:LEU:HG	1.90	0.53
1:L5:1066:G:N7	84:L5:5707:HOH:O	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1320:U:O2'	1:L5:1891:A:N1	2.38	0.53
1:L5:4188:U:H2'	1:L5:4189:U:C6	2.43	0.53
15:LM:95:ILE:O	15:LM:99:GLU:HG3	2.09	0.53
46:S2:28:U:H2'	46:S2:29:G:H8	1.74	0.53
46:S2:1348:G:H5''	46:S2:1348:G:N3	2.24	0.53
55:SL:28:THR:O	55:SL:29:GLY:C	2.52	0.53
65:Sd:6:LEU:HA	65:Sd:9:SER:HB3	1.91	0.53
1:L5:223:G:H4'	1:L5:225:G:N7	2.24	0.52
5:LB:297:LYS:HG2	5:LB:299:ILE:HG23	1.90	0.52
12:LI:110:ARG:HE	12:LI:111:LEU:HB2	1.73	0.52
46:S2:1628:C:H2'	46:S2:1629:C:C6	2.44	0.52
60:SU:94:PRO:HD2	60:SU:97:ILE:HD12	1.89	0.52
71:SN:38:TYR:CE1	71:SN:78:LYS:HG3	2.44	0.52
74:SY:97:TYR:CE2	74:SY:99:LYS:HG2	2.44	0.52
1:L5:325:U:H2'	1:L5:326:C:C6	2.44	0.52
1:L5:907:C:H2'	1:L5:908:G:H8	1.74	0.52
1:L5:1857:C:H2'	1:L5:1858:A:C8	2.44	0.52
1:L5:2865:U:OP1	84:L5:5406:HOH:O	2.19	0.52
30:Lb:101:HIS:CE1	30:Lb:104:LEU:HD13	2.44	0.52
32:Ld:23:ARG:HG2	32:Ld:121:ASN:HA	1.91	0.52
46:S2:1232:PSU:H2'	46:S2:1233:G:C8	2.43	0.52
66:Sg:215:GLN:NE2	66:Sg:231:ASP:OD1	2.41	0.52
1:L5:1877:G:O6	30:Lb:10:HIS:NE2	2.39	0.52
1:L5:2789:A:H1'	40:Ll:45:ARG:HH22	1.73	0.52
1:L5:5066:U:H2'	1:L5:5067:U:C6	2.44	0.52
8:LE:186:LEU:HD13	8:LE:212:LEU:HD11	1.92	0.52
46:S2:692:G:H1	46:S2:738:C:HO2'	1.56	0.52
47:SE:141:THR:OG1	47:SE:143:ASP:OD1	2.21	0.52
69:SJ:134:HIS:ND1	69:SJ:163:SER:OG	2.33	0.52
1:L5:1646:A:O2'	38:Lj:49:TRP:O	2.23	0.52
1:L5:2486:G:N1	1:L5:2494:U:N3	2.58	0.52
1:L5:3604:A:N6	84:L5:5650:HOH:O	2.32	0.52
24:LV:96:LEU:HD13	25:LW:20:ARG:HG2	1.91	0.52
30:Lb:28:ARG:NH1	30:Lb:29:TYR:OH	2.42	0.52
46:S2:963:A:H2'	46:S2:964:A:C8	2.44	0.52
46:S2:1667:U:H2'	46:S2:1668:U:C6	2.45	0.52
63:Sa:51:ARG:HG2	63:Sa:51:ARG:NH1	2.23	0.52
74:SY:97:TYR:HE2	74:SY:99:LYS:HG2	1.74	0.52
1:L5:1070:G:O2'	1:L5:1071:C:O5'	2.28	0.52
1:L5:4088:C:H2'	1:L5:4089:G:C8	2.44	0.52
4:LA:131:GLY:N	4:LA:169:VAL:HG23	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LN:73:ARG:HD2	16:LN:88:GLY:O	2.10	0.52
31:Lc:34:THR:HG23	31:Lc:95:ALA:HB2	1.92	0.52
46:S2:1144:A:H2'	46:S2:1145:A:C8	2.44	0.52
50:SD:75:LYS:HE2	54:SK:34:GLU:OE1	2.09	0.52
1:L5:3901:A:H2	84:L5:8875:HOH:O	1.92	0.52
1:L5:4481:U:H2'	1:L5:4482:U:C6	2.44	0.52
3:L8:148:A:H2'	3:L8:149:G:C8	2.45	0.52
31:Lc:17:ARG:HH22	31:Lc:105:ILE:HD13	1.73	0.52
46:S2:186:C:H2'	46:S2:187:G:H8	1.75	0.52
46:S2:796:G:H2'	46:S2:797:C:C6	2.45	0.52
46:S2:996:A:H2'	46:S2:997:A:C8	2.44	0.52
46:S2:1797:U:H2'	46:S2:1798:C:C6	2.45	0.52
48:SA:181:GLU:O	48:SA:185:MET:HG3	2.10	0.52
52:SH:191:GLU:CD	52:SH:191:GLU:H	2.18	0.52
68:SG:137:ARG:HD2	68:SG:178:ARG:HD2	1.91	0.52
1:L5:189:G:H22	1:L5:253:G:H22	1.56	0.52
1:L5:1072:C:H2'	1:L5:1073:G:C8	2.44	0.52
1:L5:3656:A:H2'	1:L5:3657:U:H6	1.75	0.52
1:L5:3760:A:N6	46:S2:1824:A:O3'	2.36	0.52
1:L5:3871:A:H2'	1:L5:3872:A:C8	2.44	0.52
1:L5:3910:C:H2'	1:L5:3911:C:C6	2.44	0.52
46:S2:382:C:H2'	46:S2:383:G:C8	2.43	0.52
46:S2:1589:A:N3	46:S2:1653:U:O2'	2.40	0.52
67:SC:104:ASP:OD1	67:SC:104:ASP:N	2.43	0.52
1:L5:270:U:H2'	1:L5:271:C:C6	2.45	0.52
1:L5:511:C:H5''	14:LL:165:LYS:NZ	2.25	0.52
1:L5:4232:U:H4'	1:L5:4233:A:O4'	2.09	0.52
4:LA:178:PRO:HG3	44:Lp:25:MET:HE2	1.91	0.52
26:LX:119:ILE:HD12	26:LX:140:LEU:HD21	1.91	0.52
47:SE:39:ARG:NH1	84:SE:305:HOH:O	2.38	0.52
50:SD:28:GLU:HG2	50:SD:69:LEU:HD21	1.92	0.52
51:SF:201:LYS:HG3	51:SF:204:ARG:HH21	1.74	0.52
66:Sg:11:LEU:HB2	66:Sg:307:VAL:HB	1.92	0.52
1:L5:1768:C:H2'	1:L5:1771:U:C4	2.44	0.52
1:L5:4989:U:O2'	1:L5:4991:U:OP1	2.24	0.52
7:LD:108:ARG:CZ	7:LD:253:TYR:HB2	2.39	0.52
46:S2:878:G:H22	46:S2:908:A:H2	1.57	0.52
46:S2:955:A:H61	46:S2:971:G:H1'	1.75	0.52
46:S2:1013:U:OP1	46:S2:1129:G:O2'	2.26	0.52
46:S2:1201:U:H2'	46:S2:1202:U:C6	2.45	0.52
48:SA:2:SER:HB2	48:SA:9:GLN:HE22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sg:146:SER:HA	66:Sg:177:TRP:HH2	1.73	0.52
70:SM:47:ALA:HB3	70:SM:74:ILE:HD12	1.92	0.52
73:SW:32:LYS:O	73:SW:36:ARG:HG2	2.10	0.52
1:L5:4563:U:H2'	1:L5:4564:A:H8	1.75	0.52
1:L5:4653:C:H2'	1:L5:4654:C:C6	2.45	0.52
5:LB:200:ARG:HG2	5:LB:200:ARG:HH11	1.74	0.52
5:LB:393:LYS:HE2	5:LB:397:ILE:HD11	1.91	0.52
16:LN:178:HIS:HA	16:LN:181:HIS:NE2	2.25	0.52
46:S2:399:C:N3	55:SL:104:LYS:NZ	2.53	0.52
46:S2:830:A:OP2	46:S2:846:G:N2	2.43	0.52
46:S2:831:G:N7	74:SY:11:LYS:NZ	2.54	0.52
52:SH:10:LYS:HD2	52:SH:20:GLU:HB3	1.91	0.52
69:SJ:170:PRO:HB2	69:SJ:174:LYS:HB3	1.92	0.52
72:SO:46:ASP:OD2	72:SO:48:SER:OG	2.26	0.52
1:L5:1348:U:H2'	1:L5:1349:G:C8	2.44	0.51
1:L5:3767:C:H6	1:L5:3767:C:O5'	1.93	0.51
1:L5:4936:G:C5	8:LE:183:ARG:HD3	2.46	0.51
39:Lk:34:PHE:CE2	39:Lk:56:LEU:HG	2.46	0.51
45:Lr:73:PRO:HA	45:Lr:76:SER:HB2	1.92	0.51
46:S2:1822:A:H2'	46:S2:1823:A:H8	1.74	0.51
1:L5:62:A:N3	1:L5:77:U:O2'	2.35	0.51
1:L5:1051:G:N2	84:L5:6079:HOH:O	2.42	0.51
1:L5:2814:C:H5'	1:L5:2815:A2M:OP2	2.10	0.51
1:L5:3977:C:N4	1:L5:4030:C:OP1	2.44	0.51
1:L5:4200:G:N3	12:LI:111:LEU:HD22	2.25	0.51
8:LE:99:ASP:O	8:LE:100:LYS:C	2.53	0.51
28:LZ:78:ASN:OD1	31:Lc:39:ARG:NH2	2.43	0.51
50:SD:48:ILE:HB	50:SD:86:LEU:HD22	1.92	0.51
50:SD:166:TYR:O	50:SD:200:PRO:HG3	2.09	0.51
67:SC:242:ASP:O	67:SC:246:LYS:HG2	2.09	0.51
71:SN:2:GLY:N	84:SN:203:HOH:O	2.43	0.51
1:L5:699:C:H2'	1:L5:700:G:C8	2.45	0.51
1:L5:1414:C:H2'	1:L5:1415:G:H8	1.75	0.51
1:L5:1893:C:H1'	1:L5:1937:C:O2	2.11	0.51
1:L5:2297:G:H4'	6:LC:242:PRO:HB2	1.91	0.51
1:L5:2520:C:H2'	1:L5:2521:G:H8	1.75	0.51
1:L5:4228:OMG:H5''	1:L5:4229:U:O4'	2.11	0.51
11:LH:120:GLU:CD	11:LH:124:ARG:HH12	2.18	0.51
32:Ld:50:ARG:HB3	32:Ld:51:LYS:NZ	2.25	0.51
46:S2:1189:A:H4'	62:SX:34:THR:HG21	1.91	0.51
46:S2:1520:G:O2'	46:S2:1521:C:OP1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SF:140:ASP:HB2	64:Sc:46:VAL:HG12	1.90	0.51
51:SF:145:ARG:NE	64:Sc:47:LYS:HD3	2.26	0.51
66:Sg:191:HIS:CG	66:Sg:195:LEU:HD21	2.45	0.51
46:S2:829:C:OP1	47:SE:21:ASP:HB2	2.10	0.51
49:SB:170:GLU:OE1	49:SB:174:ARG:NH1	2.44	0.51
52:SH:58:LYS:HB2	52:SH:90:LYS:HD2	1.93	0.51
53:SI:8:TRP:HA	53:SI:18:ARG:HH11	1.76	0.51
67:SC:123:ARG:NH2	84:SC:308:HOH:O	2.41	0.51
73:SW:39:THR:HA	73:SW:42:MET:HE2	1.92	0.51
1:L5:306:A:OP1	37:Li:53:TYR:HE1	1.93	0.51
1:L5:729:G:N3	1:L5:729:G:H5'	2.25	0.51
1:L5:1269:G:O2'	1:L5:1440:U:O2'	2.25	0.51
1:L5:1392:A:H2'	1:L5:1393:G:C8	2.45	0.51
1:L5:1617:G:H1'	1:L5:2513:A:N6	2.26	0.51
1:L5:5000:G:H4'	5:LB:382:MET:HE1	1.91	0.51
12:LI:169:LYS:HZ2	12:LI:169:LYS:H	1.59	0.51
46:S2:72:C:OP1	46:S2:73:C:N4	2.44	0.51
46:S2:158:A:H2'	46:S2:159:A2M:O4'	2.11	0.51
46:S2:202:G:OP1	53:SI:143:LYS:NZ	2.44	0.51
46:S2:566:U:H2'	46:S2:567:C:O4'	2.11	0.51
46:S2:928:G:H2'	46:S2:929:G:C8	2.46	0.51
46:S2:1748:G:H2'	46:S2:1749:G:C8	2.45	0.51
48:SA:22:GLY:C	48:SA:24:HIS:H	2.18	0.51
51:SF:78:MET:HB2	51:SF:159:ARG:CZ	2.40	0.51
73:SW:80:ASP:OD2	73:SW:124:LYS:NZ	2.43	0.51
1:L5:109:G:OP2	14:LL:74:ARG:NH2	2.31	0.51
1:L5:1345:A:H2'	1:L5:1346:C:C6	2.46	0.51
1:L5:3718:A2M:H2	1:L5:3934:G:O4'	2.10	0.51
1:L5:3741:C:N4	84:L5:5852:HOH:O	2.37	0.51
1:L5:4934:A:H2'	1:L5:4935:C:C6	2.45	0.51
13:LJ:57:VAL:HB	13:LJ:62:ILE:HD11	1.91	0.51
22:LT:44:GLY:HA2	22:LT:95:HIS:ND1	2.26	0.51
24:LV:46:LYS:NZ	84:LV:305:HOH:O	2.43	0.51
32:Ld:108:TYR:CE2	32:Ld:110:PRO:HG3	2.45	0.51
39:Lk:60:LEU:HD12	39:Lk:61:PRO:HD2	1.93	0.51
41:Lm:94:MET:HG2	41:Lm:105:PRO:HA	1.91	0.51
46:S2:808:A:H5''	47:SE:219:ALA:O	2.10	0.51
55:SL:120:VAL:HG22	55:SL:145:VAL:HG11	1.92	0.51
1:L5:190:G:H2'	1:L5:191:G:H8	1.76	0.51
1:L5:346:G:OP2	27:LY:13:LYS:NZ	2.34	0.51
1:L5:466:A:H2'	1:L5:467:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:485:C:O2	1:L5:485:C:H2'	2.11	0.51
1:L5:1355:G:P	19:LQ:108:ARG:HH22	2.34	0.51
1:L5:1612:G:N7	84:L5:5731:HOH:O	2.34	0.51
1:L5:5055:G:N2	32:Ld:118:GLN:OE1	2.42	0.51
20:LR:108:ARG:NH1	84:LR:210:HOH:O	2.44	0.51
31:Lc:57:LYS:NZ	84:Lc:204:HOH:O	2.36	0.51
45:Lr:97:ILE:HD13	45:Lr:107:ARG:HA	1.90	0.51
46:S2:67:C:OP1	68:SG:160:LYS:NZ	2.42	0.51
46:S2:838:G:O2'	46:S2:840:C:OP2	2.27	0.51
46:S2:1227:G:C2	46:S2:1228:A:C8	2.98	0.51
46:S2:1436:C:O2'	46:S2:1438:A:OP2	2.28	0.51
49:SB:120:MET:HG3	49:SB:142:PHE:CE2	2.46	0.51
78:Sf:140:TYR:CZ	78:Sf:142:GLY:HA2	2.46	0.51
1:L5:116:G:H2'	1:L5:117:C:C6	2.46	0.51
1:L5:163:A:H2'	1:L5:164:G:H8	1.75	0.51
1:L5:910:G:H2'	1:L5:911:U:C6	2.45	0.51
35:Lg:85:LYS:HG3	35:Lg:86:CYS:N	2.25	0.51
36:Lh:13:LYS:HE3	36:Lh:15:GLU:H	1.76	0.51
46:S2:1653:U:H2'	46:S2:1654:G:C8	2.46	0.51
48:SA:59:LEU:O	48:SA:63:ARG:HG3	2.11	0.51
50:SD:172:VAL:HG22	50:SD:185:LYS:HG2	1.92	0.51
55:SL:90:ARG:NH1	84:SL:204:HOH:O	2.43	0.51
61:SV:14:PRO:HG2	61:SV:23:ILE:HD12	1.93	0.51
69:SJ:175:ARG:O	69:SJ:179:LYS:HG3	2.11	0.51
1:L5:138:G:H2'	1:L5:139:G:C8	2.46	0.51
1:L5:268:G:H2'	1:L5:269:G:H8	1.75	0.51
1:L5:481:G:OP2	45:Lr:67:ARG:NH2	2.44	0.51
1:L5:515:C:H41	1:L5:647:G:N2	2.07	0.51
1:L5:1238:A:O2'	9:LF:52:GLU:OE1	2.29	0.51
1:L5:4584:A:H2'	1:L5:4585:U:O4'	2.10	0.51
1:L5:4625:C:O2'	1:L5:4626:A:H5'	2.11	0.51
1:L5:4988:U:H2'	1:L5:5061:A:N7	2.26	0.51
2:L7:2:U:H2'	2:L7:3:C:H6	1.76	0.51
9:LF:142:TRP:CZ2	9:LF:235:ASN:HB2	2.46	0.51
22:LT:18:PRO:HB2	22:LT:21:LYS:HG3	1.92	0.51
46:S2:1255:G:OP1	46:S2:1256:G:O2'	2.21	0.51
46:S2:1556:A:N3	46:S2:1556:A:H2'	2.26	0.51
60:SU:56:MET:HB2	60:SU:86:LYS:HB3	1.93	0.51
65:Sd:5:GLN:OE1	65:Sd:5:GLN:N	2.44	0.51
1:L5:4342:C:O3'	43:Lo:37:GLY:HA3	2.11	0.51
2:L7:22:A:H2'	2:L7:23:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LX:73:HIS:CD2	26:LX:115:LYS:HD3	2.46	0.51
33:Le:23:HIS:HA	33:Le:53:ILE:HD13	1.93	0.51
53:SI:66:SER:HA	53:SI:73:THR:HB	1.93	0.51
67:SC:64:THR:OG1	67:SC:90:GLU:OE2	2.21	0.51
1:L5:1306:C:H2'	1:L5:1307:A:C8	2.45	0.50
1:L5:3598:C:H2'	1:L5:3599:A:C8	2.46	0.50
1:L5:3656:A:H2'	1:L5:3657:U:C6	2.46	0.50
12:LI:36:LEU:HD13	12:LI:87:MET:HE3	1.93	0.50
16:LN:15:GLN:HB3	37:Li:52:PRO:HD2	1.93	0.50
46:S2:26:U:OP2	84:S2:2102:HOH:O	2.19	0.50
46:S2:1401:A:H4'	60:SU:52:GLY:HA3	1.93	0.50
46:S2:1824:A:N6	84:S2:2369:HOH:O	2.40	0.50
75:SZ:63:PRO:HA	75:SZ:97:ILE:HD11	1.93	0.50
1:L5:257:C:H2'	1:L5:258:G:C8	2.46	0.50
1:L5:260:C:N4	1:L5:261:G:O6	2.45	0.50
1:L5:1704:C:O3'	9:LF:46:ARG:NH1	2.45	0.50
1:L5:1966:C:N4	1:L5:1967:A:N3	2.59	0.50
1:L5:3760:A:N1	46:S2:1824:A:O2'	2.40	0.50
1:L5:4239:A:H2'	1:L5:4240:G:H8	1.76	0.50
1:L5:4940:C:H5'	1:L5:4941:G:H5''	1.93	0.50
37:Li:26:HIS:O	37:Li:29:ARG:HG3	2.11	0.50
46:S2:1704:C:N4	84:S2:2482:HOH:O	2.44	0.50
48:SA:205:ARG:CZ	48:SA:210:ILE:HG12	2.41	0.50
63:Sa:49:ALA:O	63:Sa:53:ILE:HG12	2.12	0.50
70:SM:20:GLU:OE1	70:SM:24:THR:OG1	2.29	0.50
1:L5:496:G:H22	1:L5:658:C:H2'	1.76	0.50
3:L8:70:G:H1'	3:L8:88:A:N6	2.26	0.50
6:LC:320:LYS:NZ	6:LC:321:ASN:HB2	2.26	0.50
8:LE:68:MET:HA	8:LE:71:ARG:HB2	1.92	0.50
14:LL:167:ARG:HH21	14:LL:173:GLU:CD	2.20	0.50
46:S2:223:C:H2'	46:S2:224:A:C8	2.46	0.50
46:S2:1088:U:H4'	46:S2:1089:G:OP2	2.11	0.50
1:L5:399:G:OP1	18:LP:20:SER:OG	2.17	0.50
1:L5:1684:A:OP1	29:La:47:LYS:NZ	2.42	0.50
1:L5:2005:G:N2	1:L5:2006:U:O4	2.45	0.50
1:L5:2705:G:H1	1:L5:2710:C:H41	1.58	0.50
1:L5:2782:U:OP2	40:LI:10:LYS:NZ	2.42	0.50
3:L8:144:U:H2'	3:L8:145:C:C6	2.46	0.50
5:LB:281:ASN:OD1	5:LB:354:GLN:NE2	2.41	0.50
46:S2:495:U:H2'	46:S2:496:C:O4'	2.12	0.50
46:S2:1845:A:H2'	46:S2:1846:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SI:124:LYS:NZ	84:SI:302:HOH:O	2.31	0.50
72:SO:17:LEU:HD23	72:SO:17:LEU:H	1.75	0.50
79:SR:100:PRO:HG2	79:SR:122:PRO:HD3	1.92	0.50
1:L5:2374:A:H5'	32:Ld:64:ILE:O	2.12	0.50
1:L5:4860:G:N2	84:L5:5747:HOH:O	2.35	0.50
23:LU:24:ASP:OD1	23:LU:26:THR:HG23	2.12	0.50
48:SA:1:MET:H2	48:SA:59:LEU:CB	2.14	0.50
50:SD:31:GLU:H	50:SD:31:GLU:CD	2.19	0.50
53:SI:113:TYR:OH	53:SI:156:ALA:O	2.20	0.50
1:L5:152:U:H5'	16:LN:56:LYS:HG3	1.93	0.50
1:L5:684:G:C5'	8:LE:100:LYS:HG3	2.38	0.50
1:L5:1273:G:H5''	30:Lb:117:ARG:HE	1.77	0.50
1:L5:2084:C:N4	84:L5:5764:HOH:O	2.35	0.50
1:L5:3933:G:N7	84:L5:5736:HOH:O	2.34	0.50
4:LA:137:ILE:HD11	4:LA:149:LYS:HB2	1.92	0.50
46:S2:115:U:H2'	46:S2:116:OMU:C6	2.42	0.50
51:SF:40:ALA:HB1	51:SF:45:TYR:CG	2.47	0.50
63:Sa:12:LYS:NZ	84:Sa:305:HOH:O	2.43	0.50
1:L5:1:C:H1'	1:L5:2:G:C8	2.46	0.50
1:L5:1975:G:O4'	1:L5:1983:A:O2'	2.27	0.50
2:L7:2:U:H2'	2:L7:3:C:C6	2.46	0.50
19:LQ:173:LYS:O	84:LQ:201:HOH:O	2.19	0.50
46:S2:306:C:C2	46:S2:308:G:C2	3.00	0.50
46:S2:575:A:H2'	46:S2:576:A2M:O4'	2.12	0.50
46:S2:1568:C:H2'	46:S2:1569:A:C8	2.46	0.50
46:S2:1668:U:OP2	57:SQ:141:TYR:OH	2.28	0.50
55:SL:154:GLN:O	71:SN:133:ARG:NH2	2.44	0.50
57:SQ:18:THR:HG22	57:SQ:75:GLY:HA2	1.93	0.50
60:SU:17:ILE:HD12	60:SU:94:PRO:HG3	1.93	0.50
79:SR:109:LEU:HG	79:SR:111:PHE:CD2	2.47	0.50
1:L5:188:G:O2'	1:L5:190:G:OP2	2.25	0.50
3:L8:6:C:H2'	3:L8:7:U:C6	2.47	0.50
12:LI:112:GLN:HA	12:LI:116:ARG:HD2	1.93	0.50
46:S2:672:A:N6	46:S2:1027:A:OP1	2.43	0.50
47:SE:158:ASP:OD2	47:SE:174:LYS:NZ	2.42	0.50
47:SE:163:ASP:OD2	47:SE:165:GLU:HG2	2.11	0.50
48:SA:141:ASN:OD1	67:SC:87:PRO:HD3	2.12	0.50
57:SQ:8:GLN:HG2	57:SQ:99:TYR:CG	2.46	0.50
1:L5:480:C:P	45:Lr:67:ARG:HH21	2.34	0.50
1:L5:991:C:H2'	1:L5:992:C:H4'	1.93	0.50
1:L5:1332:C:H2'	1:L5:1333:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1695:U:H2'	1:L5:1696:C:C6	2.47	0.50
1:L5:1836:G:N7	22:LT:116:LYS:NZ	2.57	0.50
1:L5:2256:C:H2'	1:L5:2257:C:O4'	2.12	0.50
1:L5:2611:A:H2'	1:L5:2612:G:C8	2.47	0.50
1:L5:4600:G:H1'	1:L5:4601:U:C5	2.47	0.50
8:LE:157:HIS:HB3	8:LE:160:LYS:HD2	1.92	0.50
10:LG:165:GLU:OE1	16:LN:26:ARG:NH2	2.29	0.50
33:Le:89:LEU:HD13	33:Le:118:LEU:HD22	1.94	0.50
46:S2:833:C:H2'	46:S2:834:C:C6	2.47	0.50
46:S2:1300:U:O2'	56:SP:51:ARG:NH1	2.45	0.50
70:SM:52:LEU:HD11	70:SM:62:VAL:HG12	1.92	0.50
1:L5:1866:U:H2'	1:L5:1867:A:O4'	2.12	0.49
1:L5:3684:G:H2'	1:L5:3685:C:C6	2.47	0.49
1:L5:4553:A:N7	84:L5:5745:HOH:O	2.34	0.49
1:L5:4685:U:H2'	1:L5:4686:G:C8	2.46	0.49
1:L5:4955:A:H2'	1:L5:4956:A:C8	2.47	0.49
5:LB:71:GLU:OE1	5:LB:366:LYS:HE2	2.12	0.49
21:LS:19:THR:OG1	21:LS:21:LYS:O	2.26	0.49
26:LX:155:ILE:HA	36:Lh:37:THR:HG21	1.94	0.49
29:La:84:GLU:OE2	29:La:87:ARG:NH2	2.45	0.49
37:Li:35:LYS:H	37:Li:35:LYS:CE	2.20	0.49
43:Lo:26:TYR:HB3	43:Lo:67:VAL:HB	1.93	0.49
46:S2:866:PSU:H2'	46:S2:867:OMG:H8	1.77	0.49
46:S2:1521:C:H5'	58:SS:129:LEU:HD22	1.93	0.49
46:S2:1702:G:OP1	84:S2:2103:HOH:O	2.20	0.49
52:SH:149:ASP:OD1	52:SH:151:SER:OG	2.24	0.49
66:Sg:260:ASP:O	66:Sg:264:LYS:N	2.44	0.49
79:SR:109:LEU:HG	79:SR:111:PHE:HD2	1.77	0.49
1:L5:478:G:H2'	1:L5:479:G:H8	1.75	0.49
1:L5:680:G:H2'	1:L5:681:G:C8	2.47	0.49
1:L5:1696:C:H2'	1:L5:1697:G:O4'	2.12	0.49
1:L5:2391:G:H2'	1:L5:2392:C:C6	2.48	0.49
1:L5:3584:C:N4	84:L5:5925:HOH:O	2.39	0.49
1:L5:4141:G:H5'	1:L5:4142:C:H5	1.77	0.49
1:L5:4257:A:H5''	13:LJ:54:ARG:HH22	1.76	0.49
8:LE:74:SER:HB3	30:Lb:118:LEU:HD23	1.94	0.49
10:LG:151:LYS:HB2	10:LG:151:LYS:NZ	2.27	0.49
27:LY:69:LYS:HB3	27:LY:83:GLU:OE2	2.13	0.49
46:S2:17:C:H2'	46:S2:18:C:C6	2.47	0.49
72:SO:149:ARG:HG2	72:SO:151:LEU:HD22	1.94	0.49
1:L5:991:C:N3	1:L5:992:C:O2'	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LD:158:LYS:NZ	84:LD:303:HOH:O	2.45	0.49
8:LE:162:VAL:HG12	8:LE:177:GLY:HA2	1.93	0.49
8:LE:225:PRO:O	8:LE:226:ARG:C	2.55	0.49
31:Lc:11:LEU:HD12	31:Lc:14:ILE:HD13	1.95	0.49
46:S2:1464:C:H2'	46:S2:1465:A:C8	2.47	0.49
46:S2:1678:A2M:O2'	46:S2:1679:A:H5'	2.12	0.49
47:SE:18:TRP:O	47:SE:51:ARG:NH2	2.34	0.49
67:SC:120:GLN:NE2	84:SC:312:HOH:O	2.45	0.49
1:L5:1662:C:OP2	33:Le:39:ARG:NH2	2.41	0.49
1:L5:4966:A:H2'	1:L5:4967:A:O4'	2.12	0.49
7:LD:152:ARG:HG3	7:LD:154:THR:HG23	1.94	0.49
8:LE:91:THR:HG22	8:LE:108:LYS:CB	2.42	0.49
17:LO:180:GLN:HE21	17:LO:180:GLN:C	2.20	0.49
17:LO:190:ASP:O	17:LO:194:GLU:HG2	2.13	0.49
28:LZ:14:LEU:O	35:Lg:88:ARG:HG2	2.12	0.49
28:LZ:95:VAL:HG13	28:LZ:96:VAL:HG23	1.95	0.49
48:SA:39:TYR:HE1	79:SR:108:LEU:HD12	1.77	0.49
50:SD:108:LYS:HB3	50:SD:113:LEU:HD22	1.95	0.49
50:SD:158:ILE:HG13	50:SD:164:VAL:HG12	1.95	0.49
1:L5:123:C:H2'	1:L5:124:C:C6	2.48	0.49
1:L5:2093:A:H1'	1:L5:2094:G:C5	2.48	0.49
3:L8:36:G:O2'	3:L8:103:A:N1	2.42	0.49
9:LF:80:ASN:ND2	84:LF:308:HOH:O	2.39	0.49
11:LH:137:SER:HB3	11:LH:145:ILE:HD11	1.95	0.49
46:S2:28:U:H2'	46:S2:29:G:C8	2.47	0.49
46:S2:461:U:H2'	46:S2:462:OMC:H6	1.77	0.49
46:S2:1756:C:C5	46:S2:1757:G:H8	2.31	0.49
69:SJ:64:ASP:HB3	69:SJ:67:ASP:HB3	1.94	0.49
1:L5:650:C:H2'	1:L5:651:C:C6	2.48	0.49
1:L5:1084:C:H2'	1:L5:1085:C:C6	2.48	0.49
1:L5:4138:C:C4	1:L5:4139:G:H1'	2.47	0.49
1:L5:4158:C:H2'	1:L5:4159:C:H6	1.76	0.49
13:LJ:120:ASP:HB3	13:LJ:123:ILE:HG12	1.93	0.49
17:LO:3:GLU:N	34:Lf:8:LYS:HZ1	2.10	0.49
21:LS:71:SER:O	21:LS:76:LYS:NZ	2.46	0.49
48:SA:1:MET:CA	48:SA:59:LEU:HB3	2.43	0.49
53:SI:110:ARG:HG2	53:SI:121:LEU:HB3	1.94	0.49
55:SL:24:LEU:HD23	55:SL:24:LEU:H	1.78	0.49
68:SG:213:LEU:HG	68:SG:217:MET:HE2	1.94	0.49
1:L5:749:G:N2	1:L5:912:G:O2'	2.44	0.49
1:L5:959:G:H8	1:L5:959:G:OP2	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1870:C:H2'	1:L5:1871:A2M:H8	1.95	0.49
1:L5:2078:C:OP1	33:Le:64:LYS:HG3	2.13	0.49
1:L5:2434:G:O2'	1:L5:2527:A:N1	2.42	0.49
1:L5:4981:G:O6	5:LB:21:ARG:NH2	2.46	0.49
4:LA:247:ARG:HG2	46:S2:1069:U:H4'	1.94	0.49
6:LC:230:LEU:HD11	6:LC:239:LYS:HB2	1.94	0.49
46:S2:669:A:H2'	46:S2:670:A:C8	2.46	0.49
46:S2:840:C:H5'	46:S2:841:G:H5''	1.94	0.49
46:S2:1673:U:O2'	51:SF:84:GLY:O	2.21	0.49
48:SA:63:ARG:HD3	61:SV:37:ALA:O	2.13	0.49
66:Sg:44:LYS:HB2	66:Sg:56:GLN:HB2	1.95	0.49
1:L5:1993:C:O2'	1:L5:1994:C:O4'	2.26	0.49
1:L5:4281:A:O2'	1:L5:4282:A:H2'	2.13	0.49
5:LB:122:TRP:O	5:LB:127:LYS:NZ	2.45	0.49
10:LG:50:ASP:OD1	10:LG:52:THR:HG23	2.13	0.49
12:LI:112:GLN:HG3	12:LI:116:ARG:HG2	1.95	0.49
13:LJ:95:ARG:HD3	13:LJ:98:ASN:HD21	1.78	0.49
18:LP:128:ARG:HE	18:LP:136:ILE:HG21	1.76	0.49
24:LV:27:ASN:HA	24:LV:36:ASN:HA	1.94	0.49
46:S2:190:G:H1'	46:S2:209:A:H61	1.78	0.49
46:S2:484:A2M:H8	46:S2:484:A2M:O5'	2.13	0.49
46:S2:692:G:O2'	46:S2:739:C:O2	2.29	0.49
46:S2:1164:G:O2'	46:S2:1165:G:H5'	2.11	0.49
47:SE:117:GLU:H	47:SE:117:GLU:CD	2.20	0.49
52:SH:130:LEU:HG	52:SH:177:TYR:CZ	2.48	0.49
67:SC:117:ARG:NE	84:SC:315:HOH:O	2.45	0.49
78:Sf:100:LEU:HD11	78:Sf:103:LEU:HD13	1.94	0.49
78:Sf:132:MET:HG2	78:Sf:141:CYS:HB2	1.94	0.49
1:L5:38:A:H5''	29:La:35:ALA:HB2	1.95	0.49
1:L5:457:G:H2'	1:L5:458:C:C6	2.48	0.49
1:L5:691:C:H2'	1:L5:692:A:C8	2.48	0.49
1:L5:1933:G:H2'	1:L5:1934:A:C8	2.47	0.49
1:L5:2054:U:O4	84:L5:5405:HOH:O	2.18	0.49
1:L5:3648:A:H1'	1:L5:3785:A2M:N6	2.27	0.49
2:L7:58:A:H2'	2:L7:59:G:H8	1.78	0.49
9:LF:182:TYR:CZ	9:LF:203:GLU:HG2	2.48	0.49
18:LP:14:SER:OG	18:LP:151:THR:HG22	2.13	0.49
21:LS:29:ARG:NH1	22:LT:150:LEU:HD23	2.28	0.49
39:Lk:23:VAL:HG13	39:Lk:66:VAL:HA	1.93	0.49
51:SF:73:THR:HG22	51:SF:93:VAL:HG21	1.95	0.49
58:SS:78:LYS:H	58:SS:78:LYS:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SG:152:ASP:OD2	68:SG:154:ARG:HB2	2.13	0.49
70:SM:33:ARG:HH21	70:SM:91:LEU:HD11	1.78	0.49
1:L5:657:C:O2'	1:L5:658:C:O4'	2.17	0.49
1:L5:1084:C:H2'	1:L5:1085:C:H6	1.77	0.49
1:L5:2751:G:OP2	35:Lg:69:LYS:NZ	2.46	0.49
1:L5:2864:A:H2'	1:L5:2865:U:H6	1.77	0.49
46:S2:56:G:OP1	74:SY:111:LYS:NZ	2.33	0.49
76:Sb:34:ASP:OD1	76:Sb:82:LYS:NZ	2.37	0.49
79:SR:123:THR:HG22	79:SR:125:GLY:H	1.77	0.49
1:L5:1964:A:H2'	1:L5:1965:G:O4'	2.13	0.48
6:LC:159:GLU:HA	6:LC:217:ILE:HB	1.95	0.48
46:S2:71:G:N7	68:SG:170:ARG:NH2	2.61	0.48
46:S2:318:A:N6	68:SG:186:GLN:OE1	2.46	0.48
46:S2:379:C:O2	53:SI:5:ARG:NE	2.43	0.48
47:SE:60:GLU:OE2	74:SY:20:ARG:NH1	2.37	0.48
48:SA:42:LYS:HD2	48:SA:48:ILE:HD11	1.95	0.48
48:SA:76:VAL:HG23	48:SA:87:VAL:HG13	1.94	0.48
54:SK:80:ARG:NH1	54:SK:89:ILE:O	2.46	0.48
58:SS:86:ARG:HD3	58:SS:106:LYS:HG2	1.95	0.48
67:SC:211:LYS:HG2	67:SC:215:MET:HE2	1.94	0.48
69:SJ:136:ARG:NH1	69:SJ:158:ASP:OD2	2.46	0.48
1:L5:10:A:H2'	1:L5:11:G:C8	2.48	0.48
1:L5:386:A:OP2	27:LY:89:LYS:HE2	2.14	0.48
1:L5:1333:A:H2'	1:L5:1334:A:C8	2.47	0.48
1:L5:1564:A:N1	46:S2:1029:G:O2'	2.43	0.48
1:L5:2293:U:H2'	1:L5:2294:G:C8	2.48	0.48
1:L5:4195:G:OP1	1:L5:4221:C:O2'	2.31	0.48
3:L8:77:A:H2'	3:L8:78:G:C8	2.48	0.48
3:L8:83:C:N4	27:LY:112:ASP:OD2	2.42	0.48
8:LE:226:ARG:HB2	8:LE:226:ARG:HH11	1.78	0.48
46:S2:1337:4AC:H2'	46:S2:1338:G:C8	2.48	0.48
46:S2:1597:C:H4'	46:S2:1603:G:C6	2.48	0.48
49:SB:175:GLU:O	49:SB:179:ASN:ND2	2.43	0.48
66:Sg:168:CYS:HB3	66:Sg:198:VAL:HG13	1.96	0.48
66:Sg:269:GLU:OE2	66:Sg:271:LYS:NZ	2.43	0.48
69:SJ:112:THR:HG22	69:SJ:116:LYS:HD2	1.95	0.48
1:L5:377:A:H2'	1:L5:378:A:O4'	2.14	0.48
1:L5:1480:C:O2'	1:L5:1482:G:OP2	2.30	0.48
1:L5:3738:G:O6	84:L5:5407:HOH:O	2.19	0.48
1:L5:3758:U:H2'	1:L5:3765:G:N2	2.28	0.48
1:L5:4192:A:H2'	1:L5:4193:C:H6	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LH:41:ILE:HG22	11:LH:43:VAL:HG13	1.95	0.48
23:LU:80:LYS:HG2	23:LU:110:TYR:CE2	2.49	0.48
46:S2:615:C:H2'	46:S2:616:A:O4'	2.14	0.48
56:SP:43:ARG:O	56:SP:47:ARG:HG2	2.14	0.48
57:SQ:85:ARG:HH22	57:SQ:116:ASP:CG	2.21	0.48
58:SS:78:LYS:HE2	58:SS:78:LYS:N	2.28	0.48
59:ST:116:ASP:OD1	59:ST:117:GLN:N	2.46	0.48
62:SX:60:LYS:HD3	62:SX:114:ASP:O	2.12	0.48
63:Sa:10:ARG:HB2	63:Sa:33:ASP:OD2	2.13	0.48
1:L5:382:G:H4'	1:L5:407:A:N1	2.28	0.48
1:L5:1439:C:H5'	9:LF:34:ARG:NH1	2.23	0.48
1:L5:2876:OMG:HM22	1:L5:2877:G:O5'	2.12	0.48
1:L5:4281:A:O2'	1:L5:4282:A:H8	1.97	0.48
2:L7:12:U:OP2	2:L7:67:C:O2'	2.28	0.48
5:LB:258:HIS:HA	5:LB:259:PRO:C	2.37	0.48
7:LD:142:PHE:O	7:LD:172:SER:OG	2.31	0.48
11:LH:18:ILE:HG12	11:LH:27:VAL:HG22	1.95	0.48
46:S2:29:G:H2'	46:S2:30:C:C6	2.49	0.48
46:S2:466:G:HO2'	68:SG:72:ARG:HH22	1.62	0.48
46:S2:495:U:H4'	47:SE:24:THR:HG22	1.95	0.48
46:S2:1304:U:H5''	78:Sf:94:LYS:HA	1.95	0.48
68:SG:25:ARG:HB3	68:SG:25:ARG:CZ	2.44	0.48
71:SN:25:TRP:CG	76:Sb:82:LYS:HE2	2.48	0.48
1:L5:668:C:H2'	1:L5:669:C:O4'	2.13	0.48
1:L5:674:G:H2'	1:L5:675:C:C6	2.47	0.48
1:L5:1359:G:H4'	16:LN:203:TYR:HB2	1.95	0.48
1:L5:1625:OMG:OP2	82:L5:5377:SPD:N1	2.47	0.48
1:L5:1706:A:H3'	1:L5:1707:C:H6	1.79	0.48
1:L5:2465:C:H2'	1:L5:2466:G:O4'	2.12	0.48
1:L5:4500:PSU:H6	1:L5:4500:PSU:C5'	2.25	0.48
3:L8:126:C:O2'	3:L8:127:U:O4'	2.16	0.48
5:LB:194:LEU:HD23	5:LB:194:LEU:HA	1.69	0.48
25:LW:9:SER:HB3	25:LW:51:TRP:HZ3	1.78	0.48
46:S2:634:A:H2'	46:S2:635:G:C8	2.48	0.48
63:Sa:58:VAL:HG21	72:SO:28:PHE:HZ	1.79	0.48
76:Sb:2:PRO:HB2	76:Sb:5:LYS:HE3	1.94	0.48
1:L5:1701:A:H2'	1:L5:1702:C:H5	1.78	0.48
1:L5:1824:G:OP1	22:LT:35:LYS:NZ	2.34	0.48
1:L5:2101:C:H2'	1:L5:2102:G:N7	2.28	0.48
1:L5:2547:G:H2'	1:L5:2548:C:C6	2.48	0.48
1:L5:4238:G:H2'	1:L5:4239:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4339:A:H2'	1:L5:4340:U:H6	1.79	0.48
1:L5:4524:G:C2	5:LB:252:ALA:HB1	2.48	0.48
1:L5:4688:C:O2'	11:LH:155:SER:OG	2.26	0.48
8:LE:88:VAL:O	8:LE:89:LEU:C	2.57	0.48
9:LF:105:VAL:HG13	9:LF:136:VAL:HG12	1.95	0.48
31:Lc:21:VAL:HG12	31:Lc:22:MET:HE2	1.95	0.48
46:S2:910:G:H2'	46:S2:911:C:O4'	2.14	0.48
49:SB:46:LYS:HE2	72:SO:21:VAL:HG12	1.96	0.48
60:SU:46:LYS:NZ	60:SU:101:ILE:HG12	2.29	0.48
66:Sg:124:SER:OG	66:Sg:126:ASP:OD1	2.28	0.48
78:Sf:132:MET:CE	78:Sf:139:HIS:HB3	2.44	0.48
1:L5:331:G:OP2	84:L5:5411:HOH:O	2.20	0.48
1:L5:473:C:H2'	1:L5:474:C:C6	2.49	0.48
1:L5:1245:C:H2'	1:L5:1246:G:H8	1.79	0.48
1:L5:1271:G:OP2	1:L5:1271:G:N2	2.32	0.48
1:L5:2491:C:H2'	1:L5:2492:C:O4'	2.13	0.48
1:L5:4563:U:H2'	1:L5:4564:A:C8	2.49	0.48
5:LB:168:MET:HG2	5:LB:178:ALA:HA	1.94	0.48
12:LI:75:TYR:CZ	12:LI:150:GLU:HG2	2.48	0.48
45:Lr:66:ARG:HD2	45:Lr:75:THR:O	2.14	0.48
46:S2:51:U:H2'	46:S2:52:G:C8	2.48	0.48
46:S2:822:PSU:H2'	84:S2:3372:HOH:O	2.13	0.48
46:S2:1457:U:H2'	46:S2:1458:G:C8	2.48	0.48
1:L5:74:G:O6	14:LL:103:ARG:NH2	2.41	0.48
1:L5:3837:C:H2'	1:L5:3838:U:O4'	2.14	0.48
5:LB:383:GLU:CD	5:LB:383:GLU:H	2.22	0.48
6:LC:48:ASN:ND2	84:LC:412:HOH:O	2.46	0.48
6:LC:152:LEU:HD23	6:LC:251:ILE:HG12	1.94	0.48
8:LE:67:ALA:HA	8:LE:69:TYR:CE1	2.49	0.48
22:LT:149:GLU:H	22:LT:149:GLU:CD	2.22	0.48
31:Lc:52:CYS:HA	31:Lc:92:CYS:SG	2.54	0.48
45:Lr:54:ALA:HA	45:Lr:61:VAL:HG23	1.95	0.48
46:S2:59:U:H5'	46:S2:501:C:H4'	1.95	0.48
46:S2:837:A:H62	74:SY:8:ARG:HH11	1.61	0.48
46:S2:958:G:H2'	46:S2:959:G:C8	2.48	0.48
48:SA:19:LEU:HD11	79:SR:106:LEU:HD11	1.95	0.48
51:SF:156:THR:O	51:SF:160:GLU:HG3	2.14	0.48
57:SQ:110:ASP:O	57:SQ:114:GLN:HG2	2.13	0.48
66:Sg:245:ARG:HH22	66:Sg:296:GLN:NE2	2.12	0.48
73:SW:51:GLU:OE1	76:Sb:8:LEU:HD21	2.13	0.48
1:L5:4127:A:C2	10:LG:37:LYS:HG3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4635:A:O2'	1:L5:4637:OMG:OP1	2.28	0.48
9:LF:162:ILE:HD12	9:LF:167:ILE:HB	1.94	0.48
14:LL:120:TYR:HA	14:LL:155:MET:HE1	1.96	0.48
14:LL:123:LYS:HA	36:Lh:122:LYS:HD2	1.96	0.48
31:Lc:92:CYS:HB3	84:Lc:220:HOH:O	2.14	0.48
46:S2:15:U:H2'	46:S2:16:G:O4'	2.14	0.48
46:S2:84:A:H5''	74:SY:122:LYS:HD2	1.95	0.48
46:S2:464:A:H5''	46:S2:465:A:N7	2.28	0.48
46:S2:512:A2M:H4'	46:S2:576:A2M:H2	1.95	0.48
46:S2:1017:U:H5'	71:SN:55:ARG:HD3	1.95	0.48
46:S2:1086:G:HO2'	46:S2:1088:U:H6	1.61	0.48
46:S2:1378:A:H4'	46:S2:1379:A:O5'	2.13	0.48
1:L5:233:U:O2'	1:L5:234:G:H5''	2.14	0.48
1:L5:1354:A:H5'	19:LQ:108:ARG:HH21	1.79	0.48
1:L5:1650:A:C5'	6:LC:60:HIS:HE1	2.26	0.48
1:L5:2407:G:O6	40:Ll:2:SER:N	2.47	0.48
1:L5:2411:C:H2'	1:L5:2412:A:H8	1.78	0.48
1:L5:2744:A:H2'	1:L5:2745:A:C8	2.49	0.48
1:L5:2909:C:H4'	1:L5:3586:G:H22	1.78	0.48
4:LA:206:PRO:HG3	4:LA:213:GLY:HA3	1.95	0.48
8:LE:178:PRO:HG2	8:LE:181:LEU:HG	1.96	0.48
46:S2:65:C:O5'	68:SG:174:PRO:HA	2.14	0.48
46:S2:1021:U:OP1	71:SN:132:LYS:NZ	2.47	0.48
46:S2:1402:A:H5'	60:SU:51:LYS:CE	2.43	0.48
46:S2:1438:A:H2'	46:S2:1439:A:H8	1.79	0.48
49:SB:146:ARG:NH2	84:SB:307:HOH:O	2.44	0.48
1:L5:85:G:O2'	1:L5:97:G:O6	2.31	0.47
1:L5:457:G:H2'	1:L5:458:C:H6	1.78	0.47
1:L5:4917:C:H2'	1:L5:4918:C:C6	2.48	0.47
2:L7:66:G:OP1	7:LD:10:LYS:HE3	2.14	0.47
8:LE:209:PRO:HB3	8:LE:211:HIS:CE1	2.49	0.47
46:S2:917:U:H1'	52:SH:118:ARG:NH1	2.28	0.47
51:SF:145:ARG:HE	64:Sc:47:LYS:HD3	1.80	0.47
52:SH:160:LYS:HA	52:SH:163:GLN:HB2	1.94	0.47
55:SL:72:ILE:HD13	55:SL:129:GLY:HA2	1.96	0.47
68:SG:142:ARG:HA	68:SG:147:LEU:HD12	1.95	0.47
1:L5:7:C:H2'	1:L5:8:U:C6	2.49	0.47
1:L5:1535:C:H2'	1:L5:1536:PSU:O4'	2.14	0.47
1:L5:1884:C:H4'	1:L5:2070:U:C4	2.49	0.47
1:L5:2376:A:H2'	1:L5:2377:C:C6	2.49	0.47
1:L5:3623:C:N3	84:L5:5724:HOH:O	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:3701:OMC:N4	1:L5:3745:U:H2'	2.29	0.47
1:L5:3836:A:N7	84:L5:5792:HOH:O	2.35	0.47
1:L5:3917:A:H2'	1:L5:3918:G:C8	2.49	0.47
1:L5:4196:OMG:HM23	1:L5:4196:OMG:H1'	1.67	0.47
1:L5:4704:C:H2'	1:L5:4705:A:C8	2.49	0.47
2:L7:54:A:H8	13:LJ:10:ASN:HD21	1.62	0.47
7:LD:160:PHE:HA	7:LD:163:LEU:HB3	1.96	0.47
22:LT:136:ARG:HH11	22:LT:139:HIS:HE1	1.62	0.47
28:LZ:52:LYS:O	28:LZ:65:ARG:NH2	2.30	0.47
30:Lb:63:LYS:HE2	30:Lb:63:LYS:HB3	1.81	0.47
46:S2:306:C:N3	46:S2:308:G:C2	2.83	0.47
46:S2:899:U:H3'	46:S2:900:C:H5''	1.96	0.47
46:S2:1232:PSU:H2'	46:S2:1233:G:H8	1.77	0.47
84:S2:3110:HOH:O	63:Sa:2:THR:HA	2.14	0.47
50:SD:150:MET:HE3	50:SD:152:PHE:CZ	2.48	0.47
50:SD:215:ASP:OD1	50:SD:215:ASP:N	2.46	0.47
56:SP:30:TYR:OH	56:SP:88:GLU:OE2	2.25	0.47
66:Sg:144:ASP:O	66:Sg:145:GLU:HG2	2.13	0.47
70:SM:14:VAL:HG11	70:SM:126:GLU:HG3	1.95	0.47
1:L5:35:U:H4'	1:L5:1525:A:N1	2.28	0.47
1:L5:385:A:N3	1:L5:387:G:H5''	2.29	0.47
1:L5:1371:A:N1	3:L8:28:C:O2'	2.39	0.47
1:L5:1693:U:H2'	1:L5:1694:C:O4'	2.14	0.47
1:L5:2640:G:H2'	1:L5:2641:A:C8	2.48	0.47
1:L5:3893:C:H2'	1:L5:3894:A:C8	2.49	0.47
1:L5:4254:G:C2	1:L5:4256:A:H2	2.32	0.47
8:LE:133:PHE:O	8:LE:138:ARG:NH2	2.46	0.47
45:Lr:92:SER:O	45:Lr:96:MET:HG3	2.15	0.47
46:S2:126:G:O6	68:SG:196:LYS:NZ	2.45	0.47
46:S2:1258:A:C2	46:S2:1663:A:H2'	2.49	0.47
69:SJ:46:VAL:HG23	69:SJ:102:ILE:HD11	1.96	0.47
70:SM:63:LYS:HZ2	78:Sf:108:VAL:HG21	1.78	0.47
1:L5:1185:G:O2'	7:LD:278:ASP:OD2	2.29	0.47
1:L5:2461:G:H2'	1:L5:2462:C:C6	2.48	0.47
1:L5:4130:C:H2'	1:L5:4131:G:C8	2.48	0.47
1:L5:4458:C:H2'	1:L5:4459:U:C6	2.48	0.47
12:LI:66:GLU:CD	12:LI:69:ARG:HH21	2.21	0.47
15:LM:120:ASN:HB3	15:LM:124:LYS:HE2	1.97	0.47
21:LS:74:ARG:HG2	21:LS:74:ARG:HH11	1.79	0.47
36:Lh:89:ARG:O	36:Lh:93:ARG:HG2	2.15	0.47
45:Lr:56:ASP:OD1	45:Lr:56:ASP:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:867:OMG:HM23	46:S2:867:OMG:N3	2.29	0.47
46:S2:1757:G:N2	46:S2:1758:G:H1'	2.25	0.47
48:SA:124:VAL:HG21	48:SA:134:LEU:HD21	1.96	0.47
61:SV:4:ASP:OD1	61:SV:5:ALA:N	2.48	0.47
70:SM:69:CYS:HB2	70:SM:76:LEU:HD12	1.94	0.47
1:L5:469:C:N3	8:LE:105:ARG:NH2	2.54	0.47
1:L5:1184:A:H2'	1:L5:1185:G:C8	2.49	0.47
1:L5:1677:PSU:H4'	1:L5:1680:G:N1	2.30	0.47
1:L5:1961:G:N2	1:L5:2025:A:C5	2.83	0.47
1:L5:3930:U:H2'	1:L5:3931:C:C6	2.50	0.47
11:LH:95:VAL:HG22	41:Lm:82:LEU:HB3	1.97	0.47
24:LV:90:ARG:NE	24:LV:124:GLU:OE2	2.43	0.47
46:S2:379:C:H5'	53:SI:33:ALA:HA	1.95	0.47
46:S2:1025:U:H2'	46:S2:1026:C:O4'	2.14	0.47
46:S2:1144:A:H5'	46:S2:1355:C:C5	2.50	0.47
46:S2:1283:C:O2'	46:S2:1313:A:N1	2.37	0.47
46:S2:1415:C:O2'	59:ST:132:ASP:OD2	2.21	0.47
46:S2:1538:C:H2'	46:S2:1539:U:C6	2.48	0.47
48:SA:135:THR:O	48:SA:138:SER:OG	2.26	0.47
49:SB:69:VAL:HG11	49:SB:86:LEU:HD22	1.97	0.47
52:SH:143:ARG:HB3	73:SW:51:GLU:OE2	2.15	0.47
55:SL:16:ILE:HD12	55:SL:34:PRO:HB2	1.95	0.47
66:Sg:99:ARG:HE	66:Sg:99:ARG:HB2	1.56	0.47
69:SJ:136:ARG:HA	69:SJ:141:VAL:HA	1.95	0.47
78:Sf:140:TYR:CE1	78:Sf:145:CYS:HA	2.40	0.47
79:SR:34:VAL:O	79:SR:38:ILE:HG13	2.14	0.47
1:L5:1100:U:O2'	1:L5:1167:C:N4	2.48	0.47
1:L5:1351:G:H2'	1:L5:1352:C:C6	2.49	0.47
1:L5:1409:C:O2'	1:L5:1410:U:OP1	2.29	0.47
1:L5:2622:G:O6	23:LU:81:ARG:NH2	2.48	0.47
1:L5:3619:G:H22	1:L5:3624:A:H1'	1.79	0.47
1:L5:3887:OMC:H5''	17:LO:71:TYR:CE2	2.50	0.47
12:LI:192:PRO:HA	12:LI:197:VAL:HG12	1.96	0.47
23:LU:28:PRO:HG2	23:LU:112:LEU:HD12	1.95	0.47
36:Lh:67:GLU:O	36:Lh:71:LYS:HG2	2.15	0.47
36:Lh:103:LYS:HD3	36:Lh:107:GLN:OE1	2.14	0.47
46:S2:444:G:O6	53:SI:26:LYS:HE2	2.14	0.47
46:S2:1274:G:H4'	54:SK:47:LYS:HE2	1.96	0.47
46:S2:1374:C:H2'	46:S2:1375:G:O4'	2.14	0.47
62:SX:109:GLY:O	62:SX:119:ARG:HD3	2.14	0.47
71:SN:31:ASP:O	71:SN:35:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sf:144:CYS:SG	78:Sf:146:LEU:HB2	2.55	0.47
1:L5:106:A:H2'	1:L5:107:G:O4'	2.13	0.47
1:L5:268:G:H2'	1:L5:269:G:C8	2.50	0.47
1:L5:424:U:H2'	1:L5:425:U:C6	2.49	0.47
1:L5:478:G:H2'	1:L5:479:G:C8	2.50	0.47
1:L5:689:U:H2'	1:L5:690:C:C6	2.50	0.47
1:L5:992:C:N3	1:L5:1050:C:N4	2.62	0.47
1:L5:1414:C:H2'	1:L5:1415:G:C8	2.49	0.47
1:L5:1875:C:H2'	1:L5:1876:U:C6	2.49	0.47
1:L5:1887:G:N7	84:L5:5800:HOH:O	2.36	0.47
1:L5:1955:G:H2'	1:L5:1956:A:H8	1.80	0.47
1:L5:1993:C:O2	1:L5:2002:A:N6	2.48	0.47
1:L5:2055:G:OP1	17:LO:129:LEU:HD12	2.15	0.47
1:L5:2089:G:OP2	6:LC:294:LYS:NZ	2.34	0.47
1:L5:2732:G:H2'	1:L5:2733:C:C6	2.50	0.47
1:L5:2902:G:H1'	1:L5:3597:G:H22	1.78	0.47
1:L5:3664:G:H2'	1:L5:3665:G:H8	1.79	0.47
1:L5:3723:A:C8	1:L5:3723:A:H5''	2.49	0.47
1:L5:4163:U:OP2	10:LG:53:ARG:NH1	2.34	0.47
1:L5:4173:G:H2'	1:L5:4174:U:C6	2.49	0.47
1:L5:4481:U:H2'	1:L5:4482:U:H6	1.80	0.47
1:L5:4728:U:OP1	5:LB:128:LYS:NZ	2.39	0.47
3:L8:66:A:H2'	3:L8:67:U:C6	2.50	0.47
6:LC:283:LYS:NZ	19:LQ:22:ASP:OD2	2.41	0.47
26:LX:76:ILE:HG22	26:LX:77:ILE:HD13	1.96	0.47
33:Le:19:LYS:HE3	33:Le:19:LYS:HB3	1.62	0.47
42:Ln:1:MET:HE3	46:S2:1851:MA6:H5'	1.97	0.47
46:S2:10:G:O2'	67:SC:120:GLN:HG2	2.14	0.47
46:S2:787:G:H5''	68:SG:234:LEU:HD11	1.95	0.47
46:S2:1365:G:H2'	46:S2:1366:G:H8	1.79	0.47
46:S2:1395:C:O2'	46:S2:1396:A:H5'	2.14	0.47
46:S2:1546:G:H5'	57:SQ:18:THR:HG21	1.96	0.47
48:SA:38:ILE:HD11	48:SA:150:THR:HG22	1.97	0.47
48:SA:53:ARG:HD3	61:SV:83:PHE:CE2	2.50	0.47
53:SI:57:ALA:HB2	53:SI:183:GLY:HA2	1.97	0.47
64:Sc:5:ARG:NE	72:SO:80:ASP:OD1	2.47	0.47
69:SJ:67:ASP:O	69:SJ:71:LEU:HD12	2.15	0.47
71:SN:43:LYS:HE3	71:SN:43:LYS:HB3	1.70	0.47
78:Sf:86:THR:HG23	78:Sf:87:THR:H	1.78	0.47
1:L5:2411:C:H2'	1:L5:2412:A:C8	2.50	0.47
1:L5:2517:A:H5'	35:Lg:62:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2621:A:H2'	1:L5:2622:G:C8	2.50	0.47
1:L5:3734:U:H2'	1:L5:3735:G:O4'	2.15	0.47
1:L5:4873:G:C5	17:LO:179:LYS:HE3	2.50	0.47
2:L7:6:C:O2'	7:LD:72:ASP:OD2	2.22	0.47
17:LO:77:SER:HB2	17:LO:104:VAL:HG23	1.97	0.47
21:LS:45:TRP:CD1	21:LS:56:LYS:HG3	2.50	0.47
24:LV:138:SER:C	24:LV:139:ILE:HD13	2.40	0.47
33:Le:35:TRP:CZ2	33:Le:56:PRO:HD2	2.49	0.47
46:S2:573:U:O2	46:S2:576:A2M:H8	2.15	0.47
46:S2:834:C:H2'	46:S2:835:C:C6	2.50	0.47
46:S2:1442:OMU:HM23	46:S2:1442:OMU:H1'	1.69	0.47
46:S2:1593:C:OP2	75:SZ:104:ARG:NH2	2.47	0.47
48:SA:36:GLN:O	48:SA:53:ARG:NH1	2.43	0.47
52:SH:84:GLU:HG3	52:SH:92:VAL:HG23	1.97	0.47
69:SJ:113:GLN:OE1	69:SJ:154:GLN:NE2	2.38	0.47
74:SY:8:ARG:HB2	74:SY:26:ASP:HB2	1.97	0.47
1:L5:74:G:H5'	14:LL:59:VAL:HG13	1.97	0.47
1:L5:2275:G:H2'	1:L5:2276:A:C8	2.50	0.47
1:L5:2539:C:H2'	1:L5:2540:C:H6	1.78	0.47
1:L5:2902:G:C5	1:L5:3594:C:C2	3.03	0.47
1:L5:5023:C:N4	84:L5:5408:HOH:O	2.20	0.47
7:LD:233:PRO:HA	7:LD:236:MET:HG3	1.95	0.47
10:LG:26:LYS:HG3	10:LG:28:VAL:HG22	1.96	0.47
26:LX:148:ASP:O	26:LX:152:LYS:N	2.46	0.47
28:LZ:89:ILE:HG13	28:LZ:117:LYS:HE3	1.97	0.47
46:S2:1217:A:H2'	46:S2:1218:C:O4'	2.15	0.47
46:S2:1406:G:H2'	46:S2:1407:U:C6	2.50	0.47
48:SA:7:VAL:HG23	48:SA:8:LEU:HG	1.96	0.47
61:SV:1:MET:HB3	61:SV:10:ASP:OD2	2.15	0.47
66:Sg:191:HIS:CD2	66:Sg:195:LEU:HD21	2.49	0.47
74:SY:53:ASP:OD1	74:SY:53:ASP:N	2.48	0.47
1:L5:18:C:H4'	16:LN:138:PHE:CD1	2.50	0.47
1:L5:68:U:H2'	1:L5:69:A:O4'	2.15	0.47
1:L5:419:A:N6	3:L8:15:G:H1'	2.30	0.47
1:L5:1591:U:OP2	1:L5:2856:C:O2'	2.24	0.47
1:L5:2849:A:O2'	1:L5:2855:G:N7	2.48	0.47
1:L5:3793:U:H2'	1:L5:3794:C:C6	2.50	0.47
1:L5:3869:OMC:H1'	82:L5:5378:SPD:H22	1.96	0.47
1:L5:4071:U:H2'	1:L5:4072:C:C6	2.50	0.47
1:L5:4468:U:O2	1:L5:4708:A:C8	2.68	0.47
1:L5:4887:C:H42	1:L5:4932:U:H3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:85:VAL:HG22	5:LB:204:GLN:HG3	1.97	0.47
6:LC:263:LEU:HG	6:LC:273:LEU:HD12	1.97	0.47
7:LD:135:ILE:HB	7:LD:138:GLN:HB2	1.97	0.47
10:LG:173:LEU:O	10:LG:177:MET:HG2	2.14	0.47
11:LH:15:ASN:HD21	11:LH:30:PRO:HG3	1.80	0.47
12:LI:30:LYS:HG3	12:LI:66:GLU:HG2	1.97	0.47
12:LI:103:LEU:C	12:LI:105:CYS:H	2.24	0.47
25:LW:97:LYS:HG2	25:LW:101:ARG:HE	1.80	0.47
46:S2:433:A:H5'	53:SI:22:HIS:HB3	1.96	0.47
46:S2:1101:U:H2'	46:S2:1102:G:C8	2.49	0.47
46:S2:1410:C:H2'	46:S2:1411:G:H8	1.80	0.47
48:SA:66:VAL:HG11	48:SA:185:MET:HB2	1.97	0.47
79:SR:89:SER:HB3	79:SR:92:ASP:HB2	1.97	0.47
1:L5:2384:U:H2'	1:L5:2385:U:C6	2.50	0.46
1:L5:2862:G:N3	1:L5:3624:A:H2'	2.30	0.46
1:L5:3971:G:C4	1:L5:4051:C:H1'	2.50	0.46
1:L5:4911:A:OP1	5:LB:97:ARG:NH2	2.45	0.46
3:L8:92:U:H2'	3:L8:93:C:O4'	2.14	0.46
3:L8:126:C:O2	3:L8:127:U:O2'	2.28	0.46
7:LD:128:ASP:O	7:LD:164:LYS:NZ	2.38	0.46
8:LE:72:LYS:HZ2	30:Lb:119:CYS:HA	1.80	0.46
13:LJ:160:GLU:HA	13:LJ:160:GLU:OE2	2.15	0.46
24:LV:60:MET:HE3	24:LV:129:TRP:CH2	2.50	0.46
31:Lc:26:LYS:HE2	31:Lc:98:ASP:HB2	1.96	0.46
46:S2:1035:A:H2'	46:S2:1036:A:O4'	2.16	0.46
46:S2:1307:U:O2'	78:Sf:135:HIS:ND1	2.41	0.46
46:S2:1323:U:H2'	46:S2:1324:G:H8	1.79	0.46
46:S2:1507:G:C6	78:Sf:91:ASN:HB2	2.50	0.46
55:SL:55:TYR:CD1	55:SL:115:PRO:HG2	2.50	0.46
1:L5:123:C:H2'	1:L5:124:C:H6	1.80	0.46
1:L5:190:G:H2'	1:L5:191:G:C8	2.50	0.46
1:L5:1086:C:H2'	1:L5:1087:A:C8	2.51	0.46
1:L5:4418:G:O6	1:L5:4421:C:H2'	2.14	0.46
1:L5:4759:C:H2'	1:L5:4760:G:C8	2.50	0.46
4:LA:200:ARG:NH2	4:LA:217:GLN:OE1	2.43	0.46
12:LI:190:LEU:C	12:LI:191:ILE:HD13	2.40	0.46
15:LM:41:PRO:HB3	15:LM:70:GLN:HG3	1.97	0.46
17:LO:5:GLN:H	17:LO:31:ARG:HH22	1.63	0.46
46:S2:1718:G:OP2	84:S2:2105:HOH:O	2.21	0.46
57:SQ:97:GLN:HB3	57:SQ:105:LYS:HG3	1.97	0.46
66:Sg:262:GLU:OE1	66:Sg:262:GLU:N	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SC:253:PRO:HA	67:SC:256:TRP:CE2	2.51	0.46
71:SN:127:ARG:O	71:SN:131:THR:HG23	2.15	0.46
1:L5:1194:G:O2'	84:L5:5410:HOH:O	2.20	0.46
1:L5:1327:C:H2'	1:L5:1328:G:C8	2.51	0.46
1:L5:1672:U:H2'	1:L5:1673:U:C6	2.50	0.46
1:L5:4088:C:H2'	1:L5:4089:G:H8	1.81	0.46
1:L5:4515:G:N7	84:L5:5799:HOH:O	2.36	0.46
6:LC:14:LYS:HB2	6:LC:16:GLU:OE1	2.15	0.46
10:LG:125:LYS:CG	10:LG:126:GLY:H	2.28	0.46
14:LL:209:LYS:HG2	14:LL:210:LYS:HG3	1.96	0.46
15:LM:6:PHE:H	15:LM:11:ARG:NH2	2.13	0.46
17:LO:188:LYS:HB2	17:LO:188:LYS:HE3	1.55	0.46
25:LW:19:ARG:NH2	25:LW:37:GLU:OE2	2.47	0.46
31:Lc:57:LYS:O	31:Lc:61:GLU:HG3	2.15	0.46
46:S2:1554:C:OP2	46:S2:1555:U:O2'	2.27	0.46
48:SA:126:ASP:HB3	48:SA:129:ALA:HB3	1.97	0.46
49:SB:44:ILE:HD11	49:SB:86:LEU:HD23	1.98	0.46
66:Sg:244:ASN:OD1	66:Sg:245:ARG:NH1	2.48	0.46
66:Sg:272:GLN:OE1	66:Sg:284:PRO:HG2	2.15	0.46
68:SG:225:GLN:HA	68:SG:228:ILE:HG12	1.97	0.46
77:Se:11:LYS:NZ	77:Se:15:GLN:OE1	2.42	0.46
78:Sf:102:VAL:HG12	78:Sf:104:LYS:HG3	1.96	0.46
1:L5:173:C:P	14:LL:130:LYS:HZ1	2.39	0.46
1:L5:751:G:H2'	1:L5:752:G:O4'	2.15	0.46
1:L5:1086:C:H2'	1:L5:1087:A:H8	1.80	0.46
1:L5:1743:A:N1	1:L5:1789:C:O2'	2.46	0.46
1:L5:1974:U:H5''	1:L5:1975:G:H8	1.80	0.46
1:L5:2900:U:H3'	1:L5:2901:G:H8	1.79	0.46
1:L5:4087:G:N7	4:LA:67:TYR:OH	2.41	0.46
1:L5:4158:C:H2'	1:L5:4159:C:C6	2.50	0.46
1:L5:4183:G:H2'	1:L5:4183:G:N3	2.31	0.46
5:LB:117:ARG:HA	5:LB:177:LYS:HD2	1.97	0.46
6:LC:11:TYR:OH	6:LC:148:PRO:HB2	2.16	0.46
11:LH:63:ASN:O	11:LH:67:LEU:HG	2.15	0.46
23:LU:21:PHE:CD1	23:LU:80:LYS:HG3	2.51	0.46
38:Lj:28:HIS:CG	38:Lj:31:LYS:HD3	2.50	0.46
39:Lk:60:LEU:HD12	39:Lk:60:LEU:HA	1.81	0.46
46:S2:1454:A:H5''	79:SR:3:ARG:HD2	1.98	0.46
46:S2:1643:PSU:H2'	46:S2:1644:C:C6	2.50	0.46
48:SA:18:PHE:CZ	48:SA:177:MET:HE3	2.49	0.46
58:SS:24:ARG:HB2	58:SS:29:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SC:272:HIS:O	67:SC:276:THR:OG1	2.29	0.46
79:SR:26:ASN:OD1	79:SR:59:LYS:HG2	2.15	0.46
79:SR:94:GLU:HG2	79:SR:95:ILE:HG13	1.96	0.46
1:L5:1279:A:O2'	1:L5:1281:G:N7	2.38	0.46
1:L5:2520:C:O2	1:L5:2640:G:N2	2.49	0.46
1:L5:2654:C:H2'	1:L5:2655:C:H6	1.81	0.46
1:L5:4344:U:H2'	1:L5:4345:C:C6	2.51	0.46
1:L5:4870:G:H5''	15:LM:91:TRP:CE2	2.50	0.46
5:LB:19:ARG:HB2	5:LB:234:ARG:NH2	2.30	0.46
6:LC:41:HIS:CE1	6:LC:45:ARG:HD3	2.51	0.46
10:LG:121:LYS:NZ	10:LG:127:ASP:O	2.48	0.46
14:LL:48:PRO:HB2	36:Lh:120:ALA:HB2	1.98	0.46
19:LQ:112:ARG:HG2	19:LQ:115:ARG:HH22	1.81	0.46
46:S2:179:C:H2'	46:S2:180:G:O4'	2.15	0.46
46:S2:1190:A:H2'	46:S2:1191:C:O4'	2.16	0.46
46:S2:1388:A:C2	50:SD:205:PRO:HG2	2.50	0.46
49:SB:67:PHE:CE2	72:SO:48:SER:HB3	2.50	0.46
52:SH:7:LYS:HZ1	52:SH:17:ASP:HB2	1.80	0.46
1:L5:1650:A:H5'	6:LC:60:HIS:CE1	2.50	0.46
1:L5:1687:U:H2'	1:L5:1688:G:C8	2.50	0.46
1:L5:3823:G:H5''	84:L5:7312:HOH:O	2.14	0.46
1:L5:4236:G:H4'	1:L5:4328:G:O2'	2.15	0.46
1:L5:4760:G:H2'	1:L5:4761:G:O4'	2.15	0.46
1:L5:4938:A:H61	8:LE:247:LYS:HD3	1.79	0.46
3:L8:110:U:O5'	40:Ll:8:ARG:NH2	2.48	0.46
10:LG:120:LYS:HD2	10:LG:120:LYS:N	2.30	0.46
25:LW:76:VAL:HG13	25:LW:77:LYS:HG2	1.96	0.46
29:La:89:ASN:HA	29:La:92:LYS:HG2	1.96	0.46
33:Le:35:TRP:CE2	33:Le:56:PRO:HD2	2.50	0.46
46:S2:84:A:N3	46:S2:150:A:O2'	2.49	0.46
46:S2:416:U:HO2'	46:S2:652:U:HO2'	1.62	0.46
46:S2:674:C:H2'	46:S2:675:U:C6	2.50	0.46
46:S2:1595:U:H2'	46:S2:1596:PSU:C6	2.51	0.46
59:ST:32:GLU:OE2	59:ST:32:GLU:N	2.26	0.46
66:Sg:164:ILE:HG22	66:Sg:178:ASN:HA	1.96	0.46
78:Sf:146:LEU:HG	78:Sf:147:THR:N	2.31	0.46
1:L5:739:G:OP1	1:L5:739:G:H3'	2.16	0.46
1:L5:1458:C:H2'	1:L5:1459:A:O4'	2.15	0.46
1:L5:1475:G:H2'	1:L5:1476:C:C6	2.50	0.46
1:L5:2505:C:N4	1:L5:4084:G:H4'	2.30	0.46
1:L5:4097:G:N2	1:L5:4113:U:H5'	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4225:G:P	12:LI:24:ARG:HH22	2.38	0.46
2:L7:18:C:H2'	2:L7:19:C:H6	1.81	0.46
11:LH:2:LYS:HE3	11:LH:63:ASN:HB3	1.98	0.46
18:LP:117:ILE:HD12	18:LP:148:MET:HE2	1.98	0.46
46:S2:996:A:H5''	71:SN:7:PRO:HG3	1.96	0.46
46:S2:1663:A:O2'	46:S2:1664:A:H5'	2.16	0.46
46:S2:1798:C:H2'	46:S2:1799:G:O4'	2.15	0.46
47:SE:18:TRP:HH2	47:SE:31:PRO:HD3	1.79	0.46
49:SB:48:LEU:O	72:SO:51:GLU:HG3	2.16	0.46
49:SB:179:ASN:ND2	49:SB:187:LYS:HE3	2.31	0.46
62:SX:28:LYS:HE2	62:SX:32:LEU:HD22	1.98	0.46
63:Sa:38:LYS:HD2	63:Sa:83:VAL:HG13	1.98	0.46
68:SG:56:ASN:HB2	68:SG:108:VAL:HG12	1.98	0.46
72:SO:78:ALA:HB3	72:SO:118:ALA:HB3	1.97	0.46
1:L5:137:G:C2	1:L5:138:G:N7	2.84	0.46
1:L5:267:G:H2'	1:L5:268:G:H8	1.79	0.46
1:L5:2486:G:C6	1:L5:2494:U:C2	3.04	0.46
1:L5:3911:C:H2'	1:L5:3912:U:C6	2.51	0.46
1:L5:4906:C:H2'	1:L5:4907:G:H8	1.81	0.46
18:LP:33:ALA:HB1	18:LP:117:ILE:HG12	1.97	0.46
18:LP:41:ILE:CD1	18:LP:99:GLU:HG3	2.44	0.46
29:La:71:PRO:HG2	29:La:108:TYR:HA	1.98	0.46
46:S2:799:U:H2'	46:S2:800:U:H6	1.80	0.46
46:S2:1285:G:OP2	70:SM:61:TYR:OH	2.25	0.46
48:SA:12:GLU:CD	48:SA:12:GLU:H	2.23	0.46
73:SW:11:LEU:HB3	73:SW:72:CYS:O	2.15	0.46
1:L5:677:G:H2'	1:L5:678:C:C6	2.51	0.46
1:L5:703:G:O2'	33:Le:5:ARG:NH1	2.49	0.46
1:L5:959:G:C8	8:LE:123:ARG:HG2	2.51	0.46
1:L5:1241:C:N4	30:Lb:111:ARG:HG3	2.31	0.46
1:L5:1956:A:H2'	1:L5:1957:U:C6	2.51	0.46
1:L5:3722:G:OP1	37:Li:68:ARG:HD3	2.16	0.46
1:L5:4441:A:C5'	12:LI:103:LEU:HD12	2.45	0.46
1:L5:4750:G:H2'	1:L5:4751:G:C8	2.50	0.46
3:L8:40:A:H2'	3:L8:41:A:C8	2.51	0.46
15:LM:96:GLU:O	15:LM:100:ARG:HG2	2.16	0.46
21:LS:2:LYS:HG3	21:LS:39:VAL:HG11	1.96	0.46
28:LZ:113:GLU:HA	28:LZ:116:VAL:HG22	1.98	0.46
52:SH:136:PRO:O	52:SH:162:GLN:HG3	2.16	0.46
61:SV:74:LYS:HG2	61:SV:79:VAL:HB	1.97	0.46
1:L5:387:G:O5'	27:LY:89:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:967:C:O2'	1:L5:969:C:OP2	2.25	0.46
1:L5:1269:G:H2'	1:L5:1270:A:O4'	2.16	0.46
1:L5:1271:G:N1	1:L5:2108:G:O6	2.48	0.46
1:L5:1351:G:O6	19:LQ:55:ARG:NH1	2.47	0.46
1:L5:2730:U:H2'	1:L5:2731:C:C6	2.51	0.46
1:L5:3867:A2M:HM'3	1:L5:3880:G:N2	2.31	0.46
1:L5:4504:C:H2'	1:L5:4505:C:C6	2.50	0.46
2:L7:16:A:H2'	2:L7:17:C:C6	2.51	0.46
12:LI:66:GLU:OE1	12:LI:69:ARG:NH2	2.41	0.46
17:LO:8:VAL:HG12	17:LO:117:ARG:HG3	1.98	0.46
20:LR:173:ARG:NH2	46:S2:909:G:H5'	2.31	0.46
46:S2:616:A:H1'	77:Se:12:VAL:HG23	1.98	0.46
50:SD:61:GLU:OE1	50:SD:61:GLU:HA	2.14	0.46
72:SO:54:CYS:HB2	72:SO:84:ARG:HG2	1.98	0.46
76:Sb:67:THR:OG1	76:Sb:70:LYS:O	2.26	0.46
1:L5:700:G:H2'	1:L5:701:G:H8	1.81	0.45
1:L5:979:C:H2'	1:L5:980:U:C6	2.51	0.45
1:L5:1725:U:H2'	1:L5:1726:U:H6	1.81	0.45
1:L5:2469:C:H5'	1:L5:2470:C:OP2	2.16	0.45
1:L5:2623:A:H2'	1:L5:2624:G:H8	1.81	0.45
1:L5:4130:C:H2'	1:L5:4131:G:H8	1.81	0.45
1:L5:4238:G:H2'	1:L5:4239:A:H8	1.79	0.45
1:L5:4346:U:C4'	43:Lo:82:MET:HE3	2.46	0.45
3:L8:74:U:H3'	27:LY:76:LYS:NZ	2.31	0.45
3:L8:140:C:OP1	84:L8:301:HOH:O	2.20	0.45
5:LB:246:ARG:NH1	84:LB:607:HOH:O	2.37	0.45
9:LF:226:HIS:ND1	9:LF:228:VAL:HG22	2.31	0.45
32:Ld:27:ILE:HB	32:Ld:84:ILE:HG22	1.97	0.45
46:S2:1531:A:H2'	46:S2:1532:C:C6	2.51	0.45
46:S2:1673:U:H2'	46:S2:1674:G:O4'	2.16	0.45
53:SI:76:THR:HG21	53:SI:104:ILE:HD12	1.96	0.45
66:Sg:17:TRP:HB2	66:Sg:36:ARG:HD2	1.99	0.45
1:L5:1412:G:H2'	1:L5:1413:C:O4'	2.17	0.45
1:L5:1503:A:N7	84:L5:5818:HOH:O	2.36	0.45
1:L5:1534:A2M:H2	84:Lj:241:HOH:O	2.15	0.45
1:L5:2577:C:H5''	28:LZ:111:ARG:HH12	1.82	0.45
1:L5:2602:G:H2'	1:L5:2603:C:C6	2.50	0.45
1:L5:4475:G:N7	41:Lm:125:LYS:HE3	2.32	0.45
7:LD:197:LYS:O	7:LD:202:GLN:N	2.49	0.45
14:LL:174:LYS:O	29:La:138:LYS:HE2	2.16	0.45
15:LM:32:ASP:HB2	15:LM:33:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Lc:26:LYS:HE2	31:Lc:26:LYS:HB2	1.67	0.45
46:S2:804:U:H2'	46:S2:805:U:C6	2.51	0.45
46:S2:824:C:H1'	69:SJ:144:ILE:HG21	1.98	0.45
46:S2:1272:OMC:HM23	46:S2:1272:OMC:H1'	1.72	0.45
46:S2:1589:A:H2'	46:S2:1590:C:C6	2.51	0.45
46:S2:1634:A:O2'	58:SS:142:ARG:NH2	2.48	0.45
58:SS:65:GLU:O	58:SS:69:THR:HG22	2.17	0.45
73:SW:12:LYS:HB2	73:SW:12:LYS:HE3	1.72	0.45
76:Sb:42:LYS:HE3	76:Sb:57:VAL:HG23	1.98	0.45
1:L5:398:A2M:O5'	1:L5:398:A2M:H8	2.16	0.45
1:L5:1502:G:O6	19:LQ:90:VAL:HG22	2.16	0.45
1:L5:2591:A:H2'	1:L5:2592:U:H6	1.81	0.45
1:L5:3664:G:H2'	1:L5:3665:G:C8	2.50	0.45
1:L5:4069:U:H2'	1:L5:4070:U:C6	2.52	0.45
1:L5:4420:U:H3'	1:L5:4421:C:C5	2.52	0.45
1:L5:5053:U:H5'	1:L5:5054:C:C5	2.52	0.45
1:L5:5057:C:H2'	1:L5:5058:A:C8	2.51	0.45
9:LF:88:LYS:HG2	22:LT:135:PRO:HG2	1.98	0.45
12:LI:62:SER:HA	12:LI:65:LEU:HD12	1.97	0.45
22:LT:136:ARG:NH1	84:LT:206:HOH:O	2.48	0.45
46:S2:297:A:H4'	47:SE:132:GLY:O	2.15	0.45
46:S2:496:C:OP1	47:SE:29:PRO:HD3	2.16	0.45
46:S2:903:A:H2'	46:S2:904:A:C8	2.51	0.45
62:SX:41:PHE:CZ	62:SX:102:VAL:HG23	2.51	0.45
79:SR:14:ARG:HG2	79:SR:69:ILE:HD11	1.99	0.45
1:L5:216:C:O2'	1:L5:217:C:O5'	2.29	0.45
1:L5:470:A:H61	1:L5:684:G:H1'	1.82	0.45
1:L5:1763:C:H42	1:L5:1770:A:N6	2.13	0.45
1:L5:1921:C:H1'	21:LS:160:ARG:HB3	1.99	0.45
1:L5:4322:G:N2	1:L5:4325:A:OP2	2.48	0.45
1:L5:4637:OMG:OP1	32:Ld:30:HIS:NE2	2.47	0.45
6:LC:318:PRO:HG2	9:LF:155:TYR:HB3	1.98	0.45
8:LE:46:ARG:O	8:LE:65:ARG:NH2	2.48	0.45
19:LQ:178:ARG:HA	19:LQ:184:ARG:O	2.16	0.45
20:LR:158:GLN:NE2	84:LR:211:HOH:O	2.48	0.45
32:Ld:51:LYS:HA	32:Ld:54:MET:HE3	1.98	0.45
46:S2:530:U:H3	46:S2:531:A:N6	2.13	0.45
46:S2:1541:G:N3	59:ST:12:GLN:NE2	2.64	0.45
68:SG:78:SER:HB3	68:SG:92:ARG:HG2	1.99	0.45
1:L5:28:C:H4'	1:L5:61:A:H4'	1.97	0.45
1:L5:406:C:O2'	1:L5:407:A:OP1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1692:C:O2'	19:LQ:143:ARG:NH2	2.49	0.45
1:L5:2273:G:O2'	6:LC:310:HIS:O	2.28	0.45
3:L8:75:OMG:HM23	3:L8:75:OMG:H1'	1.75	0.45
8:LE:162:VAL:HB	8:LE:175:VAL:HG13	1.99	0.45
8:LE:260:LYS:HZ3	8:LE:260:LYS:HG3	1.72	0.45
10:LG:110:LYS:HA	10:LG:113:ARG:HG2	1.98	0.45
11:LH:28:LYS:HE3	11:LH:28:LYS:HB3	1.72	0.45
12:LI:183:ASP:N	12:LI:183:ASP:OD1	2.49	0.45
20:LR:104:ARG:HD2	20:LR:108:ARG:NH2	2.31	0.45
32:Ld:75:LYS:HE3	32:Ld:79:ASN:O	2.17	0.45
46:S2:102:A:H4'	46:S2:104:A:N7	2.32	0.45
46:S2:634:A:H2'	46:S2:635:G:H8	1.81	0.45
46:S2:945:U:H2'	46:S2:946:U:C6	2.51	0.45
46:S2:955:A:N3	46:S2:956:G:H1'	2.32	0.45
46:S2:1562:C:H2'	46:S2:1563:G:H8	1.81	0.45
47:SE:10:LYS:HA	47:SE:10:LYS:HD3	1.76	0.45
62:SX:58:GLU:HG2	84:SX:230:HOH:O	2.16	0.45
67:SC:116:THR:OG1	67:SC:119:GLY:O	2.24	0.45
73:SW:11:LEU:HD12	73:SW:74:VAL:HB	1.98	0.45
76:Sb:54:VAL:HG12	76:Sb:63:LEU:HD12	1.98	0.45
1:L5:223:G:H4'	1:L5:225:G:C8	2.51	0.45
1:L5:300:A:H2'	1:L5:301:G:H8	1.82	0.45
1:L5:722:G:H2'	1:L5:723:A:O4'	2.17	0.45
1:L5:909:A:H2'	1:L5:910:G:H8	1.81	0.45
1:L5:1561:G:N2	84:L5:5442:HOH:O	2.24	0.45
1:L5:1686:C:O2'	30:Lb:18:ARG:NH1	2.49	0.45
1:L5:1927:U:OP1	1:L5:1949:U:O2'	2.29	0.45
1:L5:2045:G:O6	1:L5:3870:C:O2'	2.32	0.45
1:L5:2391:G:H2'	1:L5:2392:C:H6	1.79	0.45
1:L5:2436:U:C4	26:LX:130:PRO:HG3	2.52	0.45
1:L5:2871:A:H2'	1:L5:2872:C:O4'	2.17	0.45
1:L5:3619:G:H4'	20:LR:79:GLY:O	2.17	0.45
1:L5:4524:G:N3	5:LB:252:ALA:HB1	2.31	0.45
3:L8:141:C:H2'	3:L8:142:U:H6	1.80	0.45
6:LC:156:ASP:CG	6:LC:255:SER:HG	2.24	0.45
32:Ld:84:ILE:HG23	32:Ld:86:VAL:HG13	1.99	0.45
35:Lg:83:CYS:SG	35:Lg:86:CYS:HB2	2.56	0.45
41:Lm:98:LYS:HE2	41:Lm:115:CYS:HB2	1.99	0.45
46:S2:505:G:N7	84:S2:2280:HOH:O	2.36	0.45
46:S2:1422:G:O2'	46:S2:1424:G:OP2	2.35	0.45
46:S2:1650:A:H2'	46:S2:1651:A:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SH:113:LYS:HD2	52:SH:113:LYS:HA	1.59	0.45
69:SJ:134:HIS:HD1	69:SJ:163:SER:HG	1.56	0.45
1:L5:52:G:H4'	1:L5:1529:G:H4'	1.98	0.45
1:L5:165:A:H2'	1:L5:166:C:C6	2.52	0.45
1:L5:2571:C:H2'	1:L5:2572:C:C6	2.51	0.45
1:L5:3907:G:H5''	84:L5:8726:HOH:O	2.17	0.45
1:L5:4122:G:H4'	35:Lg:90:ARG:HG2	1.98	0.45
1:L5:4518:A:N7	5:LB:258:HIS:HE1	2.14	0.45
4:LA:46:LYS:HD2	4:LA:46:LYS:HA	1.73	0.45
5:LB:220:ILE:HB	5:LB:346:THR:HB	1.98	0.45
12:LI:33:ILE:HG23	12:LI:69:ARG:NH1	2.31	0.45
12:LI:38:ARG:NE	12:LI:83:ASP:HB3	2.29	0.45
12:LI:188:LYS:HD3	12:LI:188:LYS:HA	1.79	0.45
13:LJ:30:GLY:O	13:LJ:32:ARG:N	2.50	0.45
46:S2:140:C:H42	46:S2:313:A:H61	1.64	0.45
46:S2:805:U:H5''	73:SW:83:LEU:HD12	1.99	0.45
46:S2:1278:A:H2'	46:S2:1279:C:C6	2.52	0.45
46:S2:1377:U:O2	46:S2:1379:A:H5'	2.16	0.45
46:S2:1736:G:H2'	46:S2:1737:G:C8	2.52	0.45
48:SA:134:LEU:HD22	48:SA:144:THR:HG21	1.98	0.45
48:SA:181:GLU:OE1	48:SA:191:ARG:NH2	2.50	0.45
52:SH:12:ASN:ND2	52:SH:16:PRO:O	2.49	0.45
1:L5:10:A:H2'	1:L5:11:G:H8	1.81	0.45
1:L5:423:G:H2'	1:L5:424:U:C6	2.51	0.45
1:L5:2335:C:H2'	1:L5:2336:G:H8	1.82	0.45
1:L5:2422:OMC:OP1	18:LP:127:ARG:NH2	2.39	0.45
1:L5:2702:C:H2'	1:L5:2703:G:O4'	2.16	0.45
1:L5:3888:G:H1'	82:L5:5378:SPD:HN6	1.82	0.45
1:L5:4456:OMC:HM21	5:LB:241:PRO:HD3	1.99	0.45
1:L5:4536:OMC:HM22	1:L5:4537:C:O4'	2.17	0.45
1:L5:4921:C:N3	1:L5:4922:C:N4	2.64	0.45
1:L5:5001:PSU:H2'	1:L5:5002:U:O4'	2.16	0.45
1:L5:5055:G:H2'	1:L5:5056:A:C8	2.52	0.45
5:LB:220:ILE:HG12	5:LB:278:THR:HG23	1.99	0.45
12:LI:36:LEU:HD21	12:LI:69:ARG:NH1	2.31	0.45
13:LJ:60:PHE:O	13:LJ:62:ILE:HG23	2.16	0.45
23:LU:95:ASN:O	23:LU:99:TRP:HZ3	2.00	0.45
46:S2:1741:U:H2'	46:S2:1742:C:O4'	2.16	0.45
53:SI:110:ARG:HA	53:SI:121:LEU:HD23	1.99	0.45
60:SU:79:ARG:NH1	65:Sd:56:ASP:OXT	2.50	0.45
72:SO:34:PHE:HB3	72:SO:41:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:132:G:H2'	1:L5:133:C:H4'	1.99	0.45
1:L5:4508:C:N3	1:L5:4512:U:H5	2.15	0.45
1:L5:4928:C:H2'	1:L5:4929:C:C6	2.52	0.45
3:L8:93:C:O2'	3:L8:94:G:H8	1.99	0.45
28:LZ:53:VAL:HB	28:LZ:62:ILE:HG12	1.98	0.45
29:La:89:ASN:HA	29:La:92:LYS:HE3	1.99	0.45
46:S2:962:A:N1	46:S2:1055:A:O2'	2.47	0.45
46:S2:1759:G:O6	46:S2:1772:C:N4	2.50	0.45
47:SE:45:ILE:HA	47:SE:61:VAL:HG11	1.98	0.45
62:SX:41:PHE:HZ	62:SX:102:VAL:HG23	1.81	0.45
74:SY:102:THR:HG23	74:SY:107:ARG:HH11	1.82	0.45
1:L5:368:C:O4'	6:LC:83:GLY:HA3	2.17	0.45
1:L5:908:G:H2'	1:L5:909:A:C8	2.51	0.45
1:L5:1296:G:H2'	1:L5:1297:U:O4'	2.17	0.45
1:L5:1411:C:O2'	1:L5:1412:G:N7	2.43	0.45
1:L5:1554:A:H5'	44:Lp:9:GLY:C	2.41	0.45
1:L5:1558:A:H2'	1:L5:1559:G:C8	2.52	0.45
1:L5:1559:G:OP1	20:LR:126:LYS:NZ	2.50	0.45
1:L5:1682:A:H5''	14:LL:3:PRO:O	2.16	0.45
1:L5:2054:U:OP2	17:LO:44:SER:OG	2.31	0.45
1:L5:2065:G:H2'	1:L5:2066:C:O4'	2.17	0.45
1:L5:3604:A:H2'	1:L5:3605:C:O4'	2.17	0.45
1:L5:3934:G:H2'	1:L5:3935:C:C6	2.52	0.45
1:L5:4122:G:O2'	28:LZ:136:PHE:OXT	2.34	0.45
1:L5:4281:A:O2'	1:L5:4282:A:C8	2.70	0.45
1:L5:4653:C:H2'	1:L5:4654:C:H6	1.81	0.45
82:L5:5378:SPD:H22	17:LO:68:ARG:HH21	1.82	0.45
4:LA:102:LEU:HB2	4:LA:107:MET:HE2	1.99	0.45
6:LC:190:ARG:HA	6:LC:202:ILE:HD13	1.99	0.45
9:LF:193:GLU:OE2	9:LF:200:ARG:HB2	2.17	0.45
38:Lj:2:THR:HB	38:Lj:6:SER:OG	2.16	0.45
48:SA:1:MET:HE3	48:SA:1:MET:C	2.41	0.45
52:SH:111:LYS:HE3	52:SH:111:LYS:HB2	1.72	0.45
64:Sc:67:ARG:HH11	64:Sc:68:LEU:H	1.64	0.45
66:Sg:223:GLU:OE1	66:Sg:223:GLU:N	2.50	0.45
70:SM:87:GLU:HG3	70:SM:92:CYS:SG	2.57	0.45
1:L5:186:G:N3	1:L5:1366:G:N2	2.65	0.44
1:L5:301:G:H2'	1:L5:302:C:C6	2.52	0.44
1:L5:1082:C:O2'	1:L5:1083:U:O5'	2.29	0.44
1:L5:1365:C:N4	1:L5:1367:C:H5''	2.32	0.44
1:L5:1449:C:H2'	1:L5:1450:C:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2276:A:H2'	1:L5:2277:C:O4'	2.17	0.44
1:L5:2555:G:H2'	1:L5:2556:G:C8	2.52	0.44
1:L5:2588:C:OP1	1:L5:2768:C:O2'	2.28	0.44
1:L5:4600:G:O2'	1:L5:4601:U:P	2.75	0.44
3:L8:67:U:H2'	3:L8:68:G:H8	1.82	0.44
31:Lc:46:VAL:HB	31:Lc:71:VAL:HG22	1.99	0.44
46:S2:162:C:H2'	46:S2:163:U:O4'	2.17	0.44
46:S2:815:PSU:C4	46:S2:816:A:C8	3.06	0.44
46:S2:1365:G:H2'	46:S2:1366:G:C8	2.52	0.44
52:SH:61:ILE:HA	52:SH:93:VAL:HG23	1.99	0.44
70:SM:52:LEU:HD13	70:SM:65:VAL:HG11	1.99	0.44
1:L5:1564:A:H2'	1:L5:1565:A:C8	2.52	0.44
1:L5:1576:G:OP1	84:L5:5415:HOH:O	2.21	0.44
1:L5:1846:G:H2'	1:L5:1847:C:C6	2.52	0.44
1:L5:2279:A:O2'	33:Le:48:ARG:NH2	2.50	0.44
1:L5:2424:OMG:H8	1:L5:2424:OMG:O5'	2.00	0.44
1:L5:2496:G:H2'	1:L5:2497:C:C6	2.52	0.44
1:L5:3946:G:C2	1:L5:4068:U:H5	2.36	0.44
1:L5:5030:U:H2'	1:L5:5031:G:H8	1.83	0.44
6:LC:44:LEU:HD11	6:LC:120:LYS:HG2	1.99	0.44
7:LD:110:LEU:HD22	7:LD:115:MET:HB2	1.99	0.44
20:LR:166:THR:OG1	46:S2:873:G:OP2	2.32	0.44
28:LZ:4:PHE:HE1	28:LZ:82:PRO:HG3	1.82	0.44
29:La:103:VAL:HG23	29:La:108:TYR:O	2.16	0.44
44:Lp:7:LYS:O	44:Lp:27:LYS:NZ	2.51	0.44
46:S2:386:C:H2'	46:S2:387:C:C6	2.52	0.44
46:S2:441:C:H2'	46:S2:442:C:C6	2.52	0.44
50:SD:132:LYS:CD	50:SD:191:PRO:HA	2.47	0.44
60:SU:25:THR:HG22	60:SU:86:LYS:HG3	1.99	0.44
71:SN:25:TRP:HE1	76:Sb:83:GLN:HB2	1.82	0.44
71:SN:34:LYS:HZ2	71:SN:74:ILE:HG12	1.82	0.44
1:L5:25:A:H2'	1:L5:26:C:C6	2.51	0.44
1:L5:88:A:N7	19:LQ:173:LYS:NZ	2.65	0.44
1:L5:159:C:N4	84:L5:6546:HOH:O	2.49	0.44
1:L5:209:U:C4	1:L5:233:U:C4	3.05	0.44
1:L5:1186:U:H3'	1:L5:1187:G:H21	1.82	0.44
1:L5:1664:U:H2'	1:L5:1665:C:C6	2.52	0.44
1:L5:2306:G:H1'	1:L5:2332:A:N6	2.32	0.44
1:L5:4345:C:H2'	1:L5:4346:U:C6	2.53	0.44
2:L7:18:C:H2'	2:L7:19:C:C6	2.52	0.44
3:L8:90:C:H1'	27:LY:24:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:77:THR:HG21	5:LB:337:VAL:HG22	1.99	0.44
5:LB:356:LYS:O	5:LB:360:LEU:HD12	2.17	0.44
10:LG:248:ALA:C	10:LG:252:LYS:HE3	2.42	0.44
15:LM:120:ASN:HB3	15:LM:124:LYS:CE	2.47	0.44
23:LU:38:ASN:HA	23:LU:41:GLN:OE1	2.16	0.44
24:LV:38:TYR:CG	24:LV:66:LYS:HE2	2.52	0.44
46:S2:823:U:C6	46:S2:823:U:C5'	3.01	0.44
46:S2:1023:A:N7	84:S2:2284:HOH:O	2.36	0.44
46:S2:1149:A:H2'	46:S2:1149:A:N3	2.32	0.44
46:S2:1337:4AC:H2'	46:S2:1338:G:H8	1.82	0.44
46:S2:1402:A:H5'	60:SU:51:LYS:HE2	1.99	0.44
46:S2:1740:C:O2	84:S2:2104:HOH:O	2.20	0.44
47:SE:122:LYS:HD2	47:SE:164:LEU:HD21	2.00	0.44
48:SA:42:LYS:HE3	48:SA:44:ASP:OD1	2.17	0.44
63:Sa:65:PRO:HG3	72:SO:129:ILE:O	2.17	0.44
64:Sc:42:ILE:HD12	64:Sc:44:ARG:HD3	1.99	0.44
69:SJ:33:GLY:HA3	77:Se:38:TYR:CG	2.52	0.44
70:SM:60:MET:HE3	78:Sf:104:LYS:HD2	1.99	0.44
75:SZ:60:LYS:HE2	75:SZ:60:LYS:HB2	1.87	0.44
75:SZ:96:LEU:O	75:SZ:97:ILE:HD13	2.16	0.44
1:L5:82:U:H2'	1:L5:83:C:O4'	2.17	0.44
1:L5:153:G:H2'	1:L5:154:G:C8	2.51	0.44
1:L5:717:U:O2'	1:L5:1904:G:H4'	2.17	0.44
1:L5:963:G:H1	1:L5:2095:A:H61	1.65	0.44
1:L5:1808:C:OP1	22:LT:110:LYS:HD3	2.18	0.44
1:L5:2427:G:OP1	20:LR:5:ARG:NH2	2.46	0.44
1:L5:2448:G:H2'	1:L5:2449:A:C8	2.52	0.44
1:L5:3596:A:C5	55:SL:3:ASP:HB2	2.53	0.44
1:L5:3657:U:O4	84:L5:5409:HOH:O	2.20	0.44
1:L5:3732:A:H2'	1:L5:3733:A:H8	1.81	0.44
3:L8:18:U:OP1	84:L8:303:HOH:O	2.21	0.44
10:LG:228:ASP:OD1	10:LG:228:ASP:N	2.50	0.44
13:LJ:56:THR:CG2	13:LJ:63:ARG:HG3	2.48	0.44
13:LJ:168:GLN:OE1	13:LJ:168:GLN:N	2.51	0.44
33:Le:33:ARG:N	33:Le:33:ARG:HD2	2.32	0.44
37:Li:19:LYS:HE2	37:Li:19:LYS:H	1.83	0.44
46:S2:949:G:H2'	46:S2:950:C:C6	2.52	0.44
46:S2:1461:G:H2'	46:S2:1463:U:O2	2.17	0.44
54:SK:14:LEU:HD23	54:SK:21:MET:HE1	1.99	0.44
69:SJ:161:LEU:H	69:SJ:161:LEU:HD22	1.82	0.44
1:L5:126:C:H2'	1:L5:127:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:208:A:H2	1:L5:233:U:H5''	1.83	0.44
1:L5:230:G:OP1	27:LY:15:ARG:NH1	2.46	0.44
1:L5:455:C:C2'	1:L5:456:C:H5'	2.48	0.44
1:L5:2079:G:H2'	1:L5:2080:U:C6	2.52	0.44
1:L5:4498:OMU:H2'	1:L5:4500:PSU:OP2	2.16	0.44
1:L5:4601:U:H2'	1:L5:4602:A:H8	1.81	0.44
4:LA:158:ILE:HD12	4:LA:159:SER:O	2.18	0.44
5:LB:291:TYR:OH	5:LB:315:ASN:ND2	2.51	0.44
8:LE:223:ARG:HA	8:LE:223:ARG:HD3	1.52	0.44
28:LZ:66:SER:OG	28:LZ:123:LYS:HE3	2.17	0.44
46:S2:306:C:C4	46:S2:308:G:C2	3.06	0.44
46:S2:496:C:H2'	46:S2:497:C:C6	2.52	0.44
46:S2:595:U:H2'	46:S2:596:U:C6	2.53	0.44
46:S2:629:A:H2'	84:S2:4585:HOH:O	2.16	0.44
46:S2:1301:A:H2'	46:S2:1303:C:O2	2.18	0.44
49:SB:171:ILE:HD12	49:SB:174:ARG:HH22	1.83	0.44
52:SH:7:LYS:NZ	52:SH:17:ASP:HB2	2.32	0.44
52:SH:79:LEU:O	52:SH:83:LEU:N	2.50	0.44
69:SJ:17:ARG:NH1	84:SJ:212:HOH:O	2.50	0.44
70:SM:72:HIS:O	70:SM:73:GLN:HG2	2.18	0.44
1:L5:133:C:H2'	1:L5:134:G:O4'	2.18	0.44
1:L5:151:G:OP2	16:LN:4:TYR:OH	2.26	0.44
1:L5:680:G:H2'	1:L5:681:G:H8	1.82	0.44
1:L5:2264:C:H2'	1:L5:2265:G:O4'	2.17	0.44
1:L5:2727:C:H2'	1:L5:2728:U:C6	2.52	0.44
1:L5:3724:A2M:H1'	1:L5:3724:A2M:HM'3	1.67	0.44
1:L5:4691:A:H5'	11:LH:71:ARG:HE	1.81	0.44
3:L8:134:G:OP2	84:L8:302:HOH:O	2.21	0.44
6:LC:143:ARG:NH2	6:LC:145:GLU:OE2	2.51	0.44
8:LE:88:VAL:HB	8:LE:89:LEU:H	1.62	0.44
8:LE:244:GLU:O	8:LE:248:ILE:HG13	2.17	0.44
9:LF:174:LEU:HD23	9:LF:177:ARG:HH21	1.82	0.44
10:LG:153:GLN:OE1	10:LG:153:GLN:N	2.50	0.44
13:LJ:19:LYS:HB3	13:LJ:75:ARG:NH1	2.32	0.44
15:LM:51:PRO:HG2	15:LM:54:CYS:SG	2.58	0.44
35:Lg:78:TYR:HB3	35:Lg:82:MET:HB3	1.99	0.44
46:S2:384:U:H5'	55:SL:133:PRO:O	2.18	0.44
46:S2:433:A:H2'	46:S2:434:G:C8	2.52	0.44
46:S2:837:A:H62	74:SY:8:ARG:NH1	2.15	0.44
46:S2:1276:A:C5	46:S2:1322:G:H1'	2.53	0.44
46:S2:1293:A:H2'	46:S2:1294:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SD:193:ASP:OD2	50:SD:196:GLY:N	2.50	0.44
58:SS:92:ASP:OD1	58:SS:92:ASP:N	2.51	0.44
1:L5:362:A:N6	40:Ll:37:TYR:O	2.44	0.44
1:L5:370:U:O3'	38:Lj:25:LYS:NZ	2.50	0.44
1:L5:910:G:H2'	1:L5:911:U:H6	1.82	0.44
1:L5:1096:C:H2'	1:L5:1097:C:C6	2.53	0.44
1:L5:1450:C:H2'	1:L5:1451:G:O4'	2.17	0.44
1:L5:1650:A:C5'	6:LC:60:HIS:CE1	3.01	0.44
1:L5:2424:OMG:HM22	1:L5:2426:U:C6	2.53	0.44
1:L5:2857:A:H2'	1:L5:2858:A:O4'	2.18	0.44
1:L5:4273:A:H2'	1:L5:4274:A:C8	2.53	0.44
1:L5:4324:A:H2'	1:L5:4325:A:C8	2.52	0.44
1:L5:4606:G:H2'	1:L5:4607:A:C8	2.53	0.44
1:L5:4652:G:H2'	1:L5:4653:C:C6	2.53	0.44
2:L7:3:C:H2'	2:L7:4:U:H6	1.82	0.44
3:L8:19:C:H2'	3:L8:20:A:C8	2.53	0.44
5:LB:139:ASP:O	5:LB:143:LYS:HG3	2.18	0.44
11:LH:6:SER:OG	11:LH:67:LEU:HD22	2.18	0.44
12:LI:48:LEU:HD21	12:LI:167:ILE:HD12	1.98	0.44
46:S2:156:G:OP1	68:SG:2:LYS:NZ	2.28	0.44
46:S2:159:A2M:N1	46:S2:467:G:O2'	2.48	0.44
46:S2:496:C:H2'	46:S2:497:C:H6	1.83	0.44
46:S2:572:PSU:H5''	74:SY:60:PHE:O	2.18	0.44
46:S2:1099:G:H22	46:S2:1133:A:H2	1.66	0.44
46:S2:1695:A:N1	46:S2:1832:6MZ:O2'	2.48	0.44
49:SB:35:ALA:O	49:SB:42:ARG:NH2	2.44	0.44
58:SS:84:LEU:HD12	58:SS:95:TYR:HB3	2.00	0.44
66:Sg:244:ASN:ND2	66:Sg:295:GLY:HA3	2.25	0.44
1:L5:489:C:H3'	1:L5:490:C:C6	2.52	0.44
1:L5:1281:G:OP1	6:LC:316:LYS:NZ	2.44	0.44
1:L5:1577:G:H5'	1:L5:1578:U:H5''	1.99	0.44
1:L5:1912:G:N2	17:LO:87:MET:HE2	2.32	0.44
1:L5:4303:C:O2'	1:L5:4304:A:H2'	2.18	0.44
1:L5:4538:G:H2'	1:L5:4539:U:C6	2.53	0.44
1:L5:4719:G:O2'	1:L5:4720:C:H5''	2.17	0.44
3:L8:141:C:H5'	16:LN:113:LEU:HD11	1.99	0.44
7:LD:284:LYS:HE3	12:LI:206:LEU:HD11	2.00	0.44
8:LE:72:LYS:NZ	30:Lb:119:CYS:HA	2.33	0.44
36:Lh:18:LEU:HD23	36:Lh:18:LEU:HA	1.87	0.44
43:Lo:40:ARG:HD2	84:Lo:316:HOH:O	2.17	0.44
46:S2:1690:U:H2'	46:S2:1691:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SP:13:ARG:HA	56:SP:13:ARG:HD2	1.72	0.44
64:Sc:37:ASP:O	64:Sc:39:SER:N	2.51	0.44
76:Sb:33:MET:HE1	76:Sb:73:LEU:HD21	1.99	0.44
1:L5:938:C:OP2	84:L5:5414:HOH:O	2.21	0.44
1:L5:1078:A:H5'	1:L5:1079:C:H5	1.82	0.44
1:L5:1951:G:O2'	21:LS:95:ARG:NH1	2.36	0.44
1:L5:2072:C:O2'	9:LF:213:LEU:O	2.35	0.44
1:L5:2423:A:H2'	1:L5:2424:OMG:C8	2.53	0.44
1:L5:2568:C:H2'	1:L5:2569:G:C8	2.46	0.44
1:L5:2635:U:H2'	1:L5:2636:U:C6	2.52	0.44
1:L5:2892:C:H5'	1:L5:5018:C:H4'	2.00	0.44
1:L5:4598:C:H2'	1:L5:4611:A:N6	2.33	0.44
7:LD:164:LYS:HG2	7:LD:199:ILE:HD11	2.00	0.44
7:LD:202:GLN:HA	7:LD:205:ALA:HB3	1.99	0.44
20:LR:165:LYS:HE2	20:LR:165:LYS:HB3	1.82	0.44
46:S2:688:U:H5'	52:SH:122:LEU:HB3	1.99	0.44
46:S2:921:G:H5'	76:Sb:21:LYS:HE3	2.00	0.44
46:S2:1146:C:P	63:Sa:89:ARG:HH21	2.40	0.44
52:SH:157:HIS:HB3	52:SH:190:PRO:HG3	1.99	0.44
64:Sc:37:ASP:C	64:Sc:39:SER:H	2.26	0.44
68:SG:168:LYS:HE2	68:SG:168:LYS:HB3	1.72	0.44
78:Sf:118:ARG:HD2	78:Sf:134:SER:HB2	1.99	0.44
1:L5:659:G:H2'	1:L5:660:A:O4'	2.18	0.43
1:L5:1284:G:O4'	8:LE:130:LYS:HE2	2.17	0.43
1:L5:1628:C:OP2	4:LA:9:ARG:HD2	2.18	0.43
1:L5:2020:U:H2'	1:L5:2021:G:O4'	2.18	0.43
1:L5:2588:C:H5''	1:L5:2589:C:H5''	2.00	0.43
1:L5:2809:G:H5''	20:LR:63:CYS:SG	2.58	0.43
2:L7:19:C:H2'	2:L7:20:U:C6	2.53	0.43
3:L8:142:U:H2'	3:L8:143:G:O4'	2.17	0.43
7:LD:53:VAL:HG11	7:LD:159:VAL:HA	1.98	0.43
7:LD:166:ALA:HB1	7:LD:171:LEU:HD12	2.00	0.43
15:LM:124:LYS:O	15:LM:128:LYS:HG2	2.17	0.43
17:LO:54:TYR:OH	17:LO:73:PHE:O	2.31	0.43
17:LO:60:LYS:O	17:LO:72:HIS:NE2	2.49	0.43
36:Lh:87:LYS:HB3	36:Lh:88:THR:H	1.58	0.43
46:S2:352:U:H2'	46:S2:353:C:C6	2.53	0.43
46:S2:1578:U:H5''	46:S2:1579:A:O4'	2.18	0.43
46:S2:1737:G:H2'	46:S2:1738:C:H6	1.82	0.43
53:SI:168:GLN:NE2	84:SI:317:HOH:O	2.52	0.43
66:Sg:199:THR:HG23	66:Sg:241:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SN:38:TYR:O	71:SN:42:LYS:HG2	2.18	0.43
1:L5:978:G:H2'	1:L5:979:C:C6	2.53	0.43
1:L5:1340:OMC:HM23	1:L5:1340:OMC:H1'	1.88	0.43
1:L5:1550:G:N7	84:L5:5837:HOH:O	2.37	0.43
1:L5:1633:G:H5'	1:L5:1634:A:OP1	2.17	0.43
1:L5:1701:A:N6	1:L5:1703:C:H42	2.16	0.43
1:L5:1847:C:H2'	1:L5:1848:C:C6	2.53	0.43
1:L5:4038:C:N4	1:L5:4051:C:OP1	2.51	0.43
9:LF:241:ASN:O	9:LF:245:ARG:HG2	2.17	0.43
12:LI:55:ASP:CG	12:LI:162:ARG:HE	2.25	0.43
14:LL:105:LYS:HE2	14:LL:105:LYS:HB3	1.83	0.43
15:LM:100:ARG:HD3	17:LO:198:THR:O	2.18	0.43
22:LT:108:ARG:O	22:LT:112:ASN:N	2.43	0.43
50:SD:210:ILE:HD12	79:SR:16:ILE:HG13	2.00	0.43
51:SF:127:ARG:C	51:SF:128:ILE:HG13	2.43	0.43
53:SI:38:ILE:HA	53:SI:60:LEU:O	2.18	0.43
56:SP:130:ARG:CZ	56:SP:130:ARG:HB3	2.48	0.43
59:ST:71:GLY:O	59:ST:75:MET:HG2	2.19	0.43
68:SG:50:VAL:HG21	68:SG:111:LEU:HD13	2.00	0.43
68:SG:164:LYS:HD2	68:SG:165:GLU:HG3	2.00	0.43
79:SR:104:GLU:OE2	79:SR:107:LYS:HD3	2.18	0.43
1:L5:667:A:H1'	45:Lr:46:ARG:HE	1.82	0.43
1:L5:668:C:H4'	6:LC:6:PRO:HB3	2.00	0.43
1:L5:750:U:C2	1:L5:751:G:C8	3.06	0.43
1:L5:1249:C:H2'	1:L5:1250:C:O4'	2.19	0.43
1:L5:1703:C:C5	9:LF:36:LYS:HE3	2.53	0.43
1:L5:2688:G:H2'	1:L5:2689:C:C6	2.53	0.43
1:L5:3668:C:H5'	4:LA:8:GLN:O	2.17	0.43
3:L8:7:U:H2'	3:L8:8:U:C6	2.53	0.43
3:L8:70:G:C2	3:L8:87:G:N3	2.87	0.43
3:L8:79:G:N3	3:L8:80:A:H1'	2.33	0.43
10:LG:95:LEU:O	10:LG:99:ALA:N	2.50	0.43
10:LG:176:LYS:HE3	10:LG:176:LYS:HB2	1.76	0.43
12:LI:108:ALA:O	12:LI:110:ARG:N	2.51	0.43
28:LZ:67:LYS:HE2	28:LZ:67:LYS:HB3	1.66	0.43
43:Lo:28:LYS:NZ	43:Lo:31:ASP:OD1	2.51	0.43
46:S2:11:A:H5'	67:SC:113:GLN:OE1	2.18	0.43
46:S2:641:A:O2'	46:S2:645:C:OP1	2.36	0.43
46:S2:1203:G:H2'	46:S2:1204:A:C8	2.54	0.43
46:S2:1457:U:H2'	46:S2:1458:G:H8	1.82	0.43
46:S2:1757:G:N3	46:S2:1757:G:H2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SD:103:GLU:OE2	50:SD:173:ARG:NE	2.47	0.43
53:SI:37:LYS:HA	53:SI:37:LYS:HD3	1.76	0.43
62:SX:61:GLN:HE21	62:SX:61:GLN:HA	1.83	0.43
63:Sa:90:GLU:HA	63:Sa:90:GLU:OE2	2.18	0.43
68:SG:147:LEU:HD21	68:SG:156:TYR:CD2	2.52	0.43
1:L5:489:C:H3'	1:L5:490:C:H6	1.83	0.43
1:L5:1758:G:H2'	1:L5:1759:G:C8	2.53	0.43
1:L5:2617:G:P	20:LR:64:ARG:HH22	2.42	0.43
1:L5:4628:PSU:H4'	25:LW:16:GLY:O	2.18	0.43
1:L5:4659:G:N7	84:L5:5780:HOH:O	2.35	0.43
3:L8:14:OMU:HM23	3:L8:14:OMU:H1'	1.59	0.43
6:LC:221:PHE:HB3	6:LC:227:ILE:HG21	2.00	0.43
7:LD:179:ARG:HA	7:LD:179:ARG:HD3	1.84	0.43
12:LI:118:ALA:O	12:LI:119:PHE:C	2.61	0.43
46:S2:1197:G:OP2	84:S2:2108:HOH:O	2.21	0.43
46:S2:1407:U:H4'	57:SQ:71:ARG:NH2	2.33	0.43
46:S2:1806:A:H2'	46:S2:1807:C:O4'	2.18	0.43
49:SB:171:ILE:HD12	49:SB:174:ARG:NH2	2.34	0.43
49:SB:171:ILE:O	49:SB:175:GLU:HG2	2.19	0.43
53:SI:113:TYR:CG	53:SI:121:LEU:HD22	2.54	0.43
69:SJ:52:LYS:HE3	69:SJ:52:LYS:HB2	1.81	0.43
1:L5:217:C:OP2	1:L5:219:G:H1'	2.19	0.43
1:L5:979:C:H2'	1:L5:980:U:H6	1.82	0.43
1:L5:1283:G:H1	6:LC:312:ARG:HH21	1.67	0.43
1:L5:1356:U:H2'	1:L5:1357:C:C6	2.54	0.43
1:L5:1431:C:H2'	1:L5:1432:G:O4'	2.19	0.43
1:L5:1524:A2M:H62	1:L5:1651:G:H22	1.65	0.43
1:L5:1756:U:O2'	1:L5:1757:U:O5'	2.36	0.43
1:L5:2362:U:H2'	1:L5:2363:A2M:H8	2.01	0.43
1:L5:2809:G:O2'	1:L5:4644:G:OP1	2.31	0.43
84:L5:8247:HOH:O	6:LC:69:THR:HG21	2.17	0.43
4:LA:234:LYS:HG2	4:LA:238:ILE:HG12	1.99	0.43
7:LD:41:LYS:HB2	22:LT:68:THR:O	2.18	0.43
12:LI:87:MET:HE3	12:LI:87:MET:HB2	1.76	0.43
16:LN:3:ALA:O	16:LN:7:ILE:HG13	2.19	0.43
16:LN:126:THR:HG23	16:LN:127:TYR:CD2	2.54	0.43
16:LN:145:ASN:HB3	16:LN:148:THR:OG1	2.18	0.43
23:LU:80:LYS:HE2	23:LU:110:TYR:CE2	2.53	0.43
45:Lr:35:ARG:HG2	45:Lr:37:SER:HB3	2.00	0.43
46:S2:1017:U:H2'	46:S2:1018:U:C6	2.53	0.43
46:S2:1017:U:H2'	46:S2:1018:U:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:1777:G:H2'	46:S2:1778:C:C5	2.53	0.43
46:S2:1842:4AC:O7	46:S2:1842:4AC:H5	2.18	0.43
48:SA:63:ARG:HA	48:SA:66:VAL:HG22	2.00	0.43
48:SA:110:ASN:HB3	48:SA:113:GLN:HG3	1.99	0.43
49:SB:40:ASN:H	49:SB:75:GLN:HG2	1.82	0.43
54:SK:49:MET:HG3	54:SK:69:TRP:CE3	2.54	0.43
59:ST:107:LEU:HB3	59:ST:113:VAL:HG13	1.99	0.43
69:SJ:47:LYS:HG3	69:SJ:102:ILE:HD12	1.99	0.43
70:SM:32:ALA:HB2	70:SM:112:LYS:HD2	2.00	0.43
71:SN:110:ASP:O	71:SN:114:ARG:HG2	2.19	0.43
72:SO:59:GLY:CA	72:SO:68:GLU:HG2	2.48	0.43
1:L5:468:U:N3	1:L5:684:G:N7	2.67	0.43
1:L5:738:C:H5'	1:L5:739:G:O5'	2.18	0.43
1:L5:4131:G:H2'	1:L5:4132:C:C6	2.53	0.43
5:LB:21:ARG:HG2	5:LB:271:GLN:HG2	1.99	0.43
6:LC:140:LYS:HE3	6:LC:245:HIS:HB2	2.01	0.43
6:LC:284:MET:HE3	19:LQ:28:LEU:HD23	1.99	0.43
10:LG:120:LYS:HA	10:LG:123:ALA:O	2.18	0.43
14:LL:107:THR:OG1	37:Li:18:THR:OG1	2.27	0.43
46:S2:666:U:H2'	46:S2:667:PSU:C6	2.54	0.43
50:SD:154:ASP:OD1	50:SD:155:GLY:N	2.51	0.43
51:SF:77:MET:O	51:SF:83:ASN:ND2	2.50	0.43
53:SI:150:ASP:HA	53:SI:153:LYS:HD2	2.00	0.43
67:SC:211:LYS:O	67:SC:215:MET:HG3	2.18	0.43
68:SG:201:LYS:HE3	68:SG:201:LYS:HB3	1.87	0.43
1:L5:498:C:N4	84:L5:6661:HOH:O	2.50	0.43
1:L5:740:G:H2'	1:L5:741:C:O4'	2.18	0.43
1:L5:919:C:OP1	15:LM:69:HIS:ND1	2.49	0.43
1:L5:1733:G:N3	1:L5:4214:A:H2'	2.34	0.43
1:L5:1788:A:H2'	12:LI:22:PHE:CZ	2.54	0.43
1:L5:2303:C:H5''	33:Le:104:SER:HB3	1.99	0.43
1:L5:3925:OMU:HM23	1:L5:3925:OMU:H1'	1.84	0.43
1:L5:4253:A:H4'	1:L5:4254:G:O5'	2.19	0.43
1:L5:4297:G:C8	1:L5:4297:G:H5''	2.53	0.43
5:LB:200:ARG:HG2	5:LB:200:ARG:NH1	2.33	0.43
6:LC:22:VAL:HG22	6:LC:258:ARG:CZ	2.49	0.43
23:LU:23:LEU:HD11	23:LU:87:THR:HG21	2.01	0.43
25:LW:64:SER:O	25:LW:64:SER:OG	2.34	0.43
46:S2:1014:G:OP1	84:S2:2109:HOH:O	2.22	0.43
46:S2:1809:A:H2'	46:S2:1810:U:C6	2.53	0.43
47:SE:124:CYS:HB3	47:SE:141:THR:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SB:109:LYS:HE3	49:SB:113:MET:SD	2.58	0.43
77:Se:22:GLN:NE2	77:Se:24:LYS:HE2	2.34	0.43
1:L5:1349:G:OP1	19:LQ:54:SER:HA	2.19	0.43
1:L5:1842:G:H2'	1:L5:1843:A:O4'	2.19	0.43
1:L5:2635:U:C4	1:L5:2636:U:C4	3.06	0.43
3:L8:10:G:N7	84:L8:318:HOH:O	2.36	0.43
5:LB:80:GLU:OE1	5:LB:323:TYR:OH	2.24	0.43
6:LC:20:LYS:HB2	6:LC:20:LYS:HE2	1.83	0.43
7:LD:64:ILE:HG12	7:LD:105:LEU:HD21	2.01	0.43
7:LD:228:LYS:C	7:LD:230:SER:H	2.27	0.43
8:LE:164:PHE:CE1	8:LE:173:LEU:HB3	2.54	0.43
10:LG:88:ASP:OD1	10:LG:88:ASP:N	2.50	0.43
16:LN:6:TYR:CZ	37:Li:40:VAL:HG22	2.54	0.43
17:LO:125:LYS:HE2	17:LO:135:PHE:CZ	2.54	0.43
37:Li:76:ARG:HD3	37:Li:76:ARG:HA	1.72	0.43
46:S2:35:C:H2'	46:S2:36:PSU:H6	1.83	0.43
46:S2:1480:A:O5'	57:SQ:131:LYS:HE2	2.18	0.43
48:SA:8:LEU:HD11	61:SV:39:VAL:HG21	2.01	0.43
48:SA:78:SER:HB2	48:SA:87:VAL:HG21	2.01	0.43
49:SB:225:LEU:HD12	49:SB:225:LEU:O	2.19	0.43
50:SD:225:GLU:HG3	66:Sg:187:ASN:HB3	2.01	0.43
55:SL:80:MET:HE1	55:SL:120:VAL:O	2.18	0.43
58:SS:5:ILE:HB	75:SZ:49:LEU:O	2.18	0.43
60:SU:97:ILE:O	60:SU:101:ILE:HG13	2.19	0.43
68:SG:39:ASP:OD1	68:SG:47:GLY:N	2.31	0.43
1:L5:308:G:H1'	37:Li:31:GLY:O	2.18	0.43
1:L5:932:A:O2'	1:L5:939:G:N7	2.47	0.43
1:L5:1481:C:O2'	1:L5:1482:G:N3	2.42	0.43
1:L5:1667:G:H5'	1:L5:1688:G:OP1	2.19	0.43
1:L5:1721:G:H2'	1:L5:1722:C:C6	2.54	0.43
1:L5:1878:G:H2'	1:L5:1879:C:C6	2.53	0.43
1:L5:2010:A:C5	1:L5:2012:A:H1'	2.54	0.43
1:L5:2682:G:H2'	1:L5:2683:C:C6	2.54	0.43
1:L5:4076:G:OP1	10:LG:73:ARG:NE	2.38	0.43
84:L5:6211:HOH:O	53:SI:200:ARG:HD2	2.18	0.43
4:LA:2:GLY:HA2	4:LA:207:VAL:HG23	2.01	0.43
8:LE:43:HIS:ND1	8:LE:44:CYS:N	2.67	0.43
13:LJ:82:ILE:HG22	13:LJ:130:PHE:CE2	2.53	0.43
25:LW:74:ARG:HH21	46:S2:1748:G:H5'	1.84	0.43
28:LZ:67:LYS:HA	28:LZ:119:GLU:OE1	2.19	0.43
33:Le:16:ARG:NH1	33:Le:54:LEU:HD12	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Lh:52:LYS:HA	36:Lh:52:LYS:HD3	1.78	0.43
46:S2:563:G:N7	69:SJ:172:ARG:NH1	2.52	0.43
46:S2:1293:A:H2'	46:S2:1294:G:C8	2.54	0.43
46:S2:1730:U:H2'	46:S2:1731:A:O4'	2.18	0.43
84:S2:4515:HOH:O	47:SE:39:ARG:HG2	2.19	0.43
55:SL:25:LEU:HD13	55:SL:25:LEU:HA	1.92	0.43
66:Sg:22:ALA:HB3	66:Sg:32:LEU:HD12	2.01	0.43
69:SJ:138[A]:ARG:HB3	69:SJ:139:LYS:H	1.64	0.43
75:SZ:57:LYS:HB2	75:SZ:57:LYS:HE3	1.81	0.43
1:L5:357:U:OP1	3:L8:26:C:H4'	2.19	0.43
1:L5:908:G:H2'	1:L5:909:A:H8	1.84	0.43
1:L5:1097:C:H2'	1:L5:1098:G:C8	2.53	0.43
1:L5:1402:C:OP1	30:Lb:55:LYS:NZ	2.45	0.43
1:L5:1639:U:OP2	38:Lj:3:LYS:HD2	2.19	0.43
1:L5:1900:C:H4'	33:Le:60:TYR:CE1	2.54	0.43
1:L5:2029:A:H2'	1:L5:2030:A:C8	2.54	0.43
1:L5:2052:G:O3'	17:LO:17:GLY:HA3	2.18	0.43
1:L5:2415:OMU:H2'	1:L5:2416:G:O4'	2.19	0.43
1:L5:2415:OMU:HM23	1:L5:2415:OMU:H1'	1.77	0.43
1:L5:3723:A:H5''	1:L5:3723:A:H8	1.84	0.43
1:L5:3792:OMG:HM23	1:L5:3792:OMG:H1'	1.80	0.43
1:L5:4169:G:H4'	1:L5:4171:C:C2	2.53	0.43
1:L5:4704:C:H2'	1:L5:4705:A:H8	1.84	0.43
3:L8:5:U:H2'	3:L8:6:C:H6	1.84	0.43
6:LC:79:VAL:HG11	6:LC:86:ARG:HG3	2.01	0.43
11:LH:4:ILE:HG13	21:LS:144:GLN:CD	2.44	0.43
13:LJ:55:TYR:HA	13:LJ:64:ARG:HB2	2.01	0.43
15:LM:36:ALA:HB2	15:LM:52:PHE:CE1	2.54	0.43
17:LO:26:GLN:O	17:LO:31:ARG:HB3	2.19	0.43
46:S2:311:C:H5''	46:S2:312:G:H5''	2.01	0.43
46:S2:461:U:H2'	46:S2:462:OMC:C6	2.53	0.43
46:S2:1414:A:H2'	46:S2:1415:C:C6	2.54	0.43
55:SL:16:ILE:HD13	55:SL:16:ILE:HA	1.92	0.43
66:Sg:87:LEU:HB2	66:Sg:101:PHE:HB2	2.01	0.43
70:SM:52:LEU:HG	70:SM:53:ALA:O	2.19	0.43
74:SY:105:LYS:HA	74:SY:105:LYS:HD3	1.61	0.43
1:L5:257:C:H2'	1:L5:258:G:H8	1.83	0.42
1:L5:493:G:C6	1:L5:660:A:N1	2.87	0.42
1:L5:705:G:H2'	1:L5:706:C:C6	2.54	0.42
1:L5:1941:A:C2	1:L5:4434:C:H5'	2.54	0.42
1:L5:2046:G:OP1	17:LO:59:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4507:A:N7	84:L5:5839:HOH:O	2.37	0.42
1:L5:4943:A:OP2	1:L5:4943:A:H8	2.02	0.42
4:LA:27:ALA:HB1	4:LA:77:ILE:HG13	2.01	0.42
4:LA:83:HIS:HB3	44:Lp:64:VAL:HG22	2.01	0.42
6:LC:320:LYS:HG3	6:LC:321:ASN:N	2.34	0.42
8:LE:91:THR:HA	8:LE:107:VAL:O	2.19	0.42
10:LG:79:ALA:HB3	16:LN:18:VAL:CG2	2.49	0.42
20:LR:152:LYS:HD2	20:LR:152:LYS:C	2.44	0.42
33:Le:21:ILE:HD11	33:Le:53:ILE:HG12	2.01	0.42
39:Lk:29:LYS:H	39:Lk:29:LYS:HD3	1.84	0.42
46:S2:35:C:H2'	46:S2:36:PSU:C6	2.54	0.42
46:S2:866:PSU:O2'	46:S2:867:OMG:P	2.77	0.42
46:S2:877:C:H2'	46:S2:878:G:C8	2.54	0.42
46:S2:1231:C:O2'	46:S2:1253:A:N6	2.51	0.42
46:S2:1474:A:H2'	46:S2:1475:G:O4'	2.19	0.42
46:S2:1531:A:H4'	46:S2:1605:G:H4'	2.01	0.42
46:S2:1606:G:N2	46:S2:1632:G:H1'	2.34	0.42
46:S2:1678:A2M:H1'	46:S2:1678:A2M:HM'3	1.56	0.42
50:SD:16:ILE:HD11	65:Sd:36:LEU:HD23	2.00	0.42
53:SI:120:PRO:HB3	53:SI:123:ARG:HG3	2.00	0.42
56:SP:110:GLU:CD	56:SP:110:GLU:H	2.27	0.42
68:SG:215:LYS:O	68:SG:219:GLU:HG3	2.18	0.42
73:SW:42:MET:HE2	73:SW:42:MET:HB3	1.80	0.42
77:Se:46:VAL:HG22	77:Se:48:THR:HG23	2.01	0.42
1:L5:138:G:C6	1:L5:139:G:C6	3.07	0.42
1:L5:1241:C:OP2	8:LE:72:LYS:HE2	2.19	0.42
1:L5:1399:G:H2'	1:L5:1400:G:H8	1.84	0.42
1:L5:2749:C:H2'	1:L5:2750:G:H8	1.84	0.42
1:L5:3718:A2M:H8	1:L5:3718:A2M:O5'	2.19	0.42
1:L5:3817:A:H4'	1:L5:3818:UY1:O5'	2.19	0.42
1:L5:3873:G:H2'	1:L5:3874:G:C8	2.53	0.42
1:L5:4093:G:H2'	1:L5:4094:G:H8	1.84	0.42
1:L5:4968:A:H2'	1:L5:4969:C:H6	1.84	0.42
2:L7:4:U:H2'	2:L7:5:A:H8	1.84	0.42
2:L7:7:G:OP1	7:LD:33:ARG:HD2	2.19	0.42
11:LH:114:ILE:HB	11:LH:124:ARG:HB2	2.02	0.42
12:LI:111:LEU:HD22	12:LI:111:LEU:HA	1.84	0.42
13:LJ:96:LYS:HD2	13:LJ:163:MET:CE	2.49	0.42
15:LM:75:GLN:O	15:LM:79:LYS:HE2	2.19	0.42
20:LR:172:ARG:NH2	46:S2:908:A:O3'	2.52	0.42
22:LT:44:GLY:HA2	22:LT:95:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LT:92:ARG:HB3	22:LT:94:GLU:OE1	2.19	0.42
22:LT:120:LYS:HD3	22:LT:120:LYS:HA	1.88	0.42
23:LU:93:LYS:O	84:LU:201:HOH:O	2.21	0.42
36:Lh:13:LYS:CE	36:Lh:15:GLU:HB2	2.49	0.42
46:S2:529:A:H2'	46:S2:530:U:C6	2.54	0.42
46:S2:793:G:N2	84:S2:2816:HOH:O	2.52	0.42
46:S2:1181:A:H2'	46:S2:1182:A:C8	2.55	0.42
46:S2:1480:A:O2'	65:Sd:56:ASP:OXT	2.35	0.42
46:S2:1705:C:H2'	46:S2:1706:G:C8	2.53	0.42
48:SA:137:ALA:HB1	48:SA:142:LEU:HB3	2.01	0.42
49:SB:177:GLN:HG3	49:SB:178:THR:HG23	2.01	0.42
64:Sc:51:ARG:HG2	64:Sc:54:ASP:OD2	2.19	0.42
66:Sg:59:LEU:HB3	66:Sg:90:TRP:CE3	2.54	0.42
74:SY:110:ARG:HE	74:SY:126:GLY:CA	2.32	0.42
1:L5:60:G:H2'	1:L5:61:A:C8	2.55	0.42
1:L5:75:G:C5	14:LL:102:ARG:HA	2.55	0.42
1:L5:465:G:H2'	1:L5:466:A:C8	2.54	0.42
1:L5:677:G:H2'	1:L5:678:C:H6	1.84	0.42
1:L5:1468:C:H2'	1:L5:1469:C:C6	2.54	0.42
1:L5:1468:C:H2'	1:L5:1469:C:H6	1.84	0.42
1:L5:2097:U:H5'	1:L5:2098:G:O4'	2.18	0.42
1:L5:2417:A:OP2	1:L5:2417:A:H8	2.02	0.42
1:L5:2422:OMC:HM23	1:L5:2422:OMC:H1'	1.89	0.42
1:L5:2440:U:O2'	1:L5:2519:U:H2'	2.19	0.42
1:L5:4619:U:H2'	1:L5:4620:OMU:C6	2.49	0.42
1:L5:4899:G:C2	1:L5:4901:G:C8	3.07	0.42
1:L5:4968:A:H2'	1:L5:4969:C:C6	2.54	0.42
6:LC:5:ARG:NE	6:LC:24:LEU:O	2.31	0.42
6:LC:292:ILE:HG23	19:LQ:128:LEU:HD21	2.00	0.42
7:LD:55:VAL:HG22	7:LD:60:ILE:HG12	1.99	0.42
7:LD:79:TYR:O	7:LD:82:GLU:HG2	2.19	0.42
8:LE:161:ARG:O	8:LE:182:ASN:ND2	2.49	0.42
17:LO:189:ILE:HA	17:LO:192:TYR:HD2	1.84	0.42
18:LP:36:ILE:CG2	18:LP:114:ILE:HD13	2.49	0.42
22:LT:3:ASN:HA	84:LT:234:HOH:O	2.19	0.42
23:LU:83:LEU:O	23:LU:87:THR:HG23	2.19	0.42
28:LZ:115:LYS:O	28:LZ:119:GLU:HG3	2.19	0.42
37:Li:88:GLU:OE1	37:Li:92:ASN:ND2	2.52	0.42
39:Lk:31:ASN:HB2	39:Lk:46:VAL:HG23	2.00	0.42
45:Lr:84:LYS:HE2	45:Lr:84:LYS:HB3	1.91	0.42
46:S2:658:U:C4	62:SX:24:ASP:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SQ:13:PHE:CE1	57:SQ:15:ARG:HD2	2.54	0.42
73:SW:101:PHE:HA	73:SW:113:HIS:CE1	2.54	0.42
1:L5:110:C:H5''	84:L5:5981:HOH:O	2.19	0.42
1:L5:246:G:OP2	27:LY:132:LYS:NZ	2.53	0.42
1:L5:318:A:H2'	1:L5:319:A:C8	2.55	0.42
1:L5:760:G:N1	1:L5:903:C:O2'	2.50	0.42
1:L5:1590:C:H5''	1:L5:1591:U:O5'	2.20	0.42
1:L5:2671:C:H2'	1:L5:2672:C:C6	2.54	0.42
1:L5:2803:U:H2'	1:L5:2804:OMC:H6	1.85	0.42
1:L5:3916:G:H2'	1:L5:3917:A:C8	2.54	0.42
1:L5:4138:C:C5	1:L5:4139:G:H1'	2.55	0.42
1:L5:4254:G:H2'	1:L5:4254:G:N3	2.34	0.42
1:L5:4894:A:H3'	1:L5:4895:C:H5'	2.02	0.42
3:L8:140:C:H2'	3:L8:141:C:C6	2.53	0.42
6:LC:181:LYS:HE2	6:LC:181:LYS:HB3	1.74	0.42
14:LL:107:THR:HG1	37:Li:18:THR:HG1	1.62	0.42
46:S2:29:G:H4'	62:SX:129:SER:HB2	2.02	0.42
46:S2:344:U:H2'	46:S2:345:U:C6	2.54	0.42
46:S2:396:U:OP2	55:SL:79:LYS:NZ	2.50	0.42
46:S2:496:C:OP1	47:SE:49:ARG:NH2	2.45	0.42
46:S2:907:G:H2'	46:S2:908:A:C8	2.54	0.42
46:S2:1027:A:H4'	84:S2:3588:HOH:O	2.19	0.42
46:S2:1115:U:H1'	46:S2:1117:C:OP2	2.19	0.42
46:S2:1382:A:N6	84:S2:2348:HOH:O	2.39	0.42
46:S2:1528:G:H2'	46:S2:1529:C:C6	2.55	0.42
48:SA:141:ASN:HD21	61:SV:29:HIS:HA	1.84	0.42
48:SA:191:ARG:HD2	61:SV:43:THR:O	2.19	0.42
52:SH:17:ASP:OD1	52:SH:21:SER:N	2.52	0.42
67:SC:271:ASP:OD1	67:SC:271:ASP:N	2.52	0.42
75:SZ:97:ILE:HD13	75:SZ:97:ILE:HA	1.81	0.42
76:Sb:19:HIS:CE1	76:Sb:21:LYS:HB2	2.54	0.42
77:Se:36:MET:CE	77:Se:40:ARG:HH12	2.29	0.42
1:L5:663:G:H2'	1:L5:664:G:O4'	2.20	0.42
1:L5:703:G:H2'	1:L5:704:C:H4'	2.01	0.42
1:L5:1907:A:H5''	9:LF:220:MET:HB2	2.02	0.42
1:L5:2582:A:N1	1:L5:2681:G:O2'	2.48	0.42
1:L5:3641:U:C2	1:L5:3645:U:C4	3.08	0.42
1:L5:3970:G:O2'	1:L5:4052:C:N4	2.48	0.42
1:L5:4769:G:H5''	17:LO:176:ARG:HD3	2.01	0.42
1:L5:4880:C:OP1	15:LM:124:LYS:NZ	2.44	0.42
6:LC:180:ILE:HD11	6:LC:227:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LI:47:PRO:HG2	12:LI:142:LEU:HG	2.01	0.42
14:LL:171:GLU:HA	14:LL:174:LYS:HG2	2.02	0.42
15:LM:125:ASN:O	15:LM:129:LYS:HB2	2.19	0.42
18:LP:115:GLU:HG2	18:LP:151:THR:CG2	2.48	0.42
19:LQ:175:GLU:HA	29:La:51:GLY:C	2.44	0.42
20:LR:178:GLN:O	20:LR:182:GLU:N	2.40	0.42
22:LT:46:GLY:O	22:LT:49:GLN:NE2	2.50	0.42
28:LZ:48:ARG:HB2	28:LZ:69:LYS:HB3	2.01	0.42
30:Lb:57:MET:HE3	30:Lb:57:MET:HB2	1.78	0.42
40:Ll:12:PHE:CE2	40:Ll:51:LEU:HD22	2.55	0.42
46:S2:899:U:H3'	46:S2:900:C:C5'	2.50	0.42
46:S2:1109:C:C4	79:SR:126:MET:HE3	2.55	0.42
46:S2:1202:U:O2	67:SC:115:GLN:HB3	2.20	0.42
47:SE:44:LEU:HD21	47:SE:70:ILE:HG21	2.01	0.42
1:L5:1656:U:O2'	1:L5:3906:A:N1	2.48	0.42
1:L5:2096:G:H3'	1:L5:2096:G:N3	2.34	0.42
1:L5:2675:G:H1'	1:L5:2676:A:OP2	2.19	0.42
1:L5:4390:A:H2'	1:L5:4391:G:O4'	2.20	0.42
3:L8:41:A:H2'	3:L8:42:G:O4'	2.20	0.42
5:LB:50:LYS:HB2	5:LB:345:LEU:HD11	2.02	0.42
6:LC:13:GLU:HG2	6:LC:155:GLU:OE2	2.19	0.42
15:LM:5:ARG:NH1	15:LM:59:ASP:OD1	2.41	0.42
21:LS:20:PRO:HA	21:LS:23:HIS:HE1	1.84	0.42
35:Lg:73:HIS:CD2	35:Lg:73:HIS:C	2.98	0.42
36:Lh:5:LYS:O	36:Lh:9:LEU:HG	2.19	0.42
41:Lm:99:CYS:SG	41:Lm:101:ALA:HB2	2.59	0.42
43:Lo:12:CYS:O	43:Lo:16:GLY:N	2.51	0.42
43:Lo:30:LYS:HA	43:Lo:30:LYS:HD2	1.92	0.42
44:Lp:21:SER:O	44:Lp:25:MET:HG3	2.20	0.42
46:S2:176:U:H2'	46:S2:177:G:C8	2.54	0.42
46:S2:1046:PSU:H2'	46:S2:1047:C:O4'	2.18	0.42
46:S2:1349:G:H2'	46:S2:1350:U:C6	2.55	0.42
84:S2:4696:HOH:O	62:SX:18:ARG:HD3	2.20	0.42
47:SE:63:LYS:O	47:SE:67:GLN:NE2	2.39	0.42
55:SL:48:LYS:O	55:SL:52:GLU:HG2	2.19	0.42
66:Sg:8:ARG:HG2	66:Sg:8:ARG:HH11	1.85	0.42
66:Sg:163:PRO:HB2	66:Sg:179:LEU:HD23	2.00	0.42
72:SO:133:THR:O	72:SO:135:ILE:HG12	2.20	0.42
78:Sf:120:GLU:OE1	78:Sf:128:ALA:HA	2.19	0.42
1:L5:162:A:H2'	1:L5:163:A:C8	2.55	0.42
1:L5:462:G:H2'	1:L5:463:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1459:A:OP1	19:LQ:65:ARG:NH1	2.52	0.42
1:L5:1855:G:OP1	30:Lb:4:SER:HB2	2.20	0.42
1:L5:2654:C:H2'	1:L5:2655:C:C6	2.55	0.42
1:L5:4344:U:H2'	1:L5:4345:C:H6	1.84	0.42
1:L5:4623:OMG:HM23	1:L5:4623:OMG:H1'	1.89	0.42
1:L5:4691:A:H5'	11:LH:71:ARG:NE	2.34	0.42
1:L5:4740:G:H3'	1:L5:4741:C:H5''	2.01	0.42
4:LA:79:ALA:O	4:LA:82:ILE:HG12	2.20	0.42
5:LB:288:GLY:HA3	5:LB:330:PHE:CZ	2.55	0.42
10:LG:121:LYS:HA	10:LG:121:LYS:HD3	1.63	0.42
10:LG:143:VAL:O	10:LG:147:VAL:HG23	2.20	0.42
15:LM:113:MET:HE1	15:LM:114:LYS:HE2	2.00	0.42
15:LM:126:GLU:HG3	17:LO:185:VAL:HG13	2.02	0.42
18:LP:41:ILE:HD11	18:LP:99:GLU:HG3	2.01	0.42
28:LZ:87:VAL:HG23	28:LZ:89:ILE:HG22	2.00	0.42
43:Lo:82:MET:HE2	43:Lo:82:MET:N	2.33	0.42
46:S2:323:C:N3	46:S2:328:U:C4	2.87	0.42
46:S2:532:C:O2	46:S2:552:G:N2	2.45	0.42
46:S2:688:U:C5	52:SH:102:PRO:HA	2.55	0.42
46:S2:929:G:H2'	46:S2:930:C:O4'	2.19	0.42
46:S2:1146:C:O2'	46:S2:1150:A:N1	2.46	0.42
46:S2:1265:A:H5'	46:S2:1266:C:OP2	2.19	0.42
46:S2:1737:G:H2'	46:S2:1738:C:C6	2.55	0.42
46:S2:1737:G:P	68:SG:94:ARG:HH22	2.42	0.42
71:SN:133:ARG:NH2	84:SN:207:HOH:O	2.52	0.42
1:L5:286:U:H2'	1:L5:287:U:C6	2.55	0.42
1:L5:375:G:OP1	6:LC:62:THR:HG23	2.19	0.42
1:L5:1190:C:H2'	1:L5:1191:C:O4'	2.19	0.42
1:L5:1704:C:N4	84:L5:6830:HOH:O	2.52	0.42
1:L5:1786:A:H2'	1:L5:1789:C:C5	2.55	0.42
1:L5:2026:A:H2'	1:L5:2027:U:C6	2.55	0.42
1:L5:2549:G:H2'	1:L5:2550:G:C8	2.55	0.42
1:L5:2705:G:O6	20:LR:46:LYS:NZ	2.47	0.42
1:L5:4153:C:H2'	1:L5:4154:G:C8	2.55	0.42
1:L5:4219:A:H2'	1:L5:4220:6MZ:C8	2.49	0.42
1:L5:4688:C:H2'	1:L5:4689:PSU:C6	2.55	0.42
1:L5:4936:G:O2'	1:L5:4937:C:H5'	2.20	0.42
33:Le:124:ASN:O	84:Le:301:HOH:O	2.22	0.42
37:Li:97:MET:HE3	37:Li:97:MET:HB2	1.85	0.42
46:S2:116:OMU:HM23	46:S2:116:OMU:H1'	1.78	0.42
46:S2:1208:A:N6	84:S2:2270:HOH:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sg:5:MET:HE2	66:Sg:5:MET:HB3	1.82	0.42
74:SY:111:LYS:HE3	74:SY:111:LYS:HB3	1.87	0.42
1:L5:163:A:H2'	1:L5:164:G:C8	2.53	0.42
1:L5:206:U:H1'	1:L5:209:U:C4	2.55	0.42
1:L5:1548:G:O2'	1:L5:2812:A:N3	2.50	0.42
1:L5:1650:A:O5'	6:LC:60:HIS:CE1	2.73	0.42
1:L5:1898:C:O2'	1:L5:2279:A:H5'	2.20	0.42
1:L5:2079:G:H2'	1:L5:2080:U:H6	1.85	0.42
1:L5:2399:G:O2'	1:L5:2822:G:O2'	2.32	0.42
1:L5:2570:U:H2'	1:L5:2571:C:C6	2.55	0.42
1:L5:2745:A:H2'	1:L5:2746:A:C8	2.55	0.42
1:L5:4253:A:H5'	1:L5:4254:G:C8	2.54	0.42
1:L5:4498:OMU:O5'	1:L5:4498:OMU:H6	2.19	0.42
1:L5:5004:C:H2'	1:L5:5005:G:O4'	2.19	0.42
2:L7:45:U:H5''	7:LD:157:ASN:HD22	1.85	0.42
3:L8:94:G:H1'	38:Lj:82:THR:O	2.20	0.42
7:LD:164:LYS:HD3	7:LD:195:HIS:HE1	1.83	0.42
12:LI:34:PHE:HD2	12:LI:89:VAL:HG23	1.84	0.42
12:LI:85:PHE:HE2	12:LI:87:MET:HE2	1.85	0.42
16:LN:46:ASP:O	16:LN:50:ARG:HG3	2.20	0.42
27:LY:3:PHE:O	84:LY:201:HOH:O	2.21	0.42
39:Lk:29:LYS:HG2	39:Lk:30:ASP:N	2.35	0.42
44:Lp:38:THR:HA	44:Lp:45:THR:HA	2.02	0.42
46:S2:440:G:O2'	46:S2:1737:G:H1'	2.20	0.42
46:S2:1425:G:H2'	46:S2:1426:U:C6	2.55	0.42
52:SH:36:LEU:O	52:SH:40:LEU:HB3	2.19	0.42
53:SI:201:LYS:HZ1	55:SL:8:ARG:HA	1.85	0.42
57:SQ:18:THR:CG2	57:SQ:75:GLY:H	2.33	0.42
58:SS:108:ARG:HG2	58:SS:108:ARG:HH11	1.83	0.42
66:Sg:10:THR:HG22	66:Sg:308:ARG:HG2	2.01	0.42
68:SG:153:VAL:HG21	68:SG:179:LEU:HD13	2.02	0.42
68:SG:209:TYR:O	68:SG:213:LEU:N	2.50	0.42
73:SW:69:LEU:HD21	73:SW:72:CYS:HB3	2.01	0.42
74:SY:88:LYS:HB3	74:SY:97:TYR:CE2	2.55	0.42
1:L5:233:U:HO2'	1:L5:234:G:H8	1.67	0.42
1:L5:456:C:C2	1:L5:457:G:N7	2.88	0.42
1:L5:4348:A:C6	1:L5:4350:C:C4	3.08	0.42
3:L8:54:C:H2'	3:L8:55:PSU:O4'	2.20	0.42
7:LD:289:ARG:O	7:LD:293:ARG:HG2	2.20	0.42
18:LP:26:PHE:CE2	18:LP:121:LYS:HE2	2.55	0.42
21:LS:163:HIS:O	21:LS:164:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LW:78:PHE:HD1	25:LW:78:PHE:O	2.02	0.42
26:LX:73:HIS:NE2	26:LX:115:LYS:HD3	2.35	0.42
32:Ld:41:ARG:HB2	32:Ld:77:ILE:O	2.20	0.42
36:Lh:19:LYS:NZ	36:Lh:23:ASP:CG	2.77	0.42
46:S2:85:A:H2'	46:S2:86:C:H6	1.85	0.42
46:S2:1052:A:H2'	46:S2:1053:C:O4'	2.20	0.42
46:S2:1144:A:H5'	46:S2:1355:C:H5	1.84	0.42
46:S2:1597:C:H4'	46:S2:1603:G:O6	2.19	0.42
47:SE:92:ILE:CG2	74:SY:17:LEU:HD21	2.50	0.42
48:SA:1:MET:HE3	48:SA:2:SER:H	1.81	0.42
54:SK:53:LYS:HE2	54:SK:60:GLU:CD	2.45	0.42
70:SM:52:LEU:HD12	70:SM:107:SER:O	2.20	0.42
1:L5:420:A:C8	1:L5:421:C:C5	3.08	0.41
1:L5:423:G:H5'	18:LP:26:PHE:HZ	1.85	0.41
1:L5:473:C:H2'	1:L5:474:C:H6	1.84	0.41
1:L5:984:C:H2'	1:L5:985:C:O4'	2.20	0.41
1:L5:1183:C:H2'	1:L5:1184:A:C8	2.55	0.41
1:L5:1473:U:H2'	1:L5:1474:C:C6	2.55	0.41
1:L5:2725:A:H3'	1:L5:2726:G:C5'	2.50	0.41
3:L8:103:A:C8	3:L8:104:A:C8	3.08	0.41
5:LB:103:LYS:HD3	5:LB:103:LYS:HA	1.88	0.41
7:LD:256:LYS:HD2	7:LD:257:PRO:HD2	2.00	0.41
11:LH:18:ILE:HD11	11:LH:81:ILE:HD11	2.02	0.41
11:LH:105:ILE:HG22	11:LH:109:GLY:HA2	2.01	0.41
46:S2:96:C:O2	46:S2:473:A:O2'	2.38	0.41
46:S2:189:U:H2'	46:S2:190:G:O4'	2.20	0.41
46:S2:415:A:H2'	46:S2:416:U:O4'	2.19	0.41
46:S2:539:C:N4	84:S2:2788:HOH:O	2.52	0.41
48:SA:66:VAL:HG12	48:SA:182:VAL:HG13	2.02	0.41
49:SB:167:LYS:O	49:SB:171:ILE:HG12	2.20	0.41
49:SB:224:GLU:HB3	49:SB:227:LYS:HB2	2.02	0.41
51:SF:82:ASN:HA	51:SF:85:LYS:HD2	2.02	0.41
62:SX:140:ARG:HE	62:SX:142:ARG:NH2	2.18	0.41
68:SG:49:VAL:HB	68:SG:115:LYS:HB3	2.02	0.41
71:SN:132:LYS:HB3	71:SN:132:LYS:HE2	1.89	0.41
74:SY:110:ARG:HH21	74:SY:126:GLY:HA3	1.85	0.41
1:L5:23:C:H2'	1:L5:24:G:O4'	2.20	0.41
1:L5:400:A2M:HM'3	1:L5:400:A2M:H1'	1.81	0.41
1:L5:960:A:H3'	1:L5:961:G:H5''	2.02	0.41
1:L5:1082:C:O2'	1:L5:1083:U:O4'	2.39	0.41
1:L5:1198:G:H2'	1:L5:1199:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1416:G:H2'	1:L5:1417:C:C6	2.55	0.41
1:L5:1739:G:N3	1:L5:1742:A:N6	2.68	0.41
1:L5:1764:G:O2'	1:L5:1766:A:O5'	2.32	0.41
1:L5:3774:A:H2'	1:L5:3775:A:C8	2.56	0.41
1:L5:3939:G:O2'	1:L5:4076:G:N1	2.50	0.41
1:L5:4571:A2M:HM'3	1:L5:4571:A2M:H1'	1.81	0.41
8:LE:66:LYS:HE2	8:LE:68:MET:SD	2.60	0.41
16:LN:68:ARG:HG2	16:LN:128:LYS:HG3	2.02	0.41
21:LS:31:ARG:HH22	21:LS:102:THR:HG21	1.85	0.41
23:LU:27:HIS:HB2	23:LU:28:PRO:HD3	2.02	0.41
45:Lr:86:ALA:O	45:Lr:90:LEU:HG	2.21	0.41
46:S2:659:G:H2'	46:S2:663:C:C5	2.55	0.41
46:S2:1409:A:H2'	46:S2:1410:C:C6	2.54	0.41
53:SI:8:TRP:HA	53:SI:18:ARG:HD2	2.03	0.41
58:SS:47:LYS:HA	58:SS:47:LYS:HD3	1.91	0.41
60:SU:116:ILE:C	60:SU:118:ASP:H	2.28	0.41
66:Sg:83:TRP:HA	66:Sg:107:ASP:HB3	2.01	0.41
66:Sg:130:LYS:HG2	66:Sg:141:THR:HB	2.01	0.41
68:SG:218:LYS:O	68:SG:222:GLU:N	2.43	0.41
71:SN:25:TRP:CD2	76:Sb:82:LYS:HE2	2.55	0.41
72:SO:30:VAL:HG11	72:SO:96:LYS:HD2	2.02	0.41
73:SW:19:LYS:HG3	84:SW:236:HOH:O	2.20	0.41
1:L5:1683:PSU:H2'	1:L5:1684:A:C8	2.54	0.41
1:L5:1707:C:N4	30:Lb:102:PRO:HG2	2.35	0.41
1:L5:3765:G:O3'	1:L5:3766:A:H8	2.02	0.41
1:L5:3918:G:OP1	82:L5:5377:SPD:H82	2.19	0.41
1:L5:4178:A:H2'	1:L5:4179:G:C8	2.55	0.41
1:L5:4345:C:H2'	1:L5:4346:U:H6	1.86	0.41
1:L5:4637:OMG:HM23	1:L5:4637:OMG:H1'	1.70	0.41
6:LC:218:ILE:O	6:LC:222:ARG:HB2	2.20	0.41
7:LD:93:THR:O	7:LD:97:ALA:HB3	2.20	0.41
29:La:135:GLU:H	29:La:135:GLU:HG2	1.66	0.41
30:Lb:109:ARG:HA	30:Lb:112:ILE:HB	2.03	0.41
32:Ld:50:ARG:HG2	32:Ld:54:MET:HE2	2.01	0.41
36:Lh:4:ILE:O	36:Lh:56:ARG:NH1	2.53	0.41
36:Lh:19:LYS:HA	36:Lh:19:LYS:HD2	1.72	0.41
46:S2:51:U:H2'	46:S2:52:G:H8	1.85	0.41
46:S2:71:G:H8	46:S2:71:G:OP2	2.03	0.41
46:S2:190:G:H5''	53:SI:145:ILE:HD13	2.01	0.41
46:S2:1081:U:H5''	46:S2:1084:A:N6	2.35	0.41
46:S2:1177:PSU:H2'	46:S2:1178:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:1258:A:N1	46:S2:1663:A:H2'	2.35	0.41
46:S2:1867:U:O2'	63:Sa:38:LYS:HG2	2.20	0.41
49:SB:142:PHE:CD1	49:SB:209:ASP:HB2	2.55	0.41
51:SF:30:ILE:HD13	51:SF:39:ILE:HB	2.01	0.41
51:SF:125:SER:HA	51:SF:137:GLN:O	2.21	0.41
58:SS:94:LYS:HE2	58:SS:94:LYS:HB3	1.84	0.41
69:SJ:108:ARG:O	69:SJ:149:VAL:HG22	2.20	0.41
1:L5:406:C:HO2'	1:L5:407:A:P	2.43	0.41
1:L5:965:G:O2'	1:L5:966:A:N3	2.52	0.41
1:L5:1481:C:N4	37:Li:4:ARG:HG3	2.33	0.41
1:L5:1509:C:O3'	29:La:2:PRO:HD2	2.20	0.41
1:L5:3662:A:P	4:LA:156:LYS:HZ1	2.42	0.41
1:L5:4287:G:H2'	1:L5:4288:C:C6	2.54	0.41
1:L5:4572:U:H1'	1:L5:4720:C:C4	2.55	0.41
1:L5:4605:A:H2'	1:L5:4606:G:O4'	2.20	0.41
11:LH:121:LYS:HA	11:LH:121:LYS:HD3	1.65	0.41
12:LI:181:PHE:O	12:LI:185:VAL:HG23	2.21	0.41
19:LQ:66:MET:HE1	19:LQ:86:ILE:HD13	2.01	0.41
23:LU:63:ILE:HG12	23:LU:72:VAL:HG13	2.03	0.41
24:LV:21:PRO:HA	24:LV:54:ALA:HA	2.01	0.41
26:LX:78:LYS:HE3	26:LX:101:ASP:HA	2.03	0.41
46:S2:429:C:P	69:SJ:2:PRO:HD2	2.61	0.41
46:S2:848:U:H2'	46:S2:849:A:H8	1.85	0.41
46:S2:943:U:C2	46:S2:944:A:C8	3.08	0.41
46:S2:993:G:OP1	46:S2:1131:G:N2	2.40	0.41
46:S2:1754:G:O6	46:S2:1779:G:N1	2.53	0.41
53:SI:139:LYS:HB3	53:SI:141:ARG:NH1	2.36	0.41
66:Sg:8:ARG:N	66:Sg:309:VAL:O	2.53	0.41
69:SJ:47:LYS:HG3	69:SJ:102:ILE:CD1	2.50	0.41
72:SO:64:ALA:C	72:SO:66:ARG:H	2.28	0.41
75:SZ:91:LEU:HB3	75:SZ:97:ILE:HG12	2.02	0.41
1:L5:461:G:H2'	1:L5:462:G:C8	2.55	0.41
1:L5:683:C:H2'	1:L5:684:G:O4'	2.20	0.41
1:L5:749:G:O2'	1:L5:912:G:N1	2.49	0.41
1:L5:1566:C:H2'	1:L5:1567:U:H6	1.85	0.41
1:L5:2671:C:OP1	44:Lp:46:LYS:NZ	2.42	0.41
1:L5:3607:U:H2'	1:L5:3608:A:C8	2.56	0.41
1:L5:4393:G:O4'	1:L5:4447:5MC:HM52	2.20	0.41
1:L5:4617:G:OP2	5:LB:358:ARG:NH2	2.46	0.41
1:L5:4898:G:H2'	1:L5:4899:G:C8	2.56	0.41
4:LA:60:LYS:HB3	4:LA:60:LYS:NZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LD:223:PHE:HB3	7:LD:226:TYR:HB2	2.01	0.41
7:LD:265:ARG:HE	7:LD:265:ARG:HB3	1.74	0.41
10:LG:171:PRO:HB3	10:LG:181:TYR:CZ	2.55	0.41
12:LI:21:ARG:O	12:LI:24:ARG:NH1	2.40	0.41
17:LO:113:ASP:OD1	17:LO:113:ASP:N	2.51	0.41
19:LQ:122:THR:OG1	19:LQ:124:ASP:OD1	2.33	0.41
24:LV:62:MET:HE3	24:LV:76:VAL:HG12	2.02	0.41
46:S2:121:OMU:HM23	46:S2:121:OMU:H1'	1.72	0.41
46:S2:301:A:H2'	46:S2:302:A:O4'	2.20	0.41
46:S2:452:G:H2'	46:S2:453:C:H6	1.85	0.41
46:S2:845:G:H2'	46:S2:846:G:C8	2.55	0.41
46:S2:1077:A:H4'	84:S2:6356:HOH:O	2.20	0.41
46:S2:1616:U:H2'	46:S2:1617:G:O4'	2.21	0.41
49:SB:83:LYS:HE3	49:SB:83:LYS:HB2	1.79	0.41
55:SL:55:TYR:OH	55:SL:116:CYS:HB3	2.21	0.41
55:SL:88:ILE:HD11	55:SL:109:MET:HE2	2.01	0.41
56:SP:18:ARG:NH1	58:SS:88:LYS:O	2.52	0.41
1:L5:919:C:H2'	1:L5:920:C:H6	1.85	0.41
1:L5:2345:G:N7	29:La:9:ARG:NH2	2.69	0.41
1:L5:2525:U:OP2	20:LR:42:ARG:NH2	2.43	0.41
1:L5:3646:A:H4'	1:L5:3647:A:O5'	2.21	0.41
1:L5:4233:A:C5	1:L5:4235:G:C8	3.09	0.41
1:L5:4296:PSU:H2'	1:L5:4297:G:O4'	2.20	0.41
1:L5:4770:U:H2'	1:L5:4771:C:C6	2.55	0.41
1:L5:4881:U:H5'	1:L5:4882:U:OP1	2.19	0.41
1:L5:4926:C:H2'	1:L5:4927:G:O4'	2.21	0.41
5:LB:46:PHE:CZ	5:LB:84:MET:HG3	2.55	0.41
6:LC:168:VAL:HG12	6:LC:172:LYS:HE2	2.02	0.41
8:LE:161:ARG:NH2	15:LM:106:ASP:OD2	2.53	0.41
10:LG:160:ASP:OD1	10:LG:160:ASP:N	2.53	0.41
13:LJ:90:ARG:H	13:LJ:90:ARG:HG2	1.41	0.41
18:LP:9:GLU:OE1	18:LP:9:GLU:N	2.53	0.41
20:LR:176:ARG:CZ	20:LR:176:ARG:HB3	2.50	0.41
38:Lj:28:HIS:CD2	38:Lj:31:LYS:HD3	2.56	0.41
43:Lo:78:ARG:HA	43:Lo:78:ARG:HE	1.85	0.41
46:S2:953:C:H2'	46:S2:954:U:O4'	2.20	0.41
46:S2:1238:PSU:O4	46:S2:1242:U:C5	2.69	0.41
46:S2:1346:U:O2	46:S2:1383:A2M:H2	2.20	0.41
46:S2:1408:U:H2'	46:S2:1409:A:C8	2.56	0.41
46:S2:1559:C:H2'	46:S2:1560:U:O4'	2.20	0.41
47:SE:55:ALA:HB1	47:SE:60:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SE:188:ASN:HB3	47:SE:191:ARG:HD3	2.03	0.41
48:SA:149:ASN:HB2	48:SA:165:ASN:OD1	2.21	0.41
50:SD:1:MET:HE3	50:SD:1:MET:HB3	1.85	0.41
58:SS:22:GLY:HA2	58:SS:56:ALA:HB3	2.02	0.41
74:SY:102:THR:OG1	74:SY:103:SER:N	2.54	0.41
1:L5:99:A:H4'	16:LN:181:HIS:CD2	2.55	0.41
1:L5:2034:G:H2'	1:L5:2035:C:C6	2.55	0.41
1:L5:2557:G:O6	1:L5:2570:U:O4	2.37	0.41
1:L5:3615:G:H1'	25:LW:44:ARG:HD2	2.02	0.41
1:L5:3616:U:H3'	25:LW:44:ARG:HH12	1.85	0.41
1:L5:4346:U:H4'	43:Lo:82:MET:HE3	2.02	0.41
1:L5:4415:A:C2	1:L5:4416:G:H1'	2.56	0.41
1:L5:4919:G:H2'	1:L5:4920:C:O4'	2.20	0.41
5:LB:143:LYS:HA	5:LB:146:LEU:HD12	2.03	0.41
13:LJ:61:GLY:O	13:LJ:62:ILE:HG12	2.21	0.41
13:LJ:82:ILE:HG22	13:LJ:130:PHE:HE2	1.84	0.41
25:LW:96:GLN:O	25:LW:100:VAL:HB	2.20	0.41
29:La:76:ASP:OD1	29:La:77:LYS:N	2.54	0.41
44:Lp:13:LYS:O	84:Lp:201:HOH:O	2.22	0.41
46:S2:523:A:OP2	69:SJ:38:ARG:HD3	2.20	0.41
46:S2:1295:A:N1	46:S2:1304:U:H5	2.18	0.41
46:S2:1733:U:H2'	46:S2:1734:G:O4'	2.21	0.41
47:SE:86:PHE:O	47:SE:87:MET:HB2	2.20	0.41
48:SA:69:GLU:N	48:SA:69:GLU:OE1	2.52	0.41
51:SF:69:VAL:O	51:SF:73:THR:HG23	2.20	0.41
66:Sg:180:ALA:C	66:Sg:182:CYS:H	2.29	0.41
67:SC:252:THR:OG1	67:SC:254:ASP:OD1	2.28	0.41
79:SR:79:GLU:HG3	79:SR:83:ASN:ND2	2.36	0.41
1:L5:484:U:H4'	1:L5:485:C:H5'	2.02	0.41
1:L5:686:A:O5'	8:LE:98:GLY:HA3	2.21	0.41
1:L5:742:G:H2'	1:L5:743:G:C8	2.56	0.41
1:L5:2485:U:O2'	1:L5:2486:G:H5''	2.20	0.41
1:L5:2627:C:C2	1:L5:2628:U:C5	3.08	0.41
1:L5:2708:U:H4'	1:L5:2709:C:H5''	2.01	0.41
1:L5:3865:A:H2'	1:L5:3866:C:C6	2.56	0.41
5:LB:291:TYR:CG	5:LB:299:ILE:HG22	2.55	0.41
12:LI:77:VAL:HG22	12:LI:82:ARG:HA	2.03	0.41
20:LR:159:ALA:HA	20:LR:162:ARG:HH21	1.86	0.41
26:LX:67:ARG:NH1	84:LX:204:HOH:O	2.52	0.41
27:LY:76:LYS:HB2	27:LY:76:LYS:HE3	1.87	0.41
35:Lg:69:LYS:HD3	35:Lg:73:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Lo:11:PHE:O	43:Lo:81:ARG:NH1	2.54	0.41
46:S2:1233:G:C6	46:S2:1526:G:C6	3.09	0.41
46:S2:1240:A:H2'	46:S2:1241:A:C8	2.55	0.41
46:S2:1639:M7G:O6	84:S2:2110:HOH:O	2.22	0.41
46:S2:1713:C:H2'	46:S2:1714:U:C6	2.56	0.41
48:SA:81:ASN:HB2	48:SA:204:TYR:CE1	2.56	0.41
49:SB:62:LEU:O	49:SB:65:ARG:HG2	2.19	0.41
50:SD:35:SER:HB2	50:SD:97:CYS:SG	2.61	0.41
67:SC:176:LYS:O	67:SC:200[B]:ARG:NH2	2.54	0.41
68:SG:32:MET:HG3	68:SG:100:CYS:HB2	2.02	0.41
69:SJ:91:LYS:HA	69:SJ:91:LYS:HD3	1.93	0.41
79:SR:61:ILE:HA	79:SR:64:GLY:O	2.20	0.41
1:L5:398:A2M:HM'3	1:L5:398:A2M:H1'	1.88	0.41
1:L5:989:U:O2'	1:L5:990:C:O4'	2.39	0.41
1:L5:1415:G:H2'	1:L5:1416:G:H8	1.86	0.41
1:L5:1591:U:H5''	1:L5:4527:G:OP1	2.20	0.41
1:L5:1645:C:H2'	1:L5:1646:A:C8	2.56	0.41
1:L5:1697:G:H21	1:L5:2084:C:P	2.43	0.41
1:L5:1942:A:H2'	1:L5:1943:A:H8	1.86	0.41
1:L5:2526:C:H42	26:LX:84:GLU:CD	2.28	0.41
1:L5:2634:C:H2'	1:L5:2635:U:C6	2.55	0.41
1:L5:2662:G:H2'	1:L5:2663:G:O4'	2.21	0.41
1:L5:2722:G:H2'	1:L5:2723:U:C6	2.56	0.41
1:L5:3942:A:H2'	1:L5:3943:A:C8	2.56	0.41
1:L5:3944:G:O3'	49:SB:54:GLY:HA2	2.20	0.41
1:L5:4116:C:H5''	1:L5:4117:U:C5	2.56	0.41
84:L5:7545:HOH:O	6:LC:62:THR:HG23	2.21	0.41
3:L8:83:C:H41	27:LY:50:ARG:NH2	2.08	0.41
6:LC:266:THR:C	6:LC:268:ARG:H	2.29	0.41
8:LE:133:PHE:HA	8:LE:136:HIS:CE1	2.56	0.41
8:LE:190:HIS:HB3	8:LE:193:PHE:HD2	1.85	0.41
9:LF:155:TYR:OH	9:LF:188:GLU:OE2	2.35	0.41
13:LJ:24:ILE:HG12	13:LJ:128:LEU:HB3	2.02	0.41
14:LL:7:GLY:O	29:La:49:HIS:NE2	2.50	0.41
14:LL:111:GLN:OE1	14:LL:111:GLN:HA	2.21	0.41
23:LU:24:ASP:HB3	23:LU:111:GLU:HA	2.01	0.41
25:LW:77:LYS:HD3	25:LW:77:LYS:HA	1.90	0.41
26:LX:38:LYS:HD3	26:LX:38:LYS:HA	1.73	0.41
29:La:79:TRP:CD2	29:La:87:ARG:HD3	2.56	0.41
36:Lh:77:LYS:HE3	36:Lh:78:TYR:CZ	2.54	0.41
42:Ln:7:LYS:NZ	46:S2:1843:G:OP1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:568:C:H2'	46:S2:569:A:C8	2.55	0.41
46:S2:798:G:OP2	46:S2:799:U:H5'	2.21	0.41
46:S2:1101:U:OP1	79:SR:132:ARG:NH1	2.53	0.41
46:S2:1398:G:C2	46:S2:1399:C:C6	3.08	0.41
46:S2:1491:G:H2'	46:S2:1492:U:C6	2.56	0.41
46:S2:1617:G:N1	46:S2:1620:A:OP2	2.53	0.41
46:S2:1803:U:H2'	46:S2:1804:OMU:O4'	2.21	0.41
49:SB:126:ASP:CG	49:SB:136:ARG:HE	2.28	0.41
52:SH:57:ARG:HD2	52:SH:91:HIS:CD2	2.56	0.41
67:SC:194:ARG:NH2	84:SC:319:HOH:O	2.52	0.41
67:SC:256:TRP:CD2	73:SW:68:ARG:HD3	2.56	0.41
69:SJ:107:GLU:HA	69:SJ:112:THR:HG21	2.03	0.41
71:SN:114:ARG:HA	71:SN:114:ARG:HD3	1.93	0.41
74:SY:27:VAL:HB	74:SY:69:THR:HG23	2.02	0.41
78:Sf:118:ARG:HB3	78:Sf:131:PHE:CD1	2.56	0.41
78:Sf:139:HIS:O	78:Sf:147:THR:HA	2.21	0.41
1:L5:261:G:H2'	1:L5:262:G:O4'	2.21	0.41
1:L5:470:A:N6	1:L5:684:G:H1'	2.36	0.41
1:L5:922:C:H2'	1:L5:923:C:O4'	2.21	0.41
1:L5:1354:A:N1	1:L5:1385:G:O2'	2.52	0.41
1:L5:1784:U:P	12:LI:90:ARG:HH21	2.44	0.41
1:L5:2338:C:H4'	45:Lr:12:ASN:O	2.20	0.41
1:L5:2352:U:H2'	1:L5:2353:U:C6	2.56	0.41
1:L5:2682:G:H2'	1:L5:2683:C:H6	1.85	0.41
1:L5:2691:U:C2	1:L5:2692:U:C5	3.09	0.41
1:L5:3749:C:H4'	4:LA:221:LYS:O	2.21	0.41
1:L5:4208:U:OP2	22:LT:4:THR:OG1	2.23	0.41
1:L5:4383:U:H2'	1:L5:4384:U:C6	2.56	0.41
1:L5:4462:C:O2'	1:L5:4463:U:H5'	2.21	0.41
1:L5:4710:C:H2'	1:L5:4711:C:C6	2.56	0.41
1:L5:4942:C:H4'	8:LE:154:THR:HB	2.03	0.41
3:L8:78:G:O2'	36:Lh:42:SER:HA	2.21	0.41
5:LB:349:LYS:H	5:LB:349:LYS:HG2	1.64	0.41
7:LD:183:TYR:HB2	7:LD:190:PHE:HD1	1.86	0.41
8:LE:96:VAL:HG21	8:LE:105:ARG:HG2	2.03	0.41
46:S2:31:U:O2'	46:S2:643:A:N1	2.54	0.41
46:S2:452:G:H2'	46:S2:453:C:C6	2.56	0.41
46:S2:468:A2M:HM'3	46:S2:468:A2M:H1'	1.78	0.41
46:S2:476:A:N3	46:S2:488:U:O2'	2.49	0.41
46:S2:1445:PSU:H1'	46:S2:1580:A:N6	2.36	0.41
46:S2:1555:U:H5'	46:S2:1556:A:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:S2:1851:MA6:H5''	46:S2:1852:C:OP2	2.21	0.41
50:SD:159:HIS:C	50:SD:164:VAL:HG11	2.46	0.41
57:SQ:100:VAL:HG12	57:SQ:101:ASP:OD1	2.21	0.41
58:SS:85:ASN:N	58:SS:97:GLN:OE1	2.49	0.41
65:Sd:30:LEU:HA	65:Sd:39:CYS:HA	2.02	0.41
66:Sg:150:TRP:HE1	79:SR:37:GLU:CD	2.29	0.41
69:SJ:152:ASP:N	69:SJ:152:ASP:OD1	2.54	0.41
71:SN:102:LEU:HD11	71:SN:112:LYS:HA	2.02	0.41
1:L5:134:G:C2	36:Lh:79:LYS:HE3	2.56	0.40
1:L5:272:U:H2'	1:L5:273:U:H6	1.86	0.40
1:L5:451:C:N4	84:L5:6904:HOH:O	2.53	0.40
1:L5:461:G:H2'	1:L5:462:G:H8	1.86	0.40
1:L5:1971:C:N3	1:L5:2000:G:H2'	2.36	0.40
1:L5:2771:G:H2'	1:L5:2772:C:O4'	2.21	0.40
1:L5:3673:C:O2'	1:L5:4080:C:OP1	2.36	0.40
1:L5:4176:C:H5''	84:L5:8799:HOH:O	2.21	0.40
1:L5:4414:A:C2	1:L5:4427:G:N3	2.90	0.40
9:LF:136:VAL:O	9:LF:140:ILE:HG12	2.21	0.40
12:LI:42:LYS:HD2	12:LI:42:LYS:N	2.36	0.40
14:LL:124:LEU:HD11	36:Lh:119:TYR:HB2	2.02	0.40
18:LP:22:LEU:HB3	18:LP:90:PHE:CE2	2.56	0.40
21:LS:43:ARG:HD2	21:LS:43:ARG:HA	1.88	0.40
35:Lg:14:ASN:OD1	35:Lg:19:LYS:NZ	2.50	0.40
46:S2:53:C:O2'	46:S2:507:G:N7	2.46	0.40
46:S2:319:C:C2	46:S2:320:G:C8	3.10	0.40
46:S2:681:PSU:H4'	62:SX:9:THR:HG22	2.03	0.40
46:S2:920:A:O2'	46:S2:922:A:OP1	2.31	0.40
46:S2:980:A:H2'	46:S2:981:A:C8	2.56	0.40
46:S2:1589:A:H2'	46:S2:1590:C:H6	1.84	0.40
47:SE:51:ARG:HA	47:SE:51:ARG:HD3	1.92	0.40
50:SD:132:LYS:HD3	50:SD:191:PRO:HA	2.03	0.40
63:Sa:46:GLU:N	72:SO:113:GLN:HE22	2.19	0.40
69:SJ:131:ARG:NH1	69:SJ:143:ASN:O	2.53	0.40
79:SR:104:GLU:OE2	79:SR:104:GLU:HA	2.19	0.40
1:L5:100:C:H2'	1:L5:101:A:O4'	2.21	0.40
1:L5:136:C:N4	36:Lh:76:LYS:O	2.55	0.40
1:L5:1593:A:H5''	1:L5:2839:PSU:H5'	2.04	0.40
1:L5:1727:U:H2'	1:L5:1728:U:C6	2.57	0.40
1:L5:1852:U:H5''	29:La:22:ILE:HD12	2.02	0.40
1:L5:2519:U:C2	1:L5:2520:C:C5	3.09	0.40
1:L5:2689:C:H2'	1:L5:2690:C:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2726:G:H2'	1:L5:2727:C:C6	2.56	0.40
1:L5:3606:U:H2'	1:L5:3607:U:C6	2.56	0.40
1:L5:3635:A:H5'	84:L5:5467:HOH:O	2.21	0.40
1:L5:3779:A:H2'	1:L5:3780:G:O4'	2.21	0.40
1:L5:4568:A:O2'	1:L5:4981:G:N7	2.52	0.40
13:LJ:12:MET:O	13:LJ:137:PRO:HD2	2.21	0.40
15:LM:125:ASN:HA	15:LM:128:LYS:HG2	2.02	0.40
17:LO:55:LEU:HD23	17:LO:58:LEU:HD12	2.03	0.40
18:LP:104:LEU:HD12	18:LP:104:LEU:HA	1.89	0.40
20:LR:99:MET:HA	20:LR:99:MET:HE2	2.02	0.40
28:LZ:5:MET:HG2	28:LZ:77:TYR:CZ	2.56	0.40
29:La:93:ASN:HD21	29:La:97:ALA:HB3	1.85	0.40
44:Lp:85:ARG:HB3	44:Lp:85:ARG:NH1	2.36	0.40
46:S2:29:G:H2'	46:S2:30:C:H6	1.85	0.40
46:S2:35:C:O5'	46:S2:35:C:H6	2.03	0.40
46:S2:317:C:H2'	46:S2:318:A:H5''	2.03	0.40
46:S2:501:C:O2	46:S2:501:C:H2'	2.21	0.40
46:S2:569:A:H2'	46:S2:570:C:O4'	2.22	0.40
46:S2:639:C:H2'	46:S2:640:A:C8	2.56	0.40
46:S2:968:U:H5''	46:S2:968:U:C6	2.53	0.40
46:S2:1830:U:O4'	46:S2:1851:MA6:H2	2.20	0.40
49:SB:25:PHE:CD2	72:SO:88:LEU:HD13	2.56	0.40
56:SP:35:GLN:HA	56:SP:35:GLN:OE1	2.21	0.40
59:ST:4:VAL:HG13	59:ST:8:ASP:OD1	2.21	0.40
65:Sd:22:ARG:HG2	65:Sd:38:MET:HG2	2.03	0.40
66:Sg:164:ILE:HD11	66:Sg:221:LEU:HD13	2.03	0.40
67:SC:65:LYS:HE3	67:SC:273:LEU:HD13	2.03	0.40
69:SJ:129:LEU:HD23	69:SJ:129:LEU:HA	1.93	0.40
1:L5:282:C:H2'	1:L5:283:G:O4'	2.21	0.40
1:L5:919:C:H2'	1:L5:920:C:C6	2.57	0.40
1:L5:1534:A2M:HM'3	1:L5:1637:A:C4	2.56	0.40
1:L5:2084:C:C4	19:LQ:14:ARG:HD2	2.55	0.40
1:L5:2485:U:C2'	1:L5:2486:G:H5''	2.51	0.40
1:L5:2899:C:OP1	20:LR:108:ARG:NH2	2.53	0.40
1:L5:3748:A:H2'	1:L5:3749:C:C6	2.57	0.40
1:L5:3893:C:O2'	1:L5:4979:A:N1	2.50	0.40
1:L5:4069:U:H2'	1:L5:4070:U:H6	1.86	0.40
1:L5:4149:C:OP1	28:LZ:59:LYS:N	2.55	0.40
1:L5:4420:U:O2'	1:L5:4421:C:OP1	2.29	0.40
2:L7:1:G:H4'	7:LD:265:ARG:HG2	2.03	0.40
14:LL:90:VAL:O	14:LL:93:THR:OG1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LP:49:LYS:O	18:LP:53:LEU:HG	2.22	0.40
20:LR:154:LEU:HG	20:LR:158:GLN:HE22	1.85	0.40
27:LY:57:VAL:HB	27:LY:63:LYS:HA	2.03	0.40
28:LZ:47:ASP:N	28:LZ:69:LYS:O	2.52	0.40
33:Le:21:ILE:H	33:Le:21:ILE:HG13	1.71	0.40
38:Lj:39:TYR:CG	38:Lj:40:PRO:HA	2.57	0.40
46:S2:1431:G:H2'	46:S2:1432:U:C6	2.56	0.40
84:SF:334:HOH:O	64:Sc:63:ARG:HG2	2.21	0.40
55:SL:49:GLU:H	55:SL:49:GLU:CD	2.29	0.40
59:ST:113:VAL:HG12	59:ST:123:LEU:HD23	2.03	0.40
64:Sc:36:ASP:C	64:Sc:38:THR:H	2.29	0.40
1:L5:911:U:H3'	1:L5:912:G:C8	2.57	0.40
1:L5:1558:A:H2'	1:L5:1559:G:H8	1.87	0.40
1:L5:2018:C:O2'	84:L5:5416:HOH:O	2.21	0.40
1:L5:2804:OMC:HM23	1:L5:2804:OMC:H1'	1.91	0.40
1:L5:3789:C:O5'	1:L5:3789:C:H6	2.05	0.40
1:L5:3866:C:H2'	1:L5:3867:A2M:O4'	2.21	0.40
1:L5:4903:G:H2'	1:L5:4904:G:C8	2.56	0.40
1:L5:4960:G:H2'	1:L5:4961:G:C8	2.57	0.40
1:L5:4978:G:H2'	1:L5:4979:A:H5''	2.03	0.40
2:L7:45:U:H5''	7:LD:157:ASN:ND2	2.36	0.40
11:LH:5:LEU:HB2	11:LH:60:TRP:CZ3	2.56	0.40
11:LH:79:ASN:ND2	84:LH:204:HOH:O	2.38	0.40
11:LH:93:ARG:CZ	41:Lm:82:LEU:HD21	2.51	0.40
13:LJ:26:VAL:HG12	13:LJ:28:GLU:H	1.86	0.40
16:LN:24:ARG:HE	16:LN:24:ARG:HB3	1.53	0.40
16:LN:123:GLU:OE2	16:LN:128:LYS:HE3	2.21	0.40
24:LV:111:GLU:OE1	24:LV:131:ARG:HD3	2.21	0.40
25:LW:50:ASN:HA	25:LW:55:TYR:CD1	2.56	0.40
27:LY:130:LYS:HE2	27:LY:130:LYS:HB2	1.87	0.40
28:LZ:46:ILE:HG23	28:LZ:68:ILE:HG23	2.02	0.40
33:Le:64:LYS:HG3	33:Le:64:LYS:HZ3	1.66	0.40
37:Li:4:ARG:HE	37:Li:4:ARG:HB3	1.74	0.40
45:Lr:20:ARG:O	45:Lr:21:ASN:C	2.64	0.40
46:S2:113:G:O6	46:S2:290:U:H1'	2.21	0.40
46:S2:641:A:OP1	69:SJ:40:LYS:NZ	2.45	0.40
46:S2:1012:A:H2'	46:S2:1013:U:O4'	2.21	0.40
46:S2:1758:G:H1	46:S2:1771:G:H3'	1.86	0.40
46:S2:1781:A:N6	84:S2:2840:HOH:O	2.53	0.40
48:SA:80:ARG:O	48:SA:84:GLN:HG3	2.21	0.40
53:SI:174:CYS:HB2	53:SI:190:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SQ:146:ARG:NH2	84:SQ:208:HOH:O	2.54	0.40
58:SS:85:ASN:HB2	58:SS:97:GLN:HA	2.04	0.40
68:SG:121:ILE:H	68:SG:121:ILE:HG12	1.43	0.40
78:Sf:126:CYS:SG	78:Sf:143:LYS:HB3	2.61	0.40
1:L5:433:A:C2	1:L5:3867:A2M:H4'	2.57	0.40
1:L5:644:G:C6	1:L5:645:G:H1'	2.56	0.40
1:L5:730:G:C6	9:LF:73:ARG:HD3	2.56	0.40
1:L5:952:G:H2'	1:L5:953:C:C6	2.56	0.40
1:L5:1297:U:OP1	34:Lf:56:ASN:ND2	2.54	0.40
1:L5:2412:A:H2'	1:L5:2413:U:C6	2.55	0.40
1:L5:2725:A:H1'	20:LR:93:VAL:HG21	2.03	0.40
1:L5:2792:C:O2	38:Lj:9:GLY:HA2	2.22	0.40
1:L5:4088:C:OP1	4:LA:38:HIS:HE1	2.05	0.40
1:L5:4339:A:H2'	1:L5:4340:U:C6	2.56	0.40
1:L5:4747:C:H2'	1:L5:4748:U:O4'	2.22	0.40
1:L5:4773:C:H2'	1:L5:4774:C:C6	2.57	0.40
2:L7:54:A:C6	13:LJ:12:MET:HE2	2.56	0.40
3:L8:6:C:H2'	3:L8:7:U:H6	1.84	0.40
3:L8:39:G:H1'	3:L8:103:A:N6	2.37	0.40
5:LB:214:ASP:HB2	5:LB:283:LYS:NZ	2.37	0.40
9:LF:54:ALA:HB2	9:LF:188:GLU:HG3	2.04	0.40
10:LG:89:ARG:HG3	10:LG:89:ARG:HH11	1.86	0.40
15:LM:128:LYS:O	15:LM:132:LYS:HB2	2.21	0.40
33:Le:82:VAL:HG22	84:Le:362:HOH:O	2.21	0.40
34:Lf:51:TYR:CZ	34:Lf:68:ARG:HB2	2.56	0.40
35:Lg:24:ARG:CZ	35:Lg:30:ILE:HD11	2.52	0.40
44:Lp:41:PHE:CE2	44:Lp:62:LYS:HG2	2.57	0.40
46:S2:582:U:H2'	46:S2:583:A:H5''	2.04	0.40
46:S2:1139:C:O2	46:S2:1139:C:O4'	2.39	0.40
46:S2:1278:A:H2'	46:S2:1279:C:H6	1.86	0.40
46:S2:1499:U:H4'	50:SD:176:LEU:HD13	2.03	0.40
47:SE:47:PHE:O	47:SE:51:ARG:HB2	2.22	0.40
58:SS:36:VAL:HG21	58:SS:71:MET:HE2	2.03	0.40
62:SX:108:LYS:N	62:SX:108:LYS:HD2	2.36	0.40
62:SX:110:HIS:NE2	84:SX:203:HOH:O	2.36	0.40
70:SM:79:VAL:O	70:SM:80:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
5	LB	399/402 (99%)	387 (97%)	12 (3%)	0	100	100
6	LC	366/368 (100%)	358 (98%)	8 (2%)	0	100	100
7	LD	291/293 (99%)	279 (96%)	11 (4%)	1 (0%)	36	29
8	LE	232/247 (94%)	213 (92%)	13 (6%)	6 (3%)	4	1
9	LF	224/248 (90%)	219 (98%)	5 (2%)	0	100	100
10	LG	240/266 (90%)	227 (95%)	12 (5%)	1 (0%)	30	22
11	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
12	LI	211/214 (99%)	198 (94%)	9 (4%)	4 (2%)	6	1
13	LJ	174/178 (98%)	161 (92%)	10 (6%)	3 (2%)	7	2
14	LL	208/211 (99%)	194 (93%)	13 (6%)	1 (0%)	24	16
15	LM	137/215 (64%)	135 (98%)	2 (2%)	0	100	100
16	LN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	LO	199/203 (98%)	194 (98%)	5 (2%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
20	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
21	LS	173/176 (98%)	165 (95%)	8 (5%)	0	100	100
22	LT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	LU	99/128 (77%)	88 (89%)	11 (11%)	0	100	100
24	LV	129/140 (92%)	128 (99%)	1 (1%)	0	100	100
25	LW	120/157 (76%)	112 (93%)	8 (7%)	0	100	100
26	LX	118/156 (76%)	116 (98%)	2 (2%)	0	100	100
27	LY	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
28	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	La	144/148 (97%)	141 (98%)	2 (1%)	1 (1%)	18	10
30	Lb	95/159 (60%)	91 (96%)	4 (4%)	0	100	100
31	Lc	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
32	Ld	104/125 (83%)	100 (96%)	4 (4%)	0	100	100
33	Le	126/135 (93%)	126 (100%)	0	0	100	100
34	Lf	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
35	Lg	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
36	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	Li	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
38	Lj	84/97 (87%)	84 (100%)	0	0	100	100
39	Lk	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
44	Lp	86/92 (94%)	83 (96%)	3 (4%)	0	100	100
45	Lr	121/137 (88%)	118 (98%)	3 (2%)	0	100	100
47	SE	260/263 (99%)	259 (100%)	1 (0%)	0	100	100
48	SA	217/295 (74%)	209 (96%)	8 (4%)	0	100	100
49	SB	213/264 (81%)	204 (96%)	9 (4%)	0	100	100
50	SD	225/243 (93%)	219 (97%)	6 (3%)	0	100	100
51	SF	189/204 (93%)	173 (92%)	14 (7%)	2 (1%)	11	4
52	SH	182/194 (94%)	166 (91%)	14 (8%)	2 (1%)	11	4
53	SI	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
54	SK	95/165 (58%)	90 (95%)	5 (5%)	0	100	100
55	SL	152/158 (96%)	140 (92%)	10 (7%)	2 (1%)	9	3
56	SP	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
57	SQ	139/146 (95%)	131 (94%)	8 (6%)	0	100	100
58	SS	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
59	ST	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
60	SU	101/119 (85%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
62	SX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
63	Sa	101/115 (88%)	100 (99%)	1 (1%)	0	100	100
64	Sc	62/69 (90%)	53 (86%)	9 (14%)	0	100	100
65	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
66	Sg	311/317 (98%)	294 (94%)	17 (6%)	0	100	100
67	SC	220/293 (75%)	216 (98%)	4 (2%)	0	100	100
68	SG	232/249 (93%)	223 (96%)	8 (3%)	1 (0%)	30	22
69	SJ	181/194 (93%)	176 (97%)	5 (3%)	0	100	100
70	SM	116/132 (88%)	108 (93%)	7 (6%)	1 (1%)	14	6
71	SN	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
72	SO	132/151 (87%)	124 (94%)	8 (6%)	0	100	100
73	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
74	SY	127/133 (96%)	125 (98%)	2 (2%)	0	100	100
75	SZ	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
76	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
77	Se	56/133 (42%)	51 (91%)	5 (9%)	0	100	100
78	Sf	65/156 (42%)	52 (80%)	10 (15%)	3 (5%)	2	0
79	SR	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
All	All	11286/12657 (89%)	10866 (96%)	392 (4%)	28 (0%)	44	36

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	LE	99	ASP
10	LG	125	LYS
12	LI	110	ARG
13	LJ	62	ILE
14	LL	47	ALA
52	SH	15	LYS
70	SM	80	ASP
7	LD	88	VAL
8	LE	177	GLY
12	LI	108	ALA
13	LJ	31	ASP

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Mol	Chain	Res	Type
51	SF	128	ILE
78	Sf	125	GLU
8	LE	100	LYS
12	LI	106	ALA
12	LI	109	ASP
52	SH	192	PHE
55	SL	29	GLY
68	SG	124	LEU
8	LE	222	LEU
55	SL	25	LEU
78	Sf	102	VAL
78	Sf	128	ALA
8	LE	89	LEU
13	LJ	117	ILE
29	La	15	VAL
51	SF	79	HIS
8	LE	92	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	
4	LA	190/199 (96%)	184 (97%)	6 (3%)	34	27
5	LB	347/347 (100%)	342 (99%)	5 (1%)	59	59
6	LC	306/306 (100%)	304 (99%)	2 (1%)	76	78
7	LD	246/247 (100%)	240 (98%)	6 (2%)	43	38
8	LE	209/220 (95%)	193 (92%)	16 (8%)	12	5
9	LF	195/215 (91%)	195 (100%)	0	100	100
10	LG	204/223 (92%)	196 (96%)	8 (4%)	28	21
11	LH	169/171 (99%)	168 (99%)	1 (1%)	78	81
12	LI	181/182 (100%)	173 (96%)	8 (4%)	25	17
13	LJ	148/149 (99%)	145 (98%)	3 (2%)	48	46
14	LL	176/177 (99%)	174 (99%)	2 (1%)	65	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LM	118/161 (73%)	115 (98%)	3 (2%)	42	37
16	LN	171/172 (99%)	169 (99%)	2 (1%)	63	63
17	LO	173/174 (99%)	171 (99%)	2 (1%)	63	63
18	LP	134/163 (82%)	133 (99%)	1 (1%)	76	78
19	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	63
20	LR	166/175 (95%)	164 (99%)	2 (1%)	63	63
21	LS	156/157 (99%)	153 (98%)	3 (2%)	50	47
22	LT	139/140 (99%)	138 (99%)	1 (1%)	76	78
23	LU	91/115 (79%)	82 (90%)	9 (10%)	7	3
24	LV	101/107 (94%)	99 (98%)	2 (2%)	48	46
25	LW	101/126 (80%)	100 (99%)	1 (1%)	68	70
26	LX	108/133 (81%)	103 (95%)	5 (5%)	24	16
27	LY	123/135 (91%)	123 (100%)	0	100	100
28	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	73
29	La	119/120 (99%)	116 (98%)	3 (2%)	42	37
30	Lb	83/126 (66%)	83 (100%)	0	100	100
31	Lc	83/97 (86%)	81 (98%)	2 (2%)	43	38
32	Ld	97/110 (88%)	94 (97%)	3 (3%)	35	29
33	Le	114/121 (94%)	111 (97%)	3 (3%)	40	35
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	65	67
35	Lg	94/100 (94%)	93 (99%)	1 (1%)	65	67
36	Lh	109/110 (99%)	109 (100%)	0	100	100
37	Li	85/89 (96%)	85 (100%)	0	100	100
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	59	59
39	Lk	63/65 (97%)	59 (94%)	4 (6%)	16	8
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/116 (40%)	46 (98%)	1 (2%)	47	44
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	91/94 (97%)	90 (99%)	1 (1%)	65	67
44	Lp	71/75 (95%)	71 (100%)	0	100	100
45	Lr	107/121 (88%)	104 (97%)	3 (3%)	38	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	SE	224/225 (100%)	221 (99%)	3 (1%)	61	61
48	SA	182/243 (75%)	178 (98%)	4 (2%)	45	42
49	SB	196/231 (85%)	191 (97%)	5 (3%)	40	35
50	SD	190/202 (94%)	184 (97%)	6 (3%)	34	27
51	SF	161/170 (95%)	160 (99%)	1 (1%)	78	81
52	SH	166/174 (95%)	163 (98%)	3 (2%)	51	50
53	SI	178/180 (99%)	176 (99%)	2 (1%)	65	67
54	SK	88/136 (65%)	87 (99%)	1 (1%)	65	67
55	SL	138/142 (97%)	134 (97%)	4 (3%)	37	31
56	SP	111/130 (85%)	111 (100%)	0	100	100
57	SQ	117/121 (97%)	114 (97%)	3 (3%)	40	35
58	SS	126/132 (96%)	124 (98%)	2 (2%)	55	54
59	ST	112/114 (98%)	110 (98%)	2 (2%)	51	50
60	SU	94/107 (88%)	91 (97%)	3 (3%)	34	27
61	SV	67/67 (100%)	66 (98%)	1 (2%)	57	56
62	SX	113/115 (98%)	109 (96%)	4 (4%)	32	24
63	Sa	90/98 (92%)	88 (98%)	2 (2%)	45	42
64	Sc	57/62 (92%)	55 (96%)	2 (4%)	32	24
65	Sd	48/49 (98%)	48 (100%)	0	100	100
66	Sg	272/275 (99%)	262 (96%)	10 (4%)	30	22
67	SC	188/225 (84%)	188 (100%)	0	100	100
68	SG	204/218 (94%)	197 (97%)	7 (3%)	32	25
69	SJ	162/168 (96%)	158 (98%)	4 (2%)	42	37
70	SM	98/108 (91%)	91 (93%)	7 (7%)	13	7
71	SN	130/131 (99%)	127 (98%)	3 (2%)	44	40
72	SO	105/118 (89%)	105 (100%)	0	100	100
73	SW	112/113 (99%)	111 (99%)	1 (1%)	70	73
74	SY	111/115 (96%)	109 (98%)	2 (2%)	51	50
75	SZ	66/103 (64%)	65 (98%)	1 (2%)	57	56
76	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	61
77	Se	47/104 (45%)	46 (98%)	1 (2%)	47	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	Sf	60/140 (43%)	52 (87%)	8 (13%)	4	1
79	SR	119/122 (98%)	114 (96%)	5 (4%)	26	19
All	All	9834/10776 (91%)	9622 (98%)	212 (2%)	46	42

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	44	ILE
4	LA	84	THR
4	LA	135	THR
4	LA	208	GLU
4	LA	247	ARG
4	LA	249	THR
5	LB	60	VAL
5	LB	382	MET
5	LB	384	GLU
5	LB	386	LYS
5	LB	395	ASP
6	LC	3	CYS
6	LC	349	LEU
7	LD	37	VAL
7	LD	90	VAL
7	LD	129	GLU
7	LD	143	THR
7	LD	167	VAL
7	LD	261	VAL
8	LE	74	SER
8	LE	88	VAL
8	LE	89	LEU
8	LE	92	VAL
8	LE	100	LYS
8	LE	101	ASN
8	LE	106	VAL
8	LE	175	VAL
8	LE	194	VAL
8	LE	221	LYS
8	LE	222	LEU
8	LE	223	ARG
8	LE	224	LYS
8	LE	226	ARG
8	LE	260	LYS

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Mol	Chain	Res	Type
8	LE	274	VAL
10	LG	55	VAL
10	LG	120	LYS
10	LG	121	LYS
10	LG	125	LYS
10	LG	137[A]	ARG
10	LG	137[B]	ARG
10	LG	207	VAL
10	LG	246	SER
11	LH	45	LEU
12	LI	33	ILE
12	LI	36	LEU
12	LI	103	LEU
12	LI	104	SER
12	LI	105	CYS
12	LI	109	ASP
12	LI	110	ARG
12	LI	111	LEU
13	LJ	90	ARG
13	LJ	102	THR
13	LJ	128	LEU
14	LL	59	VAL
14	LL	130	LYS
15	LM	2	VAL
15	LM	38	VAL
15	LM	126	GLU
16	LN	60	VAL
16	LN	182	HIS
17	LO	180	GLN
17	LO	198	THR
18	LP	41	ILE
19	LQ	41	SER
19	LQ	82	VAL
20	LR	55	VAL
20	LR	177	LEU
21	LS	24	THR
21	LS	48	VAL
21	LS	88	SER
22	LT	4	THR
23	LU	18	VAL
23	LU	19	LEU
23	LU	22	THR

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Mol	Chain	Res	Type
23	LU	41	GLN
23	LU	47	ILE
23	LU	70	ILE
23	LU	72	VAL
23	LU	100	LEU
23	LU	109	SER
24	LV	27	ASN
24	LV	67	LYS
25	LW	76	VAL
26	LX	37	LYS
26	LX	38	LYS
26	LX	39	LYS
26	LX	40	ILE
26	LX	43	SER
28	LZ	5	MET
29	La	95	THR
29	La	103	VAL
29	La	120	GLN
31	Lc	21	VAL
31	Lc	69	THR
32	Ld	70	LYS
32	Ld	89	SER
32	Ld	98	SER
33	Le	53	ILE
33	Le	76	LYS
33	Le	82	VAL
34	Lf	57	THR
35	Lg	28	ASN
38	Lj	80	GLU
39	Lk	46	VAL
39	Lk	47	ILE
39	Lk	49	ASP
39	Lk	60	LEU
41	Lm	99	CYS
43	Lo	103	VAL
45	Lr	21	ASN
45	Lr	76	SER
45	Lr	80	THR
47	SE	23	LEU
47	SE	105	THR
47	SE	129	ILE
48	SA	1	MET

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Mol	Chain	Res	Type
48	SA	25	LEU
48	SA	77	ILE
48	SA	206	ASP
49	SB	47	THR
49	SB	59	SER
49	SB	63	LYS
49	SB	76	ASN
49	SB	92	GLN
50	SD	5	ILE
50	SD	44	THR
50	SD	113	LEU
50	SD	132	LYS
50	SD	136	VAL
50	SD	195	THR
51	SF	34	SER
52	SH	60	ILE
52	SH	80	VAL
52	SH	145	ARG
53	SI	73	THR
53	SI	158	ILE
54	SK	59	LYS
55	SL	28	THR
55	SL	30	LYS
55	SL	32	LYS
55	SL	144	LYS
57	SQ	18	THR
57	SQ	29	ASN
57	SQ	127	CYS
58	SS	69	THR
58	SS	98	VAL
59	ST	6	VAL
59	ST	113	VAL
60	SU	39	LEU
60	SU	93	SER
60	SU	116	ILE
61	SV	52	THR
62	SX	29	LYS
62	SX	58	GLU
62	SX	60	LYS
62	SX	61	GLN
63	Sa	45	VAL
63	Sa	93	LYS

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Mol	Chain	Res	Type
64	Sc	15	THR
64	Sc	57	THR
66	Sg	11	LEU
66	Sg	32	LEU
66	Sg	124	SER
66	Sg	134	THR
66	Sg	141	THR
66	Sg	206	LEU
66	Sg	230	LEU
66	Sg	261	LEU
66	Sg	272	GLN
66	Sg	280	LYS
68	SG	35	GLU
68	SG	41	LEU
68	SG	79	LYS
68	SG	119	LYS
68	SG	121	ILE
68	SG	126	ASP
68	SG	128	THR
69	SJ	2	PRO
69	SJ	86	VAL
69	SJ	141	VAL
69	SJ	163	SER
70	SM	46	GLN
70	SM	49	LEU
70	SM	51	VAL
70	SM	75	ASN
70	SM	91	LEU
70	SM	109	VAL
70	SM	123	VAL
71	SN	28	LEU
71	SN	32	ASP
71	SN	121	ARG
73	SW	39	THR
74	SY	6	THR
74	SY	69	THR
75	SZ	97	ILE
76	Sb	11	SER
77	Se	2	VAL
78	Sf	86	THR
78	Sf	87	THR
78	Sf	98	VAL

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Mol	Chain	Res	Type
78	Sf	143	LYS
78	Sf	144	CYS
78	Sf	145	CYS
78	Sf	146	LEU
78	Sf	147	THR
79	SR	22	THR
79	SR	45	LYS
79	SR	70	SER
79	SR	103	LYS
79	SR	124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	218	HIS
5	LB	123	HIS
6	LC	43	ASN
6	LC	89	GLN
6	LC	187	GLN
6	LC	212	ASN
6	LC	310	HIS
7	LD	229	ASN
7	LD	275	GLN
8	LE	101	ASN
10	LG	236	HIS
11	LH	15	ASN
11	LH	39	ASN
11	LH	42	ASN
11	LH	78	GLN
12	LI	59	GLN
12	LI	130	HIS
13	LJ	10	ASN
14	LL	115	GLN
15	LM	33	GLN
15	LM	34	ASN
16	LN	15	GLN
16	LN	182	HIS
17	LO	173	GLN
17	LO	184	ASN
18	LP	10	ASN
18	LP	34	GLN
18	LP	75	GLN

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Mol	Chain	Res	Type
18	LP	133	HIS
20	LR	118	HIS
20	LR	158	GLN
21	LS	125	GLN
22	LT	144	ASN
23	LU	95	ASN
23	LU	105	ASN
27	LY	14	ASN
27	LY	18	HIS
27	LY	40	GLN
29	La	67	GLN
31	Lc	72	HIS
33	Le	92	ASN
40	Ll	33	ASN
47	SE	98	ASN
47	SE	188	ASN
49	SB	92	GLN
49	SB	149	GLN
49	SB	202	GLN
50	SD	4	GLN
51	SF	82	ASN
52	SH	12	ASN
52	SH	126	HIS
52	SH	157	HIS
54	SK	66	HIS
54	SK	77	GLN
54	SK	84	HIS
59	ST	142	ASN
60	SU	47	ASN
62	SX	61	GLN
65	Sd	16	GLN
66	Sg	76	GLN
66	Sg	244	ASN
67	SC	267	GLN
67	SC	277	HIS
68	SG	81	HIS
70	SM	72	HIS
71	SN	62	GLN
74	SY	63	HIS
75	SZ	45	ASN
76	Sb	9	HIS
77	Se	44	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3705/5069 (73%)	761 (20%)	21 (0%)
2	L7	119/120 (99%)	12 (10%)	0
3	L8	155/157 (98%)	28 (18%)	0
46	S2	1713/1869 (91%)	320 (18%)	10 (0%)
All	All	5692/7215 (78%)	1121 (19%)	31 (0%)

All (1121) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	15	A
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	59	A
1	L5	64	A
1	L5	65	A
1	L5	69	A
1	L5	73	A
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	119	G
1	L5	120	A
1	L5	130	C
1	L5	131	C
1	L5	132	G
1	L5	133	C
1	L5	136	C
1	L5	144	G
1	L5	152	U
1	L5	159	C
1	L5	164	G
1	L5	183	C
1	L5	185	C
1	L5	186	G
1	L5	187	U
1	L5	188	G

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Mol	Chain	Res	Type
1	L5	189	G
1	L5	200	U
1	L5	209	U
1	L5	210	C
1	L5	213	G
1	L5	216	C
1	L5	217	C
1	L5	218	A
1	L5	219	G
1	L5	234	G
1	L5	253	G
1	L5	255	C
1	L5	256	G
1	L5	259	C
1	L5	261	G
1	L5	262	G
1	L5	264	C
1	L5	265	C
1	L5	266	C
1	L5	276	C
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	341	G
1	L5	373	G
1	L5	387	G
1	L5	396	A
1	L5	407	A
1	L5	408	A
1	L5	410	A
1	L5	412	G
1	L5	432	U
1	L5	450	G
1	L5	452	A
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	467	U

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Mol	Chain	Res	Type
1	L5	483	G
1	L5	484	U
1	L5	485	C
1	L5	486	C
1	L5	489	C
1	L5	490	C
1	L5	491	G
1	L5	497	G
1	L5	498	C
1	L5	500	G
1	L5	502	C
1	L5	503	C
1	L5	505	G
1	L5	509	A
1	L5	510	U
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	516	C
1	L5	517	C
1	L5	518	G
1	L5	519	C
1	L5	643	C
1	L5	644	G
1	L5	645	G
1	L5	653	U
1	L5	654	C
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	662	C
1	L5	663	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	669	C
1	L5	672	C
1	L5	673	C
1	L5	686	A
1	L5	687	U

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Mol	Chain	Res	Type
1	L5	696	C
1	L5	703	G
1	L5	704	C
1	L5	721	G
1	L5	730	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	740	G
1	L5	741	C
1	L5	742	G
1	L5	746	A
1	L5	904	C
1	L5	905	C
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	925	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	937	U
1	L5	941	C
1	L5	944	A
1	L5	945	U
1	L5	946	C
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	963	G
1	L5	965	G
1	L5	966	A
1	L5	967	C
1	L5	968	C
1	L5	970	G
1	L5	971	U
1	L5	972	C

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Mol	Chain	Res	Type
1	L5	981	C
1	L5	982	U
1	L5	983	C
1	L5	988	C
1	L5	989	U
1	L5	990	C
1	L5	991	C
1	L5	992	C
1	L5	995	C
1	L5	1049	C
1	L5	1050	C
1	L5	1051	G
1	L5	1070	G
1	L5	1071	C
1	L5	1072	C
1	L5	1078	A
1	L5	1079	C
1	L5	1083	U
1	L5	1168	G
1	L5	1171	G
1	L5	1173	G
1	L5	1178	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1196	G
1	L5	1198	G
1	L5	1200	G
1	L5	1202	C
1	L5	1203	G
1	L5	1205	G
1	L5	1211	G
1	L5	1215	C
1	L5	1221	G
1	L5	1222	A
1	L5	1241	C
1	L5	1248	C
1	L5	1255	A
1	L5	1260	G
1	L5	1266	G

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Mol	Chain	Res	Type
1	L5	1269	G
1	L5	1270	A
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1275	G
1	L5	1277	G
1	L5	1280	C
1	L5	1284	G
1	L5	1287	G
1	L5	1294	A
1	L5	1302	U
1	L5	1303	A
1	L5	1304	C
1	L5	1313	C
1	L5	1326	A2M
1	L5	1337	A
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1364	U
1	L5	1365	C
1	L5	1366	G
1	L5	1367	C
1	L5	1368	A
1	L5	1387	A
1	L5	1394	G
1	L5	1397	A
1	L5	1399	G
1	L5	1402	C
1	L5	1404	G
1	L5	1405	C
1	L5	1409	C
1	L5	1410	U
1	L5	1411	C
1	L5	1412	G
1	L5	1420	A
1	L5	1425	G
1	L5	1435	G
1	L5	1436	C
1	L5	1438	U
1	L5	1439	C

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Mol	Chain	Res	Type
1	L5	1442	C
1	L5	1443	A
1	L5	1445	U
1	L5	1446	C
1	L5	1452	A
1	L5	1457	G
1	L5	1477	C
1	L5	1482	G
1	L5	1483	C
1	L5	1485	C
1	L5	1498	G
1	L5	1502	G
1	L5	1516	G
1	L5	1534	A2M
1	L5	1535	C
1	L5	1547	A
1	L5	1566	C
1	L5	1578	U
1	L5	1591	U
1	L5	1596	U
1	L5	1613	A
1	L5	1624	G
1	L5	1625	OMG
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1640	C
1	L5	1641	G
1	L5	1642	A
1	L5	1654	G
1	L5	1661	C
1	L5	1676	C
1	L5	1677	PSU
1	L5	1691	G
1	L5	1694	C
1	L5	1699	A
1	L5	1700	G
1	L5	1701	A
1	L5	1702	C
1	L5	1703	C
1	L5	1704	C
1	L5	1705	G

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Mol	Chain	Res	Type
1	L5	1715	C
1	L5	1718	C
1	L5	1719	A
1	L5	1730	U
1	L5	1734	G
1	L5	1740	C
1	L5	1741	G
1	L5	1742	A
1	L5	1750	G
1	L5	1756	U
1	L5	1757	U
1	L5	1758	G
1	L5	1761	G
1	L5	1762	C
1	L5	1763	C
1	L5	1765	A
1	L5	1766	A
1	L5	1768	C
1	L5	1769	G
1	L5	1770	A
1	L5	1772	C
1	L5	1780	A
1	L5	1781	PSU
1	L5	1787	A
1	L5	1804	A
1	L5	1805	A
1	L5	1810	G
1	L5	1815	G
1	L5	1821	G
1	L5	1822	U
1	L5	1829	G
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1855	G
1	L5	1869	G
1	L5	1882	U
1	L5	1892	A
1	L5	1897	A
1	L5	1918	U
1	L5	1919	G

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Mol	Chain	Res	Type
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C
1	L5	1932	A
1	L5	1940	G
1	L5	1948	G
1	L5	1959	U
1	L5	1960	A
1	L5	1966	C
1	L5	1969	G
1	L5	1972	G
1	L5	1974	U
1	L5	1975	G
1	L5	1977	C
1	L5	1978	C
1	L5	1979	A
1	L5	1981	G
1	L5	1982	G
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1987	C
1	L5	1988	G
1	L5	1991	A
1	L5	1993	C
1	L5	1995	G
1	L5	1996	C
1	L5	1998	A
1	L5	2001	G
1	L5	2002	A
1	L5	2003	G
1	L5	2006	U
1	L5	2007	G
1	L5	2009	A
1	L5	2010	A
1	L5	2011	C
1	L5	2012	A
1	L5	2013	A
1	L5	2015	U
1	L5	2016	C
1	L5	2019	C

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Mol	Chain	Res	Type
1	L5	2020	U
1	L5	2022	C
1	L5	2024	G
1	L5	2025	A
1	L5	2026	A
1	L5	2042	A
1	L5	2046	G
1	L5	2048	U
1	L5	2052	G
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A
1	L5	2084	C
1	L5	2089	G
1	L5	2091	C
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C
1	L5	2102	G
1	L5	2104	G
1	L5	2105	A
1	L5	2106	G
1	L5	2107	C
1	L5	2108	G
1	L5	2111	G
1	L5	2112	G
1	L5	2113	G
1	L5	2252	G
1	L5	2253	A
1	L5	2255	C
1	L5	2256	C
1	L5	2258	C
1	L5	2259	G
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2313	A
1	L5	2316	G

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Mol	Chain	Res	Type
1	L5	2333	G
1	L5	2348	G
1	L5	2351	OMC
1	L5	2360	A
1	L5	2382	A
1	L5	2392	C
1	L5	2395	A
1	L5	2397	G
1	L5	2417	A
1	L5	2421	G
1	L5	2422	OMC
1	L5	2425	U
1	L5	2428	A
1	L5	2441	C
1	L5	2450	G
1	L5	2453	A
1	L5	2470	C
1	L5	2475	G
1	L5	2479	G
1	L5	2483	G
1	L5	2484	A
1	L5	2485	U
1	L5	2486	G
1	L5	2487	G
1	L5	2488	C
1	L5	2489	C
1	L5	2491	C
1	L5	2493	G
1	L5	2499	C
1	L5	2501	C
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2513	A
1	L5	2519	U
1	L5	2520	C
1	L5	2546	G
1	L5	2547	G
1	L5	2555	G
1	L5	2556	G
1	L5	2560	C
1	L5	2567	G

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Mol	Chain	Res	Type
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2627	C
1	L5	2632	PSU
1	L5	2638	G
1	L5	2652	G
1	L5	2653	C
1	L5	2662	G
1	L5	2669	C
1	L5	2676	A
1	L5	2686	G
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2703	G
1	L5	2710	C
1	L5	2711	G
1	L5	2725	A
1	L5	2726	G
1	L5	2729	C
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2769	U
1	L5	2770	C
1	L5	2788	U
1	L5	2790	U
1	L5	2794	C
1	L5	2814	C
1	L5	2815	A2M
1	L5	2826	U
1	L5	2827	G
1	L5	2829	U
1	L5	2842	G
1	L5	2855	G
1	L5	2892	C
1	L5	2899	C

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Mol	Chain	Res	Type
1	L5	2900	U
1	L5	2902	G
1	L5	2903	G
1	L5	2904	U
1	L5	2906	G
1	L5	2908	U
1	L5	2910	G
1	L5	3586	G
1	L5	3587	C
1	L5	3588	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
1	L5	3598	C
1	L5	3604	A
1	L5	3615	G
1	L5	3616	U
1	L5	3618	C
1	L5	3626	G
1	L5	3635	A
1	L5	3644	U
1	L5	3662	A
1	L5	3673	C
1	L5	3674	G
1	L5	3711	A
1	L5	3712	A
1	L5	3713	U
1	L5	3723	A
1	L5	3724	A2M
1	L5	3726	A
1	L5	3727	A
1	L5	3729	U
1	L5	3736	A
1	L5	3748	A
1	L5	3753	G
1	L5	3754	G
1	L5	3757	G
1	L5	3758	U
1	L5	3759	A
1	L5	3760	A
1	L5	3761	C
1	L5	3776	G

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Mol	Chain	Res	Type
1	L5	3777	G
1	L5	3783	A
1	L5	3786	U
1	L5	3802	U
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	UY1
1	L5	3819	G
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3844	PSU
1	L5	3851	PSU
1	L5	3876	A
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3897	G
1	L5	3898	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3945	A
1	L5	3946	G
1	L5	3947	A
1	L5	3948	C
1	L5	3949	A
1	L5	3951	G
1	L5	3956	G
1	L5	3957	U
1	L5	3960	A
1	L5	3961	G
1	L5	3963	A
1	L5	3965	A
1	L5	3966	A
1	L5	3967	G
1	L5	3969	G
1	L5	3971	G

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Mol	Chain	Res	Type
1	L5	3973	G
1	L5	3974	G
1	L5	3976	C
1	L5	3977	C
1	L5	4036	G
1	L5	4038	C
1	L5	4039	G
1	L5	4042	G
1	L5	4043	G
1	L5	4044	U
1	L5	4046	A
1	L5	4048	A
1	L5	4049	U
1	L5	4050	A
1	L5	4051	C
1	L5	4053	A
1	L5	4055	U
1	L5	4056	A
1	L5	4057	C
1	L5	4059	C
1	L5	4062	A
1	L5	4065	G
1	L5	4069	U
1	L5	4076	G
1	L5	4084	G
1	L5	4098	A
1	L5	4099	G
1	L5	4100	C
1	L5	4103	C
1	L5	4104	G
1	L5	4106	G
1	L5	4108	G
1	L5	4109	G
1	L5	4110	C
1	L5	4112	C
1	L5	4113	U
1	L5	4114	C
1	L5	4115	G
1	L5	4116	C
1	L5	4119	C
1	L5	4122	G
1	L5	4127	A

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Mol	Chain	Res	Type
1	L5	4137	C
1	L5	4139	G
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4148	C
1	L5	4150	G
1	L5	4162	C
1	L5	4163	U
1	L5	4170	A
1	L5	4177	C
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4203	A
1	L5	4222	G
1	L5	4229	U
1	L5	4233	A
1	L5	4234	A
1	L5	4249	G
1	L5	4250	G
1	L5	4251	A
1	L5	4254	G
1	L5	4258	C
1	L5	4268	A
1	L5	4273	A
1	L5	4281	A
1	L5	4291	G
1	L5	4297	G
1	L5	4298	A
1	L5	4304	A
1	L5	4305	G
1	L5	4314	C
1	L5	4330	G
1	L5	4332	C
1	L5	4339	A
1	L5	4349	C
1	L5	4373	G
1	L5	4377	G

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Mol	Chain	Res	Type
1	L5	4378	A
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
1	L5	4415	A
1	L5	4421	C
1	L5	4422	A
1	L5	4437	U
1	L5	4448	G
1	L5	4449	A
1	L5	4452	U
1	L5	4464	A
1	L5	4475	G
1	L5	4500	PSU
1	L5	4502	C
1	L5	4512	U
1	L5	4513	A
1	L5	4519	C
1	L5	4524	G
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4560	C
1	L5	4567	G
1	L5	4573	G
1	L5	4575	G
1	L5	4584	A
1	L5	4590	A2M
1	L5	4600	G
1	L5	4601	U
1	L5	4636	PSU
1	L5	4637	OMG
1	L5	4654	C
1	L5	4656	A
1	L5	4670	C
1	L5	4672	A
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4730	C

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Mol	Chain	Res	Type
1	L5	4731	G
1	L5	4734	A
1	L5	4735	G
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4746	C
1	L5	4750	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4773	C
1	L5	4775	C
1	L5	4860	G
1	L5	4870	G
1	L5	4871	C
1	L5	4874	A
1	L5	4875	G
1	L5	4882	U
1	L5	4883	C
1	L5	4889	G
1	L5	4895	C
1	L5	4896	G
1	L5	4900	C
1	L5	4901	G
1	L5	4910	A
1	L5	4912	G
1	L5	4914	C
1	L5	4923	C
1	L5	4931	G
1	L5	4934	A
1	L5	4938	A
1	L5	4941	G
1	L5	4943	A
1	L5	4955	A
1	L5	4960	G
1	L5	4961	G
1	L5	4963	G
1	L5	4966	A
1	L5	4976	U

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Mol	Chain	Res	Type
1	L5	4990	C
1	L5	4991	U
1	L5	5013	C
1	L5	5017	G
1	L5	5022	U
1	L5	5023	C
1	L5	5024	C
1	L5	5025	C
1	L5	5030	U
1	L5	5034	A
1	L5	5041	G
1	L5	5050	C
1	L5	5054	C
1	L5	5061	A
1	L5	5069	U
2	L7	22	A
2	L7	33	U
2	L7	34	C
2	L7	42	A
2	L7	50	A
2	L7	53	U
2	L7	54	A
2	L7	64	G
2	L7	97	G
2	L7	100	A
2	L7	110	G
2	L7	117	G
3	L8	34	U
3	L8	35	C
3	L8	48	A
3	L8	51	U
3	L8	52	A
3	L8	59	A
3	L8	62	A
3	L8	63	U
3	L8	71	A
3	L8	80	A
3	L8	82	A
3	L8	84	A
3	L8	85	U
3	L8	86	U
3	L8	87	G

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Mol	Chain	Res	Type
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	110	U
3	L8	112	G
3	L8	114	G
3	L8	123	U
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	128	C
3	L8	147	G
46	S2	17	C
46	S2	33	G
46	S2	46	A
46	S2	56	G
46	S2	64	A
46	S2	67	C
46	S2	68	A
46	S2	71	G
46	S2	72	C
46	S2	73	C
46	S2	74	G
46	S2	76	U
46	S2	100	PSU
46	S2	103	A
46	S2	113	G
46	S2	115	U
46	S2	126	G
46	S2	130	G
46	S2	140	C
46	S2	143	U
46	S2	155	G
46	S2	159	A2M
46	S2	160	U
46	S2	162	C
46	S2	166	A2M
46	S2	168	C
46	S2	173	A
46	S2	190	G
46	S2	198	U

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Mol	Chain	Res	Type
46	S2	200	G
46	S2	203	G
46	S2	204	G
46	S2	206	G
46	S2	209	A
46	S2	213	G
46	S2	220	U
46	S2	302	A
46	S2	306	C
46	S2	307	G
46	S2	308	G
46	S2	309	G
46	S2	318	A
46	S2	319	C
46	S2	323	C
46	S2	324	C
46	S2	325	C
46	S2	326	C
46	S2	329	G
46	S2	332	G
46	S2	335	G
46	S2	360	A
46	S2	362	C
46	S2	364	A
46	S2	368	U
46	S2	385	G
46	S2	386	C
46	S2	407	G
46	S2	408	A
46	S2	409	C
46	S2	429	C
46	S2	438	G
46	S2	448	A
46	S2	450	C
46	S2	452	G
46	S2	462	OMC
46	S2	464	A
46	S2	466	G
46	S2	471	G
46	S2	472	C
46	S2	473	A
46	S2	474	G

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Mol	Chain	Res	Type
46	S2	482	G
46	S2	487	U
46	S2	488	U
46	S2	492	C
46	S2	508	A
46	S2	509	OMG
46	S2	516	A
46	S2	525	A
46	S2	532	C
46	S2	533	A
46	S2	536	A
46	S2	537	C
46	S2	544	G
46	S2	545	A
46	S2	546	G
46	S2	547	G
46	S2	548	C
46	S2	552	G
46	S2	554	A
46	S2	556	U
46	S2	557	U
46	S2	558	G
46	S2	563	G
46	S2	564	A
46	S2	570	C
46	S2	576	A2M
46	S2	583	A
46	S2	587	A
46	S2	589	G
46	S2	591	U
46	S2	598	G
46	S2	607	U
46	S2	614	C
46	S2	617	G
46	S2	627	U
46	S2	628	A
46	S2	631	U
46	S2	632	C
46	S2	643	A
46	S2	655	A
46	S2	660	C
46	S2	668	A2M

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Mol	Chain	Res	Type
46	S2	669	A
46	S2	670	A
46	S2	671	A
46	S2	672	A
46	S2	688	U
46	S2	689	U
46	S2	692	G
46	S2	696	G
46	S2	698	G
46	S2	731	G
46	S2	732	U
46	S2	733	C
46	S2	734	C
46	S2	735	C
46	S2	736	C
46	S2	737	G
46	S2	738	C
46	S2	748	C
46	S2	749	U
46	S2	750	C
46	S2	751	G
46	S2	752	G
46	S2	753	C
46	S2	787	G
46	S2	791	C
46	S2	792	C
46	S2	793	G
46	S2	794	A
46	S2	796	G
46	S2	798	G
46	S2	799	U
46	S2	801	PSU
46	S2	811	A
46	S2	821	G
46	S2	822	PSU
46	S2	823	U
46	S2	824	C
46	S2	830	A
46	S2	836	G
46	S2	837	A
46	S2	838	G
46	S2	839	C

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Mol	Chain	Res	Type
46	S2	841	G
46	S2	842	C
46	S2	847	A
46	S2	867	OMG
46	S2	869	A
46	S2	870	A
46	S2	872	A
46	S2	881	G
46	S2	882	U
46	S2	887	U
46	S2	888	U
46	S2	891	G
46	S2	892	U
46	S2	893	U
46	S2	894	G
46	S2	895	G
46	S2	896	U
46	S2	897	U
46	S2	898	U
46	S2	900	C
46	S2	901	G
46	S2	903	A
46	S2	904	A
46	S2	909	G
46	S2	913	A
46	S2	917	U
46	S2	920	A
46	S2	922	A
46	S2	933	G
46	S2	955	A
46	S2	968	U
46	S2	971	G
46	S2	990	A
46	S2	992	A
46	S2	1017	U
46	S2	1023	A
46	S2	1027	A
46	S2	1060	A
46	S2	1061	U
46	S2	1062	A
46	S2	1081	U
46	S2	1083	A

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Mol	Chain	Res	Type
46	S2	1085	C
46	S2	1109	C
46	S2	1114	U
46	S2	1115	U
46	S2	1116	C
46	S2	1121	G
46	S2	1123	C
46	S2	1131	G
46	S2	1133	A
46	S2	1138	C
46	S2	1153	C
46	S2	1154	U
46	S2	1195	A
46	S2	1207	G
46	S2	1208	A
46	S2	1215	C
46	S2	1216	C
46	S2	1217	A
46	S2	1221	G
46	S2	1224	G
46	S2	1240	A
46	S2	1242	U
46	S2	1243	U
46	S2	1251	A
46	S2	1253	A
46	S2	1256	G
46	S2	1257	G
46	S2	1259	A
46	S2	1274	G
46	S2	1275	G
46	S2	1285	G
46	S2	1294	G
46	S2	1295	A
46	S2	1301	A
46	S2	1302	G
46	S2	1303	C
46	S2	1305	C
46	S2	1308	U
46	S2	1322	G
46	S2	1343	U
46	S2	1348	G
46	S2	1364	U

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Mol	Chain	Res	Type
46	S2	1371	U
46	S2	1372	U
46	S2	1378	A
46	S2	1397	U
46	S2	1406	G
46	S2	1419	C
46	S2	1420	G
46	S2	1421	A
46	S2	1423	C
46	S2	1424	G
46	S2	1435	C
46	S2	1436	C
46	S2	1437	C
46	S2	1438	A
46	S2	1454	A
46	S2	1463	U
46	S2	1487	A
46	S2	1489	A
46	S2	1490	OMG
46	S2	1497	G
46	S2	1498	A
46	S2	1506	A
46	S2	1508	A
46	S2	1509	U
46	S2	1521	C
46	S2	1533	A
46	S2	1547	C
46	S2	1553	C
46	S2	1556	A
46	S2	1570	G
46	S2	1579	A
46	S2	1580	A
46	S2	1588	A
46	S2	1601	A
46	S2	1604	G
46	S2	1606	G
46	S2	1621	U
46	S2	1623	A
46	S2	1647	A
46	S2	1648	G
46	S2	1654	G
46	S2	1663	A

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Mol	Chain	Res	Type
46	S2	1664	A
46	S2	1665	G
46	S2	1671	G
46	S2	1721	U
46	S2	1722	G
46	S2	1745	A
46	S2	1747	C
46	S2	1749	G
46	S2	1752	C
46	S2	1753	C
46	S2	1754	G
46	S2	1757	G
46	S2	1758	G
46	S2	1761	U
46	S2	1773	C
46	S2	1774	C
46	S2	1775	U
46	S2	1776	G
46	S2	1777	G
46	S2	1778	C
46	S2	1779	G
46	S2	1781	A
46	S2	1782	G
46	S2	1783	C
46	S2	1784	G
46	S2	1786	U
46	S2	1804	OMU
46	S2	1806	A
46	S2	1809	A
46	S2	1831	A
46	S2	1835	A
46	S2	1838	U
46	S2	1849	G
46	S2	1851	MA6
46	S2	1861	G
46	S2	1862	G
46	S2	1863	A
46	S2	1864	U
46	S2	1865	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	406	C
1	L5	509	A
1	L5	914	U
1	L5	1590	C
1	L5	1613	A
1	L5	1633	G
1	L5	1740	C
1	L5	2391	G
1	L5	2416	G
1	L5	2675	G
1	L5	2760	G
1	L5	3614	G
1	L5	3673	C
1	L5	3726	A
1	L5	3786	U
1	L5	3876	A
1	L5	4420	U
1	L5	4600	G
1	L5	4653	C
1	L5	4699	U
1	L5	4913	G
46	S2	563	G
46	S2	688	U
46	S2	823	U
46	S2	866	PSU
46	S2	1081	U
46	S2	1242	U
46	S2	1342	U
46	S2	1508	A
46	S2	1520	G
46	S2	1805	G

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

223 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
46	OMU	S2	116	46	19,22,23	1.18	3 (15%)	26,31,34	1.75	5 (19%)
46	4AC	S2	1337	46	21,24,25	1.03	1 (4%)	29,34,37	1.08	3 (10%)
1	PSU	L5	3851	1	18,21,22	1.34	2 (11%)	22,30,33	2.00	3 (13%)
1	OMG	L5	2876	1	23,26,27	1.23	3 (13%)	33,38,41	2.02	7 (21%)
46	A2M	S2	1383	46	22,25,26	1.44	4 (18%)	31,36,39	2.19	8 (25%)
3	PSU	L8	69	3	18,21,22	0.88	1 (5%)	22,30,33	0.70	0
1	PSU	L5	4552	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	OMC	L5	1340	1	19,22,23	0.78	0	26,31,34	0.62	0
46	PSU	S2	966	46	18,21,22	0.86	1 (5%)	22,30,33	0.66	0
1	PSU	L5	4521	80,1,81	18,21,22	1.29	2 (11%)	22,30,33	1.95	4 (18%)
46	PSU	S2	1244	46	18,21,22	0.88	1 (5%)	22,30,33	0.69	0
1	A2M	L5	1534	80,1	22,25,26	1.49	4 (18%)	31,36,39	2.03	9 (29%)
46	PSU	S2	609	46	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
29	V5N	La	39	29	9,11,12	2.62	2 (22%)	9,14,16	1.26	0
1	PSU	L5	4628	1	18,21,22	1.36	3 (16%)	22,30,33	1.88	3 (13%)
1	PSU	L5	4296	1	18,21,22	0.89	1 (5%)	22,30,33	0.59	0
46	PSU	S2	667	46	18,21,22	0.85	1 (5%)	22,30,33	0.61	0
46	OMU	S2	1442	46,80	19,22,23	1.20	3 (15%)	26,31,34	1.69	5 (19%)
1	PSU	L5	4353	1	18,21,22	1.38	3 (16%)	22,30,33	1.97	4 (18%)
46	A2M	S2	99	46,80	22,25,26	0.18	0	31,36,39	0.38	0
1	OMG	L5	4618	1	23,26,27	1.18	3 (13%)	33,38,41	1.98	6 (18%)
1	OMG	L5	2364	1	23,26,27	1.21	4 (17%)	33,38,41	1.86	5 (15%)
1	OMC	L5	3841	1	19,22,23	0.81	1 (5%)	26,31,34	0.88	1 (3%)
1	PSU	L5	3844	1	18,21,22	1.39	3 (16%)	22,30,33	1.97	3 (13%)
5	HIC	LB	245	5	10,11,12	1.57	1 (10%)	8,14,16	0.93	0
1	OMG	L5	3899	1	23,26,27	1.16	3 (13%)	33,38,41	1.88	8 (24%)
46	PSU	S2	1692	46	18,21,22	1.42	3 (16%)	22,30,33	1.88	3 (13%)
1	OMG	L5	1522	1	23,26,27	1.19	3 (13%)	33,38,41	2.04	8 (24%)
1	OMU	L5	2415	1	19,22,23	1.22	3 (15%)	26,31,34	1.72	5 (19%)
1	PSU	L5	4312	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
46	OMU	S2	428	46	19,22,23	1.21	2 (10%)	26,31,34	1.67	4 (15%)
1	PSU	L5	1536	1	18,21,22	1.34	2 (11%)	22,30,33	1.79	3 (13%)
1	OMU	L5	3925	1	19,22,23	1.19	2 (10%)	26,31,34	1.70	5 (19%)
1	OMG	L5	4370	1	23,26,27	1.17	3 (13%)	33,38,41	1.93	6 (18%)
46	A2M	S2	576	46	22,25,26	1.43	5 (22%)	31,36,39	2.11	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	L5	2365	80,1	19,22,23	0.78	0	26,31,34	0.75	0
1	PSU	L5	3715	1	18,21,22	1.37	3 (16%)	22,30,33	1.97	3 (13%)
1	OMC	L5	4456	1	19,22,23	0.78	0	26,31,34	0.67	0
1	A2M	L5	2401	1	22,25,26	1.46	4 (18%)	31,36,39	2.05	9 (29%)
46	PSU	S2	651	46	18,21,22	1.33	3 (16%)	22,30,33	1.92	3 (13%)
1	PSU	L5	3695	1,81	18,21,22	1.35	3 (16%)	22,30,33	1.98	4 (18%)
46	PSU	S2	34	46	18,21,22	0.86	1 (5%)	22,30,33	0.67	0
46	OMU	S2	1288	46	19,22,23	1.20	2 (10%)	26,31,34	1.71	5 (19%)
1	OMG	L5	1316	1,81	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
1	OMU	L5	4306	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)
72	IAS	SO	138	72	6,7,8	1.04	0	6,8,10	1.66	3 (50%)
46	PSU	S2	1347	46	18,21,22	0.87	1 (5%)	22,30,33	0.68	0
1	PSU	L5	1779	1	18,21,22	1.37	2 (11%)	22,30,33	1.94	5 (22%)
46	PSU	S2	686	46	18,21,22	0.86	1 (5%)	22,30,33	0.73	0
1	PSU	L5	4442	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
1	A2M	L5	1326	1	22,25,26	1.44	5 (22%)	31,36,39	2.04	9 (29%)
1	PSU	L5	3920	80,1	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
46	PSU	S2	1596	46	18,21,22	0.87	1 (5%)	22,30,33	0.62	0
1	PSU	L5	5010	1	18,21,22	0.87	1 (5%)	22,30,33	0.65	0
1	PSU	L5	5001	1	18,21,22	0.83	1 (5%)	22,30,33	0.66	0
46	OMG	S2	436	46	23,26,27	1.18	3 (13%)	33,38,41	2.01	7 (21%)
1	OMU	L5	4227	1	19,22,23	1.23	2 (10%)	26,31,34	1.72	5 (19%)
1	A2M	L5	3785	80,1	22,25,26	0.26	0	31,36,39	0.59	0
1	PSU	L5	4493	1,81	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
1	OMC	L5	2804	1	19,22,23	0.79	0	26,31,34	0.85	0
46	PSU	S2	1238	46	18,21,22	1.36	3 (16%)	22,30,33	1.99	5 (22%)
46	PSU	S2	918	46	18,21,22	1.41	3 (16%)	22,30,33	1.99	4 (18%)
1	5MC	L5	4447	1,81	18,22,23	0.36	0	26,32,35	0.61	0
1	PSU	L5	1860	1	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
46	4AC	S2	1842	46	21,24,25	0.94	1 (4%)	29,34,37	1.06	4 (13%)
1	A2M	L5	3825	1	22,25,26	1.42	4 (18%)	31,36,39	2.10	10 (32%)
46	UY1	S2	1326	46,80	19,22,23	0.20	0	22,31,34	0.42	0
46	PSU	S2	681	46	18,21,22	1.32	3 (16%)	22,30,33	2.06	4 (18%)
46	6MZ	S2	1832	46,80,81	22,25,26	1.49	5 (22%)	30,36,39	2.13	10 (33%)
46	PSU	S2	1136	46	18,21,22	0.87	1 (5%)	22,30,33	0.70	0
1	PSU	L5	4299	1	18,21,22	0.86	1 (5%)	22,30,33	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L8	55	3	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	L5	3867	1	22,25,26	1.44	4 (18%)	31,36,39	2.02	9 (29%)
1	5MC	L5	3782	80,1	18,22,23	0.94	2 (11%)	26,32,35	1.15	2 (7%)
46	PSU	S2	1045	46	18,21,22	1.41	3 (16%)	22,30,33	1.83	3 (13%)
1	OMC	L5	3887	1	19,22,23	0.82	0	26,31,34	0.89	0
46	PSU	S2	63	46	18,21,22	1.36	2 (11%)	22,30,33	1.95	4 (18%)
1	PSU	L5	1677	1	18,21,22	1.36	3 (16%)	22,30,33	2.05	5 (22%)
46	MA6	S2	1850	46	23,26,27	1.43	5 (21%)	34,38,41	2.11	11 (32%)
1	A2M	L5	1871	80,1	22,25,26	1.44	4 (18%)	31,36,39	2.15	11 (35%)
3	OMG	L8	75	3	23,26,27	1.18	3 (13%)	33,38,41	1.91	6 (18%)
46	PSU	S2	366	46	18,21,22	1.39	3 (16%)	22,30,33	2.00	4 (18%)
1	PSU	L5	1782	1	18,21,22	1.38	3 (16%)	22,30,33	1.88	4 (18%)
1	OMC	L5	3701	1,81	19,22,23	0.76	0	26,31,34	0.87	0
1	PSU	L5	4579	1	18,21,22	0.88	1 (5%)	22,30,33	0.61	0
1	PSU	L5	3770	1	18,21,22	1.44	3 (16%)	22,30,33	1.92	3 (13%)
46	A2M	S2	484	46	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
46	PSU	S2	109	46	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
46	PSU	S2	36	46	18,21,22	0.86	1 (5%)	22,30,33	0.63	0
46	PSU	S2	1625	46	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
46	OMG	S2	601	46	23,26,27	1.20	3 (13%)	33,38,41	1.89	6 (18%)
1	A2M	L5	2815	1	22,25,26	1.47	4 (18%)	31,36,39	2.09	7 (22%)
46	MA6	S2	1851	46	23,26,27	1.47	5 (21%)	34,38,41	2.16	11 (32%)
1	OMC	L5	2351	80,1	19,22,23	0.79	0	26,31,34	0.90	1 (3%)
46	PSU	S2	801	46	18,21,22	0.86	1 (5%)	22,30,33	0.62	0
1	OMG	L5	3792	1	23,26,27	1.20	3 (13%)	33,38,41	2.05	7 (21%)
1	PSU	L5	4431	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	UY1	L5	3818	1,81	19,22,23	0.22	0	22,31,34	0.50	0
46	PSU	S2	815	46	18,21,22	1.32	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	L5	1862	1	18,21,22	1.35	2 (11%)	22,30,33	1.96	4 (18%)
46	PSU	S2	649	46	18,21,22	1.38	2 (11%)	22,30,33	1.95	3 (13%)
1	PSU	L5	4972	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
46	A2M	S2	1031	46	22,25,26	1.41	4 (18%)	31,36,39	2.13	11 (35%)
46	OMG	S2	1447	46	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	L5	1781	1	18,21,22	1.33	2 (11%)	22,30,33	1.97	4 (18%)
1	OMC	L5	1881	80,1	19,22,23	0.28	0	26,31,34	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	S2	590	46	22,25,26	1.45	4 (18%)	31,36,39	2.19	8 (25%)
46	PSU	S2	822	46	18,21,22	0.87	1 (5%)	22,30,33	0.93	1 (4%)
1	OMG	L5	2424	1	23,26,27	1.21	3 (13%)	33,38,41	1.87	6 (18%)
46	A2M	S2	1678	46	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
1	OMG	L5	4637	1,81	23,26,27	1.23	3 (13%)	33,38,41	1.89	5 (15%)
1	A2M	L5	3718	1	22,25,26	1.46	5 (22%)	31,36,39	2.01	9 (29%)
3	OMU	L8	14	1,3	19,22,23	1.22	3 (15%)	26,31,34	1.67	5 (19%)
1	PSU	L5	4500	1	18,21,22	0.87	1 (5%)	22,30,33	0.60	0
46	PSU	S2	105	46	18,21,22	1.36	2 (11%)	22,30,33	1.95	3 (13%)
1	PSU	L5	3768	1	18,21,22	1.37	3 (16%)	22,30,33	1.97	3 (13%)
46	PSU	S2	814	46	18,21,22	1.35	3 (16%)	22,30,33	1.84	3 (13%)
1	PSU	L5	2843	1	18,21,22	1.36	3 (16%)	22,30,33	1.80	4 (18%)
46	OMC	S2	1272	46	19,22,23	0.81	0	26,31,34	0.86	1 (3%)
1	PSU	L5	4636	1	18,21,22	1.36	2 (11%)	22,30,33	2.01	5 (22%)
46	OMG	S2	644	46	23,26,27	1.19	3 (13%)	33,38,41	1.96	6 (18%)
1	OMG	L5	4494	1	23,26,27	1.23	3 (13%)	33,38,41	1.91	6 (18%)
46	PSU	S2	93	46	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
46	PSU	S2	1003	46	18,21,22	1.38	3 (16%)	22,30,33	1.85	3 (13%)
1	1MA	L5	1322	80,1	21,25,26	1.38	5 (23%)	31,37,40	1.65	4 (12%)
46	PSU	S2	1445	46	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
46	A2M	S2	27	46,80	22,25,26	1.41	4 (18%)	31,36,39	2.18	11 (35%)
46	PSU	S2	1046	46	18,21,22	1.39	3 (16%)	22,30,33	1.94	4 (18%)
1	A2M	L5	398	1	22,25,26	1.48	4 (18%)	31,36,39	2.13	9 (29%)
1	OMG	L5	1625	1,81	23,26,27	1.21	3 (13%)	33,38,41	1.90	6 (18%)
1	PSU	L5	1792	1,81	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	L5	3762	1	18,21,22	0.83	1 (5%)	22,30,33	0.64	0
1	OMG	L5	4196	80,1	23,26,27	1.18	3 (13%)	33,38,41	1.90	6 (18%)
1	A2M	L5	4523	80,1	22,25,26	1.46	4 (18%)	31,36,39	2.24	11 (35%)
46	PSU	S2	866	46	18,21,22	0.89	1 (5%)	22,30,33	0.96	1 (4%)
46	PSU	S2	1360	46,80,81	18,21,22	0.88	1 (5%)	22,30,33	0.80	1 (4%)
1	PSU	L5	3822	1	18,21,22	1.46	3 (16%)	22,30,33	1.93	5 (22%)
46	OMC	S2	1391	46	19,22,23	0.79	0	26,31,34	0.78	0
1	PSU	L5	4973	1	18,21,22	1.31	2 (11%)	22,30,33	1.83	3 (13%)
46	PSU	S2	119	46	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	L5	4293	1	18,21,22	0.88	1 (5%)	22,30,33	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	3730	1	18,21,22	0.87	1 (5%)	22,30,33	0.66	0
1	A2M	L5	2363	80,1	22,25,26	1.47	4 (18%)	31,36,39	2.01	9 (29%)
1	OMC	L5	2422	80,1	19,22,23	0.83	0	26,31,34	0.76	0
1	PSU	L5	4673	1,81	18,21,22	0.89	1 (5%)	22,30,33	0.56	0
1	PSU	L5	1582	1	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
46	PSU	S2	100	46,80	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
1	A2M	L5	2787	80,1	22,25,26	1.46	4 (18%)	31,36,39	2.08	8 (25%)
46	PSU	S2	218	46	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	L5	3884	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
46	OMG	S2	1328	46,81	23,26,27	0.31	0	33,38,41	0.36	0
1	PSU	L5	4689	1	18,21,22	1.33	2 (11%)	22,30,33	1.99	3 (13%)
1	PSU	L5	3764	1	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
1	A2M	L5	4590	1	22,25,26	1.46	4 (18%)	31,36,39	2.15	11 (35%)
46	PSU	S2	572	46	18,21,22	1.36	2 (11%)	22,30,33	1.84	4 (18%)
1	OMG	L5	3744	1	23,26,27	1.21	4 (17%)	33,38,41	1.93	6 (18%)
1	OMC	L5	4536	1	19,22,23	0.79	0	26,31,34	0.79	0
46	PSU	S2	1186	46	18,21,22	0.88	1 (5%)	22,30,33	0.73	0
1	OMC	L5	2824	1	19,22,23	0.79	0	26,31,34	0.68	0
1	PSU	L5	2508	1	18,21,22	1.34	3 (16%)	22,30,33	1.89	3 (13%)
46	PSU	S2	1056	46	18,21,22	1.47	3 (16%)	22,30,33	1.94	4 (18%)
46	PSU	S2	300	46	18,21,22	1.32	2 (11%)	22,30,33	1.90	4 (18%)
1	OMC	L5	3869	1	19,22,23	0.82	0	26,31,34	0.80	0
46	PSU	S2	1232	46	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	L5	4361	1	18,21,22	1.34	2 (11%)	22,30,33	1.98	4 (18%)
46	OMU	S2	121	46	19,22,23	1.20	3 (15%)	26,31,34	1.69	5 (19%)
46	A2M	S2	468	46	22,25,26	1.47	4 (18%)	31,36,39	2.07	10 (32%)
46	PSU	S2	1174	46	18,21,22	1.37	2 (11%)	22,30,33	2.04	3 (13%)
1	PSU	L5	2632	1	18,21,22	0.86	1 (5%)	22,30,33	0.60	0
46	OMG	S2	1490	46,80	23,26,27	1.18	3 (13%)	33,38,41	1.91	7 (21%)
1	OMG	L5	3627	1	23,26,27	1.18	3 (13%)	33,38,41	2.07	7 (21%)
46	A2M	S2	668	46,80	22,25,26	0.21	0	31,36,39	0.44	0
46	B8N	S2	1248	46	24,29,30	0.95	1 (4%)	29,42,45	1.53	6 (20%)
1	PSU	L5	4457	1	18,21,22	1.39	2 (11%)	22,30,33	1.96	3 (13%)
46	OMC	S2	462	46	19,22,23	0.82	0	26,31,34	0.76	0
1	A2M	L5	3724	1	22,25,26	0.18	0	31,36,39	0.32	0
1	A2M	L5	1323	1	22,25,26	1.45	4 (18%)	31,36,39	2.08	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L5	4392	1	23,26,27	1.19	3 (13%)	33,38,41	1.97	7 (21%)
46	PSU	S2	863	46	18,21,22	0.88	1 (5%)	22,30,33	0.59	0
1	PSU	L5	4403	1	18,21,22	1.33	3 (16%)	22,30,33	1.94	4 (18%)
1	PSU	L5	4471	1	18,21,22	1.40	2 (11%)	22,30,33	1.83	3 (13%)
1	OMU	L5	4620	1	19,22,23	1.20	3 (15%)	26,31,34	1.69	5 (19%)
46	OMC	S2	517	46	19,22,23	0.79	0	26,31,34	0.72	0
1	OMU	L5	2837	1	19,22,23	1.20	2 (10%)	26,31,34	1.82	5 (19%)
1	OMG	L5	4499	1	23,26,27	0.30	0	33,38,41	0.45	0
46	PSU	S2	1177	46	18,21,22	1.33	2 (11%)	22,30,33	1.97	4 (18%)
46	PSU	S2	1643	46,80	18,21,22	1.37	2 (11%)	22,30,33	1.88	4 (18%)
1	PSU	L5	2839	1	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
1	A2M	L5	400	1	22,25,26	1.47	4 (18%)	31,36,39	2.04	8 (25%)
1	PSU	L5	3853	80,1	18,21,22	1.33	2 (11%)	22,30,33	1.75	3 (13%)
46	OMU	S2	172	46	19,22,23	1.17	2 (10%)	26,31,34	1.80	5 (19%)
1	6MZ	L5	4220	1	22,25,26	1.39	4 (18%)	30,36,39	2.18	9 (30%)
1	PSU	L5	3637	1,81	18,21,22	0.86	1 (5%)	22,30,33	0.78	0
1	PSU	L5	4423	1	18,21,22	1.36	3 (16%)	22,30,33	1.92	3 (13%)
1	PSU	L5	1744	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
46	PSU	S2	1004	46	18,21,22	1.42	3 (16%)	22,30,33	1.91	3 (13%)
1	OMC	L5	3808	1	19,22,23	0.80	0	26,31,34	0.75	1 (3%)
46	PSU	S2	296	46	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	L5	4532	1	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
1	PSU	L5	4576	1	18,21,22	0.88	1 (5%)	22,30,33	0.61	0
46	PSU	S2	406	46	18,21,22	1.38	3 (16%)	22,30,33	1.89	3 (13%)
1	A2M	L5	4571	1	22,25,26	1.46	4 (18%)	31,36,39	2.06	9 (29%)
46	OMG	S2	509	46,80	23,26,27	1.20	3 (13%)	33,38,41	1.98	6 (18%)
46	A2M	S2	159	46	22,25,26	1.47	4 (18%)	31,36,39	2.15	10 (32%)
59	NMM	ST	67	59	9,11,12	1.54	1 (11%)	6,12,14	3.83	2 (33%)
46	OMC	S2	174	46	19,22,23	0.79	0	26,31,34	0.73	0
1	PSU	L5	3639	1	18,21,22	0.92	1 (5%)	22,30,33	0.63	0
46	A2M	S2	512	46	22,25,26	1.47	4 (18%)	31,36,39	2.24	9 (29%)
46	PSU	S2	1367	46	18,21,22	1.39	2 (11%)	22,30,33	1.91	4 (18%)
1	A2M	L5	1524	1	22,25,26	1.46	4 (18%)	31,36,39	2.10	7 (22%)
1	OMC	L5	2861	1	19,22,23	0.78	0	26,31,34	0.58	0
1	OMG	L5	4623	1	23,26,27	1.17	3 (13%)	33,38,41	1.91	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	S2	166	46	22,25,26	1.49	4 (18%)	31,36,39	2.14	8 (25%)
1	A2M	L5	3830	1	22,25,26	1.48	4 (18%)	31,36,39	2.20	9 (29%)
46	OMU	S2	354	46	19,22,23	1.22	2 (10%)	26,31,34	1.81	5 (19%)
46	OMG	S2	867	46	23,26,27	0.31	0	33,38,41	0.37	0
46	OMC	S2	1703	46	19,22,23	0.79	0	26,31,34	0.80	0
1	UR3	L5	4530	1	19,22,23	0.27	0	26,32,35	0.62	0
1	OMU	L5	4498	80,1	19,22,23	0.21	0	26,31,34	0.47	0
1	OMG	L5	4228	1	23,26,27	1.17	4 (17%)	33,38,41	1.92	6 (18%)
46	OMU	S2	1804	46	19,22,23	0.21	0	26,31,34	0.43	0
46	OMG	S2	683	46	23,26,27	0.30	0	33,38,41	0.50	0
1	PSU	L5	1683	1,81	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)

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
46	OMU	S2	116	46	-	1/9/27/28	0/2/2/2
46	4AC	S2	1337	46	-	0/11/29/30	0/2/2/2
1	PSU	L5	3851	1	-	2/7/25/26	0/2/2/2
1	OMG	L5	2876	1	-	0/9/27/28	0/3/3/3
46	A2M	S2	1383	46	-	3/9/27/28	0/3/3/3
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
1	PSU	L5	4552	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	1340	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	966	46	-	2/7/25/26	0/2/2/2
1	PSU	L5	4521	80,1,81	-	0/7/25/26	0/2/2/2
46	PSU	S2	1244	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	1534	80,1	-	2/9/27/28	0/3/3/3
46	PSU	S2	609	46	-	0/7/25/26	0/2/2/2
29	V5N	La	39	29	-	0/9/10/12	0/1/1/1
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4296	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	667	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	1442	46,80	-	1/9/27/28	0/2/2/2
1	PSU	L5	4353	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	99	46,80	-	0/9/27/28	0/3/3/3
1	OMG	L5	4618	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	2364	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	3841	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	3844	1	-	2/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
1	OMG	L5	3899	1	-	0/9/27/28	0/3/3/3
46	PSU	S2	1692	46	-	0/7/25/26	0/2/2/2
1	OMG	L5	1522	1	-	0/9/27/28	0/3/3/3
1	OMU	L5	2415	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	4312	1	-	0/7/25/26	0/2/2/2
46	OMU	S2	428	46	-	6/9/27/28	0/2/2/2
1	PSU	L5	1536	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	3925	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	4370	1	-	0/9/27/28	0/3/3/3
46	A2M	S2	576	46	-	2/9/27/28	0/3/3/3
1	OMC	L5	2365	80,1	-	0/9/27/28	0/2/2/2
1	PSU	L5	3715	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4456	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	2401	1	-	0/9/27/28	0/3/3/3
46	PSU	S2	651	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3695	1,81	-	0/7/25/26	0/2/2/2
46	PSU	S2	34	46	-	0/7/25/26	0/2/2/2
46	OMU	S2	1288	46	-	0/9/27/28	0/2/2/2
1	OMG	L5	1316	1,81	-	0/9/27/28	0/3/3/3
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
72	IAS	SO	138	72	-	1/7/7/8	-
46	PSU	S2	1347	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1779	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	686	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	1326	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3920	80,1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1596	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	5010	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	5001	1	-	0/7/25/26	0/2/2/2
46	OMG	S2	436	46	-	0/9/27/28	0/3/3/3
1	OMU	L5	4227	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	3785	80,1	-	1/9/27/28	0/3/3/3
1	PSU	L5	4493	1,81	-	0/7/25/26	0/2/2/2
1	OMC	L5	2804	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	1238	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	918	46	-	0/7/25/26	0/2/2/2
1	5MC	L5	4447	1,81	-	4/7/25/26	0/2/2/2
1	PSU	L5	1860	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	4AC	S2	1842	46	-	0/11/29/30	0/2/2/2
1	A2M	L5	3825	1	-	0/9/27/28	0/3/3/3
46	UY1	S2	1326	46,80	-	2/9/27/28	0/2/2/2
46	PSU	S2	681	46	-	0/7/25/26	0/2/2/2
46	6MZ	S2	1832	46,80,81	-	1/9/27/28	0/3/3/3
46	PSU	S2	1136	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4299	1	-	0/7/25/26	0/2/2/2
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2
1	A2M	L5	3867	1	-	1/9/27/28	0/3/3/3
1	5MC	L5	3782	80,1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1045	46	-	0/7/25/26	0/2/2/2
1	OMC	L5	3887	1	-	1/9/27/28	0/2/2/2
46	PSU	S2	63	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1677	1	-	2/7/25/26	0/2/2/2
46	MA6	S2	1850	46	-	0/11/29/30	0/3/3/3
1	A2M	L5	1871	80,1	-	0/9/27/28	0/3/3/3
3	OMG	L8	75	3	-	0/9/27/28	0/3/3/3
46	PSU	S2	366	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1782	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	3701	1,81	-	4/9/27/28	0/2/2/2
1	PSU	L5	4579	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3770	1	-	2/7/25/26	0/2/2/2
46	A2M	S2	484	46	-	0/9/27/28	0/3/3/3
46	PSU	S2	109	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	36	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1625	46	-	0/7/25/26	0/2/2/2
46	OMG	S2	601	46	-	0/9/27/28	0/3/3/3
1	A2M	L5	2815	1	-	4/9/27/28	0/3/3/3
46	MA6	S2	1851	46	-	3/11/29/30	0/3/3/3
1	OMC	L5	2351	80,1	-	2/9/27/28	0/2/2/2
46	PSU	S2	801	46	-	2/7/25/26	0/2/2/2
1	OMG	L5	3792	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4431	1	-	0/7/25/26	0/2/2/2
1	UY1	L5	3818	1,81	-	6/9/27/28	0/2/2/2
46	PSU	S2	815	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	1862	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	649	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4972	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	1031	46	-	1/9/27/28	0/3/3/3
46	OMG	S2	1447	46	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	1781	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	1881	80,1	-	0/9/27/28	0/2/2/2
46	A2M	S2	590	46	-	3/9/27/28	0/3/3/3
46	PSU	S2	822	46	-	2/7/25/26	0/2/2/2
1	OMG	L5	2424	1	-	0/9/27/28	0/3/3/3
46	A2M	S2	1678	46	-	1/9/27/28	0/3/3/3
1	OMG	L5	4637	1,81	-	1/9/27/28	0/3/3/3
1	A2M	L5	3718	1	-	1/9/27/28	0/3/3/3
3	OMU	L8	14	1,3	-	1/9/27/28	0/2/2/2
1	PSU	L5	4500	1	-	5/7/25/26	0/2/2/2
46	PSU	S2	105	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3768	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	814	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	2843	1	-	0/7/25/26	0/2/2/2
46	OMC	S2	1272	46	-	1/9/27/28	0/2/2/2
1	PSU	L5	4636	1	-	4/7/25/26	0/2/2/2
46	OMG	S2	644	46	-	1/9/27/28	0/3/3/3
1	OMG	L5	4494	1	-	1/9/27/28	0/3/3/3
46	PSU	S2	93	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1003	46	-	0/7/25/26	0/2/2/2
1	1MA	L5	1322	80,1	-	2/7/25/26	0/3/3/3
46	PSU	S2	1445	46	-	0/7/25/26	0/2/2/2
46	A2M	S2	27	46,80	-	1/9/27/28	0/3/3/3
46	PSU	S2	1046	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	398	1	-	1/9/27/28	0/3/3/3
1	OMG	L5	1625	1,81	-	1/9/27/28	0/3/3/3
1	PSU	L5	1792	1,81	-	1/7/25/26	0/2/2/2
1	PSU	L5	3762	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4196	80,1	-	1/9/27/28	0/3/3/3
1	A2M	L5	4523	80,1	-	0/9/27/28	0/3/3/3
46	PSU	S2	866	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1360	46,80,81	-	0/7/25/26	0/2/2/2
1	PSU	L5	3822	1	-	0/7/25/26	0/2/2/2
46	OMC	S2	1391	46	-	0/9/27/28	0/2/2/2
1	PSU	L5	4973	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	119	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3730	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2363	80,1	-	2/9/27/28	0/3/3/3
1	OMC	L5	2422	80,1	-	1/9/27/28	0/2/2/2
1	PSU	L5	4673	1,81	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	1582	1	-	2/7/25/26	0/2/2/2
46	PSU	S2	100	46,80	-	2/7/25/26	0/2/2/2
1	A2M	L5	2787	80,1	-	3/9/27/28	0/3/3/3
46	PSU	S2	218	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	3884	1	-	0/7/25/26	0/2/2/2
46	OMG	S2	1328	46,81	-	0/9/27/28	0/3/3/3
1	PSU	L5	4689	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3764	1	-	2/7/25/26	0/2/2/2
1	A2M	L5	4590	1	-	1/9/27/28	0/3/3/3
46	PSU	S2	572	46	-	0/7/25/26	0/2/2/2
1	OMG	L5	3744	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	4536	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	1186	46	-	0/7/25/26	0/2/2/2
1	OMC	L5	2824	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	2508	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1056	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	300	46	-	0/7/25/26	0/2/2/2
1	OMC	L5	3869	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	1232	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4361	1	-	0/7/25/26	0/2/2/2
46	OMU	S2	121	46	-	1/9/27/28	0/2/2/2
46	A2M	S2	468	46	-	1/9/27/28	0/3/3/3
46	PSU	S2	1174	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	2632	1	-	0/7/25/26	0/2/2/2
46	OMG	S2	1490	46,80	-	3/9/27/28	0/3/3/3
1	OMG	L5	3627	1	-	0/9/27/28	0/3/3/3
46	A2M	S2	668	46,80	-	3/9/27/28	0/3/3/3
46	B8N	S2	1248	46	-	3/16/34/35	0/2/2/2
1	PSU	L5	4457	1	-	0/7/25/26	0/2/2/2
46	OMC	S2	462	46	-	0/9/27/28	0/2/2/2
1	A2M	L5	3724	1	-	3/9/27/28	0/3/3/3
1	A2M	L5	1323	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	4392	1	-	0/9/27/28	0/3/3/3
46	PSU	S2	863	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4403	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4471	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
46	OMC	S2	517	46	-	0/9/27/28	0/2/2/2
1	OMU	L5	2837	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	4499	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PSU	S2	1177	46	-	0/7/25/26	0/2/2/2
46	PSU	S2	1643	46,80	-	0/7/25/26	0/2/2/2
1	PSU	L5	2839	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	400	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3853	80,1	-	0/7/25/26	0/2/2/2
46	OMU	S2	172	46	-	0/9/27/28	0/2/2/2
1	6MZ	L5	4220	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	3637	1,81	-	0/7/25/26	0/2/2/2
1	PSU	L5	4423	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1744	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	1004	46	-	0/7/25/26	0/2/2/2
1	OMC	L5	3808	1	-	0/9/27/28	0/2/2/2
46	PSU	S2	296	46	-	0/7/25/26	0/2/2/2
1	PSU	L5	4532	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4576	1	-	0/7/25/26	0/2/2/2
46	PSU	S2	406	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	4571	1	-	1/9/27/28	0/3/3/3
46	OMG	S2	509	46,80	-	0/9/27/28	0/3/3/3
46	A2M	S2	159	46	-	2/9/27/28	0/3/3/3
59	NMM	ST	67	59	-	0/9/11/13	-
46	OMC	S2	174	46	-	0/9/27/28	0/2/2/2
1	PSU	L5	3639	1	-	0/7/25/26	0/2/2/2
46	A2M	S2	512	46	-	2/9/27/28	0/3/3/3
46	PSU	S2	1367	46	-	0/7/25/26	0/2/2/2
1	A2M	L5	1524	1	-	1/9/27/28	0/3/3/3
1	OMC	L5	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	4623	1	-	0/9/27/28	0/3/3/3
46	A2M	S2	166	46	-	2/9/27/28	0/3/3/3
1	A2M	L5	3830	1	-	0/9/27/28	0/3/3/3
46	OMU	S2	354	46	-	0/9/27/28	0/2/2/2
46	OMG	S2	867	46	-	1/9/27/28	0/3/3/3
46	OMC	S2	1703	46	-	0/9/27/28	0/2/2/2
1	UR3	L5	4530	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	4498	80,1	-	0/9/27/28	0/2/2/2
1	OMG	L5	4228	1	-	0/9/27/28	0/3/3/3
46	OMU	S2	1804	46	-	0/9/27/28	0/2/2/2
46	OMG	S2	683	46	-	0/9/27/28	0/3/3/3
1	PSU	L5	1683	1,81	-	0/7/25/26	0/2/2/2

All (477) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	La	39	V5N	CG-ND1	-6.34	1.31	1.37
46	S2	166	A2M	C5-C4	4.65	1.47	1.39
46	S2	1832	6MZ	C5-C4	4.55	1.47	1.39
46	S2	159	A2M	C5-C4	4.53	1.47	1.39
46	S2	484	A2M	C5-C4	4.50	1.47	1.39
1	L5	1534	A2M	C5-C4	4.48	1.47	1.39
1	L5	2815	A2M	C5-C4	4.46	1.47	1.39
1	L5	398	A2M	C5-C4	4.45	1.47	1.39
1	L5	2401	A2M	C5-C4	4.44	1.47	1.39
1	L5	3718	A2M	C5-C4	4.44	1.47	1.39
1	L5	4523	A2M	C5-C4	4.43	1.47	1.39
1	L5	400	A2M	C5-C4	4.43	1.47	1.39
1	L5	4590	A2M	C5-C4	4.43	1.47	1.39
46	S2	1678	A2M	C5-C4	4.42	1.47	1.39
46	S2	1851	MA6	C5-C4	4.40	1.47	1.39
1	L5	1524	A2M	C5-C4	4.39	1.47	1.39
1	L5	4220	6MZ	C5-C4	4.39	1.47	1.39
1	L5	4571	A2M	C5-C4	4.39	1.47	1.39
1	L5	3867	A2M	C5-C4	4.37	1.47	1.39
46	S2	1383	A2M	C5-C4	4.37	1.47	1.39
1	L5	2787	A2M	C5-C4	4.37	1.47	1.39
46	S2	512	A2M	C5-C4	4.37	1.47	1.39
46	S2	590	A2M	C5-C4	4.35	1.47	1.39
1	L5	2363	A2M	C5-C4	4.35	1.47	1.39
1	L5	1871	A2M	C5-C4	4.34	1.47	1.39
1	L5	1323	A2M	C5-C4	4.34	1.47	1.39
46	S2	468	A2M	C5-C4	4.34	1.47	1.39
1	L5	1326	A2M	C5-C4	4.32	1.47	1.39
1	L5	3830	A2M	C5-C4	4.28	1.47	1.39
46	S2	576	A2M	C5-C4	4.16	1.46	1.39
46	S2	27	A2M	C5-C4	4.15	1.46	1.39
46	S2	1850	MA6	C5-C4	4.14	1.46	1.39
59	ST	67	NMM	CZ-NH2	4.14	1.44	1.34
1	L5	3825	A2M	C5-C4	4.13	1.46	1.39
46	S2	1031	A2M	C5-C4	4.01	1.46	1.39
29	La	39	V5N	CD2-NE2	-3.90	1.31	1.37
1	L5	3639	PSU	C6-C5	3.60	1.39	1.35
46	S2	866	PSU	C6-C5	3.44	1.39	1.35
1	L5	4296	PSU	C6-C5	3.44	1.39	1.35
3	L8	69	PSU	C6-C5	3.43	1.39	1.35
1	L5	4293	PSU	C6-C5	3.42	1.39	1.35
46	S2	863	PSU	C6-C5	3.41	1.39	1.35
1	L5	4579	PSU	C6-C5	3.41	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4576	PSU	C6-C5	3.41	1.39	1.35
1	L5	4532	PSU	C6-C5	3.40	1.39	1.35
46	S2	1244	PSU	C6-C5	3.40	1.39	1.35
46	S2	1360	PSU	C6-C5	3.39	1.39	1.35
46	S2	1596	PSU	C6-C5	3.38	1.39	1.35
1	L5	3764	PSU	C6-C5	3.38	1.39	1.35
46	S2	609	PSU	C6-C5	3.37	1.39	1.35
46	S2	822	PSU	C6-C5	3.37	1.39	1.35
1	L5	2632	PSU	C6-C5	3.37	1.39	1.35
1	L5	4673	PSU	C6-C5	3.37	1.39	1.35
46	S2	34	PSU	C6-C5	3.36	1.39	1.35
1	L5	3822	PSU	C4-N3	-3.36	1.32	1.38
1	L5	5010	PSU	C6-C5	3.36	1.39	1.35
1	L5	4493	PSU	C6-C5	3.36	1.39	1.35
46	S2	1347	PSU	C6-C5	3.36	1.39	1.35
1	L5	4299	PSU	C6-C5	3.35	1.39	1.35
46	S2	667	PSU	C6-C5	3.35	1.39	1.35
46	S2	1136	PSU	C6-C5	3.35	1.39	1.35
46	S2	100	PSU	C6-C5	3.34	1.39	1.35
1	L5	2839	PSU	C6-C5	3.33	1.39	1.35
46	S2	1056	PSU	C4-N3	-3.33	1.32	1.38
46	S2	801	PSU	C6-C5	3.33	1.39	1.35
46	S2	1186	PSU	C6-C5	3.32	1.39	1.35
1	L5	3884	PSU	C6-C5	3.32	1.39	1.35
1	L5	4500	PSU	C6-C5	3.31	1.39	1.35
1	L5	3730	PSU	C6-C5	3.31	1.39	1.35
46	S2	966	PSU	C6-C5	3.31	1.39	1.35
1	L5	3637	PSU	C6-C5	3.30	1.39	1.35
46	S2	36	PSU	C6-C5	3.29	1.39	1.35
1	L5	4552	PSU	C6-C5	3.29	1.39	1.35
46	S2	1174	PSU	C6-C5	3.25	1.39	1.35
46	S2	686	PSU	C6-C5	3.24	1.39	1.35
1	L5	5001	PSU	C6-C5	3.24	1.39	1.35
46	S2	296	PSU	C6-C5	3.22	1.39	1.35
46	S2	1232	PSU	C6-C5	3.21	1.39	1.35
1	L5	3762	PSU	C6-C5	3.20	1.39	1.35
1	L5	4457	PSU	C6-C5	3.20	1.39	1.35
1	L5	4353	PSU	C6-C5	3.20	1.39	1.35
46	S2	1692	PSU	C6-C5	3.20	1.39	1.35
46	S2	93	PSU	C6-C5	3.19	1.39	1.35
1	L5	4471	PSU	C6-C5	3.19	1.39	1.35
1	L5	1536	PSU	C6-C5	3.17	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3770	PSU	C6-C5	3.17	1.39	1.35
1	L5	1779	PSU	C6-C5	3.16	1.39	1.35
46	S2	406	PSU	C6-C5	3.15	1.39	1.35
1	L5	1782	PSU	C6-C5	3.15	1.39	1.35
46	S2	109	PSU	C6-C5	3.14	1.39	1.35
1	L5	4423	PSU	C6-C5	3.13	1.39	1.35
46	S2	1238	PSU	C6-C5	3.12	1.39	1.35
1	L5	1792	PSU	C6-C5	3.12	1.39	1.35
1	L5	3920	PSU	C6-C5	3.12	1.39	1.35
3	L8	55	PSU	C6-C5	3.11	1.38	1.35
1	L5	3851	PSU	C6-C5	3.11	1.38	1.35
46	S2	1248	B8N	C6-C5	3.11	1.39	1.34
46	S2	1445	PSU	C6-C5	3.10	1.38	1.35
1	L5	1625	OMG	C5-C4	3.10	1.47	1.38
46	S2	649	PSU	C6-C5	3.10	1.38	1.35
1	L5	4431	PSU	C6-C5	3.10	1.38	1.35
1	L5	4494	OMG	C5-C4	3.08	1.47	1.38
1	L5	4637	OMG	C5-C4	3.08	1.47	1.38
1	L5	4973	PSU	C6-C5	3.06	1.38	1.35
46	S2	1367	PSU	C4-N3	-3.06	1.33	1.38
46	S2	1447	OMG	C5-C4	3.05	1.47	1.38
46	S2	1625	PSU	C6-C5	3.05	1.38	1.35
1	L5	3715	PSU	C4-N3	-3.05	1.33	1.38
1	L5	4636	PSU	C6-C5	3.05	1.38	1.35
3	L8	75	OMG	C5-C4	3.04	1.47	1.38
1	L5	3899	OMG	C5-C4	3.03	1.47	1.38
1	L5	3844	PSU	C6-C5	3.02	1.38	1.35
1	L5	1683	PSU	C6-C5	3.02	1.38	1.35
1	L5	4196	OMG	C5-C4	3.02	1.47	1.38
1	L5	1862	PSU	C6-C5	3.02	1.38	1.35
1	L5	4628	PSU	C6-C5	3.02	1.38	1.35
46	S2	63	PSU	C6-C5	3.01	1.38	1.35
1	L5	3770	PSU	C4-N3	-3.01	1.33	1.38
46	S2	366	PSU	C4-N3	-3.01	1.33	1.38
46	S2	1045	PSU	C4-N3	-3.00	1.33	1.38
1	L5	4972	PSU	C6-C5	3.00	1.38	1.35
1	L5	2843	PSU	C6-C5	3.00	1.38	1.35
1	L5	1744	PSU	C6-C5	2.99	1.38	1.35
5	LB	245	HIC	CD2-CG	2.99	1.41	1.36
46	S2	509	OMG	C5-C4	2.99	1.47	1.38
1	L5	4442	PSU	C6-C5	2.99	1.38	1.35
46	S2	601	OMG	C5-C4	2.98	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	2424	OMG	C5-C4	2.98	1.47	1.38
1	L5	1860	PSU	C6-C5	2.98	1.38	1.35
46	S2	1643	PSU	C6-C5	2.98	1.38	1.35
46	S2	218	PSU	C6-C5	2.97	1.38	1.35
46	S2	300	PSU	C6-C5	2.97	1.38	1.35
1	L5	4392	OMG	C5-C4	2.97	1.47	1.38
1	L5	4493	PSU	C4-N3	-2.96	1.33	1.38
46	S2	572	PSU	C6-C5	2.96	1.38	1.35
46	S2	644	OMG	C5-C4	2.96	1.47	1.38
46	S2	63	PSU	C4-N3	-2.95	1.33	1.38
46	S2	1238	PSU	C4-N3	-2.95	1.33	1.38
1	L5	4361	PSU	C6-C5	2.95	1.38	1.35
46	S2	1004	PSU	C6-C5	2.94	1.38	1.35
46	S2	1367	PSU	C6-C5	2.94	1.38	1.35
1	L5	2364	OMG	C5-C4	2.94	1.46	1.38
1	L5	1322	1MA	C6-N6	2.93	1.35	1.28
1	L5	4370	OMG	C5-C4	2.93	1.46	1.38
46	S2	1046	PSU	C6-C5	2.93	1.38	1.35
1	L5	1860	PSU	C4-N3	-2.93	1.33	1.38
1	L5	1322	1MA	C5-C4	2.92	1.46	1.38
46	S2	814	PSU	C6-C5	2.92	1.38	1.35
1	L5	1316	OMG	C5-C4	2.92	1.46	1.38
1	L5	1781	PSU	C6-C5	2.91	1.38	1.35
1	L5	3853	PSU	C6-C5	2.91	1.38	1.35
46	S2	815	PSU	C6-C5	2.91	1.38	1.35
1	L5	3768	PSU	C4-N3	-2.91	1.33	1.38
46	S2	1177	PSU	C4-N3	-2.91	1.33	1.38
46	S2	436	OMG	C5-C4	2.91	1.46	1.38
46	S2	119	PSU	C6-C5	2.91	1.38	1.35
1	L5	4618	OMG	C5-C4	2.90	1.46	1.38
1	L5	3844	PSU	C4-N3	-2.89	1.33	1.38
46	S2	1031	A2M	C5-N7	-2.89	1.33	1.39
1	L5	1677	PSU	C6-C5	2.89	1.38	1.35
46	S2	1003	PSU	C6-C5	2.89	1.38	1.35
46	S2	105	PSU	C6-C5	2.88	1.38	1.35
1	L5	4228	OMG	C5-C4	2.88	1.46	1.38
46	S2	918	PSU	C6-C5	2.88	1.38	1.35
1	L5	2839	PSU	C4-N3	-2.88	1.33	1.38
1	L5	1779	PSU	C4-N3	-2.88	1.33	1.38
46	S2	366	PSU	C6-C5	2.87	1.38	1.35
46	S2	1004	PSU	C4-N3	-2.87	1.33	1.38
1	L5	2876	OMG	C5-C4	2.87	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	93	PSU	C4-N3	-2.86	1.33	1.38
1	L5	2508	PSU	C4-N3	-2.86	1.33	1.38
1	L5	2843	PSU	C4-N3	-2.86	1.33	1.38
1	L5	1582	PSU	C6-C5	2.86	1.38	1.35
46	S2	1046	PSU	C4-N3	-2.86	1.33	1.38
46	S2	1692	PSU	C4-N3	-2.86	1.33	1.38
1	L5	4521	PSU	C6-C5	2.85	1.38	1.35
46	S2	296	PSU	C4-N3	-2.85	1.33	1.38
1	L5	4623	OMG	C5-C4	2.85	1.46	1.38
1	L5	1862	PSU	C4-N3	-2.84	1.33	1.38
1	L5	2508	PSU	C6-C5	2.84	1.38	1.35
46	S2	649	PSU	C4-N3	-2.84	1.33	1.38
1	L5	1522	OMG	C5-C4	2.84	1.46	1.38
46	S2	651	PSU	C6-C5	2.84	1.38	1.35
46	S2	1851	MA6	C5-C6	2.84	1.49	1.41
46	S2	1445	PSU	C4-N3	-2.83	1.33	1.38
1	L5	4972	PSU	C4-N3	-2.83	1.33	1.38
1	L5	3744	OMG	C6-N1	-2.83	1.33	1.38
1	L5	3695	PSU	C6-C5	2.82	1.38	1.35
46	S2	1174	PSU	C4-N3	-2.82	1.33	1.38
46	S2	1003	PSU	C4-N3	-2.82	1.33	1.38
1	L5	4521	PSU	C4-N3	-2.82	1.33	1.38
46	S2	484	A2M	C5-C6	2.82	1.48	1.41
1	L5	3792	OMG	C6-N1	-2.81	1.33	1.38
46	S2	651	PSU	C4-N3	-2.81	1.33	1.38
1	L5	1782	PSU	C4-N3	-2.81	1.33	1.38
1	L5	4312	PSU	C6-C5	2.81	1.38	1.35
3	L8	55	PSU	C4-N3	-2.81	1.33	1.38
1	L5	1781	PSU	C4-N3	-2.81	1.33	1.38
46	S2	1045	PSU	C6-C5	2.80	1.38	1.35
46	S2	918	PSU	C4-N3	-2.80	1.33	1.38
1	L5	3822	PSU	C6-C5	2.80	1.38	1.35
46	S2	814	PSU	C4-N3	-2.79	1.33	1.38
46	S2	105	PSU	C4-N3	-2.79	1.33	1.38
46	S2	1490	OMG	C5-C4	2.79	1.46	1.38
1	L5	3768	PSU	C6-C5	2.79	1.38	1.35
1	L5	4403	PSU	C6-C5	2.78	1.38	1.35
1	L5	4353	PSU	C4-N3	-2.78	1.33	1.38
1	L5	4423	PSU	C4-N3	-2.78	1.33	1.38
46	S2	681	PSU	C4-N3	-2.78	1.33	1.38
1	L5	1744	PSU	C4-N3	-2.78	1.33	1.38
46	S2	1643	PSU	C4-N3	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	681	PSU	C6-C5	2.77	1.38	1.35
1	L5	3695	PSU	C4-N3	-2.77	1.33	1.38
46	S2	109	PSU	C4-N3	-2.76	1.33	1.38
1	L5	4689	PSU	C6-C5	2.76	1.38	1.35
1	L5	1582	PSU	C4-N3	-2.76	1.33	1.38
1	L5	4637	OMG	C6-N1	-2.75	1.33	1.38
46	S2	354	OMU	C4-N3	-2.75	1.33	1.38
46	S2	300	PSU	C4-N3	-2.75	1.33	1.38
46	S2	572	PSU	C4-N3	-2.73	1.33	1.38
1	L5	3830	A2M	C5-N7	-2.73	1.33	1.39
1	L5	4403	PSU	C4-N3	-2.73	1.33	1.38
1	L5	1536	PSU	C4-N3	-2.72	1.33	1.38
1	L5	1625	OMG	C6-N1	-2.72	1.33	1.38
1	L5	4628	PSU	C4-N3	-2.71	1.33	1.38
1	L5	4442	PSU	C4-N3	-2.71	1.33	1.38
1	L5	3920	PSU	C4-N3	-2.71	1.33	1.38
1	L5	3782	5MC	C6-C5	2.71	1.39	1.34
1	L5	4431	PSU	C4-N3	-2.71	1.33	1.38
1	L5	3825	A2M	C5-N7	-2.71	1.33	1.39
1	L5	4306	OMU	C4-N3	-2.70	1.33	1.38
1	L5	4552	PSU	C4-N3	-2.70	1.33	1.38
1	L5	4471	PSU	C4-N3	-2.70	1.33	1.38
1	L5	3744	OMG	C5-C4	2.70	1.46	1.38
1	L5	3792	OMG	C5-C4	2.70	1.46	1.38
46	S2	1625	PSU	C4-N3	-2.70	1.33	1.38
1	L5	4361	PSU	C4-N3	-2.70	1.33	1.38
1	L5	4636	PSU	C4-N3	-2.70	1.33	1.38
46	S2	428	OMU	C4-N3	-2.69	1.33	1.38
1	L5	4689	PSU	C4-N3	-2.69	1.33	1.38
1	L5	4457	PSU	C4-N3	-2.69	1.33	1.38
46	S2	406	PSU	C4-N3	-2.69	1.33	1.38
1	L5	2363	A2M	C5-C6	2.69	1.48	1.41
1	L5	2787	A2M	C5-C6	2.68	1.48	1.41
1	L5	398	A2M	C5-C6	2.67	1.48	1.41
1	L5	4312	PSU	C4-N3	-2.67	1.33	1.38
1	L5	1534	A2M	C5-C6	2.67	1.48	1.41
46	S2	121	OMU	C4-N3	-2.67	1.33	1.38
46	S2	1832	6MZ	C5-C6	2.66	1.48	1.41
1	L5	4227	OMU	C4-N3	-2.66	1.33	1.38
1	L5	3830	A2M	C5-C6	2.66	1.48	1.41
1	L5	1524	A2M	C5-C6	2.66	1.48	1.41
1	L5	2424	OMG	C6-N1	-2.66	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1232	PSU	C4-N3	-2.66	1.33	1.38
1	L5	4571	A2M	C5-C6	2.65	1.48	1.41
46	S2	512	A2M	C5-C6	2.65	1.48	1.41
1	L5	1792	PSU	C4-N3	-2.65	1.33	1.38
1	L5	4590	A2M	C5-C6	2.64	1.48	1.41
46	S2	218	PSU	C4-N3	-2.64	1.33	1.38
1	L5	3627	OMG	C5-C4	2.64	1.46	1.38
1	L5	4494	OMG	C6-N1	-2.64	1.33	1.38
46	S2	1177	PSU	C6-C5	2.63	1.38	1.35
1	L5	4973	PSU	C4-N3	-2.62	1.34	1.38
1	L5	3884	PSU	C4-N3	-2.62	1.34	1.38
46	S2	119	PSU	C4-N3	-2.61	1.34	1.38
46	S2	468	A2M	C5-C6	2.61	1.48	1.41
1	L5	3853	PSU	C4-N3	-2.61	1.34	1.38
46	S2	1850	MA6	C4-N9	-2.61	1.31	1.37
3	L8	14	OMU	C4-N3	-2.61	1.33	1.38
1	L5	1323	A2M	C5-C6	2.61	1.48	1.41
1	L5	2837	OMU	C4-N3	-2.60	1.33	1.38
46	S2	1850	MA6	C5-C6	2.60	1.48	1.41
46	S2	644	OMG	C6-N1	-2.60	1.34	1.38
1	L5	1677	PSU	C4-N3	-2.60	1.34	1.38
46	S2	1383	A2M	C5-C6	2.60	1.48	1.41
46	S2	601	OMG	C6-N1	-2.60	1.34	1.38
46	S2	509	OMG	C6-N1	-2.59	1.34	1.38
1	L5	2876	OMG	C5-N7	-2.59	1.34	1.39
46	S2	1337	4AC	C4-N4	-2.59	1.36	1.39
46	S2	1442	OMU	C4-N3	-2.59	1.33	1.38
46	S2	590	A2M	C5-C6	2.58	1.48	1.41
46	S2	1678	A2M	C5-C6	2.58	1.48	1.41
1	L5	3627	OMG	C6-N1	-2.57	1.34	1.38
1	L5	1683	PSU	C4-N3	-2.57	1.34	1.38
46	S2	166	A2M	C5-C6	2.57	1.48	1.41
46	S2	172	OMU	C4-N3	-2.57	1.34	1.38
46	S2	436	OMG	C6-N1	-2.57	1.34	1.38
1	L5	4392	OMG	C6-N1	-2.57	1.34	1.38
1	L5	2815	A2M	C5-C6	2.57	1.48	1.41
1	L5	2415	OMU	C4-N3	-2.57	1.34	1.38
1	L5	2401	A2M	C5-C6	2.56	1.48	1.41
1	L5	4523	A2M	C5-C6	2.56	1.48	1.41
1	L5	3718	A2M	C5-C6	2.56	1.48	1.41
1	L5	3867	A2M	C5-C6	2.55	1.48	1.41
1	L5	4620	OMU	C4-N3	-2.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3792	OMG	C5-N7	-2.55	1.34	1.39
1	L5	2876	OMG	C6-N1	-2.54	1.34	1.38
46	S2	1056	PSU	C6-C5	2.54	1.38	1.35
46	S2	576	A2M	C5-C6	2.54	1.48	1.41
46	S2	815	PSU	C4-N3	-2.54	1.34	1.38
46	S2	27	A2M	C5-C6	2.53	1.48	1.41
1	L5	1871	A2M	C5-C6	2.53	1.48	1.41
46	S2	1288	OMU	C4-N3	-2.53	1.34	1.38
1	L5	1326	A2M	C5-C6	2.52	1.48	1.41
1	L5	3851	PSU	C4-N3	-2.52	1.34	1.38
46	S2	159	A2M	C5-C6	2.51	1.48	1.41
46	S2	1447	OMG	C6-N1	-2.51	1.34	1.38
1	L5	3715	PSU	C6-C5	2.50	1.38	1.35
1	L5	2364	OMG	C6-N1	-2.50	1.34	1.38
1	L5	3627	OMG	C5-N7	-2.50	1.34	1.39
46	S2	354	OMU	C2-N3	-2.49	1.33	1.38
3	L8	75	OMG	C6-N1	-2.48	1.34	1.38
46	S2	1383	A2M	C5-N7	-2.48	1.34	1.39
1	L5	1322	1MA	C5-N7	-2.48	1.34	1.39
46	S2	159	A2M	C5-N7	-2.48	1.34	1.39
1	L5	2424	OMG	C5-N7	-2.47	1.34	1.39
46	S2	918	PSU	O4'-C1'	-2.47	1.40	1.43
1	L5	3925	OMU	C4-N3	-2.47	1.34	1.38
46	S2	1490	OMG	C6-N1	-2.47	1.34	1.38
1	L5	400	A2M	C5-C6	2.47	1.48	1.41
1	L5	1316	OMG	C6-N1	-2.46	1.34	1.38
46	S2	116	OMU	C4-N3	-2.46	1.34	1.38
46	S2	590	A2M	C5-N7	-2.45	1.34	1.39
1	L5	1522	OMG	C6-N1	-2.44	1.34	1.38
1	L5	2815	A2M	C5-N7	-2.43	1.34	1.39
46	S2	576	A2M	C5-N7	-2.42	1.34	1.39
1	L5	4196	OMG	C6-N1	-2.42	1.34	1.38
1	L5	3822	PSU	C2-N3	-2.42	1.33	1.37
46	S2	1056	PSU	C2-N3	-2.42	1.33	1.37
46	S2	512	A2M	C8-N7	2.41	1.36	1.31
1	L5	4618	OMG	C6-N1	-2.40	1.34	1.38
1	L5	1323	A2M	C8-N7	2.39	1.36	1.31
1	L5	2363	A2M	C5-N7	-2.38	1.34	1.39
1	L5	1524	A2M	C5-N7	-2.37	1.34	1.39
46	S2	1678	A2M	C5-N7	-2.37	1.34	1.39
1	L5	4494	OMG	C5-N7	-2.36	1.34	1.39
1	L5	398	A2M	C5-N7	-2.36	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4227	OMU	C2-N3	-2.36	1.33	1.38
1	L5	398	A2M	C8-N7	2.35	1.36	1.31
1	L5	4523	A2M	C5-N7	-2.35	1.34	1.39
1	L5	4228	OMG	C6-N1	-2.35	1.34	1.38
46	S2	27	A2M	C8-N7	2.35	1.36	1.31
1	L5	4306	OMU	C2-N3	-2.35	1.33	1.38
1	L5	3718	A2M	C5-N7	-2.35	1.34	1.39
1	L5	1326	A2M	C5-N7	-2.34	1.34	1.39
1	L5	3867	A2M	C8-N7	2.34	1.36	1.31
46	S2	1842	4AC	C4-N4	-2.33	1.36	1.39
1	L5	3744	OMG	C5-N7	-2.33	1.34	1.39
1	L5	1322	1MA	C2-N3	2.33	1.35	1.30
1	L5	4590	A2M	C5-N7	-2.33	1.34	1.39
1	L5	3825	A2M	C5-C6	2.32	1.47	1.41
1	L5	2401	A2M	C5-N7	-2.31	1.34	1.39
1	L5	4220	6MZ	C5-C6	2.31	1.47	1.41
1	L5	2787	A2M	C5-N7	-2.31	1.34	1.39
1	L5	4623	OMG	C6-N1	-2.31	1.34	1.38
1	L5	4571	A2M	C8-N7	2.31	1.36	1.31
46	S2	1045	PSU	C2-N3	-2.30	1.33	1.37
46	S2	1447	OMG	C5-N7	-2.30	1.34	1.39
46	S2	468	A2M	C8-N7	2.30	1.35	1.31
1	L5	4220	6MZ	C5-N7	-2.30	1.34	1.39
46	S2	484	A2M	C5-N7	-2.29	1.34	1.39
46	S2	644	OMG	C5-N7	-2.29	1.34	1.39
1	L5	1625	OMG	C5-N7	-2.29	1.34	1.39
46	S2	512	A2M	C5-N7	-2.29	1.34	1.39
1	L5	4196	OMG	C5-N7	-2.29	1.34	1.39
46	S2	166	A2M	C5-N7	-2.28	1.34	1.39
1	L5	4370	OMG	C6-N1	-2.28	1.34	1.38
46	S2	601	OMG	C5-N7	-2.28	1.34	1.39
1	L5	2415	OMU	C2-N3	-2.28	1.33	1.38
3	L8	14	OMU	C2-N3	-2.28	1.33	1.38
1	L5	1677	PSU	O4'-C1'	-2.28	1.40	1.43
1	L5	400	A2M	C8-N7	2.28	1.35	1.31
1	L5	3782	5MC	C6-N1	-2.28	1.34	1.38
46	S2	1832	6MZ	C5-N7	-2.27	1.34	1.39
1	L5	1534	A2M	C5-N7	-2.27	1.34	1.39
1	L5	400	A2M	C5-N7	-2.27	1.34	1.39
1	L5	2843	PSU	C2-N3	-2.27	1.33	1.37
1	L5	4590	A2M	C8-N7	2.27	1.35	1.31
46	S2	1490	OMG	C5-N7	-2.27	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	509	OMG	C5-N7	-2.26	1.34	1.39
1	L5	1534	A2M	C8-N7	2.26	1.35	1.31
1	L5	2401	A2M	C8-N7	2.26	1.35	1.31
46	S2	1851	MA6	C4-N9	-2.26	1.32	1.37
1	L5	1582	PSU	C2-N3	-2.26	1.33	1.37
46	S2	1442	OMU	C2-N3	-2.25	1.34	1.38
1	L5	1524	A2M	C8-N7	2.25	1.35	1.31
46	S2	590	A2M	C8-N7	2.24	1.35	1.31
1	L5	3899	OMG	C4-N9	-2.24	1.32	1.38
1	L5	4370	OMG	C5-N7	-2.24	1.34	1.39
46	S2	1850	MA6	C5-N7	-2.24	1.34	1.39
46	S2	172	OMU	C2-N3	-2.24	1.34	1.38
1	L5	1871	A2M	C8-N7	2.24	1.35	1.31
1	L5	3867	A2M	C5-N7	-2.24	1.34	1.39
46	S2	468	A2M	C5-N7	-2.24	1.34	1.39
46	S2	428	OMU	C2-N3	-2.24	1.34	1.38
46	S2	484	A2M	C8-N7	2.23	1.35	1.31
1	L5	2787	A2M	C8-N7	2.23	1.35	1.31
1	L5	4493	PSU	C2-N3	-2.23	1.33	1.37
46	S2	1832	6MZ	C4-N9	-2.22	1.32	1.37
1	L5	2837	OMU	C2-N3	-2.22	1.34	1.38
1	L5	1316	OMG	C5-N7	-2.22	1.34	1.39
1	L5	1871	A2M	C5-N7	-2.22	1.34	1.39
46	S2	121	OMU	C2-N3	-2.21	1.34	1.38
1	L5	4228	OMG	C5-N7	-2.20	1.34	1.39
46	S2	1031	A2M	C5-C6	2.20	1.47	1.41
1	L5	2363	A2M	C8-N7	2.20	1.35	1.31
1	L5	2815	A2M	C8-N7	2.20	1.35	1.31
1	L5	4571	A2M	C5-N7	-2.19	1.34	1.39
46	S2	1003	PSU	C2-N3	-2.19	1.33	1.37
46	S2	576	A2M	C4-N9	-2.19	1.32	1.37
1	L5	2364	OMG	C4-N9	-2.18	1.32	1.38
46	S2	166	A2M	C8-N7	2.18	1.35	1.31
46	S2	576	A2M	C8-N7	2.18	1.35	1.31
1	L5	4623	OMG	C5-N7	-2.17	1.34	1.39
1	L5	2364	OMG	C5-N7	-2.17	1.34	1.39
46	S2	1004	PSU	C2-N3	-2.17	1.33	1.37
46	S2	1031	A2M	C4-N9	-2.16	1.32	1.37
1	L5	4618	OMG	C5-N7	-2.16	1.34	1.39
1	L5	1522	OMG	C5-N7	-2.15	1.34	1.39
46	S2	1238	PSU	C2-N3	-2.15	1.33	1.37
46	S2	1851	MA6	C5-N7	-2.15	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1046	PSU	C2-N3	-2.15	1.33	1.37
1	L5	4392	OMG	C5-N7	-2.15	1.34	1.39
46	S2	436	OMG	C5-N7	-2.15	1.34	1.39
1	L5	4637	OMG	C5-N7	-2.13	1.35	1.39
1	L5	3718	A2M	C8-N7	2.13	1.35	1.31
46	S2	1288	OMU	C2-N3	-2.13	1.34	1.38
46	S2	681	PSU	C2-N3	-2.13	1.33	1.37
1	L5	4620	OMU	C2-N3	-2.12	1.34	1.38
1	L5	3718	A2M	C4-N9	-2.12	1.33	1.37
46	S2	1832	6MZ	C8-N7	2.12	1.35	1.31
1	L5	3925	OMU	C2-N3	-2.12	1.34	1.38
1	L5	1782	PSU	C2-N3	-2.12	1.33	1.37
1	L5	4228	OMG	C4-N9	-2.12	1.32	1.38
3	L8	75	OMG	C5-N7	-2.11	1.35	1.39
1	L5	1326	A2M	C4-N9	-2.11	1.33	1.37
46	S2	366	PSU	C2-N3	-2.11	1.33	1.37
1	L5	1323	A2M	C5-N7	-2.11	1.35	1.39
46	S2	1850	MA6	C8-N7	2.10	1.35	1.31
46	S2	1851	MA6	C8-N7	2.10	1.35	1.31
1	L5	2415	OMU	C5-C4	-2.09	1.39	1.43
3	L8	14	OMU	C2-N1	2.09	1.41	1.38
1	L5	3899	OMG	C6-N1	-2.09	1.35	1.38
1	L5	4523	A2M	C8-N7	2.09	1.35	1.31
46	S2	1692	PSU	C2-N3	-2.09	1.33	1.37
1	L5	4620	OMU	C5-C4	-2.09	1.39	1.43
1	L5	3825	A2M	C4-N9	-2.08	1.33	1.37
46	S2	159	A2M	C8-N7	2.08	1.35	1.31
46	S2	1678	A2M	C8-N7	2.08	1.35	1.31
1	L5	1322	1MA	C4-N9	-2.08	1.32	1.38
1	L5	3841	OMC	C6-C5	2.07	1.39	1.35
46	S2	27	A2M	C5-N7	-2.07	1.35	1.39
1	L5	3768	PSU	C2-N3	-2.07	1.34	1.37
46	S2	93	PSU	C2-N3	-2.07	1.34	1.37
46	S2	121	OMU	C5-C4	-2.06	1.39	1.43
1	L5	3844	PSU	C2-N3	-2.06	1.34	1.37
1	L5	3770	PSU	C2-N3	-2.06	1.34	1.37
1	L5	3715	PSU	C2-N1	-2.05	1.33	1.36
1	L5	3830	A2M	C8-N7	2.05	1.35	1.31
1	L5	3744	OMG	C4-N9	-2.05	1.32	1.38
1	L5	4353	PSU	C2-N3	-2.05	1.34	1.37
1	L5	4423	PSU	C2-N3	-2.05	1.34	1.37
1	L5	2508	PSU	C2-N3	-2.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	S2	1383	A2M	C8-N7	2.03	1.35	1.31
46	S2	814	PSU	C2-N3	-2.03	1.34	1.37
1	L5	4220	6MZ	C8-N7	2.03	1.35	1.31
46	S2	406	PSU	C2-N3	-2.03	1.34	1.37
46	S2	651	PSU	C2-N3	-2.03	1.34	1.37
1	L5	2839	PSU	C2-N3	-2.02	1.34	1.37
1	L5	1326	A2M	C8-N7	2.01	1.35	1.31
46	S2	116	OMU	C2-N3	-2.01	1.34	1.38
46	S2	116	OMU	C5-C4	-2.01	1.39	1.43
1	L5	4306	OMU	C5-C4	-2.01	1.39	1.43
46	S2	1442	OMU	C5-C4	-2.01	1.39	1.43
1	L5	4403	PSU	C2-N3	-2.01	1.34	1.37
1	L5	3695	PSU	C2-N3	-2.00	1.34	1.37
1	L5	4628	PSU	C2-N3	-2.00	1.34	1.37

All (823) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	ST	67	NMM	NE-CZ-NH2	-8.35	111.82	119.48
1	L5	3830	A2M	C5-C4-N3	-6.69	118.02	126.75
46	S2	1383	A2M	C5-C4-N3	-6.68	118.04	126.75
46	S2	590	A2M	C5-C4-N3	-6.67	118.05	126.75
1	L5	398	A2M	C5-C4-N3	-6.48	118.30	126.75
46	S2	166	A2M	C5-C4-N3	-6.42	118.38	126.75
46	S2	1174	PSU	N1-C2-N3	6.41	122.39	115.13
1	L5	2815	A2M	C5-C4-N3	-6.41	118.39	126.75
46	S2	1056	PSU	N1-C2-N3	6.39	122.37	115.13
1	L5	1677	PSU	N1-C2-N3	6.37	122.35	115.13
46	S2	366	PSU	N1-C2-N3	6.34	122.31	115.13
46	S2	484	A2M	C5-C4-N3	-6.32	118.50	126.75
1	L5	3770	PSU	N1-C2-N3	6.30	122.27	115.13
46	S2	509	OMG	C5-C4-N3	-6.29	118.25	128.46
1	L5	1524	A2M	C5-C4-N3	-6.29	118.54	126.75
1	L5	3792	OMG	C5-C4-N3	-6.29	118.26	128.46
1	L5	3822	PSU	N1-C2-N3	6.29	122.25	115.13
1	L5	3715	PSU	N1-C2-N3	6.28	122.25	115.13
46	S2	105	PSU	N1-C2-N3	6.27	122.23	115.13
46	S2	644	OMG	C5-C4-N3	-6.26	118.31	128.46
1	L5	3851	PSU	N1-C2-N3	6.24	122.20	115.13
1	L5	4353	PSU	N1-C2-N3	6.24	122.20	115.13
46	S2	1678	A2M	C5-C4-N3	-6.22	118.63	126.75
46	S2	1447	OMG	C5-C4-N3	-6.22	118.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4361	PSU	N1-C2-N3	6.21	122.16	115.13
1	L5	1860	PSU	N1-C2-N3	6.20	122.16	115.13
1	L5	1862	PSU	N1-C2-N3	6.20	122.15	115.13
1	L5	4636	PSU	N1-C2-N3	6.20	122.15	115.13
1	L5	4220	6MZ	C5-C4-N3	-6.19	118.67	126.75
1	L5	400	A2M	C5-C4-N3	-6.19	118.67	126.75
46	S2	109	PSU	N1-C2-N3	6.18	122.13	115.13
1	L5	4403	PSU	N1-C2-N3	6.18	122.13	115.13
46	S2	296	PSU	N1-C2-N3	6.17	122.12	115.13
1	L5	4457	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	1779	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	3768	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	4689	PSU	N1-C2-N3	6.16	122.11	115.13
1	L5	3920	PSU	N1-C2-N3	6.15	122.10	115.13
1	L5	3844	PSU	N1-C2-N3	6.15	122.10	115.13
46	S2	159	A2M	C5-C4-N3	-6.14	118.74	126.75
46	S2	406	PSU	N1-C2-N3	6.13	122.08	115.13
46	S2	1367	PSU	N1-C2-N3	6.13	122.07	115.13
46	S2	63	PSU	N1-C2-N3	6.12	122.07	115.13
1	L5	1781	PSU	N1-C2-N3	6.12	122.06	115.13
1	L5	2424	OMG	C5-C4-N3	-6.12	118.54	128.46
1	L5	4423	PSU	N1-C2-N3	6.10	122.05	115.13
1	L5	4521	PSU	N1-C2-N3	6.10	122.04	115.13
46	S2	1177	PSU	N1-C2-N3	6.10	122.04	115.13
46	S2	512	A2M	C5-C4-N3	-6.10	118.79	126.75
1	L5	3718	A2M	C5-C4-N3	-6.09	118.80	126.75
1	L5	1744	PSU	N1-C2-N3	6.09	122.03	115.13
1	L5	4590	A2M	C5-C4-N3	-6.08	118.81	126.75
46	S2	681	PSU	N1-C2-N3	6.08	122.02	115.13
3	L8	55	PSU	N1-C2-N3	6.07	122.01	115.13
1	L5	2839	PSU	N1-C2-N3	6.06	122.00	115.13
1	L5	3867	A2M	C5-C4-N3	-6.06	118.85	126.75
1	L5	1323	A2M	C5-C4-N3	-6.06	118.85	126.75
46	S2	1445	PSU	N1-C2-N3	6.05	121.99	115.13
46	S2	300	PSU	N1-C2-N3	6.05	121.98	115.13
1	L5	4494	OMG	C5-C4-N3	-6.05	118.65	128.46
46	S2	649	PSU	N1-C2-N3	6.04	121.97	115.13
1	L5	2508	PSU	N1-C2-N3	6.03	121.97	115.13
46	S2	436	OMG	C5-C4-N3	-6.03	118.67	128.46
46	S2	1692	PSU	N1-C2-N3	6.03	121.96	115.13
46	S2	918	PSU	N1-C2-N3	6.03	121.96	115.13
1	L5	2363	A2M	C5-C4-N3	-6.02	118.89	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1004	PSU	N1-C2-N3	6.02	121.95	115.13
1	L5	3884	PSU	N1-C2-N3	6.02	121.95	115.13
1	L5	1625	OMG	C5-C4-N3	-6.02	118.70	128.46
1	L5	2401	A2M	C5-C4-N3	-6.00	118.92	126.75
1	L5	4571	A2M	C5-C4-N3	-6.00	118.93	126.75
1	L5	4637	OMG	C5-C4-N3	-6.00	118.73	128.46
46	S2	1046	PSU	N1-C2-N3	5.99	121.92	115.13
1	L5	3695	PSU	N1-C2-N3	5.98	121.91	115.13
1	L5	2876	OMG	C5-C4-N3	-5.98	118.77	128.46
46	S2	1643	PSU	N1-C2-N3	5.97	121.89	115.13
1	L5	3627	OMG	C5-C4-N3	-5.96	118.80	128.46
1	L5	4196	OMG	C5-C4-N3	-5.96	118.80	128.46
1	L5	4628	PSU	N1-C2-N3	5.95	121.87	115.13
1	L5	1782	PSU	N1-C2-N3	5.95	121.87	115.13
46	S2	93	PSU	N1-C2-N3	5.94	121.86	115.13
1	L5	1792	PSU	N1-C2-N3	5.93	121.85	115.13
46	S2	601	OMG	C5-C4-N3	-5.93	118.84	128.46
3	L8	75	OMG	C5-C4-N3	-5.93	118.84	128.46
46	S2	651	PSU	N1-C2-N3	5.92	121.84	115.13
1	L5	2787	A2M	C5-C4-N3	-5.92	119.02	126.75
1	L5	4392	OMG	C5-C4-N3	-5.92	118.86	128.46
1	L5	4972	PSU	N1-C2-N3	5.91	121.83	115.13
46	S2	814	PSU	N1-C2-N3	5.90	121.82	115.13
46	S2	1232	PSU	N1-C2-N3	5.90	121.81	115.13
1	L5	4471	PSU	N1-C2-N3	5.90	121.81	115.13
1	L5	4442	PSU	N1-C2-N3	5.89	121.81	115.13
1	L5	1522	OMG	C5-C4-N3	-5.88	118.92	128.46
1	L5	4552	PSU	N1-C2-N3	5.88	121.79	115.13
46	S2	1238	PSU	N1-C2-N3	5.87	121.78	115.13
46	S2	218	PSU	N1-C2-N3	5.86	121.77	115.13
46	S2	572	PSU	N1-C2-N3	5.85	121.76	115.13
1	L5	4431	PSU	N1-C2-N3	5.85	121.76	115.13
46	S2	1625	PSU	N1-C2-N3	5.84	121.75	115.13
46	S2	1045	PSU	N1-C2-N3	5.84	121.75	115.13
1	L5	3825	A2M	C5-C4-N3	-5.84	119.13	126.75
1	L5	4523	A2M	C5-C4-N3	-5.84	119.13	126.75
1	L5	4493	PSU	N1-C2-N3	5.83	121.73	115.13
1	L5	1683	PSU	N1-C2-N3	5.81	121.72	115.13
1	L5	4618	OMG	C5-C4-N3	-5.81	119.04	128.46
1	L5	1871	A2M	C5-C4-N3	-5.79	119.20	126.75
1	L5	1326	A2M	C5-C4-N3	-5.79	119.20	126.75
1	L5	1534	A2M	C5-C4-N3	-5.78	119.21	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	119	PSU	N1-C2-N3	5.78	121.67	115.13
46	S2	576	A2M	C5-C4-N3	-5.77	119.23	126.75
46	S2	1490	OMG	C5-C4-N3	-5.76	119.11	128.46
1	L5	4312	PSU	N1-C2-N3	5.75	121.65	115.13
1	L5	3744	OMG	C5-C4-N3	-5.74	119.14	128.46
46	S2	468	A2M	C5-C4-N3	-5.73	119.28	126.75
46	S2	27	A2M	C5-C4-N3	-5.71	119.30	126.75
46	S2	815	PSU	N1-C2-N3	5.69	121.57	115.13
1	L5	3792	OMG	C2-N3-C4	5.69	122.43	112.30
46	S2	1003	PSU	N1-C2-N3	5.68	121.57	115.13
1	L5	4370	OMG	C5-C4-N3	-5.67	119.27	128.46
1	L5	4973	PSU	N1-C2-N3	5.65	121.54	115.13
1	L5	1536	PSU	N1-C2-N3	5.61	121.49	115.13
1	L5	1316	OMG	C5-C4-N3	-5.56	119.44	128.46
1	L5	1582	PSU	N1-C2-N3	5.56	121.42	115.13
1	L5	2843	PSU	N1-C2-N3	5.55	121.42	115.13
46	S2	1031	A2M	C5-C4-N3	-5.53	119.54	126.75
1	L5	4623	OMG	C5-C4-N3	-5.47	119.58	128.46
1	L5	3853	PSU	N1-C2-N3	5.43	121.28	115.13
1	L5	2364	OMG	C5-C4-N3	-5.42	119.66	128.46
46	S2	1832	6MZ	C5-C4-N3	-5.37	119.75	126.75
1	L5	4220	6MZ	N3-C4-N9	5.26	135.74	127.08
46	S2	1851	MA6	C5-C4-N3	-5.26	119.89	126.75
1	L5	4228	OMG	C5-C4-N3	-5.23	119.98	128.46
46	S2	590	A2M	N3-C4-N9	5.20	135.66	127.08
1	L5	3627	OMG	C2-N3-C4	5.19	121.54	112.30
46	S2	1383	A2M	N3-C4-N9	5.17	135.60	127.08
46	S2	644	OMG	C2-N3-C4	5.15	121.47	112.30
46	S2	436	OMG	C2-N3-C4	5.14	121.45	112.30
1	L5	2815	A2M	N3-C4-N9	5.13	135.53	127.08
1	L5	2876	OMG	C2-N3-C4	5.12	121.43	112.30
1	L5	1522	OMG	C2-N3-C4	5.11	121.41	112.30
46	S2	1248	B8N	C4-N3-C2	-5.11	118.99	125.46
46	S2	1678	A2M	N3-C4-N9	5.09	135.46	127.08
1	L5	3830	A2M	N3-C4-N9	5.07	135.44	127.08
1	L5	4392	OMG	C2-N3-C4	5.04	121.28	112.30
1	L5	4618	OMG	C2-N3-C4	5.01	121.23	112.30
1	L5	3899	OMG	C5-C4-N3	-5.01	120.33	128.46
1	L5	1524	A2M	N3-C4-N9	4.99	135.31	127.08
46	S2	509	OMG	C2-N3-C4	4.98	121.17	112.30
1	L5	4196	OMG	C2-N3-C4	4.97	121.15	112.30
46	S2	166	A2M	N3-C4-N9	4.94	135.22	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1447	OMG	C2-N3-C4	4.92	121.07	112.30
1	L5	1322	1MA	C5-C4-N3	-4.90	119.95	127.26
46	S2	172	OMU	C4-N3-C2	-4.88	120.14	126.58
1	L5	3792	OMG	N9-C4-N3	4.88	135.73	125.94
46	S2	601	OMG	C2-N3-C4	4.88	120.99	112.30
1	L5	3744	OMG	C2-N3-C4	4.87	120.97	112.30
1	L5	4590	A2M	N3-C4-N9	4.85	135.08	127.08
1	L5	1625	OMG	N9-C4-N3	4.85	135.68	125.94
46	S2	644	OMG	N9-C4-N3	4.84	135.67	125.94
1	L5	4494	OMG	C2-N3-C4	4.82	120.89	112.30
3	L8	75	OMG	C2-N3-C4	4.82	120.88	112.30
1	L5	1316	OMG	C2-N3-C4	4.81	120.87	112.30
1	L5	4523	A2M	N3-C4-N9	4.81	135.01	127.08
46	S2	1850	MA6	C5-C4-N3	-4.81	120.48	126.75
1	L5	400	A2M	N3-C4-N9	4.81	135.00	127.08
1	L5	1326	A2M	N3-C4-N9	4.79	134.97	127.08
46	S2	1490	OMG	C2-N3-C4	4.79	120.83	112.30
1	L5	398	A2M	N3-C4-N9	4.79	134.97	127.08
1	L5	4637	OMG	C2-N3-C4	4.78	120.81	112.30
1	L5	4370	OMG	C2-N3-C4	4.78	120.81	112.30
46	S2	509	OMG	N9-C4-N3	4.77	135.51	125.94
1	L5	2424	OMG	C2-N3-C4	4.77	120.79	112.30
1	L5	4228	OMG	C2-N3-C4	4.75	120.76	112.30
1	L5	4623	OMG	C2-N3-C4	4.73	120.74	112.30
46	S2	484	A2M	N3-C4-N9	4.72	134.86	127.08
1	L5	2837	OMU	C4-N3-C2	-4.71	120.37	126.58
46	S2	512	A2M	N3-C4-N9	4.71	134.84	127.08
46	S2	512	A2M	C2'-C1'-N9	-4.70	105.62	113.53
1	L5	2424	OMG	N9-C4-N3	4.70	135.37	125.94
1	L5	2401	A2M	N3-C4-N9	4.69	134.81	127.08
46	S2	681	PSU	C4-N3-C2	-4.68	119.60	126.34
46	S2	354	OMU	C4-N3-C2	-4.68	120.41	126.58
1	L5	3899	OMG	C2-N3-C4	4.68	120.63	112.30
46	S2	1850	MA6	C2-N1-C6	4.67	122.77	111.75
1	L5	4227	OMU	C4-N3-C2	-4.64	120.45	126.58
1	L5	4571	A2M	N3-C4-N9	4.64	134.73	127.08
46	S2	1031	A2M	N3-C4-N9	4.64	134.72	127.08
1	L5	3825	A2M	N3-C4-N9	4.62	134.70	127.08
46	S2	159	A2M	N3-C4-N9	4.61	134.69	127.08
1	L5	3867	A2M	N3-C4-N9	4.61	134.68	127.08
46	S2	1851	MA6	C2-N1-C6	4.60	122.63	111.75
46	S2	116	OMU	C4-N3-C2	-4.60	120.51	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1323	A2M	N3-C4-N9	4.59	134.65	127.08
1	L5	1625	OMG	C2-N3-C4	4.59	120.48	112.30
1	L5	4523	A2M	C2'-C1'-N9	-4.59	105.80	113.53
46	S2	1447	OMG	N9-C4-N3	4.58	135.13	125.94
46	S2	1238	PSU	C4-N3-C2	-4.58	119.74	126.34
46	S2	1442	OMU	C4-N3-C2	-4.57	120.55	126.58
1	L5	4494	OMG	N9-C4-N3	4.55	135.08	125.94
1	L5	2364	OMG	C2-N3-C4	4.55	120.41	112.30
46	S2	436	OMG	N9-C4-N3	4.54	135.05	125.94
46	S2	1288	OMU	C4-N3-C2	-4.53	120.61	126.58
1	L5	2363	A2M	N3-C4-N9	4.52	134.54	127.08
1	L5	2876	OMG	N9-C4-N3	4.52	135.02	125.94
46	S2	1490	OMG	N9-C4-N3	4.52	135.01	125.94
1	L5	1871	A2M	N3-C4-N9	4.52	134.53	127.08
1	L5	3718	A2M	N3-C4-N9	4.52	134.53	127.08
1	L5	4306	OMU	C4-N3-C2	-4.50	120.64	126.58
1	L5	1322	1MA	C2-N3-C4	4.49	121.23	112.41
1	L5	1677	PSU	C4-N3-C2	-4.48	119.89	126.34
1	L5	1534	A2M	N3-C4-N9	4.48	134.46	127.08
1	L5	3925	OMU	C4-N3-C2	-4.46	120.70	126.58
1	L5	3627	OMG	N9-C4-N3	4.45	134.87	125.94
3	L8	75	OMG	N9-C4-N3	4.44	134.86	125.94
1	L5	3744	OMG	N9-C4-N3	4.43	134.83	125.94
1	L5	2415	OMU	C4-N3-C2	-4.42	120.75	126.58
46	S2	1851	MA6	C4-C5-N7	-4.41	105.25	110.62
46	S2	428	OMU	C4-N3-C2	-4.41	120.76	126.58
46	S2	468	A2M	N3-C4-N9	4.41	134.35	127.08
46	S2	116	OMU	N3-C2-N1	4.40	120.74	114.89
46	S2	1177	PSU	C4-N3-C2	-4.39	120.01	126.34
46	S2	1832	6MZ	C6-C5-N7	4.38	137.13	132.39
46	S2	354	OMU	N3-C2-N1	4.38	120.70	114.89
1	L5	2837	OMU	N3-C2-N1	4.38	120.70	114.89
46	S2	576	A2M	N3-C4-N9	4.37	134.29	127.08
46	S2	601	OMG	N9-C4-N3	4.37	134.71	125.94
1	L5	4636	PSU	C4-N3-C2	-4.36	120.05	126.34
46	S2	172	OMU	N3-C2-N1	4.36	120.68	114.89
46	S2	121	OMU	C4-N3-C2	-4.35	120.84	126.58
1	L5	4392	OMG	N9-C4-N3	4.35	134.68	125.94
46	S2	27	A2M	N3-C4-N9	4.34	134.24	127.08
1	L5	3925	OMU	N3-C2-N1	4.34	120.65	114.89
1	L5	1781	PSU	C4-N3-C2	-4.34	120.09	126.34
1	L5	3851	PSU	C4-N3-C2	-4.33	120.09	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L8	14	OMU	C4-N3-C2	-4.33	120.87	126.58
1	L5	4227	OMU	N3-C2-N1	4.32	120.62	114.89
1	L5	4196	OMG	N9-C4-N3	4.32	134.61	125.94
46	S2	1046	PSU	C4-N3-C2	-4.32	120.12	126.34
1	L5	4306	OMU	N3-C2-N1	4.30	120.59	114.89
46	S2	576	A2M	C2'-C1'-N9	-4.29	106.30	113.53
1	L5	3830	A2M	C2'-C1'-N9	-4.27	106.35	113.53
1	L5	4637	OMG	N9-C4-N3	4.25	134.48	125.94
1	L5	4361	PSU	C4-N3-C2	-4.25	120.22	126.34
1	L5	2787	A2M	N3-C4-N9	4.25	134.09	127.08
46	S2	366	PSU	C4-N3-C2	-4.24	120.22	126.34
46	S2	1832	6MZ	N3-C4-N9	4.24	134.07	127.08
1	L5	4353	PSU	C4-N3-C2	-4.24	120.23	126.34
46	S2	649	PSU	C4-N3-C2	-4.23	120.25	126.34
59	ST	67	NMM	NE-CZ-NH1	4.22	128.18	120.26
1	L5	1316	OMG	N9-C4-N3	4.22	134.42	125.94
46	S2	1174	PSU	C4-N3-C2	-4.21	120.27	126.34
1	L5	4689	PSU	C4-N3-C2	-4.20	120.29	126.34
1	L5	4618	OMG	N9-C4-N3	4.19	134.36	125.94
46	S2	121	OMU	N3-C2-N1	4.16	120.41	114.89
1	L5	4370	OMG	N9-C4-N3	4.16	134.29	125.94
1	L5	1522	OMG	N9-C4-N3	4.15	134.28	125.94
1	L5	4620	OMU	C4-N3-C2	-4.15	121.11	126.58
46	S2	1442	OMU	N3-C2-N1	4.13	120.38	114.89
1	L5	3695	PSU	C4-N3-C2	-4.13	120.38	126.34
1	L5	4972	PSU	C4-N3-C2	-4.12	120.40	126.34
46	S2	63	PSU	C4-N3-C2	-4.12	120.41	126.34
1	L5	1862	PSU	C4-N3-C2	-4.11	120.42	126.34
1	L5	4493	PSU	C4-N3-C2	-4.11	120.42	126.34
1	L5	4521	PSU	C4-N3-C2	-4.11	120.42	126.34
1	L5	4620	OMU	N3-C2-N1	4.10	120.33	114.89
46	S2	1288	OMU	N3-C2-N1	4.08	120.31	114.89
46	S2	296	PSU	C4-N3-C2	-4.08	120.46	126.34
46	S2	590	A2M	C2-N3-C4	4.08	121.39	111.75
46	S2	815	PSU	C4-N3-C2	-4.06	120.49	126.34
46	S2	651	PSU	C4-N3-C2	-4.06	120.49	126.34
1	L5	1744	PSU	C4-N3-C2	-4.04	120.52	126.34
46	S2	105	PSU	C4-N3-C2	-4.04	120.52	126.34
1	L5	2508	PSU	C4-N3-C2	-4.04	120.52	126.34
1	L5	3768	PSU	C4-N3-C2	-4.04	120.52	126.34
46	S2	300	PSU	C4-N3-C2	-4.04	120.52	126.34
1	L5	2415	OMU	N3-C2-N1	4.03	120.25	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3920	PSU	C4-N3-C2	-4.03	120.53	126.34
1	L5	1779	PSU	C4-N3-C2	-4.03	120.53	126.34
46	S2	1850	MA6	C4-C5-N7	-4.00	105.75	110.62
1	L5	4403	PSU	C4-N3-C2	-4.00	120.58	126.34
46	S2	27	A2M	C2-N3-C4	4.00	121.19	111.75
46	S2	1004	PSU	C4-N3-C2	-3.99	120.58	126.34
1	L5	4423	PSU	C4-N3-C2	-3.99	120.59	126.34
1	L5	2787	A2M	C2-N3-C4	3.99	121.17	111.75
1	L5	1782	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L5	3822	PSU	C4-N3-C2	-3.98	120.61	126.34
1	L5	3884	PSU	C4-N3-C2	-3.97	120.62	126.34
46	S2	218	PSU	C4-N3-C2	-3.96	120.63	126.34
1	L5	4552	PSU	C4-N3-C2	-3.96	120.63	126.34
3	L8	55	PSU	C4-N3-C2	-3.96	120.64	126.34
1	L5	3715	PSU	C4-N3-C2	-3.96	120.64	126.34
1	L5	3695	PSU	O2-C2-N1	-3.96	118.43	122.79
1	L5	4220	6MZ	C2-N3-C4	3.96	121.09	111.75
46	S2	1056	PSU	C4-N3-C2	-3.95	120.64	126.34
1	L5	4457	PSU	C4-N3-C2	-3.95	120.65	126.34
1	L5	1323	A2M	C2-N3-C4	3.94	121.06	111.75
1	L5	4312	PSU	C4-N3-C2	-3.94	120.66	126.34
3	L8	14	OMU	C5-C4-N3	3.94	120.73	114.84
1	L5	4442	PSU	C4-N3-C2	-3.93	120.67	126.34
46	S2	484	A2M	C2-N3-C4	3.93	121.04	111.75
46	S2	512	A2M	C2-N3-C4	3.93	121.04	111.75
1	L5	3844	PSU	C4-N3-C2	-3.92	120.69	126.34
1	L5	3830	A2M	C2-N3-C4	3.92	121.01	111.75
1	L5	4431	PSU	C4-N3-C2	-3.92	120.70	126.34
1	L5	2815	A2M	C2-N3-C4	3.92	121.00	111.75
1	L5	398	A2M	C2-N3-C4	3.91	121.00	111.75
1	L5	1582	PSU	C4-N3-C2	-3.91	120.70	126.34
46	S2	1232	PSU	C4-N3-C2	-3.91	120.71	126.34
1	L5	4623	OMG	N9-C4-N3	3.91	133.79	125.94
46	S2	1678	A2M	C2-N3-C4	3.90	120.96	111.75
1	L5	1326	A2M	C2-N3-C4	3.90	120.96	111.75
1	L5	1683	PSU	C4-N3-C2	-3.90	120.73	126.34
1	L5	400	A2M	C2-N3-C4	3.90	120.95	111.75
1	L5	2364	OMG	C6-C5-N7	3.89	137.49	130.25
46	S2	93	PSU	C4-N3-C2	-3.89	120.73	126.34
1	L5	1524	A2M	C2-N3-C4	3.89	120.94	111.75
46	S2	1445	PSU	C4-N3-C2	-3.89	120.74	126.34
46	S2	428	OMU	N3-C2-N1	3.89	120.05	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	918	PSU	C4-N3-C2	-3.88	120.75	126.34
46	S2	109	PSU	C4-N3-C2	-3.88	120.75	126.34
46	S2	166	A2M	C2-N3-C4	3.87	120.89	111.75
1	L5	1860	PSU	C4-N3-C2	-3.87	120.76	126.34
46	S2	1031	A2M	N3-C2-N1	-3.87	122.55	128.60
46	S2	1367	PSU	C4-N3-C2	-3.86	120.77	126.34
46	S2	1643	PSU	C4-N3-C2	-3.86	120.78	126.34
46	S2	1003	PSU	C4-N3-C2	-3.86	120.78	126.34
1	L5	1792	PSU	C4-N3-C2	-3.85	120.79	126.34
1	L5	4628	PSU	C4-N3-C2	-3.85	120.80	126.34
1	L5	2843	PSU	C4-N3-C2	-3.84	120.81	126.34
1	L5	2401	A2M	C2-N3-C4	3.82	120.78	111.75
46	S2	814	PSU	C4-N3-C2	-3.82	120.83	126.34
1	L5	4228	OMG	C6-C5-N7	3.81	137.34	130.25
1	L5	3867	A2M	C2-N3-C4	3.81	120.74	111.75
46	S2	1625	PSU	C4-N3-C2	-3.80	120.86	126.34
1	L5	4689	PSU	O2-C2-N1	-3.80	118.61	122.79
46	S2	1383	A2M	C2-N3-C4	3.80	120.72	111.75
1	L5	3770	PSU	C4-N3-C2	-3.79	120.88	126.34
46	S2	1031	A2M	C2-N3-C4	3.79	120.70	111.75
1	L5	4571	A2M	C2-N3-C4	3.79	120.70	111.75
1	L5	2839	PSU	C4-N3-C2	-3.78	120.89	126.34
46	S2	428	OMU	C5-C4-N3	3.78	120.50	114.84
1	L5	1522	OMG	C6-C5-N7	3.78	137.27	130.25
1	L5	4973	PSU	C4-N3-C2	-3.78	120.90	126.34
1	L5	4590	A2M	C2-N3-C4	3.78	120.67	111.75
46	S2	354	OMU	C5-C4-N3	3.77	120.48	114.84
1	L5	3768	PSU	O2-C2-N1	-3.77	118.64	122.79
1	L5	1683	PSU	O2-C2-N1	-3.76	118.65	122.79
46	S2	119	PSU	C4-N3-C2	-3.76	120.92	126.34
46	S2	468	A2M	C2-N3-C4	3.75	120.62	111.75
1	L5	1792	PSU	O2-C2-N1	-3.75	118.67	122.79
1	L5	1871	A2M	C2-N3-C4	3.74	120.60	111.75
1	L5	4228	OMG	N9-C4-N3	3.74	133.45	125.94
1	L5	4471	PSU	C4-N3-C2	-3.74	120.95	126.34
1	L5	3782	5MC	C5-C6-N1	-3.73	119.50	123.34
46	S2	1692	PSU	C4-N3-C2	-3.73	120.96	126.34
46	S2	27	A2M	N3-C2-N1	-3.73	122.77	128.60
1	L5	4312	PSU	O2-C2-N1	-3.72	118.69	122.79
46	S2	572	PSU	C4-N3-C2	-3.72	120.98	126.34
1	L5	2837	OMU	C5-C4-N3	3.71	120.40	114.84
46	S2	1174	PSU	O2-C2-N1	-3.71	118.71	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	406	PSU	C4-N3-C2	-3.69	121.03	126.34
46	S2	1832	6MZ	C2-N3-C4	3.68	120.45	111.75
46	S2	1851	MA6	C2-N3-C4	3.68	120.45	111.75
46	S2	1442	OMU	C5-C4-N3	3.68	120.34	114.84
1	L5	1860	PSU	O2-C2-N1	-3.67	118.75	122.79
46	S2	1288	OMU	C5-C4-N3	3.67	120.33	114.84
1	L5	4636	PSU	O2-C2-N1	-3.67	118.75	122.79
46	S2	159	A2M	C2-N3-C4	3.67	120.42	111.75
1	L5	1871	A2M	C2'-C1'-N9	-3.66	107.36	113.53
1	L5	4392	OMG	C6-C5-N7	3.66	137.06	130.25
46	S2	172	OMU	C5-C4-N3	3.66	120.31	114.84
1	L5	3718	A2M	C2-N3-C4	3.66	120.39	111.75
46	S2	484	A2M	C4-C5-N7	-3.65	106.17	110.62
1	L5	2787	A2M	C4-C5-N7	-3.64	106.18	110.62
1	L5	4523	A2M	C2-N3-C4	3.64	120.36	111.75
1	L5	2415	OMU	C5-C4-N3	3.64	120.28	114.84
1	L5	3715	PSU	O2-C2-N1	-3.63	118.80	122.79
1	L5	3825	A2M	C2-N3-C4	3.62	120.31	111.75
46	S2	1851	MA6	N3-C4-N9	3.62	133.04	127.08
1	L5	4227	OMU	C5-C4-N3	3.61	120.25	114.84
1	L5	2364	OMG	N9-C4-N3	3.61	133.19	125.94
46	S2	1832	6MZ	N1-C2-N3	-3.61	122.96	128.60
1	L5	1536	PSU	C4-N3-C2	-3.61	121.14	126.34
46	S2	1850	MA6	C2-N3-C4	3.60	120.26	111.75
1	L5	1862	PSU	O2-C2-N1	-3.60	118.82	122.79
1	L5	2363	A2M	C2-N3-C4	3.60	120.26	111.75
1	L5	4457	PSU	O2-C2-N1	-3.60	118.83	122.79
46	S2	116	OMU	C5-C4-N3	3.60	120.22	114.84
46	S2	822	PSU	C3'-C2'-C1'	3.59	105.81	101.64
1	L5	4620	OMU	C5-C4-N3	3.59	120.20	114.84
1	L5	3899	OMG	N9-C4-N3	3.59	133.14	125.94
1	L5	4306	OMU	C5-C4-N3	3.58	120.19	114.84
1	L5	4618	OMG	C6-C5-N7	3.57	136.89	130.25
46	S2	406	PSU	O2-C2-N1	-3.57	118.86	122.79
46	S2	651	PSU	O2-C2-N1	-3.56	118.87	122.79
1	L5	3899	OMG	C6-C5-N7	3.56	136.86	130.25
1	L5	4361	PSU	O2-C2-N1	-3.56	118.88	122.79
1	L5	4623	OMG	C6-C5-N7	3.56	136.86	130.25
46	S2	218	PSU	O2-C2-N1	-3.56	118.88	122.79
46	S2	121	OMU	C5-C4-N3	3.55	120.16	114.84
1	L5	2876	OMG	C6-C5-N7	3.55	136.86	130.25
46	S2	105	PSU	O2-C2-N1	-3.55	118.88	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1850	MA6	N1-C2-N3	-3.55	123.05	128.60
46	S2	576	A2M	C2-N3-C4	3.54	120.12	111.75
1	L5	3851	PSU	O2-C2-N1	-3.54	118.89	122.79
1	L5	2363	A2M	C4-C5-N7	-3.52	106.33	110.62
3	L8	14	OMU	N3-C2-N1	3.52	119.56	114.89
46	S2	436	OMG	C6-C5-N7	3.51	136.78	130.25
46	S2	1850	MA6	N3-C4-N9	3.51	132.87	127.08
46	S2	681	PSU	O2-C2-N1	-3.50	118.94	122.79
1	L5	1534	A2M	C4-C5-N7	-3.50	106.36	110.62
46	S2	1045	PSU	C4-N3-C2	-3.49	121.30	126.34
1	L5	4972	PSU	O2-C2-N1	-3.49	118.95	122.79
46	S2	468	A2M	C4-C5-N7	-3.49	106.37	110.62
1	L5	3844	PSU	O2-C2-N1	-3.49	118.95	122.79
1	L5	1677	PSU	O2-C2-N1	-3.49	118.95	122.79
1	L5	3853	PSU	C4-N3-C2	-3.48	121.32	126.34
1	L5	398	A2M	C4-C5-N7	-3.48	106.38	110.62
1	L5	4628	PSU	O2-C2-N1	-3.48	118.96	122.79
1	L5	4973	PSU	O2-C2-N1	-3.48	118.96	122.79
1	L5	1534	A2M	C2-N3-C4	3.47	119.96	111.75
1	L5	2787	A2M	N3-C2-N1	-3.47	123.18	128.60
46	S2	1832	6MZ	C4-C5-N7	-3.47	106.40	110.62
1	L5	1322	1MA	N9-C4-N3	3.46	135.00	126.94
46	S2	27	A2M	C4-C5-N7	-3.45	106.41	110.62
46	S2	576	A2M	C4-C5-N7	-3.44	106.42	110.62
1	L5	4403	PSU	O2-C2-N1	-3.43	119.01	122.79
1	L5	3825	A2M	C2'-C1'-N9	-3.43	107.75	113.53
1	L5	1316	OMG	C6-C5-N7	3.43	136.62	130.25
1	L5	4471	PSU	O2-C2-N1	-3.42	119.02	122.79
46	S2	1383	A2M	C2'-C1'-N9	-3.42	107.77	113.53
1	L5	1779	PSU	O2-C2-N1	-3.42	119.03	122.79
1	L5	4521	PSU	O2-C2-N1	-3.42	119.03	122.79
46	S2	1851	MA6	C5-N7-C8	3.41	108.36	103.51
46	S2	1367	PSU	O2-C2-N1	-3.41	119.03	122.79
46	S2	159	A2M	C2'-C1'-N9	-3.41	107.78	113.53
1	L5	3925	OMU	C5-C4-N3	3.41	119.94	114.84
46	S2	1003	PSU	O2-C2-N1	-3.41	119.04	122.79
1	L5	1323	A2M	C4-C5-N7	-3.41	106.47	110.62
1	L5	4370	OMG	C6-C5-N7	3.39	136.56	130.25
46	S2	119	PSU	O2-C2-N1	-3.39	119.06	122.79
1	L5	4571	A2M	C4-C5-N7	-3.39	106.50	110.62
46	S2	918	PSU	O2-C2-N1	-3.38	119.07	122.79
46	S2	1445	PSU	O2-C2-N1	-3.38	119.07	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1177	PSU	O2-C2-N1	-3.38	119.07	122.79
1	L5	4637	OMG	C6-C5-N7	3.38	136.53	130.25
46	S2	296	PSU	O2-C2-N1	-3.38	119.07	122.79
1	L5	4220	6MZ	N1-C2-N3	-3.37	123.33	128.60
46	S2	1625	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L5	3718	A2M	C4-C5-N7	-3.37	106.52	110.62
1	L5	4552	PSU	O2-C2-N1	-3.37	119.08	122.79
1	L5	4431	PSU	O2-C2-N1	-3.37	119.08	122.79
46	S2	1232	PSU	O2-C2-N1	-3.37	119.08	122.79
46	S2	1850	MA6	C4-N9-C8	3.37	109.38	105.73
1	L5	1871	A2M	N3-C2-N1	-3.35	123.36	128.60
1	L5	1781	PSU	O2-C2-N1	-3.35	119.11	122.79
1	L5	1323	A2M	N3-C2-N1	-3.34	123.38	128.60
46	S2	109	PSU	O2-C2-N1	-3.34	119.11	122.79
46	S2	1004	PSU	O2-C2-N1	-3.34	119.11	122.79
46	S2	512	A2M	N3-C2-N1	-3.34	123.38	128.60
1	L5	3770	PSU	O2-C2-N1	-3.33	119.12	122.79
1	L5	3830	A2M	C4-C5-N7	-3.33	106.56	110.62
1	L5	4353	PSU	O2-C2-N1	-3.33	119.12	122.79
1	L5	3627	OMG	C6-C5-N7	3.32	136.41	130.25
1	L5	4590	A2M	C4-C5-N7	-3.31	106.58	110.62
1	L5	1871	A2M	C4-C5-N7	-3.31	106.58	110.62
46	S2	159	A2M	C4-C5-N7	-3.31	106.59	110.62
1	L5	3867	A2M	C4-C5-N7	-3.31	106.59	110.62
46	S2	468	A2M	N3-C2-N1	-3.31	123.43	128.60
46	S2	815	PSU	O2-C2-N1	-3.29	119.17	122.79
1	L5	3744	OMG	C6-C5-N7	3.29	136.36	130.25
46	S2	1383	A2M	C4-C5-N7	-3.28	106.62	110.62
46	S2	1643	PSU	O2-C2-N1	-3.28	119.18	122.79
46	S2	1850	MA6	C5-N7-C8	3.27	108.16	103.51
1	L5	400	A2M	N3-C2-N1	-3.26	123.51	128.60
1	L5	3792	OMG	C6-C5-N7	3.26	136.30	130.25
1	L5	1326	A2M	N3-C2-N1	-3.25	123.52	128.60
1	L5	4442	PSU	O2-C2-N1	-3.25	119.21	122.79
1	L5	4423	PSU	O2-C2-N1	-3.25	119.22	122.79
46	S2	649	PSU	O2-C2-N1	-3.25	119.22	122.79
1	L5	2415	OMU	O4-C4-C5	-3.24	119.46	125.16
46	S2	512	A2M	C4-C5-N7	-3.24	106.67	110.62
46	S2	601	OMG	C6-C5-N7	3.24	136.27	130.25
1	L5	4196	OMG	C6-C5-N7	3.23	136.26	130.25
1	L5	4523	A2M	N3-C2-N1	-3.23	123.55	128.60
1	L5	4590	A2M	N3-C2-N1	-3.23	123.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L8	75	OMG	C6-C5-N7	3.23	136.25	130.25
46	S2	1692	PSU	O2-C2-N1	-3.22	119.24	122.79
46	S2	572	PSU	O2-C2-N1	-3.22	119.25	122.79
1	L5	2401	A2M	C4-C5-N7	-3.22	106.70	110.62
46	S2	590	A2M	N3-C2-N1	-3.21	123.58	128.60
46	S2	1851	MA6	N1-C2-N3	-3.21	123.58	128.60
3	L8	55	PSU	O2-C2-N1	-3.21	119.26	122.79
1	L5	400	A2M	C4-C5-N7	-3.21	106.71	110.62
1	L5	3825	A2M	N3-C2-N1	-3.21	123.59	128.60
1	L5	1744	PSU	O2-C2-N1	-3.20	119.26	122.79
1	L5	4571	A2M	N3-C2-N1	-3.20	123.59	128.60
1	L5	3884	PSU	O2-C2-N1	-3.20	119.27	122.79
1	L5	3825	A2M	C4-C5-N7	-3.19	106.73	110.62
1	L5	1524	A2M	C4-C5-N7	-3.18	106.75	110.62
46	S2	1490	OMG	C6-C5-N7	3.18	136.16	130.25
46	S2	366	PSU	O2-C2-N1	-3.17	119.30	122.79
1	L5	3867	A2M	N3-C2-N1	-3.16	123.66	128.60
1	L5	3853	PSU	O2-C2-N1	-3.16	119.31	122.79
1	L5	2837	OMU	O4-C4-C5	-3.16	119.61	125.16
46	S2	1678	A2M	N3-C2-N1	-3.15	123.67	128.60
46	S2	63	PSU	O2-C2-N1	-3.15	119.32	122.79
1	L5	2815	A2M	C4-C5-N7	-3.15	106.79	110.62
46	S2	590	A2M	C4-C5-N7	-3.14	106.79	110.62
46	S2	166	A2M	C4-C5-N7	-3.14	106.80	110.62
46	S2	1046	PSU	O2-C2-N1	-3.13	119.34	122.79
1	L5	3920	PSU	O2-C2-N1	-3.13	119.35	122.79
1	L5	2401	A2M	N3-C2-N1	-3.11	123.74	128.60
1	L5	2815	A2M	N3-C2-N1	-3.11	123.74	128.60
1	L5	1524	A2M	N3-C2-N1	-3.10	123.75	128.60
46	S2	1678	A2M	C4-C5-N7	-3.10	106.84	110.62
46	S2	166	A2M	N3-C2-N1	-3.09	123.77	128.60
46	S2	484	A2M	N3-C2-N1	-3.09	123.77	128.60
3	L8	14	OMU	O4-C4-C5	-3.08	119.75	125.16
46	S2	1447	OMG	C6-C5-N7	3.08	135.97	130.25
1	L5	4523	A2M	C4-C5-N7	-3.07	106.88	110.62
1	L5	1582	PSU	O2-C2-N1	-3.05	119.43	122.79
46	S2	300	PSU	O2-C2-N1	-3.05	119.44	122.79
46	S2	116	OMU	O4-C4-C5	-3.04	119.81	125.16
1	L5	2364	OMG	C4-C5-N7	-3.03	105.93	110.72
46	S2	1288	OMU	O4-C4-C5	-3.03	119.83	125.16
46	S2	484	A2M	C5-N7-C8	3.03	107.81	103.51
1	L5	4494	OMG	C6-C5-N7	3.02	135.87	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1782	PSU	O2-C2-N1	-3.01	119.47	122.79
46	S2	509	OMG	C6-C5-N7	3.01	135.85	130.25
46	S2	814	PSU	O2-C2-N1	-3.00	119.48	122.79
1	L5	4220	6MZ	C6-C5-N7	3.00	135.64	132.39
46	S2	644	OMG	C6-C5-N7	3.00	135.82	130.25
46	S2	1850	MA6	C6-C5-N7	2.99	138.31	133.28
46	S2	1031	A2M	C2'-C1'-N9	-2.99	108.49	113.53
1	L5	1536	PSU	O2-C2-N1	-2.99	119.50	122.79
1	L5	398	A2M	N3-C2-N1	-2.99	123.93	128.60
1	L5	1522	OMG	C4-C5-N7	-2.99	105.99	110.72
1	L5	1326	A2M	C4-C5-N7	-2.98	106.99	110.62
46	S2	1832	6MZ	C4-N9-C8	2.98	108.96	105.73
46	S2	1442	OMU	O4-C4-C5	-2.97	119.94	125.16
1	L5	1326	A2M	C4-N9-C8	2.97	108.94	105.73
46	S2	121	OMU	O4-C4-C5	-2.97	119.94	125.16
46	S2	27	A2M	C5-N7-C8	2.97	107.72	103.51
46	S2	1031	A2M	C4-C5-N7	-2.96	107.01	110.62
46	S2	1851	MA6	C6-C5-N7	2.96	138.26	133.28
1	L5	2508	PSU	O2-C2-N1	-2.96	119.53	122.79
1	L5	2363	A2M	C5-N7-C8	2.96	107.71	103.51
46	S2	1031	A2M	C4-N9-C8	2.96	108.93	105.73
46	S2	1056	PSU	O2-C2-N1	-2.95	119.54	122.79
1	L5	4306	OMU	O4-C4-C5	-2.94	119.98	125.16
46	S2	27	A2M	C4-N9-C8	2.94	108.91	105.73
1	L5	4620	OMU	O4-C4-C5	-2.94	120.00	125.16
46	S2	172	OMU	O4-C4-C5	-2.93	120.01	125.16
46	S2	1383	A2M	C5-N7-C8	2.92	107.66	103.51
1	L5	4590	A2M	C5-N7-C8	2.91	107.65	103.51
46	S2	354	OMU	O4-C4-C5	-2.91	120.04	125.16
1	L5	3718	A2M	C2'-C1'-N9	-2.90	108.64	113.53
46	S2	27	A2M	C2'-C1'-N9	-2.90	108.65	113.53
1	L5	2787	A2M	C5-N7-C8	2.90	107.62	103.51
46	S2	468	A2M	C5-N7-C8	2.89	107.62	103.51
1	L5	4571	A2M	C5-N7-C8	2.89	107.61	103.51
1	L5	4227	OMU	O4-C4-C5	-2.88	120.09	125.16
1	L5	4220	6MZ	C4-N9-C8	2.88	108.85	105.73
46	S2	428	OMU	O4-C4-C5	-2.88	120.10	125.16
46	S2	1031	A2M	C5-N7-C8	2.87	107.59	103.51
1	L5	4523	A2M	C4-N9-C8	2.86	108.83	105.73
1	L5	1534	A2M	C5-N7-C8	2.86	107.57	103.51
1	L5	2837	OMU	O2-C2-N1	-2.86	118.99	122.79
1	L5	3925	OMU	O4-C4-C5	-2.84	120.17	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1850	MA6	N9-C8-N7	-2.83	110.05	113.91
1	L5	4590	A2M	C4-N9-C8	2.83	108.79	105.73
1	L5	1871	A2M	C5-N7-C8	2.81	107.51	103.51
46	S2	1832	6MZ	C5-N7-C8	2.81	107.50	103.51
46	S2	93	PSU	O2-C2-N1	-2.81	119.69	122.79
46	S2	1238	PSU	O2-C2-N1	-2.81	119.69	122.79
46	S2	576	A2M	N3-C2-N1	-2.81	124.21	128.60
46	S2	576	A2M	C5-N7-C8	2.81	107.50	103.51
1	L5	1323	A2M	C5-N7-C8	2.80	107.49	103.51
1	L5	398	A2M	C5-N7-C8	2.80	107.49	103.51
1	L5	4220	6MZ	C4-C5-N7	-2.80	107.21	110.62
1	L5	2839	PSU	O2-C2-N1	-2.80	119.71	122.79
1	L5	1625	OMG	C6-C5-N7	2.79	135.45	130.25
46	S2	1337	4AC	C6-C5-C4	2.79	120.38	116.96
1	L5	2363	A2M	N3-C2-N1	-2.79	124.25	128.60
1	L5	4590	A2M	C2'-C1'-N9	-2.78	108.84	113.53
46	S2	1851	MA6	C4-N9-C8	2.78	108.74	105.73
46	S2	1678	A2M	C5-N7-C8	2.78	107.45	103.51
1	L5	4618	OMG	C4-C5-N7	-2.77	106.33	110.72
1	L5	3830	A2M	N3-C2-N1	-2.77	124.27	128.60
1	L5	4637	OMG	C4-C5-N7	-2.75	106.36	110.72
46	S2	159	A2M	N3-C2-N1	-2.75	124.30	128.60
1	L5	3825	A2M	C5-N7-C8	2.75	107.41	103.51
1	L5	4571	A2M	C4-N9-C8	2.74	108.70	105.73
1	L5	1524	A2M	C5-N7-C8	2.74	107.40	103.51
1	L5	4523	A2M	C5-N7-C8	2.74	107.39	103.51
1	L5	4392	OMG	C4-C5-N7	-2.73	106.40	110.72
46	S2	172	OMU	O2-C2-N1	-2.72	119.16	122.79
1	L5	1534	A2M	N3-C2-N1	-2.72	124.34	128.60
46	S2	1383	A2M	N3-C2-N1	-2.72	124.35	128.60
1	L5	1323	A2M	C4-N9-C8	2.72	108.67	105.73
1	L5	3718	A2M	N3-C2-N1	-2.71	124.36	128.60
46	S2	1678	A2M	C4-N9-C8	2.71	108.67	105.73
46	S2	468	A2M	C4-N9-C8	2.71	108.67	105.73
1	L5	3867	A2M	C5-N7-C8	2.71	107.36	103.51
46	S2	576	A2M	C4-N9-C8	2.71	108.66	105.73
46	S2	590	A2M	C5-N7-C8	2.71	107.35	103.51
1	L5	1871	A2M	C4-N9-C8	2.70	108.66	105.73
46	S2	1248	B8N	N3-C2-N1	2.70	120.57	116.76
1	L5	2815	A2M	C5-N7-C8	2.70	107.34	103.51
1	L5	2424	OMG	C6-C5-N7	2.70	135.26	130.25
46	S2	354	OMU	O2-C2-N1	-2.69	119.20	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1045	PSU	O2-C2-N1	-2.69	119.82	122.79
1	L5	4228	OMG	C4-C5-N7	-2.69	106.46	110.72
1	L5	3782	5MC	C5-C4-N3	-2.69	118.77	121.67
46	S2	1447	OMG	C4-C5-N7	-2.68	106.48	110.72
46	S2	27	A2M	C6-C5-N7	2.68	137.01	132.02
1	L5	2876	OMG	C4-C5-N7	-2.67	106.49	110.72
1	L5	1534	A2M	C4-N9-C8	2.67	108.62	105.73
46	S2	436	OMG	C4-C5-N7	-2.67	106.50	110.72
1	L5	4623	OMG	C4-C5-N7	-2.66	106.52	110.72
1	L5	4370	OMG	C4-C5-N7	-2.65	106.52	110.72
46	S2	1842	4AC	C6-C5-C4	2.65	120.20	116.96
1	L5	2401	A2M	C5-N7-C8	2.65	107.27	103.51
1	L5	398	A2M	C2'-C1'-N9	-2.65	109.07	113.53
46	S2	512	A2M	C5-N7-C8	2.65	107.27	103.51
46	S2	918	PSU	O4'-C1'-C2'	2.63	108.85	105.14
1	L5	3830	A2M	C5-N7-C8	2.62	107.23	103.51
46	S2	601	OMG	C4-C5-N7	-2.61	106.59	110.72
3	L8	75	OMG	C4-C5-N7	-2.60	106.61	110.72
1	L5	400	A2M	C5-N7-C8	2.59	107.19	103.51
46	S2	159	A2M	C5-N7-C8	2.58	107.18	103.51
1	L5	3627	OMG	C4-C5-N7	-2.58	106.64	110.72
1	L5	1326	A2M	C5-N7-C8	2.58	107.17	103.51
1	L5	4196	OMG	C4-C5-N7	-2.57	106.65	110.72
46	S2	1678	A2M	C2'-C1'-N9	2.56	117.85	113.53
1	L5	4220	6MZ	C5-N7-C8	2.56	107.14	103.51
46	S2	1031	A2M	C2-N1-C6	2.55	123.14	118.77
1	L5	2876	OMG	O6-C6-C5	-2.55	119.84	126.60
46	S2	1851	MA6	N1-C6-N6	2.54	119.87	117.08
1	L5	400	A2M	C4-N9-C8	2.54	108.48	105.73
46	S2	512	A2M	C4-N9-C8	2.54	108.48	105.73
46	S2	116	OMU	O2-C2-N1	-2.54	119.42	122.79
1	L5	2787	A2M	C6-C5-N7	2.54	136.74	132.02
1	L5	3718	A2M	C5-N7-C8	2.53	107.11	103.51
1	L5	3825	A2M	C4-N9-C8	2.52	108.46	105.73
46	S2	484	A2M	C2'-C1'-N9	-2.52	109.29	113.53
46	S2	509	OMG	C4-C5-N7	-2.52	106.74	110.72
46	S2	468	A2M	C6-C5-N7	2.50	136.68	132.02
46	S2	27	A2M	N9-C8-N7	-2.50	110.49	113.91
1	L5	2363	A2M	C4-N9-C8	2.50	108.44	105.73
1	L5	4220	6MZ	C9-N6-C6	-2.48	120.73	122.87
1	L5	2401	A2M	C4-N9-C8	2.48	108.42	105.73
1	L5	3867	A2M	C4-N9-C8	2.48	108.41	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1323	A2M	C6-C5-N7	2.48	136.63	132.02
1	L5	2815	A2M	C4-N9-C8	2.48	108.41	105.73
46	S2	1238	PSU	C5-C6-N1	-2.45	118.43	122.11
1	L5	2415	OMU	C1'-N1-C2	2.45	122.01	117.57
1	L5	1524	A2M	C4-N9-C8	2.45	108.38	105.73
1	L5	3744	OMG	C4-C5-N7	-2.45	106.84	110.72
46	S2	1832	6MZ	C2-N1-C6	2.45	123.46	115.25
1	L5	1316	OMG	C4-C5-N7	-2.44	106.86	110.72
46	S2	166	A2M	C5-N7-C8	2.44	106.97	103.51
46	S2	1851	MA6	N9-C8-N7	-2.43	110.59	113.91
46	S2	484	A2M	C6-C5-N7	2.43	136.55	132.02
1	L5	1316	OMG	O6-C6-C5	-2.43	120.16	126.60
46	S2	1842	4AC	C5-C4-N3	-2.41	118.71	122.59
1	L5	4493	PSU	O2-C2-N1	-2.41	120.14	122.79
46	S2	1490	OMG	O6-C6-C5	-2.41	120.22	126.60
1	L5	3822	PSU	C5-C6-N1	-2.40	118.50	122.11
1	L5	4306	OMU	O2-C2-N1	-2.39	119.61	122.79
46	S2	121	OMU	O2-C2-N1	-2.39	119.61	122.79
1	L5	3792	OMG	O6-C6-C5	-2.39	120.27	126.60
1	L5	4370	OMG	O6-C6-C5	-2.39	120.27	126.60
46	S2	366	PSU	C5-C6-N1	-2.39	118.53	122.11
1	L5	1781	PSU	C5-C6-N1	-2.38	118.53	122.11
46	S2	166	A2M	C2'-C1'-N9	-2.38	109.52	113.53
1	L5	1625	OMG	O6-C6-C5	-2.37	120.31	126.60
1	L5	2351	OMC	O2-C2-N3	-2.37	118.48	122.33
3	L8	14	OMU	C1'-N1-C2	2.37	121.85	117.57
1	L5	1871	A2M	C6-C5-N7	2.37	136.43	132.02
1	L5	3825	A2M	C2-N1-C6	2.36	122.82	118.77
46	S2	1337	4AC	C5-C4-N3	-2.36	118.79	122.59
1	L5	4494	OMG	C4-C5-N7	-2.36	106.98	110.72
1	L5	1322	1MA	N1-C2-N3	-2.35	123.20	126.00
1	L5	3627	OMG	C2'-C1'-N9	-2.34	109.68	114.22
1	L5	1326	A2M	C6-C5-N7	2.34	136.38	132.02
1	L5	2843	PSU	O2-C2-N1	-2.34	120.22	122.79
1	L5	3822	PSU	O2-C2-N1	-2.34	120.22	122.79
1	L5	3899	OMG	O6-C6-C5	-2.34	120.40	126.60
46	S2	1360	PSU	C3'-C2'-C1'	2.34	104.36	101.64
1	L5	1625	OMG	C4-C5-N7	-2.33	107.03	110.72
1	L5	3841	OMC	O2-C2-N3	-2.33	118.54	122.33
1	L5	2424	OMG	O6-C6-C5	-2.33	120.42	126.60
1	L5	4228	OMG	O6-C6-C5	-2.33	120.42	126.60
1	L5	4636	PSU	C5-C6-N1	-2.33	118.62	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1031	A2M	N9-C8-N7	-2.33	110.73	113.91
1	L5	4623	OMG	O6-C6-C5	-2.33	120.42	126.60
46	S2	1490	OMG	C4-C5-N7	-2.33	107.04	110.72
46	S2	644	OMG	C4-C5-N7	-2.32	107.05	110.72
1	L5	3867	A2M	C6-C5-N7	2.30	136.31	132.02
46	S2	484	A2M	C4-N9-C8	2.30	108.22	105.73
72	SO	138	IAS	OD1-CG-CB	-2.30	118.74	125.43
1	L5	4620	OMU	O2-C2-N1	-2.29	119.74	122.79
46	S2	1337	4AC	O7-C7-N4	2.28	125.52	121.82
1	L5	4227	OMU	O2-C2-N1	-2.28	119.75	122.79
46	S2	512	A2M	C6-C5-N7	2.28	136.27	132.02
1	L5	3822	PSU	O2-C2-N3	-2.27	117.53	121.82
1	L5	3744	OMG	O6-C6-C5	-2.27	120.57	126.60
1	L5	3627	OMG	O6-C6-C5	-2.27	120.57	126.60
1	L5	4571	A2M	C6-C5-N7	2.27	136.25	132.02
1	L5	2401	A2M	C6-C5-N7	2.27	136.25	132.02
1	L5	3792	OMG	C4-C5-N7	-2.27	107.13	110.72
1	L5	3899	OMG	C2'-C1'-N9	-2.26	109.84	114.22
46	S2	866	PSU	C2'-C3'-C4'	-2.26	98.26	102.64
1	L5	2363	A2M	C6-C5-N7	2.25	136.22	132.02
46	S2	1442	OMU	O2-C2-N1	-2.25	119.79	122.79
46	S2	1046	PSU	C5-C6-N1	-2.25	118.74	122.11
1	L5	4571	A2M	N9-C8-N7	-2.24	110.85	113.91
46	S2	166	A2M	C5'-C4'-C3'	-2.24	106.78	115.18
1	L5	4353	PSU	C5-C6-N1	-2.24	118.75	122.11
1	L5	1534	A2M	C6-C5-N7	2.24	136.19	132.02
1	L5	4494	OMG	O6-C6-C5	-2.24	120.67	126.60
1	L5	1582	PSU	C6-C5-C4	-2.23	116.64	118.20
46	S2	509	OMG	O6-C6-C5	-2.23	120.68	126.60
46	S2	644	OMG	O6-C6-C5	-2.23	120.69	126.60
1	L5	1323	A2M	N9-C8-N7	-2.23	110.87	113.91
1	L5	1677	PSU	C5-C6-N1	-2.23	118.77	122.11
46	S2	681	PSU	C5-C6-N1	-2.23	118.77	122.11
1	L5	4590	A2M	N9-C8-N7	-2.23	110.87	113.91
46	S2	159	A2M	C5'-C4'-C3'	-2.22	106.84	115.18
1	L5	4493	PSU	C5-C6-N1	-2.22	118.77	122.11
1	L5	4196	OMG	O6-C6-C5	-2.21	120.74	126.60
46	S2	63	PSU	C5-C6-N1	-2.21	118.79	122.11
46	S2	590	A2M	O4'-C1'-N9	2.21	112.41	108.06
1	L5	3792	OMG	C5-C6-N1	2.21	118.80	113.19
1	L5	400	A2M	C6-C5-N7	2.21	136.13	132.02
46	S2	1177	PSU	C5-C6-N1	-2.21	118.80	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	398	A2M	C6-C5-N7	2.20	136.12	132.02
46	S2	590	A2M	C4-N9-C8	2.20	108.11	105.73
1	L5	3718	A2M	C6-C5-N7	2.20	136.12	132.02
46	S2	576	A2M	C6-C5-N7	2.20	136.11	132.02
1	L5	4442	PSU	O4'-C1'-C2'	2.19	108.23	105.14
1	L5	2424	OMG	C4-C5-N7	-2.19	107.25	110.72
1	L5	1862	PSU	C5-C6-N1	-2.19	118.83	122.11
1	L5	1522	OMG	O6-C6-C5	-2.18	120.81	126.60
46	S2	576	A2M	N9-C8-N7	-2.18	110.93	113.91
1	L5	1782	PSU	C5-C6-N1	-2.18	118.84	122.11
1	L5	4403	PSU	O4'-C1'-C2'	2.18	108.21	105.14
46	S2	436	OMG	O6-C6-C5	-2.18	120.83	126.60
72	SO	138	IAS	OXT-C-O	-2.17	119.17	124.09
1	L5	2363	A2M	N9-C8-N7	-2.16	110.95	113.91
46	S2	1272	OMC	O2-C2-N3	-2.16	118.81	122.33
46	S2	1832	6MZ	N9-C8-N7	-2.16	110.96	113.91
1	L5	4361	PSU	C5-C6-N1	-2.16	118.87	122.11
46	S2	468	A2M	N9-C8-N7	-2.15	110.97	113.91
1	L5	1871	A2M	N9-C8-N7	-2.15	110.97	113.91
1	L5	3695	PSU	C5-C6-N1	-2.14	118.90	122.11
1	L5	3808	OMC	O2-C2-N3	-2.14	118.85	122.33
1	L5	3899	OMG	C4-C5-N7	-2.14	107.33	110.72
1	L5	4590	A2M	C6-C5-N7	2.14	136.01	132.02
1	L5	4392	OMG	O6-C6-C5	-2.14	120.92	126.60
1	L5	4618	OMG	O6-C6-C5	-2.13	120.94	126.60
46	S2	1447	OMG	O6-C6-C5	-2.13	120.94	126.60
1	L5	1779	PSU	C5-C6-N1	-2.13	118.91	122.11
1	L5	3718	A2M	C4-N9-C8	2.13	108.04	105.73
1	L5	2876	OMG	C5-C6-N1	2.13	118.60	113.19
1	L5	4972	PSU	C5-C6-N1	-2.13	118.92	122.11
3	L8	75	OMG	O6-C6-C5	-2.13	120.96	126.60
1	L5	2401	A2M	C2'-C1'-N9	-2.12	109.95	113.53
46	S2	1850	MA6	C4-N9-C1'	-2.12	121.54	126.59
46	S2	1383	A2M	C4-N9-C8	2.11	108.02	105.73
1	L5	4523	A2M	N9-C8-N7	-2.11	111.02	113.91
1	L5	1677	PSU	O4'-C1'-C2'	2.11	108.12	105.14
46	S2	1056	PSU	O4'-C1'-C2'	2.11	108.12	105.14
1	L5	4523	A2M	C2-N1-C6	2.11	122.38	118.77
1	L5	4521	PSU	C5-C6-N1	-2.11	118.95	122.11
46	S2	1288	OMU	C1'-N1-C2	2.11	121.38	117.57
46	S2	572	PSU	O4'-C1'-C2'	2.10	108.10	105.14
46	S2	1031	A2M	C6-C5-N7	2.10	135.93	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	159	A2M	C6-C5-N7	2.09	135.92	132.02
46	S2	1842	4AC	N4-C4-N3	2.09	117.36	113.85
1	L5	3830	A2M	C6-C5-N7	2.09	135.91	132.02
1	L5	2787	A2M	C4-N9-C8	2.09	107.99	105.73
46	S2	300	PSU	C5-C6-N1	-2.09	118.98	122.11
1	L5	2843	PSU	C5-C6-N1	-2.09	118.98	122.11
1	L5	1871	A2M	C2-N1-C6	2.08	122.34	118.77
46	S2	1248	B8N	O4'-C1'-C2'	2.08	108.08	105.14
1	L5	1326	A2M	N9-C8-N7	-2.08	111.07	113.91
1	L5	4392	OMG	C5-C6-N1	2.08	118.47	113.19
46	S2	468	A2M	C2-N1-C6	2.08	122.33	118.77
46	S2	1248	B8N	C31-N3-C2	2.08	120.78	117.67
46	S2	1248	B8N	O36-C34-O35	-2.07	119.38	124.09
1	L5	1779	PSU	O4'-C1'-C2'	2.07	108.06	105.14
46	S2	1238	PSU	O4-C4-C5	-2.06	118.65	124.05
46	S2	1678	A2M	C6-C5-N7	2.06	135.85	132.02
46	S2	601	OMG	O6-C6-C5	-2.06	121.14	126.60
1	L5	1522	OMG	C8-N7-C5	2.05	107.96	104.24
46	S2	1367	PSU	C5-C6-N1	-2.05	119.03	122.11
1	L5	398	A2M	C4-N9-C8	2.05	107.95	105.73
1	L5	4590	A2M	C2-N1-C6	2.05	122.29	118.77
46	S2	436	OMG	C5-C6-N1	2.05	118.40	113.19
46	S2	1490	OMG	C5-C6-N1	2.05	118.39	113.19
1	L5	3925	OMU	O2-C2-N1	-2.05	120.06	122.79
1	L5	1534	A2M	N9-C8-N7	-2.05	111.11	113.91
1	L5	4523	A2M	C6-C5-N7	2.04	135.83	132.02
46	S2	1842	4AC	O7-C7-N4	2.04	125.12	121.82
72	SO	138	IAS	OXT-C-CA	2.04	120.33	113.38
46	S2	296	PSU	C5-C6-N1	-2.04	119.05	122.11
46	S2	1678	A2M	N9-C8-N7	-2.03	111.13	113.91
46	S2	159	A2M	C2'-C3'-C4'	2.03	106.40	101.99
46	S2	27	A2M	C2-N1-C6	2.02	122.24	118.77
1	L5	2839	PSU	C5-C6-N1	-2.02	119.08	122.11
1	L5	3830	A2M	O2'-C2'-C1'	2.02	113.02	109.08
46	S2	484	A2M	N9-C8-N7	-2.02	111.15	113.91
1	L5	3825	A2M	C6-C5-N7	2.01	135.77	132.02
1	L5	4636	PSU	O4'-C1'-C2'	2.01	107.98	105.14
1	L5	3899	OMG	C5-C6-N1	2.01	118.30	113.19
46	S2	93	PSU	C5-C6-N1	-2.01	119.10	122.11
46	S2	1643	PSU	O4'-C1'-C2'	2.01	107.97	105.14
1	L5	3867	A2M	N9-C8-N7	-2.01	111.17	113.91
1	L5	1522	OMG	C2'-C1'-N9	-2.01	110.33	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	S2	1248	B8N	O36-C34-C33	2.00	120.20	113.38

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	14	OMU	C1'-C2'-O2'-CM2
1	L5	1582	PSU	O4'-C1'-C5-C4
1	L5	1582	PSU	O4'-C1'-C5-C6
1	L5	1677	PSU	C2'-C1'-C5-C6
1	L5	2824	OMC	C1'-C2'-O2'-CM2
1	L5	3701	OMC	C2'-C1'-N1-C6
1	L5	3724	A2M	C1'-C2'-O2'-CM'
1	L5	3770	PSU	C3'-C4'-C5'-O5'
1	L5	3818	UY1	C1'-C2'-O2'-CM2
1	L5	3851	PSU	C3'-C4'-C5'-O5'
1	L5	4196	OMG	C1'-C2'-O2'-CM2
1	L5	4500	PSU	C3'-C4'-C5'-O5'
1	L5	4500	PSU	O4'-C4'-C5'-O5'
1	L5	4571	A2M	C1'-C2'-O2'-CM'
1	L5	4590	A2M	C4'-C5'-O5'-P
1	L5	4636	PSU	C2'-C1'-C5-C6
1	L5	4636	PSU	C3'-C4'-C5'-O5'
1	L5	4637	OMG	C1'-C2'-O2'-CM2
46	S2	121	OMU	C1'-C2'-O2'-CM2
46	S2	166	A2M	C3'-C4'-C5'-O5'
46	S2	468	A2M	C1'-C2'-O2'-CM'
46	S2	576	A2M	C3'-C4'-C5'-O5'
46	S2	801	PSU	C3'-C4'-C5'-O5'
46	S2	822	PSU	C3'-C4'-C5'-O5'
46	S2	1031	A2M	C1'-C2'-O2'-CM'
46	S2	1272	OMC	C1'-C2'-O2'-CM2
46	S2	1326	UY1	C2'-C1'-C5-C4
46	S2	1383	A2M	C1'-C2'-O2'-CM'
46	S2	1442	OMU	C1'-C2'-O2'-CM2
46	S2	1490	OMG	O4'-C4'-C5'-O5'
46	S2	1678	A2M	C1'-C2'-O2'-CM'
46	S2	1851	MA6	O4'-C4'-C5'-O5'
72	SO	138	IAS	CA-CB-CG-OD1
1	L5	2815	A2M	O4'-C4'-C5'-O5'
1	L5	2815	A2M	C3'-C4'-C5'-O5'
1	L5	3770	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L5	3818	UY1	O4'-C4'-C5'-O5'
46	S2	100	PSU	O4'-C4'-C5'-O5'
46	S2	668	A2M	O4'-C4'-C5'-O5'
46	S2	668	A2M	C3'-C4'-C5'-O5'
46	S2	1851	MA6	C3'-C4'-C5'-O5'
1	L5	3818	UY1	C3'-C4'-C5'-O5'
1	L5	4636	PSU	O4'-C4'-C5'-O5'
46	S2	100	PSU	C3'-C4'-C5'-O5'
46	S2	159	A2M	C3'-C4'-C5'-O5'
46	S2	166	A2M	O4'-C4'-C5'-O5'
46	S2	576	A2M	O4'-C4'-C5'-O5'
46	S2	801	PSU	O4'-C4'-C5'-O5'
46	S2	822	PSU	O4'-C4'-C5'-O5'
1	L5	1625	OMG	C3'-C2'-O2'-CM2
1	L5	3701	OMC	C2'-C1'-N1-C2
1	L5	3867	A2M	C3'-C4'-C5'-O5'
1	L5	3851	PSU	O4'-C4'-C5'-O5'
46	S2	159	A2M	O4'-C4'-C5'-O5'
1	L5	4447	5MC	C2'-C1'-N1-C6
1	L5	2787	A2M	C2'-C1'-N9-C8
46	S2	1248	B8N	N34-C33-C34-O36
1	L5	2787	A2M	C2'-C1'-N9-C4
46	S2	1248	B8N	N34-C33-C34-O35
1	L5	3818	UY1	C4'-C5'-O5'-P
46	S2	512	A2M	O4'-C4'-C5'-O5'
1	L5	400	A2M	C1'-C2'-O2'-CM'
46	S2	116	OMU	C1'-C2'-O2'-CM2
1	L5	1326	A2M	C4'-C5'-O5'-P
46	S2	1490	OMG	C4'-C5'-O5'-P
46	S2	590	A2M	C3'-C4'-C5'-O5'
46	S2	1248	B8N	C31-C32-C33-C34
1	L5	4500	PSU	C4'-C5'-O5'-P
1	L5	3764	PSU	C3'-C4'-C5'-O5'
46	S2	428	OMU	O4'-C4'-C5'-O5'
46	S2	1447	OMG	C3'-C4'-C5'-O5'
1	L5	3701	OMC	O4'-C1'-N1-C6
1	L5	4447	5MC	O4'-C1'-N1-C6
1	L5	1534	A2M	C4'-C5'-O5'-P
1	L5	3701	OMC	O4'-C1'-N1-C2
1	L5	3764	PSU	O4'-C4'-C5'-O5'
46	S2	512	A2M	C3'-C4'-C5'-O5'
1	L5	4447	5MC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
46	S2	428	OMU	C2'-C1'-N1-C6
46	S2	644	OMG	C4'-C5'-O5'-P
1	L5	3724	A2M	O4'-C4'-C5'-O5'
46	S2	966	PSU	O4'-C4'-C5'-O5'
1	L5	4494	OMG	C3'-C2'-O2'-CM2
1	L5	2815	A2M	C4'-C5'-O5'-P
1	L5	4447	5MC	O4'-C1'-N1-C2
1	L5	3844	PSU	C4'-C5'-O5'-P
46	S2	1851	MA6	C4'-C5'-O5'-P
46	S2	1383	A2M	C3'-C4'-C5'-O5'
46	S2	1490	OMG	C3'-C4'-C5'-O5'
1	L5	3818	UY1	O4'-C1'-C5-C4
1	L5	4500	PSU	O4'-C1'-C5-C4
46	S2	1326	UY1	O4'-C1'-C5-C4
46	S2	1383	A2M	O4'-C4'-C5'-O5'
46	S2	1832	6MZ	N1-C6-N6-C9
1	L5	2787	A2M	O4'-C1'-N9-C8
46	S2	590	A2M	O4'-C1'-N9-C8
1	L5	1322	1MA	C2'-C1'-N9-C8
46	S2	428	OMU	O4'-C1'-N1-C6
46	S2	867	OMG	O4'-C4'-C5'-O5'
1	L5	398	A2M	C1'-C2'-O2'-CM'
1	L5	2363	A2M	C1'-C2'-O2'-CM'
1	L5	2415	OMU	C1'-C2'-O2'-CM2
1	L5	2815	A2M	C1'-C2'-O2'-CM'
1	L5	3718	A2M	C1'-C2'-O2'-CM'
46	S2	27	A2M	C1'-C2'-O2'-CM'
1	L5	1524	A2M	C3'-C2'-O2'-CM'
1	L5	2363	A2M	C3'-C2'-O2'-CM'
1	L5	1322	1MA	C2'-C1'-N9-C4
1	L5	3724	A2M	C3'-C4'-C5'-O5'
46	S2	428	OMU	C3'-C4'-C5'-O5'
1	L5	1677	PSU	O4'-C1'-C5-C6
1	L5	3818	UY1	O4'-C1'-C5-C6
1	L5	4500	PSU	O4'-C1'-C5-C6
1	L5	4636	PSU	O4'-C1'-C5-C6
1	L5	2351	OMC	C2'-C1'-N1-C2
1	L5	1534	A2M	O4'-C4'-C5'-O5'
1	L5	1792	PSU	C3'-C4'-C5'-O5'
1	L5	2351	OMC	O4'-C4'-C5'-O5'
1	L5	2422	OMC	O4'-C4'-C5'-O5'
1	L5	3785	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L5	3844	PSU	O4'-C4'-C5'-O5'
46	S2	966	PSU	C3'-C4'-C5'-O5'
1	L5	3887	OMC	C4'-C5'-O5'-P
46	S2	428	OMU	C3'-C2'-O2'-CM2
46	S2	428	OMU	O4'-C1'-N1-C2
46	S2	590	A2M	C2'-C1'-N9-C8
46	S2	668	A2M	C2'-C1'-N9-C8

There are no ring outliers.

91 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	S2	116	OMU	2	0
46	S2	1337	4AC	2	0
1	L5	2876	OMG	1	0
46	S2	1383	A2M	1	0
1	L5	1340	OMC	2	0
1	L5	1534	A2M	2	0
1	L5	4628	PSU	1	0
1	L5	4296	PSU	1	0
46	S2	667	PSU	1	0
46	S2	1442	OMU	1	0
46	S2	99	A2M	1	0
1	L5	1522	OMG	1	0
1	L5	2415	OMU	2	0
1	L5	1536	PSU	1	0
1	L5	3925	OMU	1	0
46	S2	576	A2M	3	0
1	L5	4456	OMC	1	0
46	S2	686	PSU	2	0
1	L5	1326	A2M	1	0
46	S2	1596	PSU	1	0
1	L5	5001	PSU	1	0
1	L5	3785	A2M	1	0
1	L5	2804	OMC	2	0
46	S2	1238	PSU	2	0
1	L5	4447	5MC	1	0
46	S2	1842	4AC	1	0
46	S2	681	PSU	1	0
46	S2	1832	6MZ	1	0
3	L8	55	PSU	1	0
1	L5	3867	A2M	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	3887	OMC	1	0
1	L5	1677	PSU	1	0
1	L5	1871	A2M	1	0
3	L8	75	OMG	1	0
1	L5	3701	OMC	1	0
46	S2	484	A2M	1	0
46	S2	36	PSU	2	0
1	L5	2815	A2M	1	0
46	S2	1851	MA6	3	0
1	L5	2351	OMC	1	0
1	L5	3792	OMG	1	0
1	L5	3818	UY1	1	0
46	S2	815	PSU	1	0
46	S2	822	PSU	1	0
1	L5	2424	OMG	3	0
46	S2	1678	A2M	2	0
1	L5	4637	OMG	3	0
1	L5	3718	A2M	4	0
3	L8	14	OMU	1	0
1	L5	4500	PSU	3	0
46	S2	1272	OMC	1	0
1	L5	1322	1MA	1	0
46	S2	1445	PSU	1	0
46	S2	1046	PSU	1	0
1	L5	398	A2M	2	0
1	L5	1625	OMG	1	0
1	L5	3762	PSU	1	0
1	L5	4196	OMG	1	0
46	S2	866	PSU	2	0
1	L5	4293	PSU	1	0
1	L5	2363	A2M	1	0
1	L5	2422	OMC	2	0
1	L5	4689	PSU	1	0
46	S2	572	PSU	1	0
1	L5	4536	OMC	1	0
1	L5	3869	OMC	1	0
46	S2	1232	PSU	2	0
46	S2	121	OMU	2	0
46	S2	468	A2M	3	0
1	L5	2632	PSU	2	0
1	L5	4457	PSU	1	0
46	S2	462	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	3724	A2M	1	0
1	L5	4620	OMU	2	0
46	S2	1177	PSU	1	0
46	S2	1643	PSU	1	0
1	L5	2839	PSU	1	0
1	L5	400	A2M	1	0
1	L5	4220	6MZ	1	0
1	L5	4571	A2M	1	0
46	S2	509	OMG	1	0
46	S2	159	A2M	4	0
46	S2	512	A2M	1	0
1	L5	1524	A2M	1	0
1	L5	4623	OMG	1	0
46	S2	166	A2M	1	0
46	S2	867	OMG	3	0
1	L5	4498	OMU	3	0
1	L5	4228	OMG	1	0
46	S2	1804	OMU	1	0
1	L5	1683	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 410 ligands modelled in this entry, 408 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
82	SPD	L5	5377	-	9,9,9	0.33	0	8,8,8	0.76	0
82	SPD	L5	5378	-	9,9,9	0.34	0	8,8,8	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	SPD	L5	5377	-	-	3/7/7/7	-
82	SPD	L5	5378	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	L5	5378	SPD	N6-C7-C8-C9
82	L5	5377	SPD	C3-C4-C5-N6
82	L5	5378	SPD	C8-C7-N6-C5
82	L5	5378	SPD	C2-C3-C4-C5
82	L5	5377	SPD	N6-C7-C8-C9
82	L5	5377	SPD	N1-C2-C3-C4
82	L5	5378	SPD	C3-C4-C5-N6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	L5	5377	SPD	2	0
82	L5	5378	SPD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

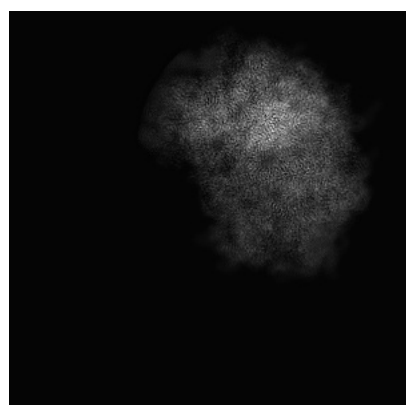
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18539. These allow visual inspection of the internal detail of the map and identification of artifacts.

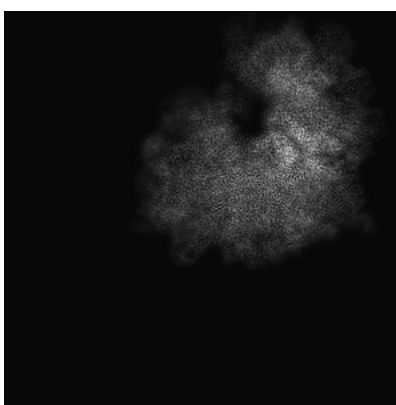
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

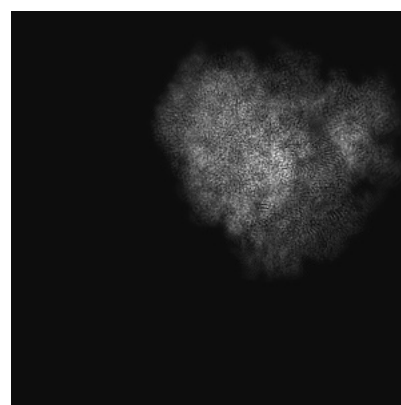
6.1.1 Primary map



X



Y

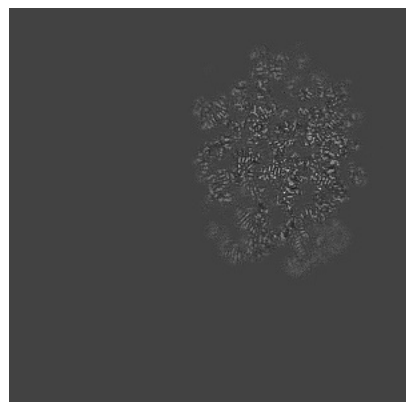


Z

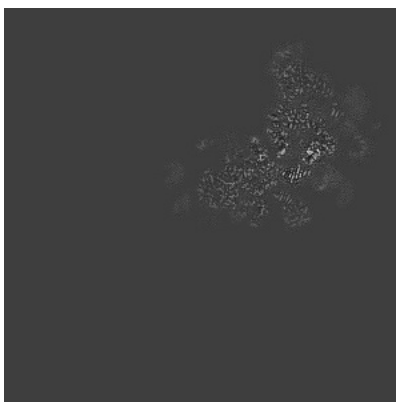
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices [i](#)

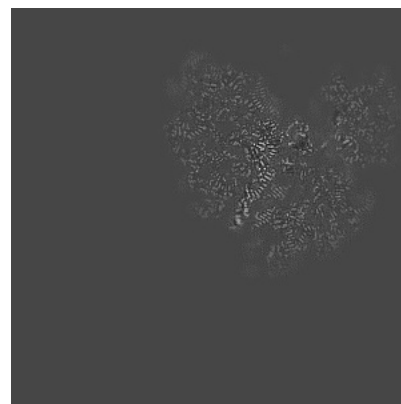
6.3.1 Primary map



X Index: 306



Y Index: 326

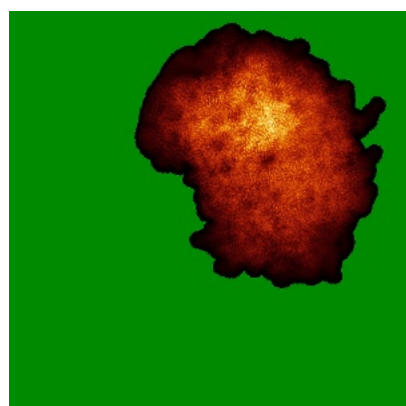


Z Index: 363

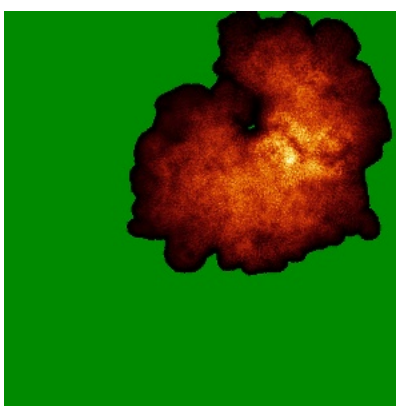
The images above show the largest variance slices of the map in three orthogonal directions.

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

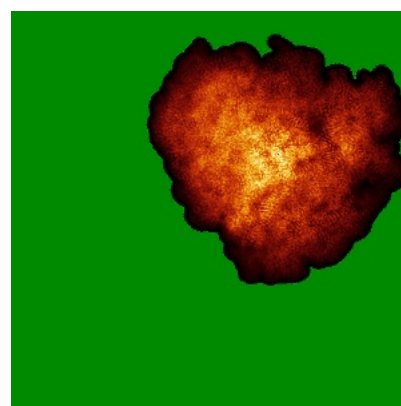
6.4.1 Primary map



X



Y

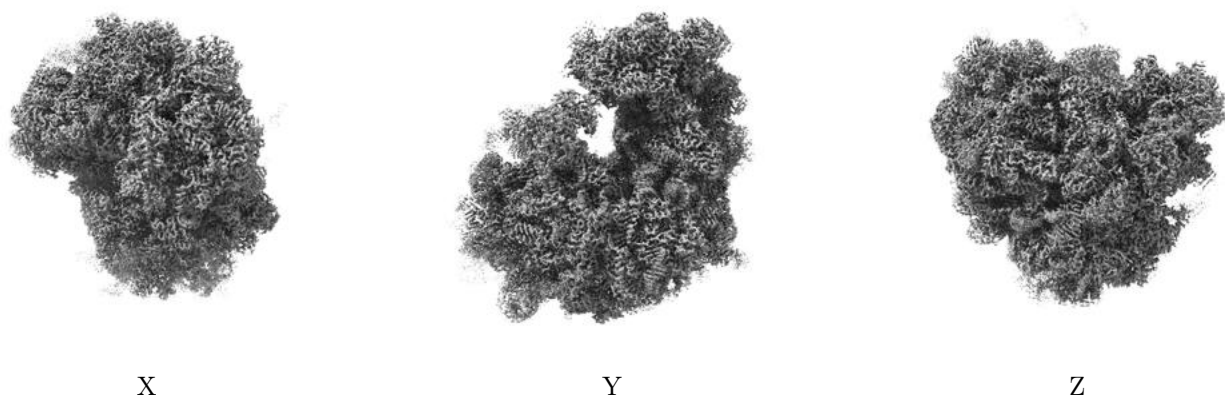


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0266. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

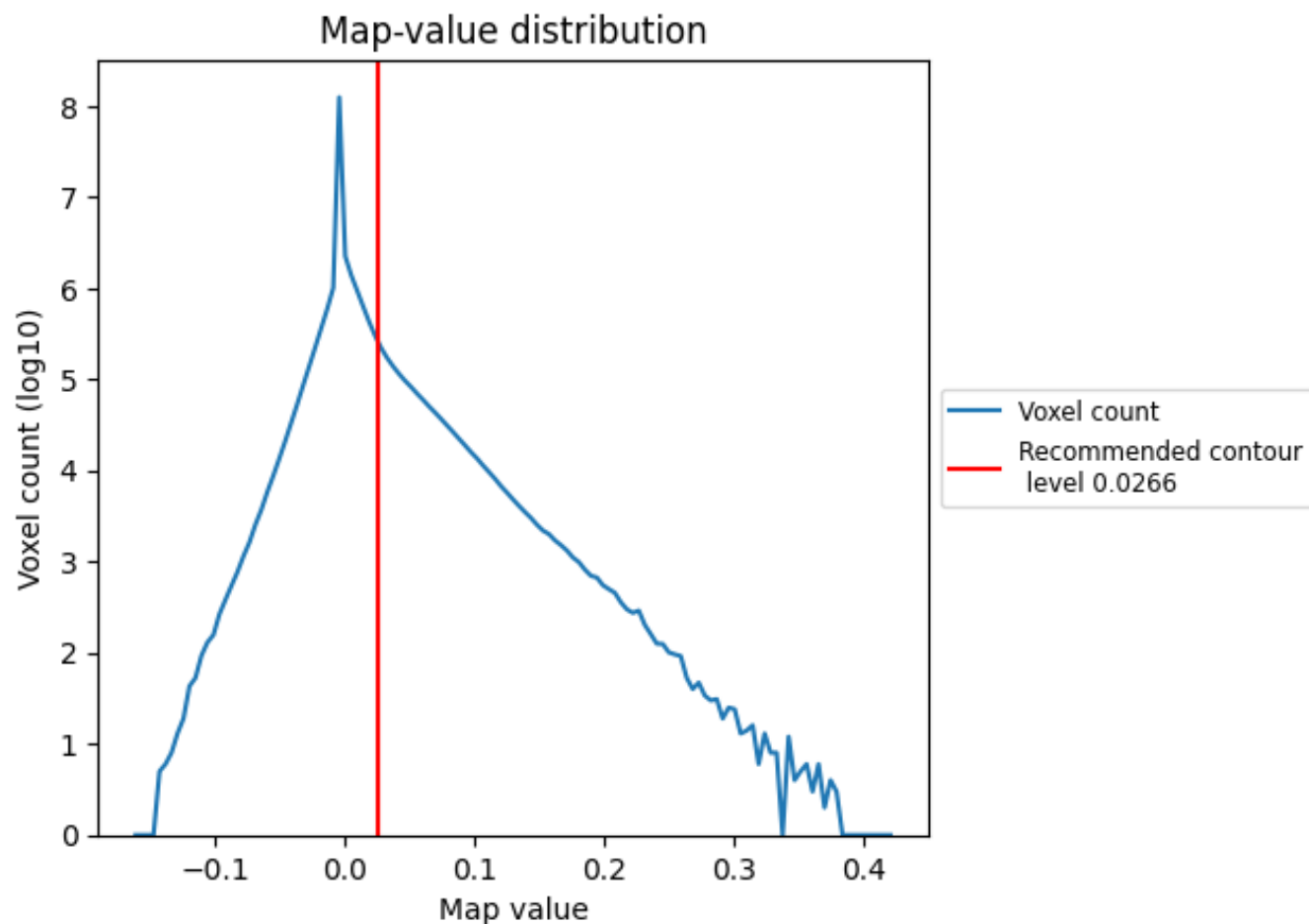
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

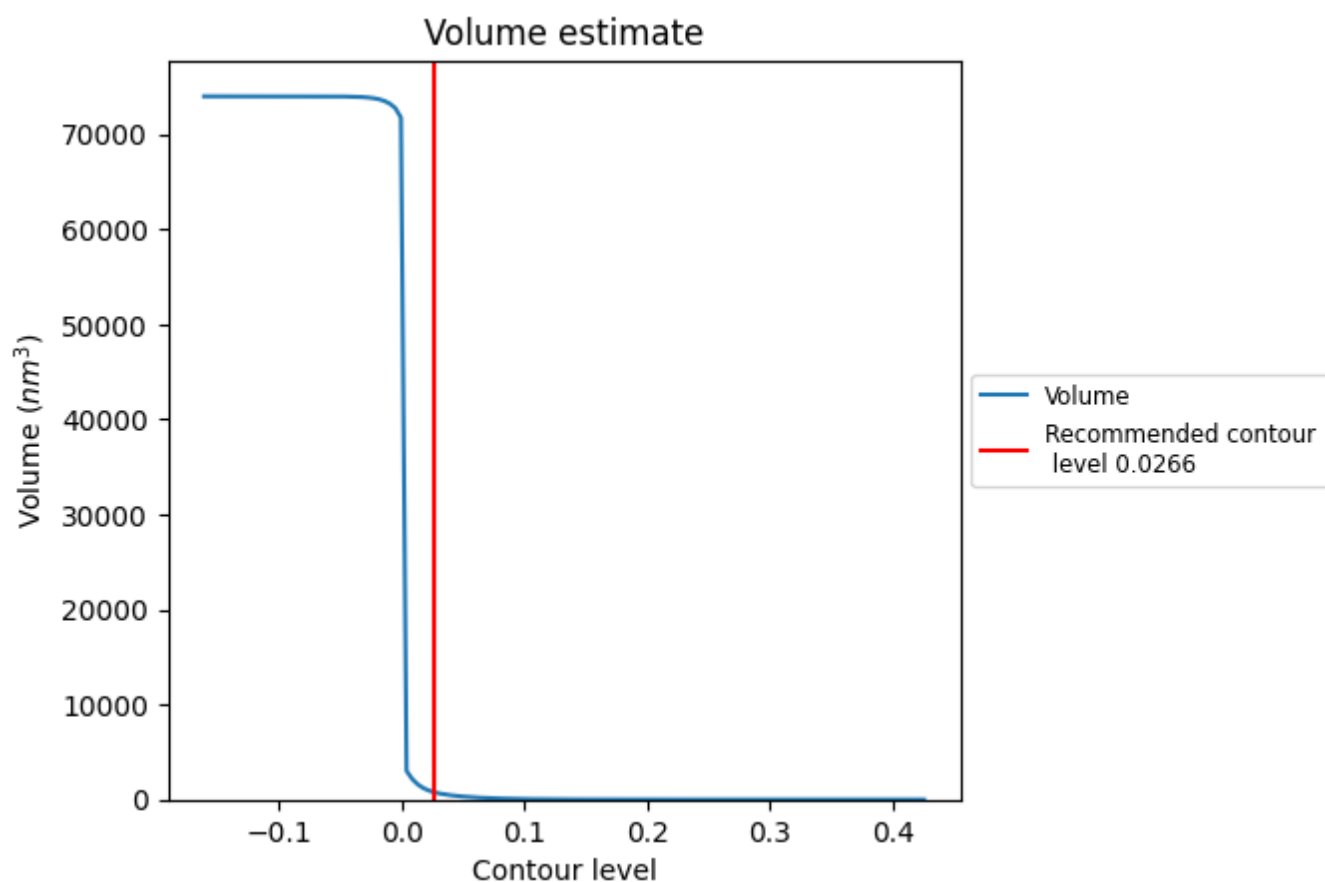
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

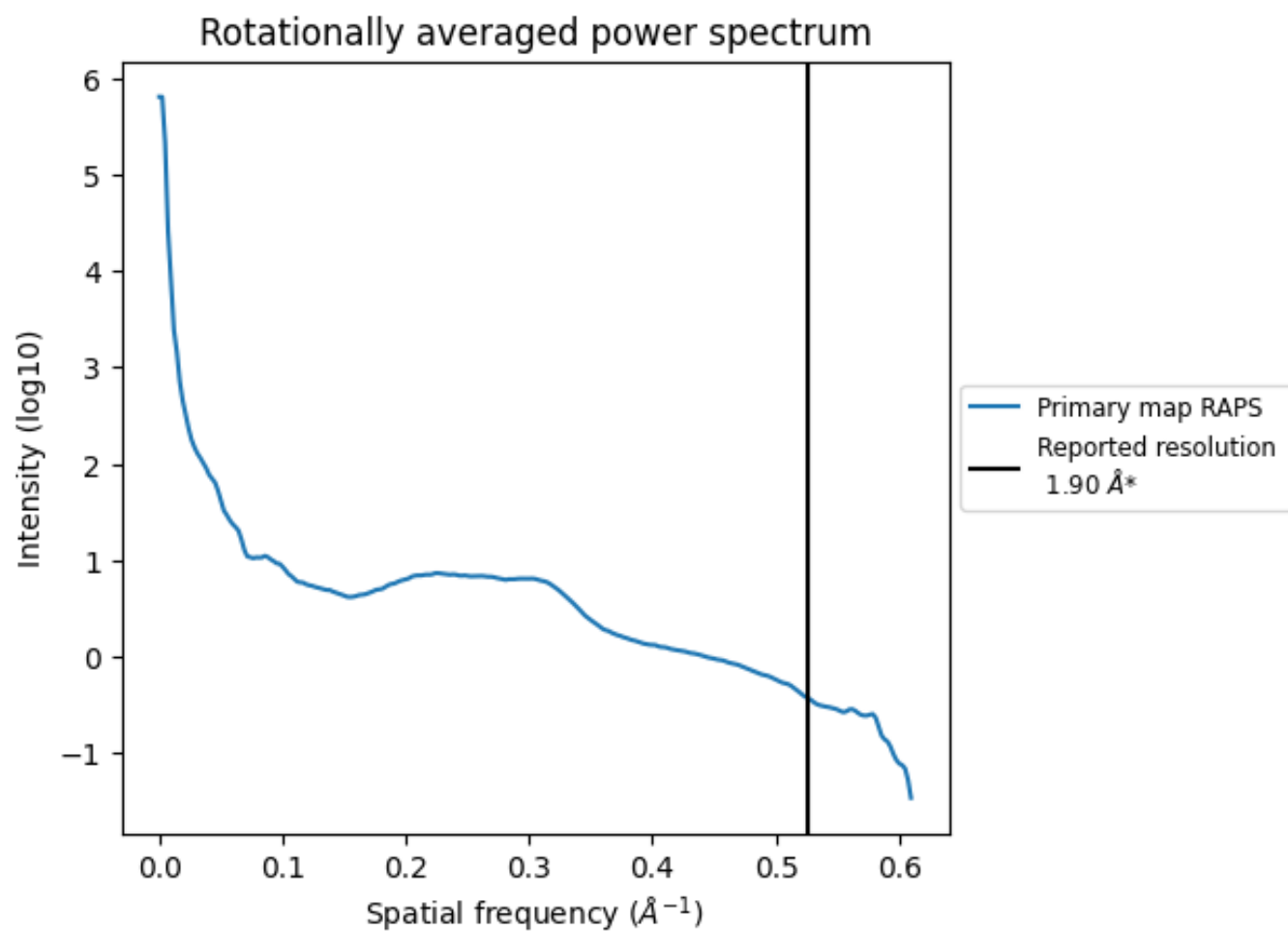
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 776 nm³; this corresponds to an approximate mass of 701 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 0.526 Å⁻¹

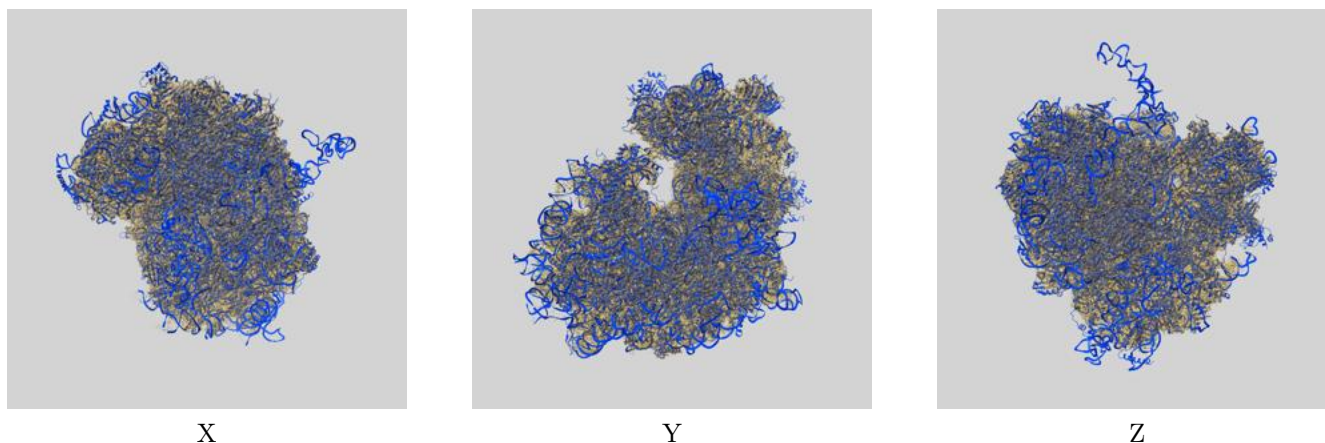
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

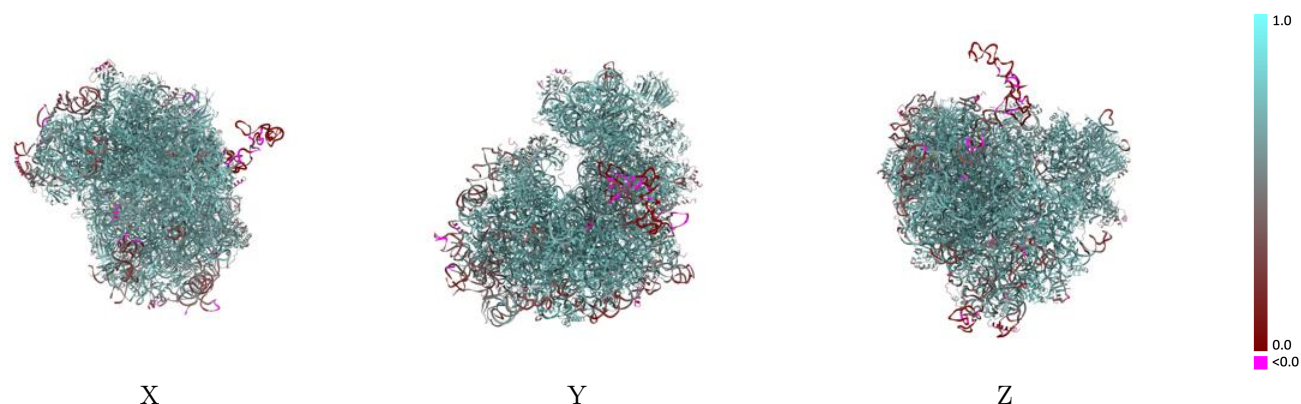
This section contains information regarding the fit between EMDB map EMD-18539 and PDB model 8QOI. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



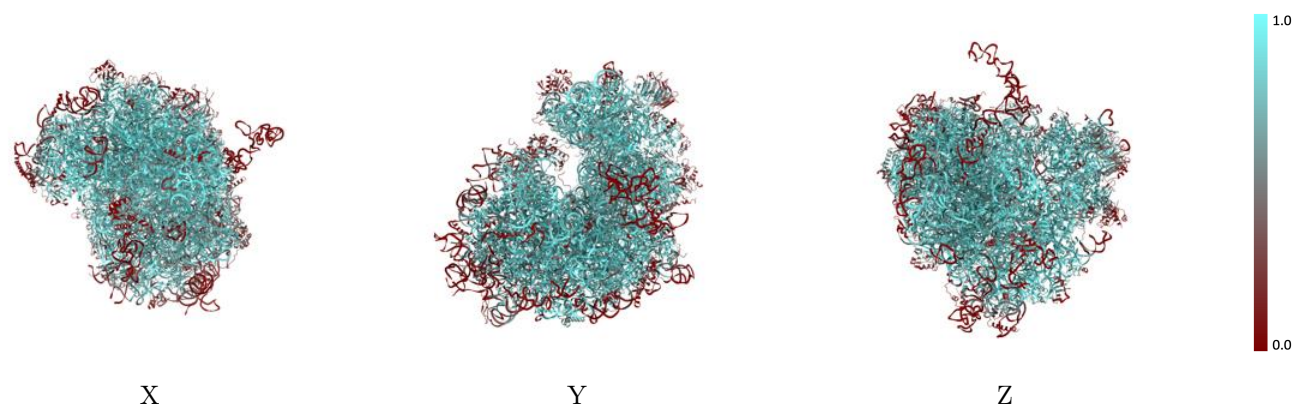
The images above show the 3D surface view of the map at the recommended contour level 0.0266 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



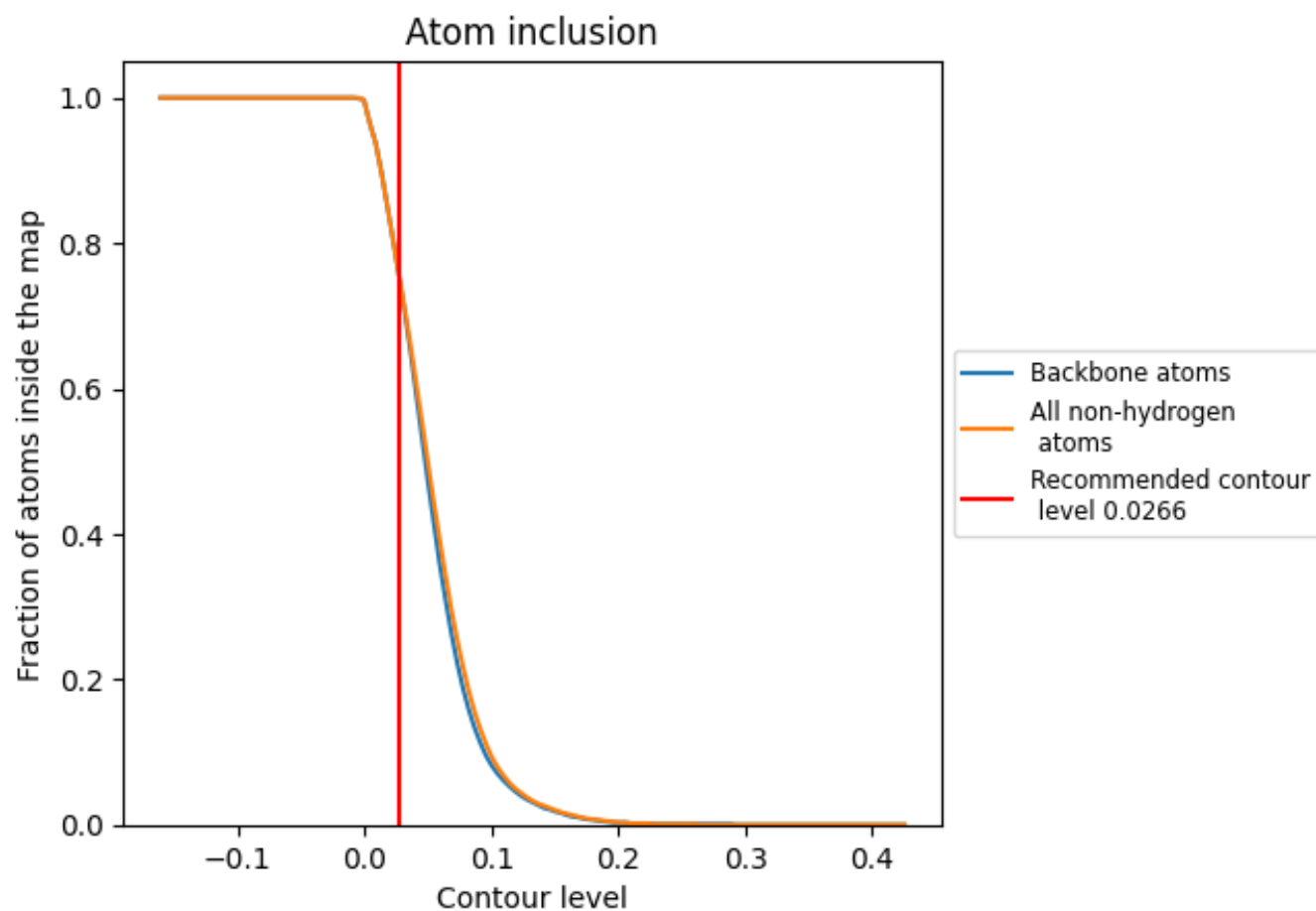
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0266).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.0266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.6690
L5	 0.7500	 0.6420
L7	 0.8910	 0.7000
L8	 0.8520	 0.6880
LA	 0.9720	 0.7900
LB	 0.8180	 0.7300
LC	 0.8300	 0.7310
LD	 0.5970	 0.6380
LE	 0.5300	 0.5970
LF	 0.8590	 0.7570
LG	 0.5650	 0.6050
LH	 0.6550	 0.6850
LI	 0.6850	 0.6830
LJ	 0.4600	 0.5790
LL	 0.7000	 0.6660
LM	 0.7880	 0.6920
LN	 0.9670	 0.7880
LO	 0.8460	 0.7410
LP	 0.8700	 0.7660
LQ	 0.8760	 0.7740
LR	 0.7860	 0.6910
LS	 0.8670	 0.7480
LT	 0.7820	 0.7160
LU	 0.3610	 0.5570
LV	 0.9200	 0.7640
LW	 0.5050	 0.5020
LX	 0.7840	 0.7180
LY	 0.7960	 0.7250
LZ	 0.7110	 0.6750
La	 0.8820	 0.7630
Lb	 0.5640	 0.6440
Lc	 0.8720	 0.7000
Ld	 0.7720	 0.7060
Le	 0.8720	 0.7690
Lf	 0.9190	 0.7720



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Chain	Atom inclusion	Q-score
Lg	 0.8470	 0.7210
Lh	 0.7700	 0.7160
Li	 0.6880	 0.6900
Lj	 0.9540	 0.7920
Lk	 0.4920	 0.5970
Ll	 0.8320	 0.7400
Lm	 0.7810	 0.7290
Ln	 0.9950	 0.7810
Lo	 0.7210	 0.7220
Lp	 0.9740	 0.7810
Lr	 0.8270	 0.7330
S2	 0.8310	 0.6640
SA	 0.7790	 0.6830
SB	 0.8420	 0.7050
SC	 0.8400	 0.7280
SD	 0.7260	 0.6640
SE	 0.8430	 0.7180
SF	 0.8190	 0.7090
SG	 0.5280	 0.6140
SH	 0.3970	 0.5370
SI	 0.7950	 0.6850
SJ	 0.8150	 0.7130
SK	 0.6960	 0.6760
SL	 0.8230	 0.7070
SM	 0.0380	 0.4540
SN	 0.8920	 0.7300
SO	 0.8730	 0.7040
SP	 0.7340	 0.6990
SQ	 0.8360	 0.7240
SR	 0.6830	 0.6390
SS	 0.7530	 0.7050
ST	 0.8210	 0.7210
SU	 0.5530	 0.6430
SV	 0.7480	 0.6930
SW	 0.9450	 0.7600
SX	 0.9250	 0.7620
SY	 0.7100	 0.6700
SZ	 0.6230	 0.6660
Sa	 0.8580	 0.7170
Sb	 0.6450	 0.6570
Sc	 0.7860	 0.6150
Sd	 0.8870	 0.7390

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Chain	Atom inclusion	Q-score
Se	 0.6280	 0.6400
Sf	 0.1090	 0.5240
Sg	 0.5000	 0.6450