



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 10:45 PM EDT

PDB ID : 9C3H / pdb_00009c3h
EMDB ID : EMD-45170
Title : Structure of the CNOT3-bound human 80S ribosome with tRNA-ARG in the P-site.
Authors : Erzberger, J.P.; Cruz, V.E.
Deposited on : 2024-06-01
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

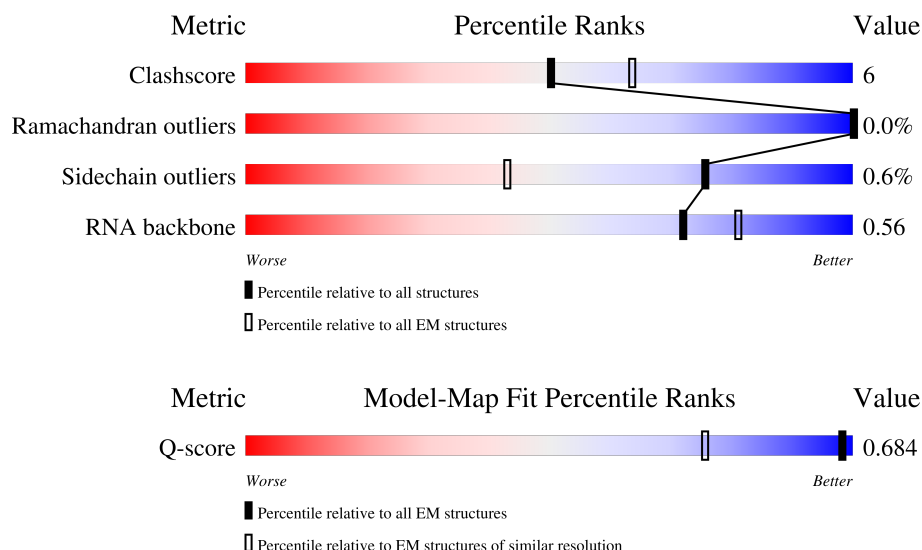
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.00 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.



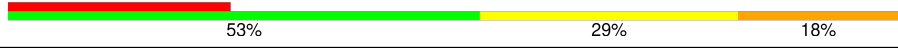
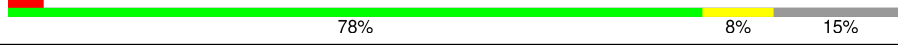
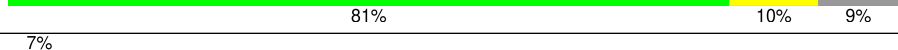
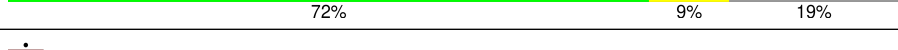
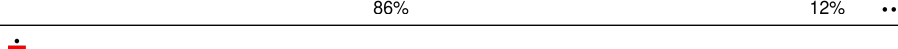
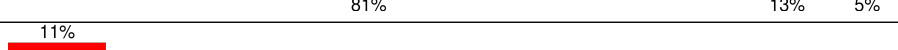
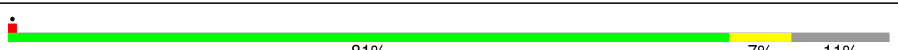
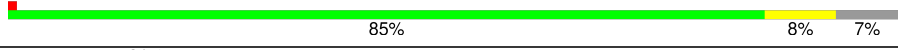
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1659 (1.50 - 2.50)

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	L1	157	
2	L5	5069	
3	L8	297	

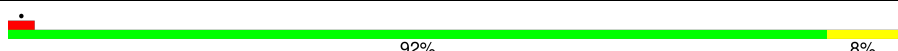
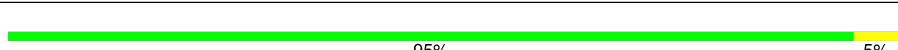
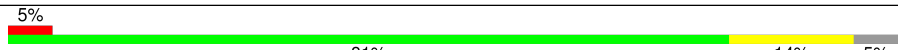
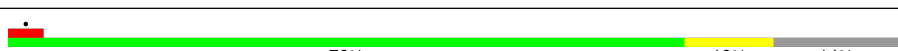
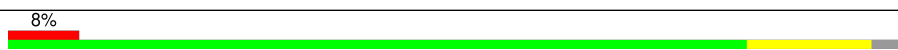
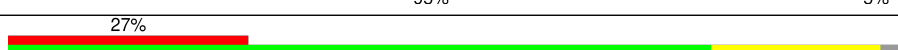
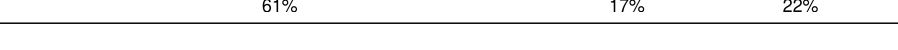
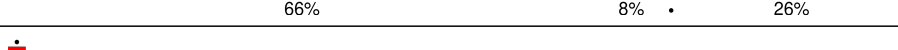
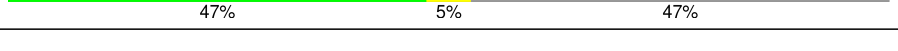
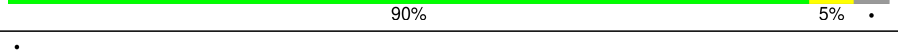
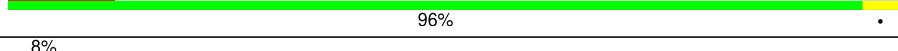
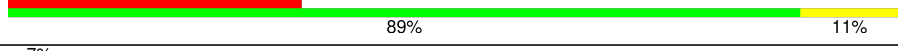
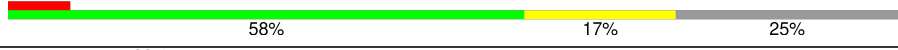
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Mol	Chain	Length	Quality of chain
4	L9	121	
5	LB	403	
6	S4	76	
7	LC	427	
8	LD	257	
9	LE	145	
10	LF	248	
11	LG	266	
12	LH	192	
13	LI	135	
14	LJ	178	
15	LK	288	
16	LM	215	
17	LN	204	
18	LO	123	
19	LP	97	
20	LQ	211	
21	LR	196	
22	LS	176	
23	LT	160	
24	LU	51	
25	LV	140	
26	LW	157	
27	LY	203	
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	106	
34	Lf	110	
35	Lg	117	
36	Lh	184	
37	Li	105	
38	Lj	188	
39	Lk	70	
40	Ll	137	
41	Lm	128	
42	Ln	156	
43	Lo	99	
44	Lp	92	
45	Lz	214	
46	NC	25	
47	S1	264	
48	S2	1869	
49	S5	9	
50	SA	295	
51	SB	609	
52	SC	293	
53	SD	204	

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

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Mol	Chain	Length	Quality of chain
79	Sf	56	9%84%12%••
80	Sg	317	70%63%32%•
81	So	25	•96%•
82	Sy	132	92%65%26%•8%
83	Sz	156	47%28%18%•53%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 222228 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 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	148	Total	C	N	O	P	0	0
			3153	1408	563	1035	147		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3531	Total	C	N	O	P	0	0
			75768	33782	13851	24605	3530		

- Molecule 3 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	293	Total	C	N	O	S	0	0
			2386	1510	435	427	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L9	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	401	Total	C	N	O	S	0	0
			3234	2058	607	555	14		

- Molecule 6 is a RNA chain called tRNA-ARG,CCG-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S4	76	Total	C	N	O	P	0	0
			1634	732	290	536	76		

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 8 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD	248	Total	C	N	O	S	0	0
			1899	1189	389	315	6		

- Molecule 9 is a protein called Large ribosomal subunit protein uL24.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LF	173	SER	ALA	conflict	UNP P18124

- Molecule 11 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	216	Total	C	N	O	S	0	0
			1752	1117	337	294	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 13 is a protein called Large ribosomal subunit protein eL32.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	167	Total	C	N	O	S	0	0
			1340	848	250	236	6		

- Molecule 15 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LK	222	Total	C	N	O	S	0	0
			1780	1147	337	292	4		

- Molecule 16 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 17 is a protein called Large ribosomal subunit protein eL15.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 19 is a protein called Large ribosomal subunit protein eL37.

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

- Molecule 20 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 21 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	186	Total	C	N	O	S	0	0
			1558	965	335	249	9		

- Molecule 22 is a protein called Large ribosomal subunit protein eL20.

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

- Molecule 23 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 24 is a protein called Large ribosomal subunit protein eL39.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 26 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LW	110	Total	C	N	O	S	0	0
			893	560	180	150	3		

- Molecule 27 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	198	Total	C	N	O	S	0	0
			1624	1048	317	254	5		

- Molecule 28 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	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
			1162	736	237	186	3		

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	104	Total	C	N	O	S	0	0
			848	526	186	132	4		

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	101	Total	C	N	O	S	0	0
			785	498	138	142	7		

- Molecule 32 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	104	Total	C	N	O	S	0	0
			862	546	167	147	2		

- Molecule 33 is a protein called Large ribosomal subunit protein eL42.

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

- Molecule 34 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	109	Total	C	N	O	S	0	0
			875	555	174	143	3		

- Molecule 35 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	111	Total	C	N	O	S	0	0
			882	552	182	142	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lh	159	Total	C	N	O	S	0	0
			1289	808	249	223	9		

- Molecule 37 is a protein called Large ribosomal subunit protein eL36.

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

- Molecule 38 is a protein called Large ribosomal subunit protein eL18.

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

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

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 Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	124	Total	C	N	O	S	0	0
			990	614	205	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ll	2	ACE	-	acetylation	UNP P46779

- Molecule 41 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	100	Total	C	N	O	S	0	0
			816	524	142	148	2		

- Molecule 42 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	116	Total	C	N	O	S	0	0
			949	606	178	164	1		

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	PRO	deletion	UNP P62987
Lo	?	-	PRO	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	ARG	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	PHE	deletion	UNP P62987
Lo	?	-	ALA	deletion	UNP P62987
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	LYS	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	GLU	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	GLY	deletion	UNP P62987
Lo	?	-	ARG	deletion	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
Lo	?	-	THR	deletion	UNP P62987
Lo	?	-	LEU	deletion	UNP P62987
Lo	?	-	SER	deletion	UNP P62987
Lo	?	-	ASP	deletion	UNP P62987
Lo	?	-	TYR	deletion	UNP P62987
Lo	?	-	ASN	deletion	UNP P62987
Lo	?	-	ILE	deletion	UNP P62987
Lo	?	-	GLN	deletion	UNP P62987
Lo	?	-	LYS	deletion	UNP P62987

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

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 Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lz	211	Total	C	N	O	S	0	0
			1705	1081	329	281	14		

- Molecule 46 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	NC	25	Total	C	N	O	0	0
			227	134	52	41		

- Molecule 47 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S1	221	Total	C	N	O	S	0	0
			1790	1135	323	318	14		

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1660	Total	C	N	O	P	0	0
			35485	15869	6358	11599	1659		

- Molecule 49 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S5	9	Total	C	N	O	P	0	0
			191	85	33	64	9		

- Molecule 50 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SA	220	Total	C	N	O	S	0	0
			1731	1099	303	321	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	2	ACE	-	acetylation	UNP P08865

- Molecule 51 is a protein called CCR4-NOT transcription complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SB	232	Total	C	N	O	S	0	0
			1937	1204	344	383	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SB	608	PRO	-	expression tag	UNP O75175
SB	609	ARG	-	expression tag	UNP O75175

- Molecule 52 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SC	219	Total	C	N	O	S	0	0
			1700	1100	292	298	10		

- Molecule 53 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SD	184	Total	C	N	O	S	0	0
			1463	917	276	263	7		

- Molecule 54 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SE	262	Total	C	N	O	S	0	0
			2075	1324	386	357	8		

- Molecule 55 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SG	229	Total	C	N	O	S	0	0
			1853	1158	369	319	7		

- Molecule 56 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH	187	Total	C	N	O	S	0	0
			1509	963	277	268	1		

- Molecule 57 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SI	207	Total	C	N	O	S	0	0
			1695	1064	334	292	5		

- Molecule 58 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SJ	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 59 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SK	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 60 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SL	143	Total	C	N	O	S	0	0
			1180	754	223	197	6		

- Molecule 61 is a protein called Small ribosomal subunit protein eS10.

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

- Molecule 62 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 63 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SO	127	Total	C	N	O	S	0	0
			956	585	189	176	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 64 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SP	125	Total	C	N	O	S	0	0
			1021	647	192	175	7		

- Molecule 65 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ	139	Total	C	N	O	S	0	0
			1108	704	210	191	3		

- Molecule 66 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	ST	147	Total	C	N	O	S	0	0
			1208	758	244	205	1		

- Molecule 68 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SU	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 69 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 70 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 71 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 72 is a protein called Isoform 3 of Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SY	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 73 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 74 is a protein called Small ribosomal subunit protein eS26.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 76 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sc	83	Total	C	N	O	S	0	0
			670	431	125	113	1		

- Molecule 77 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sd	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 78 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Se	55	Total	C	N	O	S	0	0
			437	271	95	70	1		

- Molecule 79 is a protein called Small ribosomal subunit protein uS14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sg	303	Total	C	N	O	S	0	0
			2364	1492	412	448	12		

- Molecule 81 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sy	121	Total	C	N	O	S	0	0
			939	590	166	174	9		

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sz	74	Total	C	N	O	S	0	0
			607	384	116	100	7		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	L1	4	Total	Mg	0
			4	4	
84	L5	204	Total	Mg	0
			204	204	
84	L9	3	Total	Mg	0
			3	3	
84	S4	6	Total	Mg	0
			6	6	
84	LD	1	Total	Mg	0
			1	1	
84	LI	2	Total	Mg	0
			2	2	
84	LN	1	Total	Mg	0
			1	1	
84	LR	2	Total	Mg	0
			2	2	
84	LV	1	Total	Mg	0
			1	1	
84	La	1	Total	Mg	0
			1	1	
84	Lh	1	Total	Mg	0
			1	1	
84	S2	97	Total	Mg	0
			97	97	

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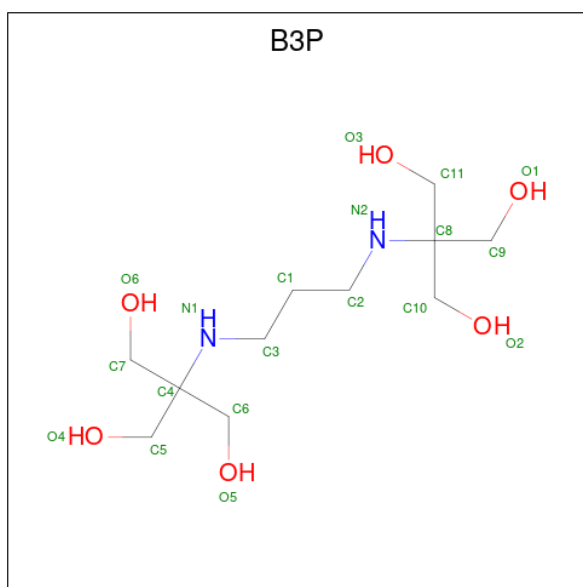
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Mol	Chain	Residues	Atoms		AltConf
84	SG	1	Total 1	Mg 1	0
84	ST	1	Total 1	Mg 1	0
84	SX	1	Total 1	Mg 1	0

- Molecule 85 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
85	L1	3	Total 3	K 3	0
85	L5	42	Total 42	K 42	0
85	L9	1	Total 1	K 1	0
85	LC	1	Total 1	K 1	0
85	LD	2	Total 2	K 2	0
85	LV	1	Total 1	K 1	0
85	Lz	1	Total 1	K 1	0
85	S2	39	Total 39	K 39	0
85	SE	1	Total 1	K 1	0
85	SO	1	Total 1	K 1	0
85	ST	1	Total 1	K 1	0
85	Sf	1	Total 1	K 1	0

- Molecule 86 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				AltConf
86	L5	1	Total	C	N	O	0
			19	11	2	6	

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	LP	1	Total	Zn	0
			1	1	
87	Le	1	Total	Zn	0
			1	1	
87	Lg	1	Total	Zn	0
			1	1	
87	Lo	1	Total	Zn	0
			1	1	
87	Lp	1	Total	Zn	0
			1	1	
87	Sa	1	Total	Zn	0
			1	1	
87	Sf	1	Total	Zn	0
			1	1	
87	Sz	1	Total	Zn	0
			1	1	

- Molecule 88 is water.

Mol	Chain	Residues	Atoms		AltConf
88	L1	153	Total 153	O 153	0
88	L5	4961	Total 4961	O 4961	0
88	L8	25	Total 25	O 25	0
88	L9	93	Total 93	O 93	0
88	LB	85	Total 85	O 85	0
88	S4	52	Total 52	O 52	0
88	LC	104	Total 104	O 104	0
88	LD	91	Total 91	O 91	0
88	LE	10	Total 10	O 10	0
88	LF	52	Total 52	O 52	0
88	LG	16	Total 16	O 16	0
88	LH	18	Total 18	O 18	0
88	LI	64	Total 64	O 64	0
88	LJ	3	Total 3	O 3	0
88	LK	12	Total 12	O 12	0
88	LM	7	Total 7	O 7	0
88	LN	89	Total 89	O 89	0
88	LO	13	Total 13	O 13	0
88	LP	33	Total 33	O 33	0
88	LQ	45	Total 45	O 45	0
88	LR	23	Total 23	O 23	0
88	LS	39	Total 39	O 39	0

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Mol	Chain	Residues	Atoms		AltConf
88	LT	41	Total 41	O 41	0
88	LU	10	Total 10	O 10	0
88	LV	27	Total 27	O 27	0
88	LW	7	Total 7	O 7	0
88	LY	42	Total 42	O 42	0
88	LZ	10	Total 10	O 10	0
88	La	46	Total 46	O 46	0
88	Lb	15	Total 15	O 15	0
88	Lc	8	Total 8	O 8	0
88	Ld	15	Total 15	O 15	0
88	Le	19	Total 19	O 19	0
88	Lf	33	Total 33	O 33	0
88	Lg	30	Total 30	O 30	0
88	Lh	42	Total 42	O 42	0
88	Li	4	Total 4	O 4	0
88	Lj	69	Total 69	O 69	0
88	Lk	4	Total 4	O 4	0
88	Ll	27	Total 27	O 27	0
88	Lm	1	Total 1	O 1	0
88	Ln	18	Total 18	O 18	0
88	Lo	3	Total 3	O 3	0

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Mol	Chain	Residues	Atoms		AltConf
88	Lp	25	Total 25	O 25	0
88	Lz	16	Total 16	O 16	0
88	S1	25	Total 25	O 25	0
88	S2	2334	Total 2334	O 2334	0
88	S5	11	Total 11	O 11	0
88	SA	9	Total 9	O 9	0
88	SB	9	Total 9	O 9	0
88	SC	36	Total 36	O 36	0
88	SD	25	Total 25	O 25	0
88	SE	45	Total 45	O 45	0
88	SG	16	Total 16	O 16	0
88	SH	6	Total 6	O 6	0
88	SI	31	Total 31	O 31	0
88	SJ	34	Total 34	O 34	0
88	SK	6	Total 6	O 6	0
88	SL	43	Total 43	O 43	0
88	SM	4	Total 4	O 4	0
88	SN	32	Total 32	O 32	0
88	SO	33	Total 33	O 33	0
88	SP	14	Total 14	O 14	0
88	SQ	32	Total 32	O 32	0

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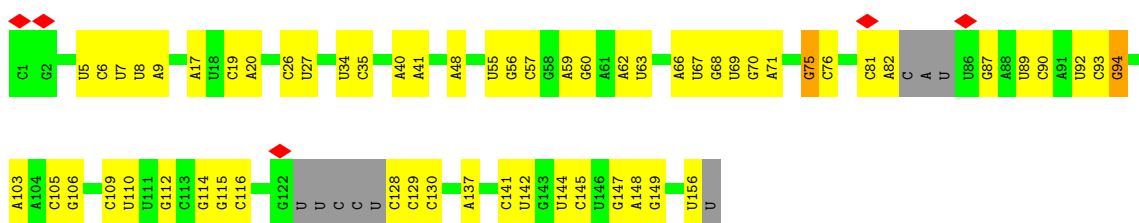
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88	SS	5	Total 5	O 5	0
88	ST	23	Total 23	O 23	0
88	SU	20	Total 20	O 20	0
88	SV	8	Total 8	O 8	0
88	SW	39	Total 39	O 39	0
88	SX	47	Total 47	O 47	0
88	SY	10	Total 10	O 10	0
88	SZ	12	Total 12	O 12	0
88	Sa	38	Total 38	O 38	0
88	Sb	11	Total 11	O 11	0
88	Sc	3	Total 3	O 3	0
88	Sd	2	Total 2	O 2	0
88	Se	10	Total 10	O 10	0
88	Sf	8	Total 8	O 8	0
88	Sg	1	Total 1	O 1	0
88	So	3	Total 3	O 3	0

3 Residue-property plots

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

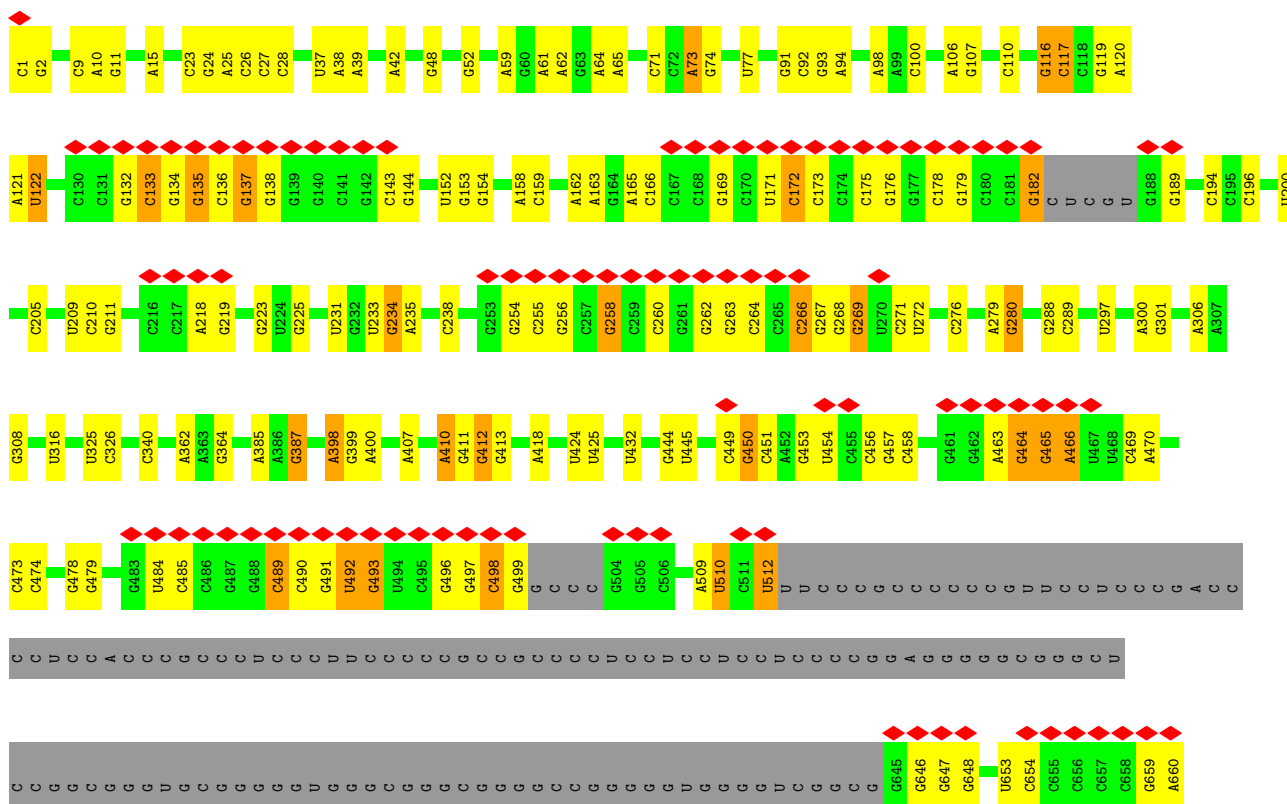
• Molecule 1: 5.8S rRNA

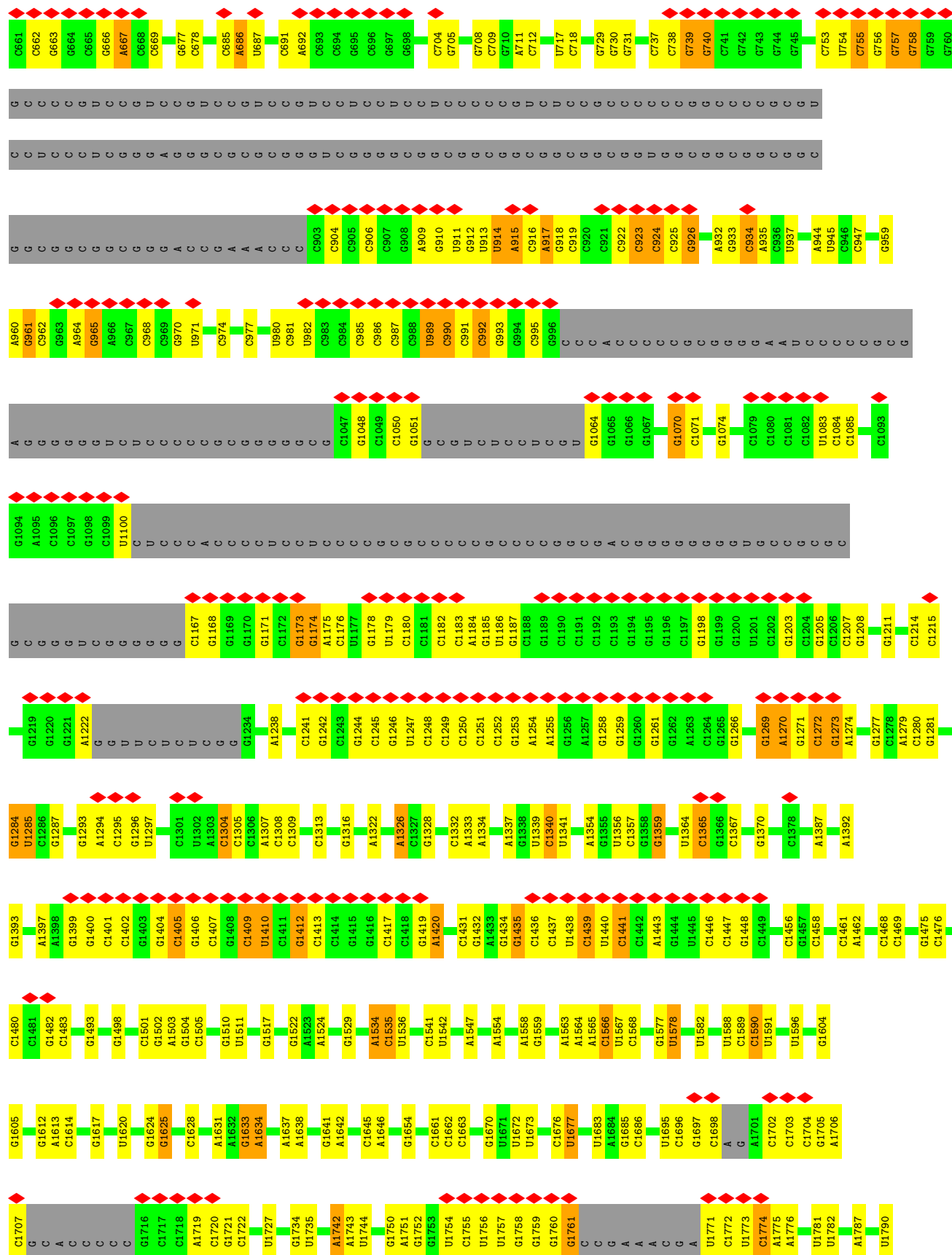
Chain L1: 



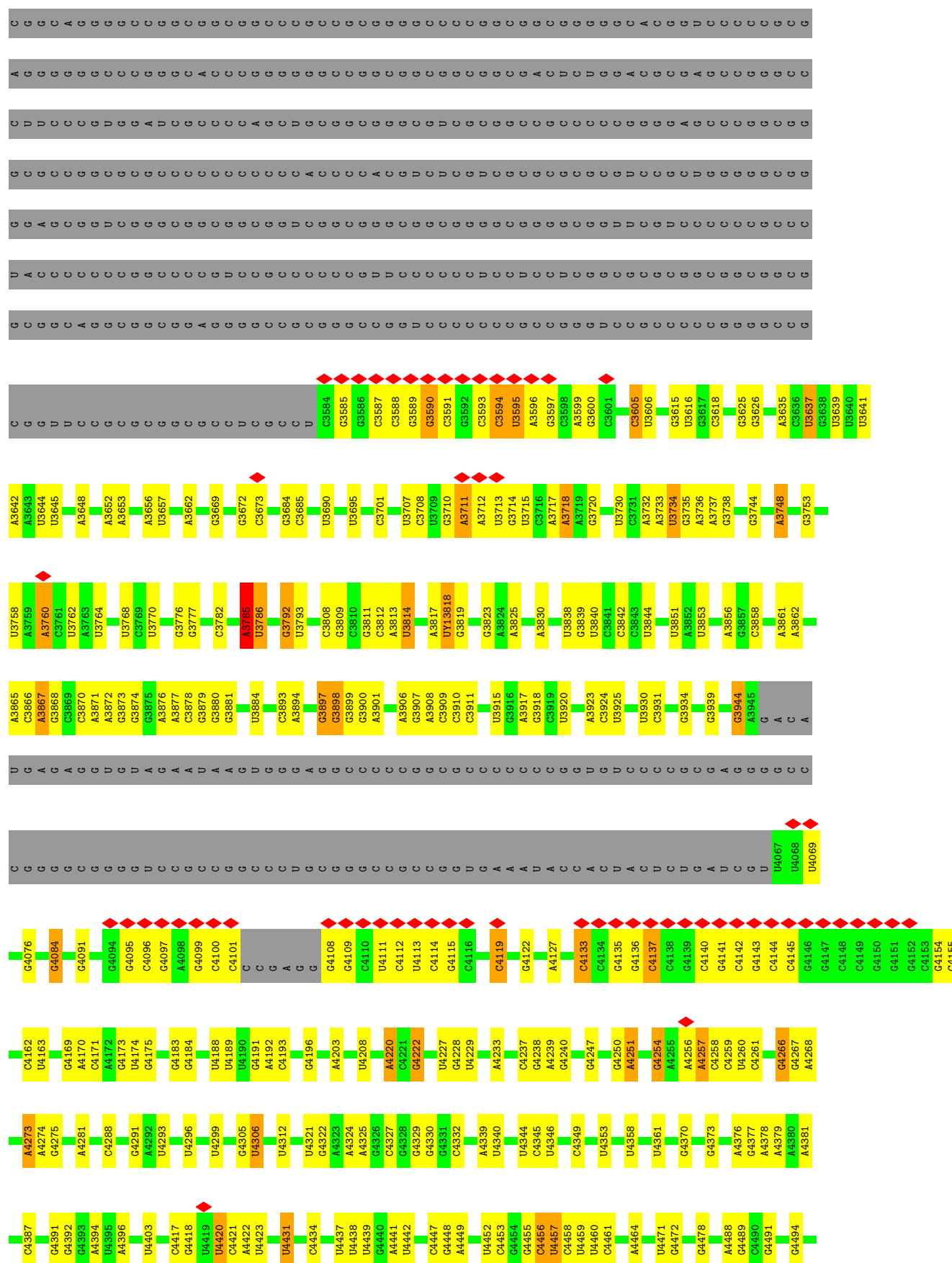
• Molecule 2: 28S rRNA

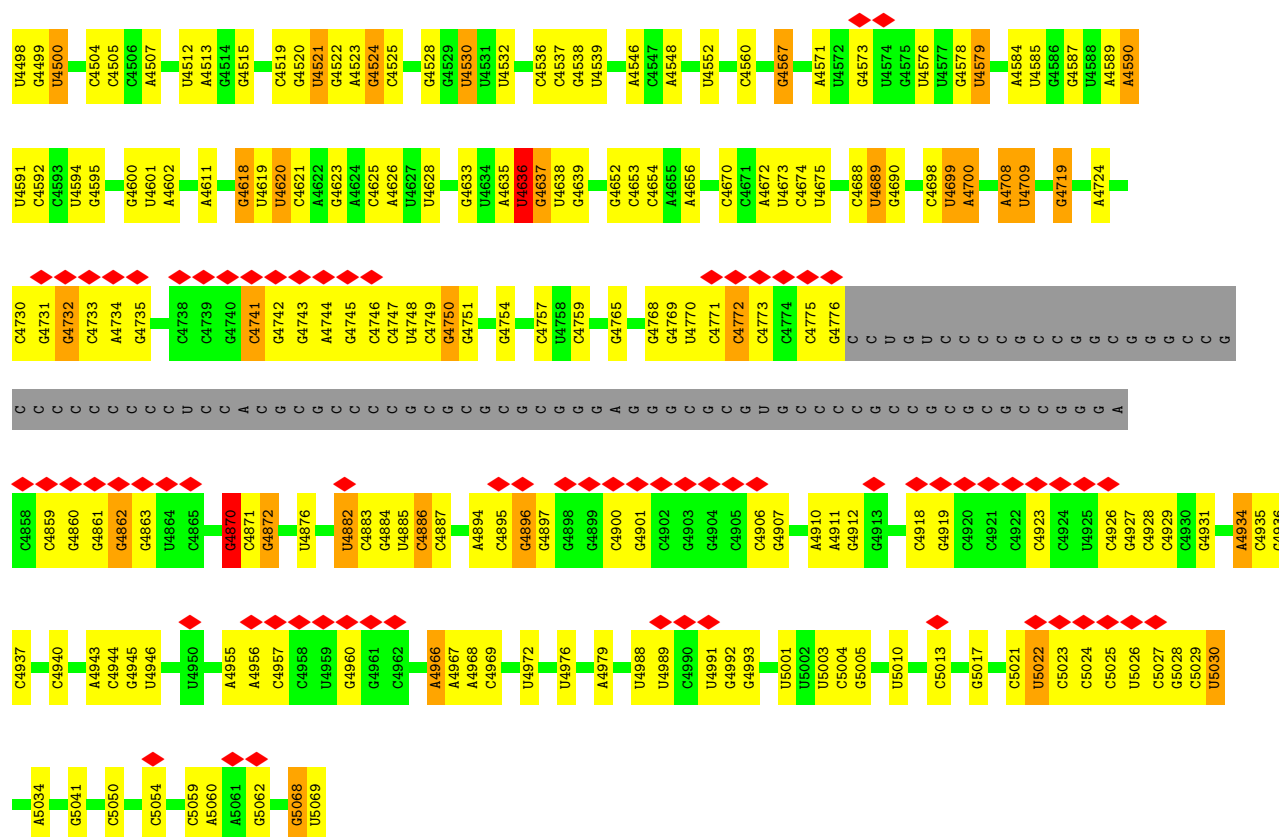
Chain L5: 



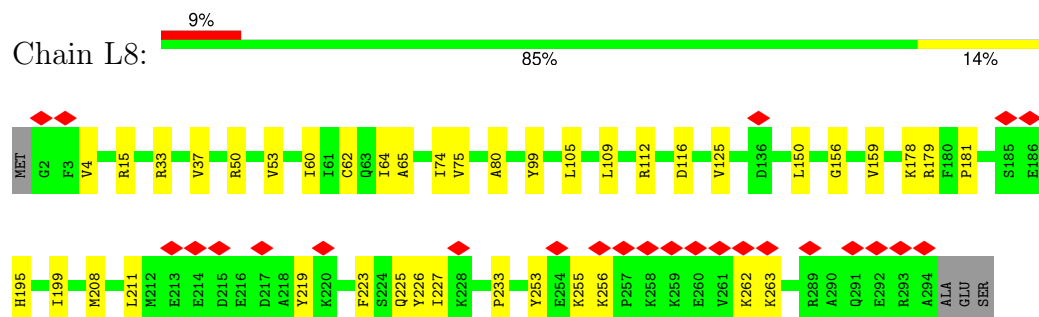




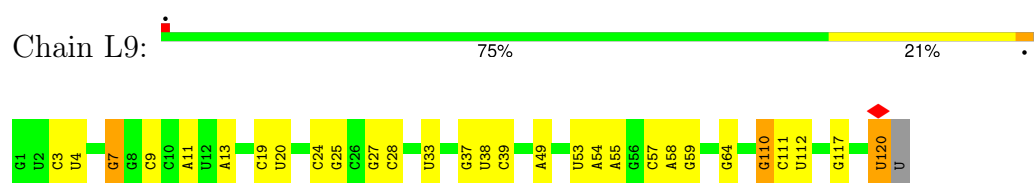




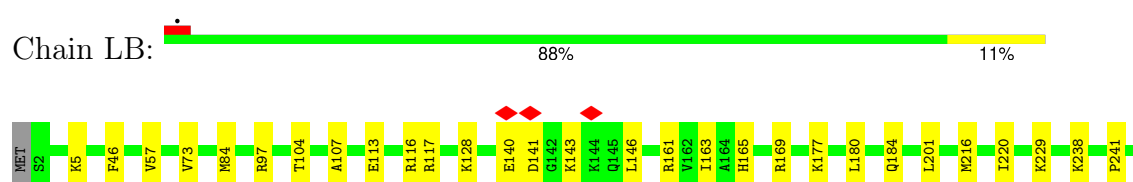
• Molecule 3: Large ribosomal subunit protein uL18



• Molecule 4: 5S rRNA



• Molecule 5: Large ribosomal subunit protein uL3

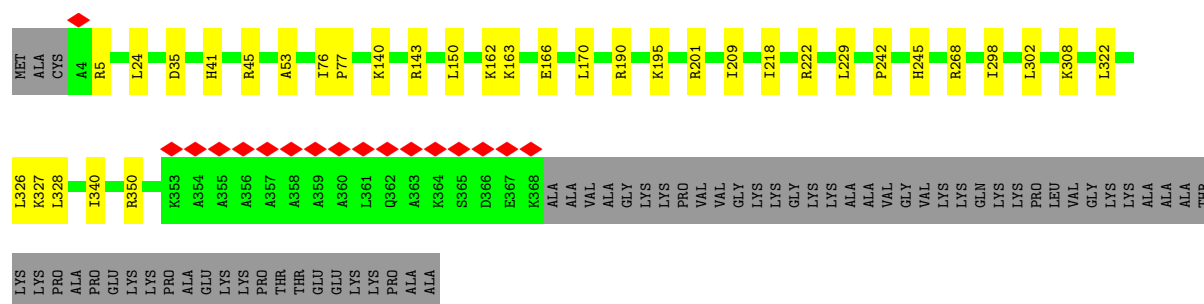
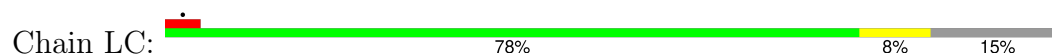




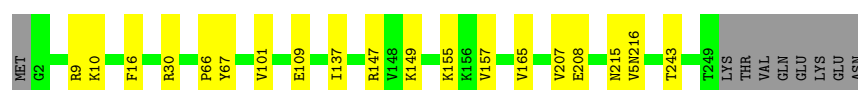
• Molecule 6: tRNA-ARG,CCG-1



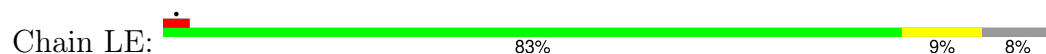
• Molecule 7: Large ribosomal subunit protein uL4



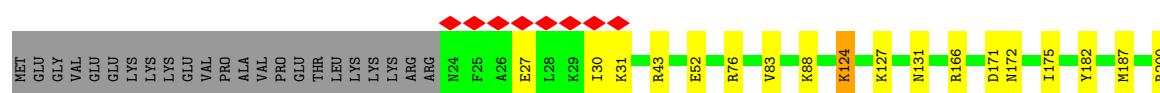
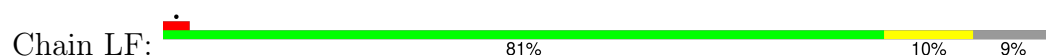
• Molecule 8: Large ribosomal subunit protein uL2



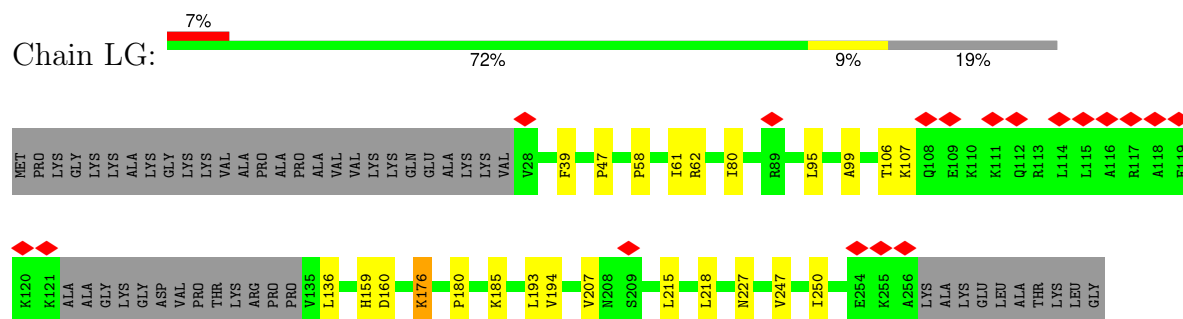
• Molecule 9: Large ribosomal subunit protein uL24



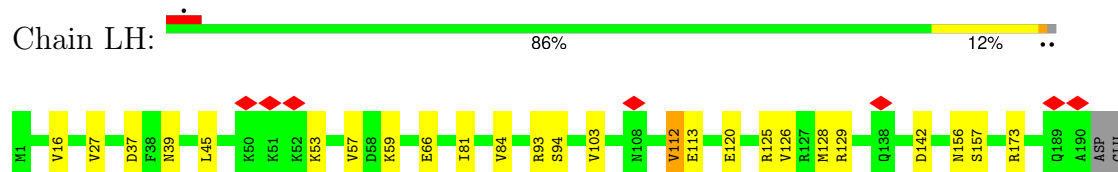
• Molecule 10: Large ribosomal subunit protein uL30



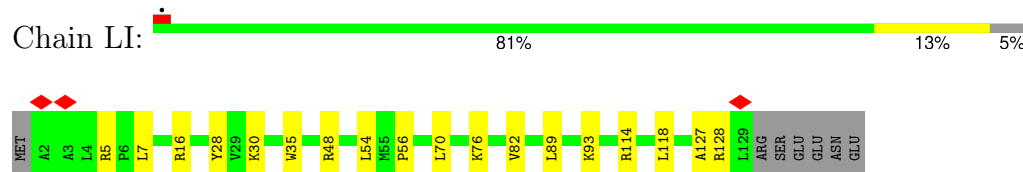
- Molecule 11: Large ribosomal subunit protein eL8



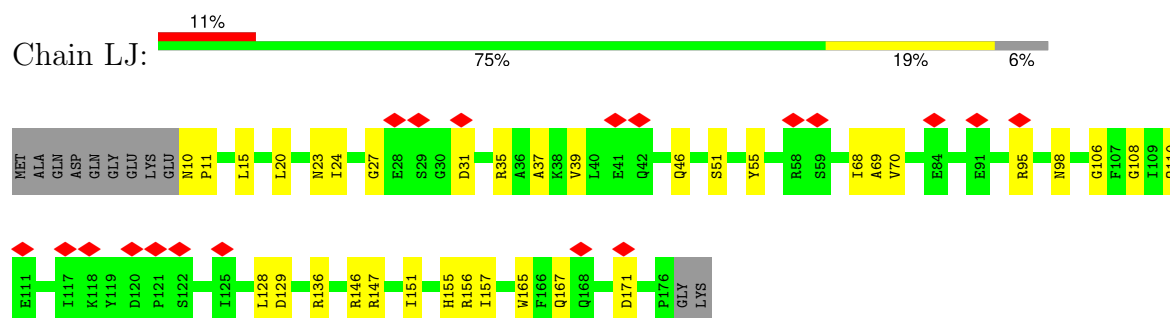
- Molecule 12: Large ribosomal subunit protein uL6



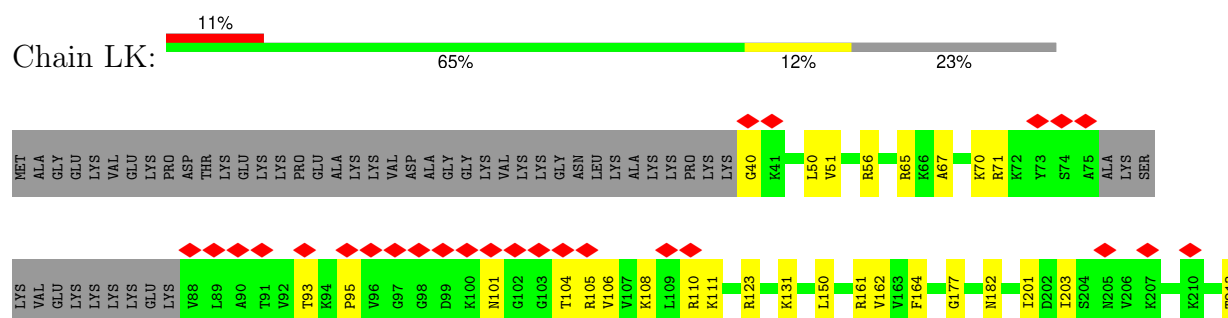
- Molecule 13: Large ribosomal subunit protein eL32

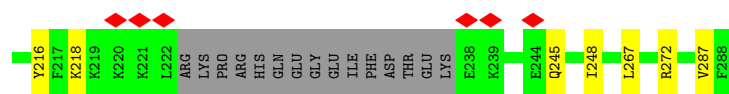


- Molecule 14: Large ribosomal subunit protein uL5

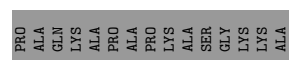
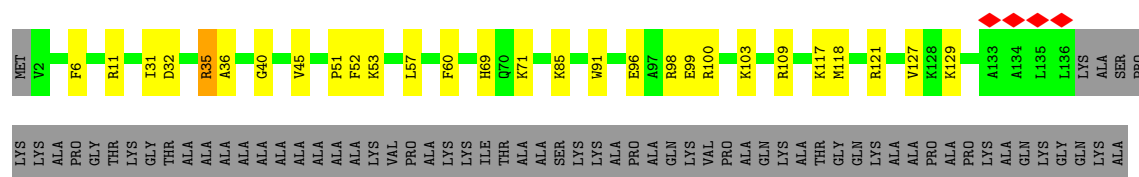


- Molecule 15: Large ribosomal subunit protein eL6





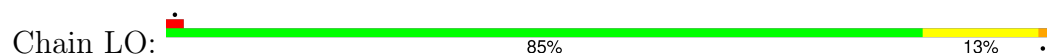
- Molecule 16: Large ribosomal subunit protein eL14



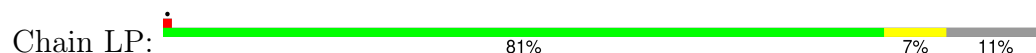
- Molecule 17: Large ribosomal subunit protein eL15



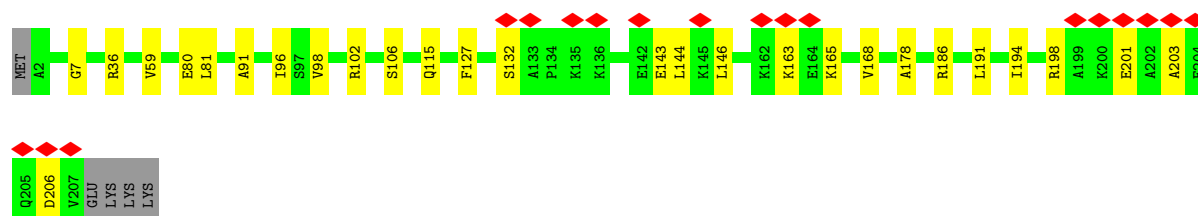
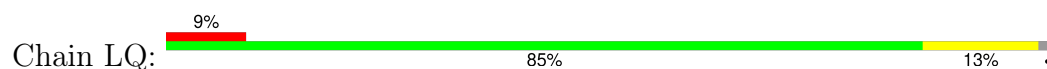
- Molecule 18: Large ribosomal subunit protein uL29



- Molecule 19: Large ribosomal subunit protein eL37

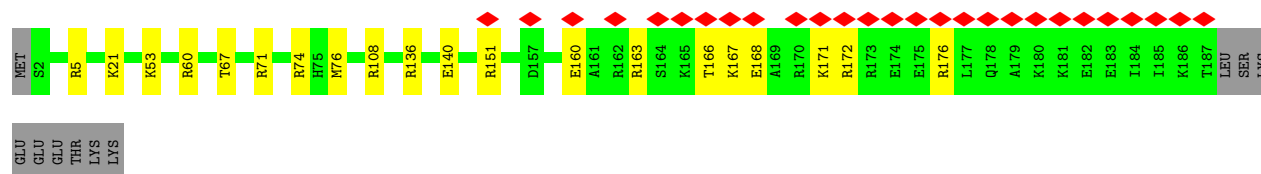


- Molecule 20: Large ribosomal subunit protein eL13

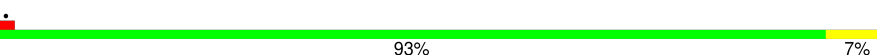


- Molecule 21: Large ribosomal subunit protein eL19

Chain LR: 

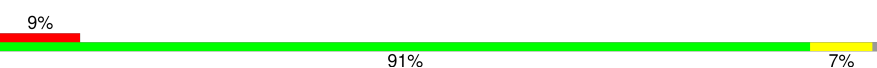


- Molecule 22: Large ribosomal subunit protein eL20

Chain LS: 



- Molecule 23: Large ribosomal subunit protein eL21

Chain LT: 



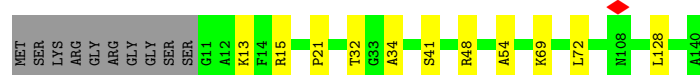
- Molecule 24: Large ribosomal subunit protein eL39

Chain LU: 



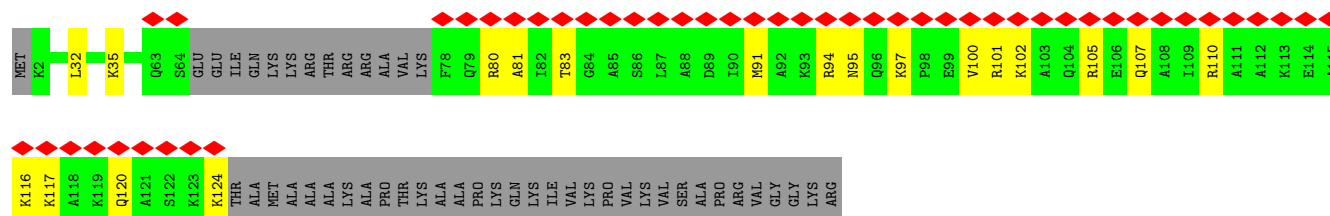
- Molecule 25: Large ribosomal subunit protein uL14

Chain LV: 



- Molecule 26: Large ribosomal subunit protein eL24

Chain LW: 



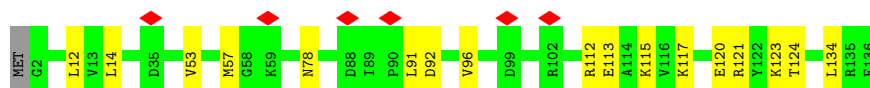
- Molecule 27: Large ribosomal subunit protein uL13

Chain LY:  90% 8%



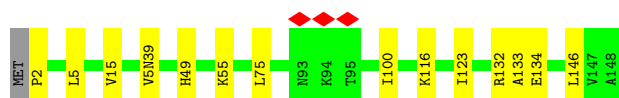
- Molecule 28: Large ribosomal subunit protein eL27

Chain LZ:  87% 12%



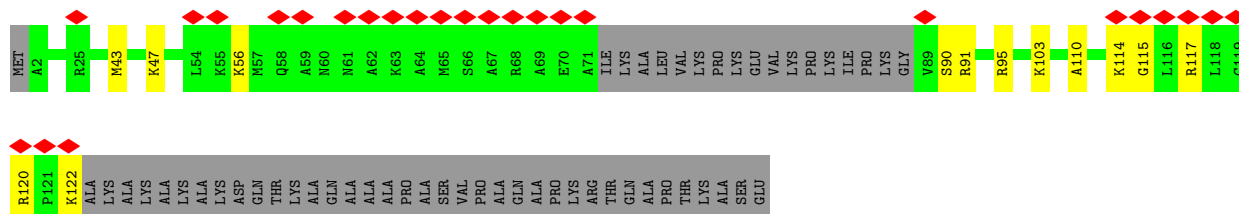
- Molecule 29: Large ribosomal subunit protein uL15

Chain La:  90% 9%



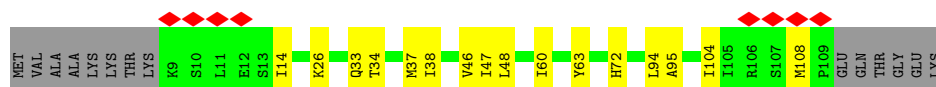
- Molecule 30: Large ribosomal subunit protein eL29

Chain Lb:  16% 57% 8% 35%



- Molecule 31: Large ribosomal subunit protein eL30

Chain Lc:  7% 74% 14% 12%



- Molecule 32: Large ribosomal subunit protein eL31

Chain Ld:  7% 73% 10% 17%



- Molecule 33: Large ribosomal subunit protein eL42

Chain Le:  92% 8%



- Molecule 34: Large ribosomal subunit protein eL33

Chain Lf:  95% 5%



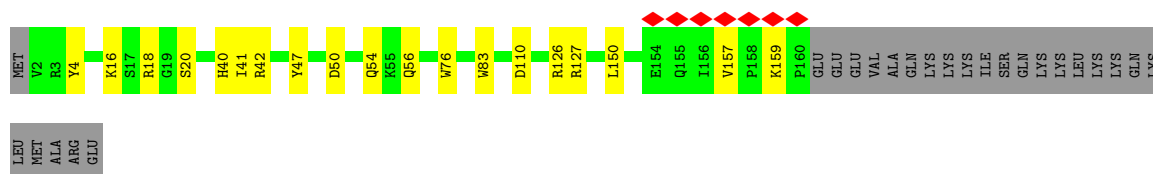
- Molecule 35: Large ribosomal subunit protein eL34

Chain Lg:  5% 81% 14% 5%



- Molecule 36: Large ribosomal subunit protein uL22

Chain Lh:  76% 10% 14%

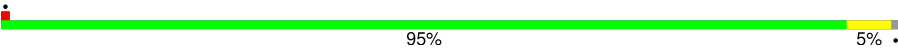


- Molecule 37: Large ribosomal subunit protein eL36

Chain Li:  8% 83% 14%



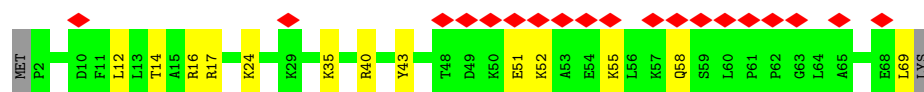
- Molecule 38: Large ribosomal subunit protein eL18

Chain Lj:  95% 5%

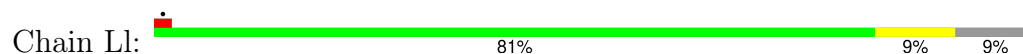


- Molecule 39: Large ribosomal subunit protein eL38

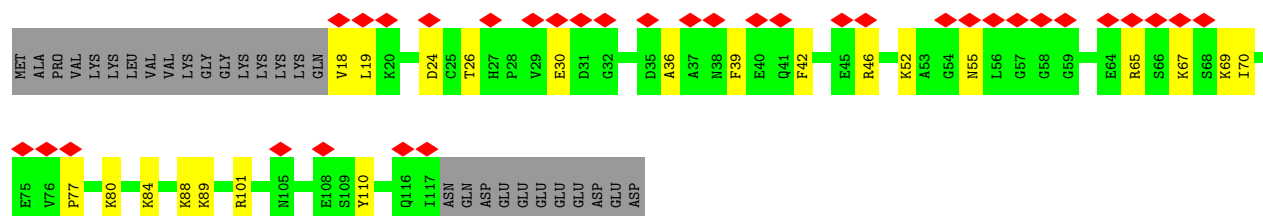
Chain Lk:  27% 79% 19%



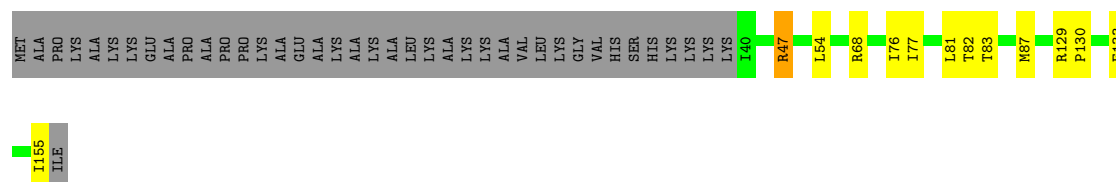
- Molecule 40: Large ribosomal subunit protein eL28



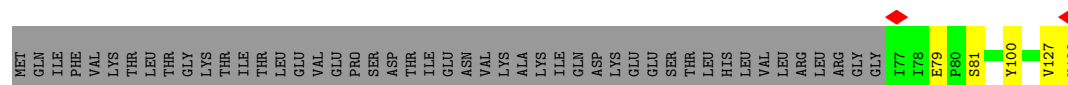
- Molecule 41: Large ribosomal subunit protein eL22



- Molecule 42: Large ribosomal subunit protein uL23



- Molecule 43: Large ribosomal subunit protein eL40



- Molecule 44: Large ribosomal subunit protein eL43

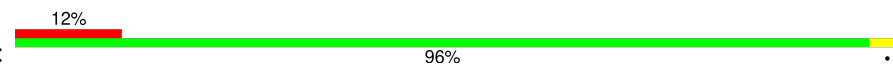


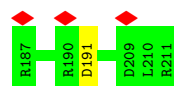
- Molecule 45: Large ribosomal subunit protein uL16

Chain Lz: 



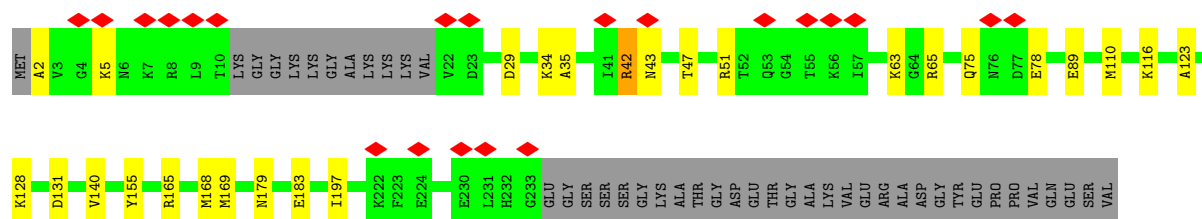
- Molecule 46: Nascent chain

Chain NC: 

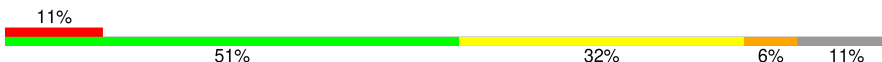


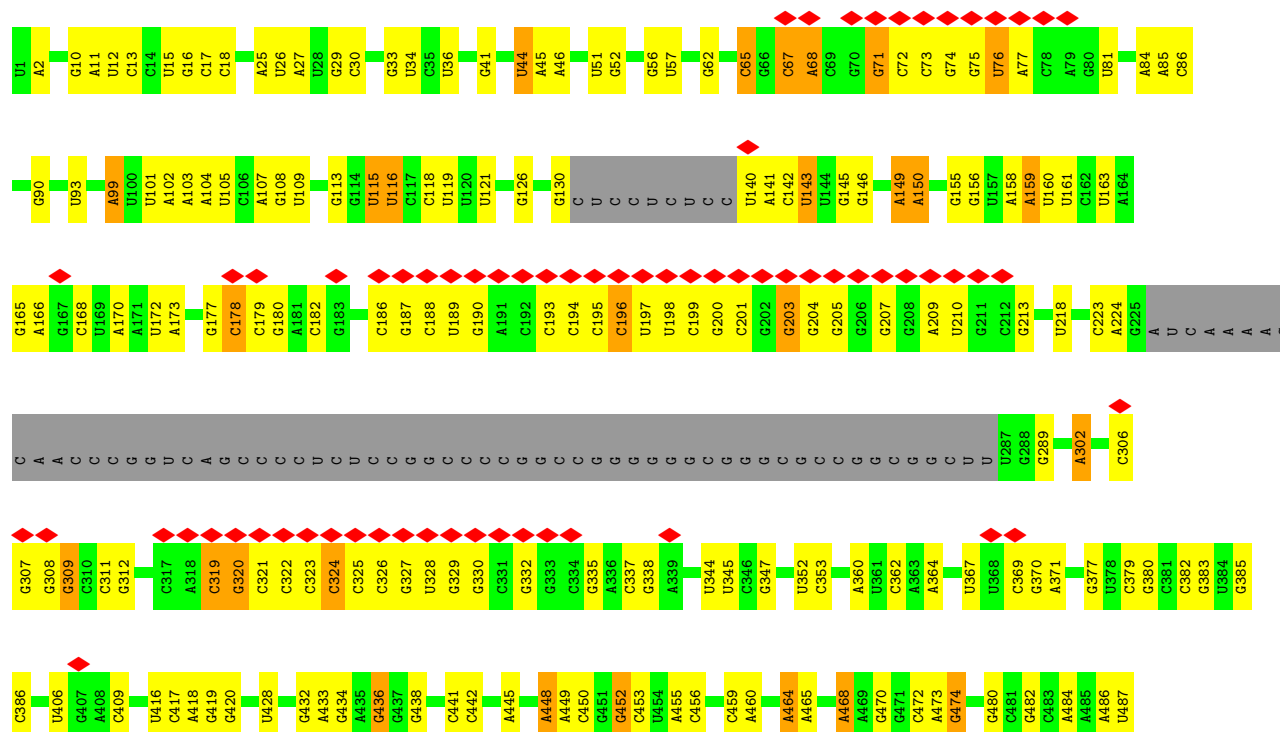
- Molecule 47: Small ribosomal subunit protein eS1

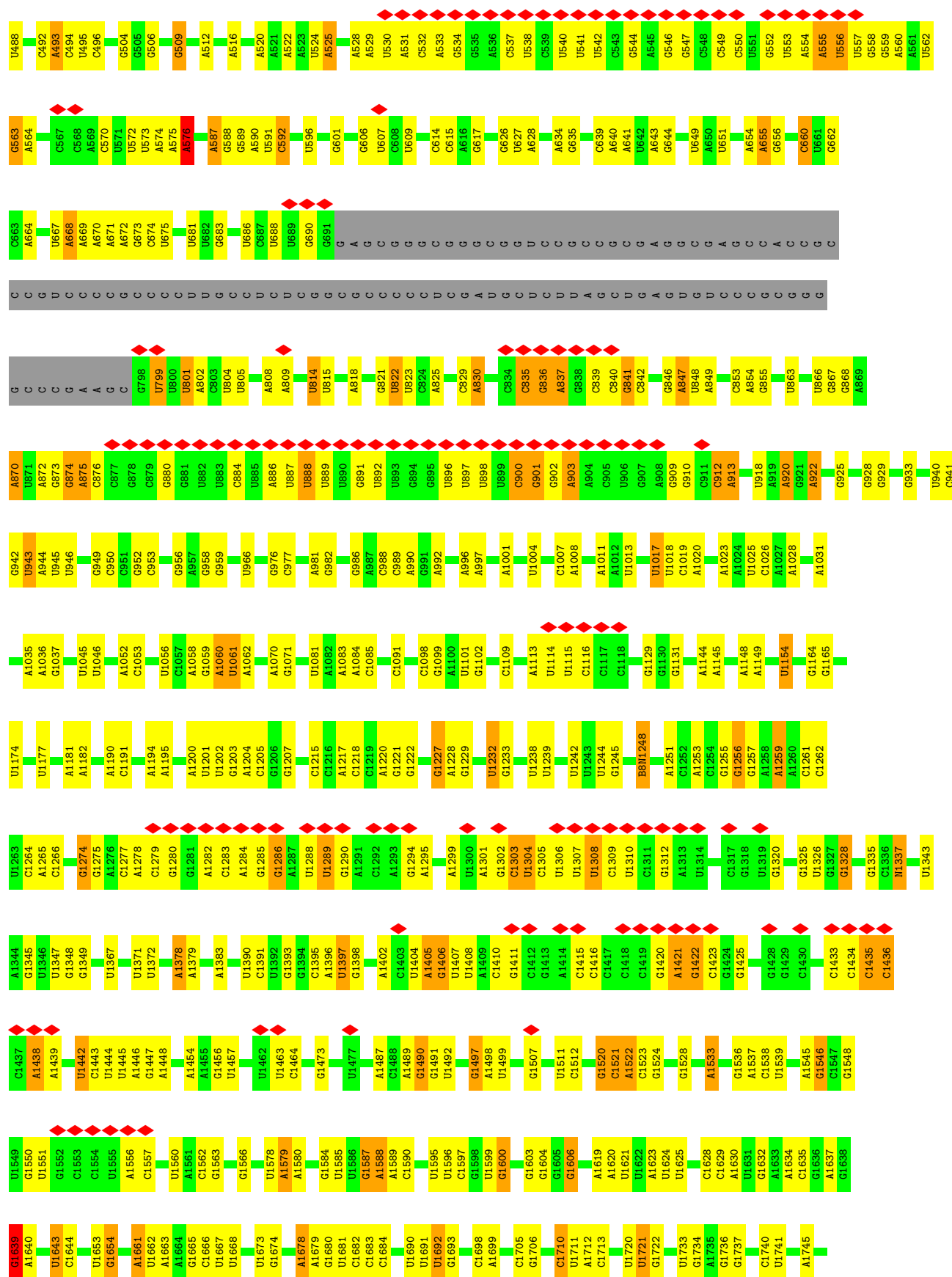
Chain S1: 

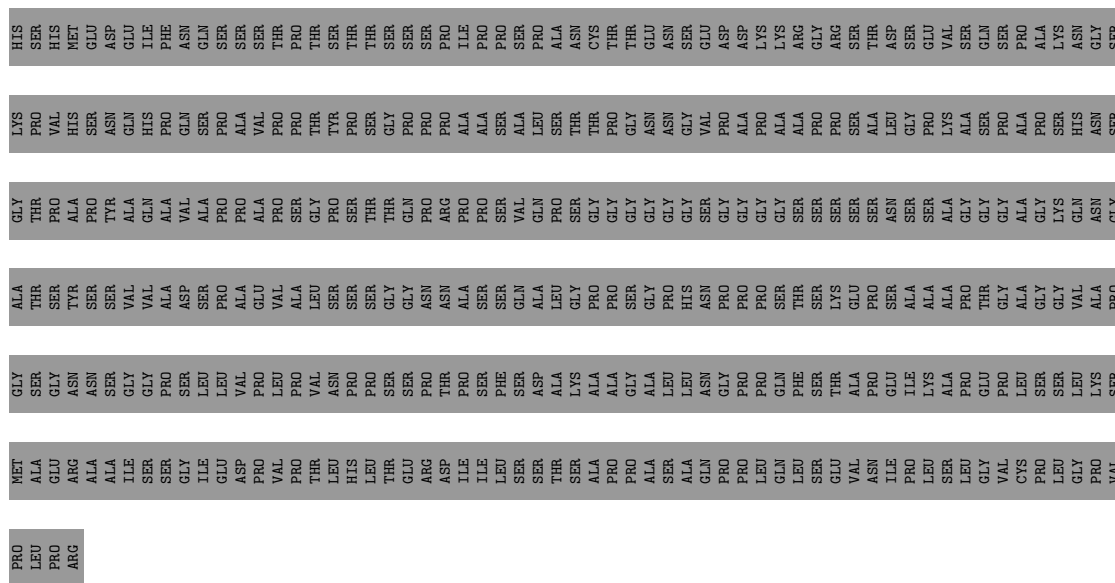


- Molecule 48: 18S rRNA

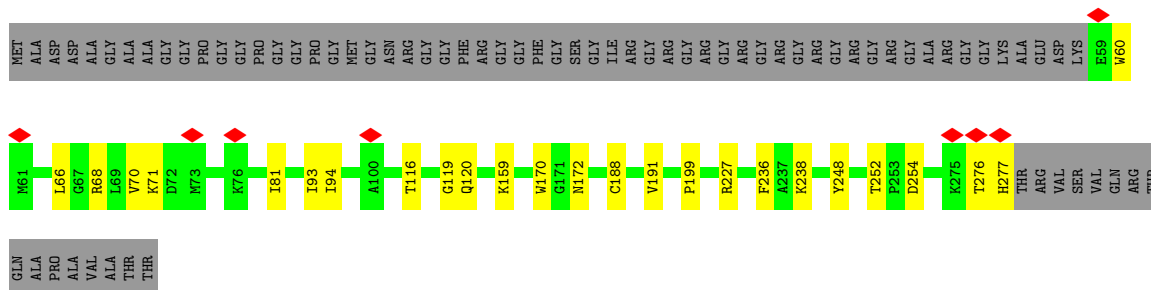
Chain S2: 



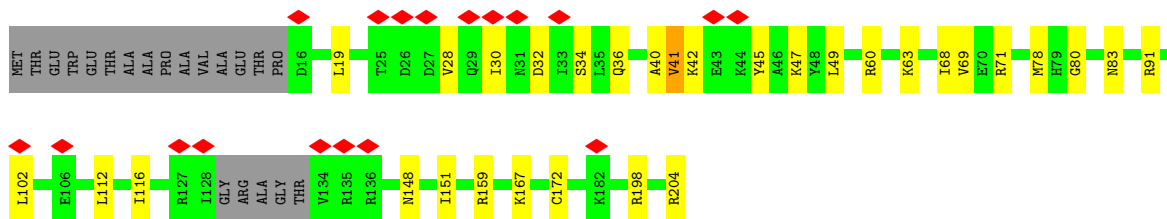
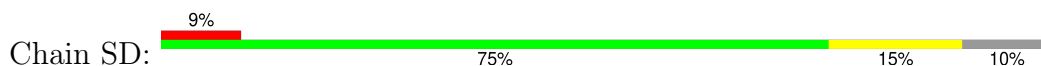




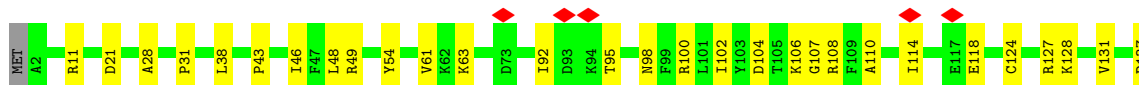
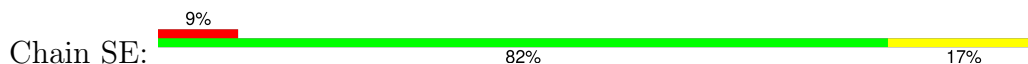
- Molecule 52: Small ribosomal subunit protein uS5

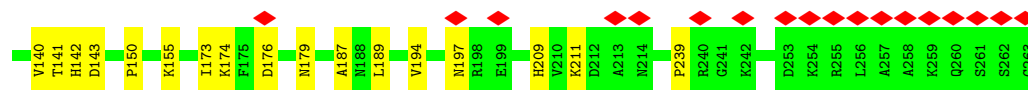


- Molecule 53: Small ribosomal subunit protein uS7

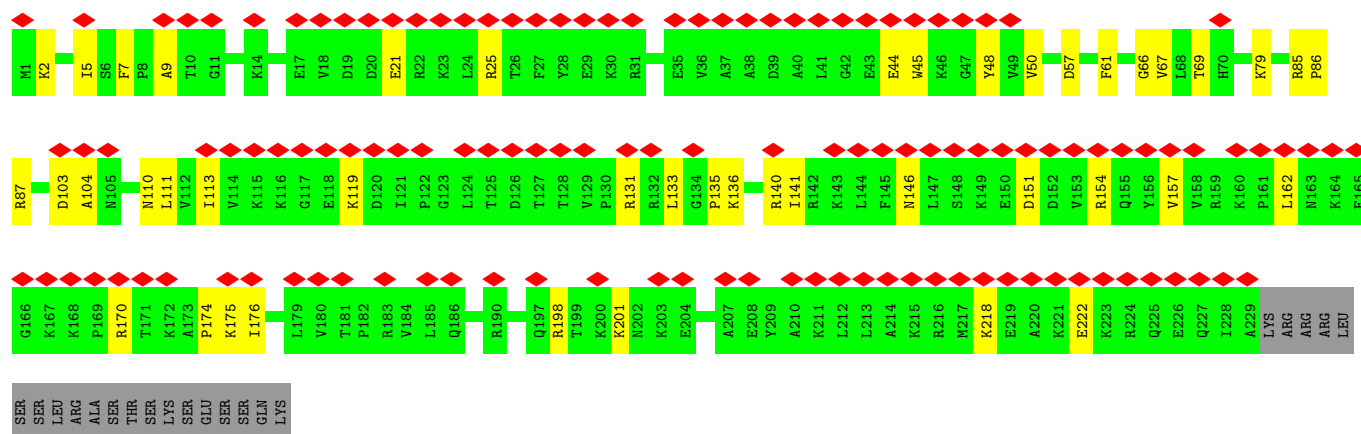
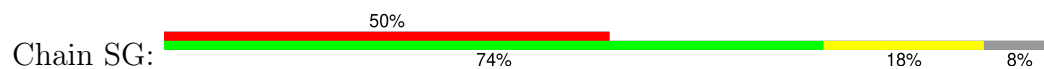


- Molecule 54: Small ribosomal subunit protein eS4, X isoform

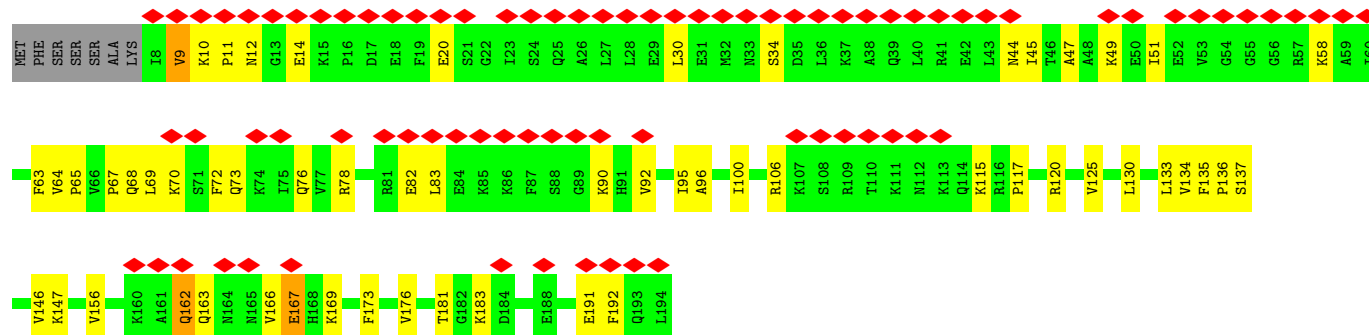
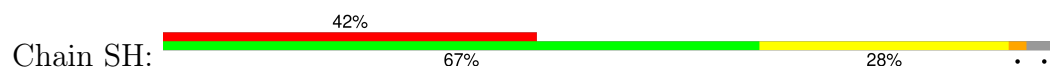




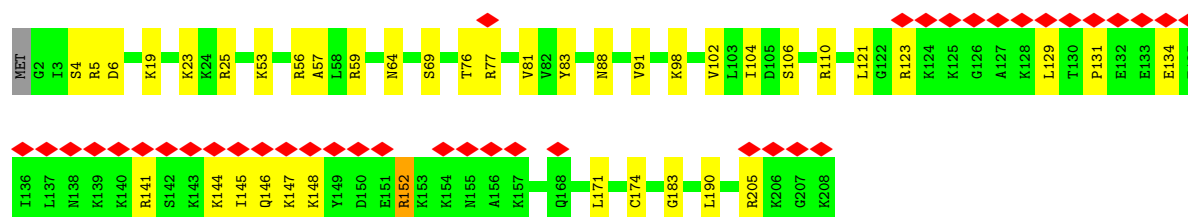
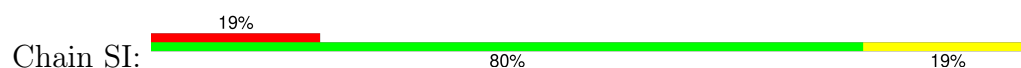
• Molecule 55: Small ribosomal subunit protein eS6



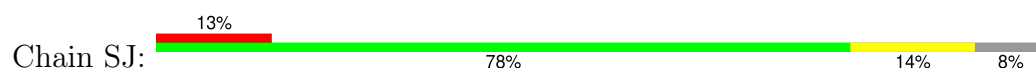
• Molecule 56: Small ribosomal subunit protein eS7

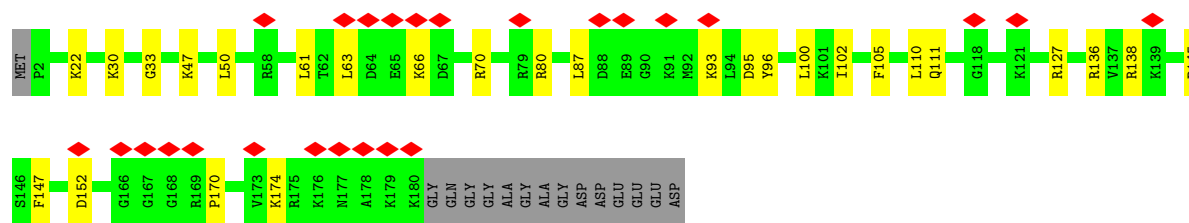


• Molecule 57: Small ribosomal subunit protein eS8



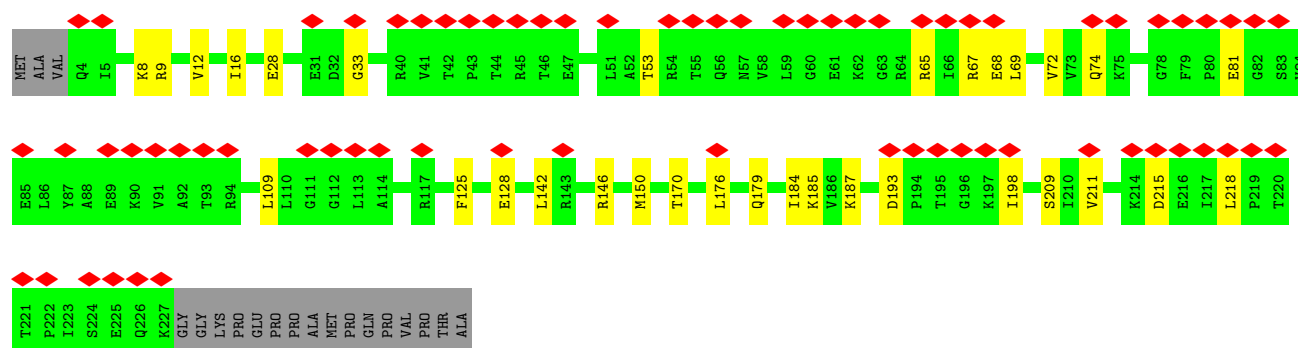
• Molecule 58: Small ribosomal subunit protein uS4





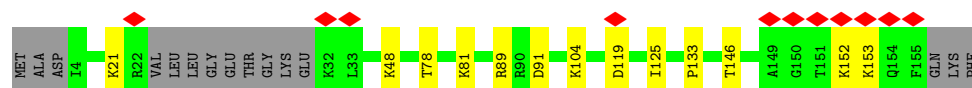
- Molecule 59: Small ribosomal subunit protein uS3

Chain SK:



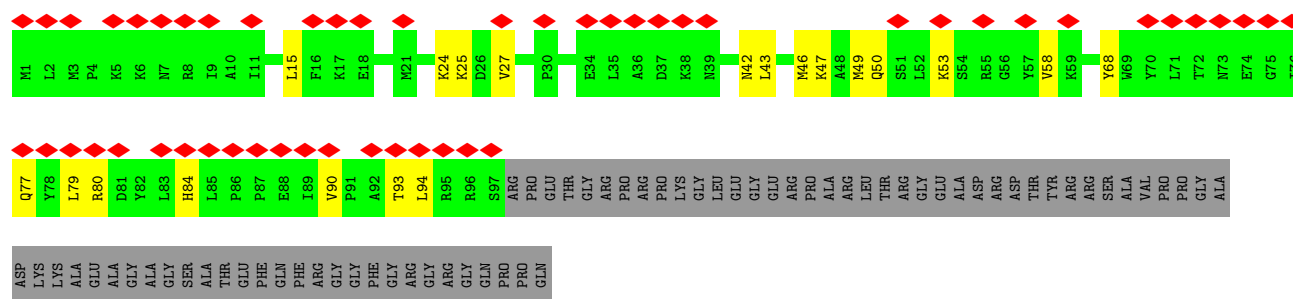
- Molecule 60: Small ribosomal subunit protein uS17

Chain SL:



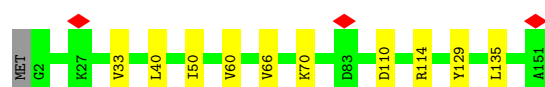
- Molecule 61: Small ribosomal subunit protein eS10

Chain SM:



- Molecule 62: Small ribosomal subunit protein uS15

Chain SN:



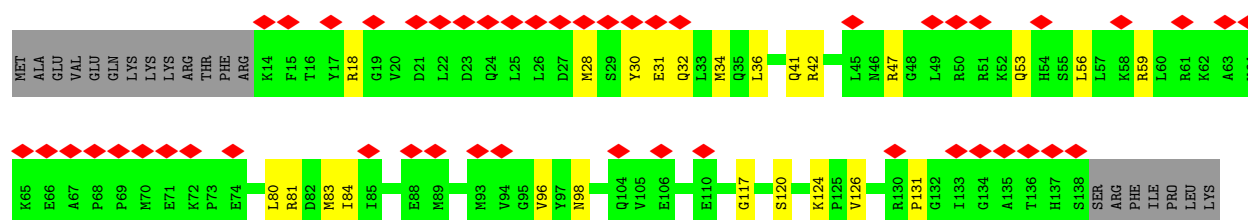
- Molecule 63: Small ribosomal subunit protein uS11

Chain SO: 



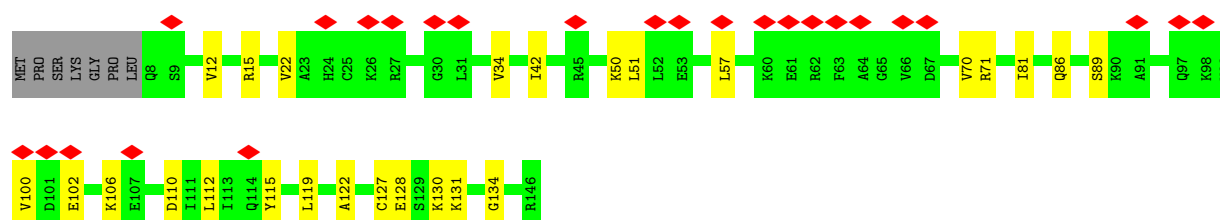
- Molecule 64: Small ribosomal subunit protein uS19

Chain SP: 



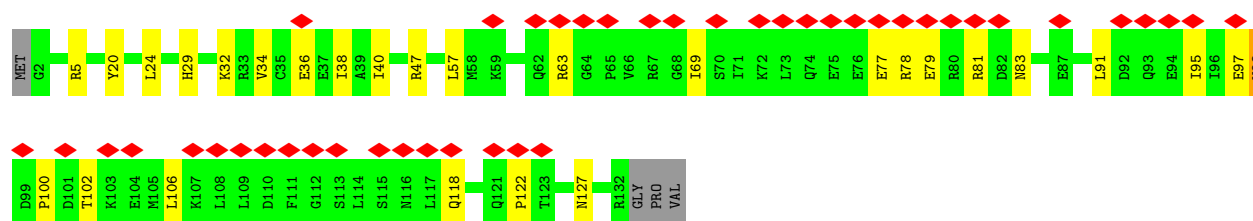
- Molecule 65: Small ribosomal subunit protein uS9

Chain SQ: 



- Molecule 66: Small ribosomal subunit protein eS17

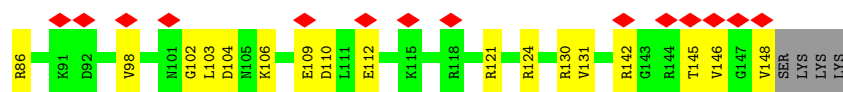
Chain SS: 



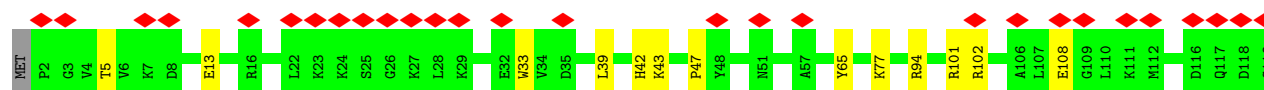
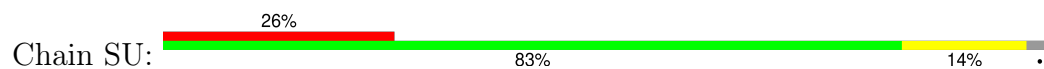
- Molecule 67: Small ribosomal subunit protein uS13

Chain ST: 

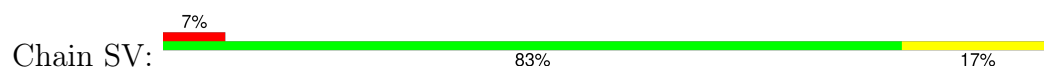




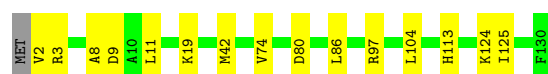
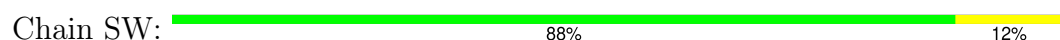
- Molecule 68: Small ribosomal subunit protein eS19



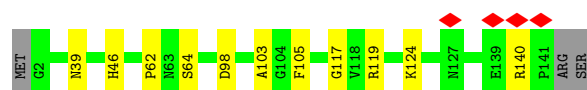
- Molecule 69: Small ribosomal subunit protein eS21



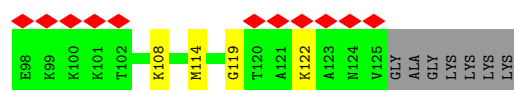
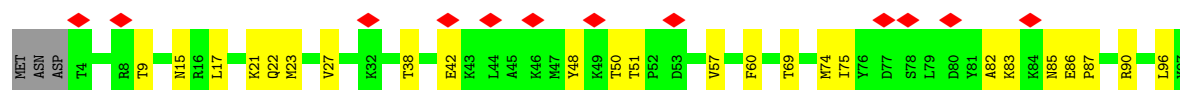
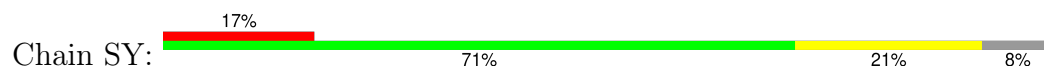
- Molecule 70: Small ribosomal subunit protein uS8



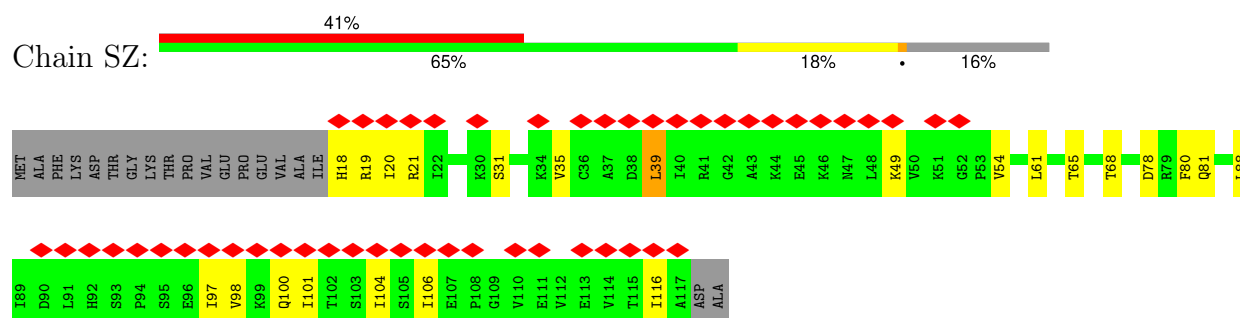
- Molecule 71: Small ribosomal subunit protein uS12



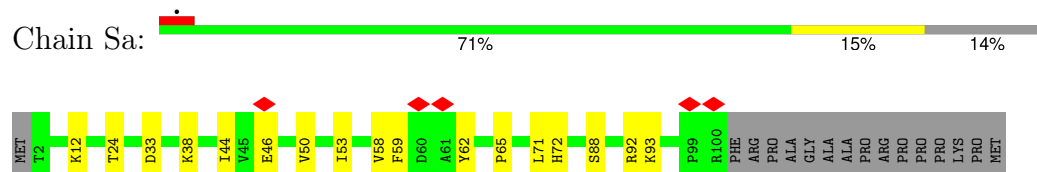
- Molecule 72: Isoform 3 of Small ribosomal subunit protein eS24



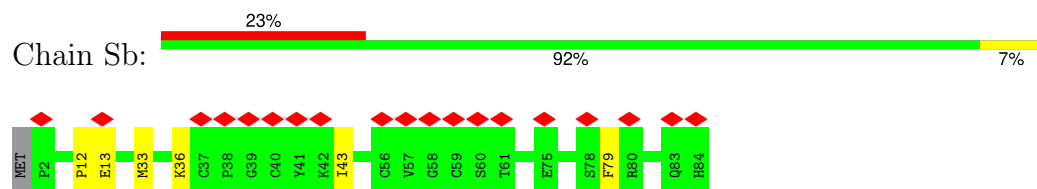
- Molecule 73: Small ribosomal subunit protein uS10



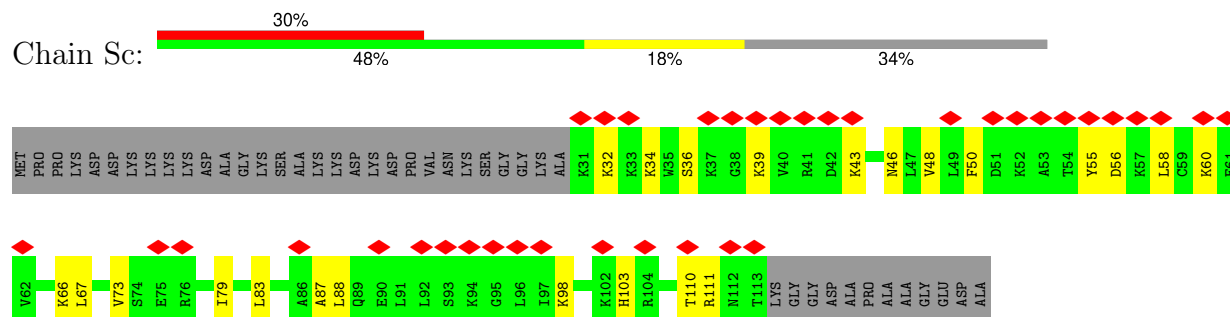
- Molecule 74: Small ribosomal subunit protein eS26



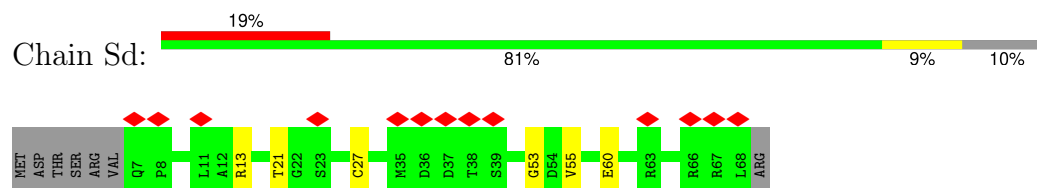
- Molecule 75: Small ribosomal subunit protein eS27



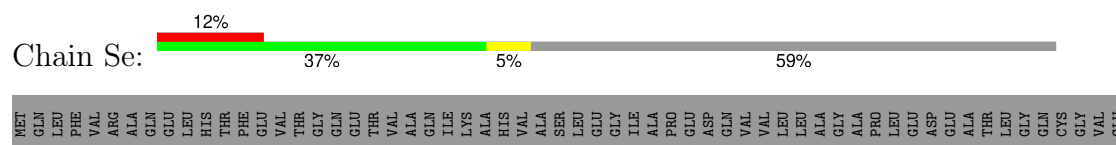
- Molecule 76: Small ribosomal subunit protein eS25



- Molecule 77: Small ribosomal subunit protein eS28

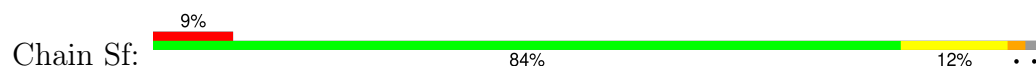


- Molecule 78: FAU ubiquitin-like and ribosomal protein S30

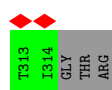
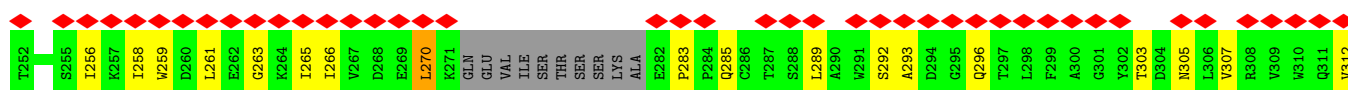
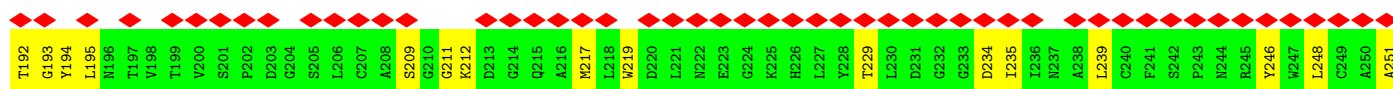
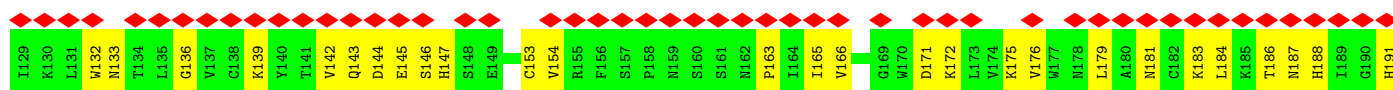
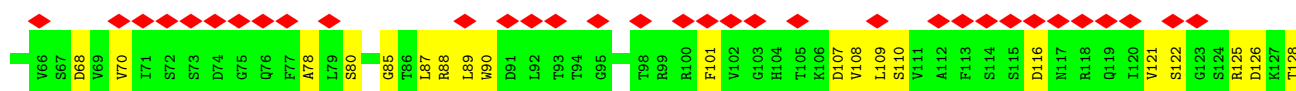
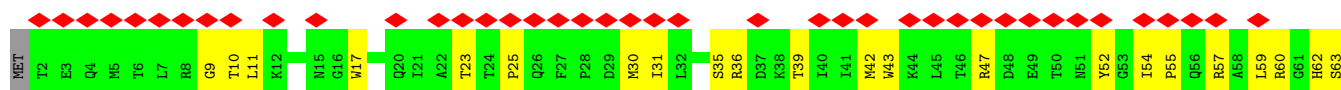




- Molecule 79: Small ribosomal subunit protein uS14



- Molecule 80: Receptor of activated protein C kinase 1



- Molecule 81: Small ribosomal subunit protein eS32

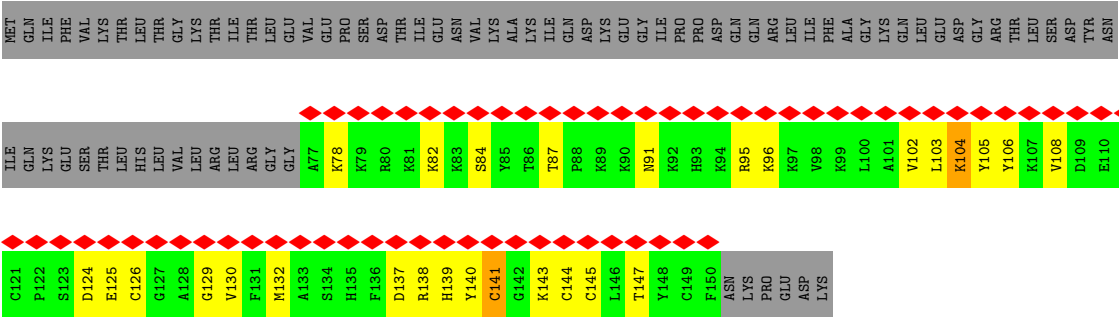
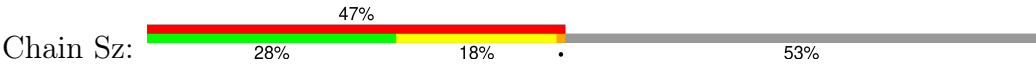


- Molecule 82: Small ribosomal subunit protein eS12





● Molecule 83: Ubiquitin-40S ribosomal protein S27a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	17	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0175	Depositor
Map size ($\text{\AA}$)	419.328, 419.328, 419.328	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.936, 0.936, 0.936	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, ACE, 1MG, K, 4AC, PSU, UY1, B8N, MA6, H2U, JMH, OMG, 1MA, A2M, 5MC, OMU, 7MG, 2MG, V5N, UR3, OMC, 5MU, 6MZ, M3L, MG, M2G, MLZ, HIC, IAS, ZN, HY3

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	L1	0.25	0/3450	0.31	0/5372
2	L5	0.26	2/81683 (0.0%)	0.34	0/127409
3	L8	0.14	0/2432	0.32	0/3256
4	L9	0.24	0/2858	0.29	0/4455
5	LB	0.16	0/3289	0.35	0/4399
6	S4	0.70	0/1530	0.86	0/2384
7	LC	0.16	0/2962	0.35	0/3977
8	LD	0.16	0/1924	0.40	0/2578
9	LE	0.13	0/1132	0.31	0/1504
10	LF	0.18	0/1905	0.36	0/2540
11	LG	0.15	0/1781	0.33	0/2397
12	LH	0.15	0/1537	0.32	0/2066
13	LI	0.18	0/1071	0.38	0/1429
14	LJ	0.15	0/1363	0.37	0/1824
15	LK	0.13	0/1814	0.32	0/2435
16	LM	0.15	0/1133	0.33	0/1516
17	LN	0.17	0/1745	0.38	0/2338
18	LO	0.15	0/1022	0.30	0/1351
19	LP	0.17	0/720	0.39	0/952
20	LQ	0.14	0/1695	0.31	0/2270
21	LR	0.15	0/1574	0.30	0/2080
22	LS	0.15	0/1500	0.34	0/2013
23	LT	0.14	0/1312	0.33	0/1753
24	LU	0.16	0/453	0.32	0/599
25	LV	0.15	0/986	0.36	0/1324
26	LW	0.14	0/907	0.31	0/1202
27	LY	0.18	0/1656	0.36	0/2216
28	LZ	0.14	0/1129	0.31	0/1507
29	La	0.17	0/1178	0.37	0/1573
30	Lb	0.15	0/850	0.30	0/1121
31	Lc	0.19	0/796	0.35	0/1068

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.16	0/877	0.35	0/1181
33	Le	0.16	0/866	0.32	0/1141
34	Lf	0.17	0/894	0.34	0/1198
35	Lg	0.15	0/892	0.33	0/1189
36	Lh	0.16	0/1317	0.36	0/1769
37	Li	0.13	0/843	0.27	0/1115
38	Lj	0.17	0/1536	0.38	0/2052
39	Lk	0.13	0/565	0.26	0/750
40	Ll	0.19	0/1003	0.35	0/1346
41	Lm	0.14	0/830	0.36	0/1114
42	Ln	0.14	0/966	0.32	0/1301
43	Lo	0.14	0/433	0.31	0/575
44	Lp	0.16	0/691	0.37	0/919
45	Lz	0.15	0/1744	0.31	0/2331
46	NC	0.13	0/226	0.30	0/299
47	S1	0.13	0/1816	0.30	0/2427
48	S2	0.28	3/37683 (0.0%)	0.31	0/58736
49	S5	0.21	0/212	0.29	0/328
50	SA	0.15	0/1766	0.30	0/2399
51	SB	0.34	0/1959	0.68	0/2618
52	SC	0.14	0/1737	0.31	0/2347
53	SD	0.13	0/1483	0.30	0/1993
54	SE	0.13	0/2117	0.30	0/2849
55	SG	0.13	0/1876	0.30	0/2499
56	SH	0.14	0/1532	0.31	0/2053
57	SI	0.13	0/1724	0.30	0/2298
58	SJ	0.13	0/1520	0.30	0/2030
59	SK	0.12	0/1773	0.32	0/2387
60	SL	0.14	0/1201	0.31	0/1604
61	SM	0.12	0/840	0.30	0/1133
62	SN	0.14	0/1231	0.31	0/1656
63	SO	0.14	0/959	0.32	0/1284
64	SP	0.12	0/1041	0.29	0/1392
65	SQ	0.14	0/1125	0.31	0/1506
66	SS	0.13	0/1078	0.30	0/1447
67	ST	0.12	0/1226	0.30	0/1643
68	SU	0.12	0/1113	0.29	0/1493
69	SV	0.12	0/643	0.30	0/860
70	SW	0.15	0/1050	0.32	0/1406
71	SX	0.13	0/1096	0.32	0/1461
72	SY	0.12	0/1019	0.28	0/1354
73	SZ	0.14	0/805	0.33	0/1081
74	Sa	0.14	0/805	0.32	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Sb	0.12	0/664	0.28	0/891
76	Sc	0.11	0/678	0.27	0/906
77	Sd	0.11	0/490	0.27	0/656
78	Se	0.11	0/442	0.28	0/582
79	Sf	0.12	0/469	0.30	0/623
80	Sg	0.12	0/2420	0.35	0/3294
81	So	0.18	0/240	0.33	0/305
82	Sy	0.14	0/949	0.34	0/1273
83	Sz	0.14	0/619	0.39	0/818
All	All	0.23	5/222471 (0.0%)	0.34	0/325899

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
16	LM	0	1
51	SB	0	4
57	SI	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1288	OMU	O3'-P	5.14	1.61	1.56
48	S2	1383	A2M	O3'-P	5.11	1.61	1.56
2	L5	1773	OMU	O3'-P	5.06	1.61	1.56
48	S2	576	A2M	O3'-P	5.03	1.61	1.56
2	L5	2837	OMU	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	LM	35	ARG	Sidechain
51	SB	13	ARG	Sidechain
51	SB	177	ARG	Sidechain
51	SB	57	ARG	Sidechain
51	SB	90	ARG	Sidechain

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Mol	Chain	Res	Type	Group
57	SI	152	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	L1	3153	0	1603	40	0
2	L5	75768	0	38369	657	0
3	L8	2386	0	2421	29	0
4	L9	2558	0	1295	18	0
5	LB	3234	0	3372	31	0
6	S4	1634	0	839	15	0
7	LC	2908	0	3082	25	0
8	LD	1899	0	1985	12	0
9	LE	1115	0	1205	11	0
10	LF	1870	0	1996	23	0
11	LG	1752	0	1877	15	0
12	LH	1518	0	1601	21	0
13	LI	1053	0	1147	10	0
14	LJ	1340	0	1377	23	0
15	LK	1780	0	1938	26	0
16	LM	1111	0	1174	24	0
17	LN	1700	0	1749	14	0
18	LO	1014	0	1148	12	0
19	LP	705	0	736	7	0
20	LQ	1664	0	1773	19	0
21	LR	1558	0	1718	14	0
22	LS	1460	0	1502	18	0
23	LT	1284	0	1352	7	0
24	LU	443	0	483	6	0
25	LV	972	0	1034	7	0
26	LW	893	0	936	25	0
27	LY	1624	0	1771	22	0
28	LZ	1106	0	1182	12	0
29	La	1162	0	1206	9	0
30	Lb	848	0	918	14	0
31	Lc	785	0	825	10	0
32	Ld	862	0	912	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Le	863	0	929	4	0
34	Lf	875	0	912	4	0
35	Lg	882	0	972	12	0
36	Lh	1289	0	1324	15	0
37	Li	832	0	917	10	0
38	Lj	1512	0	1628	5	0
39	Lk	559	0	624	8	0
40	Ll	990	0	1054	10	0
41	Lm	816	0	842	15	0
42	Ln	949	0	1016	10	0
43	Lo	436	0	477	13	0
44	Lp	681	0	731	4	0
45	Lz	1705	0	1757	14	0
46	NC	227	0	236	1	0
47	S1	1790	0	1873	18	0
48	S2	35485	0	17959	399	0
49	S5	191	0	98	0	0
50	SA	1731	0	1734	34	0
51	SB	1937	0	1951	42	0
52	SC	1700	0	1784	14	0
53	SD	1463	0	1517	24	0
54	SE	2075	0	2177	32	0
55	SG	1853	0	2005	41	0
56	SH	1509	0	1604	35	0
57	SI	1695	0	1785	30	0
58	SJ	1495	0	1615	17	0
59	SK	1745	0	1839	27	0
60	SL	1180	0	1253	11	0
61	SM	816	0	841	15	0
62	SN	1207	0	1293	7	0
63	SO	956	0	981	11	0
64	SP	1021	0	1065	18	0
65	SQ	1108	0	1174	17	0
66	SS	1064	0	1118	19	0
67	ST	1208	0	1270	20	0
68	SU	1094	0	1120	15	0
69	SV	636	0	637	8	0
70	SW	1033	0	1080	15	0
71	SX	1088	0	1149	6	0
72	SY	1002	0	1075	24	0
73	SZ	795	0	862	18	0
74	Sa	792	0	841	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	Sb	650	0	672	3	0
76	Sc	670	0	745	25	0
77	Sd	488	0	514	4	0
78	Se	437	0	484	4	0
79	Sf	458	0	448	8	0
80	Sg	2364	0	2318	65	0
81	So	239	0	289	2	0
82	Sy	939	0	974	36	0
83	Sz	607	0	633	31	0
84	L1	4	0	0	0	0
84	L5	204	0	0	0	0
84	L9	3	0	0	0	0
84	LD	1	0	0	0	0
84	LI	2	0	0	0	0
84	LN	1	0	0	0	0
84	LR	2	0	0	0	0
84	LV	1	0	0	0	0
84	La	1	0	0	0	0
84	Lh	1	0	0	0	0
84	S2	97	0	0	0	0
84	S4	6	0	0	0	0
84	SG	1	0	0	0	0
84	ST	1	0	0	0	0
84	SX	1	0	0	0	0
85	L1	3	0	0	0	0
85	L5	42	0	0	0	0
85	L9	1	0	0	0	0
85	LC	1	0	0	0	0
85	LD	2	0	0	0	0
85	LV	1	0	0	0	0
85	Lz	1	0	0	0	0
85	S2	39	0	0	0	0
85	SE	1	0	0	0	0
85	SO	1	0	0	0	0
85	ST	1	0	0	0	0
85	Sf	1	0	0	0	0
86	L5	19	0	26	0	0
87	LP	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lg	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	Sa	1	0	0	0	0
87	Sf	1	0	0	0	0
87	Sz	1	0	0	0	0
88	L1	153	0	0	0	0
88	L5	4961	0	0	15	0
88	L8	25	0	0	0	0
88	L9	93	0	0	0	0
88	LB	85	0	0	0	0
88	LC	104	0	0	2	0
88	LD	91	0	0	1	0
88	LE	10	0	0	0	0
88	LF	52	0	0	0	0
88	LG	16	0	0	0	0
88	LH	18	0	0	0	0
88	LI	64	0	0	0	0
88	LJ	3	0	0	0	0
88	LK	12	0	0	0	0
88	LM	7	0	0	1	0
88	LN	89	0	0	0	0
88	LO	13	0	0	0	0
88	LP	33	0	0	1	0
88	LQ	45	0	0	1	0
88	LR	23	0	0	0	0
88	LS	39	0	0	0	0
88	LT	41	0	0	0	0
88	LU	10	0	0	0	0
88	LV	27	0	0	0	0
88	LW	7	0	0	0	0
88	LY	42	0	0	0	0
88	LZ	10	0	0	0	0
88	La	46	0	0	0	0
88	Lb	15	0	0	1	0
88	Lc	8	0	0	0	0
88	Ld	15	0	0	0	0
88	Le	19	0	0	0	0
88	Lf	33	0	0	0	0
88	Lg	30	0	0	0	0
88	Lh	42	0	0	0	0
88	Li	4	0	0	1	0
88	Lj	69	0	0	0	0
88	Lk	4	0	0	1	0
88	Ll	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	Lm	1	0	0	0	0
88	Ln	18	0	0	1	0
88	Lo	3	0	0	0	0
88	Lp	25	0	0	0	0
88	Lz	16	0	0	0	0
88	S1	25	0	0	0	0
88	S2	2334	0	0	18	0
88	S4	52	0	0	0	0
88	S5	11	0	0	0	0
88	SA	9	0	0	0	0
88	SB	9	0	0	1	0
88	SC	36	0	0	0	0
88	SD	25	0	0	0	0
88	SE	45	0	0	0	0
88	SG	16	0	0	0	0
88	SH	6	0	0	0	0
88	SI	31	0	0	1	0
88	SJ	34	0	0	2	0
88	SK	6	0	0	0	0
88	SL	43	0	0	1	0
88	SM	4	0	0	1	0
88	SN	32	0	0	2	0
88	SO	33	0	0	0	0
88	SP	14	0	0	0	0
88	SQ	32	0	0	0	0
88	SS	5	0	0	1	0
88	ST	23	0	0	0	0
88	SU	20	0	0	0	0
88	SV	8	0	0	0	0
88	SW	39	0	0	0	0
88	SX	47	0	0	1	0
88	SY	10	0	0	0	0
88	SZ	12	0	0	0	0
88	Sa	38	0	0	1	0
88	Sb	11	0	0	0	0
88	Sc	3	0	0	0	0
88	Sd	2	0	0	0	0
88	Se	10	0	0	0	0
88	Sf	8	0	0	0	0
88	Sg	1	0	0	0	0
88	So	3	0	0	0	0
All	All	222228	0	158748	2057	0

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

All (2057) 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)
40:Ll:30:ASN:OD1	40:Ll:50:GLY:HA3	1.51	1.10
50:SA:206:ASP:OD1	50:SA:207:PRO:HD2	1.53	1.07
43:Lo:127:VAL:CG1	43:Lo:128:LYS:HE2	1.85	1.06
26:LW:97:LYS:HD3	55:SG:146:ASN:ND2	1.72	1.03
80:Sg:109:LEU:CD2	80:Sg:125:ARG:HG3	1.87	1.03
59:SK:193:ASP:OD2	59:SK:198:ILE:HG12	1.61	1.01
43:Lo:127:VAL:HG12	43:Lo:128:LYS:CE	1.90	1.00
80:Sg:109:LEU:HD21	80:Sg:125:ARG:CG	1.91	1.00
80:Sg:109:LEU:HD21	80:Sg:125:ARG:HG3	1.00	0.99
43:Lo:127:VAL:HG12	43:Lo:128:LYS:HE2	1.43	0.97
67:ST:98:VAL:HG11	67:ST:106:LYS:HG3	1.47	0.94
83:Sz:103:LEU:HD12	83:Sz:104:LYS:N	1.81	0.94
51:SB:29:TRP:CZ3	51:SB:94:VAL:HG21	2.01	0.94
48:S2:870:A:OP2	60:SL:153:LYS:HE3	1.69	0.91
50:SA:206:ASP:CG	50:SA:207:PRO:HD2	1.96	0.90
72:SY:50:THR:HG22	72:SY:51:THR:H	1.36	0.88
26:LW:97:LYS:HD3	55:SG:146:ASN:HD22	1.38	0.86
82:Sy:36:ARG:HD2	83:Sz:103:LEU:CD2	2.05	0.85
2:L5:3944:OMG:HN1	2:L5:4069:U:H3	1.24	0.84
2:L5:2611:A:H5'	2:L5:2688:G:H4'	1.59	0.83
48:S2:835:C:O5'	48:S2:836:G:N2	2.13	0.82
72:SY:9:THR:HB	72:SY:23:MET:SD	2.20	0.82
1:L1:156:U:H3	2:L5:1:C:H42	1.28	0.81
48:S2:928:G:H1	48:S2:1013:U:H3	1.27	0.81
82:Sy:20:GLU:HG3	82:Sy:119:GLN:HG2	1.62	0.81
72:SY:50:THR:HG22	72:SY:51:THR:N	1.95	0.81
2:L5:2557:G:H1	2:L5:2570:U:H3	1.28	0.80
55:SG:79:LYS:HG2	55:SG:86:PRO:HG3	1.61	0.80
48:S2:1507:G:H21	83:Sz:87:THR:HB	1.47	0.80
40:Ll:30:ASN:CG	40:Ll:50:GLY:HA3	2.06	0.80
22:LS:168:THR:HA	27:LY:118:MET:HE1	1.64	0.80
2:L5:1271:G:H8	10:LF:30:ILE:HD11	1.44	0.80
2:L5:182:G:H1	2:L5:254:G:H22	1.29	0.79
43:Lo:127:VAL:HG11	43:Lo:128:LYS:HE2	1.63	0.79
56:SH:30:LEU:O	56:SH:34:SER:HB3	1.83	0.79
82:Sy:32:ALA:HB1	82:Sy:37:GLU:HB3	1.65	0.79
22:LS:168:THR:N	27:LY:118:MET:HE3	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1271:G:C8	10:LF:30:ILE:HD11	2.19	0.78
2:L5:2469:C:H5	2:L5:2471:G:H1	1.27	0.78
2:L5:964:A:H2'	2:L5:965:G:H4'	1.65	0.78
48:S2:925:G:H1	48:S2:1017:U:H3	1.27	0.78
2:L5:1271:G:H22	2:L5:2106:G:H1	1.32	0.77
80:Sg:184:LEU:HD21	80:Sg:187:ASN:HD21	1.48	0.77
22:LS:168:THR:CA	27:LY:118:MET:HE1	2.15	0.76
43:Lo:127:VAL:HG12	43:Lo:128:LYS:HE3	1.67	0.76
25:LV:13:LYS:HD3	25:LV:128:LEU:HD11	1.67	0.76
26:LW:80:ARG:HH21	55:SG:131:ARG:HE	1.33	0.76
16:LM:31:ILE:CG2	16:LM:35:ARG:HH21	2.00	0.75
3:L8:256:LYS:HD2	4:L9:117:G:H5''	1.67	0.74
16:LM:31:ILE:HG21	16:LM:35:ARG:HH21	1.50	0.74
26:LW:97:LYS:CD	55:SG:146:ASN:ND2	2.50	0.74
15:LK:93:THR:HG22	15:LK:106:VAL:HG22	1.70	0.74
22:LS:168:THR:N	27:LY:118:MET:CE	2.52	0.73
2:L5:492:U:H4'	2:L5:493:G:H5''	1.70	0.73
80:Sg:54:ILE:HG13	80:Sg:55:PRO:HD2	1.71	0.73
2:L5:1271:G:H8	10:LF:30:ILE:CD1	2.02	0.73
43:Lo:127:VAL:CG1	43:Lo:128:LYS:CE	2.55	0.73
51:SB:135:LEU:HD21	51:SB:211:VAL:HG22	1.70	0.73
22:LS:169:THR:HG22	27:LY:118:MET:SD	2.29	0.72
2:L5:3823:G:OP2	2:L5:3823:G:N2	2.19	0.72
2:L5:2495:U:H2'	2:L5:2496:G:H8	1.53	0.72
33:Le:11:PHE:O	33:Le:81:ARG:NH2	2.22	0.72
47:S1:35:ALA:O	47:S1:42:ARG:NH1	2.23	0.72
2:L5:1921:C:O2'	22:LS:160:ARG:NH1	2.22	0.71
2:L5:2562:G:N2	2:L5:2565:A:OP2	2.23	0.70
2:L5:980:U:HO2'	15:LK:40:GLY:N	1.89	0.70
2:L5:1754:U:H3	2:L5:1776:A:H61	1.39	0.70
70:SW:80:ASP:OD1	70:SW:124:LYS:NZ	2.21	0.70
48:S2:1228:A:H2'	48:S2:1229:G:C8	2.25	0.70
48:S2:1637:A:OP2	76:Sc:39:LYS:NZ	2.24	0.70
64:SP:31:GLU:HA	64:SP:34:MET:HE2	1.72	0.70
59:SK:170:THR:HG23	59:SK:187:LYS:HG2	1.73	0.70
2:L5:1365:C:H41	2:L5:1370:G:H22	1.38	0.70
72:SY:50:THR:CG2	72:SY:51:THR:H	2.04	0.70
26:LW:117:LYS:HD2	48:S2:327:G:H8	1.57	0.70
64:SP:56:LEU:HD23	64:SP:83:MET:HE3	1.74	0.69
2:L5:1339:U:H2'	2:L5:1340:OMC:C6	2.27	0.69
50:SA:10:MET:HE2	50:SA:55:TRP:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LS:167:PHE:C	27:LY:118:MET:CE	2.65	0.69
2:L5:1100:U:O3'	2:L5:1167:C:N4	2.26	0.69
48:S2:1285:G:H22	82:Sy:57:ASP:HB3	1.58	0.69
60:SL:81:LYS:HE2	88:SL:239:HOH:O	1.93	0.69
2:L5:1175:A:H2	2:L5:1185:G:H1	1.40	0.69
80:Sg:87:LEU:HB2	80:Sg:101:PHE:HB2	1.75	0.69
16:LM:51:PRO:HB2	16:LM:53:LYS:HG2	1.73	0.69
48:S2:1435:C:O2	48:S2:1436:C:N4	2.26	0.68
2:L5:1070:G:OP2	15:LK:65:ARG:NH1	2.25	0.68
48:S2:1550:G:H3'	48:S2:1579:A:H61	1.58	0.68
2:L5:1176:C:H42	2:L5:1184:A:H61	1.40	0.68
5:LB:286:LYS:NZ	5:LB:302:ASN:O	2.26	0.68
48:S2:1521:C:H5'	64:SP:126:VAL:HB	1.74	0.68
48:S2:874:G:H2'	48:S2:875:A:H8	1.59	0.68
2:L5:137:G:H2'	2:L5:138:G:C8	2.29	0.68
48:S2:1473:G:N7	88:S2:2129:HOH:O	2.26	0.68
80:Sg:31:ILE:HG12	80:Sg:43:TRP:HB2	1.76	0.68
82:Sy:36:ARG:HD2	83:Sz:103:LEU:HD22	1.76	0.68
83:Sz:126:CYS:SG	83:Sz:144:CYS:HB3	2.34	0.68
67:ST:102:GLY:O	67:ST:106:LYS:HG2	1.94	0.68
26:LW:102:LYS:HD3	26:LW:105:ARG:HH21	1.59	0.67
54:SE:95:THR:O	54:SE:95:THR:HG22	1.92	0.67
15:LK:50:LEU:HD23	15:LK:56:ARG:HA	1.77	0.67
2:L5:4992:G:H2'	2:L5:4993:G:C8	2.29	0.67
48:S2:189:U:OP1	57:SI:152:ARG:NH2	2.28	0.67
68:SU:33:TRP:HZ2	68:SU:102:ARG:HG3	1.59	0.67
40:Ll:48:THR:HG22	40:Ll:65:LYS:HB2	1.75	0.67
48:S2:1277:C:H2'	48:S2:1278:A:H8	1.60	0.67
48:S2:1536:G:H2'	48:S2:1537:A:H8	1.59	0.67
48:S2:1566:G:N7	68:SU:101:ARG:NH2	2.42	0.67
7:LC:140:LYS:HE2	7:LC:245:HIS:HB2	1.75	0.67
48:S2:1588:A:H2'	48:S2:1589:A:C8	2.28	0.67
83:Sz:103:LEU:HD12	83:Sz:104:LYS:O	1.95	0.67
60:SL:152:LYS:O	60:SL:153:LYS:HG2	1.94	0.67
2:L5:4537:C:H2'	2:L5:4538:G:C8	2.30	0.67
2:L5:2601:A:N6	2:L5:2744:A:OP2	2.28	0.66
5:LB:216:MET:HG3	5:LB:281:ASN:HA	1.77	0.66
26:LW:97:LYS:HA	26:LW:101:ARG:HG3	1.77	0.66
48:S2:84:A:H5''	72:SY:122:LYS:HD3	1.76	0.66
48:S2:801:PSU:O2	56:SH:106:ARG:NH2	2.28	0.66
48:S2:953:C:O2	63:SO:55:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1396:A:O2'	48:S2:1398:G:N7	2.27	0.66
57:SI:91:VAL:HG21	57:SI:205:ARG:HH12	1.59	0.66
2:L5:2262:G:OP2	40:L1:98:ARG:NH1	2.28	0.66
54:SE:128:LYS:HB3	54:SE:140:VAL:HB	1.78	0.66
48:S2:1398:G:H1'	80:Sg:63:SER:HB3	1.78	0.66
2:L5:3717:A:OP2	2:L5:3735:G:N2	2.27	0.66
54:SE:100:ARG:HH21	54:SE:118:GLU:HG2	1.61	0.65
80:Sg:87:LEU:HD21	80:Sg:122:SER:HB3	1.78	0.65
20:LQ:191:LEU:HD22	20:LQ:194:ILE:HD11	1.78	0.65
80:Sg:212:LYS:HA	80:Sg:235:ILE:HG13	1.76	0.65
48:S2:1444:U:OP1	65:SQ:15:ARG:NH2	2.30	0.65
65:SQ:128:GLU:OE2	65:SQ:131:LYS:NZ	2.29	0.65
16:LM:98:ARG:NH1	88:LM:301:HOH:O	2.29	0.65
48:S2:145:G:H2'	48:S2:146:G:C8	2.32	0.65
59:SK:142:LEU:HD13	59:SK:150:MET:HE3	1.78	0.65
2:L5:3717:A:H2'	2:L5:3718:A2M:H8	1.79	0.65
2:L5:2351:OMC:HM22	2:L5:2352:U:H5'	1.77	0.65
2:L5:1727:U:OP1	10:LF:131:ASN:ND2	2.29	0.65
2:L5:1774:C:H2'	2:L5:1775:A:H8	1.62	0.64
2:L5:4967:A:H2'	2:L5:4968:A:H8	1.61	0.64
2:L5:1187:G:OP2	2:L5:1187:G:N2	2.25	0.64
2:L5:3717:A:H2'	2:L5:3718:A2M:C8	2.28	0.64
2:L5:4431:PSU:OP2	45:Lz:3:ARG:NH2	2.24	0.64
48:S2:1410:C:H2'	48:S2:1411:G:H8	1.61	0.64
12:LH:16:VAL:HG21	12:LH:81:ILE:HG23	1.79	0.64
12:LH:173:ARG:HB2	43:Lo:127:VAL:CG2	2.27	0.64
48:S2:434:G:N7	88:S2:2156:HOH:O	2.29	0.64
2:L5:711:A:H2'	2:L5:712:C:C6	2.32	0.64
52:SC:172:ASN:ND2	58:SJ:95:ASP:OD2	2.31	0.64
48:S2:1579:A:N7	88:S2:2168:HOH:O	2.29	0.64
69:SV:38:GLU:OE2	69:SV:51:LYS:NZ	2.31	0.64
2:L5:1761:G:H1	2:L5:1771:U:H3	1.44	0.63
12:LH:94:SER:HB2	12:LH:142:ASP:HB3	1.79	0.63
48:S2:107:A:H2'	48:S2:108:G:C8	2.33	0.63
48:S2:1325:G:N3	88:S2:2176:HOH:O	2.30	0.63
22:LS:168:THR:CA	27:LY:118:MET:CE	2.76	0.63
82:Sy:36:ARG:HD2	83:Sz:103:LEU:HD23	1.79	0.63
2:L5:4267:G:N7	88:L5:5477:HOH:O	2.30	0.63
30:Lb:90:SER:OG	30:Lb:95:ARG:NH1	2.30	0.63
48:S2:44:U:O2'	48:S2:45:A:H2'	1.98	0.63
48:S2:901:G:H2'	48:S2:902:G:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:109:C:O2'	19:LP:20:ARG:NH2	2.30	0.63
2:L5:2572:C:O2'	28:LZ:112:ARG:NH2	2.32	0.63
48:S2:981:A:H2'	48:S2:982:G:C8	2.34	0.63
48:S2:1536:G:H2'	48:S2:1537:A:C8	2.33	0.63
50:SA:77:ILE:HG12	50:SA:99:ILE:HB	1.78	0.63
51:SB:101:LYS:HB2	51:SB:104:SER:HB3	1.79	0.63
2:L5:135:G:N2	18:LO:95:LEU:O	2.30	0.63
41:Lm:65:ARG:HG2	41:Lm:67:LYS:H	1.62	0.63
48:S2:474:G:N7	88:S2:2172:HOH:O	2.30	0.63
2:L5:235:A:OP1	7:LC:201:ARG:NH2	2.27	0.63
38:Lj:49:LYS:HG2	38:Lj:53:MET:HE3	1.80	0.63
51:SB:160:LYS:NZ	51:SB:164:ASP:OD1	2.31	0.63
54:SE:124:CYS:HB3	54:SE:141:THR:HB	1.81	0.63
15:LK:101:ASN:O	15:LK:105:ARG:NH1	2.29	0.63
55:SG:50:VAL:HG12	55:SG:113:ILE:HD13	1.80	0.63
47:S1:63:LYS:NZ	47:S1:89:GLU:O	2.32	0.63
51:SB:169:LEU:O	51:SB:173:ILE:HG13	1.98	0.63
66:SS:95:ILE:HD11	66:SS:118:GLN:HB2	1.80	0.63
2:L5:2478:C:N3	2:L5:2591:A:O2'	2.29	0.63
2:L5:4260:U:H2'	2:L5:4261:C:C6	2.34	0.63
48:S2:1262:C:O2'	79:Sf:12:ARG:NH1	2.32	0.62
82:Sy:15:ASN:O	82:Sy:19:GLN:HG2	1.99	0.62
2:L5:268:G:H2'	2:L5:269:G:H8	1.63	0.62
2:L5:1812:C:H5''	30:Lb:56:LYS:HE3	1.81	0.62
82:Sy:116:LYS:HZ2	82:Sy:119:GLN:H	1.47	0.62
2:L5:1419:G:O2'	29:La:116:LYS:NZ	2.29	0.62
54:SE:176:ASP:OD1	54:SE:179:ASN:ND2	2.33	0.62
1:L1:19:C:H2'	1:L1:20:A:C8	2.34	0.62
45:Lz:30:LYS:NZ	45:Lz:66:GLU:OE1	2.32	0.62
51:SB:192:ASN:HA	53:SD:198:ARG:HH21	1.63	0.62
20:LQ:80:GLU:OE2	20:LQ:102:ARG:NH2	2.30	0.62
48:S2:190:G:OP2	57:SI:148:LYS:NZ	2.32	0.62
48:S2:322:C:O2'	48:S2:324:C:N4	2.32	0.62
48:S2:1277:C:H2'	48:S2:1278:A:C8	2.34	0.62
2:L5:4966:A:H5'	5:LB:128:LYS:HG3	1.81	0.62
48:S2:1533:A:H2	48:S2:1536:G:N3	1.96	0.62
80:Sg:163:PRO:HB2	80:Sg:179:LEU:HB3	1.82	0.62
3:L8:62:CYS:HB3	3:L8:105:LEU:HD22	1.82	0.62
2:L5:757:G:H2'	2:L5:758:G:H8	1.64	0.62
48:S2:928:G:H2'	48:S2:929:G:C8	2.35	0.62
48:S2:1533:A:C8	48:S2:1604:G:H1'	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:737:C:OP2	16:LM:71:LYS:NZ	2.32	0.61
42:Ln:76:ILE:HG22	42:Ln:77:ILE:HD12	1.82	0.61
48:S2:1548:G:N3	88:S2:2190:HOH:O	2.31	0.61
48:S2:1745:A:H1'	55:SG:66:GLY:HA2	1.81	0.61
70:SW:8:ALA:HA	70:SW:74:VAL:HG11	1.82	0.61
48:S2:68:A:H62	48:S2:81:U:H3	1.47	0.61
48:S2:506:G:OP1	72:SY:108:LYS:NZ	2.33	0.61
48:S2:528:A:H2'	48:S2:529:A:C8	2.35	0.61
55:SG:21:GLU:OE1	55:SG:25:ARG:NH2	2.26	0.61
70:SW:11:LEU:HD12	70:SW:74:VAL:CG1	2.29	0.61
35:Lg:45:ALA:HB3	35:Lg:82:MET:HG2	1.82	0.61
54:SE:197:ASN:HB3	54:SE:209:HIS:HB2	1.82	0.61
12:LH:93:ARG:NH1	12:LH:142:ASP:O	2.34	0.61
17:LN:20:ARG:HH21	17:LN:24:ARG:HH21	1.49	0.61
53:SD:102:LEU:HD23	76:Sc:67:LEU:HD12	1.83	0.61
2:L5:4274:A:H2'	2:L5:4275:G:C8	2.35	0.61
51:SB:29:TRP:CZ3	51:SB:94:VAL:CG2	2.79	0.61
2:L5:4522:G:O2'	2:L5:4525:C:OP2	2.13	0.61
80:Sg:142:VAL:HG12	80:Sg:146:SER:HB3	1.83	0.61
2:L5:3923:A:H2'	2:L5:3924:C:C6	2.35	0.61
48:S2:532:C:O2	48:S2:552:G:N2	2.34	0.61
48:S2:1548:G:H1	48:S2:1584:G:H1	1.48	0.61
72:SY:23:MET:HE1	72:SY:48:TYR:CZ	2.36	0.61
2:L5:4882:U:OP1	16:LM:117:LYS:NZ	2.34	0.60
2:L5:4911:A:N7	88:L5:5493:HOH:O	2.31	0.60
48:S2:379:C:O2	57:SI:5:ARG:NE	2.34	0.60
80:Sg:107:ASP:HB2	80:Sg:125:ARG:HD2	1.82	0.60
2:L5:4861:G:H2'	2:L5:4862:G:H8	1.67	0.60
2:L5:465:G:O2'	2:L5:466:A:OP1	2.19	0.60
2:L5:755:C:H2'	2:L5:756:G:H8	1.66	0.60
48:S2:165:G:OP2	48:S2:165:G:N2	2.28	0.60
1:L1:156:U:H3	2:L5:1:C:N4	2.00	0.60
11:LG:106:THR:HG22	11:LG:107:LYS:N	2.17	0.60
54:SE:31:PRO:HG2	54:SE:38:LEU:HG	1.83	0.60
12:LH:173:ARG:CB	43:Lo:127:VAL:HG23	2.32	0.60
37:Li:41:ARG:NH1	88:Li:201:HOH:O	2.34	0.60
48:S2:367:U:H4'	48:S2:371:A:C8	2.37	0.60
48:S2:1299:A:OP1	64:SP:59:ARG:NH1	2.35	0.60
2:L5:1662:C:H2'	2:L5:1663:C:C6	2.36	0.60
2:L5:4537:C:H2'	2:L5:4538:G:H8	1.66	0.60
48:S2:809:A:OP1	54:SE:187:ALA:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:3718:A2M:H2	2:L5:3934:G:O4'	2.01	0.60
6:S4:18:OMG:HN22	6:S4:19:A:H62	1.48	0.60
26:LW:97:LYS:NZ	55:SG:146:ASN:HD21	2.00	0.60
48:S2:496:C:OP1	54:SE:49:ARG:NH2	2.33	0.60
55:SG:57:ASP:OD1	55:SG:61:PHE:N	2.33	0.60
58:SJ:170:PRO:HB3	58:SJ:174:LYS:HD2	1.84	0.60
2:L5:1332:C:H2'	2:L5:1333:A:H8	1.65	0.59
2:L5:4591:U:H2'	2:L5:4592:C:C6	2.37	0.59
28:LZ:113:GLU:OE2	28:LZ:117:LYS:NZ	2.32	0.59
48:S2:309:G:OP2	57:SI:53:LYS:NZ	2.31	0.59
48:S2:377:G:H5'	57:SI:98:LYS:HB3	1.84	0.59
2:L5:1774:C:H2'	2:L5:1775:A:C8	2.37	0.59
48:S2:1113:A:H2'	48:S2:1114:U:C6	2.37	0.59
18:LO:95:LEU:HB3	18:LO:99:GLU:HG3	1.83	0.59
32:Ld:91:LYS:HG2	32:Ld:92:ARG:N	2.17	0.59
73:SZ:39:LEU:HD23	73:SZ:101:ILE:HG22	1.83	0.59
2:L5:1503:A:H4'	2:L5:1504:G:H5'	1.84	0.59
30:Lb:47:LYS:NZ	88:Lb:201:HOH:O	2.35	0.59
48:S2:1794:C:N3	88:S2:2184:HOH:O	2.31	0.59
70:SW:3:ARG:NH1	70:SW:9:ASP:OD2	2.36	0.59
75:Sb:33:MET:HB3	75:Sb:79:PHE:HB2	1.84	0.59
82:Sy:71:GLU:HG3	83:Sz:114:ILE:HG12	1.84	0.59
2:L5:4894:A:OP1	16:LM:129:LYS:NZ	2.32	0.59
48:S2:640:A:H2'	48:S2:641:A:C8	2.37	0.59
75:Sb:36:LYS:HB2	75:Sb:43:ILE:HD13	1.85	0.59
2:L5:3910:C:H2'	2:L5:3911:C:C6	2.38	0.59
2:L5:4472:G:O2'	43:Lo:100:TYR:O	2.20	0.59
2:L5:4946:U:HO2'	34:Lf:2:SER:N	2.00	0.59
2:L5:4967:A:H2'	2:L5:4968:A:C8	2.36	0.59
11:LG:99:ALA:HB1	11:LG:136:LEU:HD11	1.84	0.59
13:LI:82:VAL:HG13	13:LI:114:ARG:HG2	1.85	0.59
26:LW:97:LYS:NZ	55:SG:146:ASN:ND2	2.50	0.59
26:LW:116:LYS:HB3	26:LW:117:LYS:HZ2	1.67	0.59
48:S2:1803:U:H2'	48:S2:1804:OMU:H6	1.83	0.59
52:SC:60:TRP:O	52:SC:71:LYS:NZ	2.29	0.59
59:SK:109:LEU:HD12	59:SK:184:ILE:HD11	1.85	0.59
9:LE:47:MET:HE1	9:LE:118:ILE:HG13	1.85	0.59
48:S2:434:G:H5''	57:SI:23:LYS:HE2	1.85	0.59
72:SY:9:THR:CB	72:SY:23:MET:SD	2.88	0.59
2:L5:1400:G:H2'	2:L5:1401:C:C6	2.37	0.59
22:LS:9:GLU:OE2	22:LS:31:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1497:G:N7	61:SM:25:LYS:NZ	2.46	0.59
51:SB:138:GLN:OE1	51:SB:176:HIS:NE2	2.30	0.59
2:L5:4239:A:H2'	2:L5:4240:G:C8	2.38	0.59
48:S2:1446:A:HO2'	48:S2:1447:G:H8	1.51	0.59
72:SY:9:THR:CG2	72:SY:23:MET:SD	2.91	0.59
16:LM:100:ARG:HA	16:LM:103:LYS:HG2	1.85	0.59
48:S2:562:U:H2'	48:S2:563:G:C8	2.37	0.59
48:S2:1335:G:OP1	59:SK:185:LYS:NZ	2.36	0.59
51:SB:186:ILE:HG23	51:SB:195:ILE:HD13	1.83	0.59
55:SG:135:PRO:HG2	55:SG:141:ILE:HG12	1.84	0.59
80:Sg:239:LEU:HD22	80:Sg:248:LEU:HD11	1.85	0.59
82:Sy:26:LEU:HD12	82:Sy:30:GLY:HA2	1.85	0.59
82:Sy:36:ARG:CD	83:Sz:103:LEU:CD2	2.79	0.59
2:L5:1279:A:OP1	15:LK:131:LYS:NZ	2.24	0.58
2:L5:3736:A:H2'	2:L5:3737:A:C8	2.37	0.58
32:Ld:91:LYS:HG2	32:Ld:92:ARG:H	1.68	0.58
48:S2:12:U:H2'	48:S2:13:C:C6	2.38	0.58
80:Sg:176:VAL:HB	80:Sg:186:THR:HB	1.85	0.58
2:L5:1271:G:C8	10:LF:30:ILE:CD1	2.82	0.58
61:SM:27:VAL:HG13	61:SM:43:LEU:HD13	1.84	0.58
8:LD:147:ARG:HG2	8:LD:157:VAL:HG22	1.84	0.58
48:S2:1061:U:O2'	48:S2:1848:U:O2'	2.22	0.58
48:S2:1712:A:H2'	48:S2:1713:C:C6	2.39	0.58
2:L5:1703:C:O2'	10:LF:43:ARG:NH2	2.36	0.58
48:S2:664:A:O2'	48:S2:670:A:N1	2.33	0.58
48:S2:848:U:H2'	48:S2:849:A:H8	1.68	0.58
2:L5:93:G:H2'	2:L5:94:A:C8	2.38	0.58
2:L5:1307:A:H2'	2:L5:1308:C:C6	2.38	0.58
2:L5:1942:A:H2'	2:L5:1943:A:C8	2.39	0.58
2:L5:4260:U:H2'	2:L5:4261:C:H6	1.69	0.58
2:L5:980:U:H2'	2:L5:981:C:C6	2.38	0.58
45:Lz:36:LEU:HD11	45:Lz:69:ARG:HH11	1.68	0.58
48:S2:555:A:OP2	78:Se:99:LYS:NZ	2.35	0.58
48:S2:1279:C:H2'	48:S2:1280:G:H8	1.68	0.58
2:L5:691:C:H2'	2:L5:692:A:C8	2.39	0.58
2:L5:1965:G:C2	2:L5:1966:C:H1'	2.38	0.58
2:L5:4719:G:N7	88:L5:5511:HOH:O	2.32	0.58
27:LY:197:LYS:NZ	27:LY:203:VAL:O	2.36	0.58
73:SZ:20:ILE:HG12	73:SZ:116:ILE:HG12	1.84	0.58
2:L5:2583:C:OP2	35:Lg:76:ARG:NH1	2.36	0.58
2:L5:2876:OMG:HM22	2:L5:2877:G:H5'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LJ:15:LEU:HD12	14:LJ:165:TRP:HB2	1.84	0.58
51:SB:49:LYS:HG3	51:SB:53:LYS:HE2	1.84	0.58
62:SN:33:VAL:HG21	62:SN:66:VAL:HG11	1.85	0.58
67:ST:24:ARG:HB2	67:ST:29:ALA:HB2	1.85	0.58
59:SK:74:GLN:NE2	59:SK:81:GLU:O	2.35	0.58
2:L5:4884:G:O6	15:LK:272:ARG:NH2	2.37	0.57
48:S2:1434:C:H1'	73:SZ:19:ARG:HD3	1.87	0.57
48:S2:1578:U:O2	59:SK:9:ARG:NH2	2.31	0.57
48:S2:115:U:H2'	48:S2:116:OMU:C6	2.33	0.57
50:SA:127:PRO:HA	50:SA:134:LEU:HD11	1.86	0.57
83:Sz:103:LEU:CD1	83:Sz:104:LYS:O	2.52	0.57
2:L5:2267:U:OP1	40:Ll:37:SER:HB2	2.05	0.57
22:LS:169:THR:CG2	27:LY:118:MET:SD	2.91	0.57
48:S2:1420:G:H21	48:S2:1421:A:H1'	1.69	0.57
48:S2:1801:A:H2'	48:S2:1802:C:C6	2.39	0.57
53:SD:91:ARG:HD2	76:Sc:103:HIS:CE1	2.39	0.57
61:SM:77:GLN:OE1	61:SM:80:ARG:NH1	2.37	0.57
7:LC:163:LYS:O	7:LC:166:GLU:HG2	2.04	0.57
48:S2:847:A:OP1	54:SE:108:ARG:NH1	2.38	0.57
51:SB:29:TRP:CH2	51:SB:94:VAL:CG2	2.88	0.57
51:SB:29:TRP:CH2	51:SB:94:VAL:HG21	2.38	0.57
2:L5:740:G:N2	2:L5:924:C:H42	2.03	0.57
48:S2:1706:G:H5'	81:So:1:MET:HB2	1.87	0.57
67:ST:34:LYS:NZ	67:ST:104:ASP:OD1	2.30	0.57
68:SU:13:GLU:OE1	68:SU:142:ASN:ND2	2.36	0.57
2:L5:267:G:OP1	18:LO:109:ARG:NH2	2.26	0.57
12:LH:16:VAL:O	12:LH:53:LYS:NZ	2.37	0.57
38:Lj:112:ARG:HG2	38:Lj:115:ARG:HH22	1.69	0.57
72:SY:114:MET:O	72:SY:122:LYS:NZ	2.37	0.57
25:LV:32:THR:O	25:LV:69:LYS:NZ	2.35	0.57
47:S1:75:GLN:HG2	47:S1:78:GLU:HG3	1.86	0.57
52:SC:68:ARG:HH21	52:SC:276:THR:HB	1.68	0.57
66:SS:78:ARG:HH21	66:SS:79:GLU:HG2	1.70	0.57
2:L5:3786:U:O2	2:L5:3814:U:H4'	2.05	0.57
48:S2:51:U:H2'	48:S2:52:G:H8	1.70	0.57
48:S2:1557:C:H1'	48:S2:1661:A:H5'	1.87	0.57
2:L5:492:U:H1'	7:LC:268:ARG:HH21	1.70	0.57
2:L5:934:C:H41	7:LC:350:ARG:HH21	1.53	0.57
2:L5:3711:A:H2'	2:L5:3712:A:H8	1.69	0.57
10:LF:127:LYS:HB2	23:LT:133:ALA:HB3	1.87	0.57
13:LI:70:LEU:HD11	13:LI:76:LYS:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1091:C:HO2'	70:SW:2:VAL:N	2.02	0.56
2:L5:510:U:OP1	20:LQ:163:LYS:NZ	2.38	0.56
2:L5:2422:OMC:OP1	36:Lh:127:ARG:NH2	2.37	0.56
2:L5:74:G:H5'	20:LQ:59:VAL:HB	1.86	0.56
2:L5:662:C:H2'	2:L5:663:G:H8	1.69	0.56
2:L5:4633:G:N7	88:L5:5515:HOH:O	2.33	0.56
6:S4:26:M2G:HM12	6:S4:44:A:H2	1.70	0.56
48:S2:420:G:O2'	48:S2:660:C:N3	2.39	0.56
2:L5:739:G:HO2'	2:L5:740:G:H8	1.51	0.56
47:S1:34:LYS:NZ	47:S1:43:ASN:OD1	2.38	0.56
50:SA:198:MET:HG2	50:SA:200:ASP:H	1.70	0.56
60:SL:152:LYS:O	60:SL:153:LYS:CG	2.52	0.56
16:LM:40:GLY:HA3	16:LM:45:VAL:HB	1.86	0.56
36:Lh:54:GLN:HA	36:Lh:83:TRP:CD1	2.41	0.56
48:S2:65:C:C2	55:SG:174:PRO:HG3	2.40	0.56
2:L5:1308:C:H2'	2:L5:1309:C:C6	2.40	0.56
2:L5:1332:C:H2'	2:L5:1333:A:C8	2.41	0.56
2:L5:2091:C:O2	2:L5:2094:G:O2'	2.17	0.56
2:L5:3880:G:H2'	2:L5:3881:G:C8	2.41	0.56
48:S2:836:G:H1'	48:S2:837:A:H5''	1.86	0.56
58:SJ:63:LEU:O	58:SJ:70:ARG:NH1	2.38	0.56
60:SL:91:ASP:HB3	60:SL:104:LYS:HE2	1.88	0.56
67:ST:86:ARG:NH2	67:ST:110:ASP:OD2	2.35	0.56
82:Sy:116:LYS:NZ	82:Sy:119:GLN:H	2.03	0.56
1:L1:94:G:OP2	19:LP:72:ARG:NH1	2.36	0.56
2:L5:2602:G:H2'	2:L5:2603:C:C6	2.41	0.56
21:LR:168:GLU:OE1	21:LR:172:ARG:NH2	2.39	0.56
48:S2:30:C:O2'	48:S2:596:U:OP1	2.23	0.56
48:S2:1464:C:OP2	66:SS:63:ARG:NH2	2.38	0.56
58:SJ:47:LYS:HG3	58:SJ:102:ILE:HD12	1.88	0.56
59:SK:215:ASP:OD1	59:SK:215:ASP:N	2.36	0.56
2:L5:469:C:N3	15:LK:105:ARG:NH2	2.48	0.56
2:L5:2640:G:H2'	2:L5:2641:A:C8	2.40	0.56
36:Lh:126:ARG:NH1	46:NC:191:ASP:OD2	2.38	0.56
54:SE:107:GLY:HA2	54:SE:189:LEU:HG	1.87	0.56
61:SM:42:ASN:ND2	61:SM:46:MET:SD	2.79	0.56
73:SZ:20:ILE:HD12	73:SZ:98:VAL:HG21	1.87	0.56
2:L5:325:U:H2'	2:L5:326:C:C6	2.41	0.56
6:S4:61:C:H2'	6:S4:62:C:C6	2.40	0.56
26:LW:107:GLN:HB2	26:LW:110:ARG:HH21	1.69	0.56
41:Lm:80:LYS:HG2	41:Lm:110:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SZ:80:PHE:HB3	79:Sf:52:PHE:HB3	1.87	0.56
2:L5:1940:G:N2	2:L5:4434:C:OP1	2.37	0.56
2:L5:2458:C:H5''	17:LN:67:ARG:HD2	1.88	0.56
2:L5:4339:A:H2'	2:L5:4340:U:H6	1.70	0.56
1:L1:148:A:H2'	1:L1:149:G:C8	2.41	0.55
2:L5:4111:U:H2'	2:L5:4112:C:C6	2.42	0.55
26:LW:80:ARG:HG2	26:LW:81:ALA:H	1.71	0.55
32:Ld:24:GLU:HG3	32:Ld:122:VAL:HG21	1.88	0.55
47:S1:29:ASP:OD1	47:S1:51:ARG:NH2	2.33	0.55
48:S2:1228:A:H2'	48:S2:1229:G:H8	1.70	0.55
63:SO:28:PHE:HZ	74:Sa:58:VAL:HG21	1.71	0.55
2:L5:989:U:O2	2:L5:1064:G:O6	2.23	0.55
2:L5:2864:A:H2'	2:L5:2865:U:C6	2.41	0.55
26:LW:94:ARG:HD2	55:SG:146:ASN:HB2	1.88	0.55
26:LW:120:GLN:O	26:LW:124:LYS:HB2	2.05	0.55
2:L5:4934:A:H2'	2:L5:4935:C:C6	2.41	0.55
3:L8:116:ASP:N	3:L8:116:ASP:OD1	2.38	0.55
26:LW:91:MET:O	26:LW:95:ASN:ND2	2.40	0.55
35:Lg:104:VAL:HG12	35:Lg:108:LYS:HE2	1.89	0.55
48:S2:1310:U:H4'	83:Sz:143:LYS:HB2	1.87	0.55
56:SH:30:LEU:O	56:SH:34:SER:CB	2.52	0.55
67:ST:98:VAL:CG1	67:ST:106:LYS:HG3	2.30	0.55
2:L5:264:C:O2	18:LO:112:ARG:NH2	2.39	0.55
12:LH:45:LEU:HD22	12:LH:57:VAL:HG22	1.88	0.55
48:S2:51:U:H2'	48:S2:52:G:C8	2.41	0.55
48:S2:1037:G:H4'	48:S2:1845:A:H4'	1.89	0.55
53:SD:28:VAL:O	53:SD:42:LYS:NZ	2.29	0.55
54:SE:104:ASP:HB3	54:SE:110:ALA:HB2	1.89	0.55
2:L5:4251:A:H5''	14:LJ:108:GLY:HA3	1.87	0.55
2:L5:4455:G:H5''	5:LB:5:LYS:HE2	1.89	0.55
7:LC:209:ILE:HB	7:LC:229:LEU:HD13	1.88	0.55
12:LH:37:ASP:OD1	12:LH:39:ASN:ND2	2.38	0.55
55:SG:7:PHE:HE1	55:SG:9:ALA:HB3	1.72	0.55
2:L5:4594:U:H2'	2:L5:4595:G:H8	1.71	0.55
3:L8:150:LEU:HD12	14:LJ:146:ARG:HG3	1.89	0.55
37:Li:70:LEU:HB2	37:Li:87:ARG:NH1	2.22	0.55
2:L5:2520:C:O2	2:L5:2640:G:N2	2.39	0.55
22:LS:167:PHE:C	27:LY:118:MET:HE3	2.31	0.55
2:L5:662:C:H2'	2:L5:663:G:C8	2.42	0.55
2:L5:4724:A:O2'	5:LB:104:THR:HG22	2.07	0.55
48:S2:1285:G:H3'	48:S2:1286:G:H5''	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sy:36:ARG:CD	83:Sz:103:LEU:HD22	2.36	0.55
1:L1:141:C:H2'	1:L1:142:U:C6	2.42	0.55
2:L5:647:G:H2'	2:L5:648:G:H8	1.71	0.55
2:L5:2504:C:OP2	42:Ln:47:ARG:NH2	2.37	0.55
2:L5:4173:G:H2'	2:L5:4174:U:C6	2.42	0.55
2:L5:4238:G:H2'	2:L5:4239:A:C8	2.42	0.55
48:S2:1407:U:H2'	48:S2:1408:U:C6	2.42	0.55
51:SB:114:VAL:HG12	51:SB:115:ASP:N	2.22	0.55
64:SP:41:GLN:HG3	64:SP:84:ILE:HD13	1.89	0.55
73:SZ:78:ASP:OD1	79:Sf:54:LYS:NZ	2.26	0.55
48:S2:102:A:H4'	48:S2:104:A:C8	2.42	0.55
48:S2:1710:OMC:HM22	48:S2:1711:U:H5'	1.89	0.55
56:SH:10:LYS:HE3	56:SH:20:GLU:HB3	1.89	0.55
68:SU:77:LYS:HB2	68:SU:94:ARG:HH21	1.72	0.55
74:Sa:59:PHE:HB2	74:Sa:62:TYR:HB2	1.88	0.55
2:L5:478:G:H2'	2:L5:479:G:H8	1.72	0.54
48:S2:874:G:H2'	48:S2:875:A:C8	2.40	0.54
65:SQ:89:SER:HB3	65:SQ:112:LEU:HD13	1.89	0.54
2:L5:4621:C:OP1	25:LV:48:ARG:HD2	2.07	0.54
15:LK:108:LYS:HE3	15:LK:111:LYS:HA	1.90	0.54
64:SP:53:GLN:HG3	64:SP:83:MET:HE1	1.88	0.54
2:L5:1604:G:H2'	2:L5:1605:G:C8	2.42	0.54
5:LB:57:VAL:HG22	5:LB:73:VAL:HG22	1.89	0.54
48:S2:495:U:H2'	48:S2:496:C:O4'	2.07	0.54
48:S2:888:U:N3	48:S2:900:C:N3	2.56	0.54
48:S2:902:G:O2'	48:S2:903:A:O4'	2.25	0.54
48:S2:942:G:H2'	48:S2:943:U:C6	2.42	0.54
50:SA:108:PHE:HB2	50:SA:136:GLU:HG2	1.88	0.54
67:ST:16:LEU:HD12	67:ST:33:ILE:HD13	1.89	0.54
2:L5:2280:G:OP1	13:LI:48:ARG:NH2	2.40	0.54
52:SC:252:THR:OG1	52:SC:254:ASP:OD1	2.23	0.54
59:SK:218:LEU:HD13	80:Sg:192:THR:HB	1.88	0.54
2:L5:5026:U:O2'	57:SI:77:ARG:NH1	2.40	0.54
36:Lh:4:TYR:CZ	36:Lh:18:ARG:HG3	2.43	0.54
48:S2:15:U:H2'	48:S2:16:G:O4'	2.08	0.54
48:S2:156:G:OP1	55:SG:2:LYS:NZ	2.31	0.54
50:SA:145:ILE:HG12	50:SA:159:ILE:HB	1.90	0.54
53:SD:102:LEU:HD21	76:Sc:67:LEU:HA	1.89	0.54
54:SE:63:LYS:NZ	72:SY:85:ASN:O	2.40	0.54
21:LR:160:GLU:OE1	21:LR:163:ARG:NH2	2.41	0.54
48:S2:322:C:HO2'	48:S2:324:C:N4	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1595:U:H2'	48:S2:1596:U:C6	2.43	0.54
54:SE:137:PRO:HB2	54:SE:150:PRO:HD2	1.90	0.54
61:SM:49:MET:HE1	61:SM:58:VAL:HG11	1.89	0.54
80:Sg:145:GLU:O	80:Sg:175:LYS:NZ	2.40	0.54
2:L5:4768:G:OP1	27:LY:168:TYR:OH	2.21	0.54
2:L5:5029:C:O2'	2:L5:5030:U:O5'	2.24	0.54
10:LF:182:TYR:HB3	10:LF:200:ARG:HG3	1.88	0.54
41:Lm:52:LYS:HB2	41:Lm:55:ASN:HB3	1.89	0.54
45:Lz:201:PRO:HB2	45:Lz:203:ARG:HG2	1.89	0.54
2:L5:3871:A:H2'	2:L5:3872:A:C8	2.42	0.54
26:LW:105:ARG:NH1	55:SG:151:ASP:OD1	2.39	0.54
2:L5:3589:G:N2	2:L5:3590:G:N7	2.47	0.54
2:L5:4699:U:H1'	2:L5:4700:A:H5''	1.90	0.54
16:LM:127:VAL:HG21	27:LY:178:ARG:HG2	1.89	0.54
48:S2:141:A:H4'	48:S2:142:C:H3'	1.90	0.54
48:S2:1239:U:H5''	64:SP:124:LYS:HD2	1.90	0.54
72:SY:9:THR:HG21	72:SY:23:MET:SD	2.48	0.54
72:SY:22:GLN:HB3	72:SY:74:MET:HE1	1.89	0.54
74:Sa:44:ILE:HD12	74:Sa:65:PRO:HG2	1.89	0.54
12:LH:173:ARG:HB2	43:Lo:127:VAL:HG23	1.90	0.54
20:LQ:186:ARG:NH1	88:LQ:303:HOH:O	2.40	0.54
20:LQ:198:ARG:HA	20:LQ:201:GLU:HG2	1.90	0.54
39:Lk:40:ARG:NH2	88:Lk:101:HOH:O	2.39	0.54
48:S2:1405:A:H2'	48:S2:1406:G:O4'	2.07	0.54
73:SZ:54:VAL:HB	73:SZ:88:LEU:HB2	1.90	0.54
80:Sg:23:THR:HG21	80:Sg:292:SER:HA	1.90	0.54
80:Sg:54:ILE:CG1	80:Sg:55:PRO:HD2	2.38	0.54
2:L5:280:G:H5''	17:LN:14:LYS:HE2	1.90	0.53
2:L5:4136:G:H2'	2:L5:4137:C:O4'	2.07	0.53
2:L5:4934:A:H2'	2:L5:4935:C:H6	1.72	0.53
3:L8:33:ARG:NH1	4:L9:7:G:OP1	2.39	0.53
11:LG:193:LEU:HD12	11:LG:194:VAL:HG13	1.90	0.53
63:SO:34:PHE:HB3	63:SO:41:PHE:HB2	1.89	0.53
66:SS:79:GLU:O	66:SS:83:ASN:ND2	2.37	0.53
2:L5:73:A:OP1	20:LQ:106:SER:HB2	2.08	0.53
2:L5:3656:A:H2'	2:L5:3657:U:H6	1.71	0.53
2:L5:4256:A:HO2'	14:LJ:55:TYR:HH	1.54	0.53
2:L5:4926:C:H2'	2:L5:4927:G:O4'	2.08	0.53
48:S2:170:A:OP2	55:SG:140:ARG:NH1	2.41	0.53
48:S2:804:U:H2'	48:S2:805:U:C6	2.43	0.53
50:SA:124:VAL:HG21	50:SA:134:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SH:47:ALA:HB3	56:SH:63:PHE:HB2	1.91	0.53
2:L5:411:G:H4'	2:L5:412:G:H5''	1.89	0.53
2:L5:1173:G:H2'	2:L5:1174:G:C8	2.43	0.53
2:L5:4111:U:H2'	2:L5:4112:C:H6	1.72	0.53
28:LZ:91:LEU:HB3	28:LZ:96:VAL:HG21	1.89	0.53
48:S2:319:C:H2'	48:S2:320:G:C8	2.43	0.53
56:SH:117:PRO:HG2	56:SH:120:ARG:HD3	1.90	0.53
82:Sy:68:LEU:O	82:Sy:72:HIS:ND1	2.40	0.53
48:S2:1404:U:P	73:SZ:21:ARG:HH12	2.31	0.53
17:LN:138:PHE:HA	17:LN:143:ARG:HD2	1.89	0.53
56:SH:83:LEU:HB3	56:SH:92:VAL:HG21	1.90	0.53
58:SJ:138:ARG:NH2	58:SJ:152:ASP:O	2.42	0.53
2:L5:194:C:O2	9:LE:121:ARG:NH2	2.41	0.53
51:SB:201:ARG:HA	51:SB:204:LYS:HB2	1.91	0.53
64:SP:53:GLN:HA	64:SP:83:MET:HE1	1.91	0.53
37:Li:56:ARG:HD2	37:Li:72:PHE:CZ	2.44	0.53
48:S2:1410:C:H2'	48:S2:1411:G:C8	2.42	0.53
53:SD:102:LEU:HD23	76:Sc:67:LEU:CD1	2.38	0.53
2:L5:424:U:H2'	2:L5:425:U:C6	2.43	0.53
2:L5:917:A:H2'	2:L5:918:G:O4'	2.09	0.53
2:L5:1751:A:H2'	2:L5:1752:G:C8	2.44	0.53
4:L9:111:C:H2'	4:L9:112:U:O4'	2.09	0.53
31:Lc:47:ILE:HD12	31:Lc:94:LEU:HD11	1.90	0.53
48:S2:615:C:OP2	71:SX:64:SER:OG	2.26	0.53
48:S2:1203:G:H2'	48:S2:1204:A:C8	2.43	0.53
74:Sa:93:LYS:NZ	88:Sa:305:HOH:O	2.40	0.53
3:L8:125:VAL:HG11	3:L8:199:ILE:HG21	1.91	0.53
48:S2:57:U:OP1	48:S2:504:G:O2'	2.27	0.53
48:S2:118:C:H1'	48:S2:445:A:C5	2.44	0.53
54:SE:141:THR:OG1	54:SE:143:ASP:OD1	2.24	0.53
70:SW:11:LEU:HD12	70:SW:74:VAL:HG12	1.90	0.53
29:La:2:PRO:HD2	29:La:5:LEU:HD12	1.90	0.53
35:Lg:83:CYS:SG	35:Lg:86:CYS:HB2	2.49	0.53
48:S2:455:A:H2'	48:S2:456:C:C6	2.44	0.53
72:SY:50:THR:CG2	72:SY:51:THR:N	2.64	0.53
2:L5:469:C:H2'	2:L5:470:A:C8	2.44	0.52
2:L5:3732:A:H2'	2:L5:3733:A:C8	2.44	0.52
2:L5:3917:A:H2'	2:L5:3918:G:H8	1.74	0.52
48:S2:29:G:H2'	48:S2:30:C:C6	2.44	0.52
48:S2:115:U:H2'	48:S2:116:OMU:H6	1.92	0.52
54:SE:54:TYR:O	72:SY:15:ASN:ND2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SI:148:LYS:HD3	57:SI:152:ARG:HH21	1.73	0.52
2:L5:2101:C:N4	2:L5:2102:G:O6	2.42	0.52
47:S1:5:LYS:NZ	48:S2:958:G:O6	2.42	0.52
48:S2:1784:G:H2'	48:S2:1785:C:C6	2.44	0.52
51:SB:25:PHE:HE2	51:SB:90:ARG:HE	1.56	0.52
2:L5:132:G:H2'	2:L5:133:C:H4'	1.92	0.52
2:L5:1645:C:H2'	2:L5:1646:A:C8	2.44	0.52
2:L5:2050:OMG:HM22	2:L5:2051:C:O4'	2.10	0.52
2:L5:3711:A:H2'	2:L5:3712:A:C8	2.45	0.52
2:L5:4478:G:O2'	2:L5:4602:A:N1	2.40	0.52
2:L5:4935:C:H2'	2:L5:4936:G:C8	2.45	0.52
8:LD:149:LYS:HD2	8:LD:155:LYS:HE3	1.90	0.52
16:LM:96:GLU:O	16:LM:100:ARG:HG2	2.09	0.52
21:LR:151:ARG:NH1	60:SL:119:ASP:OD1	2.43	0.52
2:L5:755:C:H2'	2:L5:756:G:C8	2.43	0.52
2:L5:2613:C:H4'	35:Lg:2:VAL:HG21	1.90	0.52
48:S2:533:A:H2'	48:S2:534:G:C8	2.44	0.52
1:L1:128:C:H2'	1:L1:129:C:C6	2.44	0.52
2:L5:1071:C:N4	15:LK:67:ALA:HB2	2.25	0.52
2:L5:1801:A:H4'	23:LT:102:ARG:HH21	1.74	0.52
2:L5:4344:U:H2'	2:L5:4345:C:C6	2.45	0.52
48:S2:1712:A:H2'	48:S2:1713:C:H6	1.73	0.52
2:L5:968:C:H5'	15:LK:110:ARG:HD2	1.92	0.52
2:L5:1271:G:N2	2:L5:2106:G:H22	2.08	0.52
2:L5:3923:A:H2'	2:L5:3924:C:H6	1.75	0.52
48:S2:101:U:H5''	57:SI:19:LYS:HE3	1.92	0.52
54:SE:174:LYS:O	54:SE:179:ASN:ND2	2.43	0.52
57:SI:123:ARG:HD2	57:SI:129:LEU:HD11	1.92	0.52
80:Sg:101:PHE:CE2	80:Sg:136:GLY:HA2	2.44	0.52
2:L5:218:A:H2'	2:L5:218:A:N3	2.25	0.52
2:L5:4173:G:H2'	2:L5:4174:U:H6	1.74	0.52
2:L5:4928:C:O2	16:LM:118:MET:HE1	2.10	0.52
48:S2:16:G:H2'	48:S2:17:C:C6	2.44	0.52
48:S2:195:C:H2'	48:S2:196:C:C6	2.45	0.52
66:SS:34:VAL:O	66:SS:38:ILE:HG13	2.09	0.52
2:L5:1707:C:H3'	30:Lb:103:LYS:HG3	1.90	0.52
22:LS:168:THR:N	27:LY:118:MET:HE1	2.25	0.52
27:LY:8:VAL:HG12	27:LY:117:ARG:HG3	1.92	0.52
48:S2:85:A:H2'	48:S2:86:C:H6	1.75	0.52
48:S2:85:A:O2'	48:S2:149:A:N3	2.41	0.52
48:S2:464:A:H5''	48:S2:465:A:N7	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sy:19:GLN:HE22	82:Sy:88:TRP:CG	2.28	0.52
1:L1:26:C:O2'	7:LC:53:ALA:O	2.27	0.52
1:L1:144:U:H2'	1:L1:145:C:C6	2.45	0.52
2:L5:456:C:H2'	2:L5:457:G:H8	1.74	0.52
4:L9:110:G:H2'	4:L9:111:C:C6	2.44	0.52
5:LB:220:ILE:HG12	5:LB:278:THR:HG23	1.92	0.52
7:LC:218:ILE:O	7:LC:222:ARG:HB2	2.09	0.52
41:Lm:26:THR:O	41:Lm:30:GLU:HG2	2.10	0.52
47:S1:2:ALA:N	63:SO:68:GLU:OE2	2.43	0.52
47:S1:168:MET:HG2	47:S1:197:ILE:HG21	1.92	0.52
48:S2:473:A:N7	88:S2:2231:HOH:O	2.34	0.52
70:SW:104:LEU:HD23	70:SW:125:ILE:HA	1.92	0.52
82:Sy:86:GLY:HA3	82:Sy:105:GLY:HA2	1.92	0.52
1:L1:128:C:H2'	1:L1:129:C:H6	1.74	0.51
2:L5:1186:U:H2'	2:L5:1187:G:N3	2.26	0.51
2:L5:1440:U:H2'	2:L5:1441:C:C6	2.45	0.51
48:S2:868:G:C6	56:SH:115:LYS:HD3	2.45	0.51
48:S2:1407:U:H2'	48:S2:1408:U:H6	1.75	0.51
2:L5:1279:A:O2'	2:L5:1281:G:N7	2.38	0.51
2:L5:4108:G:H2'	2:L5:4109:G:C8	2.45	0.51
2:L5:4288:C:O2'	2:L5:4321:U:OP1	2.24	0.51
6:S4:17:G:H1'	6:S4:57:G:N2	2.25	0.51
45:Lz:87:ILE:HG12	45:Lz:138:ILE:HG12	1.91	0.51
62:SN:40:LEU:HD12	62:SN:50:ILE:HG23	1.92	0.51
2:L5:92:C:C2	29:La:55:LYS:HE2	2.46	0.51
2:L5:3910:C:H2'	2:L5:3911:C:H6	1.74	0.51
2:L5:4238:G:H2'	2:L5:4239:A:H8	1.73	0.51
2:L5:268:G:H2'	2:L5:269:G:C8	2.44	0.51
2:L5:1270:A:H8	2:L5:2105:A:H2	1.58	0.51
2:L5:1751:A:H2'	2:L5:1752:G:H8	1.75	0.51
2:L5:4208:U:OP2	23:LT:4:THR:OG1	2.27	0.51
10:LF:27:GLU:O	10:LF:31:LYS:HG3	2.11	0.51
26:LW:97:LYS:CD	55:SG:146:ASN:HD22	2.13	0.51
48:S2:382:C:H2'	48:S2:383:G:H8	1.76	0.51
48:S2:1309:C:O2'	83:Sz:141:CYS:O	2.28	0.51
48:S2:1538:C:H2'	48:S2:1539:U:C6	2.46	0.51
51:SB:199:ALA:HB1	51:SB:229:LEU:HD11	1.92	0.51
57:SI:144:LYS:HA	57:SI:147:LYS:HE2	1.92	0.51
68:SU:77:LYS:HB2	68:SU:94:ARG:NH2	2.25	0.51
2:L5:4638:U:H2'	2:L5:4639:G:N3	2.26	0.51
2:L5:5003:U:H2'	2:L5:5004:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LH:129:ARG:NE	12:LH:156:ASN:OD1	2.39	0.51
48:S2:690:G:OP2	48:S2:690:G:N2	2.35	0.51
48:S2:1801:A:H2'	48:S2:1802:C:H6	1.76	0.51
61:SM:84:HIS:CD2	82:Sy:27:ILE:HG13	2.46	0.51
80:Sg:191:HIS:CG	80:Sg:195:LEU:HD21	2.46	0.51
2:L5:659:G:H2'	2:L5:660:A:H8	1.75	0.51
2:L5:1247:U:H2'	2:L5:1248:C:C6	2.45	0.51
2:L5:4274:A:H2'	2:L5:4275:G:H8	1.75	0.51
48:S2:522:A:H5''	58:SJ:145:PRO:HD2	1.93	0.51
48:S2:530:U:H2'	48:S2:531:A:C8	2.46	0.51
48:S2:1011:A:N1	88:S2:2219:HOH:O	2.34	0.51
50:SA:206:ASP:CG	50:SA:207:PRO:CD	2.77	0.51
58:SJ:22:LYS:NZ	88:SJ:204:HOH:O	2.34	0.51
78:Se:96:GLN:O	78:Se:98:LYS:NZ	2.31	0.51
2:L5:489:C:O2'	2:L5:667:A:N1	2.42	0.51
3:L8:211:LEU:HB3	3:L8:219:TYR:HB2	1.91	0.51
39:Lk:52:LYS:HA	39:Lk:55:LYS:HD2	1.92	0.51
48:S2:25:A:HO2'	48:S2:26:U:H6	1.59	0.51
48:S2:952:G:H2'	48:S2:953:C:C6	2.46	0.51
51:SB:49:LYS:HD3	51:SB:91:PHE:HZ	1.76	0.51
70:SW:11:LEU:HD12	70:SW:74:VAL:HG13	1.91	0.51
2:L5:756:G:N1	2:L5:757:G:O6	2.44	0.51
2:L5:1207:C:H2'	2:L5:1208:G:H8	1.76	0.51
2:L5:3707:U:H2'	2:L5:3708:C:C6	2.46	0.51
48:S2:1533:A:N3	48:S2:1533:A:H2'	2.26	0.51
48:S2:1797:U:H2'	48:S2:1798:C:C6	2.46	0.51
83:Sz:137:ASP:OD1	83:Sz:138:ARG:N	2.44	0.51
2:L5:121:A:H3'	2:L5:122:U:H5'	1.93	0.51
2:L5:974:C:O2'	7:LC:327:LYS:NZ	2.44	0.51
2:L5:2864:A:H2'	2:L5:2865:U:H6	1.76	0.51
48:S2:943:U:O2'	63:SO:135:ILE:O	2.27	0.51
48:S2:996:A:H2'	48:S2:997:A:C8	2.45	0.51
48:S2:1563:G:OP1	68:SU:121:ARG:NH1	2.44	0.51
57:SI:131:PRO:HA	57:SI:134:GLU:HG2	1.93	0.51
22:LS:167:PHE:C	27:LY:118:MET:HE1	2.36	0.51
47:S1:116:LYS:HG2	48:S2:988:C:H5''	1.92	0.51
48:S2:1007:C:H2'	48:S2:1008:A:C8	2.45	0.51
48:S2:1201:U:H2'	48:S2:1202:U:C6	2.46	0.51
1:L1:71:A:N1	1:L1:81:C:O2'	2.41	0.50
2:L5:23:C:H2'	2:L5:24:G:O4'	2.11	0.50
2:L5:464:G:H2'	2:L5:465:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1662:C:H2'	2:L5:1663:C:H6	1.76	0.50
2:L5:1910:G:N7	88:L5:5548:HOH:O	2.35	0.50
41:Lm:24:ASP:HB2	41:Lm:69:LYS:NZ	2.26	0.50
48:S2:418:A:H2'	48:S2:419:G:C8	2.46	0.50
50:SA:59:LEU:HD22	50:SA:181:GLU:HG2	1.94	0.50
66:SS:29:HIS:O	66:SS:32:LYS:HG2	2.11	0.50
67:ST:23:ARG:HB3	76:Sc:48:VAL:HG11	1.92	0.50
2:L5:4546:A:N7	8:LD:215:ASN:ND2	2.56	0.50
2:L5:4918:C:H2'	2:L5:4919:G:C8	2.46	0.50
26:LW:97:LYS:HZ2	55:SG:146:ASN:HD21	1.58	0.50
48:S2:588:G:OP2	48:S2:588:G:N2	2.34	0.50
2:L5:646:G:H2'	2:L5:647:G:C8	2.47	0.50
2:L5:647:G:H2'	2:L5:648:G:C8	2.46	0.50
2:L5:4174:U:H2'	2:L5:4175:G:H8	1.76	0.50
80:Sg:116:ASP:OD1	80:Sg:116:ASP:N	2.44	0.50
48:S2:1600:G:N3	48:S2:1600:G:H2'	2.26	0.50
76:Sc:73:VAL:HG21	76:Sc:88:LEU:HD21	1.94	0.50
76:Sc:79:ILE:HB	76:Sc:83:LEU:HD23	1.92	0.50
2:L5:424:U:H2'	2:L5:425:U:H6	1.75	0.50
2:L5:2620:G:H2'	2:L5:2621:A:H8	1.76	0.50
2:L5:3652:A:H2'	2:L5:3653:A:C5	2.46	0.50
2:L5:4743:G:H2'	2:L5:4744:A:C8	2.47	0.50
2:L5:4927:G:OP2	2:L5:4927:G:N2	2.29	0.50
7:LC:328:LEU:HD13	10:LF:187:MET:HE2	1.92	0.50
32:Ld:75:LYS:HE3	32:Ld:79:ASN:O	2.11	0.50
48:S2:1255:G:OP1	48:S2:1256:G:O2'	2.14	0.50
48:S2:1653:U:H2'	48:S2:1654:G:C8	2.47	0.50
50:SA:164:ASN:O	50:SA:170:SER:OG	2.26	0.50
52:SC:68:ARG:HG3	52:SC:277:HIS:NE2	2.26	0.50
56:SH:100:ILE:HG12	56:SH:125:VAL:HG21	1.93	0.50
2:L5:463:A:H2	2:L5:692:A:N1	2.10	0.50
2:L5:1241:C:C6	30:Lb:115:GLY:HA2	2.47	0.50
2:L5:1249:C:H2'	2:L5:1250:C:C6	2.46	0.50
2:L5:2520:C:H2'	2:L5:2521:G:C8	2.47	0.50
2:L5:2539:C:H2'	2:L5:2540:C:C6	2.46	0.50
2:L5:4567:G:N7	88:L5:5558:HOH:O	2.35	0.50
3:L8:208:MET:HE3	3:L8:233:PRO:HG3	1.93	0.50
7:LC:162:LYS:N	7:LC:166:GLU:OE2	2.41	0.50
48:S2:196:C:N4	48:S2:203:G:O6	2.45	0.50
48:S2:223:C:H2'	48:S2:224:A:C8	2.47	0.50
48:S2:1683:C:H2'	48:S2:1684:C:H6	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SA:80:ARG:NH1	50:SA:165:ASN:O	2.40	0.50
51:SB:49:LYS:HD3	51:SB:91:PHE:CZ	2.47	0.50
56:SH:78:ARG:O	56:SH:82:GLU:HG2	2.12	0.50
82:Sy:26:LEU:HA	82:Sy:30:GLY:HA2	1.92	0.50
82:Sy:89:VAL:HG11	82:Sy:109:VAL:HG11	1.94	0.50
2:L5:753:C:H42	2:L5:910:G:H1	1.60	0.50
5:LB:317:LEU:HD11	5:LB:382:MET:HG2	1.94	0.50
7:LC:298:ILE:O	7:LC:302:LEU:HG	2.11	0.50
40:L1:30:ASN:HD21	40:L1:63:VAL:HB	1.77	0.50
48:S2:1679:A:OP1	53:SD:60:ARG:NH2	2.42	0.50
62:SN:110:ASP:O	62:SN:114:ARG:HG2	2.12	0.50
2:L5:4741:C:N4	2:L5:4743:G:OP1	2.45	0.50
14:LJ:95:ARG:O	14:LJ:98:ASN:HB2	2.12	0.50
20:LQ:178:ALA:N	29:La:134:GLU:OE2	2.39	0.50
48:S2:1628:C:H2'	48:S2:1629:C:C6	2.47	0.50
54:SE:102:ILE:HD12	54:SE:239:PRO:HD3	1.93	0.50
83:Sz:102:VAL:HG13	83:Sz:104:LYS:HG2	1.92	0.50
2:L5:4344:U:H2'	2:L5:4345:C:H6	1.77	0.50
48:S2:493:A:H1'	48:S2:574:A:H5'	1.94	0.50
48:S2:1523:C:H4'	67:ST:145:THR:HA	1.93	0.50
65:SQ:106:LYS:NZ	65:SQ:110:ASP:OD2	2.45	0.50
66:SS:97:GLU:OE1	66:SS:97:GLU:N	2.42	0.50
1:L1:89:U:H2'	1:L1:90:C:C6	2.47	0.49
2:L5:469:C:H2'	2:L5:470:A:H8	1.77	0.49
2:L5:1685:G:H2'	2:L5:1686:C:C6	2.47	0.49
2:L5:4222:G:N7	88:L5:5559:HOH:O	2.35	0.49
48:S2:533:A:H2'	48:S2:534:G:H8	1.77	0.49
67:ST:44:VAL:HG11	67:ST:71:MET:HG3	1.94	0.49
76:Sc:34:LYS:HG3	76:Sc:36:SER:H	1.76	0.49
76:Sc:73:VAL:HG12	76:Sc:79:ILE:HD11	1.94	0.49
82:Sy:52:LEU:HD23	82:Sy:78:LYS:HZ2	1.76	0.49
2:L5:1246:G:H2'	2:L5:1247:U:C6	2.47	0.49
2:L5:1420:A:H2'	2:L5:1420:A:N3	2.27	0.49
5:LB:161:ARG:HG2	5:LB:184:GLN:HA	1.93	0.49
36:Lh:40:HIS:NE2	36:Lh:110:ASP:O	2.43	0.49
48:S2:1667:U:H2'	48:S2:1668:U:C6	2.47	0.49
57:SI:110:ARG:HG2	57:SI:121:LEU:HB3	1.94	0.49
2:L5:271:C:H2'	2:L5:272:U:C6	2.48	0.49
2:L5:1249:C:H2'	2:L5:1250:C:H6	1.77	0.49
48:S2:1511:U:H2'	48:S2:1512:C:C6	2.47	0.49
48:S2:1562:C:H2'	48:S2:1563:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SK:12:VAL:HG21	79:Sf:34:TYR:HB3	1.94	0.49
2:L5:1646:A:O2'	19:LP:49:TRP:O	2.26	0.49
2:L5:2620:G:H2'	2:L5:2621:A:C8	2.47	0.49
2:L5:2702:C:OP1	41:Lm:101:ARG:NH2	2.44	0.49
2:L5:4491:G:H5''	2:L5:4620:OMU:HM21	1.94	0.49
2:L5:4896:G:H2'	2:L5:4897:G:H8	1.76	0.49
22:LS:69:GLU:HG2	22:LS:101:THR:HG22	1.95	0.49
47:S1:47:THR:OG1	47:S1:65:ARG:NH1	2.45	0.49
48:S2:940:U:H2'	48:S2:941:C:C6	2.48	0.49
48:S2:1692:PSU:H2'	48:S2:1693:G:C8	2.48	0.49
52:SC:116:THR:OG1	52:SC:119:GLY:O	2.27	0.49
56:SH:58:LYS:HB2	56:SH:90:LYS:HG2	1.93	0.49
12:LH:112:VAL:HG13	12:LH:126:VAL:HB	1.94	0.49
19:LP:14:LYS:NZ	88:LP:205:HOH:O	2.41	0.49
50:SA:149:ASN:HD22	50:SA:166:LYS:HE2	1.77	0.49
51:SB:198:ASP:O	51:SB:202:LYS:HG3	2.12	0.49
54:SE:92:ILE:HG21	72:SY:17:LEU:HD11	1.94	0.49
2:L5:1241:C:N3	30:Lb:120:ARG:NH2	2.59	0.49
2:L5:1468:C:H2'	2:L5:1469:C:H6	1.77	0.49
2:L5:1685:G:H2'	2:L5:1686:C:H6	1.78	0.49
2:L5:3669:G:H21	2:L5:3672:G:H21	1.61	0.49
2:L5:4420:PSU:H2'	2:L5:4421:C:C5	2.47	0.49
15:LK:287:VAL:O	16:LM:109:ARG:NH2	2.46	0.49
43:Lo:79:GLU:OE1	43:Lo:81:SER:OG	2.23	0.49
51:SB:49:LYS:NZ	88:SB:702:HOH:O	2.33	0.49
60:SL:152:LYS:C	60:SL:153:LYS:HG2	2.37	0.49
2:L5:691:C:H2'	2:L5:692:A:H8	1.75	0.49
2:L5:1895:G:H2'	2:L5:1896:A:O4'	2.13	0.49
2:L5:2602:G:H2'	2:L5:2603:C:H6	1.77	0.49
5:LB:378:ARG:HG2	26:LW:32:LEU:HD21	1.95	0.49
18:LO:89:ARG:O	18:LO:93:ARG:HG2	2.13	0.49
40:L1:26:SER:OG	40:L1:28:GLU:OE1	2.24	0.49
48:S2:1259:A:H1'	48:S2:1264:C:N4	2.28	0.49
48:S2:1528:G:O2'	48:S2:1666:C:OP1	2.27	0.49
48:S2:1597:C:H4'	48:S2:1603:G:O6	2.13	0.49
57:SI:106:SER:HB3	57:SI:171:LEU:HG	1.93	0.49
80:Sg:42:MET:HB3	80:Sg:57:ARG:HB3	1.94	0.49
2:L5:362:A:N6	24:LU:37:TYR:O	2.44	0.49
2:L5:456:C:H2'	2:L5:457:G:C8	2.47	0.49
2:L5:753:C:N4	2:L5:910:G:H1	2.11	0.49
2:L5:909:A:H2'	2:L5:910:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:919:C:OP1	16:LM:69:HIS:ND1	2.46	0.49
2:L5:3893:C:H2'	2:L5:3894:A:C8	2.47	0.49
2:L5:4169:G:H4'	2:L5:4171:C:C2	2.48	0.49
2:L5:4524:G:N3	5:LB:252:ALA:HB1	2.28	0.49
2:L5:4594:U:H2'	2:L5:4595:G:C8	2.48	0.49
2:L5:4619:U:H2'	2:L5:4620:OMU:H6	1.94	0.49
36:Lh:4:TYR:CZ	36:Lh:16:LYS:HB2	2.48	0.49
48:S2:1285:G:H1	82:Sy:57:ASP:HB3	1.78	0.49
50:SA:6:ASP:HA	50:SA:9:GLN:HG2	1.95	0.49
53:SD:40:ALA:HB1	53:SD:45:TYR:CG	2.48	0.49
56:SH:9:VAL:HG12	56:SH:44:ASN:HA	1.93	0.49
2:L5:153:G:H2'	2:L5:154:G:H8	1.77	0.49
48:S2:829:C:OP1	54:SE:21:ASP:HB2	2.13	0.49
48:S2:1227:G:C2	48:S2:1228:A:C8	3.01	0.49
48:S2:1390:U:H2'	48:S2:1391:OMC:C6	2.48	0.49
48:S2:1845:A:H2'	48:S2:1846:G:C8	2.48	0.49
53:SD:34:SER:HA	77:Sd:55:VAL:HB	1.95	0.49
56:SH:95:ILE:HD11	56:SH:133:LEU:HD13	1.95	0.49
72:SY:83:LYS:HE3	72:SY:96:LEU:HD13	1.95	0.49
82:Sy:36:ARG:CD	83:Sz:103:LEU:HD23	2.41	0.49
2:L5:135:G:O6	18:LO:97:LYS:HE2	2.12	0.49
2:L5:3656:A:H2'	2:L5:3657:U:C6	2.47	0.49
3:L8:195:HIS:O	3:L8:199:ILE:HG12	2.13	0.49
6:S4:6:C:H2'	6:S4:7:G:C8	2.48	0.49
8:LD:101:VAL:HG22	8:LD:165:VAL:HG22	1.93	0.49
13:LI:89:LEU:HD13	13:LI:118:LEU:HD22	1.94	0.49
17:LN:20:ARG:HH21	17:LN:24:ARG:NH2	2.10	0.49
31:Lc:104:ILE:O	31:Lc:108:MET:HG2	2.13	0.49
45:Lz:38:ARG:NH2	45:Lz:45:GLU:OE2	2.36	0.49
47:S1:110:MET:HE1	47:S1:140:VAL:HG21	1.95	0.49
48:S2:830:A:OP2	48:S2:846:G:N2	2.46	0.49
48:S2:1279:C:H2'	48:S2:1280:G:C8	2.47	0.49
48:S2:1822:A:H2'	48:S2:1823:A:C8	2.47	0.49
50:SA:122:LEU:HB3	50:SA:144:THR:HG22	1.95	0.49
51:SB:55:LEU:HA	51:SB:58:LEU:HD12	1.95	0.49
2:L5:3684:G:H2'	2:L5:3685:C:C6	2.48	0.48
5:LB:163:ILE:HG22	5:LB:180:LEU:HD11	1.95	0.48
48:S2:99:A2M:H8	48:S2:99:A2M:O5'	2.13	0.48
54:SE:95:THR:O	54:SE:95:THR:CG2	2.60	0.48
66:SS:77:GLU:HB3	66:SS:81:ARG:NH1	2.28	0.48
2:L5:478:G:H2'	2:L5:479:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1870:C:H2'	2:L5:1871:A2M:H8	1.95	0.48
2:L5:2838:G:H5'	5:LB:247:GLY:HA2	1.94	0.48
7:LC:35:ASP:OD1	88:LC:602:HOH:O	2.20	0.48
7:LC:195:LYS:O	88:LC:601:HOH:O	2.20	0.48
42:Ln:129:ARG:NH2	42:Ln:133:GLU:OE2	2.45	0.48
48:S2:1217:A:H2'	48:S2:1218:C:C6	2.49	0.48
48:S2:1301:A:OP2	79:Sf:2:GLY:N	2.46	0.48
83:Sz:103:LEU:HD11	83:Sz:106:TYR:CE2	2.48	0.48
2:L5:464:G:O2'	2:L5:465:G:OP1	2.27	0.48
2:L5:677:G:H2'	2:L5:678:C:C6	2.49	0.48
2:L5:3599:A:H2'	2:L5:3600:G:C8	2.48	0.48
2:L5:4859:C:O3'	27:LY:169:ARG:NH1	2.47	0.48
2:L5:5068:G:N2	2:L5:5069:U:O4	2.34	0.48
5:LB:165:HIS:HB3	5:LB:180:LEU:HD13	1.94	0.48
23:LT:115:LYS:HA	23:LT:118:GLU:HG2	1.95	0.48
45:Lz:36:LEU:HD11	45:Lz:69:ARG:NH1	2.26	0.48
2:L5:444:G:H2'	2:L5:445:U:C6	2.48	0.48
2:L5:911:U:H2'	2:L5:912:G:O4'	2.13	0.48
2:L5:1468:C:OP1	29:La:132:ARG:NH2	2.43	0.48
2:L5:1577:G:O2'	2:L5:1612:G:H4'	2.13	0.48
2:L5:4769:G:OP1	27:LY:176:ARG:NH2	2.46	0.48
6:S4:47:H2U:H1'	6:S4:48:U:C5	2.47	0.48
45:Lz:76:MET:HE1	45:Lz:148:VAL:HA	1.94	0.48
83:Sz:140:TYR:HE1	83:Sz:145:CYS:HA	1.77	0.48
2:L5:4381:A:P	51:SB:1:MET:H3	2.36	0.48
3:L8:156:GLY:HA2	3:L8:181:PRO:HD3	1.95	0.48
8:LD:207:VAL:HG13	8:LD:208:GLU:OE1	2.14	0.48
12:LH:37:ASP:CG	12:LH:39:ASN:HD22	2.22	0.48
48:S2:10:G:O2'	52:SC:120:GLN:HG2	2.12	0.48
48:S2:382:C:H2'	48:S2:383:G:C8	2.48	0.48
74:Sa:88:SER:O	74:Sa:92:ARG:HG3	2.12	0.48
2:L5:1251:C:H2'	2:L5:1252:C:C5	2.49	0.48
2:L5:1672:U:H2'	2:L5:1673:U:C6	2.47	0.48
2:L5:1857:C:H2'	2:L5:1858:A:H8	1.78	0.48
48:S2:1098:C:H2'	48:S2:1099:G:C8	2.49	0.48
56:SH:169:LYS:HG3	56:SH:173:PHE:CZ	2.49	0.48
58:SJ:110:LEU:HB2	58:SJ:147:PHE:HB3	1.95	0.48
80:Sg:9:GLY:C	80:Sg:10:THR:HG23	2.39	0.48
1:L1:67:U:H2'	1:L1:68:G:H8	1.79	0.48
2:L5:3893:C:O2'	2:L5:4979:A:N1	2.46	0.48
11:LG:207:VAL:HG21	11:LG:215:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1551:U:OP2	59:SK:9:ARG:NH1	2.47	0.48
68:SU:108:GLU:CD	68:SU:121:ARG:HE	2.22	0.48
80:Sg:283:PRO:O	80:Sg:285:GLN:NE2	2.47	0.48
82:Sy:19:GLN:HE22	82:Sy:88:TRP:CD1	2.31	0.48
83:Sz:82:LYS:NZ	83:Sz:84:SER:OG	2.47	0.48
2:L5:1468:C:H2'	2:L5:1469:C:C6	2.48	0.48
2:L5:1617:G:H1'	2:L5:2513:A:N6	2.29	0.48
2:L5:4258:C:H2'	2:L5:4259:C:H6	1.77	0.48
7:LC:218:ILE:HD13	7:LC:229:LEU:HG	1.94	0.48
48:S2:1020:A:N6	88:S2:2418:HOH:O	2.46	0.48
48:S2:1261:C:O2	79:Sf:10:HIS:NE2	2.46	0.48
55:SG:67:VAL:HG12	55:SG:69:THR:HG22	1.96	0.48
57:SI:88:ASN:OD1	57:SI:205:ARG:NH2	2.47	0.48
2:L5:205:C:N3	2:L5:209:U:H5	2.12	0.48
2:L5:1771:U:H2'	2:L5:1772:C:C6	2.48	0.48
48:S2:875:A:H2'	48:S2:876:C:H6	1.79	0.48
63:SO:120:ALA:HB2	74:Sa:53:ILE:HD13	1.94	0.48
71:SX:117:GLY:C	71:SX:119:ARG:HH21	2.21	0.48
83:Sz:126:CYS:HB3	83:Sz:130:VAL:HG11	1.96	0.48
2:L5:1244:G:H2'	2:L5:1245:C:C6	2.48	0.48
2:L5:1742:A:N1	2:L5:1790:U:O2'	2.43	0.48
2:L5:2424:OMG:HM22	2:L5:2426:U:C6	2.49	0.48
2:L5:3707:U:H2'	2:L5:3708:C:H6	1.78	0.48
2:L5:4188:U:H2'	2:L5:4189:U:C6	2.49	0.48
2:L5:4746:C:H2'	2:L5:4747:C:C6	2.49	0.48
2:L5:4746:C:H2'	2:L5:4747:C:H6	1.79	0.48
5:LB:216:MET:HE3	5:LB:359:ALA:HA	1.96	0.48
48:S2:549:C:H2'	48:S2:550:C:C6	2.49	0.48
56:SH:63:PHE:HA	56:SH:95:ILE:O	2.14	0.48
82:Sy:14:VAL:HG22	82:Sy:126:GLU:HB2	1.96	0.48
1:L1:115:G:H2'	1:L1:116:C:C6	2.49	0.47
2:L5:709:C:OP1	34:Lf:89:ARG:NH2	2.47	0.47
2:L5:730:G:OP2	10:LF:76:ARG:NE	2.37	0.47
2:L5:1696:C:H2'	2:L5:1697:G:C8	2.49	0.47
2:L5:2300:A:N7	7:LC:143:ARG:NH1	2.62	0.47
2:L5:3710:G:N3	2:L5:3711:A:N6	2.62	0.47
2:L5:4174:U:H2'	2:L5:4175:G:C8	2.49	0.47
2:L5:4266:G:N3	2:L5:4266:G:H2'	2.28	0.47
48:S2:17:C:O2'	48:S2:1194:A:N1	2.40	0.47
2:L5:3594:C:H5''	2:L5:3595:U:H5	1.79	0.47
2:L5:4239:A:H2'	2:L5:4240:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LZ:112:ARG:HH11	28:LZ:115:LYS:HD3	1.79	0.47
33:Le:2:VAL:N	33:Le:90:HIS:O	2.47	0.47
47:S1:165:ARG:HG2	47:S1:169:MET:HE3	1.95	0.47
48:S2:495:U:OP1	54:SE:49:ARG:NH1	2.47	0.47
48:S2:1397:U:O4	65:SQ:12:VAL:HA	2.14	0.47
1:L1:112:G:OP1	2:L5:2779:C:O2'	2.20	0.47
2:L5:158:A:N1	2:L5:276:C:O2'	2.44	0.47
2:L5:2293:U:H2'	2:L5:2294:G:C8	2.49	0.47
2:L5:3587:C:H2'	2:L5:3588:C:C6	2.49	0.47
2:L5:3642:A:C4	19:LP:3:LYS:HB3	2.50	0.47
2:L5:4115:G:OP2	2:L5:4115:G:N2	2.34	0.47
23:LT:51:GLY:HA3	23:LT:92:ARG:HG3	1.97	0.47
48:S2:179:C:H2'	48:S2:180:G:O4'	2.14	0.47
48:S2:1606:G:N2	48:S2:1632:G:H1'	2.28	0.47
53:SD:49:LEU:HD12	65:SQ:50:LYS:HG2	1.96	0.47
55:SG:103:ASP:OD1	55:SG:104:ALA:N	2.42	0.47
57:SI:4:SER:OG	57:SI:6:ASP:OD2	2.30	0.47
64:SP:96:VAL:HB	64:SP:120:SER:HB2	1.96	0.47
73:SZ:20:ILE:HG21	73:SZ:98:VAL:HG11	1.94	0.47
74:Sa:46:GLU:O	74:Sa:50:VAL:HG23	2.14	0.47
80:Sg:217:MET:HG2	80:Sg:229:THR:HG23	1.95	0.47
2:L5:1238:A:O2'	10:LF:52:GLU:OE2	2.31	0.47
2:L5:1269:G:O2'	2:L5:1270:A:O5'	2.26	0.47
2:L5:1480:C:H1'	2:L5:1482:G:N2	2.30	0.47
25:LV:21:PRO:HA	25:LV:54:ALA:HA	1.96	0.47
28:LZ:121:ARG:O	28:LZ:124:THR:OG1	2.27	0.47
30:Lb:43:MET:HE2	30:Lb:47:LYS:HZ1	1.79	0.47
51:SB:55:LEU:HB3	51:SB:84:ILE:HG23	1.95	0.47
82:Sy:68:LEU:HD22	82:Sy:72:HIS:HE1	1.78	0.47
1:L1:19:C:H2'	1:L1:20:A:H8	1.79	0.47
2:L5:1564:A:H2'	2:L5:1565:A:C8	2.48	0.47
2:L5:1857:C:H2'	2:L5:1858:A:C8	2.49	0.47
2:L5:3861:A:H2'	2:L5:3862:A:C8	2.50	0.47
32:Ld:36:VAL:HG23	32:Ld:41:ARG:HG2	1.95	0.47
48:S2:634:A:H2'	48:S2:635:G:H8	1.79	0.47
53:SD:30:ILE:HD11	53:SD:41:VAL:HG11	1.96	0.47
72:SY:87:PRO:HG2	72:SY:90:ARG:HG3	1.96	0.47
1:L1:87:G:P	18:LO:7:ARG:HH22	2.38	0.47
2:L5:2412:A:H2'	2:L5:2413:U:C6	2.50	0.47
2:L5:2498:C:H2'	2:L5:2499:C:H6	1.79	0.47
2:L5:2505:C:N4	2:L5:4084:G:H4'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4339:A:H2'	2:L5:4340:U:C6	2.47	0.47
4:L9:39:C:O2'	14:LJ:46:GLN:HB3	2.15	0.47
29:La:100:ILE:HG13	29:La:123:ILE:HB	1.95	0.47
41:Lm:19:LEU:HD23	41:Lm:19:LEU:H	1.79	0.47
48:S2:11:A:N1	48:S2:1200:A:H2	2.12	0.47
56:SH:73:GLN:HA	56:SH:76:GLN:HB2	1.96	0.47
1:L1:6:C:H2'	1:L1:7:U:C6	2.50	0.47
1:L1:8:U:H2'	1:L1:9:A:C8	2.50	0.47
2:L5:175:C:H2'	2:L5:176:G:H8	1.79	0.47
2:L5:451:C:OP2	2:L5:1294:A:N6	2.47	0.47
2:L5:1412:G:H2'	2:L5:1413:C:C6	2.50	0.47
2:L5:1434:G:H2'	2:L5:1435:G:O4'	2.14	0.47
2:L5:1695:U:H2'	2:L5:1696:C:C6	2.50	0.47
2:L5:2362:U:H2'	2:L5:2363:A2M:H8	1.97	0.47
2:L5:3858:C:OP1	88:L5:5401:HOH:O	2.21	0.47
2:L5:4968:A:H2'	2:L5:4969:C:H6	1.79	0.47
7:LC:76:ILE:HD12	7:LC:77:PRO:HD2	1.96	0.47
31:Lc:33:GLN:O	31:Lc:37:MET:HG2	2.15	0.47
48:S2:199:C:O2'	48:S2:201:C:OP2	2.29	0.47
48:S2:452:G:H2'	48:S2:453:C:H6	1.80	0.47
48:S2:524:U:H5''	48:S2:525:A:O4'	2.14	0.47
48:S2:801:PSU:H2'	48:S2:802:A:H8	1.78	0.47
48:S2:1245:G:O2'	48:S2:1492:U:OP1	2.30	0.47
50:SA:144:THR:OG1	50:SA:156:TYR:O	2.27	0.47
54:SE:127:ARG:HG3	54:SE:142:HIS:HA	1.97	0.47
56:SH:11:PRO:HD2	56:SH:44:ASN:HD22	1.80	0.47
56:SH:69:LEU:HG	56:SH:96:ALA:HB2	1.96	0.47
65:SQ:57:LEU:HD11	65:SQ:115:TYR:CD2	2.50	0.47
69:SV:40:ASP:OD1	69:SV:41:LYS:N	2.47	0.47
73:SZ:97:ILE:O	73:SZ:101:ILE:HG13	2.15	0.47
76:Sc:110:THR:OG1	76:Sc:111:ARG:N	2.48	0.47
80:Sg:246:TYR:CE2	80:Sg:261:LEU:HB2	2.50	0.47
80:Sg:259:TRP:CD1	80:Sg:266:ILE:HG12	2.50	0.47
82:Sy:121:LYS:O	82:Sy:125:GLU:HG2	2.14	0.47
2:L5:980:U:H2'	2:L5:981:C:H6	1.80	0.47
2:L5:2632:PSU:H2'	2:L5:2633:U:C6	2.50	0.47
2:L5:4861:G:H2'	2:L5:4862:G:C8	2.47	0.47
3:L8:99:TYR:CD2	3:L8:199:ILE:HD12	2.50	0.47
47:S1:131:ASP:OD1	47:S1:131:ASP:N	2.35	0.47
48:S2:958:G:H2'	48:S2:959:G:C8	2.49	0.47
48:S2:1025:U:H2'	48:S2:1026:C:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SH:181:THR:HG22	56:SH:183:LYS:HG3	1.96	0.47
2:L5:2862:G:H4'	2:L5:3625:G:N7	2.29	0.47
14:LJ:31:ASP:OD2	14:LJ:35:ARG:NH2	2.47	0.47
48:S2:71:G:O6	55:SG:170:ARG:NH1	2.48	0.47
48:S2:920:A:O2'	48:S2:922:A:OP1	2.21	0.47
50:SA:44:ASP:OD1	50:SA:44:ASP:N	2.40	0.47
55:SG:5:ILE:HG12	55:SG:111:LEU:HB2	1.96	0.47
2:L5:27:C:OP1	17:LN:193:ARG:NH1	2.48	0.47
2:L5:2476:G:H2'	2:L5:2477:A:C8	2.49	0.47
29:La:75:LEU:HD11	29:La:133:ALA:HA	1.97	0.47
45:Lz:76:MET:HG3	45:Lz:85:PHE:CD1	2.50	0.47
48:S2:178:C:H2'	48:S2:179:C:H6	1.80	0.47
48:S2:1533:A:N7	48:S2:1604:G:H1'	2.30	0.47
51:SB:56:GLN:HG2	51:SB:88:MET:HE3	1.96	0.47
52:SC:170:TRP:CE2	52:SC:199:PRO:HG3	2.49	0.47
2:L5:934:C:H41	7:LC:350:ARG:NH2	2.13	0.46
2:L5:961:G:O6	15:LK:123:ARG:NH1	2.38	0.46
2:L5:2693:G:H2'	2:L5:2694:G:N2	2.30	0.46
7:LC:340:ILE:HG21	15:LK:50:LEU:HD13	1.97	0.46
11:LG:58:PRO:HD2	11:LG:61:ILE:HD12	1.97	0.46
48:S2:141:A:N6	48:S2:177:G:O2'	2.48	0.46
50:SA:52:LYS:O	50:SA:56:GLU:HG2	2.15	0.46
67:ST:34:LYS:HB3	67:ST:103:LEU:HD23	1.96	0.46
68:SU:42:HIS:NE2	68:SU:43:LYS:HE2	2.30	0.46
71:SX:39:ASN:O	88:SX:301:HOH:O	2.20	0.46
1:L1:115:G:H2'	1:L1:116:C:H6	1.80	0.46
2:L5:1271:G:H22	2:L5:2106:G:H22	1.63	0.46
2:L5:2292:C:H2'	2:L5:2293:U:C6	2.49	0.46
2:L5:4456:OMC:HM21	5:LB:241:PRO:HD3	1.97	0.46
6:S4:11:C:H2'	6:S4:12:C:C6	2.50	0.46
48:S2:909:G:H2'	48:S2:910:G:C8	2.50	0.46
48:S2:1232:PSU:H2'	48:S2:1233:G:C8	2.51	0.46
66:SS:102:THR:O	66:SS:106:LEU:HG	2.15	0.46
68:SU:65:TYR:HB2	68:SU:131:LEU:HD22	1.97	0.46
76:Sc:50:PHE:CZ	76:Sc:58:LEU:HD22	2.50	0.46
2:L5:3720:G:H22	2:L5:3733:A:H2	1.63	0.46
2:L5:4220:6MZ:O5'	2:L5:4220:6MZ:H8	2.15	0.46
2:L5:4453:C:H6	2:L5:4453:C:O5'	1.98	0.46
2:L5:4748:U:H5''	34:Lf:54:LYS:NZ	2.30	0.46
3:L8:253:TYR:OH	4:L9:117:G:OP1	2.29	0.46
15:LK:213:THR:H	15:LK:216:TYR:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:17:C:H2'	48:S2:18:C:C6	2.50	0.46
48:S2:634:A:H2'	48:S2:635:G:C8	2.50	0.46
48:S2:1289:U:H2'	48:S2:1290:G:C8	2.50	0.46
48:S2:1434:C:H5''	73:SZ:49:LYS:HZ3	1.80	0.46
65:SQ:130:LYS:NZ	65:SQ:134:GLY:O	2.45	0.46
2:L5:162:A:H2'	2:L5:163:A:C8	2.50	0.46
2:L5:914:U:H4'	2:L5:915:A:O5'	2.16	0.46
2:L5:1567:U:H2'	2:L5:1568:C:C6	2.50	0.46
2:L5:2411:C:H2'	2:L5:2412:A:C8	2.51	0.46
2:L5:2515:G:OP1	35:Lg:37:LYS:NZ	2.32	0.46
11:LG:106:THR:CG2	11:LG:107:LYS:N	2.79	0.46
31:Lc:38:ILE:HD11	31:Lc:46:VAL:HG21	1.98	0.46
36:Lh:50:ASP:OD2	36:Lh:56:GLN:NE2	2.38	0.46
45:Lz:101:LYS:NZ	45:Lz:102:MET:O	2.33	0.46
48:S2:528:A:H2'	48:S2:529:A:H8	1.76	0.46
48:S2:1285:G:H3'	48:S2:1286:G:C5'	2.45	0.46
54:SE:11:ARG:HA	54:SE:28:ALA:HB2	1.96	0.46
55:SG:157:VAL:HB	55:SG:176:ILE:HD11	1.96	0.46
56:SH:146:VAL:HG12	70:SW:42:MET:HE1	1.98	0.46
59:SK:193:ASP:OD2	59:SK:198:ILE:CG1	2.48	0.46
66:SS:127:ASN:OD1	66:SS:127:ASN:N	2.49	0.46
2:L5:162:A:H2'	2:L5:163:A:H8	1.80	0.46
2:L5:450:G:H2'	2:L5:451:C:C6	2.50	0.46
2:L5:757:G:H2'	2:L5:758:G:C8	2.48	0.46
2:L5:1942:A:H2'	2:L5:1943:A:H8	1.79	0.46
2:L5:2745:A:H2'	2:L5:2746:A:C8	2.50	0.46
8:LD:30:ARG:HG2	88:LD:462:HOH:O	2.16	0.46
22:LS:81:TRP:CE3	22:LS:128:LYS:HG3	2.51	0.46
47:S1:155:TYR:OH	48:S2:989:C:OP2	2.28	0.46
48:S2:45:A:N1	48:S2:480:G:O2'	2.44	0.46
48:S2:1520:G:O2'	48:S2:1521:C:OP1	2.26	0.46
48:S2:1643:PSU:H2'	48:S2:1644:C:C6	2.51	0.46
48:S2:1690:U:H2'	48:S2:1691:U:C6	2.50	0.46
51:SB:140:ASP:OD1	76:Sc:66:LYS:HG3	2.16	0.46
51:SB:162:LYS:HE2	51:SB:162:LYS:HB2	1.63	0.46
58:SJ:87:LEU:HD13	58:SJ:100:LEU:HD21	1.96	0.46
64:SP:28:MET:HB3	64:SP:32:GLN:HB2	1.97	0.46
65:SQ:112:LEU:HD22	65:SQ:119:LEU:HD13	1.97	0.46
68:SU:39:LEU:HG	68:SU:47:PRO:HG3	1.98	0.46
2:L5:10:A:H2'	2:L5:11:G:C8	2.51	0.46
2:L5:1242:G:H1'	30:Lb:120:ARG:HE	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4247:G:H5'	3:L8:4:VAL:HG21	1.97	0.46
4:L9:3:C:H2'	4:L9:4:U:C6	2.51	0.46
26:LW:117:LYS:HE2	48:S2:327:G:H1'	1.96	0.46
48:S2:29:G:OP1	71:SX:124:LYS:NZ	2.39	0.46
57:SI:141:ARG:O	57:SI:146:GLN:NE2	2.49	0.46
1:L1:66:A:H2'	1:L1:67:U:C6	2.50	0.46
2:L5:464:G:HO2'	2:L5:465:G:P	2.38	0.46
2:L5:981:C:OP2	15:LK:71:ARG:NH2	2.47	0.46
2:L5:1356:U:H2'	2:L5:1357:C:C6	2.51	0.46
2:L5:1633:G:H5'	2:L5:1634:A:OP1	2.15	0.46
2:L5:1920:C:H3'	2:L5:1921:C:H5''	1.97	0.46
2:L5:3669:G:H21	2:L5:3672:G:N2	2.13	0.46
12:LH:103:VAL:HG13	12:LH:112:VAL:HG23	1.96	0.46
12:LH:173:ARG:HB3	43:Lo:127:VAL:HG23	1.97	0.46
39:Lk:24:LYS:HD3	39:Lk:69:LEU:HD11	1.97	0.46
48:S2:818:A:OP1	58:SJ:80:ARG:NH1	2.44	0.46
50:SA:184:ARG:HD3	50:SA:191:ARG:HG3	1.98	0.46
52:SC:188:CYS:SG	52:SC:238:LYS:HE3	2.55	0.46
56:SH:45:ILE:HG22	56:SH:64:VAL:HG12	1.97	0.46
59:SK:69:LEU:HA	59:SK:72:VAL:HG22	1.97	0.46
2:L5:685:C:O2'	2:L5:686:A:N7	2.42	0.46
2:L5:1721:G:H2'	2:L5:1722:C:C6	2.50	0.46
2:L5:4771:C:H2'	2:L5:4772:C:C6	2.50	0.46
2:L5:4928:C:H2'	2:L5:4929:C:H6	1.81	0.46
20:LQ:143:GLU:HA	20:LQ:146:LEU:HG	1.98	0.46
21:LR:166:THR:HG21	48:S2:873:G:C5'	2.46	0.46
48:S2:943:U:C2	48:S2:944:A:C8	3.03	0.46
48:S2:1285:G:H1	82:Sy:57:ASP:H	1.64	0.46
48:S2:1286:G:N2	48:S2:1312:G:O2'	2.45	0.46
80:Sg:234:ASP:OD1	80:Sg:235:ILE:N	2.49	0.46
80:Sg:256:ILE:O	80:Sg:270:LEU:HD12	2.16	0.46
2:L5:300:A:H2'	2:L5:301:G:H8	1.81	0.46
2:L5:3861:A:H2'	2:L5:3862:A:H8	1.81	0.46
2:L5:4457:PSU:H1'	5:LB:252:ALA:HB3	1.98	0.46
2:L5:4862:G:H2'	2:L5:4863:G:C8	2.51	0.46
2:L5:4906:C:H2'	2:L5:4907:G:C8	2.51	0.46
37:Li:59:GLU:O	37:Li:63:VAL:HG22	2.16	0.46
37:Li:65:LYS:HB3	37:Li:68:ARG:HB3	1.98	0.46
39:Lk:55:LYS:O	39:Lk:58:GLN:HG2	2.15	0.46
48:S2:194:C:H2'	48:S2:195:C:C6	2.51	0.46
59:SK:65:ARG:O	59:SK:68:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sz:95:ARG:HG2	83:Sz:96:LYS:N	2.31	0.46
83:Sz:105:TYR:HA	83:Sz:117:LEU:HD12	1.97	0.46
1:L1:82:A:H61	9:LE:50:ARG:HH22	1.65	0.46
2:L5:28:C:H4'	2:L5:61:A:H4'	1.98	0.46
2:L5:1775:A:H2'	2:L5:1776:A:O4'	2.16	0.46
2:L5:4254:G:H2'	2:L5:4254:G:N3	2.30	0.46
7:LC:190:ARG:O	7:LC:195:LYS:HD3	2.15	0.46
26:LW:117:LYS:HD2	48:S2:327:G:C8	2.45	0.46
30:Lb:122:LYS:HB2	30:Lb:122:LYS:HE3	1.79	0.46
37:Li:29:ARG:HE	37:Li:32:ARG:NH2	2.15	0.46
48:S2:416:U:H2'	48:S2:417:C:O4'	2.14	0.46
50:SA:177:MET:SD	50:SA:180:ARG:NH2	2.89	0.46
51:SB:28:ILE:HD13	51:SB:47:ASP:HB3	1.98	0.46
51:SB:228:ASP:OD1	51:SB:229:LEU:N	2.47	0.46
70:SW:8:ALA:HA	70:SW:74:VAL:CG1	2.44	0.46
71:SX:98:ASP:OD2	71:SX:140:ARG:NH1	2.37	0.46
82:Sy:61:TYR:HA	82:Sy:64:LEU:HB3	1.98	0.46
2:L5:1566:C:H2'	2:L5:1567:U:H6	1.81	0.45
2:L5:4345:C:H2'	2:L5:4346:U:C6	2.51	0.45
12:LH:112:VAL:HG12	12:LH:128:MET:HE3	1.98	0.45
14:LJ:136:ARG:HG3	14:LJ:157:ILE:HD11	1.98	0.45
16:LM:31:ILE:CG2	16:LM:35:ARG:NH2	2.77	0.45
48:S2:575:A:H2'	48:S2:576:A2M:O4'	2.16	0.45
48:S2:1328:OMG:H4'	83:Sz:78:LYS:HE3	1.98	0.45
51:SB:49:LYS:O	51:SB:52:ILE:HG22	2.16	0.45
53:SD:68:ILE:HD11	53:SD:151:ILE:HD11	1.98	0.45
53:SD:78:MET:HB2	53:SD:159:ARG:NH2	2.31	0.45
56:SH:65:PRO:HG2	56:SH:68:GLN:HB2	1.98	0.45
2:L5:175:C:H2'	2:L5:176:G:C8	2.50	0.45
2:L5:677:G:H2'	2:L5:678:C:H6	1.81	0.45
2:L5:1567:U:H2'	2:L5:1568:C:H6	1.80	0.45
2:L5:2500:U:H2'	2:L5:2501:C:C6	2.52	0.45
2:L5:4635:A:H3'	2:L5:4636:PSU:H4'	1.98	0.45
30:Lb:43:MET:HE2	30:Lb:47:LYS:NZ	2.31	0.45
31:Lc:47:ILE:HB	31:Lc:94:LEU:HG	1.97	0.45
48:S2:436:OMG:OP2	88:S2:2101:HOH:O	2.21	0.45
53:SD:19:LEU:HD21	53:SD:69:VAL:HG21	1.99	0.45
2:L5:1359:G:N7	88:L5:5570:HOH:O	2.36	0.45
2:L5:2264:C:H2'	2:L5:2265:G:O4'	2.17	0.45
2:L5:2461:G:H2'	2:L5:2462:C:C6	2.51	0.45
2:L5:4358:U:OP1	20:LQ:194:ILE:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4524:G:C2	5:LB:252:ALA:HB1	2.50	0.45
9:LE:130:LYS:HD3	9:LE:130:LYS:HA	1.70	0.45
16:LM:99:GLU:HG2	16:LM:103:LYS:NZ	2.31	0.45
17:LN:119:TYR:CE1	17:LN:131:GLU:HB2	2.51	0.45
48:S2:344:U:H2'	48:S2:345:U:C6	2.52	0.45
48:S2:468:A2M:HM'3	48:S2:468:A2M:H1'	1.80	0.45
48:S2:1589:A:H2'	48:S2:1590:C:H6	1.81	0.45
48:S2:1681:U:H2'	48:S2:1682:C:C6	2.52	0.45
51:SB:112:GLN:OE1	51:SB:114:VAL:CG2	2.64	0.45
60:SL:78:THR:HG21	60:SL:89:ARG:HB2	1.97	0.45
2:L5:659:G:H2'	2:L5:660:A:C8	2.51	0.45
2:L5:4885:U:H2'	2:L5:4886:C:O4'	2.17	0.45
4:L9:3:C:H2'	4:L9:4:U:H6	1.81	0.45
8:LD:109:GLU:H	8:LD:109:GLU:CD	2.24	0.45
10:LF:166:ARG:NH2	10:LF:212:LYS:HD3	2.31	0.45
48:S2:814:PSU:OP2	88:S2:2102:HOH:O	2.21	0.45
48:S2:1390:U:H2'	48:S2:1391:OMC:H6	1.81	0.45
48:S2:1690:U:H2'	48:S2:1691:U:H6	1.81	0.45
51:SB:51:GLU:HA	51:SB:54:LYS:HD2	1.98	0.45
51:SB:185:THR:HG23	51:SB:188:ARG:HH21	1.81	0.45
64:SP:18:ARG:HB2	64:SP:36:LEU:HD22	1.98	0.45
65:SQ:102:GLU:HB2	80:Sg:55:PRO:O	2.15	0.45
69:SV:22:ARG:NH2	70:SW:19:LYS:O	2.49	0.45
2:L5:464:G:H2'	2:L5:465:G:C8	2.51	0.45
2:L5:3813:A:N3	2:L5:4538:G:O2'	2.40	0.45
2:L5:3917:A:H2'	2:L5:3918:G:C8	2.51	0.45
2:L5:4536:OMC:HM22	2:L5:4537:C:O4'	2.16	0.45
2:L5:4911:A:OP1	5:LB:97:ARG:NH2	2.40	0.45
18:LO:6:ALA:O	18:LO:10:ARG:HG3	2.17	0.45
48:S2:1395:C:O2'	48:S2:1396:A:H5'	2.17	0.45
48:S2:1798:C:H2'	48:S2:1799:G:O4'	2.16	0.45
55:SG:45:TRP:HZ3	55:SG:113:ILE:HD11	1.81	0.45
76:Sc:56:ASP:O	76:Sc:60:LYS:HB2	2.17	0.45
76:Sc:58:LEU:HD21	76:Sc:87:ALA:HB1	1.98	0.45
80:Sg:184:LEU:HD21	80:Sg:187:ASN:ND2	2.25	0.45
2:L5:1244:G:H2'	2:L5:1245:C:H6	1.81	0.45
2:L5:4251:A:O2'	14:LJ:110:GLN:OE1	2.32	0.45
2:L5:4441:A:H4'	45:Lz:102:MET:HE3	1.98	0.45
2:L5:4538:G:H2'	2:L5:4539:U:C6	2.51	0.45
2:L5:4749:C:H2'	2:L5:4750:G:O4'	2.17	0.45
12:LH:59:LYS:HE3	12:LH:66:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ld:91:LYS:CG	32:Ld:92:ARG:H	2.29	0.45
48:S2:1084:A:OP1	48:S2:1858:G:O2'	2.31	0.45
48:S2:1221:G:H2'	48:S2:1222:G:C8	2.52	0.45
48:S2:1673:U:H2'	48:S2:1674:G:O4'	2.17	0.45
65:SQ:34:VAL:HG22	65:SQ:70:VAL:HB	1.99	0.45
76:Sc:50:PHE:HB3	76:Sc:55:TYR:HB2	1.99	0.45
1:L1:6:C:H2'	1:L1:7:U:H6	1.81	0.45
2:L5:2045:G:O6	2:L5:3870:C:O2'	2.31	0.45
2:L5:2411:C:H2'	2:L5:2412:A:H8	1.81	0.45
2:L5:2654:C:H2'	2:L5:2655:C:H6	1.81	0.45
2:L5:2793:G:O6	88:L5:5402:HOH:O	2.21	0.45
20:LQ:91:ALA:HB1	20:LQ:96:ILE:HB	1.98	0.45
21:LR:176:ARG:NH2	48:S2:909:G:H5''	2.32	0.45
48:S2:85:A:H2'	48:S2:86:C:C6	2.52	0.45
48:S2:188:C:H2'	48:S2:189:U:C6	2.51	0.45
80:Sg:128:THR:HG22	80:Sg:143:GLN:HG2	1.98	0.45
2:L5:990:C:C4	2:L5:992:C:H1'	2.52	0.45
2:L5:2335:C:H2'	2:L5:2336:G:H8	1.82	0.45
2:L5:4906:C:H2'	2:L5:4907:G:H8	1.82	0.45
2:L5:4968:A:H2'	2:L5:4969:C:C6	2.52	0.45
4:L9:58:A:H2'	4:L9:59:G:C8	2.52	0.45
10:LF:175:ILE:HD11	10:LF:187:MET:SD	2.57	0.45
11:LG:159:HIS:ND1	11:LG:185:LYS:HA	2.32	0.45
15:LK:201:ILE:HD11	15:LK:267:LEU:HD21	1.99	0.45
32:Ld:37:GLY:O	32:Ld:41:ARG:HG3	2.17	0.45
48:S2:186:C:H2'	48:S2:187:G:C8	2.51	0.45
48:S2:1306:U:H2'	48:S2:1307:U:O4'	2.17	0.45
50:SA:76:VAL:HG23	50:SA:87:VAL:HG13	1.99	0.45
56:SH:51:ILE:HD11	56:SH:176:VAL:HG22	1.98	0.45
74:Sa:24:THR:HG23	74:Sa:72:HIS:H	1.82	0.45
78:Se:97:GLU:H	78:Se:97:GLU:CD	2.25	0.45
2:L5:385:A:N3	2:L5:387:G:H5''	2.32	0.45
2:L5:1340:OMC:HM22	2:L5:1341:U:O4'	2.17	0.45
2:L5:1431:C:H2'	2:L5:1432:G:O4'	2.17	0.45
2:L5:1439:C:H42	2:L5:2105:A:N6	2.15	0.45
2:L5:1907:A:H2'	2:L5:1908:A:C8	2.51	0.45
2:L5:3641:U:C6	2:L5:3645:U:C4	3.05	0.45
2:L5:4133:C:OP1	2:L5:4144:C:N4	2.41	0.45
2:L5:4460:U:H2'	2:L5:4461:C:C6	2.51	0.45
2:L5:4734:A:H2'	2:L5:4735:G:C8	2.52	0.45
30:Lb:117:ARG:HA	30:Lb:117:ARG:HD3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:107:A:H2'	48:S2:108:G:H8	1.81	0.45
53:SD:102:LEU:HD21	76:Sc:66:LYS:O	2.17	0.45
55:SG:85:ARG:O	55:SG:87:ARG:NH1	2.50	0.45
56:SH:130:LEU:HD21	56:SH:156:VAL:HG21	1.97	0.45
57:SI:83:TYR:HA	57:SI:205:ARG:NH1	2.32	0.45
59:SK:28:GLU:HG2	59:SK:69:LEU:HD21	1.99	0.45
67:ST:124:ARG:NE	67:ST:130:ARG:O	2.42	0.45
82:Sy:92:CYS:HB2	82:Sy:103:VAL:HG23	1.99	0.45
83:Sz:132:MET:HG2	83:Sz:141:CYS:HA	1.98	0.45
2:L5:465:G:HO2'	2:L5:466:A:P	2.39	0.45
2:L5:1697:G:H2'	2:L5:1698:C:O4'	2.16	0.45
2:L5:1866:U:H2'	2:L5:1867:A:O4'	2.17	0.45
2:L5:3748:A:H5''	8:LD:243:THR:HB	1.99	0.45
2:L5:3873:G:H2'	2:L5:3874:G:C8	2.52	0.45
2:L5:4745:G:H1	2:L5:4955:A:H61	1.64	0.45
2:L5:5026:U:H4'	2:L5:5027:C:H5'	1.98	0.45
48:S2:383:G:O2'	60:SL:133:PRO:O	2.34	0.45
48:S2:912:C:H4'	48:S2:913:A:OP2	2.16	0.45
48:S2:1836:G:OP2	48:S2:1839:U:O2'	2.35	0.45
50:SA:180:ARG:HD3	50:SA:184:ARG:CZ	2.47	0.45
55:SG:48:TYR:OH	55:SG:119:LYS:O	2.20	0.45
64:SP:81:ARG:NH2	64:SP:117:GLY:O	2.50	0.45
67:ST:15:VAL:HB	67:ST:20:ILE:HD13	1.98	0.45
68:SU:130:ASP:O	68:SU:134:ILE:HG12	2.17	0.45
2:L5:1438:U:O2	2:L5:2099:G:H3'	2.17	0.44
21:LR:176:ARG:HH22	48:S2:910:G:P	2.40	0.44
36:Lh:40:HIS:CE1	36:Lh:157:VAL:HB	2.53	0.44
48:S2:90:G:N7	88:S2:2264:HOH:O	2.36	0.44
48:S2:559:G:O2'	48:S2:560:A:H5''	2.17	0.44
48:S2:804:U:H2'	48:S2:805:U:H6	1.82	0.44
48:S2:986:G:N7	88:S2:2265:HOH:O	2.36	0.44
48:S2:1265:A:H5'	48:S2:1266:C:OP2	2.17	0.44
48:S2:1589:A:H2'	48:S2:1590:C:C6	2.52	0.44
54:SE:176:ASP:OD1	54:SE:176:ASP:N	2.49	0.44
59:SK:8:LYS:HG2	73:SZ:61:LEU:HD11	1.99	0.44
2:L5:717:U:H2'	2:L5:718:C:C6	2.52	0.44
2:L5:2520:C:H2'	2:L5:2521:G:H8	1.82	0.44
2:L5:3733:A:H2'	2:L5:3734:PSU:O4'	2.17	0.44
2:L5:4133:C:P	2:L5:4144:C:H42	2.40	0.44
2:L5:4578:G:H2'	2:L5:4579:PSU:C6	2.53	0.44
4:L9:57:C:H2'	4:L9:58:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LC:41:HIS:CE1	7:LC:45:ARG:HD3	2.51	0.44
17:LN:178:HIS:HA	17:LN:181:HIS:NE2	2.33	0.44
48:S2:302:A:N3	57:SI:64:ASN:ND2	2.65	0.44
48:S2:530:U:H2'	48:S2:531:A:H8	1.83	0.44
50:SA:7:VAL:HG21	69:SV:42:VAL:O	2.17	0.44
53:SD:102:LEU:CD2	76:Sc:67:LEU:HA	2.47	0.44
56:SH:65:PRO:HB2	56:SH:67:PRO:HD2	1.98	0.44
66:SS:57:LEU:HD13	66:SS:69:ILE:HD11	1.97	0.44
80:Sg:188:HIS:HB3	80:Sg:219:TRP:CZ3	2.52	0.44
1:L1:144:U:H2'	1:L1:145:C:H6	1.82	0.44
2:L5:211:G:H5'	2:L5:234:G:O2'	2.17	0.44
2:L5:444:G:H2'	2:L5:445:U:H6	1.82	0.44
2:L5:922:C:H2'	2:L5:923:C:O4'	2.17	0.44
2:L5:3865:A:H2'	2:L5:3866:C:C6	2.53	0.44
2:L5:4589:A:N1	2:L5:4621:C:O2'	2.46	0.44
3:L8:263:LYS:H	3:L8:263:LYS:HG2	1.58	0.44
16:LM:6:PHE:H	16:LM:11:ARG:NH2	2.15	0.44
48:S2:160:U:O2'	48:S2:161:U:H3'	2.17	0.44
57:SI:57:ALA:HB2	57:SI:183:GLY:HA2	1.98	0.44
62:SN:114:ARG:NH1	88:SN:202:HOH:O	2.44	0.44
2:L5:1284:G:O2'	2:L5:1285:U:H5''	2.17	0.44
2:L5:1824:G:H5''	23:LT:35:LYS:HE2	1.99	0.44
2:L5:4458:C:H2'	2:L5:4459:U:C6	2.52	0.44
2:L5:4652:G:H2'	2:L5:4653:C:C6	2.52	0.44
5:LB:258:HIS:HA	5:LB:259:PRO:C	2.43	0.44
12:LH:27:VAL:HG12	12:LH:84:VAL:HG21	2.00	0.44
41:Lm:24:ASP:OD1	41:Lm:26:THR:OG1	2.30	0.44
45:Lz:153:ARG:HA	45:Lz:156:LYS:HE2	2.00	0.44
48:S2:532:C:H2'	48:S2:533:A:C8	2.53	0.44
48:S2:909:G:H2'	48:S2:910:G:H8	1.83	0.44
48:S2:1407:U:H4'	65:SQ:71:ARG:NH2	2.32	0.44
48:S2:1415:C:O2'	68:SU:132:ASP:OD2	2.23	0.44
48:S2:1421:A:OP1	48:S2:1422:G:N2	2.50	0.44
48:S2:1662:U:O4	48:S2:1663:A:N6	2.45	0.44
48:S2:1736:G:H2'	48:S2:1737:G:C8	2.52	0.44
50:SA:8:LEU:HD11	69:SV:39:VAL:HG21	1.99	0.44
83:Sz:103:LEU:HD12	83:Sz:104:LYS:CA	2.46	0.44
2:L5:512:U:OP2	20:LQ:165:LYS:HD2	2.18	0.44
2:L5:1578:U:OP1	2:L5:3637:PSU:O2'	2.36	0.44
2:L5:1846:G:H2'	2:L5:1847:C:C6	2.53	0.44
2:L5:4928:C:H2'	2:L5:4929:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LD:66:PRO:HG2	8:LD:67:TYR:CE2	2.53	0.44
20:LQ:81:LEU:HD11	20:LQ:98:VAL:HG22	2.00	0.44
32:Ld:91:LYS:CG	32:Ld:92:ARG:N	2.81	0.44
35:Lg:41:ALA:O	35:Lg:52:ARG:HD3	2.18	0.44
48:S2:1378:A:H4'	48:S2:1379:A:O5'	2.17	0.44
50:SA:132:GLN:HB3	50:SA:133:PRO:HD3	2.00	0.44
59:SK:67:ARG:HB3	61:SM:93:THR:HG22	2.00	0.44
76:Sc:98:LYS:HB3	76:Sc:110:THR:HG23	1.98	0.44
80:Sg:17:TRP:CE2	80:Sg:303:THR:HG23	2.52	0.44
2:L5:1328:G:O2'	2:L5:2349:A:OP1	2.29	0.44
2:L5:2414:G:H2'	2:L5:2415:OMU:H6	2.00	0.44
2:L5:2495:U:H2'	2:L5:2496:G:C8	2.42	0.44
2:L5:2562:G:O2'	2:L5:2565:A:N6	2.50	0.44
2:L5:2836:A:H4'	5:LB:229:LYS:HA	1.98	0.44
31:Lc:34:THR:HG23	31:Lc:95:ALA:HB2	1.99	0.44
36:Lh:42:ARG:NH2	36:Lh:159:LYS:HD3	2.33	0.44
39:Lk:12:LEU:HD22	39:Lk:16:ARG:HH12	1.82	0.44
44:Lp:8:VAL:O	44:Lp:11:VAL:HG22	2.18	0.44
48:S2:158:A:H2'	48:S2:159:A2M:O4'	2.17	0.44
48:S2:178:C:H2'	48:S2:179:C:C6	2.52	0.44
48:S2:1802:C:H2'	48:S2:1803:U:C6	2.52	0.44
61:SM:15:LEU:HD23	61:SM:79:LEU:HD11	1.99	0.44
2:L5:25:A:H2'	2:L5:26:C:C6	2.52	0.44
2:L5:52:G:H4'	2:L5:1529:G:H4'	2.00	0.44
2:L5:947:C:H5''	15:LK:51:VAL:HG21	1.98	0.44
2:L5:1272:C:H4'	2:L5:1273:G:OP1	2.18	0.44
2:L5:1333:A:H2'	2:L5:1334:A:C8	2.53	0.44
2:L5:1480:C:O2'	2:L5:1482:G:OP2	2.29	0.44
2:L5:2876:OMG:C8	44:Lp:16:THR:HG22	2.53	0.44
2:L5:3930:U:H2'	2:L5:3931:C:C6	2.53	0.44
2:L5:4258:C:H5'	14:LJ:68:ILE:HD11	2.00	0.44
2:L5:4324:A:H2'	2:L5:4325:A:C8	2.53	0.44
21:LR:67:THR:O	21:LR:71:ARG:HG3	2.18	0.44
48:S2:841:G:H2'	48:S2:842:C:C6	2.52	0.44
70:SW:8:ALA:CA	70:SW:74:VAL:HG11	2.47	0.44
74:Sa:38:LYS:NZ	74:Sa:71:LEU:HD12	2.33	0.44
80:Sg:258:ILE:HD11	80:Sg:270:LEU:HD11	2.00	0.44
2:L5:62:A:N3	2:L5:77:U:O2'	2.42	0.44
2:L5:4653:C:H2'	2:L5:4654:C:C6	2.53	0.44
3:L8:37:VAL:HG12	3:L8:50:ARG:HD3	2.00	0.44
41:Lm:18:VAL:HG21	41:Lm:77:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:639:C:H2'	48:S2:640:A:C8	2.53	0.44
48:S2:1113:A:H2'	48:S2:1114:U:H6	1.83	0.44
48:S2:1619:A:P	64:SP:47:ARG:HE	2.40	0.44
48:S2:1839:U:H2'	48:S2:1840:U:C6	2.53	0.44
68:SU:129:ARG:O	68:SU:133:ARG:HG3	2.17	0.44
80:Sg:85:GLY:HA2	80:Sg:108:VAL:HG23	1.99	0.44
2:L5:182:G:H1	2:L5:254:G:N2	2.06	0.44
2:L5:266:C:H2'	2:L5:267:G:H8	1.83	0.44
2:L5:2708:U:H4'	2:L5:2709:C:H5''	1.99	0.44
2:L5:3648:A:H1'	2:L5:3785:A2M:N6	2.33	0.44
2:L5:4345:C:H2'	2:L5:4346:U:H6	1.82	0.44
2:L5:4488:A:H4'	2:L5:4489:G:C8	2.53	0.44
2:L5:4584:A:H2'	2:L5:4585:U:O4'	2.17	0.44
15:LK:150:LEU:HD11	15:LK:164:PHE:HB2	2.00	0.44
26:LW:97:LYS:HG2	26:LW:101:ARG:NH1	2.33	0.44
42:Ln:83:THR:O	42:Ln:87:MET:HG2	2.18	0.44
48:S2:1736:G:H2'	48:S2:1737:G:H8	1.83	0.44
51:SB:81:ARG:HH22	51:SB:82:LYS:HZ3	1.66	0.44
80:Sg:144:ASP:O	80:Sg:145:GLU:HG2	2.18	0.44
2:L5:1458:C:H5''	38:Lj:69:LYS:HD2	2.00	0.43
2:L5:1563:A:N6	48:S2:1028:A:N1	2.66	0.43
2:L5:2079:G:H2'	2:L5:2080:U:C6	2.53	0.43
2:L5:2529:A:O2'	2:L5:2531:C:OP2	2.36	0.43
2:L5:4459:U:H2'	2:L5:4460:U:C6	2.53	0.43
2:L5:4734:A:H2'	2:L5:4735:G:H8	1.83	0.43
2:L5:4935:C:H2'	2:L5:4936:G:H8	1.81	0.43
14:LJ:10:ASN:HB3	14:LJ:11:PRO:HD3	2.00	0.43
14:LJ:35:ARG:O	14:LJ:39:VAL:HG23	2.17	0.43
48:S2:84:A:N3	48:S2:150:A:O2'	2.51	0.43
48:S2:352:U:H2'	48:S2:353:C:C6	2.53	0.43
48:S2:945:U:H2'	48:S2:946:U:C6	2.53	0.43
53:SD:71:ARG:NH2	53:SD:148:ASN:OD1	2.47	0.43
59:SK:125:PHE:O	59:SK:128:GLU:HG2	2.18	0.43
66:SS:98:VAL:HG13	66:SS:102:THR:HB	2.00	0.43
2:L5:288:G:H2'	2:L5:289:C:C6	2.53	0.43
2:L5:1446:C:H2'	2:L5:1447:C:O4'	2.18	0.43
2:L5:1558:A:H2'	2:L5:1559:G:C8	2.53	0.43
2:L5:1588:U:H2'	2:L5:1589:C:C6	2.53	0.43
2:L5:2326:G:H5''	13:LI:127:ALA:HB2	1.99	0.43
2:L5:4192:A:H2'	2:L5:4193:C:H6	1.83	0.43
2:L5:4273:A:H2'	2:L5:4274:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L8:60:ILE:HB	3:L8:80:ALA:HB2	2.00	0.43
15:LK:95:PRO:HA	15:LK:104:THR:HG22	2.00	0.43
28:LZ:53:VAL:HG12	28:LZ:57:MET:HE1	1.99	0.43
48:S2:432:G:H2'	48:S2:433:A:C8	2.53	0.43
48:S2:573:U:O2	48:S2:576:A2M:H8	2.18	0.43
48:S2:1148:A:H4'	48:S2:1149:A:O4'	2.18	0.43
48:S2:1416:C:OP1	68:SU:129:ARG:HG3	2.17	0.43
48:S2:1425:G:H21	68:SU:5:THR:CG2	2.31	0.43
48:S2:1785:C:H2'	48:S2:1786:U:O4'	2.18	0.43
50:SA:61:ALA:HB1	50:SA:145:ILE:HD13	2.00	0.43
73:SZ:18:HIS:ND1	73:SZ:116:ILE:HD13	2.33	0.43
73:SZ:31:SER:O	73:SZ:35:VAL:HG23	2.18	0.43
80:Sg:195:LEU:HA	80:Sg:211:GLY:HA3	1.99	0.43
2:L5:1251:C:H2'	2:L5:1252:C:C6	2.54	0.43
2:L5:4633:G:N2	88:L5:6094:HOH:O	2.51	0.43
10:LF:124:LYS:HB2	10:LF:124:LYS:HE3	1.88	0.43
48:S2:1456:G:H2'	48:S2:1457:U:C6	2.53	0.43
50:SA:80:ARG:HH22	50:SA:166:LYS:HA	1.83	0.43
52:SC:191:VAL:HG11	52:SC:236:PHE:HA	2.00	0.43
53:SD:32:ASP:O	53:SD:36:GLN:HG3	2.19	0.43
56:SH:162:GLN:O	56:SH:166:VAL:HG22	2.18	0.43
61:SM:90:VAL:HB	61:SM:94:LEU:HB2	2.00	0.43
82:Sy:123:VAL:O	82:Sy:126:GLU:HG2	2.18	0.43
1:L1:106:G:H4'	1:L1:137:A:H5'	2.00	0.43
2:L5:9:C:OP2	17:LN:40:PRO:HG3	2.17	0.43
2:L5:1475:G:H2'	2:L5:1476:C:C6	2.54	0.43
2:L5:4114:C:O2'	2:L5:4115:G:H5'	2.17	0.43
27:LY:185:VAL:O	27:LY:189:ILE:HG12	2.18	0.43
34:Lf:106:TYR:HA	34:Lf:107:PRO:C	2.43	0.43
35:Lg:82:MET:HE2	35:Lg:82:MET:HB3	1.72	0.43
48:S2:944:A:H5''	63:SO:134:PRO:HB3	2.01	0.43
48:S2:1013:U:OP1	48:S2:1129:G:O2'	2.36	0.43
48:S2:1299:A:H2	79:Sf:6:LEU:HD11	1.83	0.43
48:S2:1587:G:OP1	48:S2:1587:G:N2	2.49	0.43
53:SD:80:GLY:HA2	53:SD:83:ASN:ND2	2.33	0.43
59:SK:179:GLN:OE1	59:SK:179:GLN:N	2.51	0.43
65:SQ:51:LEU:HD12	65:SQ:51:LEU:HA	1.85	0.43
80:Sg:191:HIS:NE2	80:Sg:209:SER:OG	2.47	0.43
2:L5:407:A:O2'	2:L5:410:A:OP1	2.21	0.43
2:L5:925:C:H2'	2:L5:926:G:H4'	1.99	0.43
2:L5:1441:C:O2	2:L5:2104:G:N2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1720:C:H2'	2:L5:1721:G:O4'	2.18	0.43
2:L5:2557:G:H2'	2:L5:2558:C:C6	2.53	0.43
2:L5:2611:A:H2'	2:L5:2612:G:C8	2.54	0.43
2:L5:2706:G:N2	2:L5:2708:U:H5'	2.33	0.43
2:L5:4587:G:OP1	27:LY:61:ARG:HD2	2.19	0.43
3:L8:191:ASN:HB3	3:L8:194:VAL:HG13	1.99	0.43
9:LE:113:LYS:HE3	9:LE:113:LYS:HB2	1.90	0.43
11:LG:80:ILE:HD11	17:LN:18:VAL:HG23	2.00	0.43
48:S2:140:U:O2'	48:S2:143:U:OP1	2.36	0.43
48:S2:875:A:H2'	48:S2:876:C:C6	2.53	0.43
55:SG:201:LYS:HB3	55:SG:201:LYS:HE3	1.82	0.43
56:SH:12:ASN:ND2	56:SH:14:GLU:O	2.50	0.43
58:SJ:66:LYS:HD2	58:SJ:66:LYS:HA	1.86	0.43
69:SV:15:ARG:NH1	69:SV:33:GLN:HB2	2.34	0.43
80:Sg:110:SER:HB2	80:Sg:153:CYS:HA	1.99	0.43
2:L5:196:C:H4'	9:LE:126:ARG:CG	2.49	0.43
2:L5:491:G:O2'	2:L5:493:G:O4'	2.27	0.43
2:L5:498:C:N4	2:L5:499:G:O6	2.52	0.43
2:L5:924:C:H2'	2:L5:925:C:O4'	2.18	0.43
2:L5:1207:C:H2'	2:L5:1208:G:C8	2.53	0.43
2:L5:1504:G:H2'	2:L5:1505:C:C6	2.53	0.43
2:L5:3865:A:H2'	2:L5:3866:C:H6	1.83	0.43
2:L5:4095:G:H1	2:L5:4113:U:H3	1.65	0.43
2:L5:4625:C:O2'	2:L5:4626:A:H5'	2.18	0.43
88:L5:8999:HOH:O	11:LG:62:ARG:HD3	2.18	0.43
18:LO:12:LYS:HE2	18:LO:12:LYS:HB3	1.90	0.43
33:Le:59:LYS:NZ	33:Le:61:LYS:O	2.44	0.43
48:S2:65:C:C2	55:SG:133:LEU:HD22	2.54	0.43
48:S2:486:A:N1	88:S2:2270:HOH:O	2.37	0.43
48:S2:667:U:OP1	88:S2:2103:HOH:O	2.21	0.43
48:S2:1070:A:H2'	48:S2:1071:G:O4'	2.18	0.43
48:S2:1164:G:O2'	48:S2:1165:G:H5'	2.18	0.43
54:SE:43:PRO:HG2	54:SE:46:ILE:HG12	2.01	0.43
56:SH:192:PHE:CG	75:Sb:12:PRO:HB3	2.53	0.43
60:SL:125:ILE:HB	60:SL:146:THR:OG1	2.19	0.43
80:Sg:25:PRO:HA	80:Sg:293:ALA:HB2	2.00	0.43
80:Sg:147:HIS:HD1	80:Sg:171:ASP:CG	2.26	0.43
80:Sg:181:ASN:O	80:Sg:183:LYS:HG3	2.18	0.43
2:L5:453:G:H2'	2:L5:705:G:C8	2.54	0.43
2:L5:2808:G:O3'	21:LR:60:ARG:NH1	2.52	0.43
6:S4:21:A:N7	6:S4:47:H2U:C2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LF:171:ASP:OD1	10:LF:172:ASN:N	2.52	0.43
15:LK:245:GLN:HA	15:LK:248:ILE:HG12	2.00	0.43
19:LP:14:LYS:HE3	24:LU:51:LEU:C	2.44	0.43
37:Li:54:GLU:O	37:Li:58:MET:HG3	2.18	0.43
48:S2:949:G:H2'	48:S2:950:C:C6	2.53	0.43
50:SA:80:ARG:O	50:SA:84:GLN:HG3	2.17	0.43
57:SI:174:CYS:HB2	57:SI:190:LEU:HD21	1.99	0.43
72:SY:119:GLY:O	72:SY:122:LYS:HG3	2.19	0.43
82:Sy:71:GLU:O	82:Sy:73:GLN:NE2	2.52	0.43
2:L5:258:G:OP2	20:LQ:132:SER:HB2	2.19	0.43
2:L5:399:G:OP1	36:Lh:20:SER:OG	2.31	0.43
2:L5:1921:C:C6	22:LS:161:ARG:HD3	2.54	0.43
2:L5:2079:G:H2'	2:L5:2080:U:H6	1.84	0.43
3:L8:262:LYS:HD2	4:L9:120:U:O3'	2.19	0.43
17:LN:5:LYS:NZ	37:Li:37:THR:OG1	2.36	0.43
48:S2:1733:U:H2'	48:S2:1734:G:O4'	2.19	0.43
48:S2:1749:G:H2'	48:S2:1750:C:C6	2.54	0.43
53:SD:112:LEU:O	53:SD:116:ILE:HG12	2.19	0.43
57:SI:81:VAL:HG22	57:SI:102:VAL:HG12	2.00	0.43
80:Sg:194:TYR:CE2	80:Sg:212:LYS:HD2	2.54	0.43
1:L1:60:G:P	42:Ln:68:ARG:HH22	2.42	0.43
2:L5:1084:C:H2'	2:L5:1085:C:H6	1.83	0.43
2:L5:1405:C:H2'	2:L5:1406:G:C8	2.53	0.43
2:L5:1558:A:H2'	2:L5:1559:G:H8	1.84	0.43
2:L5:1589:C:H2'	2:L5:1590:C:C6	2.54	0.43
3:L8:223:PHE:HB3	3:L8:226:TYR:HB2	2.01	0.43
8:LD:137:ILE:HD11	8:LD:149:LYS:HB2	1.99	0.43
14:LJ:51:SER:OG	14:LJ:69:ALA:HB3	2.19	0.43
48:S2:150:A:N3	48:S2:150:A:H2'	2.34	0.43
48:S2:170:A:H4'	55:SG:136:LYS:HD3	2.00	0.43
48:S2:654:A:OP2	48:S2:655:A:O2'	2.34	0.43
48:S2:886:A:H2'	48:S2:887:U:O4'	2.19	0.43
56:SH:70:LYS:HA	56:SH:70:LYS:HD2	1.90	0.43
56:SH:135:PHE:CG	56:SH:136:PRO:HA	2.54	0.43
1:L1:87:G:OP1	18:LO:5:LYS:HE3	2.19	0.43
2:L5:2029:A:H2'	2:L5:2030:A:C8	2.53	0.43
2:L5:2729:C:H2'	2:L5:2730:U:O4'	2.19	0.43
2:L5:3732:A:H2'	2:L5:3733:A:H8	1.84	0.43
2:L5:3856:A:H5''	36:Lh:83:TRP:O	2.19	0.43
3:L8:179:ARG:HA	3:L8:179:ARG:HD3	1.83	0.43
5:LB:113:GLU:OE2	5:LB:169:ARG:N	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Lc:48:LEU:HD21	31:Lc:60:ILE:HG21	2.00	0.43
32:Ld:115:LYS:HA	32:Ld:115:LYS:HD2	1.95	0.43
39:Lk:14:THR:HA	39:Lk:17:ARG:HD3	2.01	0.43
42:Ln:54:LEU:HD23	42:Ln:54:LEU:H	1.84	0.43
48:S2:142:C:H41	48:S2:330:G:P	2.42	0.43
48:S2:558:G:H2'	48:S2:559:G:C8	2.54	0.43
48:S2:573:U:O2'	48:S2:575:A:N7	2.51	0.43
48:S2:1144:A:H2'	48:S2:1145:A:C8	2.54	0.43
48:S2:1154:U:O4	52:SC:227:ARG:HD2	2.19	0.43
48:S2:1600:G:H4'	76:Sc:43:LYS:NZ	2.33	0.43
48:S2:1795:G:N7	88:S2:2266:HOH:O	2.36	0.43
48:S2:1850:MA6:H103	48:S2:1851:MA6:N6	2.33	0.43
80:Sg:251:ALA:N	80:Sg:289:LEU:HD11	2.33	0.43
83:Sz:139:HIS:O	83:Sz:147:THR:HA	2.18	0.43
2:L5:473:C:H2'	2:L5:474:C:C6	2.54	0.42
2:L5:3808:OMC:HM22	2:L5:3809:G:H5'	2.01	0.42
5:LB:303:ALA:HB2	5:LB:314:ILE:HA	2.01	0.42
11:LG:176:LYS:HG3	37:Li:43:MET:HE1	2.00	0.42
41:Lm:39:PHE:CD2	41:Lm:70:ILE:HD12	2.54	0.42
48:S2:656:G:H5'	48:S2:662:G:N2	2.33	0.42
48:S2:1101:U:H2'	48:S2:1102:G:C8	2.54	0.42
80:Sg:172:LYS:HG2	80:Sg:193:GLY:C	2.44	0.42
80:Sg:263:GLY:O	80:Sg:265:ILE:HG23	2.18	0.42
2:L5:172:C:H5'	2:L5:173:C:OP2	2.19	0.42
2:L5:453:G:H5''	2:L5:454:U:O5'	2.19	0.42
2:L5:1409:C:O2'	2:L5:1410:U:OP1	2.33	0.42
2:L5:1493:G:OP1	88:L5:5403:HOH:O	2.22	0.42
2:L5:2323:C:H2'	2:L5:2324:C:C6	2.53	0.42
2:L5:2385:U:OP1	21:LR:5:ARG:NH2	2.53	0.42
2:L5:4257:A:H2	14:LJ:27:GLY:HA3	1.84	0.42
2:L5:5059:C:H2'	2:L5:5060:A:C8	2.53	0.42
3:L8:208:MET:HG2	3:L8:223:PHE:CE2	2.54	0.42
4:L9:9:C:OP1	23:LT:26:PRO:HB2	2.19	0.42
40:Ll:97:ILE:HD13	40:Ll:107:ARG:HA	2.01	0.42
41:Lm:84:LYS:HG2	41:Lm:88:LYS:HE2	2.01	0.42
48:S2:380:G:P	57:SI:56:ARG:HH22	2.42	0.42
48:S2:1630:A:H5'	67:ST:37:GLY:N	2.34	0.42
50:SA:149:ASN:ND2	50:SA:166:LYS:HG2	2.34	0.42
52:SC:66:LEU:HD11	52:SC:81:ILE:HG12	2.01	0.42
58:SJ:61:LEU:CD2	58:SJ:95:ASP:OD1	2.67	0.42
80:Sg:9:GLY:O	80:Sg:10:THR:CG2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:Sg:47:ARG:HG2	80:Sg:52:TYR:CZ	2.54	0.42
1:L1:40:A:H2'	1:L1:41:A:C8	2.53	0.42
2:L5:37:U:H2'	2:L5:38:A:O4'	2.19	0.42
2:L5:308:G:O6	17:LN:12:ARG:NH1	2.53	0.42
2:L5:653:U:H2'	2:L5:654:C:C6	2.54	0.42
2:L5:1923:A:OP1	22:LS:160:ARG:NH2	2.51	0.42
2:L5:2413:U:H2'	2:L5:2414:G:H8	1.84	0.42
4:L9:55:A:H4'	14:LJ:155:HIS:HB2	2.01	0.42
5:LB:46:PHE:CZ	5:LB:84:MET:HG3	2.54	0.42
15:LK:162:VAL:HA	15:LK:177:GLY:HA3	2.01	0.42
16:LM:11:ARG:HG2	16:LM:57:LEU:HD22	2.01	0.42
32:Ld:64:ILE:HG23	32:Ld:68:LEU:HD23	2.01	0.42
48:S2:77:A:H2	55:SG:175:LYS:HG3	1.83	0.42
48:S2:496:C:P	54:SE:49:ARG:HH22	2.42	0.42
53:SD:47:LYS:NZ	65:SQ:115:TYR:O	2.52	0.42
61:SM:50:GLN:HA	61:SM:53:LYS:HG2	2.01	0.42
66:SS:20:TYR:O	66:SS:24:LEU:HD13	2.20	0.42
66:SS:36:GLU:HB3	66:SS:47:ARG:HD2	2.01	0.42
67:ST:26:ILE:HG13	67:ST:45:LEU:HD11	2.01	0.42
1:L1:141:C:H2'	1:L1:142:U:H6	1.82	0.42
2:L5:2022:C:H2'	2:L5:2023:C:O4'	2.19	0.42
2:L5:2565:A:H3'	2:L5:2566:G:H8	1.83	0.42
2:L5:4688:C:H2'	2:L5:4689:PSU:C6	2.55	0.42
2:L5:4690:G:O6	2:L5:4698:C:H5''	2.20	0.42
2:L5:4708:A:N3	2:L5:4709:U:H5'	2.35	0.42
2:L5:4744:A:H2'	2:L5:4745:G:O4'	2.20	0.42
2:L5:5021:C:H2'	2:L5:5022:U:O4'	2.20	0.42
6:S4:54:5MU:H2'	6:S4:55:PSU:O4'	2.19	0.42
15:LK:50:LEU:HD12	15:LK:51:VAL:N	2.34	0.42
24:LU:20:ASN:ND2	24:LU:42:ARG:O	2.48	0.42
25:LV:34:ALA:HB2	25:LV:72:LEU:HD13	2.01	0.42
48:S2:289:G:OP1	54:SE:155:LYS:NZ	2.43	0.42
48:S2:639:C:H2'	48:S2:640:A:H8	1.84	0.42
48:S2:1035:A:H2'	48:S2:1036:A:O4'	2.20	0.42
48:S2:1220:A:H2'	48:S2:1221:G:O4'	2.18	0.42
48:S2:1232:PSU:H2'	48:S2:1233:G:H8	1.83	0.42
80:Sg:11:LEU:HB2	80:Sg:307:VAL:HB	2.01	0.42
83:Sz:103:LEU:HD12	83:Sz:103:LEU:C	2.39	0.42
83:Sz:103:LEU:CD1	83:Sz:104:LYS:N	2.67	0.42
2:L5:1247:U:H2'	2:L5:1248:C:H6	1.83	0.42
2:L5:2474:G:N2	2:L5:2503:G:H5''	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:2838:G:H5'	5:LB:247:GLY:CA	2.49	0.42
2:L5:3842:C:OP1	5:LB:238:LYS:NZ	2.48	0.42
2:L5:3867:A2M:HM'3	2:L5:3880:G:N2	2.35	0.42
10:LF:209:TRP:CD1	10:LF:210:PRO:HD2	2.55	0.42
11:LG:247:VAL:O	11:LG:250:ILE:HG12	2.19	0.42
14:LJ:146:ARG:HG2	14:LJ:147:ARG:HG3	2.02	0.42
31:Lc:26:LYS:HD3	31:Lc:26:LYS:HA	1.85	0.42
45:Lz:48:LEU:O	45:Lz:139:ARG:HA	2.19	0.42
47:S1:123:ALA:HB2	47:S1:165:ARG:HG3	2.00	0.42
48:S2:1181:A:H2'	48:S2:1182:A:C8	2.54	0.42
56:SH:147:LYS:HE2	56:SH:147:LYS:HB2	1.93	0.42
59:SK:211:VAL:O	66:SS:20:TYR:OH	2.24	0.42
64:SP:34:MET:HB3	64:SP:42:ARG:HG3	2.00	0.42
67:ST:109:GLU:O	67:ST:112:GLU:HG3	2.19	0.42
1:L1:70:G:H5''	9:LE:27:ARG:CZ	2.49	0.42
2:L5:1818:G:O2'	2:L5:1820:C:OP2	2.32	0.42
2:L5:1847:C:H2'	2:L5:1848:C:C6	2.55	0.42
2:L5:2371:U:OP1	2:L5:2826:U:O2'	2.26	0.42
2:L5:2436:U:C4	42:Ln:130:PRO:HG3	2.55	0.42
2:L5:2538:U:H2'	2:L5:2539:C:C6	2.54	0.42
2:L5:2640:G:H2'	2:L5:2641:A:H8	1.84	0.42
2:L5:3605:C:H2'	2:L5:3606:U:O4'	2.20	0.42
2:L5:4520:G:H2'	2:L5:4521:PSU:O4'	2.20	0.42
2:L5:4674:C:H2'	2:L5:4675:U:C6	2.55	0.42
2:L5:4772:C:H2'	2:L5:4773:C:C6	2.54	0.42
6:S4:18:OMG:HN22	6:S4:19:A:N6	2.15	0.42
14:LJ:37:ALA:HA	14:LJ:70:VAL:HG21	2.01	0.42
14:LJ:151:ILE:HD11	14:LJ:156:ARG:HG3	2.01	0.42
20:LQ:7:GLY:O	29:La:49:HIS:NE2	2.51	0.42
21:LR:167:LYS:O	21:LR:171:LYS:HG2	2.20	0.42
28:LZ:14:LEU:O	35:Lg:88:ARG:HG2	2.19	0.42
28:LZ:92:ASP:O	28:LZ:96:VAL:HG22	2.19	0.42
30:Lb:91:ARG:HE	30:Lb:91:ARG:HB2	1.73	0.42
40:Ll:30:ASN:HD21	40:Ll:63:VAL:CG1	2.32	0.42
42:Ln:82:THR:HG22	42:Ln:155:ILE:HG23	2.01	0.42
48:S2:165:G:H1'	55:SG:110:ASN:HD22	1.84	0.42
48:S2:1149:A:H2'	48:S2:1149:A:N3	2.34	0.42
51:SB:59:ARG:O	51:SB:63:LYS:HG3	2.19	0.42
53:SD:167:LYS:HE3	53:SD:172:CYS:SG	2.60	0.42
55:SG:7:PHE:CE1	55:SG:9:ALA:HB3	2.54	0.42
55:SG:44:GLU:HG2	55:SG:45:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SJ:50:LEU:HD13	58:SJ:105:PHE:CE1	2.55	0.42
63:SO:92:ALA:HB2	63:SO:125:LYS:HB2	2.02	0.42
69:SV:35:ASN:OD1	69:SV:52:THR:HG22	2.19	0.42
76:Sc:60:LYS:HB3	76:Sc:60:LYS:HE3	1.81	0.42
2:L5:223:G:H4'	2:L5:225:G:C8	2.55	0.42
2:L5:2554:U:H1'	2:L5:2574:G:N2	2.34	0.42
2:L5:2898:G:H2'	2:L5:2899:C:C6	2.54	0.42
2:L5:4928:C:H5'	16:LM:121:ARG:HH12	1.85	0.42
4:L9:19:C:H2'	4:L9:20:U:C6	2.54	0.42
13:LI:128:ARG:HA	13:LI:128:ARG:HD3	1.72	0.42
14:LJ:23:ASN:HB3	14:LJ:129:ASP:OD1	2.20	0.42
14:LJ:24:ILE:HG12	14:LJ:128:LEU:HB3	2.00	0.42
18:LO:88:THR:O	18:LO:92:ARG:HG3	2.19	0.42
20:LQ:127:PHE:CD2	20:LQ:144:LEU:HD22	2.54	0.42
26:LW:83:THR:HG23	55:SG:131:ARG:O	2.20	0.42
30:Lb:110:ALA:O	30:Lb:114:LYS:HG3	2.19	0.42
48:S2:587:A:H5'	48:S2:592:C:H41	1.85	0.42
54:SE:48:LEU:HD12	54:SE:61:VAL:HG13	2.00	0.42
56:SH:72:PHE:O	56:SH:76:GLN:HB2	2.20	0.42
65:SQ:51:LEU:HD13	65:SQ:81:ILE:HG23	2.02	0.42
2:L5:116:G:OP2	17:LN:2:GLY:N	2.53	0.42
2:L5:909:A:H2'	2:L5:910:G:C8	2.55	0.42
2:L5:2065:G:H2'	2:L5:2066:C:O4'	2.19	0.42
2:L5:2909:C:O2'	2:L5:2910:G:N7	2.49	0.42
2:L5:4956:A:H2'	2:L5:4957:C:C6	2.55	0.42
36:Lh:41:ILE:HD13	36:Lh:150:LEU:HD21	2.02	0.42
48:S2:193:C:H2'	48:S2:194:C:H6	1.85	0.42
48:S2:674:C:H2'	48:S2:675:U:C6	2.55	0.42
48:S2:1446:A:O2'	48:S2:1447:G:H8	2.03	0.42
48:S2:1720:U:H5''	48:S2:1721:U:OP2	2.19	0.42
50:SA:127:PRO:HA	50:SA:134:LEU:CD1	2.50	0.42
51:SB:149:LEU:HD22	51:SB:162:LYS:HG3	2.01	0.42
57:SI:69:SER:HB2	60:SL:21:LYS:HG3	2.02	0.42
2:L5:1510:G:H2'	2:L5:1511:U:C6	2.54	0.42
2:L5:1727:U:P	10:LF:131:ASN:HD22	2.42	0.42
2:L5:2297:G:H4'	7:LC:242:PRO:HB2	2.02	0.42
2:L5:2789:A:H1'	24:LU:45:ARG:HH22	1.84	0.42
2:L5:4872:2MG:HM21	27:LY:201:LEU:C	2.45	0.42
15:LK:161:ARG:O	15:LK:182:ASN:ND2	2.52	0.42
48:S2:321:C:H2'	48:S2:322:C:C6	2.55	0.42
48:S2:1335:G:H5''	59:SK:185:LYS:HZ2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1620:A:H1'	48:S2:1624:U:OP2	2.20	0.42
51:SB:160:LYS:HA	51:SB:160:LYS:HD2	1.85	0.42
54:SE:106:LYS:O	54:SE:108:ARG:HG3	2.19	0.42
57:SI:148:LYS:HD3	57:SI:152:ARG:NH2	2.33	0.42
61:SM:53:LYS:HB3	61:SM:58:VAL:HG23	2.01	0.42
70:SW:8:ALA:HB2	70:SW:74:VAL:HG21	2.02	0.42
70:SW:86:LEU:HD21	70:SW:113:HIS:HB2	2.02	0.42
76:Sc:39:LYS:HB2	76:Sc:39:LYS:HE2	1.82	0.42
2:L5:106:A:H2'	2:L5:107:G:O4'	2.20	0.42
2:L5:231:U:H4'	9:LE:100:HIS:CD2	2.54	0.42
2:L5:271:C:H2'	2:L5:272:U:H6	1.83	0.42
2:L5:1174:G:H1	2:L5:1186:U:H3	1.68	0.42
2:L5:2100:A:O2'	2:L5:2101:C:O5'	2.32	0.42
2:L5:2480:G:H2'	2:L5:2481:G:H8	1.85	0.42
2:L5:2673:G:H5''	2:L5:2675:G:O4'	2.19	0.42
2:L5:4119:C:H41	35:Lg:100:GLN:HG2	1.85	0.42
2:L5:4731:G:H4'	2:L5:4732:G:O4'	2.20	0.42
2:L5:4743:G:H2'	2:L5:4744:A:H8	1.85	0.42
2:L5:4870:OMG:H5''	16:LM:91:TRP:CD2	2.55	0.42
28:LZ:123:LYS:HE3	28:LZ:123:LYS:HB3	1.82	0.42
38:Lj:88:ASP:OD1	38:Lj:89:ASP:N	2.53	0.42
41:Lm:80:LYS:HE2	41:Lm:110:TYR:CZ	2.54	0.42
42:Ln:129:ARG:NH1	88:Ln:202:HOH:O	2.53	0.42
48:S2:77:A:N7	55:SG:154:ARG:HD2	2.35	0.42
48:S2:455:A:H2'	48:S2:456:C:H6	1.83	0.42
48:S2:459:C:H2'	48:S2:460:A:O4'	2.20	0.42
51:SB:112:GLN:OE1	51:SB:114:VAL:HG22	2.20	0.42
54:SE:98:ASN:HB2	54:SE:114:ILE:O	2.20	0.42
58:SJ:111:GLN:NE2	58:SJ:127:ARG:HB2	2.34	0.42
59:SK:72:VAL:HB	61:SM:68:TYR:HD2	1.85	0.42
64:SP:131:PRO:HG2	67:ST:148:VAL:HG12	2.02	0.42
80:Sg:62:HIS:CE1	80:Sg:88:ARG:HD2	2.55	0.42
1:L1:17:A:H1'	2:L5:418:A:C2	2.55	0.41
2:L5:178:C:H2'	2:L5:179:G:C8	2.55	0.41
2:L5:2384:U:H2'	2:L5:2385:U:C6	2.55	0.41
2:L5:2539:C:H2'	2:L5:2540:C:H6	1.85	0.41
2:L5:4460:U:H2'	2:L5:4461:C:H6	1.85	0.41
3:L8:64:ILE:HG13	3:L8:109:LEU:HD22	2.02	0.41
5:LB:288:GLY:HA3	5:LB:330:PHE:CZ	2.55	0.41
6:S4:15:A:O5'	6:S4:15:A:H8	2.03	0.41
9:LE:76:LYS:HD3	24:LU:31:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LF:241:ASN:O	10:LF:245:ARG:HG2	2.19	0.41
47:S1:51:ARG:HE	47:S1:51:ARG:HB3	1.70	0.41
48:S2:494:C:N4	48:S2:509:OMG:HN22	2.17	0.41
48:S2:1499:U:H4'	59:SK:176:LEU:HD22	2.02	0.41
51:SB:126:GLN:HA	51:SB:129:THR:OG1	2.20	0.41
56:SH:49:LYS:HE2	56:SH:49:LYS:HB3	1.89	0.41
61:SM:24:LYS:O	61:SM:42:ASN:ND2	2.51	0.41
62:SN:129:TYR:HB3	62:SN:135:LEU:HG	2.01	0.41
66:SS:100:PRO:HG2	66:SS:122:PRO:HD3	2.02	0.41
72:SY:21:LYS:HB2	72:SY:75:ILE:HB	2.01	0.41
80:Sg:35:SER:OG	80:Sg:36:ARG:N	2.53	0.41
80:Sg:39:THR:HG21	80:Sg:60:ARG:NH1	2.35	0.41
82:Sy:89:VAL:HG11	82:Sy:109:VAL:HG21	2.02	0.41
82:Sy:116:LYS:HD3	82:Sy:119:GLN:HB3	2.02	0.41
2:L5:1241:C:C5	30:Lb:115:GLY:HA2	2.55	0.41
2:L5:1461:C:H2'	2:L5:1462:A:C8	2.54	0.41
2:L5:4611:A:H2	12:LH:120:GLU:HG2	1.86	0.41
7:LC:322:LEU:O	7:LC:326:LEU:HG	2.20	0.41
12:LH:173:ARG:CB	43:Lo:127:VAL:CG2	2.93	0.41
20:LQ:178:ALA:HB1	29:La:146:LEU:HD21	2.02	0.41
21:LR:21:LYS:HA	21:LR:53:LYS:HE3	2.02	0.41
31:Lc:38:ILE:HG21	31:Lc:63:TYR:HB3	2.01	0.41
48:S2:65:C:OP1	55:SG:136:LYS:NZ	2.49	0.41
48:S2:337:C:H2'	48:S2:338:G:C8	2.55	0.41
48:S2:1217:A:H2'	48:S2:1218:C:H6	1.84	0.41
48:S2:1348:G:C8	48:S2:1349:G:C8	3.08	0.41
50:SA:203:PHE:HZ	66:SS:91:LEU:HD11	1.86	0.41
54:SE:174:LYS:HB3	54:SE:174:LYS:HE3	1.84	0.41
58:SJ:33:GLY:HA3	78:Se:112:TYR:CG	2.55	0.41
64:SP:30:TYR:O	64:SP:34:MET:HG3	2.20	0.41
80:Sg:121:VAL:HG21	80:Sg:165:ILE:HG21	2.02	0.41
2:L5:2480:G:H2'	2:L5:2481:G:C8	2.56	0.41
2:L5:2758:G:O2'	2:L5:2765:A:N3	2.45	0.41
2:L5:2762:G:H2'	2:L5:2764:A:H5''	2.02	0.41
2:L5:2899:C:P	21:LR:108:ARG:HH22	2.43	0.41
2:L5:5004:C:OP1	26:LW:35:LYS:HD3	2.20	0.41
11:LG:180:PRO:HA	11:LG:227:ASN:OD1	2.19	0.41
12:LH:113:GLU:HG2	12:LH:125:ARG:HG2	2.02	0.41
14:LJ:167:GLN:O	14:LJ:171:ASP:HA	2.20	0.41
15:LK:203:ILE:O	15:LK:203:ILE:HG22	2.20	0.41
48:S2:441:C:H2'	48:S2:442:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:452:G:H2'	48:S2:453:C:C6	2.55	0.41
48:S2:1634:A:H2'	48:S2:1635:C:O4'	2.20	0.41
72:SY:27:VAL:HB	72:SY:69:THR:HG23	2.02	0.41
1:L1:56:G:H2'	1:L1:57:C:O4'	2.20	0.41
2:L5:223:G:H4'	2:L5:225:G:N7	2.36	0.41
2:L5:1535:C:N3	2:L5:1637:A:H5'	2.35	0.41
2:L5:1743:A:O4'	3:L8:15:ARG:HD2	2.19	0.41
2:L5:2902:G:H5'	2:L5:2903:G:OP2	2.20	0.41
3:L8:53:VAL:HG11	3:L8:159:VAL:HA	2.01	0.41
3:L8:75:VAL:O	3:L8:112:ARG:NH2	2.53	0.41
13:LI:7:LEU:HB2	13:LI:93:LYS:HB3	2.03	0.41
18:LO:98:HIS:O	18:LO:102:LEU:HG	2.21	0.41
28:LZ:12:LEU:HD22	28:LZ:134:LEU:HD22	2.03	0.41
45:Lz:212:LEU:HD23	45:Lz:212:LEU:HA	1.82	0.41
48:S2:67:C:C5	55:SG:162:LEU:HB3	2.55	0.41
48:S2:1256:G:O6	73:SZ:65:THR:HG22	2.20	0.41
48:S2:1545:A:H2'	48:S2:1546:G:C8	2.55	0.41
48:S2:1599:U:OP2	76:Sc:46:ASN:ND2	2.53	0.41
51:SB:114:VAL:CG1	51:SB:115:ASP:N	2.83	0.41
52:SC:70:VAL:HG21	52:SC:93:ILE:HG23	2.02	0.41
63:SO:58:GLY:O	63:SO:62:VAL:HG22	2.20	0.41
65:SQ:22:VAL:HG11	65:SQ:71:ARG:NH2	2.36	0.41
72:SY:82:ALA:O	72:SY:86:GLU:HB2	2.19	0.41
80:Sg:30:MET:HE2	80:Sg:30:MET:HB3	1.97	0.41
1:L1:7:U:H2'	1:L1:8:U:C6	2.56	0.41
1:L1:75:OMG:HM22	1:L1:76:C:O4'	2.21	0.41
2:L5:1702:C:H5''	7:LC:308:LYS:HD2	2.02	0.41
2:L5:2448:G:H2'	2:L5:2449:A:C8	2.55	0.41
2:L5:2890:C:H2'	2:L5:2891:U:C6	2.55	0.41
2:L5:3690:U:H5'	2:L5:3818:UY1:OP2	2.19	0.41
2:L5:3909:C:O2	2:L5:4396:A:N1	2.53	0.41
2:L5:4578:G:H2'	2:L5:4579:PSU:H6	1.84	0.41
2:L5:4956:A:H2'	2:L5:4957:C:H6	1.85	0.41
4:L9:24:C:H2'	4:L9:25:G:O4'	2.20	0.41
5:LB:116:ARG:O	5:LB:177:LYS:HD3	2.21	0.41
6:S4:16:H2U:O4'	51:SB:59:ARG:NH2	2.54	0.41
36:Lh:4:TYR:OH	36:Lh:18:ARG:HG3	2.21	0.41
41:Lm:42:PHE:CE1	41:Lm:46:ARG:HD2	2.55	0.41
48:S2:1802:C:H2'	48:S2:1803:U:H6	1.84	0.41
63:SO:44:VAL:HG12	63:SO:53:ILE:HB	2.02	0.41
71:SX:46:HIS:CD2	71:SX:103:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sy:40:LYS:HD3	83:Sz:129:GLY:HA3	2.02	0.41
2:L5:100:C:OP2	88:L5:5405:HOH:O	2.22	0.41
2:L5:1554:A:H5'	44:Lp:9:GLY:C	2.45	0.41
2:L5:1964:A:C4	2:L5:1965:G:C8	3.09	0.41
2:L5:2293:U:H2'	2:L5:2294:G:H8	1.86	0.41
2:L5:3893:C:H2'	2:L5:3894:A:H8	1.86	0.41
2:L5:4250:G:H4'	14:LJ:106:GLY:C	2.45	0.41
2:L5:4322:G:N2	2:L5:4325:A:OP2	2.52	0.41
2:L5:4507:A:HO2'	25:LV:41:SER:HG	1.64	0.41
2:L5:4601:U:H2'	2:L5:4602:A:H8	1.85	0.41
2:L5:4966:A:H2'	2:L5:4967:A:O4'	2.20	0.41
4:L9:11:A:O2'	4:L9:13:A:OP2	2.35	0.41
6:S4:47:H2U:O2	6:S4:48:U:H5	2.03	0.41
16:LM:32:ASP:OD1	16:LM:35:ARG:HG3	2.21	0.41
35:Lg:106:VAL:O	35:Lg:110:GLN:HG2	2.20	0.41
48:S2:193:C:H2'	48:S2:194:C:C6	2.55	0.41
48:S2:1264:C:H4'	48:S2:1265:A:O4'	2.21	0.41
48:S2:1307:U:H2'	48:S2:1308:U:C6	2.56	0.41
48:S2:1678:A2M:O2'	48:S2:1679:A:H5'	2.21	0.41
65:SQ:86:GLN:HE22	65:SQ:122:ALA:HA	1.85	0.41
67:ST:27:ALA:HB2	67:ST:52:LEU:HD12	2.01	0.41
80:Sg:126:ASP:O	80:Sg:128:THR:HG23	2.20	0.41
83:Sz:103:LEU:HD12	83:Sz:104:LYS:C	2.46	0.41
1:L1:5:U:H2'	1:L1:6:C:H6	1.85	0.41
2:L5:238:C:OP2	9:LE:45:ARG:NH2	2.54	0.41
2:L5:986:C:H2'	2:L5:987:C:C6	2.55	0.41
2:L5:2352:U:H2'	2:L5:2353:U:C6	2.56	0.41
2:L5:4530:UR3:O5'	2:L5:4530:UR3:H6	2.21	0.41
5:LB:140:GLU:HG3	5:LB:141:ASP:N	2.35	0.41
9:LE:54:GLU:HG3	9:LE:108:ARG:HB3	2.03	0.41
10:LF:83:VAL:HG22	22:LS:62:VAL:HA	2.01	0.41
11:LG:39:PHE:CD1	11:LG:47:PRO:HD3	2.56	0.41
12:LH:128:MET:SD	12:LH:157:SER:HB3	2.60	0.41
21:LR:74:ARG:O	21:LR:76:MET:HG2	2.21	0.41
32:Ld:36:VAL:CG2	32:Ld:41:ARG:HG2	2.51	0.41
37:Li:70:LEU:HB2	37:Li:87:ARG:HH11	1.86	0.41
48:S2:520:A:O2'	48:S2:825:A:N3	2.49	0.41
48:S2:1018:U:H2'	48:S2:1019:C:C6	2.56	0.41
48:S2:1060:A:H4'	48:S2:1061:U:H5''	2.01	0.41
48:S2:1438:A:H2'	48:S2:1439:A:C8	2.55	0.41
50:SA:30:LEU:HD11	50:SA:35:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SV:3:ASN:HD21	69:SV:7:GLU:HB2	1.84	0.41
80:Sg:59:LEU:HB3	80:Sg:90:TRP:CE3	2.56	0.41
1:L1:67:U:H2'	1:L1:68:G:C8	2.55	0.41
2:L5:25:A:H2'	2:L5:26:C:H6	1.84	0.41
2:L5:457:G:H2'	2:L5:458:C:C6	2.55	0.41
2:L5:1802:A:H5''	2:L5:1803:G:H5'	2.02	0.41
2:L5:3738:G:N7	88:L5:5598:HOH:O	2.37	0.41
2:L5:3930:U:H2'	2:L5:3931:C:H6	1.85	0.41
2:L5:4504:C:H2'	2:L5:4505:C:C6	2.56	0.41
2:L5:4618:OMG:H5''	25:LV:15:ARG:HB2	2.02	0.41
7:LC:5:ARG:HD2	7:LC:24:LEU:O	2.21	0.41
10:LF:88:LYS:HE3	10:LF:88:LYS:HB2	1.86	0.41
19:LP:64:MET:O	19:LP:68:LYS:HG2	2.20	0.41
21:LR:136:ARG:O	21:LR:140:GLU:HG2	2.21	0.41
48:S2:1274:G:H5''	61:SM:47:LYS:HE2	2.03	0.41
48:S2:1522:A:C8	67:ST:146:VAL:HG21	2.55	0.41
48:S2:1536:G:C2	48:S2:1537:A:C5	3.08	0.41
48:S2:1822:A:H2'	48:S2:1823:A:H8	1.84	0.41
67:ST:121:ARG:HG3	67:ST:131:VAL:HB	2.02	0.41
74:Sa:12:LYS:HB2	74:Sa:33:ASP:OD2	2.21	0.41
80:Sg:154:VAL:HA	80:Sg:166:VAL:O	2.21	0.41
82:Sy:49:LEU:HB2	82:Sy:114:TYR:OH	2.21	0.41
1:L1:26:C:H2'	1:L1:27:U:C6	2.56	0.41
1:L1:92:U:H2'	1:L1:93:C:O4'	2.20	0.41
2:L5:398:A2M:HM'3	2:L5:398:A2M:H1'	1.90	0.41
2:L5:1084:C:H2'	2:L5:1085:C:C6	2.56	0.41
2:L5:1704:C:H5'	10:LF:43:ARG:HH22	1.85	0.41
2:L5:1893:C:H1'	2:L5:1937:C:O2	2.20	0.41
2:L5:2276:A:H2'	2:L5:2277:C:O4'	2.21	0.41
2:L5:2323:C:H2'	2:L5:2324:C:H6	1.86	0.41
2:L5:2377:C:H2'	2:L5:2378:G:O4'	2.21	0.41
2:L5:2434:G:O2'	2:L5:2527:A:N1	2.50	0.41
2:L5:2588:C:OP1	2:L5:2768:C:O2'	2.32	0.41
2:L5:2759:G:O2'	2:L5:2760:G:O4'	2.20	0.41
2:L5:4438:U:H2'	2:L5:4439:U:O4'	2.20	0.41
2:L5:4488:A:H4'	2:L5:4489:G:H8	1.85	0.41
2:L5:5004:C:H2'	2:L5:5005:G:O4'	2.20	0.41
3:L8:178:LYS:HE3	3:L8:179:ARG:NH2	2.35	0.41
4:L9:27:G:H2'	4:L9:28:C:C6	2.55	0.41
5:LB:107:ALA:HB2	5:LB:201:LEU:HD22	2.03	0.41
5:LB:117:ARG:HA	5:LB:177:LYS:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S4:43:A:H2'	6:S4:44:A:C8	2.56	0.41
10:LF:217:ARG:O	10:LF:246:ARG:HD2	2.21	0.41
20:LQ:203:ALA:HA	20:LQ:206:ASP:HB3	2.03	0.41
24:LU:24:PRO:HD2	24:LU:27:ILE:HG13	2.03	0.41
28:LZ:120:GLU:O	28:LZ:124:THR:HG23	2.21	0.41
48:S2:808:A:H2	48:S2:855:G:H22	1.68	0.41
48:S2:1058:A:H2'	48:S2:1059:G:C8	2.55	0.41
48:S2:1442:OMU:HM22	48:S2:1443:C:O4'	2.21	0.41
48:S2:1491:G:H2'	48:S2:1492:U:C6	2.56	0.41
48:S2:1639:7MG:H2'	48:S2:1640:A:C8	2.55	0.41
50:SA:104:THR:O	50:SA:107:THR:OG1	2.28	0.41
52:SC:94:ILE:HG13	52:SC:159:LYS:O	2.21	0.41
55:SG:218:LYS:O	55:SG:222:GLU:HG2	2.21	0.41
58:SJ:93:LYS:HB2	58:SJ:96:TYR:HD2	1.85	0.41
64:SP:98:ASN:HB3	64:SP:120:SER:OG	2.21	0.41
77:Sd:13:ARG:NH1	77:Sd:53:GLY:O	2.54	0.41
77:Sd:21:THR:HG23	77:Sd:27:CYS:HB2	2.03	0.41
79:Sf:56:ASP:N	79:Sf:56:ASP:OD1	2.52	0.41
80:Sg:133:ASN:HB3	80:Sg:139:LYS:HD2	2.03	0.41
80:Sg:172:LYS:HE2	80:Sg:193:GLY:HA2	2.02	0.41
82:Sy:52:LEU:HD23	82:Sy:78:LYS:NZ	2.36	0.41
2:L5:116:G:H2'	2:L5:117:C:C6	2.55	0.41
2:L5:1364:U:OP2	20:LQ:36:ARG:NH2	2.45	0.41
2:L5:1620:U:H6	2:L5:1620:U:H5''	1.85	0.41
11:LG:95:LEU:HD13	11:LG:218:LEU:HD13	2.02	0.41
11:LG:160:ASP:OD1	11:LG:160:ASP:N	2.54	0.41
36:Lh:16:LYS:HE2	36:Lh:16:LYS:HB3	1.80	0.41
47:S1:128:LYS:HE3	47:S1:128:LYS:HB3	1.91	0.41
47:S1:179:ASN:HB3	47:S1:183:GLU:HB2	2.03	0.41
48:S2:853:C:C2	48:S2:854:A:C8	3.09	0.41
48:S2:976:G:H2'	48:S2:977:C:C6	2.56	0.41
48:S2:1204:A:H2'	48:S2:1205:C:C6	2.56	0.41
48:S2:1228:A:H5''	76:Sc:32:LYS:HD2	2.02	0.41
48:S2:1337:4AC:O2'	73:SZ:68:THR:HB	2.21	0.41
48:S2:1740:C:H2'	48:S2:1741:U:C6	2.56	0.41
51:SB:157:LYS:HE3	51:SB:157:LYS:HB2	1.84	0.41
59:SK:33:GLY:HA3	59:SK:53:THR:HG22	2.03	0.41
76:Sc:32:LYS:HB2	76:Sc:32:LYS:HE2	1.90	0.41
83:Sz:124:ASP:OD1	83:Sz:125:GLU:N	2.54	0.41
2:L5:1296:G:H2'	2:L5:1297:U:O4'	2.21	0.40
2:L5:1304:C:H2'	2:L5:1305:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4154:G:H2'	2:L5:4155:C:C6	2.56	0.40
2:L5:4237:C:OP1	2:L5:4327:C:O2'	2.35	0.40
2:L5:4256:A:O2'	14:LJ:55:TYR:OH	2.29	0.40
3:L8:223:PHE:O	3:L8:227:ILE:HG12	2.21	0.40
16:LM:36:ALA:HB2	16:LM:52:PHE:CE1	2.56	0.40
48:S2:1018:U:H2'	48:S2:1019:C:H6	1.86	0.40
56:SH:134:VAL:O	56:SH:137:SER:OG	2.36	0.40
63:SO:45:THR:HG22	63:SO:52:THR:HA	2.03	0.40
66:SS:5:ARG:NH1	88:SS:201:HOH:O	2.54	0.40
70:SW:8:ALA:CB	70:SW:74:VAL:HG21	2.51	0.40
2:L5:1392:A:H2'	2:L5:1393:G:C8	2.57	0.40
2:L5:1628:C:OP2	8:LD:9:ARG:HD2	2.21	0.40
2:L5:1670:G:C8	2:L5:1855:G:C8	3.10	0.40
2:L5:2374:A:P	32:Ld:50:ARG:HH22	2.44	0.40
3:L8:225:GLN:HB2	4:L9:49:A:OP1	2.22	0.40
6:S4:30:G:OP1	48:S2:1524:G:O2'	2.39	0.40
16:LM:60:PHE:HE1	16:LM:85:LYS:HE2	1.85	0.40
26:LW:97:LYS:CE	55:SG:146:ASN:ND2	2.85	0.40
33:Le:70:LEU:O	33:Le:80:LYS:HA	2.21	0.40
38:Lj:34:PHE:CE1	38:Lj:38:ARG:HG3	2.56	0.40
39:Lk:35:LYS:HA	39:Lk:43:TYR:O	2.21	0.40
48:S2:17:C:OP2	88:S2:2105:HOH:O	2.21	0.40
48:S2:75:G:C4	48:S2:76:U:H5	2.38	0.40
48:S2:1190:A:H2'	48:S2:1191:C:O4'	2.20	0.40
48:S2:1852:C:OP2	81:So:1:MET:HG3	2.21	0.40
51:SB:81:ARG:HH12	51:SB:82:LYS:HG3	1.85	0.40
57:SI:76:THR:HG21	57:SI:104:ILE:HD12	2.03	0.40
59:SK:209:SER:HB2	66:SS:40:ILE:HB	2.04	0.40
61:SM:42:ASN:N	88:SM:202:HOH:O	2.54	0.40
62:SN:60:VAL:HG13	62:SN:66:VAL:HG21	2.03	0.40
62:SN:70:LYS:NZ	88:SN:207:HOH:O	2.54	0.40
80:Sg:78:ALA:O	80:Sg:89:LEU:HD12	2.21	0.40
1:L1:129:C:H2'	1:L1:130:C:C6	2.56	0.40
2:L5:1307:A:H2'	2:L5:1308:C:H6	1.82	0.40
2:L5:1541:C:H2'	2:L5:1542:U:C6	2.57	0.40
2:L5:2500:U:H2'	2:L5:2501:C:H6	1.86	0.40
2:L5:3897:G:O2'	2:L5:3898:G:OP2	2.36	0.40
2:L5:4770:U:H2'	2:L5:4771:C:C5	2.56	0.40
13:LI:16:ARG:NH1	13:LI:54:LEU:HD12	2.36	0.40
13:LI:28:TYR:HB3	13:LI:30:LYS:HG2	2.03	0.40
16:LM:6:PHE:H	16:LM:11:ARG:HH21	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Lm:36:ALA:HB1	41:Lm:65:ARG:HD2	2.03	0.40
48:S2:448:A:H5'	57:SI:25:ARG:HA	2.04	0.40
48:S2:1052:A:H2'	48:S2:1053:C:O4'	2.21	0.40
48:S2:1305:C:C2	48:S2:1306:U:C5	3.09	0.40
57:SI:19:LYS:O	88:SI:301:HOH:O	2.22	0.40
59:SK:12:VAL:O	59:SK:16:ILE:HG12	2.22	0.40
72:SY:38:THR:O	72:SY:42:GLU:HG2	2.20	0.40
72:SY:57:VAL:HB	72:SY:60:PHE:CE2	2.56	0.40
73:SZ:100:GLN:O	73:SZ:104:ILE:HG13	2.20	0.40
80:Sg:68:ASP:O	80:Sg:80:SER:HA	2.21	0.40
2:L5:279:A:N1	2:L5:306:A:H5''	2.36	0.40
2:L5:1721:G:H2'	2:L5:1722:C:H6	1.85	0.40
2:L5:2424:OMG:H8	2:L5:2424:OMG:O5'	2.03	0.40
2:L5:3792:OMG:H2'	2:L5:3793:U:C6	2.56	0.40
2:L5:3868:G:H22	2:L5:3900:G:H1'	1.85	0.40
2:L5:4417:C:H2'	2:L5:4418:G:O4'	2.21	0.40
2:L5:4437:U:C2	2:L5:4515:G:H4'	2.56	0.40
3:L8:65:ALA:HB2	3:L8:74:ILE:HD13	2.03	0.40
13:LI:35:TRP:CE2	13:LI:56:PRO:HD2	2.57	0.40
27:LY:51:LYS:O	27:LY:55:LEU:HG	2.21	0.40
36:Lh:47:TYR:CE1	36:Lh:76:TRP:HZ2	2.39	0.40
39:Lk:51:GLU:O	39:Lk:55:LYS:HG3	2.21	0.40
41:Lm:89:LYS:HE3	41:Lm:89:LYS:HB3	1.94	0.40
42:Ln:81:LEU:HD12	42:Ln:81:LEU:HA	1.94	0.40
48:S2:556:U:H2'	48:S2:557:U:C6	2.56	0.40
48:S2:1303:C:H2'	48:S2:1304:U:H6	1.87	0.40
48:S2:1398:G:H22	48:S2:1448:A:H2	1.68	0.40
64:SP:56:LEU:HD22	64:SP:80:LEU:HD12	2.03	0.40
80:Sg:296:GLN:HG3	80:Sg:312:VAL:HG21	2.03	0.40
2:L5:667:A:H8	2:L5:667:A:O5'	2.05	0.40
2:L5:1566:C:H2'	2:L5:1567:U:C6	2.57	0.40
2:L5:1927:U:OP1	2:L5:1949:U:O2'	2.36	0.40
2:L5:2656:U:OP1	28:LZ:78:ASN:ND2	2.55	0.40
2:L5:2726:G:H2'	2:L5:2727:C:C6	2.56	0.40
8:LD:10:LYS:HA	8:LD:16:PHE:CD2	2.57	0.40
15:LK:67:ALA:HB1	15:LK:70:LYS:HE2	2.02	0.40
17:LN:84:PRO:HA	17:LN:87:HIS:CG	2.57	0.40
27:LY:166:ILE:HD12	27:LY:169:ARG:HH21	1.87	0.40
31:Lc:14:ILE:HD13	31:Lc:72:HIS:CE1	2.56	0.40
35:Lg:50:PRO:HG3	44:Lp:61:MET:HE3	2.02	0.40
40:Ll:17:LEU:HD21	40:Ll:19:LYS:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:1434:C:H2'	48:S2:1435:C:C6	2.56	0.40
48:S2:1678:A2M:HM'3	48:S2:1678:A2M:H1'	1.63	0.40
48:S2:1705:C:H2'	48:S2:1706:G:C8	2.56	0.40
53:SD:63:LYS:HD3	53:SD:71:ARG:NH2	2.36	0.40
53:SD:204:ARG:HD3	77:Sd:60:GLU:HG3	2.02	0.40
56:SH:163:GLN:O	56:SH:167:GLU:HB2	2.22	0.40
57:SI:141:ARG:HD3	57:SI:145:ILE:HG22	2.03	0.40
58:SJ:136:ARG:NH1	88:SJ:206:HOH:O	2.53	0.40
59:SK:146:ARG:HD2	59:SK:146:ARG:HA	1.91	0.40
73:SZ:61:LEU:O	73:SZ:81:GLN:HA	2.22	0.40
80:Sg:9:GLY:O	80:Sg:10:THR:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L8	291/297 (98%)	282 (97%)	9 (3%)	0	100	100
5	LB	398/403 (99%)	394 (99%)	4 (1%)	0	100	100
7	LC	363/427 (85%)	352 (97%)	11 (3%)	0	100	100
8	LD	245/257 (95%)	237 (97%)	8 (3%)	0	100	100
9	LE	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
10	LF	223/248 (90%)	218 (98%)	5 (2%)	0	100	100
11	LG	212/266 (80%)	209 (99%)	3 (1%)	0	100	100
12	LH	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
13	LI	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
14	LJ	165/178 (93%)	163 (99%)	2 (1%)	0	100	100
15	LK	216/288 (75%)	210 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	LM	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
17	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
18	LO	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
19	LP	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
20	LQ	204/211 (97%)	202 (99%)	2 (1%)	0	100	100
21	LR	184/196 (94%)	183 (100%)	1 (0%)	0	100	100
22	LS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
23	LT	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
24	LU	48/51 (94%)	48 (100%)	0	0	100	100
25	LV	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
26	LW	106/157 (68%)	103 (97%)	3 (3%)	0	100	100
27	LY	196/203 (97%)	193 (98%)	3 (2%)	0	100	100
28	LZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	La	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	18	14
30	Lb	99/159 (62%)	97 (98%)	2 (2%)	0	100	100
31	Lc	99/115 (86%)	99 (100%)	0	0	100	100
32	Ld	102/125 (82%)	102 (100%)	0	0	100	100
33	Le	102/106 (96%)	102 (100%)	0	0	100	100
34	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
35	Lg	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
36	Lh	157/184 (85%)	153 (98%)	4 (2%)	0	100	100
37	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
38	Lj	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
39	Lk	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
40	Ll	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
41	Lm	98/128 (77%)	91 (93%)	7 (7%)	0	100	100
42	Ln	114/156 (73%)	113 (99%)	1 (1%)	0	100	100
43	Lo	50/99 (50%)	50 (100%)	0	0	100	100
44	Lp	86/92 (94%)	82 (95%)	4 (5%)	0	100	100
45	Lz	209/214 (98%)	209 (100%)	0	0	100	100
46	NC	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	S1	217/264 (82%)	214 (99%)	3 (1%)	0	100	100
50	SA	218/295 (74%)	217 (100%)	1 (0%)	0	100	100
51	SB	230/609 (38%)	219 (95%)	10 (4%)	1 (0%)	30	27
52	SC	217/293 (74%)	211 (97%)	6 (3%)	0	100	100
53	SD	180/204 (88%)	172 (96%)	8 (4%)	0	100	100
54	SE	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
55	SG	227/249 (91%)	222 (98%)	5 (2%)	0	100	100
56	SH	185/194 (95%)	177 (96%)	8 (4%)	0	100	100
57	SI	205/208 (99%)	203 (99%)	2 (1%)	0	100	100
58	SJ	177/194 (91%)	173 (98%)	4 (2%)	0	100	100
59	SK	222/243 (91%)	217 (98%)	5 (2%)	0	100	100
60	SL	139/158 (88%)	137 (99%)	2 (1%)	0	100	100
61	SM	95/165 (58%)	91 (96%)	4 (4%)	0	100	100
62	SN	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
63	SO	123/151 (82%)	120 (98%)	3 (2%)	0	100	100
64	SP	123/145 (85%)	121 (98%)	2 (2%)	0	100	100
65	SQ	137/146 (94%)	135 (98%)	2 (2%)	0	100	100
66	SS	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
67	ST	145/152 (95%)	142 (98%)	3 (2%)	0	100	100
68	SU	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
69	SV	81/83 (98%)	81 (100%)	0	0	100	100
70	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
71	SX	137/143 (96%)	136 (99%)	1 (1%)	0	100	100
72	SY	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
73	SZ	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
74	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
75	Sb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
76	Sc	81/125 (65%)	78 (96%)	3 (4%)	0	100	100
77	Sd	60/69 (87%)	60 (100%)	0	0	100	100
78	Se	53/133 (40%)	53 (100%)	0	0	100	100
79	Sf	53/56 (95%)	52 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	Sg	299/317 (94%)	284 (95%)	15 (5%)	0	100	100
81	So	23/25 (92%)	23 (100%)	0	0	100	100
82	Sy	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
83	Sz	72/156 (46%)	63 (88%)	8 (11%)	1 (1%)	9	4
All	All	11414/13366 (85%)	11166 (98%)	245 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	SB	97	GLU
83	Sz	91	ASN
29	La	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L8	247/250 (99%)	245 (99%)	2 (1%)	73	80
5	LB	347/348 (100%)	345 (99%)	2 (1%)	78	85
7	LC	304/348 (87%)	302 (99%)	2 (1%)	76	82
8	LD	189/198 (96%)	189 (100%)	0	100	100
9	LE	124/135 (92%)	124 (100%)	0	100	100
10	LF	195/216 (90%)	194 (100%)	1 (0%)	81	87
11	LG	187/223 (84%)	186 (100%)	1 (0%)	81	87
12	LH	169/171 (99%)	168 (99%)	1 (1%)	78	85
13	LI	114/121 (94%)	113 (99%)	1 (1%)	70	78
14	LJ	141/149 (95%)	140 (99%)	1 (1%)	76	82
15	LK	196/252 (78%)	195 (100%)	1 (0%)	81	87
16	LM	115/161 (71%)	115 (100%)	0	100	100
17	LN	171/172 (99%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	LO	109/110 (99%)	107 (98%)	2 (2%)	51	58
19	LP	73/80 (91%)	73 (100%)	0	100	100
20	LQ	172/177 (97%)	170 (99%)	2 (1%)	63	70
21	LR	165/175 (94%)	165 (100%)	0	100	100
22	LS	157/157 (100%)	156 (99%)	1 (1%)	78	85
23	LT	138/140 (99%)	136 (99%)	2 (1%)	59	66
24	LU	47/48 (98%)	47 (100%)	0	100	100
25	LV	100/107 (94%)	100 (100%)	0	100	100
26	LW	90/126 (71%)	89 (99%)	1 (1%)	65	73
27	LY	170/174 (98%)	170 (100%)	0	100	100
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	119/120 (99%)	119 (100%)	0	100	100
30	Lb	85/125 (68%)	85 (100%)	0	100	100
31	Lc	86/97 (89%)	86 (100%)	0	100	100
32	Ld	95/110 (86%)	95 (100%)	0	100	100
33	Le	92/93 (99%)	92 (100%)	0	100	100
34	Lf	88/89 (99%)	88 (100%)	0	100	100
35	Lg	95/100 (95%)	95 (100%)	0	100	100
36	Lh	140/163 (86%)	140 (100%)	0	100	100
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	164/165 (99%)	164 (100%)	0	100	100
39	Lk	63/65 (97%)	63 (100%)	0	100	100
40	Ll	107/120 (89%)	107 (100%)	0	100	100
41	Lm	90/115 (78%)	90 (100%)	0	100	100
42	Ln	104/133 (78%)	103 (99%)	1 (1%)	68	75
43	Lo	48/90 (53%)	48 (100%)	0	100	100
44	Lp	71/75 (95%)	71 (100%)	0	100	100
45	Lz	179/181 (99%)	178 (99%)	1 (1%)	78	85
46	NC	25/25 (100%)	25 (100%)	0	100	100
47	S1	200/231 (87%)	199 (100%)	1 (0%)	81	87
50	SA	182/242 (75%)	181 (100%)	1 (0%)	81	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	SB	215/509 (42%)	212 (99%)	3 (1%)	59	66
52	SC	185/225 (82%)	184 (100%)	1 (0%)	81	87
53	SD	157/170 (92%)	156 (99%)	1 (1%)	78	85
54	SE	224/225 (100%)	220 (98%)	4 (2%)	51	58
55	SG	199/218 (91%)	198 (100%)	1 (0%)	81	87
56	SH	168/174 (97%)	164 (98%)	4 (2%)	43	47
57	SI	179/180 (99%)	178 (99%)	1 (1%)	78	85
58	SJ	160/168 (95%)	159 (99%)	1 (1%)	78	85
59	SK	188/202 (93%)	188 (100%)	0	100	100
60	SL	130/142 (92%)	129 (99%)	1 (1%)	73	80
61	SM	88/136 (65%)	88 (100%)	0	100	100
62	SN	130/131 (99%)	130 (100%)	0	100	100
63	SO	99/118 (84%)	99 (100%)	0	100	100
64	SP	111/130 (85%)	111 (100%)	0	100	100
65	SQ	115/121 (95%)	112 (97%)	3 (3%)	40	44
66	SS	119/122 (98%)	118 (99%)	1 (1%)	73	80
67	ST	127/132 (96%)	126 (99%)	1 (1%)	73	80
68	SU	111/115 (96%)	111 (100%)	0	100	100
69	SV	67/67 (100%)	66 (98%)	1 (2%)	57	64
70	SW	112/113 (99%)	111 (99%)	1 (1%)	70	78
71	SX	111/114 (97%)	110 (99%)	1 (1%)	70	78
72	SY	107/114 (94%)	107 (100%)	0	100	100
73	SZ	92/107 (86%)	90 (98%)	2 (2%)	45	50
74	Sa	86/98 (88%)	86 (100%)	0	100	100
75	Sb	75/76 (99%)	74 (99%)	1 (1%)	61	68
76	Sc	74/103 (72%)	74 (100%)	0	100	100
77	Sd	55/62 (89%)	55 (100%)	0	100	100
78	Se	45/104 (43%)	44 (98%)	1 (2%)	45	50
79	Sf	48/49 (98%)	47 (98%)	1 (2%)	47	52
80	Sg	263/275 (96%)	259 (98%)	4 (2%)	57	64
81	So	24/24 (100%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
82	Sy	103/108 (95%)	102 (99%)	1 (1%)	68	75
83	Sz	66/140 (47%)	63 (96%)	3 (4%)	24	23
All	All	9989/11356 (88%)	9927 (99%)	62 (1%)	76	85

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L8	194	VAL
3	L8	255	LYS
5	LB	143	LYS
5	LB	146	LEU
7	LC	150	LEU
7	LC	170	LEU
10	LF	124	LYS
11	LG	176	LYS
12	LH	112	VAL
13	LI	5	ARG
14	LJ	20	LEU
15	LK	218	LYS
18	LO	46	LYS
18	LO	98	HIS
20	LQ	115	GLN
20	LQ	168	VAL
22	LS	150	ILE
23	LT	97	LYS
23	LT	121	GLU
26	LW	100	VAL
42	Ln	47	ARG
45	Lz	129	VAL
47	S1	42	ARG
50	SA	13	GLU
51	SB	1	MET
51	SB	81	ARG
51	SB	225	LEU
52	SC	248	TYR
53	SD	41	VAL
54	SE	131	VAL
54	SE	173	ILE
54	SE	194	VAL
54	SE	211	LYS
55	SG	198	ARG

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Mol	Chain	Res	Type
56	SH	9	VAL
56	SH	162	GLN
56	SH	167	GLU
56	SH	191	GLU
57	SI	59	ARG
58	SJ	30	LYS
60	SL	48	LYS
65	SQ	42	ILE
65	SQ	100	VAL
65	SQ	127	CYS
66	SS	98	VAL
67	ST	142	ARG
69	SV	81	LYS
70	SW	97	ARG
71	SX	105	PHE
73	SZ	39	LEU
73	SZ	106	ILE
75	Sb	13	GLU
78	Se	126	LYS
79	Sf	56	ASP
80	Sg	70	VAL
80	Sg	132	TRP
80	Sg	270	LEU
80	Sg	305	ASN
82	Sy	20	GLU
83	Sz	104	LYS
83	Sz	108	VAL
83	Sz	141	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
3	L8	45	ASN
3	L8	229	ASN
5	LB	184	GLN
7	LC	38	ASN
7	LC	329	ASN
9	LE	14	ASN
10	LF	126	ASN
10	LF	205	ASN
12	LH	15	ASN
12	LH	98	HIS

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Mol	Chain	Res	Type
13	LI	80	HIS
16	LM	34	ASN
16	LM	44	GLN
19	LP	48	ASN
27	LY	150	GLN
27	LY	180	GLN
28	LZ	78	ASN
29	La	120	GLN
31	Lc	19	GLN
32	Ld	69	ASN
36	Lh	21	ASN
36	Lh	28	ASN
36	Lh	56	GLN
36	Lh	133	HIS
40	Li	30	ASN
40	Li	70	GLN
41	Lm	50	ASN
41	Lm	55	ASN
41	Lm	116	GLN
42	Ln	69	ASN
42	Ln	151	ASN
45	Lz	73	ASN
45	Lz	144	ASN
45	Lz	213	HIS
47	S1	53	GLN
47	S1	158	HIS
50	SA	36	GLN
51	SB	163	GLN
51	SB	222	ASN
53	SD	203	ASN
54	SE	36	HIS
54	SE	161	GLN
54	SE	216	ASN
55	SG	146	ASN
60	SL	94	HIS
61	SM	28	HIS
61	SM	61	GLN
61	SM	84	HIS
64	SP	54	HIS
64	SP	79	HIS
64	SP	103	ASN
65	SQ	142	GLN

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Mol	Chain	Res	Type
66	SS	62	GLN
66	SS	74	GLN
67	ST	11	HIS
67	ST	19	ASN
70	SW	70	ASN
71	SX	23	HIS
80	Sg	187	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	145/157 (92%)	12 (8%)	0
2	L5	3511/5069 (69%)	519 (14%)	10 (0%)
4	L9	119/121 (98%)	9 (7%)	0
48	S2	1655/1869 (88%)	248 (14%)	4 (0%)
49	S5	8/9 (88%)	1 (12%)	0
6	S4	75/76 (98%)	24 (32%)	2 (2%)
All	All	5513/7301 (75%)	813 (14%)	16 (0%)

All (813) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	34	U
1	L1	35	C
1	L1	48	A
1	L1	59	A
1	L1	62	A
1	L1	63	U
1	L1	94	G
1	L1	103	A
1	L1	105	C
1	L1	110	U
1	L1	114	G
1	L1	147	G
2	L5	2	G
2	L5	15	A
2	L5	39	A
2	L5	48	G
2	L5	59	A
2	L5	64	A
2	L5	65	A

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Mol	Chain	Res	Type
2	L5	71	C
2	L5	73	A
2	L5	91	G
2	L5	98	A
2	L5	110	C
2	L5	116	G
2	L5	117	C
2	L5	119	G
2	L5	120	A
2	L5	122	U
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	136	C
2	L5	137	G
2	L5	143	C
2	L5	144	G
2	L5	152	U
2	L5	159	C
2	L5	165	A
2	L5	166	C
2	L5	169	G
2	L5	171	U
2	L5	172	C
2	L5	182	G
2	L5	189	G
2	L5	200	U
2	L5	210	C
2	L5	219	G
2	L5	233	U
2	L5	234	G
2	L5	255	C
2	L5	256	G
2	L5	258	G
2	L5	260	C
2	L5	262	G
2	L5	263	G
2	L5	266	C
2	L5	269	G
2	L5	280	G
2	L5	297	U
2	L5	316	U

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Mol	Chain	Res	Type
2	L5	340	C
2	L5	364	G
2	L5	387	G
2	L5	410	A
2	L5	412	G
2	L5	413	G
2	L5	432	U
2	L5	449	C
2	L5	450	G
2	L5	465	G
2	L5	466	A
2	L5	484	U
2	L5	485	C
2	L5	489	C
2	L5	490	C
2	L5	492	U
2	L5	493	G
2	L5	496	G
2	L5	497	G
2	L5	498	C
2	L5	509	A
2	L5	510	U
2	L5	512	U
2	L5	666	G
2	L5	667	A
2	L5	669	C
2	L5	686	A
2	L5	687	U
2	L5	704	C
2	L5	708	G
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	740	G
2	L5	754	U
2	L5	755	C
2	L5	757	G
2	L5	758	G
2	L5	904	C
2	L5	906	C
2	L5	913	U
2	L5	914	U

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Mol	Chain	Res	Type
2	L5	915	A
2	L5	916	C
2	L5	917	A
2	L5	923	C
2	L5	924	C
2	L5	926	G
2	L5	932	A
2	L5	933	G
2	L5	934	C
2	L5	935	A
2	L5	937	U
2	L5	944	A
2	L5	945	U
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	965	G
2	L5	970	G
2	L5	971	U
2	L5	977	C
2	L5	982	U
2	L5	985	C
2	L5	989	U
2	L5	990	C
2	L5	991	C
2	L5	992	C
2	L5	993	G
2	L5	995	C
2	L5	1048	G
2	L5	1050	C
2	L5	1051	G
2	L5	1070	G
2	L5	1074	G
2	L5	1083	U
2	L5	1168	G
2	L5	1171	G
2	L5	1173	G
2	L5	1174	G
2	L5	1178	G
2	L5	1179	U
2	L5	1180	C

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Mol	Chain	Res	Type
2	L5	1182	C
2	L5	1183	C
2	L5	1198	G
2	L5	1203	G
2	L5	1205	G
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1222	A
2	L5	1253	G
2	L5	1254	A
2	L5	1255	A
2	L5	1258	G
2	L5	1259	G
2	L5	1261	G
2	L5	1266	G
2	L5	1269	G
2	L5	1270	A
2	L5	1272	C
2	L5	1273	G
2	L5	1274	A
2	L5	1277	G
2	L5	1280	C
2	L5	1284	G
2	L5	1285	U
2	L5	1287	G
2	L5	1293	G
2	L5	1295	C
2	L5	1304	C
2	L5	1313	C
2	L5	1326	A2M
2	L5	1337	A
2	L5	1354	A
2	L5	1359	G
2	L5	1365	C
2	L5	1367	C
2	L5	1387	A
2	L5	1397	A
2	L5	1399	G
2	L5	1402	C
2	L5	1404	G
2	L5	1405	C

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Mol	Chain	Res	Type
2	L5	1407	C
2	L5	1409	C
2	L5	1410	U
2	L5	1412	G
2	L5	1417	C
2	L5	1420	A
2	L5	1435	G
2	L5	1436	C
2	L5	1437	C
2	L5	1439	C
2	L5	1441	C
2	L5	1443	A
2	L5	1448	G
2	L5	1483	C
2	L5	1498	G
2	L5	1501	C
2	L5	1502	G
2	L5	1534	A2M
2	L5	1535	C
2	L5	1547	A
2	L5	1566	C
2	L5	1578	U
2	L5	1591	U
2	L5	1596	U
2	L5	1613	A
2	L5	1614	C
2	L5	1624	G
2	L5	1625	OMG
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1638	A
2	L5	1641	G
2	L5	1642	A
2	L5	1654	G
2	L5	1661	C
2	L5	1676	C
2	L5	1677	PSU
2	L5	1705	G
2	L5	1706	A
2	L5	1719	A
2	L5	1734	G

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Mol	Chain	Res	Type
2	L5	1735	U
2	L5	1742	A
2	L5	1750	G
2	L5	1755	C
2	L5	1756	U
2	L5	1757	U
2	L5	1758	G
2	L5	1759	G
2	L5	1761	G
2	L5	1774	C
2	L5	1787	A
2	L5	1804	A
2	L5	1805	A
2	L5	1810	G
2	L5	1821	G
2	L5	1822	U
2	L5	1834	U
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1843	A
2	L5	1855	G
2	L5	1869	G
2	L5	1897	A
2	L5	1918	U
2	L5	1919	G
2	L5	1921	C
2	L5	1922	G
2	L5	1925	G
2	L5	1931	C
2	L5	1932	A
2	L5	1948	G
2	L5	1959	U
2	L5	1960	A
2	L5	1962	A
2	L5	1966	C
2	L5	2025	A
2	L5	2026	A
2	L5	2046	G
2	L5	2048	U
2	L5	2055	G
2	L5	2056	G

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Mol	Chain	Res	Type
2	L5	2069	A
2	L5	2084	C
2	L5	2085	G
2	L5	2092	G
2	L5	2095	A
2	L5	2096	G
2	L5	2097	U
2	L5	2098	G
2	L5	2101	C
2	L5	2102	G
2	L5	2103	G
2	L5	2106	G
2	L5	2260	C
2	L5	2277	C
2	L5	2289	C
2	L5	2300	A
2	L5	2301	G
2	L5	2313	A
2	L5	2348	G
2	L5	2351	OMC
2	L5	2360	A
2	L5	2395	A
2	L5	2397	G
2	L5	2417	A
2	L5	2421	G
2	L5	2422	OMC
2	L5	2450	G
2	L5	2475	G
2	L5	2503	G
2	L5	2504	C
2	L5	2505	C
2	L5	2506	G
2	L5	2513	A
2	L5	2519	U
2	L5	2520	C
2	L5	2529	A
2	L5	2530	U
2	L5	2554	U
2	L5	2565	A
2	L5	2573	A
2	L5	2583	C
2	L5	2587	A

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Mol	Chain	Res	Type
2	L5	2589	C
2	L5	2601	A
2	L5	2627	C
2	L5	2631	U
2	L5	2638	G
2	L5	2653	C
2	L5	2662	G
2	L5	2669	C
2	L5	2687	U
2	L5	2695	A
2	L5	2696	A
2	L5	2703	G
2	L5	2705	G
2	L5	2711	G
2	L5	2712	G
2	L5	2725	A
2	L5	2726	G
2	L5	2743	A
2	L5	2756	G
2	L5	2763	U
2	L5	2764	A
2	L5	2788	U
2	L5	2790	U
2	L5	2796	G
2	L5	2798	A
2	L5	2814	C
2	L5	2826	U
2	L5	2827	G
2	L5	2829	U
2	L5	2838	G
2	L5	2855	G
2	L5	2877	G
2	L5	2903	G
2	L5	2905	C
2	L5	2906	G
2	L5	2907	G
2	L5	2908	U
2	L5	3585	G
2	L5	3590	G
2	L5	3591	C
2	L5	3593	C
2	L5	3594	C

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Mol	Chain	Res	Type
2	L5	3595	U
2	L5	3596	A
2	L5	3597	G
2	L5	3605	C
2	L5	3615	G
2	L5	3616	U
2	L5	3618	C
2	L5	3626	G
2	L5	3635	A
2	L5	3644	U
2	L5	3662	A
2	L5	3673	C
2	L5	3711	A
2	L5	3713	U
2	L5	3714	G
2	L5	3748	A
2	L5	3753	G
2	L5	3760	A2M
2	L5	3776	G
2	L5	3777	G
2	L5	3785	A2M
2	L5	3786	U
2	L5	3811	G
2	L5	3812	C
2	L5	3814	U
2	L5	3817	A
2	L5	3819	G
2	L5	3838	U
2	L5	3839	G
2	L5	3840	U
2	L5	3876	A
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3897	G
2	L5	3898	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3939	G

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Mol	Chain	Res	Type
2	L5	4076	G
2	L5	4084	G
2	L5	4091	G
2	L5	4096	C
2	L5	4097	G
2	L5	4099	G
2	L5	4100	C
2	L5	4101	C
2	L5	4119	C
2	L5	4122	G
2	L5	4127	A
2	L5	4133	C
2	L5	4135	G
2	L5	4137	C
2	L5	4140	C
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4145	C
2	L5	4162	C
2	L5	4163	U
2	L5	4170	A
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4203	A
2	L5	4222	G
2	L5	4229	U
2	L5	4233	A
2	L5	4251	A
2	L5	4254	G
2	L5	4257	A
2	L5	4266	G
2	L5	4268	A
2	L5	4273	A
2	L5	4281	A
2	L5	4291	G
2	L5	4305	G
2	L5	4306	OMU
2	L5	4329	G
2	L5	4330	G
2	L5	4332	C

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Mol	Chain	Res	Type
2	L5	4349	C
2	L5	4373	G
2	L5	4376	A
2	L5	4377	G
2	L5	4378	A
2	L5	4379	A
2	L5	4387	C
2	L5	4391	G
2	L5	4394	A
2	L5	4422	A
2	L5	4448	G
2	L5	4449	A
2	L5	4452	U
2	L5	4464	A
2	L5	4500	PSU
2	L5	4512	U
2	L5	4513	A
2	L5	4519	C
2	L5	4524	G
2	L5	4528	G
2	L5	4548	A
2	L5	4560	C
2	L5	4567	G
2	L5	4573	G
2	L5	4590	A2M
2	L5	4600	G
2	L5	4636	PSU
2	L5	4637	OMG
2	L5	4656	A
2	L5	4670	C
2	L5	4672	A
2	L5	4700	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4730	C
2	L5	4732	G
2	L5	4733	C
2	L5	4741	C
2	L5	4742	G
2	L5	4750	G
2	L5	4751	G

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Mol	Chain	Res	Type
2	L5	4754	G
2	L5	4757	C
2	L5	4759	C
2	L5	4765	G
2	L5	4772	C
2	L5	4775	C
2	L5	4776	G
2	L5	4860	G
2	L5	4862	G
2	L5	4870	OMG
2	L5	4871	C
2	L5	4876	U
2	L5	4882	U
2	L5	4883	C
2	L5	4886	C
2	L5	4887	C
2	L5	4895	C
2	L5	4896	G
2	L5	4900	C
2	L5	4901	G
2	L5	4910	A
2	L5	4912	G
2	L5	4923	C
2	L5	4931	G
2	L5	4934	A
2	L5	4937	C
2	L5	4940	C
2	L5	4943	A
2	L5	4944	C
2	L5	4945	G
2	L5	4960	G
2	L5	4966	A
2	L5	4976	U
2	L5	4988	U
2	L5	4989	U
2	L5	4991	U
2	L5	5013	C
2	L5	5017	G
2	L5	5022	U
2	L5	5023	C
2	L5	5024	C
2	L5	5025	C

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Mol	Chain	Res	Type
2	L5	5028	G
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5050	C
2	L5	5054	C
2	L5	5062	G
2	L5	5068	G
4	L9	7	G
4	L9	33	U
4	L9	37	G
4	L9	38	U
4	L9	53	U
4	L9	54	A
4	L9	64	G
4	L9	110	G
4	L9	120	U
6	S4	5	G
6	S4	7	G
6	S4	8	U
6	S4	9	1MG
6	S4	11	C
6	S4	13	U
6	S4	14	A
6	S4	16	H2U
6	S4	17	G
6	S4	18	OMG
6	S4	19	A
6	S4	20	H2U
6	S4	21	A
6	S4	28	C
6	S4	42	G
6	S4	47	H2U
6	S4	48	U
6	S4	49	G
6	S4	52	G
6	S4	60	U
6	S4	61	C
6	S4	62	C
6	S4	69	G
6	S4	74	C
48	S2	2	A

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Mol	Chain	Res	Type
48	S2	33	G
48	S2	41	G
48	S2	44	U
48	S2	46	A
48	S2	56	G
48	S2	62	G
48	S2	65	C
48	S2	67	C
48	S2	68	A
48	S2	71	G
48	S2	72	C
48	S2	73	C
48	S2	74	G
48	S2	76	U
48	S2	103	A
48	S2	113	G
48	S2	115	U
48	S2	126	G
48	S2	130	G
48	S2	143	U
48	S2	149	A
48	S2	150	A
48	S2	155	G
48	S2	163	U
48	S2	168	C
48	S2	173	A
48	S2	178	C
48	S2	182	C
48	S2	196	C
48	S2	197	U
48	S2	198	U
48	S2	200	G
48	S2	203	G
48	S2	204	G
48	S2	205	G
48	S2	207	G
48	S2	209	A
48	S2	213	G
48	S2	302	A
48	S2	306	C
48	S2	307	G
48	S2	308	G

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Mol	Chain	Res	Type
48	S2	309	G
48	S2	311	C
48	S2	312	G
48	S2	319	C
48	S2	320	G
48	S2	323	C
48	S2	324	C
48	S2	325	C
48	S2	326	C
48	S2	328	U
48	S2	329	G
48	S2	332	G
48	S2	335	G
48	S2	347	G
48	S2	360	A
48	S2	362	C
48	S2	364	A
48	S2	369	C
48	S2	370	G
48	S2	385	G
48	S2	386	C
48	S2	409	C
48	S2	438	G
48	S2	448	A
48	S2	449	A
48	S2	450	C
48	S2	452	G
48	S2	464	A
48	S2	470	G
48	S2	472	C
48	S2	474	G
48	S2	482	G
48	S2	487	U
48	S2	488	U
48	S2	492	C
48	S2	493	A
48	S2	516	A
48	S2	525	A
48	S2	537	C
48	S2	538	U
48	S2	540	U
48	S2	541	U

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Mol	Chain	Res	Type
48	S2	542	U
48	S2	544	G
48	S2	546	G
48	S2	547	G
48	S2	553	U
48	S2	554	A
48	S2	555	A
48	S2	556	U
48	S2	563	G
48	S2	564	A
48	S2	570	C
48	S2	576	A2M
48	S2	587	A
48	S2	589	G
48	S2	591	U
48	S2	592	C
48	S2	606	G
48	S2	607	U
48	S2	614	C
48	S2	617	G
48	S2	626	G
48	S2	628	A
48	S2	643	A
48	S2	655	A
48	S2	660	C
48	S2	668	A2M
48	S2	669	A
48	S2	671	A
48	S2	672	A
48	S2	673	G
48	S2	688	U
48	S2	799	OMU
48	S2	821	G
48	S2	822	PSU
48	S2	830	A
48	S2	835	C
48	S2	836	G
48	S2	837	A
48	S2	839	C
48	S2	840	C
48	S2	841	G
48	S2	847	A

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Mol	Chain	Res	Type
48	S2	870	A
48	S2	872	A
48	S2	875	A
48	S2	880	G
48	S2	884	C
48	S2	888	U
48	S2	889	U
48	S2	891	G
48	S2	892	U
48	S2	896	U
48	S2	897	U
48	S2	898	U
48	S2	900	C
48	S2	901	G
48	S2	903	A
48	S2	913	A
48	S2	920	A
48	S2	922	A
48	S2	933	G
48	S2	943	U
48	S2	956	G
48	S2	990	A
48	S2	992	A
48	S2	1001	A
48	S2	1017	U
48	S2	1023	A
48	S2	1060	A
48	S2	1061	U
48	S2	1062	A
48	S2	1083	A
48	S2	1085	C
48	S2	1109	C
48	S2	1115	U
48	S2	1116	C
48	S2	1131	G
48	S2	1154	U
48	S2	1195	A
48	S2	1207	G
48	S2	1215	C
48	S2	1227	G
48	S2	1242	U
48	S2	1248	B8N

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Mol	Chain	Res	Type
48	S2	1251	A
48	S2	1253	A
48	S2	1256	G
48	S2	1257	G
48	S2	1259	A
48	S2	1274	G
48	S2	1275	G
48	S2	1282	A
48	S2	1283	C
48	S2	1284	A
48	S2	1286	G
48	S2	1289	U
48	S2	1294	G
48	S2	1295	A
48	S2	1302	G
48	S2	1303	C
48	S2	1304	U
48	S2	1308	U
48	S2	1320	G
48	S2	1343	U
48	S2	1345	G
48	S2	1371	U
48	S2	1372	U
48	S2	1378	A
48	S2	1393	G
48	S2	1397	U
48	S2	1402	A
48	S2	1405	A
48	S2	1406	G
48	S2	1421	A
48	S2	1422	G
48	S2	1423	C
48	S2	1433	C
48	S2	1435	C
48	S2	1436	C
48	S2	1438	A
48	S2	1454	A
48	S2	1463	U
48	S2	1487	A
48	S2	1489	A
48	S2	1490	OMG
48	S2	1497	G

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Mol	Chain	Res	Type
48	S2	1498	A
48	S2	1521	C
48	S2	1522	A
48	S2	1533	A
48	S2	1546	G
48	S2	1556	A
48	S2	1560	U
48	S2	1579	A
48	S2	1580	A
48	S2	1585	U
48	S2	1587	G
48	S2	1588	A
48	S2	1600	G
48	S2	1606	G
48	S2	1621	U
48	S2	1623	A
48	S2	1639	7MG
48	S2	1654	G
48	S2	1661	A
48	S2	1665	G
48	S2	1680	G
48	S2	1698	C
48	S2	1699	A
48	S2	1721	U
48	S2	1722	G
48	S2	1825	A
48	S2	1826	G
48	S2	1829	G
48	S2	1838	U
48	S2	1849	G
48	S2	1851	MA6
48	S2	1852	C
48	S2	1861	G
48	S2	1862	G
48	S2	1863	A
48	S2	1864	U
48	S2	1865	C
49	S5	40	G

All (16) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
2	L5	42	A
2	L5	464	G
2	L5	465	G
2	L5	1590	C
2	L5	1613	A
2	L5	1633	G
2	L5	2529	A
2	L5	2587	A
2	L5	3876	A
2	L5	4699	U
6	S4	19	A
6	S4	60	U
48	S2	836	G
48	S2	874	G
48	S2	912	C
48	S2	1520	G

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

235 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	1MG	S4	37	6	23,26,27	0.61	0	33,39,42	0.71	1 (3%)
48	OMC	S2	462	48	19,22,23	0.80	0	25,31,34	0.85	0
71	HY3	SX	62	71,85	7,8,9	0.98	0	7,10,12	1.08	1 (14%)
2	A2M	L5	1524	2	22,25,26	1.41	2 (9%)	30,36,39	0.94	2 (6%)
48	PSU	S2	36	48	18,21,22	1.39	3 (16%)	21,30,33	1.97	4 (19%)
48	OMU	S2	1442	48	19,22,23	1.24	4 (21%)	25,31,34	1.80	4 (16%)
2	PSU	L5	4972	2	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
48	OMU	S2	116	48	19,22,23	1.20	3 (15%)	25,31,34	1.82	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4420	2	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
48	OMC	S2	174	48	19,22,23	0.79	0	25,31,34	0.83	0
48	PSU	S2	1244	48	18,21,22	1.36	2 (11%)	21,30,33	2.06	3 (14%)
48	OMU	S2	1288	48	19,22,23	1.21	2 (10%)	25,31,34	1.90	6 (24%)
48	PSU	S2	918	48	18,21,22	1.40	3 (16%)	21,30,33	2.10	5 (23%)
2	PSU	L5	3884	2	18,21,22	1.40	3 (16%)	21,30,33	2.03	4 (19%)
2	OMG	L5	4623	2	23,26,27	1.20	3 (13%)	32,38,41	2.08	5 (15%)
6	H2U	S4	16	6	18,21,22	0.63	0	19,30,33	0.54	0
2	OMC	L5	1340	2	19,22,23	0.80	0	25,31,34	0.85	1 (4%)
2	PSU	L5	4689	2	18,21,22	1.42	3 (16%)	21,30,33	2.04	4 (19%)
2	OMG	L5	1522	2	23,26,27	1.17	2 (8%)	32,38,41	2.07	7 (21%)
48	PSU	S2	1347	48	18,21,22	1.36	2 (11%)	21,30,33	2.16	4 (19%)
48	A2M	S2	1031	48	22,25,26	1.30	1 (4%)	30,36,39	1.03	1 (3%)
6	1MA	S4	58	6	21,25,26	0.41	0	30,37,40	0.55	0
6	5MU	S4	54	6	19,22,23	0.25	0	27,32,35	0.31	0
48	PSU	S2	801	48	18,21,22	1.39	3 (16%)	21,30,33	2.07	5 (23%)
48	6MZ	S2	1832	84,85,48	22,25,26	1.54	4 (18%)	29,36,39	2.09	9 (31%)
2	A2M	L5	3825	2	22,25,26	1.34	2 (9%)	30,36,39	0.95	1 (3%)
48	OMC	S2	1391	48	19,22,23	0.79	0	25,31,34	0.81	0
2	PSU	L5	2508	2	18,21,22	1.32	3 (16%)	21,30,33	2.00	4 (19%)
48	A2M	S2	99	84,48	22,25,26	1.31	1 (4%)	30,36,39	1.01	2 (6%)
2	A2M	L5	2787	2	22,25,26	1.44	2 (9%)	30,36,39	0.99	1 (3%)
48	PSU	S2	93	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	3 (14%)
2	OMG	L5	3944	2	23,26,27	1.21	3 (13%)	32,38,41	1.96	6 (18%)
2	PSU	L5	4471	2	18,21,22	1.44	3 (16%)	21,30,33	1.95	4 (19%)
48	MA6	S2	1850	48	23,26,27	1.58	5 (21%)	33,38,41	2.26	14 (42%)
48	PSU	S2	814	48	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
48	OMC	S2	1710	48	19,22,23	0.80	0	25,31,34	0.96	1 (4%)
2	5MC	L5	3782	2,84	19,22,23	1.65	3 (15%)	26,32,35	1.04	2 (7%)
2	A2M	L5	3867	2	22,25,26	1.30	1 (4%)	30,36,39	0.95	2 (6%)
2	PSU	L5	3920	2,84	18,21,22	1.38	2 (11%)	21,30,33	2.13	6 (28%)
2	OMU	L5	3925	2	19,22,23	1.23	2 (10%)	25,31,34	1.85	5 (20%)
2	PSU	L5	3853	2,84	18,21,22	1.40	2 (11%)	21,30,33	2.01	3 (14%)
2	PSU	L5	4431	2	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
2	OMG	L5	2364	2	23,26,27	1.14	3 (13%)	32,38,41	2.02	7 (21%)
2	OMG	L5	3744	2	23,26,27	1.17	3 (13%)	32,38,41	1.96	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	L5	4456	2	19,22,23	0.78	0	25,31,34	0.88	1 (4%)
48	A2M	S2	1383	48	22,25,26	1.30	2 (9%)	30,36,39	1.16	5 (16%)
48	OMG	S2	867	48	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
2	OMC	L5	3701	85,2	19,22,23	0.77	0	25,31,34	0.87	1 (4%)
2	PSU	L5	4552	2	18,21,22	1.33	2 (11%)	21,30,33	2.21	3 (14%)
2	PSU	L5	2632	2	18,21,22	1.42	3 (16%)	21,30,33	2.02	3 (14%)
2	PSU	L5	4457	2	18,21,22	1.33	2 (11%)	21,30,33	2.08	4 (19%)
48	OMG	S2	683	48	23,26,27	1.16	2 (8%)	32,38,41	2.04	6 (18%)
2	UY1	L5	3818	85,2	19,22,23	1.55	5 (26%)	21,31,34	1.88	5 (23%)
2	PSU	L5	4521	85,2,84	18,21,22	1.36	2 (11%)	21,30,33	2.11	4 (19%)
48	PSU	S2	210	48	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
2	OMG	L5	4618	2	23,26,27	1.17	3 (13%)	32,38,41	2.03	6 (18%)
2	PSU	L5	1792	85,2	18,21,22	1.32	2 (11%)	21,30,33	1.98	3 (14%)
48	A2M	S2	468	48	22,25,26	1.41	2 (9%)	30,36,39	0.98	2 (6%)
43	M3L	Lo	98	43	10,11,12	1.04	0	9,14,16	0.67	0
2	OMC	L5	3808	2	19,22,23	0.75	0	25,31,34	0.78	0
48	OMU	S2	1326	84,48	19,22,23	1.21	3 (15%)	25,31,34	1.84	5 (20%)
2	6MZ	L5	4220	2	22,25,26	1.56	4 (18%)	29,36,39	2.14	9 (31%)
2	OMG	L5	2050	2	23,26,27	1.17	3 (13%)	32,38,41	1.95	5 (15%)
2	A2M	L5	1534	2,84	22,25,26	1.33	2 (9%)	30,36,39	1.07	1 (3%)
8	V5N	LD	216	8	8,11,12	1.62	2 (25%)	8,14,16	1.77	3 (37%)
2	PSU	L5	4299	2	18,21,22	1.39	3 (16%)	21,30,33	1.96	4 (19%)
2	A2M	L5	2815	2	22,25,26	1.34	2 (9%)	30,36,39	0.90	1 (3%)
2	OMC	L5	4536	2	19,22,23	0.76	0	25,31,34	0.87	0
2	JMH	L5	1456	2	18,22,23	2.83	6 (33%)	23,32,35	0.91	1 (4%)
48	PSU	S2	1445	48	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
2	PSU	L5	4423	2	18,21,22	1.34	2 (11%)	21,30,33	2.09	4 (19%)
48	PSU	S2	866	48	18,21,22	1.39	2 (11%)	21,30,33	2.05	3 (14%)
2	OMG	L5	1316	2	23,26,27	1.21	4 (17%)	32,38,41	1.94	6 (18%)
48	A2M	S2	484	48	22,25,26	1.34	3 (13%)	30,36,39	0.90	1 (3%)
2	OMG	L5	1625	85,2	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
2	PSU	L5	3768	2	18,21,22	1.37	2 (11%)	21,30,33	2.20	4 (19%)
2	PSU	L5	4628	2	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
48	PSU	S2	218	48	18,21,22	1.38	3 (16%)	21,30,33	1.96	4 (19%)
48	OMU	S2	428	48	19,22,23	1.18	2 (10%)	25,31,34	1.84	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	1643	84,48	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)
2	2MG	L5	1517	2	23,26,27	1.31	2 (8%)	33,38,41	1.44	4 (12%)
2	OMC	L5	2365	2	19,22,23	0.75	0	25,31,34	0.78	0
2	OMU	L5	1773	2	19,22,23	1.22	3 (15%)	25,31,34	1.84	5 (20%)
48	PSU	S2	681	48	18,21,22	1.32	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	L5	4579	2	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
48	PSU	S2	1232	48	18,21,22	1.38	2 (11%)	21,30,33	2.02	3 (14%)
2	PSU	L5	5001	2	18,21,22	1.35	2 (11%)	21,30,33	2.09	3 (14%)
2	PSU	L5	4500	2	18,21,22	1.36	2 (11%)	21,30,33	2.11	5 (23%)
2	PSU	L5	1683	85,2	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
48	PSU	S2	1625	48	18,21,22	1.36	2 (11%)	21,30,33	2.02	3 (14%)
48	4AC	S2	1842	85,48	21,24,25	3.13	11 (52%)	28,34,37	0.98	1 (3%)
2	A2M	L5	2401	2	22,25,26	1.36	2 (9%)	30,36,39	0.94	1 (3%)
2	A2M	L5	1871	2,84	22,25,26	1.36	3 (13%)	30,36,39	1.06	1 (3%)
2	PSU	L5	3637	85,2	18,21,22	1.34	2 (11%)	21,30,33	2.13	4 (19%)
2	OMC	L5	3869	2	19,22,23	0.76	0	25,31,34	0.71	0
6	M2G	S4	26	6	24,27,28	0.42	0	33,40,43	0.44	0
2	OMG	L5	4499	2	23,26,27	1.16	3 (13%)	32,38,41	2.09	7 (21%)
48	PSU	S2	1692	48	18,21,22	1.40	2 (11%)	21,30,33	2.06	4 (19%)
2	OMC	L5	1881	2,84	19,22,23	0.77	0	25,31,34	0.96	1 (4%)
48	PSU	S2	966	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	4 (19%)
2	OMC	L5	3887	2	19,22,23	0.78	0	25,31,34	0.83	0
2	OMC	L5	2824	2	19,22,23	0.78	0	25,31,34	0.74	0
48	7MG	S2	1639	6,48	23,26,27	1.09	1 (4%)	27,39,42	0.85	2 (7%)
2	OMU	L5	2837	2	19,22,23	1.25	3 (15%)	25,31,34	1.90	5 (20%)
2	PSU	L5	4353	2	18,21,22	1.32	3 (16%)	21,30,33	2.05	4 (19%)
2	OMU	L5	4306	2	19,22,23	1.24	3 (15%)	25,31,34	1.75	4 (16%)
48	PSU	S2	1174	85,48	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
48	PSU	S2	1238	48	18,21,22	1.39	2 (11%)	21,30,33	2.13	4 (19%)
48	PSU	S2	1367	48	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
48	PSU	S2	406	48	18,21,22	1.38	3 (16%)	21,30,33	2.11	4 (19%)
2	OMG	L5	3899	2	23,26,27	1.18	3 (13%)	32,38,41	2.10	6 (18%)
48	OMG	S2	436	48	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
2	OMU	L5	4498	2	19,22,23	1.20	3 (15%)	25,31,34	1.91	5 (20%)
2	PSU	L5	3851	2	18,21,22	1.39	2 (11%)	21,30,33	1.98	5 (23%)
6	PSU	S4	27	6	18,21,22	0.92	1 (5%)	21,30,33	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	3715	2	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
48	A2M	S2	1678	48	22,25,26	1.42	3 (13%)	30,36,39	1.00	2 (6%)
2	PSU	L5	5010	2	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
1	OMG	L1	75	1	23,26,27	1.17	3 (13%)	32,38,41	2.00	6 (18%)
30	MLZ	Lb	5	30	8,9,10	0.65	0	4,9,11	0.96	0
2	A2M	L5	398	2	22,25,26	1.42	2 (9%)	30,36,39	0.99	3 (10%)
48	PSU	S2	863	48	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	L5	3730	2	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
2	OMG	L5	4870	2	23,26,27	1.18	3 (13%)	32,38,41	1.93	6 (18%)
2	OMU	L5	4620	2	19,22,23	1.23	3 (15%)	25,31,34	1.64	5 (20%)
1	PSU	L1	69	1	18,21,22	1.44	2 (11%)	21,30,33	2.14	5 (23%)
2	2MG	L5	4872	2	23,26,27	1.28	2 (8%)	33,38,41	1.43	4 (12%)
2	PSU	L5	4673	2	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
48	MA6	S2	1851	48	23,26,27	1.56	4 (17%)	33,38,41	2.30	13 (39%)
48	PSU	S2	1046	48	18,21,22	1.35	2 (11%)	21,30,33	1.91	4 (19%)
2	PSU	L5	1781	2	18,21,22	1.43	3 (16%)	21,30,33	1.99	3 (14%)
2	PSU	L5	4403	2	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
2	A2M	L5	3785	2	22,25,26	1.36	3 (13%)	30,36,39	1.30	3 (10%)
2	PSU	L5	3770	2	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
2	OMC	L5	2351	2,84	19,22,23	0.78	0	25,31,34	0.92	1 (4%)
2	OMG	L5	2876	2	23,26,27	1.17	3 (13%)	32,38,41	1.99	6 (18%)
48	OMU	S2	121	48	19,22,23	1.19	3 (15%)	25,31,34	1.80	5 (20%)
48	PSU	S2	686	48	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
48	PSU	S2	822	48	18,21,22	1.36	2 (11%)	21,30,33	1.97	4 (19%)
48	A2M	S2	166	48	22,25,26	1.40	3 (13%)	30,36,39	1.05	2 (6%)
2	OMG	L5	2424	2	23,26,27	1.20	3 (13%)	32,38,41	1.94	6 (18%)
48	OMU	S2	172	48	19,22,23	1.20	2 (10%)	25,31,34	1.89	5 (20%)
48	OMG	S2	1328	85,48	23,26,27	1.17	3 (13%)	32,38,41	1.94	6 (18%)
6	1MG	S4	9	6,84	23,26,27	0.63	0	33,39,42	0.78	1 (3%)
2	A2M	L5	3718	2	22,25,26	1.27	2 (9%)	30,36,39	1.01	2 (6%)
6	PSU	S4	55	6	18,21,22	0.92	1 (5%)	21,30,33	0.72	0
2	A2M	L5	4590	2	22,25,26	1.34	2 (9%)	30,36,39	1.03	1 (3%)
48	PSU	S2	109	48	18,21,22	1.37	3 (16%)	21,30,33	2.01	3 (14%)
48	PSU	S2	609	48	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
48	PSU	S2	1004	48	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	PSU	S2	1056	48	18,21,22	1.37	3 (16%)	21,30,33	1.97	4 (19%)
48	A2M	S2	159	48	22,25,26	1.38	3 (13%)	30,36,39	1.03	3 (10%)
2	OMG	L5	3792	85,2	23,26,27	1.22	3 (13%)	32,38,41	2.02	6 (18%)
2	PSU	L5	3764	2	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
48	OMC	S2	517	48	19,22,23	0.78	0	25,31,34	0.83	0
2	OMG	L5	4392	2	23,26,27	1.17	4 (17%)	32,38,41	2.00	6 (18%)
48	PSU	S2	815	48	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
5	HIC	LB	245	5	10,11,12	1.25	0	9,14,16	2.58	3 (33%)
2	A2M	L5	4571	2	22,25,26	1.38	2 (9%)	30,36,39	0.94	2 (6%)
2	PSU	L5	4361	2	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
1	PSU	L1	55	1	18,21,22	1.39	3 (16%)	21,30,33	2.13	4 (19%)
2	PSU	L5	1582	2	18,21,22	1.41	2 (11%)	21,30,33	2.05	3 (14%)
2	PSU	L5	4532	2	18,21,22	1.42	3 (16%)	21,30,33	2.03	3 (14%)
2	PSU	L5	3734	2	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)
29	V5N	La	39	29	8,11,12	1.56	1 (12%)	8,14,16	1.94	3 (37%)
48	A2M	S2	576	85,48	22,25,26	1.31	2 (9%)	30,36,39	1.04	2 (6%)
48	PSU	S2	823	48	18,21,22	1.35	2 (11%)	21,30,33	2.11	5 (23%)
48	PSU	S2	1177	48	18,21,22	1.34	2 (11%)	21,30,33	2.19	4 (19%)
48	OMC	S2	1703	84,48	19,22,23	0.76	0	25,31,34	0.78	0
2	PSU	L5	4312	2	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
6	H2U	S4	47	6	18,21,22	0.63	0	19,30,33	0.45	0
2	OMG	L5	4228	2	23,26,27	1.20	3 (13%)	32,38,41	2.02	6 (18%)
48	OMG	S2	509	84,48	23,26,27	1.21	3 (13%)	32,38,41	1.96	5 (15%)
2	2MG	L5	729	2	23,26,27	1.30	2 (8%)	33,38,41	1.44	4 (12%)
48	OMG	S2	1490	84,48	23,26,27	1.18	3 (13%)	32,38,41	1.90	6 (18%)
2	A2M	L5	1326	2	22,25,26	1.36	2 (9%)	30,36,39	0.95	2 (6%)
48	PSU	S2	649	48	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
2	OMC	L5	2861	2	19,22,23	0.78	0	25,31,34	0.80	0
2	OMG	L5	4196	6,2	23,26,27	1.17	3 (13%)	32,38,41	2.03	7 (21%)
48	A2M	S2	512	48	22,25,26	1.38	2 (9%)	30,36,39	1.02	1 (3%)
48	A2M	S2	27	84,48	22,25,26	1.32	1 (4%)	30,36,39	0.99	1 (3%)
2	PSU	L5	4576	2	18,21,22	1.36	2 (11%)	21,30,33	2.08	3 (14%)
48	OMG	S2	601	48	23,26,27	1.18	3 (13%)	32,38,41	1.98	6 (18%)
2	OMC	L5	2804	2	19,22,23	0.79	1 (5%)	25,31,34	0.75	0
48	PSU	S2	1045	48	18,21,22	1.37	2 (11%)	21,30,33	2.09	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	3695	85,2,84	18,21,22	1.35	2 (11%)	21,30,33	2.15	5 (23%)
48	PSU	S2	119	48	18,21,22	1.37	2 (11%)	21,30,33	2.04	3 (14%)
48	PSU	S2	572	85,48	18,21,22	1.41	2 (11%)	21,30,33	2.08	4 (19%)
2	PSU	L5	1862	2	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
2	OMG	L5	4370	2	23,26,27	1.15	3 (13%)	32,38,41	2.09	7 (21%)
6	2MG	S4	10	6	23,26,27	0.36	0	33,38,41	0.44	0
2	PSU	L5	4442	2	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
48	OMU	S2	799	48	19,22,23	1.25	4 (21%)	25,31,34	1.78	5 (20%)
2	OMU	L5	2415	2	19,22,23	1.25	4 (21%)	25,31,34	1.72	5 (20%)
2	OMU	L5	4227	2	19,22,23	1.24	3 (15%)	25,31,34	1.83	5 (20%)
6	OMG	S4	18	6	23,26,27	0.33	0	32,38,41	0.44	0
48	OMU	S2	1804	48	19,22,23	1.24	3 (15%)	25,31,34	1.82	4 (16%)
48	A2M	S2	668	84,48	22,25,26	1.48	5 (22%)	30,36,39	1.00	1 (3%)
48	PSU	S2	105	48	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
2	PSU	L5	3758	2	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)
2	A2M	L5	400	2	22,25,26	1.36	2 (9%)	30,36,39	0.91	0
2	PSU	L5	3639	2	18,21,22	1.41	2 (11%)	21,30,33	2.08	6 (28%)
2	PSU	L5	1782	2	18,21,22	1.36	2 (11%)	21,30,33	2.09	3 (14%)
2	OMC	L5	3841	2	19,22,23	0.78	0	25,31,34	0.79	0
2	OMG	L5	4494	2	23,26,27	1.18	2 (8%)	32,38,41	1.97	6 (18%)
63	IAS	SO	138	63	6,7,8	1.10	0	3,8,10	2.15	1 (33%)
2	PSU	L5	1860	2	18,21,22	1.37	3 (16%)	21,30,33	1.92	4 (19%)
2	5MC	L5	4447	85,2	19,22,23	1.70	3 (15%)	26,32,35	1.27	2 (7%)
2	A2M	L5	4523	2,84	22,25,26	1.43	4 (18%)	30,36,39	1.15	2 (6%)
2	PSU	L5	1536	2	18,21,22	1.37	2 (11%)	21,30,33	1.99	4 (19%)
2	PSU	L5	4296	2	18,21,22	1.40	2 (11%)	21,30,33	2.08	4 (19%)
6	H2U	S4	20	6	18,21,22	0.68	1 (5%)	19,30,33	0.51	0
2	PSU	L5	3762	2	18,21,22	1.42	2 (11%)	21,30,33	2.10	4 (19%)
2	A2M	L5	2363	2,84	22,25,26	1.32	2 (9%)	30,36,39	0.95	2 (6%)
2	PSU	L5	3844	2	18,21,22	1.38	3 (16%)	21,30,33	2.03	3 (14%)
2	UR3	L5	4530	2	19,22,23	0.94	0	26,32,35	1.70	2 (7%)
2	A2M	L5	3830	2	22,25,26	1.40	2 (9%)	30,36,39	1.05	2 (6%)
2	1MA	L5	1322	2,84	21,25,26	0.78	1 (4%)	30,37,40	1.15	3 (10%)
2	OMG	L5	1760	2	23,26,27	1.19	3 (13%)	32,38,41	2.01	6 (18%)
48	A2M	S2	590	48	22,25,26	1.48	3 (13%)	30,36,39	1.02	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4636	2	18,21,22	1.41	3 (16%)	21,30,33	2.04	4 (19%)
48	PSU	S2	34	48	18,21,22	1.39	3 (16%)	21,30,33	2.02	4 (19%)
2	A2M	L5	3760	2,48	22,25,26	1.44	3 (13%)	30,36,39	0.99	1 (3%)
48	OMG	S2	644	48	23,26,27	1.20	3 (13%)	32,38,41	2.02	6 (18%)
2	PSU	L5	4293	2	18,21,22	1.38	2 (11%)	21,30,33	2.01	3 (14%)
48	PSU	S2	651	48	18,21,22	1.36	2 (11%)	21,30,33	2.12	4 (19%)
2	PSU	L5	1744	85,2	18,21,22	1.33	2 (11%)	21,30,33	2.08	4 (19%)
48	B8N	S2	1248	48	25,29,30	3.33	8 (32%)	28,42,45	2.04	8 (28%)
2	PSU	L5	1677	2	18,21,22	1.44	3 (16%)	21,30,33	2.08	4 (19%)
48	PSU	S2	1081	48	18,21,22	1.42	2 (11%)	21,30,33	2.09	5 (23%)
48	4AC	S2	1337	48	21,24,25	3.20	11 (52%)	28,34,37	1.08	3 (10%)
48	OMU	S2	627	48	19,22,23	1.20	2 (10%)	25,31,34	1.77	5 (20%)
2	OMC	L5	2422	2,84	19,22,23	0.79	0	25,31,34	0.74	0
33	MLZ	Le	53	33	8,9,10	0.68	0	4,9,11	0.80	0
2	OMG	L5	4637	85,2	23,26,27	1.16	3 (13%)	32,38,41	2.05	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1MG	S4	37	6	-	0/7/25/26	0/3/3/3
48	OMC	S2	462	48	-	0/9/27/28	0/2/2/2
71	HY3	SX	62	71,85	-	0/1/12/14	0/1/1/1
2	A2M	L5	1524	2	-	1/9/27/28	0/3/3/3
48	PSU	S2	36	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	1442	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
48	OMU	S2	116	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	4420	2	-	0/7/25/26	0/2/2/2
48	OMC	S2	174	48	-	1/9/27/28	0/2/2/2
48	PSU	S2	1244	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	1288	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	918	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
6	H2U	S4	16	6	-	3/7/38/39	0/2/2/2
2	OMC	L5	1340	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
48	PSU	S2	1347	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	1031	48	-	0/9/27/28	0/3/3/3
6	1MA	S4	58	6	-	2/7/25/26	0/3/3/3
6	5MU	S4	54	6	-	0/7/25/26	0/2/2/2
48	PSU	S2	801	48	-	0/7/25/26	0/2/2/2
48	6MZ	S2	1832	84,85,48	-	2/9/27/28	0/3/3/3
2	A2M	L5	3825	2	-	0/9/27/28	0/3/3/3
48	OMC	S2	1391	48	-	0/9/27/28	0/2/2/2
2	PSU	L5	2508	2	-	0/7/25/26	0/2/2/2
48	A2M	S2	99	84,48	-	1/9/27/28	0/3/3/3
2	A2M	L5	2787	2	-	4/9/27/28	0/3/3/3
48	PSU	S2	93	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	3944	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
48	MA6	S2	1850	48	-	1/11/29/30	0/3/3/3
48	PSU	S2	814	48	-	0/7/25/26	0/2/2/2
48	OMC	S2	1710	48	-	0/9/27/28	0/2/2/2
2	5MC	L5	3782	2,84	-	0/7/25/26	0/2/2/2
2	A2M	L5	3867	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	3920	2,84	-	0/7/25/26	0/2/2/2
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3853	2,84	-	0/7/25/26	0/2/2/2
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2364	2	-	1/9/27/28	0/3/3/3
2	OMG	L5	3744	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
48	A2M	S2	1383	48	-	1/9/27/28	0/3/3/3
48	OMG	S2	867	48	-	0/9/27/28	0/3/3/3
2	OMC	L5	3701	85,2	-	4/9/27/28	0/2/2/2
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	2632	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
48	OMG	S2	683	48	-	1/9/27/28	0/3/3/3
2	UY1	L5	3818	85,2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4521	85,2,84	-	0/7/25/26	0/2/2/2
48	PSU	S2	210	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	4618	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1792	85,2	-	0/7/25/26	0/2/2/2
48	A2M	S2	468	48	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	M3L	Lo	98	43	-	0/9/10/12	-
2	OMC	L5	3808	2	-	0/9/27/28	0/2/2/2
48	OMU	S2	1326	84,48	-	0/9/27/28	0/2/2/2
2	6MZ	L5	4220	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	2050	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	1534	2,84	-	1/9/27/28	0/3/3/3
8	V5N	LD	216	8	-	1/9/10/12	0/1/1/1
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2815	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	JMH	L5	1456	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1445	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4423	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	866	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	1316	2	-	0/9/27/28	0/3/3/3
48	A2M	S2	484	48	-	0/9/27/28	0/3/3/3
2	OMG	L5	1625	85,2	-	1/9/27/28	0/3/3/3
2	PSU	L5	3768	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	218	48	-	0/7/25/26	0/2/2/2
48	OMU	S2	428	48	-	4/9/27/28	0/2/2/2
48	PSU	S2	1643	84,48	-	0/7/25/26	0/2/2/2
2	2MG	L5	1517	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2365	2	-	0/9/27/28	0/2/2/2
2	OMU	L5	1773	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	681	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1232	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
2	PSU	L5	1683	85,2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1625	48	-	0/7/25/26	0/2/2/2
48	4AC	S2	1842	85,48	-	0/11/29/30	0/2/2/2
2	A2M	L5	2401	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	1871	2,84	-	0/9/27/28	0/3/3/3
2	PSU	L5	3637	85,2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3869	2	-	1/9/27/28	0/2/2/2
6	M2G	S4	26	6	-	0/11/29/30	0/3/3/3
2	OMG	L5	4499	2	-	1/9/27/28	0/3/3/3
48	PSU	S2	1692	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	1881	2,84	-	0/9/27/28	0/2/2/2
48	PSU	S2	966	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L5	3887	2	-	0/9/27/28	0/2/2/2
2	OMC	L5	2824	2	-	0/9/27/28	0/2/2/2
48	7MG	S2	1639	6,48	-	2/7/37/38	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	1174	85,48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1238	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1367	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	406	48	-	0/7/25/26	0/2/2/2
2	OMG	L5	3899	2	-	0/9/27/28	0/3/3/3
48	OMG	S2	436	48	-	0/9/27/28	0/3/3/3
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3851	2	-	2/7/25/26	0/2/2/2
6	PSU	S4	27	6	-	0/7/25/26	0/2/2/2
2	PSU	L5	3715	2	-	0/7/25/26	0/2/2/2
48	A2M	S2	1678	48	-	1/9/27/28	0/3/3/3
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
1	OMG	L1	75	1	-	0/9/27/28	0/3/3/3
30	MLZ	Lb	5	30	-	2/7/8/10	-
2	A2M	L5	398	2	-	0/9/27/28	0/3/3/3
48	PSU	S2	863	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3730	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4870	2	-	3/9/27/28	0/3/3/3
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
1	PSU	L1	69	1	-	0/7/25/26	0/2/2/2
2	2MG	L5	4872	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4673	2	-	0/7/25/26	0/2/2/2
48	MA6	S2	1851	48	-	4/11/29/30	0/3/3/3
48	PSU	S2	1046	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	1781	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3785	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	3770	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2351	2,84	-	2/9/27/28	0/2/2/2
2	OMG	L5	2876	2	-	0/9/27/28	0/3/3/3
48	OMU	S2	121	48	-	0/9/27/28	0/2/2/2
48	PSU	S2	686	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	822	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	166	48	-	0/9/27/28	0/3/3/3
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	S2	172	48	-	0/9/27/28	0/2/2/2
48	OMG	S2	1328	85,48	-	0/9/27/28	0/3/3/3
6	1MG	S4	9	6,84	-	1/7/25/26	0/3/3/3
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3
6	PSU	S4	55	6	-	0/7/25/26	0/2/2/2
2	A2M	L5	4590	2	-	1/9/27/28	0/3/3/3
48	PSU	S2	109	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	609	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1004	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1056	48	-	0/7/25/26	0/2/2/2
48	A2M	S2	159	48	-	0/9/27/28	0/3/3/3
2	OMG	L5	3792	85,2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3764	2	-	0/7/25/26	0/2/2/2
48	OMC	S2	517	48	-	0/9/27/28	0/2/2/2
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
48	PSU	S2	815	48	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
1	PSU	L1	55	1	-	0/7/25/26	0/2/2/2
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3734	2	-	0/7/25/26	0/2/2/2
29	V5N	La	39	29	-	0/9/10/12	0/1/1/1
48	A2M	S2	576	85,48	-	2/9/27/28	0/3/3/3
48	PSU	S2	823	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	1177	48	-	0/7/25/26	0/2/2/2
48	OMC	S2	1703	84,48	-	0/9/27/28	0/2/2/2
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
6	H2U	S4	47	6	-	2/7/38/39	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
48	OMG	S2	509	84,48	-	0/9/27/28	0/3/3/3
2	2MG	L5	729	2	-	0/9/27/28	0/3/3/3
48	OMG	S2	1490	84,48	-	1/9/27/28	0/3/3/3
2	A2M	L5	1326	2	-	2/9/27/28	0/3/3/3
48	PSU	S2	649	48	-	0/7/25/26	0/2/2/2
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4196	6,2	-	0/9/27/28	0/3/3/3
48	A2M	S2	512	48	-	2/9/27/28	0/3/3/3
48	A2M	S2	27	84,48	-	0/9/27/28	0/3/3/3
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMG	S2	601	48	-	0/9/27/28	0/3/3/3
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
48	PSU	S2	1045	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3695	85,2,84	-	0/7/25/26	0/2/2/2
48	PSU	S2	119	48	-	0/7/25/26	0/2/2/2
48	PSU	S2	572	85,48	-	0/7/25/26	0/2/2/2
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3
6	2MG	S4	10	6	-	0/9/27/28	0/3/3/3
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
48	OMU	S2	799	48	-	1/9/27/28	0/2/2/2
2	OMU	L5	2415	2	-	0/9/27/28	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
6	OMG	S4	18	6	-	2/9/27/28	0/3/3/3
48	OMU	S2	1804	48	-	0/9/27/28	0/2/2/2
48	A2M	S2	668	84,48	-	2/9/27/28	0/3/3/3
48	PSU	S2	105	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	3758	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	400	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3841	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4494	2	-	0/9/27/28	0/3/3/3
63	IAS	SO	138	63	-	1/7/7/8	-
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	5MC	L5	4447	85,2	-	4/7/25/26	0/2/2/2
2	A2M	L5	4523	2,84	-	0/9/27/28	0/3/3/3
2	PSU	L5	1536	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
6	H2U	S4	20	6	-	2/7/38/39	0/2/2/2
2	PSU	L5	3762	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2363	2,84	-	1/9/27/28	0/3/3/3
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3830	2	-	0/9/27/28	0/3/3/3
2	1MA	L5	1322	2,84	-	2/7/25/26	0/3/3/3
2	OMG	L5	1760	2	-	0/9/27/28	0/3/3/3
48	A2M	S2	590	48	-	3/9/27/28	0/3/3/3
2	PSU	L5	4636	2	-	2/7/25/26	0/2/2/2
48	PSU	S2	34	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	L5	3760	2,48	-	5/9/27/28	0/3/3/3
48	OMG	S2	644	48	-	1/9/27/28	0/3/3/3
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	651	48	-	0/7/25/26	0/2/2/2
2	PSU	L5	1744	85,2	-	0/7/25/26	0/2/2/2
48	B8N	S2	1248	48	-	4/16/34/35	0/2/2/2
2	PSU	L5	1677	2	-	0/7/25/26	0/2/2/2
48	PSU	S2	1081	48	-	1/7/25/26	0/2/2/2
48	4AC	S2	1337	48	-	0/11/29/30	0/2/2/2
48	OMU	S2	627	48	-	2/9/27/28	0/2/2/2
2	OMC	L5	2422	2,84	-	0/9/27/28	0/2/2/2
33	MLZ	Le	53	33	-	2/7/8/10	-
2	OMG	L5	4637	85,2	-	0/9/27/28	0/3/3/3

All (513) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1248	B8N	C4-N3	-8.14	1.26	1.40
48	S2	1248	B8N	C6-N1	7.66	1.55	1.36
2	L5	1456	JMH	C2-N1	7.61	1.49	1.38
48	S2	1337	4AC	C4-N3	7.02	1.44	1.32
48	S2	1248	B8N	C4-C5	6.97	1.63	1.47
48	S2	1842	4AC	C4-N3	6.69	1.44	1.32
2	L5	1456	JMH	C6-C5	6.68	1.50	1.35
48	S2	1337	4AC	C6-C5	6.36	1.49	1.35
48	S2	1842	4AC	C6-C5	6.32	1.49	1.35
48	S2	1337	4AC	C2-N3	6.07	1.48	1.36
2	L5	3782	5MC	C5-C4	5.98	1.48	1.44
2	L5	4447	5MC	C5-C4	5.96	1.48	1.44
48	S2	1842	4AC	C2-N3	5.69	1.47	1.36
48	S2	1248	B8N	C2-N1	5.58	1.55	1.39
48	S2	1248	B8N	C6-C5	5.40	1.42	1.35
2	L5	4220	6MZ	C5-C4	4.92	1.47	1.39
48	S2	1850	MA6	C5-C4	4.86	1.47	1.39
48	S2	1851	MA6	C5-C4	4.86	1.47	1.39
48	S2	1832	6MZ	C5-C4	4.82	1.47	1.39
48	S2	1248	B8N	C1'-C5	-4.75	1.39	1.50
2	L5	1456	JMH	C2-N3	4.59	1.48	1.39
2	L5	729	2MG	C2-N2	4.52	1.42	1.33
2	L5	1517	2MG	C2-N2	4.51	1.42	1.33
2	L5	4872	2MG	C2-N2	4.46	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	1639	7MG	C5-N7	4.45	1.41	1.35
2	L5	1871	A2M	O5'-C5'	-4.28	1.31	1.44
2	L5	2787	A2M	O5'-C5'	-4.27	1.31	1.44
48	S2	1842	4AC	C2-N1	4.17	1.48	1.40
2	L5	3760	A2M	O5'-C5'	-4.16	1.32	1.44
2	L5	3830	A2M	O5'-C5'	-4.14	1.32	1.44
48	S2	1337	4AC	C2-N1	4.11	1.48	1.40
2	L5	4523	A2M	O5'-C5'	-4.02	1.32	1.44
2	L5	3825	A2M	O5'-C5'	-4.01	1.32	1.44
2	L5	3785	A2M	O5'-C5'	-3.98	1.32	1.44
2	L5	2401	A2M	O5'-C5'	-3.96	1.32	1.44
2	L5	2815	A2M	O5'-C5'	-3.93	1.32	1.44
2	L5	2363	A2M	O5'-C5'	-3.93	1.32	1.44
48	S2	1383	A2M	O5'-C5'	-3.92	1.32	1.44
48	S2	1842	4AC	C5-C4	3.92	1.49	1.41
48	S2	99	A2M	O5'-C5'	-3.91	1.32	1.44
48	S2	27	A2M	O5'-C5'	-3.91	1.32	1.44
2	L5	1326	A2M	O5'-C5'	-3.90	1.32	1.44
2	L5	398	A2M	O5'-C5'	-3.88	1.32	1.44
2	L5	3867	A2M	O5'-C5'	-3.88	1.32	1.44
2	L5	1524	A2M	O5'-C5'	-3.86	1.32	1.44
48	S2	468	A2M	O5'-C5'	-3.86	1.33	1.44
48	S2	512	A2M	O5'-C5'	-3.81	1.33	1.44
48	S2	1337	4AC	C5-C4	3.80	1.49	1.41
2	L5	4571	A2M	O5'-C5'	-3.78	1.33	1.44
2	L5	1534	A2M	O5'-C5'	-3.77	1.33	1.44
48	S2	668	A2M	O5'-C5'	-3.76	1.33	1.44
2	L5	400	A2M	O5'-C5'	-3.75	1.33	1.44
48	S2	1031	A2M	O5'-C5'	-3.72	1.33	1.44
48	S2	1842	4AC	O2-C2	-3.72	1.16	1.23
48	S2	1678	A2M	O5'-C5'	-3.69	1.33	1.44
2	L5	3639	PSU	C6-C5	3.69	1.39	1.35
2	L5	4403	PSU	C6-C5	3.68	1.39	1.35
48	S2	166	A2M	O5'-C5'	-3.66	1.33	1.44
2	L5	3718	A2M	O5'-C5'	-3.65	1.33	1.44
48	S2	1337	4AC	C7-N4	3.63	1.44	1.37
6	S4	55	PSU	C6-C5	3.62	1.39	1.35
48	S2	484	A2M	O5'-C5'	-3.60	1.33	1.44
48	S2	159	A2M	O5'-C5'	-3.59	1.33	1.44
2	L5	3884	PSU	C6-C5	3.57	1.39	1.35
48	S2	1232	PSU	C6-C5	3.56	1.39	1.35
2	L5	1781	PSU	C6-C5	3.56	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4532	PSU	C6-C5	3.56	1.39	1.35
2	L5	2632	PSU	C6-C5	3.56	1.39	1.35
6	S4	27	PSU	C6-C5	3.54	1.39	1.35
2	L5	3853	PSU	C6-C5	3.53	1.39	1.35
2	L5	4590	A2M	O5'-C5'	-3.53	1.33	1.44
2	L5	3818	UY1	C4-N3	-3.52	1.32	1.38
2	L5	3770	PSU	C6-C5	3.51	1.39	1.35
48	S2	590	A2M	O5'-C5'	-3.51	1.34	1.44
48	S2	1367	PSU	C6-C5	3.50	1.39	1.35
2	L5	4673	PSU	C6-C5	3.50	1.39	1.35
48	S2	1692	PSU	C6-C5	3.49	1.39	1.35
48	S2	572	PSU	C6-C5	3.48	1.39	1.35
1	L1	69	PSU	C6-C5	3.48	1.39	1.35
2	L5	1536	PSU	C6-C5	3.47	1.39	1.35
2	L5	3762	PSU	C6-C5	3.47	1.39	1.35
2	L5	3844	PSU	C6-C5	3.47	1.39	1.35
48	S2	1238	PSU	C6-C5	3.46	1.39	1.35
48	S2	649	PSU	C6-C5	3.46	1.39	1.35
48	S2	576	A2M	O5'-C5'	-3.46	1.34	1.44
2	L5	4296	PSU	C6-C5	3.45	1.39	1.35
2	L5	4636	PSU	C6-C5	3.45	1.39	1.35
48	S2	866	PSU	C6-C5	3.45	1.39	1.35
48	S2	1842	4AC	C7-N4	3.45	1.44	1.37
2	L5	4299	PSU	C6-C5	3.44	1.39	1.35
48	S2	1174	PSU	C6-C5	3.44	1.39	1.35
48	S2	1337	4AC	O2-C2	-3.42	1.17	1.23
48	S2	210	PSU	C6-C5	3.42	1.39	1.35
48	S2	918	PSU	C6-C5	3.42	1.39	1.35
2	L5	4471	PSU	C6-C5	3.41	1.39	1.35
2	L5	4361	PSU	C6-C5	3.41	1.39	1.35
48	S2	1337	4AC	C4-N4	3.40	1.45	1.39
2	L5	4579	PSU	C6-C5	3.40	1.39	1.35
2	L5	4521	PSU	C6-C5	3.38	1.39	1.35
48	S2	966	PSU	C6-C5	3.38	1.39	1.35
48	S2	1004	PSU	C6-C5	3.38	1.39	1.35
48	S2	36	PSU	C6-C5	3.37	1.39	1.35
2	L5	3734	PSU	C6-C5	3.37	1.39	1.35
2	L5	3637	PSU	C6-C5	3.37	1.39	1.35
48	S2	1081	PSU	C6-C5	3.37	1.39	1.35
48	S2	93	PSU	C6-C5	3.36	1.39	1.35
2	L5	3920	PSU	C6-C5	3.35	1.39	1.35
48	S2	1046	PSU	C6-C5	3.33	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4293	PSU	C6-C5	3.33	1.39	1.35
48	S2	119	PSU	C6-C5	3.32	1.39	1.35
48	S2	801	PSU	C6-C5	3.32	1.39	1.35
2	L5	3730	PSU	C6-C5	3.32	1.39	1.35
48	S2	815	PSU	C6-C5	3.31	1.39	1.35
2	L5	3851	PSU	C6-C5	3.31	1.39	1.35
48	S2	651	PSU	C6-C5	3.31	1.39	1.35
48	S2	863	PSU	C6-C5	3.30	1.38	1.35
2	L5	3768	PSU	C6-C5	3.30	1.38	1.35
48	S2	609	PSU	C6-C5	3.30	1.38	1.35
48	S2	1056	PSU	C6-C5	3.30	1.38	1.35
48	S2	1842	4AC	C6-N1	3.29	1.45	1.38
2	L5	3695	PSU	C6-C5	3.28	1.38	1.35
2	L5	1860	PSU	C6-C5	3.27	1.38	1.35
2	L5	5010	PSU	C6-C5	3.27	1.38	1.35
2	L5	3792	OMG	C5-C4	3.27	1.47	1.38
2	L5	4689	PSU	C6-C5	3.27	1.38	1.35
2	L5	4972	PSU	C6-C5	3.27	1.38	1.35
2	L5	4457	PSU	C6-C5	3.27	1.38	1.35
2	L5	1683	PSU	C6-C5	3.25	1.38	1.35
48	S2	686	PSU	C6-C5	3.24	1.38	1.35
48	S2	1045	PSU	C6-C5	3.23	1.38	1.35
48	S2	1445	PSU	C6-C5	3.23	1.38	1.35
48	S2	1625	PSU	C6-C5	3.23	1.38	1.35
2	L5	1862	PSU	C6-C5	3.23	1.38	1.35
2	L5	3764	PSU	C6-C5	3.22	1.38	1.35
48	S2	34	PSU	C6-C5	3.22	1.38	1.35
2	L5	3715	PSU	C6-C5	3.22	1.38	1.35
2	L5	4442	PSU	C6-C5	3.22	1.38	1.35
2	L5	4312	PSU	C6-C5	3.21	1.38	1.35
2	L5	1782	PSU	C6-C5	3.20	1.38	1.35
2	L5	4196	OMG	C5-C4	3.20	1.47	1.38
1	L1	55	PSU	C6-C5	3.19	1.38	1.35
2	L5	1625	OMG	C5-C4	3.19	1.47	1.38
48	S2	406	PSU	C6-C5	3.18	1.38	1.35
2	L5	1760	OMG	C5-C4	3.18	1.47	1.38
2	L5	4552	PSU	C6-C5	3.18	1.38	1.35
48	S2	105	PSU	C6-C5	3.18	1.38	1.35
2	L5	4576	PSU	C6-C5	3.17	1.38	1.35
2	L5	4431	PSU	C6-C5	3.16	1.38	1.35
48	S2	681	PSU	C6-C5	3.16	1.38	1.35
48	S2	823	PSU	C6-C5	3.16	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4423	PSU	C6-C5	3.16	1.38	1.35
2	L5	5001	PSU	C6-C5	3.16	1.38	1.35
48	S2	822	PSU	C6-C5	3.16	1.38	1.35
48	S2	1337	4AC	C6-N1	3.15	1.45	1.38
2	L5	4494	OMG	C5-C4	3.15	1.47	1.38
48	S2	218	PSU	C6-C5	3.15	1.38	1.35
2	L5	3944	OMG	C5-C4	3.14	1.47	1.38
29	La	39	V5N	CE1-ND1	3.14	1.40	1.35
2	L5	1582	PSU	C6-C5	3.14	1.38	1.35
2	L5	4392	OMG	C5-C4	3.14	1.47	1.38
48	S2	1643	PSU	C6-C5	3.14	1.38	1.35
48	S2	1347	PSU	C6-C5	3.13	1.38	1.35
48	S2	601	OMG	C5-C4	3.13	1.47	1.38
2	L5	3758	PSU	C6-C5	3.13	1.38	1.35
2	L5	1744	PSU	C6-C5	3.13	1.38	1.35
2	L5	4353	PSU	C6-C5	3.12	1.38	1.35
2	L5	4447	5MC	C6-C5	3.12	1.39	1.34
48	S2	1177	PSU	C6-C5	3.12	1.38	1.35
48	S2	109	PSU	C6-C5	3.12	1.38	1.35
2	L5	4623	OMG	C5-C4	3.11	1.47	1.38
2	L5	4628	PSU	C6-C5	3.11	1.38	1.35
2	L5	2050	OMG	C5-C4	3.11	1.47	1.38
2	L5	1316	OMG	C5-C4	3.10	1.47	1.38
48	S2	814	PSU	C6-C5	3.10	1.38	1.35
48	S2	1244	PSU	C6-C5	3.10	1.38	1.35
2	L5	2876	OMG	C5-C4	3.09	1.47	1.38
48	S2	1851	MA6	C5-C6	3.09	1.49	1.41
2	L5	4500	PSU	C6-C5	3.09	1.38	1.35
1	L1	75	OMG	C5-C4	3.09	1.47	1.38
2	L5	3744	OMG	C5-C4	3.09	1.47	1.38
48	S2	644	OMG	C5-C4	3.08	1.47	1.38
48	S2	867	OMG	C5-C4	3.08	1.47	1.38
2	L5	2424	OMG	C5-C4	3.07	1.47	1.38
48	S2	1328	OMG	C5-C4	3.07	1.47	1.38
48	S2	436	OMG	C5-C4	3.06	1.47	1.38
2	L5	4618	OMG	C5-C4	3.06	1.47	1.38
2	L5	1522	OMG	C5-C4	3.04	1.47	1.38
48	S2	509	OMG	C5-C4	3.04	1.47	1.38
2	L5	4870	OMG	C5-C4	3.03	1.47	1.38
48	S2	1850	MA6	C5-C6	3.03	1.49	1.41
2	L5	2508	PSU	C6-C5	3.02	1.38	1.35
48	S2	1490	OMG	C5-C4	3.01	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4228	OMG	C5-C4	3.00	1.47	1.38
2	L5	4420	PSU	C6-C5	3.00	1.38	1.35
2	L5	4370	OMG	C5-C4	2.99	1.46	1.38
2	L5	3899	OMG	C5-C4	2.98	1.46	1.38
2	L5	4637	OMG	C5-C4	2.97	1.46	1.38
48	S2	683	OMG	C5-C4	2.97	1.46	1.38
1	L1	69	PSU	C4-N3	-2.96	1.33	1.38
1	L1	55	PSU	C4-N3	-2.96	1.33	1.38
2	L5	4499	OMG	C5-C4	2.95	1.46	1.38
2	L5	4220	6MZ	C5-C6	2.94	1.49	1.41
2	L5	1677	PSU	C6-C5	2.93	1.38	1.35
48	S2	1842	4AC	C4-N4	2.92	1.44	1.39
8	LD	216	V5N	CE1-ND1	2.92	1.39	1.35
2	L5	2364	OMG	C5-C4	2.91	1.46	1.38
48	S2	801	PSU	C4-N3	-2.89	1.33	1.38
48	S2	814	PSU	C4-N3	-2.89	1.33	1.38
2	L5	3920	PSU	C4-N3	-2.89	1.33	1.38
2	L5	1677	PSU	C4-N3	-2.86	1.33	1.38
2	L5	3715	PSU	C4-N3	-2.86	1.33	1.38
2	L5	3758	PSU	C4-N3	-2.84	1.33	1.38
2	L5	3639	PSU	C4-N3	-2.84	1.33	1.38
2	L5	1792	PSU	C6-C5	2.84	1.38	1.35
48	S2	406	PSU	C4-N3	-2.82	1.33	1.38
2	L5	4299	PSU	C4-N3	-2.82	1.33	1.38
2	L5	4471	PSU	C4-N3	-2.82	1.33	1.38
2	L5	1781	PSU	C4-N3	-2.81	1.33	1.38
2	L5	3925	OMU	C4-N3	-2.81	1.33	1.38
48	S2	93	PSU	C4-N3	-2.81	1.33	1.38
2	L5	2837	OMU	C4-N3	-2.80	1.33	1.38
48	S2	1832	6MZ	C5-C6	2.80	1.48	1.41
48	S2	966	PSU	C4-N3	-2.80	1.33	1.38
2	L5	3851	PSU	C4-N3	-2.80	1.33	1.38
2	L5	3818	UY1	C4-C5	-2.79	1.36	1.44
2	L5	4689	PSU	C4-N3	-2.79	1.33	1.38
2	L5	3782	5MC	C6-C5	2.79	1.39	1.34
48	S2	1347	PSU	C4-N3	-2.79	1.33	1.38
2	L5	4579	PSU	C4-N3	-2.79	1.33	1.38
2	L5	4442	PSU	C4-N3	-2.78	1.33	1.38
2	L5	4293	PSU	C4-N3	-2.77	1.33	1.38
2	L5	1582	PSU	C4-N3	-2.76	1.33	1.38
48	S2	815	PSU	C4-N3	-2.76	1.33	1.38
2	L5	4673	PSU	C4-N3	-2.75	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	609	PSU	C4-N3	-2.75	1.33	1.38
2	L5	3695	PSU	C4-N3	-2.75	1.33	1.38
48	S2	36	PSU	C4-N3	-2.75	1.33	1.38
48	S2	1045	PSU	C4-N3	-2.75	1.33	1.38
48	S2	509	OMG	C6-N1	-2.74	1.33	1.38
2	L5	4500	PSU	C4-N3	-2.74	1.33	1.38
48	S2	34	PSU	C4-N3	-2.74	1.33	1.38
48	S2	1081	PSU	C4-N3	-2.74	1.33	1.38
2	L5	4620	OMU	C4-N3	-2.73	1.33	1.38
2	L5	4431	PSU	C4-N3	-2.73	1.33	1.38
2	L5	1683	PSU	C4-N3	-2.73	1.33	1.38
2	L5	1782	PSU	C4-N3	-2.73	1.33	1.38
48	S2	109	PSU	C4-N3	-2.73	1.33	1.38
48	S2	218	PSU	C4-N3	-2.72	1.33	1.38
48	S2	105	PSU	C4-N3	-2.72	1.33	1.38
48	S2	686	PSU	C4-N3	-2.72	1.33	1.38
2	L5	4498	OMU	C4-N3	-2.72	1.34	1.38
48	S2	572	PSU	C4-N3	-2.72	1.33	1.38
2	L5	4636	PSU	C4-N3	-2.72	1.33	1.38
2	L5	4312	PSU	C4-N3	-2.72	1.33	1.38
2	L5	2632	PSU	C4-N3	-2.72	1.33	1.38
48	S2	1238	PSU	C4-N3	-2.72	1.33	1.38
48	S2	799	OMU	C4-N3	-2.71	1.34	1.38
48	S2	1692	PSU	C4-N3	-2.71	1.33	1.38
48	S2	1804	OMU	C4-N3	-2.71	1.34	1.38
48	S2	1004	PSU	C4-N3	-2.71	1.33	1.38
48	S2	1232	PSU	C4-N3	-2.71	1.33	1.38
2	L5	3637	PSU	C4-N3	-2.70	1.33	1.38
2	L5	4296	PSU	C4-N3	-2.70	1.33	1.38
48	S2	651	PSU	C4-N3	-2.70	1.33	1.38
48	S2	210	PSU	C4-N3	-2.69	1.33	1.38
48	S2	1445	PSU	C4-N3	-2.69	1.33	1.38
48	S2	1244	PSU	C4-N3	-2.69	1.33	1.38
2	L5	3768	PSU	C4-N3	-2.68	1.33	1.38
48	S2	918	PSU	C4-N3	-2.68	1.33	1.38
2	L5	4576	PSU	C4-N3	-2.68	1.33	1.38
2	L5	2415	OMU	C4-N3	-2.68	1.34	1.38
2	L5	3762	PSU	C4-N3	-2.68	1.33	1.38
2	L5	3770	PSU	C4-N3	-2.68	1.33	1.38
2	L5	4972	PSU	C4-N3	-2.68	1.33	1.38
2	L5	4420	PSU	C4-N3	-2.67	1.33	1.38
48	S2	649	PSU	C4-N3	-2.67	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	3730	PSU	C4-N3	-2.67	1.33	1.38
2	L5	4628	PSU	C4-N3	-2.67	1.33	1.38
48	S2	1174	PSU	C4-N3	-2.67	1.33	1.38
2	L5	4227	OMU	C4-N3	-2.66	1.34	1.38
48	S2	866	PSU	C4-N3	-2.66	1.33	1.38
48	S2	1177	PSU	C4-N3	-2.66	1.33	1.38
2	L5	5010	PSU	C4-N3	-2.66	1.33	1.38
2	L5	1860	PSU	C4-N3	-2.66	1.33	1.38
48	S2	1442	OMU	C4-N3	-2.65	1.34	1.38
2	L5	4361	PSU	C4-N3	-2.65	1.33	1.38
2	L5	3844	PSU	C4-N3	-2.65	1.33	1.38
48	S2	121	OMU	C4-N3	-2.65	1.34	1.38
2	L5	4306	OMU	C4-N3	-2.64	1.34	1.38
2	L5	3734	PSU	C4-N3	-2.64	1.33	1.38
48	S2	1625	PSU	C4-N3	-2.64	1.33	1.38
48	S2	1046	PSU	C4-N3	-2.64	1.33	1.38
2	L5	4423	PSU	C4-N3	-2.64	1.33	1.38
2	L5	3884	PSU	C4-N3	-2.63	1.33	1.38
48	S2	681	PSU	C4-N3	-2.63	1.33	1.38
2	L5	1536	PSU	C4-N3	-2.63	1.33	1.38
48	S2	119	PSU	C4-N3	-2.63	1.33	1.38
2	L5	5001	PSU	C4-N3	-2.63	1.33	1.38
48	S2	822	PSU	C4-N3	-2.62	1.33	1.38
48	S2	1288	OMU	C4-N3	-2.62	1.34	1.38
48	S2	1367	PSU	C4-N3	-2.62	1.33	1.38
48	S2	627	OMU	C4-N3	-2.61	1.34	1.38
2	L5	2508	PSU	C4-N3	-2.61	1.34	1.38
48	S2	116	OMU	C4-N3	-2.61	1.34	1.38
48	S2	1326	OMU	C4-N3	-2.61	1.34	1.38
2	L5	4457	PSU	C4-N3	-2.61	1.34	1.38
2	L5	3853	PSU	C4-N3	-2.60	1.34	1.38
48	S2	1056	PSU	C4-N3	-2.60	1.34	1.38
2	L5	1792	PSU	C4-N3	-2.60	1.34	1.38
2	L5	3760	A2M	C8-N9	2.60	1.42	1.37
2	L5	1744	PSU	C4-N3	-2.60	1.34	1.38
2	L5	1456	JMH	O2-C2	-2.59	1.17	1.22
2	L5	1625	OMG	C6-N1	-2.59	1.34	1.38
48	S2	823	PSU	C4-N3	-2.59	1.34	1.38
48	S2	863	PSU	C4-N3	-2.58	1.34	1.38
2	L5	1773	OMU	C4-N3	-2.58	1.34	1.38
2	L5	1862	PSU	C4-N3	-2.58	1.34	1.38
48	S2	428	OMU	C4-N3	-2.57	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	3764	PSU	C4-N3	-2.57	1.34	1.38
48	S2	172	OMU	C4-N3	-2.57	1.34	1.38
2	L5	1677	PSU	O4'-C1'	-2.56	1.40	1.43
2	L5	4552	PSU	C4-N3	-2.56	1.34	1.38
2	L5	3792	OMG	C6-N1	-2.56	1.34	1.38
2	L5	4403	PSU	C4-N3	-2.56	1.34	1.38
48	S2	644	OMG	C6-N1	-2.56	1.34	1.38
48	S2	1643	PSU	C4-N3	-2.55	1.34	1.38
2	L5	4353	PSU	C4-N3	-2.55	1.34	1.38
2	L5	2424	OMG	C6-N1	-2.54	1.34	1.38
48	S2	668	A2M	O4'-C4'	-2.54	1.39	1.45
2	L5	1456	JMH	C5-C4	2.53	1.48	1.42
2	L5	4521	PSU	C4-N3	-2.53	1.34	1.38
2	L5	4228	OMG	C6-N1	-2.53	1.34	1.38
2	L5	1456	JMH	C6-N1	2.51	1.44	1.38
2	L5	4494	OMG	C6-N1	-2.50	1.34	1.38
2	L5	1760	OMG	C6-N1	-2.49	1.34	1.38
48	S2	1832	6MZ	C5-N7	-2.49	1.34	1.39
48	S2	867	OMG	C6-N1	-2.49	1.34	1.38
48	S2	436	OMG	C6-N1	-2.49	1.34	1.38
2	L5	3818	UY1	O4-C4	-2.48	1.18	1.23
48	S2	1490	OMG	C6-N1	-2.48	1.34	1.38
2	L5	4623	OMG	C6-N1	-2.47	1.34	1.38
2	L5	4618	OMG	C6-N1	-2.47	1.34	1.38
2	L5	1524	A2M	C2'-C1'	2.46	1.59	1.53
48	S2	683	OMG	C6-N1	-2.46	1.34	1.38
2	L5	4532	PSU	C4-N3	-2.45	1.34	1.38
48	S2	1328	OMG	C6-N1	-2.45	1.34	1.38
2	L5	4637	OMG	C6-N1	-2.44	1.34	1.38
2	L5	3944	OMG	C6-N1	-2.44	1.34	1.38
2	L5	1316	OMG	C6-N1	-2.44	1.34	1.38
2	L5	3744	OMG	C6-N1	-2.44	1.34	1.38
2	L5	1326	A2M	C5-C4	2.44	1.43	1.39
2	L5	4523	A2M	C8-N9	2.43	1.41	1.37
2	L5	2876	OMG	C6-N1	-2.43	1.34	1.38
2	L5	1522	OMG	C6-N1	-2.43	1.34	1.38
2	L5	4870	OMG	C6-N1	-2.43	1.34	1.38
2	L5	4499	OMG	C6-N1	-2.42	1.34	1.38
48	S2	601	OMG	C6-N1	-2.42	1.34	1.38
48	S2	590	A2M	C5-C4	2.40	1.43	1.39
2	L5	4220	6MZ	C5-N7	-2.40	1.34	1.39
2	L5	1517	2MG	C4-N3	2.40	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	3830	A2M	C5-C4	2.40	1.43	1.39
1	L1	75	OMG	C6-N1	-2.40	1.34	1.38
2	L5	2050	OMG	C6-N1	-2.39	1.34	1.38
48	S2	1851	MA6	C4-N9	-2.39	1.32	1.37
2	L5	4370	OMG	C6-N1	-2.39	1.34	1.38
2	L5	4306	OMU	C2-N3	-2.38	1.33	1.38
2	L5	2787	A2M	C2'-C1'	2.38	1.59	1.53
2	L5	2364	OMG	C6-N1	-2.37	1.34	1.38
48	S2	1842	4AC	O7-C7	-2.36	1.18	1.23
2	L5	2401	A2M	C5-C4	2.35	1.43	1.39
48	S2	668	A2M	C8-N9	2.35	1.41	1.37
2	L5	3818	UY1	O2-C2	-2.34	1.18	1.23
2	L5	2415	OMU	C2-N3	-2.34	1.33	1.38
2	L5	2424	OMG	C5-N7	-2.34	1.34	1.39
2	L5	4620	OMU	C2-N3	-2.34	1.33	1.38
2	L5	3792	OMG	C5-N7	-2.34	1.34	1.39
48	S2	1248	B8N	O4-C4	-2.32	1.18	1.23
48	S2	159	A2M	C5-C4	2.32	1.43	1.39
2	L5	729	2MG	C4-N3	2.32	1.39	1.34
2	L5	4227	OMU	C2-N3	-2.31	1.33	1.38
2	L5	398	A2M	C5-C4	2.30	1.43	1.39
2	L5	4498	OMU	C2-N3	-2.29	1.34	1.38
2	L5	4447	5MC	C6-N1	-2.29	1.34	1.38
2	L5	3899	OMG	C6-N1	-2.29	1.34	1.38
48	S2	1326	OMU	C2-N3	-2.28	1.34	1.38
8	LD	216	V5N	CG-ND1	2.27	1.39	1.37
48	S2	644	OMG	C5-N7	-2.27	1.34	1.39
2	L5	3925	OMU	C2-N3	-2.27	1.34	1.38
48	S2	468	A2M	C5-C4	2.26	1.43	1.39
2	L5	4196	OMG	C5-N7	-2.26	1.34	1.39
48	S2	590	A2M	C2'-C1'	2.25	1.58	1.53
2	L5	2815	A2M	C5-C4	2.25	1.43	1.39
48	S2	159	A2M	C5'-C4'	2.25	1.58	1.51
2	L5	3718	A2M	C5-C4	2.25	1.43	1.39
2	L5	2876	OMG	C5-N7	-2.25	1.34	1.39
2	L5	4196	OMG	C6-N1	-2.25	1.34	1.38
48	S2	1804	OMU	C2-N3	-2.24	1.34	1.38
1	L1	75	OMG	C5-N7	-2.23	1.34	1.39
2	L5	4523	A2M	C5-C4	2.23	1.43	1.39
48	S2	1850	MA6	C5-N7	-2.23	1.35	1.39
2	L5	3782	5MC	C6-N1	-2.23	1.34	1.38
2	L5	4870	OMG	C5-N7	-2.23	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	799	OMU	C2-N3	-2.22	1.34	1.38
48	S2	1678	A2M	C8-N9	2.22	1.41	1.37
48	S2	1442	OMU	C2-N3	-2.22	1.34	1.38
2	L5	4872	2MG	C4-N3	2.22	1.39	1.34
48	S2	1337	4AC	CM7-C7	2.21	1.55	1.50
48	S2	116	OMU	C5-C4	-2.21	1.38	1.43
2	L5	3944	OMG	C5-N7	-2.21	1.34	1.39
2	L5	2050	OMG	C5-N7	-2.21	1.34	1.39
48	S2	601	OMG	C5-N7	-2.21	1.34	1.39
48	S2	172	OMU	C2-N3	-2.21	1.34	1.38
48	S2	116	OMU	C2-N3	-2.20	1.34	1.38
2	L5	1316	OMG	C5-N7	-2.20	1.34	1.39
2	L5	3818	UY1	C6-N1	-2.20	1.32	1.36
48	S2	1850	MA6	C4-N9	-2.20	1.33	1.37
48	S2	1288	OMU	C2-N3	-2.19	1.34	1.38
48	S2	1337	4AC	O7-C7	-2.19	1.18	1.23
2	L5	4392	OMG	C6-N1	-2.19	1.34	1.38
48	S2	627	OMU	C2-N3	-2.18	1.34	1.38
2	L5	4299	PSU	C2-N3	-2.18	1.33	1.37
48	S2	1490	OMG	C5-N7	-2.18	1.34	1.39
6	S4	20	H2U	C2-N3	-2.18	1.34	1.38
48	S2	484	A2M	C5-C4	2.18	1.43	1.39
48	S2	121	OMU	C2-N3	-2.18	1.34	1.38
2	L5	3899	OMG	C5-N7	-2.18	1.34	1.39
48	S2	1442	OMU	C5-C4	-2.17	1.39	1.43
48	S2	1850	MA6	C8-N7	2.17	1.35	1.31
2	L5	3760	A2M	C5-C4	2.16	1.42	1.39
2	L5	400	A2M	C5-C4	2.15	1.42	1.39
48	S2	1248	B8N	O2-C2	-2.15	1.18	1.22
2	L5	2837	OMU	C2-N1	2.15	1.41	1.38
48	S2	484	A2M	C2'-C1'	2.14	1.58	1.53
2	L5	1773	OMU	C2-N3	-2.14	1.34	1.38
2	L5	1534	A2M	C5-C4	2.14	1.42	1.39
48	S2	801	PSU	C2-N3	-2.14	1.34	1.37
2	L5	4220	6MZ	C8-N7	2.13	1.35	1.31
48	S2	867	OMG	C5-N7	-2.13	1.34	1.39
48	S2	509	OMG	C5-N7	-2.13	1.34	1.39
48	S2	799	OMU	C2-N1	2.12	1.41	1.38
48	S2	406	PSU	C2-N3	-2.12	1.34	1.37
2	L5	2415	OMU	C2-N1	2.12	1.41	1.38
2	L5	1860	PSU	C2-N3	-2.12	1.34	1.37
2	L5	4571	A2M	C5-C4	2.12	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4392	OMG	C5-N7	-2.12	1.34	1.39
1	L1	55	PSU	C2-N3	-2.11	1.34	1.37
2	L5	4532	PSU	C2-N1	-2.11	1.33	1.36
48	S2	34	PSU	C2-N3	-2.11	1.34	1.37
48	S2	436	OMG	C5-N7	-2.11	1.34	1.39
2	L5	1322	1MA	C2-N1	2.11	1.40	1.35
48	S2	576	A2M	C5-C4	2.11	1.42	1.39
2	L5	2363	A2M	C5-C4	2.10	1.42	1.39
2	L5	1625	OMG	C5-N7	-2.10	1.34	1.39
2	L5	2804	OMC	C6-C5	2.10	1.40	1.35
48	S2	218	PSU	C2-N3	-2.10	1.34	1.37
2	L5	1871	A2M	C5-C4	2.10	1.42	1.39
2	L5	3785	A2M	C5-C4	2.10	1.42	1.39
48	S2	166	A2M	C8-N9	2.10	1.41	1.37
48	S2	1842	4AC	CM7-C7	2.10	1.54	1.50
2	L5	4471	PSU	C2-N3	-2.10	1.34	1.37
2	L5	4689	PSU	C2-N3	-2.09	1.34	1.37
48	S2	1832	6MZ	C8-N7	2.09	1.35	1.31
48	S2	36	PSU	C2-N3	-2.09	1.34	1.37
2	L5	4370	OMG	C5-N7	-2.09	1.34	1.39
2	L5	4523	A2M	C2'-C1'	2.09	1.58	1.53
2	L5	1871	A2M	C8-N9	2.09	1.41	1.37
48	S2	121	OMU	C5-C4	-2.08	1.39	1.43
48	S2	1678	A2M	C5-C4	2.07	1.42	1.39
48	S2	1804	OMU	C5-C4	-2.07	1.39	1.43
48	S2	1851	MA6	C8-N7	2.07	1.35	1.31
2	L5	2415	OMU	C5-C4	-2.07	1.39	1.43
48	S2	1328	OMG	C5-N7	-2.07	1.34	1.39
48	S2	428	OMU	C2-N3	-2.07	1.34	1.38
2	L5	4498	OMU	C5-C4	-2.07	1.39	1.43
48	S2	668	A2M	C2'-C1'	2.06	1.58	1.53
48	S2	668	A2M	C5-C4	2.06	1.42	1.39
2	L5	1781	PSU	C2-N3	-2.06	1.34	1.37
2	L5	3884	PSU	C2-N3	-2.06	1.34	1.37
48	S2	166	A2M	C5-C4	2.06	1.42	1.39
2	L5	4353	PSU	C2-N3	-2.06	1.34	1.37
2	L5	4499	OMG	C5-N7	-2.06	1.34	1.39
2	L5	1316	OMG	C4-N9	-2.05	1.32	1.38
2	L5	3785	A2M	C8-N9	2.05	1.41	1.37
48	S2	918	PSU	O4'-C1'	-2.05	1.41	1.43
2	L5	3825	A2M	C8-N9	2.05	1.41	1.37
2	L5	4228	OMG	C5-N7	-2.05	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4306	OMU	C2-N1	2.05	1.41	1.38
48	S2	1383	A2M	C5-C4	2.05	1.42	1.39
2	L5	4590	A2M	C5-C4	2.04	1.42	1.39
48	S2	109	PSU	C2-N3	-2.04	1.34	1.37
2	L5	3744	OMG	C5-N7	-2.04	1.35	1.39
2	L5	4636	PSU	C2-N3	-2.04	1.34	1.37
2	L5	2837	OMU	C2-N3	-2.04	1.34	1.38
2	L5	4227	OMU	C2-N1	2.04	1.41	1.38
48	S2	1056	PSU	C2-N3	-2.03	1.34	1.37
48	S2	799	OMU	C5-C4	-2.03	1.39	1.43
48	S2	1326	OMU	C5-C4	-2.03	1.39	1.43
2	L5	4620	OMU	C5-C4	-2.03	1.39	1.43
2	L5	3758	PSU	C2-N3	-2.02	1.34	1.37
2	L5	1760	OMG	C5-N7	-2.02	1.35	1.39
2	L5	1773	OMU	C2-N1	2.02	1.41	1.38
48	S2	93	PSU	C2-N3	-2.02	1.34	1.37
48	S2	966	PSU	C2-N3	-2.02	1.34	1.37
2	L5	4623	OMG	C5-N7	-2.02	1.35	1.39
2	L5	2364	OMG	C5-N7	-2.02	1.35	1.39
48	S2	1442	OMU	C2-N1	2.01	1.41	1.38
2	L5	4637	OMG	C5-N7	-2.01	1.35	1.39
2	L5	4392	OMG	C4-N9	-2.01	1.32	1.38
2	L5	2632	PSU	C2-N3	-2.01	1.34	1.37
2	L5	4618	OMG	C5-N7	-2.01	1.35	1.39
2	L5	2508	PSU	C2-N3	-2.01	1.34	1.37
2	L5	3844	PSU	C2-N3	-2.00	1.34	1.37
48	S2	512	A2M	C5-C4	2.00	1.42	1.39

All (805) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3920	PSU	N1-C2-N3	6.85	122.39	115.17
1	L1	55	PSU	N1-C2-N3	6.77	122.31	115.17
2	L5	4530	UR3	C4-N3-C2	-6.77	119.13	124.58
2	L5	3768	PSU	N1-C2-N3	6.77	122.31	115.17
48	S2	1177	PSU	N1-C2-N3	6.73	122.27	115.17
2	L5	3762	PSU	N1-C2-N3	6.69	122.23	115.17
1	L1	69	PSU	N1-C2-N3	6.69	122.22	115.17
2	L5	3695	PSU	N1-C2-N3	6.67	122.20	115.17
48	S2	1347	PSU	N1-C2-N3	6.66	122.20	115.17
2	L5	3639	PSU	N1-C2-N3	6.66	122.19	115.17
48	S2	1238	PSU	N1-C2-N3	6.64	122.17	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4673	PSU	N1-C2-N3	6.63	122.17	115.17
2	L5	1782	PSU	N1-C2-N3	6.61	122.14	115.17
48	S2	801	PSU	N1-C2-N3	6.61	122.14	115.17
2	L5	3637	PSU	N1-C2-N3	6.59	122.12	115.17
48	S2	572	PSU	N1-C2-N3	6.58	122.11	115.17
48	S2	1081	PSU	N1-C2-N3	6.57	122.10	115.17
2	L5	4521	PSU	N1-C2-N3	6.57	122.10	115.17
48	S2	1045	PSU	N1-C2-N3	6.56	122.09	115.17
2	L5	4552	PSU	N1-C2-N3	6.56	122.09	115.17
2	L5	4457	PSU	N1-C2-N3	6.55	122.08	115.17
2	L5	3792	OMG	C5-C4-N3	-6.55	117.97	128.39
2	L5	4442	PSU	N1-C2-N3	6.55	122.08	115.17
5	LB	245	HIC	NE2-CE1-ND1	-6.54	110.16	112.66
2	L5	4500	PSU	N1-C2-N3	6.53	122.06	115.17
2	L5	4296	PSU	N1-C2-N3	6.53	122.06	115.17
48	S2	651	PSU	N1-C2-N3	6.51	122.04	115.17
48	S2	815	PSU	N1-C2-N3	6.51	122.03	115.17
2	L5	4636	PSU	N1-C2-N3	6.50	122.02	115.17
2	L5	4423	PSU	N1-C2-N3	6.49	122.02	115.17
2	L5	4576	PSU	N1-C2-N3	6.49	122.02	115.17
2	L5	5001	PSU	N1-C2-N3	6.47	121.99	115.17
48	S2	406	PSU	N1-C2-N3	6.47	121.99	115.17
48	S2	1445	PSU	N1-C2-N3	6.47	121.99	115.17
48	S2	814	PSU	N1-C2-N3	6.46	121.98	115.17
2	L5	4431	PSU	N1-C2-N3	6.45	121.98	115.17
48	S2	966	PSU	N1-C2-N3	6.44	121.97	115.17
2	L5	1760	OMG	C5-C4-N3	-6.44	118.14	128.39
2	L5	4579	PSU	N1-C2-N3	6.43	121.95	115.17
2	L5	1781	PSU	N1-C2-N3	6.43	121.95	115.17
48	S2	1692	PSU	N1-C2-N3	6.42	121.94	115.17
48	S2	823	PSU	N1-C2-N3	6.42	121.94	115.17
48	S2	1004	PSU	N1-C2-N3	6.42	121.94	115.17
48	S2	119	PSU	N1-C2-N3	6.41	121.93	115.17
2	L5	3734	PSU	N1-C2-N3	6.41	121.93	115.17
48	S2	644	OMG	C5-C4-N3	-6.41	118.19	128.39
2	L5	1677	PSU	N1-C2-N3	6.40	121.92	115.17
2	L5	3770	PSU	N1-C2-N3	6.39	121.91	115.17
48	S2	866	PSU	N1-C2-N3	6.38	121.90	115.17
2	L5	1582	PSU	N1-C2-N3	6.38	121.90	115.17
48	S2	105	PSU	N1-C2-N3	6.38	121.89	115.17
48	S2	681	PSU	N1-C2-N3	6.38	121.89	115.17
2	L5	3853	PSU	N1-C2-N3	6.37	121.89	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	34	PSU	N1-C2-N3	6.37	121.89	115.17
48	S2	1367	PSU	N1-C2-N3	6.37	121.89	115.17
48	S2	918	PSU	N1-C2-N3	6.37	121.88	115.17
2	L5	3884	PSU	N1-C2-N3	6.36	121.88	115.17
48	S2	93	PSU	N1-C2-N3	6.36	121.88	115.17
48	S2	863	PSU	N1-C2-N3	6.35	121.86	115.17
2	L5	4370	OMG	C5-C4-N3	-6.35	118.29	128.39
2	L5	4532	PSU	N1-C2-N3	6.33	121.85	115.17
2	L5	4499	OMG	C5-C4-N3	-6.33	118.32	128.39
48	S2	649	PSU	N1-C2-N3	6.32	121.84	115.17
48	S2	1625	PSU	N1-C2-N3	6.32	121.83	115.17
2	L5	3851	PSU	N1-C2-N3	6.32	121.83	115.17
48	S2	1244	PSU	N1-C2-N3	6.31	121.82	115.17
48	S2	609	PSU	N1-C2-N3	6.30	121.82	115.17
2	L5	1625	OMG	C5-C4-N3	-6.30	118.36	128.39
2	L5	4972	PSU	N1-C2-N3	6.30	121.81	115.17
2	L5	1862	PSU	N1-C2-N3	6.29	121.81	115.17
48	S2	1232	PSU	N1-C2-N3	6.29	121.81	115.17
48	S2	686	PSU	N1-C2-N3	6.29	121.80	115.17
2	L5	2632	PSU	N1-C2-N3	6.28	121.80	115.17
2	L5	3844	PSU	N1-C2-N3	6.28	121.79	115.17
48	S2	1174	PSU	N1-C2-N3	6.28	121.79	115.17
2	L5	3758	PSU	N1-C2-N3	6.27	121.79	115.17
2	L5	4196	OMG	C5-C4-N3	-6.27	118.41	128.39
2	L5	4471	PSU	N1-C2-N3	6.27	121.78	115.17
48	S2	109	PSU	N1-C2-N3	6.27	121.78	115.17
2	L5	4628	PSU	N1-C2-N3	6.26	121.78	115.17
2	L5	1744	PSU	N1-C2-N3	6.25	121.76	115.17
2	L5	5010	PSU	N1-C2-N3	6.25	121.76	115.17
48	S2	210	PSU	N1-C2-N3	6.25	121.76	115.17
2	L5	4637	OMG	C5-C4-N3	-6.24	118.46	128.39
2	L5	4353	PSU	N1-C2-N3	6.22	121.73	115.17
2	L5	2424	OMG	C5-C4-N3	-6.22	118.50	128.39
48	S2	867	OMG	C5-C4-N3	-6.22	118.50	128.39
2	L5	4293	PSU	N1-C2-N3	6.20	121.70	115.17
2	L5	3715	PSU	N1-C2-N3	6.19	121.70	115.17
48	S2	1643	PSU	N1-C2-N3	6.18	121.69	115.17
2	L5	3730	PSU	N1-C2-N3	6.18	121.69	115.17
2	L5	4312	PSU	N1-C2-N3	6.18	121.68	115.17
2	L5	1683	PSU	N1-C2-N3	6.16	121.67	115.17
2	L5	4361	PSU	N1-C2-N3	6.15	121.66	115.17
48	S2	509	OMG	C5-C4-N3	-6.14	118.61	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4618	OMG	C5-C4-N3	-6.13	118.63	128.39
48	S2	36	PSU	N1-C2-N3	6.13	121.63	115.17
48	S2	1056	PSU	N1-C2-N3	6.13	121.63	115.17
48	S2	601	OMG	C5-C4-N3	-6.13	118.64	128.39
48	S2	683	OMG	C5-C4-N3	-6.12	118.65	128.39
2	L5	4403	PSU	N1-C2-N3	6.11	121.62	115.17
2	L5	4689	PSU	N1-C2-N3	6.11	121.62	115.17
1	L1	75	OMG	C5-C4-N3	-6.11	118.66	128.39
2	L5	4299	PSU	N1-C2-N3	6.10	121.60	115.17
2	L5	4420	PSU	N1-C2-N3	6.10	121.60	115.17
48	S2	218	PSU	N1-C2-N3	6.09	121.59	115.17
2	L5	2508	PSU	N1-C2-N3	6.09	121.59	115.17
48	S2	822	PSU	N1-C2-N3	6.08	121.58	115.17
2	L5	3944	OMG	C5-C4-N3	-6.08	118.72	128.39
2	L5	2876	OMG	C5-C4-N3	-6.07	118.73	128.39
2	L5	4623	OMG	C5-C4-N3	-6.07	118.73	128.39
2	L5	1860	PSU	N1-C2-N3	6.06	121.56	115.17
2	L5	3744	OMG	C5-C4-N3	-6.04	118.78	128.39
48	S2	1328	OMG	C5-C4-N3	-6.03	118.80	128.39
2	L5	3764	PSU	N1-C2-N3	6.03	121.53	115.17
2	L5	1792	PSU	N1-C2-N3	6.02	121.52	115.17
2	L5	2364	OMG	C5-C4-N3	-6.02	118.82	128.39
2	L5	3899	OMG	C5-C4-N3	-5.98	118.88	128.39
2	L5	4494	OMG	C5-C4-N3	-5.97	118.89	128.39
2	L5	1536	PSU	N1-C2-N3	5.97	121.46	115.17
2	L5	4870	OMG	C5-C4-N3	-5.91	118.98	128.39
2	L5	4392	OMG	C5-C4-N3	-5.89	119.01	128.39
48	S2	436	OMG	C5-C4-N3	-5.87	119.06	128.39
2	L5	4220	6MZ	C5-C4-N3	-5.86	118.64	126.72
2	L5	2050	OMG	C5-C4-N3	-5.86	119.06	128.39
48	S2	1046	PSU	N1-C2-N3	5.86	121.35	115.17
2	L5	4228	OMG	C5-C4-N3	-5.84	119.09	128.39
2	L5	1522	OMG	C5-C4-N3	-5.83	119.11	128.39
2	L5	1316	OMG	C5-C4-N3	-5.78	119.20	128.39
48	S2	1490	OMG	C5-C4-N3	-5.70	119.32	128.39
48	S2	1832	6MZ	C5-C4-N3	-5.61	118.99	126.72
2	L5	3899	OMG	C2-N3-C4	5.40	121.60	112.30
2	L5	4370	OMG	C2-N3-C4	5.38	121.56	112.30
2	L5	4623	OMG	C2-N3-C4	5.35	121.52	112.30
2	L5	4499	OMG	C2-N3-C4	5.35	121.52	112.30
2	L5	2876	OMG	C2-N3-C4	5.31	121.44	112.30
2	L5	4637	OMG	C2-N3-C4	5.30	121.43	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4196	OMG	C2-N3-C4	5.28	121.39	112.30
48	S2	1850	MA6	C5-C4-N3	-5.25	119.48	126.72
48	S2	1248	B8N	C5-C4-N3	5.24	125.67	116.15
2	L5	4618	OMG	C2-N3-C4	5.20	121.26	112.30
2	L5	1522	OMG	C2-N3-C4	5.20	121.26	112.30
2	L5	2364	OMG	C2-N3-C4	5.19	121.23	112.30
48	S2	172	OMU	C4-N3-C2	-5.16	120.20	126.61
48	S2	601	OMG	C2-N3-C4	5.16	121.19	112.30
48	S2	644	OMG	C2-N3-C4	5.15	121.17	112.30
2	L5	3792	OMG	C2-N3-C4	5.14	121.15	112.30
48	S2	683	OMG	C2-N3-C4	5.13	121.14	112.30
2	L5	1760	OMG	C2-N3-C4	5.13	121.14	112.30
2	L5	4494	OMG	C2-N3-C4	5.07	121.03	112.30
2	L5	4392	OMG	C2-N3-C4	5.07	121.02	112.30
48	S2	436	OMG	C2-N3-C4	5.05	121.00	112.30
1	L1	75	OMG	C2-N3-C4	5.03	120.95	112.30
2	L5	3744	OMG	C2-N3-C4	5.00	120.92	112.30
48	S2	867	OMG	C2-N3-C4	5.00	120.92	112.30
2	L5	4498	OMU	C4-N3-C2	-5.00	120.41	126.61
2	L5	1625	OMG	C2-N3-C4	5.00	120.91	112.30
2	L5	3944	OMG	C2-N3-C4	5.00	120.91	112.30
48	S2	1328	OMG	C2-N3-C4	5.00	120.90	112.30
2	L5	2424	OMG	C2-N3-C4	4.99	120.90	112.30
48	S2	428	OMU	C4-N3-C2	-4.99	120.42	126.61
2	L5	4228	OMG	C2-N3-C4	4.95	120.83	112.30
48	S2	1326	OMU	C4-N3-C2	-4.94	120.47	126.61
48	S2	1851	MA6	C10-N6-C6	-4.89	108.08	120.52
48	S2	1851	MA6	C5-C4-N3	-4.89	119.99	126.72
48	S2	509	OMG	C2-N3-C4	4.89	120.72	112.30
2	L5	1760	OMG	N9-C4-N3	4.88	135.71	125.95
2	L5	4227	OMU	C4-N3-C2	-4.88	120.56	126.61
2	L5	2050	OMG	C2-N3-C4	4.87	120.69	112.30
2	L5	3925	OMU	C4-N3-C2	-4.87	120.56	126.61
2	L5	3792	OMG	N9-C4-N3	4.87	135.68	125.95
48	S2	1490	OMG	C2-N3-C4	4.87	120.68	112.30
2	L5	4870	OMG	C2-N3-C4	4.85	120.65	112.30
2	L5	4370	OMG	N9-C4-N3	4.84	135.63	125.95
2	L5	4552	PSU	O2-C2-N1	-4.84	117.80	122.79
2	L5	4196	OMG	N9-C4-N3	4.84	135.62	125.95
2	L5	2837	OMU	C4-N3-C2	-4.83	120.62	126.61
2	L5	3818	UY1	N1-C2-N3	4.81	120.24	115.17
2	L5	1625	OMG	N9-C4-N3	4.81	135.57	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1773	OMU	C4-N3-C2	-4.77	120.69	126.61
48	S2	1442	OMU	C4-N3-C2	-4.77	120.69	126.61
48	S2	1804	OMU	C4-N3-C2	-4.75	120.72	126.61
2	L5	1316	OMG	C2-N3-C4	4.75	120.48	112.30
2	L5	4872	2MG	CM2-N2-C2	-4.74	113.46	123.65
48	S2	627	OMU	C4-N3-C2	-4.74	120.73	126.61
2	L5	4499	OMG	N9-C4-N3	4.73	135.42	125.95
48	S2	116	OMU	C4-N3-C2	-4.72	120.75	126.61
48	S2	1248	B8N	C4-N3-C2	-4.71	119.82	125.62
48	S2	644	OMG	N9-C4-N3	4.70	135.35	125.95
2	L5	3818	UY1	C4-N3-C2	-4.67	119.94	126.37
2	L5	4306	OMU	C4-N3-C2	-4.66	120.83	126.61
48	S2	121	OMU	C4-N3-C2	-4.66	120.83	126.61
2	L5	2837	OMU	N3-C2-N1	4.65	120.94	114.89
2	L5	2424	OMG	N9-C4-N3	4.64	135.23	125.95
48	S2	867	OMG	N9-C4-N3	4.64	135.22	125.95
48	S2	1177	PSU	C4-N3-C2	-4.64	119.99	126.37
2	L5	2876	OMG	N9-C4-N3	4.63	135.20	125.95
48	S2	1288	OMU	C4-N3-C2	-4.62	120.88	126.61
2	L5	4227	OMU	N3-C2-N1	4.61	120.89	114.89
2	L5	4220	6MZ	N3-C4-N9	4.59	134.97	127.17
2	L5	4637	OMG	N9-C4-N3	4.59	135.13	125.95
2	L5	3944	OMG	N9-C4-N3	4.59	135.12	125.95
2	L5	729	2MG	CM2-N2-C2	-4.57	113.82	123.65
48	S2	799	OMU	C4-N3-C2	-4.57	120.94	126.61
48	S2	1832	6MZ	N3-C4-N9	4.56	134.93	127.17
2	L5	3768	PSU	C4-N3-C2	-4.55	120.10	126.37
2	L5	1316	OMG	N9-C4-N3	4.55	135.05	125.95
48	S2	601	OMG	N9-C4-N3	4.54	135.03	125.95
48	S2	681	PSU	C4-N3-C2	-4.53	120.13	126.37
48	S2	1850	MA6	C2-N1-C6	4.48	122.78	111.83
48	S2	1490	OMG	N9-C4-N3	4.48	134.91	125.95
1	L1	75	OMG	N9-C4-N3	4.48	134.91	125.95
2	L5	4498	OMU	N3-C2-N1	4.48	120.72	114.89
2	L5	3637	PSU	C4-N3-C2	-4.47	120.21	126.37
2	L5	4870	OMG	N9-C4-N3	4.47	134.90	125.95
2	L5	3925	OMU	N3-C2-N1	4.47	120.71	114.89
2	L5	4353	PSU	C4-N3-C2	-4.47	120.22	126.37
48	S2	1347	PSU	C4-N3-C2	-4.46	120.22	126.37
2	L5	1517	2MG	CM2-N2-C2	-4.46	114.06	123.65
2	L5	3744	OMG	N9-C4-N3	4.45	134.85	125.95
48	S2	509	OMG	N9-C4-N3	4.45	134.84	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1851	MA6	C2-N1-C6	4.44	122.68	111.83
2	L5	4552	PSU	C4-N3-C2	-4.43	120.27	126.37
2	L5	3695	PSU	C4-N3-C2	-4.42	120.28	126.37
48	S2	651	PSU	C4-N3-C2	-4.42	120.29	126.37
48	S2	406	PSU	C4-N3-C2	-4.41	120.29	126.37
2	L5	2415	OMU	C4-N3-C2	-4.40	121.15	126.61
48	S2	683	OMG	N9-C4-N3	4.39	134.74	125.95
48	S2	172	OMU	N3-C2-N1	4.39	120.60	114.89
2	L5	4447	5MC	C5-C6-N1	-4.38	118.55	123.31
2	L5	4494	OMG	N9-C4-N3	4.38	134.72	125.95
2	L5	4618	OMG	N9-C4-N3	4.37	134.69	125.95
48	S2	436	OMG	N9-C4-N3	4.37	134.69	125.95
48	S2	863	PSU	C4-N3-C2	-4.37	120.35	126.37
2	L5	1744	PSU	C4-N3-C2	-4.37	120.36	126.37
2	L5	4423	PSU	C4-N3-C2	-4.36	120.36	126.37
48	S2	1326	OMU	N3-C2-N1	4.36	120.56	114.89
2	L5	4420	PSU	C4-N3-C2	-4.35	120.38	126.37
2	L5	4403	PSU	C4-N3-C2	-4.35	120.38	126.37
2	L5	2364	OMG	N9-C4-N3	4.33	134.60	125.95
2	L5	4500	PSU	C4-N3-C2	-4.32	120.42	126.37
2	L5	2050	OMG	N9-C4-N3	4.32	134.59	125.95
48	S2	823	PSU	C4-N3-C2	-4.32	120.42	126.37
2	L5	1862	PSU	C4-N3-C2	-4.31	120.43	126.37
48	S2	1328	OMG	N9-C4-N3	4.31	134.56	125.95
48	S2	1238	PSU	C4-N3-C2	-4.29	120.46	126.37
2	L5	1677	PSU	C4-N3-C2	-4.27	120.48	126.37
48	S2	1851	MA6	C4-C5-N7	-4.27	105.70	110.58
2	L5	5001	PSU	C4-N3-C2	-4.25	120.52	126.37
2	L5	1773	OMU	N3-C2-N1	4.24	120.41	114.89
48	S2	627	OMU	N3-C2-N1	4.23	120.40	114.89
48	S2	1442	OMU	N3-C2-N1	4.23	120.40	114.89
2	L5	3884	PSU	C4-N3-C2	-4.22	120.56	126.37
2	L5	4521	PSU	C4-N3-C2	-4.22	120.56	126.37
48	S2	799	OMU	N3-C2-N1	4.22	120.38	114.89
48	S2	1692	PSU	C4-N3-C2	-4.21	120.57	126.37
2	L5	1683	PSU	O2-C2-N1	-4.21	118.45	122.79
2	L5	4576	PSU	C4-N3-C2	-4.21	120.58	126.37
48	S2	801	PSU	C4-N3-C2	-4.21	120.58	126.37
48	S2	649	PSU	C4-N3-C2	-4.19	120.59	126.37
48	S2	815	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	3920	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	4457	PSU	C4-N3-C2	-4.19	120.60	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4431	PSU	C4-N3-C2	-4.19	120.60	126.37
48	S2	1244	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	3758	PSU	C4-N3-C2	-4.19	120.60	126.37
2	L5	4296	PSU	C4-N3-C2	-4.19	120.60	126.37
48	S2	105	PSU	C4-N3-C2	-4.18	120.61	126.37
2	L5	3768	PSU	O2-C2-N1	-4.18	118.48	122.79
2	L5	2508	PSU	C4-N3-C2	-4.18	120.61	126.37
1	L1	69	PSU	C4-N3-C2	-4.18	120.61	126.37
2	L5	4673	PSU	C4-N3-C2	-4.17	120.62	126.37
48	S2	1850	MA6	C10-N6-C6	-4.17	109.91	120.52
2	L5	4623	OMG	N9-C4-N3	4.16	134.28	125.95
2	L5	1782	PSU	C4-N3-C2	-4.16	120.64	126.37
2	L5	3715	PSU	C4-N3-C2	-4.16	120.65	126.37
1	L1	55	PSU	C4-N3-C2	-4.15	120.65	126.37
2	L5	4306	OMU	N3-C2-N1	4.15	120.29	114.89
48	S2	1804	OMU	N3-C2-N1	4.15	120.29	114.89
2	L5	1683	PSU	C4-N3-C2	-4.15	120.66	126.37
48	S2	1045	PSU	C4-N3-C2	-4.14	120.66	126.37
48	S2	1081	PSU	C4-N3-C2	-4.14	120.67	126.37
2	L5	4392	OMG	N9-C4-N3	4.14	134.22	125.95
2	L5	3844	PSU	C4-N3-C2	-4.12	120.69	126.37
2	L5	4689	PSU	C4-N3-C2	-4.12	120.69	126.37
2	L5	3762	PSU	C4-N3-C2	-4.12	120.69	126.37
48	S2	572	PSU	C4-N3-C2	-4.12	120.69	126.37
48	S2	686	PSU	C4-N3-C2	-4.12	120.70	126.37
48	S2	428	OMU	N3-C2-N1	4.11	120.25	114.89
48	S2	866	PSU	C4-N3-C2	-4.11	120.71	126.37
48	S2	1174	PSU	C4-N3-C2	-4.11	120.71	126.37
2	L5	3730	PSU	C4-N3-C2	-4.11	120.71	126.37
2	L5	4972	PSU	C4-N3-C2	-4.11	120.71	126.37
2	L5	1522	OMG	N9-C4-N3	4.11	134.16	125.95
48	S2	814	PSU	C4-N3-C2	-4.10	120.72	126.37
48	S2	1004	PSU	C4-N3-C2	-4.10	120.72	126.37
2	L5	3851	PSU	C4-N3-C2	-4.10	120.72	126.37
2	L5	1582	PSU	C4-N3-C2	-4.10	120.72	126.37
48	S2	1445	PSU	C4-N3-C2	-4.09	120.73	126.37
48	S2	1850	MA6	N3-C4-N9	4.09	134.13	127.17
48	S2	1347	PSU	O2-C2-N1	-4.08	118.58	122.79
2	L5	5010	PSU	C4-N3-C2	-4.07	120.76	126.37
48	S2	121	OMU	N3-C2-N1	4.07	120.19	114.89
2	L5	1792	PSU	C4-N3-C2	-4.06	120.77	126.37
2	L5	4442	PSU	C4-N3-C2	-4.06	120.78	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3899	OMG	N9-C4-N3	4.05	134.06	125.95
2	L5	4361	PSU	C4-N3-C2	-4.05	120.79	126.37
2	L5	4228	OMG	N9-C4-N3	4.05	134.06	125.95
48	S2	966	PSU	C4-N3-C2	-4.05	120.79	126.37
48	S2	1288	OMU	N3-C2-N1	4.05	120.16	114.89
2	L5	1517	2MG	N1-C2-N2	-4.05	112.43	116.56
48	S2	93	PSU	C4-N3-C2	-4.04	120.80	126.37
48	S2	1643	PSU	C4-N3-C2	-4.04	120.80	126.37
48	S2	918	PSU	C4-N3-C2	-4.04	120.80	126.37
2	L5	3770	PSU	C4-N3-C2	-4.04	120.81	126.37
48	S2	34	PSU	C4-N3-C2	-4.04	120.81	126.37
48	S2	119	PSU	C4-N3-C2	-4.04	120.81	126.37
2	L5	3734	PSU	C4-N3-C2	-4.03	120.81	126.37
2	L5	4579	PSU	C4-N3-C2	-4.03	120.81	126.37
48	S2	1367	PSU	C4-N3-C2	-4.03	120.82	126.37
48	S2	823	PSU	O2-C2-N1	-4.03	118.64	122.79
48	S2	1056	PSU	C4-N3-C2	-4.00	120.86	126.37
48	S2	116	OMU	C5-C4-N3	4.00	120.41	114.80
48	S2	210	PSU	C4-N3-C2	-4.00	120.86	126.37
48	S2	1850	MA6	C4-C5-N7	-3.99	106.02	110.58
2	L5	3764	PSU	C4-N3-C2	-3.99	120.87	126.37
2	L5	1536	PSU	C4-N3-C2	-3.98	120.88	126.37
2	L5	4312	PSU	C4-N3-C2	-3.98	120.89	126.37
2	L5	2632	PSU	C4-N3-C2	-3.98	120.89	126.37
2	L5	4293	PSU	C4-N3-C2	-3.97	120.90	126.37
48	S2	1625	PSU	C4-N3-C2	-3.96	120.92	126.37
48	S2	36	PSU	C4-N3-C2	-3.96	120.92	126.37
2	L5	729	2MG	N1-C2-N2	-3.95	112.53	116.56
48	S2	609	PSU	C4-N3-C2	-3.95	120.93	126.37
2	L5	4532	PSU	C4-N3-C2	-3.94	120.94	126.37
48	S2	1232	PSU	C4-N3-C2	-3.94	120.94	126.37
2	L5	1522	OMG	C6-C5-N7	3.94	137.46	130.29
2	L5	4299	PSU	C4-N3-C2	-3.94	120.94	126.37
48	S2	1804	OMU	C5-C4-N3	3.94	120.32	114.80
2	L5	4498	OMU	C5-C4-N3	3.94	120.32	114.80
2	L5	4628	PSU	C4-N3-C2	-3.94	120.95	126.37
48	S2	1445	PSU	O2-C2-N1	-3.94	118.73	122.79
2	L5	4620	OMU	N3-C2-N1	3.93	120.01	114.89
48	S2	116	OMU	N3-C2-N1	3.93	120.01	114.89
48	S2	1244	PSU	O2-C2-N1	-3.93	118.74	122.79
48	S2	651	PSU	O2-C2-N1	-3.93	118.74	122.79
2	L5	3639	PSU	C4-N3-C2	-3.93	120.96	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	109	PSU	C4-N3-C2	-3.92	120.97	126.37
2	L5	4521	PSU	O2-C2-N1	-3.92	118.74	122.79
2	L5	4620	OMU	C4-N3-C2	-3.92	121.74	126.61
48	S2	1177	PSU	O2-C2-N1	-3.91	118.75	122.79
2	L5	3899	OMG	C6-C5-N7	3.91	137.40	130.29
2	L5	3853	PSU	C4-N3-C2	-3.90	121.00	126.37
48	S2	121	OMU	C5-C4-N3	3.90	120.26	114.80
48	S2	1248	B8N	C1'-C5-C4	3.89	123.52	117.61
48	S2	822	PSU	C4-N3-C2	-3.89	121.01	126.37
2	L5	1744	PSU	O2-C2-N1	-3.88	118.79	122.79
48	S2	172	OMU	C5-C4-N3	3.88	120.23	114.80
2	L5	1781	PSU	C4-N3-C2	-3.87	121.04	126.37
2	L5	1582	PSU	O2-C2-N1	-3.87	118.80	122.79
48	S2	1625	PSU	O2-C2-N1	-3.86	118.81	122.79
48	S2	1046	PSU	C4-N3-C2	-3.86	121.05	126.37
2	L5	4306	OMU	C5-C4-N3	3.86	120.21	114.80
2	L5	4636	PSU	C4-N3-C2	-3.86	121.06	126.37
2	L5	2415	OMU	N3-C2-N1	3.86	119.91	114.89
48	S2	1288	OMU	C5-C4-N3	3.85	120.20	114.80
2	L5	1862	PSU	O2-C2-N1	-3.85	118.82	122.79
2	L5	4623	OMG	C6-C5-N7	3.85	137.29	130.29
2	L5	3762	PSU	O2-C2-N1	-3.84	118.83	122.79
48	S2	428	OMU	C5-C4-N3	3.84	120.17	114.80
2	L5	4431	PSU	O2-C2-N1	-3.83	118.83	122.79
2	L5	4532	PSU	O2-C2-N1	-3.83	118.84	122.79
48	S2	218	PSU	C4-N3-C2	-3.83	121.09	126.37
2	L5	2415	OMU	C5-C4-N3	3.83	120.16	114.80
2	L5	3925	OMU	C5-C4-N3	3.83	120.16	114.80
48	S2	1326	OMU	C5-C4-N3	3.82	120.15	114.80
2	L5	5001	PSU	O2-C2-N1	-3.82	118.85	122.79
29	La	39	V5N	O-C-CA	-3.81	114.97	124.77
2	L5	4471	PSU	C4-N3-C2	-3.81	121.12	126.37
2	L5	1860	PSU	C4-N3-C2	-3.80	121.13	126.37
48	S2	1045	PSU	O2-C2-N1	-3.80	118.87	122.79
2	L5	4228	OMG	C6-C5-N7	3.80	137.21	130.29
48	S2	1442	OMU	C5-C4-N3	3.80	120.12	114.80
2	L5	1773	OMU	C5-C4-N3	3.79	120.11	114.80
48	S2	1174	PSU	O2-C2-N1	-3.78	118.89	122.79
2	L5	4872	2MG	N1-C2-N2	-3.76	112.72	116.56
48	S2	627	OMU	C5-C4-N3	3.76	120.06	114.80
2	L5	4423	PSU	O2-C2-N1	-3.75	118.92	122.79
48	S2	572	PSU	O2-C2-N1	-3.75	118.92	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	799	OMU	C5-C4-N3	3.74	120.05	114.80
2	L5	1782	PSU	O2-C2-N1	-3.73	118.94	122.79
48	S2	109	PSU	O2-C2-N1	-3.73	118.94	122.79
48	S2	1081	PSU	O2-C2-N1	-3.73	118.94	122.79
2	L5	4689	PSU	O2-C2-N1	-3.72	118.95	122.79
48	S2	1238	PSU	O2-C2-N1	-3.72	118.95	122.79
48	S2	1851	MA6	N3-C4-N9	3.71	133.47	127.17
48	S2	863	PSU	O2-C2-N1	-3.70	118.97	122.79
2	L5	4500	PSU	O2-C2-N1	-3.70	118.97	122.79
2	L5	4220	6MZ	C2-N3-C4	3.69	120.85	111.83
2	L5	4227	OMU	C5-C4-N3	3.69	119.97	114.80
2	L5	4220	6MZ	C4-C5-N7	-3.69	106.36	110.58
48	S2	1248	B8N	N3-C2-N1	3.68	121.21	116.72
1	L1	55	PSU	O2-C2-N1	-3.68	119.00	122.79
2	L5	4636	PSU	O2-C2-N1	-3.67	119.00	122.79
2	L5	1792	PSU	O2-C2-N1	-3.67	119.00	122.79
2	L5	4628	PSU	O2-C2-N1	-3.66	119.01	122.79
48	S2	119	PSU	O2-C2-N1	-3.66	119.02	122.79
2	L5	3853	PSU	O2-C2-N1	-3.65	119.02	122.79
48	S2	866	PSU	O2-C2-N1	-3.65	119.03	122.79
2	L5	4576	PSU	O2-C2-N1	-3.65	119.03	122.79
48	S2	918	PSU	O2-C2-N1	-3.63	119.05	122.79
2	L5	3695	PSU	O2-C2-N1	-3.62	119.05	122.79
63	SO	138	IAS	OD1-CG-CB	-3.61	114.88	125.38
2	L5	3734	PSU	O2-C2-N1	-3.61	119.07	122.79
2	L5	4420	PSU	O2-C2-N1	-3.60	119.07	122.79
48	S2	1232	PSU	O2-C2-N1	-3.60	119.08	122.79
48	S2	686	PSU	O2-C2-N1	-3.59	119.09	122.79
2	L5	4312	PSU	O2-C2-N1	-3.58	119.10	122.79
2	L5	2508	PSU	O2-C2-N1	-3.57	119.11	122.79
2	L5	3637	PSU	O2-C2-N1	-3.55	119.12	122.79
2	L5	4293	PSU	O2-C2-N1	-3.55	119.12	122.79
48	S2	406	PSU	O2-C2-N1	-3.54	119.14	122.79
48	S2	1004	PSU	O2-C2-N1	-3.53	119.15	122.79
2	L5	4392	OMG	C6-C5-N7	3.52	136.70	130.29
2	L5	2632	PSU	O2-C2-N1	-3.52	119.16	122.79
2	L5	3730	PSU	O2-C2-N1	-3.52	119.16	122.79
2	L5	4296	PSU	O2-C2-N1	-3.51	119.16	122.79
2	L5	3764	PSU	O2-C2-N1	-3.51	119.17	122.79
2	L5	5010	PSU	O2-C2-N1	-3.51	119.17	122.79
48	S2	1832	6MZ	C2-N3-C4	3.51	120.41	111.83
48	S2	1850	MA6	C2-N3-C4	3.51	120.40	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	69	PSU	O2-C2-N1	-3.51	119.17	122.79
48	S2	1643	PSU	O2-C2-N1	-3.50	119.18	122.79
2	L5	4579	PSU	O2-C2-N1	-3.50	119.18	122.79
2	L5	3770	PSU	O2-C2-N1	-3.49	119.19	122.79
48	S2	683	OMG	C6-C5-N7	3.49	136.64	130.29
2	L5	4618	OMG	C6-C5-N7	3.49	136.64	130.29
2	L5	2364	OMG	C6-C5-N7	3.49	136.64	130.29
48	S2	649	PSU	O2-C2-N1	-3.49	119.19	122.79
48	S2	815	PSU	O2-C2-N1	-3.48	119.20	122.79
48	S2	116	OMU	O4-C4-C5	-3.48	119.16	125.16
48	S2	814	PSU	O2-C2-N1	-3.47	119.21	122.79
2	L5	4442	PSU	O2-C2-N1	-3.47	119.22	122.79
48	S2	1692	PSU	O2-C2-N1	-3.46	119.22	122.79
2	L5	3844	PSU	O2-C2-N1	-3.45	119.23	122.79
2	L5	1677	PSU	O2-C2-N1	-3.45	119.23	122.79
2	L5	4530	UR3	C5-C4-N3	3.45	119.58	115.04
48	S2	1832	6MZ	C4-C5-N7	-3.45	106.64	110.58
2	L5	2837	OMU	C5-C4-N3	3.44	119.62	114.80
2	L5	4494	OMG	C6-C5-N7	3.44	136.55	130.29
48	S2	34	PSU	O2-C2-N1	-3.44	119.25	122.79
48	S2	436	OMG	C6-C5-N7	3.43	136.54	130.29
2	L5	4403	PSU	O2-C2-N1	-3.43	119.25	122.79
48	S2	218	PSU	O2-C2-N1	-3.43	119.25	122.79
48	S2	1832	6MZ	N1-C2-N3	-3.43	123.40	128.58
2	L5	4457	PSU	O2-C2-N1	-3.42	119.26	122.79
2	L5	2050	OMG	C6-C5-N7	3.41	136.50	130.29
2	L5	4620	OMU	C5-C4-N3	3.40	119.57	114.80
48	S2	822	PSU	O2-C2-N1	-3.40	119.28	122.79
2	L5	4220	6MZ	N1-C2-N3	-3.39	123.45	128.58
48	S2	1328	OMG	C6-C5-N7	3.38	136.44	130.29
48	S2	105	PSU	O2-C2-N1	-3.37	119.32	122.79
2	L5	4220	6MZ	C6-C5-N7	3.36	136.09	132.43
2	L5	3715	PSU	O2-C2-N1	-3.36	119.33	122.79
2	L5	4673	PSU	O2-C2-N1	-3.36	119.33	122.79
2	L5	4637	OMG	C6-C5-N7	3.36	136.40	130.29
48	S2	1850	MA6	N1-C2-N3	-3.34	123.52	128.58
2	L5	3758	PSU	O2-C2-N1	-3.34	119.34	122.79
48	S2	1851	MA6	C2-N3-C4	3.34	119.99	111.83
48	S2	1367	PSU	O2-C2-N1	-3.34	119.35	122.79
48	S2	609	PSU	O2-C2-N1	-3.31	119.37	122.79
2	L5	3744	OMG	C6-C5-N7	3.30	136.29	130.29
48	S2	428	OMU	O4-C4-C5	-3.29	119.48	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	601	OMG	C6-C5-N7	3.29	136.28	130.29
2	L5	1536	PSU	O2-C2-N1	-3.29	119.39	122.79
2	L5	4498	OMU	O4-C4-C5	-3.28	119.50	125.16
48	S2	1056	PSU	O2-C2-N1	-3.28	119.40	122.79
2	L5	4972	PSU	O2-C2-N1	-3.28	119.41	122.79
48	S2	93	PSU	O2-C2-N1	-3.27	119.41	122.79
2	L5	2876	OMG	C6-C5-N7	3.27	136.24	130.29
2	L5	4499	OMG	C6-C5-N7	3.27	136.23	130.29
8	LD	216	V5N	O-C-CA	-3.26	116.38	124.77
1	L1	75	OMG	C6-C5-N7	3.26	136.22	130.29
48	S2	509	OMG	C6-C5-N7	3.26	136.22	130.29
48	S2	1851	MA6	C4-N9-C8	3.24	109.14	105.74
48	S2	36	PSU	O2-C2-N1	-3.23	119.45	122.79
2	L5	4196	OMG	C6-C5-N7	3.23	136.17	130.29
2	L5	4370	OMG	C6-C5-N7	3.20	136.12	130.29
48	S2	1490	OMG	C6-C5-N7	3.20	136.11	130.29
48	S2	966	PSU	O2-C2-N1	-3.18	119.51	122.79
29	La	39	V5N	O2-CB-CA	3.18	114.48	107.49
48	S2	121	OMU	O4-C4-C5	-3.16	119.72	125.16
48	S2	210	PSU	O2-C2-N1	-3.15	119.54	122.79
2	L5	4361	PSU	O2-C2-N1	-3.14	119.55	122.79
2	L5	3899	OMG	C4-C5-N7	-3.14	105.70	110.67
2	L5	1781	PSU	O2-C2-N1	-3.13	119.56	122.79
2	L5	3884	PSU	O2-C2-N1	-3.12	119.57	122.79
48	S2	681	PSU	O2-C2-N1	-3.12	119.57	122.79
48	S2	1442	OMU	O4-C4-C5	-3.12	119.78	125.16
48	S2	867	OMG	C6-C5-N7	3.11	135.95	130.29
48	S2	1851	MA6	N1-C2-N3	-3.10	123.88	128.58
48	S2	1832	6MZ	C6-C5-N7	3.10	135.81	132.43
48	S2	1046	PSU	O2-C2-N1	-3.10	119.60	122.79
48	S2	1804	OMU	O4-C4-C5	-3.09	119.83	125.16
2	L5	1860	PSU	O2-C2-N1	-3.09	119.60	122.79
2	L5	1625	OMG	C6-C5-N7	3.09	135.91	130.29
2	L5	3944	OMG	C6-C5-N7	3.08	135.90	130.29
48	S2	644	OMG	C6-C5-N7	3.08	135.90	130.29
2	L5	4870	OMG	C6-C5-N7	3.08	135.90	130.29
2	L5	4353	PSU	O2-C2-N1	-3.08	119.61	122.79
2	L5	3639	PSU	O2-C2-N1	-3.08	119.62	122.79
2	L5	4498	OMU	O2-C2-N1	-3.06	118.81	122.80
48	S2	1850	MA6	C4-N9-C8	3.05	108.94	105.74
2	L5	3782	5MC	C5-C6-N1	-3.02	120.03	123.31
48	S2	1288	OMU	O4-C4-C5	-3.02	119.95	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	801	PSU	O2-C2-N1	-3.02	119.67	122.79
2	L5	1322	1MA	N1-C6-N6	3.02	127.29	119.71
2	L5	3785	A2M	C2'-C1'-N9	-3.02	108.79	113.75
2	L5	1522	OMG	C4-C5-N7	-3.00	105.92	110.67
2	L5	4299	PSU	O2-C2-N1	-2.99	119.70	122.79
48	S2	1326	OMU	O4-C4-C5	-2.99	120.00	125.16
2	L5	1760	OMG	C6-C5-N7	2.98	135.71	130.29
2	L5	4471	PSU	O2-C2-N1	-2.97	119.73	122.79
2	L5	4623	OMG	C4-C5-N7	-2.96	105.97	110.67
2	L5	1316	OMG	C6-C5-N7	2.96	135.67	130.29
48	S2	172	OMU	O4-C4-C5	-2.94	120.09	125.16
2	L5	2415	OMU	O4-C4-C5	-2.94	120.09	125.16
2	L5	1773	OMU	O4-C4-C5	-2.94	120.10	125.16
2	L5	3792	OMG	C6-C5-N7	2.93	135.62	130.29
2	L5	4228	OMG	C4-C5-N7	-2.93	106.03	110.67
48	S2	1851	MA6	C5-N7-C8	2.93	108.05	103.45
2	L5	2837	OMU	O4-C4-C5	-2.93	120.12	125.16
2	L5	2424	OMG	C6-C5-N7	2.92	135.61	130.29
2	L5	4392	OMG	C4-C5-N7	-2.89	106.09	110.67
2	L5	1322	1MA	C6-C5-N7	-2.88	127.07	132.16
48	S2	1248	B8N	C31-N3-C4	2.88	121.25	117.18
2	L5	4306	OMU	O4-C4-C5	-2.88	120.20	125.16
2	L5	1534	A2M	C3'-C2'-C1'	-2.87	97.31	102.81
8	LD	216	V5N	O2-CB-CA	2.87	113.79	107.49
48	S2	1288	OMU	O3'-C3'-C2'	2.86	119.18	111.19
48	S2	627	OMU	O4-C4-C5	-2.85	120.24	125.16
48	S2	799	OMU	O4-C4-C5	-2.83	120.29	125.16
2	L5	3925	OMU	O4-C4-C5	-2.82	120.30	125.16
48	S2	683	OMG	C4-C5-N7	-2.82	106.20	110.67
48	S2	1850	MA6	C5-N7-C8	2.82	107.88	103.45
2	L5	1322	1MA	CM1-N1-C6	-2.78	115.84	120.15
48	S2	172	OMU	O2-C2-N1	-2.77	119.19	122.80
2	L5	1871	A2M	C2'-C1'-N9	-2.77	109.20	113.75
2	L5	4618	OMG	C4-C5-N7	-2.76	106.29	110.67
2	L5	3851	PSU	O2-C2-N1	-2.76	119.94	122.79
2	L5	3782	5MC	C5-C4-N3	-2.74	118.94	121.75
2	L5	4523	A2M	C3'-C2'-C1'	-2.72	97.60	102.81
2	L5	3920	PSU	O2-C2-N1	-2.70	120.00	122.79
2	L5	4227	OMU	O4-C4-C5	-2.69	120.52	125.16
5	LB	245	HIC	CZ-NE2-CD2	-2.69	122.50	126.03
2	L5	4220	6MZ	C5-N7-C8	2.69	107.67	103.45
48	S2	1851	MA6	C9-N6-C6	-2.68	113.72	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	75	OMG	C4-C5-N7	-2.66	106.45	110.67
2	L5	2050	OMG	C4-C5-N7	-2.66	106.46	110.67
48	S2	1710	OMC	O2-C2-N3	-2.66	118.14	122.33
48	S2	1328	OMG	C4-C5-N7	-2.65	106.47	110.67
48	S2	1851	MA6	C6-C5-N7	2.65	137.66	133.43
48	S2	644	OMG	C4-C5-N7	-2.65	106.48	110.67
48	S2	1337	4AC	C6-C5-C4	2.61	120.15	117.00
2	L5	3925	OMU	O2-C2-N1	-2.61	119.40	122.80
2	L5	1536	PSU	C6-C5-C4	-2.61	116.41	118.17
2	L5	3792	OMG	C4-C5-N7	-2.60	106.54	110.67
48	S2	509	OMG	C4-C5-N7	-2.60	106.55	110.67
48	S2	1832	6MZ	C4-N9-C8	2.60	108.46	105.74
2	L5	2364	OMG	C4-C5-N7	-2.59	106.56	110.67
2	L5	3744	OMG	C4-C5-N7	-2.57	106.60	110.67
48	S2	918	PSU	O4'-C1'-C2'	2.57	108.70	105.15
48	S2	406	PSU	C5-C6-N1	-2.57	118.58	122.14
2	L5	4499	OMG	C4-C5-N7	-2.57	106.60	110.67
2	L5	3637	PSU	C5-C6-N1	-2.55	118.60	122.14
48	S2	116	OMU	O2-C2-N1	-2.55	119.48	122.80
48	S2	436	OMG	C4-C5-N7	-2.54	106.64	110.67
2	L5	4637	OMG	C4-C5-N7	-2.54	106.64	110.67
2	L5	3818	UY1	C6-N1-C2	-2.54	120.33	122.69
48	S2	1248	B8N	O4-C4-C5	-2.54	118.19	122.58
48	S2	601	OMG	C4-C5-N7	-2.53	106.66	110.67
2	L5	4494	OMG	C4-C5-N7	-2.53	106.66	110.67
2	L5	2837	OMU	O2-C2-N1	-2.52	119.51	122.80
2	L5	1625	OMG	C4-C5-N7	-2.52	106.67	110.67
48	S2	576	A2M	C2'-C1'-N9	-2.52	109.60	113.75
48	S2	1851	MA6	C10-N6-C9	-2.52	108.08	116.18
2	L5	1677	PSU	C5-C6-N1	-2.52	118.64	122.14
2	L5	4420	PSU	C5-C6-N1	-2.52	118.64	122.14
2	L5	4196	OMG	C4-C5-N7	-2.51	106.69	110.67
2	L5	4447	5MC	C5-C4-N3	-2.51	119.19	121.75
48	S2	428	OMU	O2-C2-N1	-2.50	119.54	122.80
48	S2	1383	A2M	C3'-C2'-C1'	-2.50	98.03	102.81
2	L5	3785	A2M	C4'-O4'-C1'	-2.49	103.96	109.47
2	L5	1760	OMG	C4-C5-N7	-2.49	106.72	110.67
2	L5	4227	OMU	O2-C2-N1	-2.48	119.56	122.80
2	L5	4590	A2M	C2'-C1'-N9	-2.48	109.68	113.75
48	S2	1832	6MZ	C5-N7-C8	2.47	107.34	103.45
48	S2	867	OMG	C4-C5-N7	-2.47	106.76	110.67
48	S2	1031	A2M	C2'-C1'-N9	-2.46	109.70	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1850	MA6	C9-N6-C6	-2.45	114.28	120.52
2	L5	4353	PSU	C5-C6-N1	-2.45	118.74	122.14
2	L5	4370	OMG	C4-C5-N7	-2.44	106.80	110.67
48	S2	681	PSU	C5-C6-N1	-2.44	118.75	122.14
2	L5	4220	6MZ	C4-N9-C8	2.44	108.30	105.74
2	L5	3718	A2M	N3-C2-N1	2.44	132.27	128.58
48	S2	1383	A2M	C2'-C1'-N9	-2.44	109.74	113.75
48	S2	590	A2M	N3-C4-N9	2.43	131.30	127.17
2	L5	4872	2MG	N1-C2-N3	2.42	127.75	123.68
48	S2	799	OMU	C1'-N1-C2	2.41	121.92	117.59
2	L5	3758	PSU	C5-C6-N1	-2.41	118.80	122.14
48	S2	1238	PSU	C5-C6-N1	-2.41	118.80	122.14
48	S2	1832	6MZ	C2-N1-C6	2.41	123.22	115.24
2	L5	2876	OMG	O6-C6-C5	-2.41	120.18	126.53
2	L5	3944	OMG	C4-C5-N7	-2.41	106.86	110.67
2	L5	3695	PSU	C5-C6-N1	-2.40	118.81	122.14
2	L5	1326	A2M	N3-C4-N9	2.40	131.25	127.17
1	L1	69	PSU	O4'-C1'-C2'	2.40	108.47	105.15
2	L5	3920	PSU	O2-C2-N3	-2.39	117.61	121.86
2	L5	729	2MG	N1-C2-N3	2.38	127.69	123.68
48	S2	1248	B8N	O4-C4-N3	-2.38	116.12	119.99
48	S2	1639	7MG	C5-C4-N9	2.38	109.38	106.33
48	S2	1639	7MG	C4-C5-N7	2.37	108.18	105.38
48	S2	1851	MA6	N9-C8-N7	-2.37	110.57	113.94
1	L1	69	PSU	C5-C6-N1	-2.37	118.85	122.14
2	L5	4620	OMU	O2-C2-N1	-2.37	119.71	122.80
48	S2	801	PSU	C5-C6-N1	-2.36	118.86	122.14
48	S2	627	OMU	O2-C2-N1	-2.36	119.72	122.80
2	L5	4870	OMG	C4-C5-N7	-2.36	106.94	110.67
2	L5	2364	OMG	O6-C6-C5	-2.35	120.32	126.53
2	L5	2876	OMG	C4-C5-N7	-2.35	106.95	110.67
2	L5	4296	PSU	C5-C6-N1	-2.35	118.88	122.14
2	L5	2424	OMG	C4-C5-N7	-2.35	106.95	110.67
48	S2	1177	PSU	C5-C6-N1	-2.35	118.89	122.14
48	S2	1326	OMU	O2-C2-N1	-2.34	119.75	122.80
2	L5	4637	OMG	O6-C6-C5	-2.34	120.35	126.53
2	L5	1517	2MG	N1-C2-N3	2.33	127.60	123.68
2	L5	4620	OMU	O4-C4-C5	-2.33	121.14	125.16
2	L5	2415	OMU	C1'-N1-C2	2.33	121.77	117.59
2	L5	4499	OMG	O6-C6-C5	-2.32	120.41	126.53
48	S2	668	A2M	O4'-C1'-N9	-2.31	103.66	108.09
48	S2	815	PSU	C5-C6-N1	-2.30	118.94	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S4	9	1MG	N2-C2-N1	-2.30	116.94	118.79
2	L5	1524	A2M	N3-C4-N9	2.30	131.08	127.17
2	L5	4442	PSU	O4'-C1'-C2'	2.30	108.33	105.15
48	S2	1347	PSU	C5-C6-N1	-2.29	118.96	122.14
2	L5	4500	PSU	C5-C6-N1	-2.29	118.96	122.14
2	L5	4392	OMG	O6-C6-C5	-2.29	120.48	126.53
1	L1	75	OMG	O6-C6-C5	-2.29	120.50	126.53
2	L5	3768	PSU	C5-C6-N1	-2.28	118.97	122.14
48	S2	1337	4AC	C5-C4-N3	-2.28	119.03	122.60
48	S2	867	OMG	O6-C6-C5	-2.28	120.52	126.53
48	S2	651	PSU	C5-C6-N1	-2.28	118.98	122.14
2	L5	1316	OMG	O6-C6-C5	-2.27	120.53	126.53
2	L5	2424	OMG	O6-C6-C5	-2.27	120.55	126.53
48	S2	1850	MA6	C6-C5-N7	2.26	137.05	133.43
5	LB	245	HIC	CD2-NE2-CE1	2.25	107.60	106.71
2	L5	3920	PSU	C5-C6-N1	-2.25	119.01	122.14
2	L5	3818	UY1	O2-C2-N1	-2.25	120.47	122.79
48	S2	1383	A2M	C2'-C3'-C4'	-2.24	97.17	101.99
2	L5	398	A2M	N3-C4-N9	2.24	130.98	127.17
2	L5	4370	OMG	O6-C6-C5	-2.24	120.61	126.53
2	L5	3899	OMG	C8-N7-C5	2.24	108.25	104.26
48	S2	822	PSU	O4'-C1'-C2'	2.24	108.25	105.15
48	S2	1056	PSU	C5-C6-N1	-2.24	119.04	122.14
2	L5	4870	OMG	O6-C6-C5	-2.23	120.63	126.53
2	L5	3830	A2M	C2'-C1'-N9	-2.23	110.08	113.75
6	S4	37	1MG	N2-C2-N1	-2.23	116.99	118.79
2	L5	3639	PSU	C5-C6-N1	-2.23	119.05	122.14
2	L5	3867	A2M	N3-C4-N9	2.23	130.96	127.17
48	S2	1850	MA6	N9-C8-N7	-2.23	110.78	113.94
2	L5	1316	OMG	C4-C5-N7	-2.23	107.14	110.67
2	L5	1326	A2M	C5-C4-N3	-2.22	123.65	126.72
2	L5	3770	PSU	C5-C6-N1	-2.22	119.05	122.14
2	L5	4196	OMG	O6-C6-C5	-2.22	120.67	126.53
2	L5	4220	6MZ	C2-N1-C6	2.22	122.60	115.24
2	L5	3701	OMC	O2-C2-N3	-2.21	118.84	122.33
2	L5	3785	A2M	O4'-C1'-N9	2.21	112.34	108.09
48	S2	644	OMG	O6-C6-C5	-2.21	120.69	126.53
2	L5	729	2MG	C6-C5-C4	2.21	122.16	118.83
48	S2	1490	OMG	C4-C5-N7	-2.21	107.17	110.67
2	L5	4403	PSU	C5-C6-N1	-2.21	119.08	122.14
8	LD	216	V5N	O2-CB-CG	-2.21	104.24	109.90
2	L5	4523	A2M	C2'-C1'-N9	-2.20	110.13	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1517	2MG	C6-C5-C4	2.20	122.14	118.83
1	L1	55	PSU	C5-C6-N1	-2.20	119.09	122.14
48	S2	1490	OMG	O6-C6-C5	-2.20	120.74	126.53
48	S2	601	OMG	O6-C6-C5	-2.19	120.74	126.53
48	S2	686	PSU	C5-C6-N1	-2.19	119.10	122.14
2	L5	3884	PSU	C5-C6-N1	-2.19	119.10	122.14
2	L5	1773	OMU	O2'-C2'-C1'	2.19	113.14	108.99
48	S2	1678	A2M	C2-N1-C6	-2.19	115.14	118.73
48	S2	512	A2M	N3-C4-N9	2.18	130.88	127.17
48	S2	590	A2M	C2-N1-C6	-2.18	115.14	118.73
48	S2	159	A2M	C3'-C2'-C1'	-2.18	98.63	102.81
2	L5	3744	OMG	O6-C6-C5	-2.18	120.78	126.53
2	L5	4872	2MG	C6-C5-C4	2.18	122.11	118.83
48	S2	1045	PSU	C5-C6-N1	-2.18	119.12	122.14
48	S2	1678	A2M	N3-C4-N9	2.17	130.87	127.17
2	L5	4628	PSU	O4'-C1'-C2'	2.17	108.15	105.15
2	L5	3715	PSU	C5-C6-N1	-2.17	119.13	122.14
2	L5	3851	PSU	C5-C6-N1	-2.17	119.13	122.14
2	L5	2401	A2M	N3-C4-N9	2.16	130.84	127.17
48	S2	1248	B8N	O4'-C1'-C2'	2.16	108.13	105.15
48	S2	823	PSU	C5-C6-N1	-2.15	119.15	122.14
2	L5	3718	A2M	C2-N1-C6	-2.15	115.19	118.73
48	S2	166	A2M	N3-C4-N9	2.15	130.82	127.17
2	L5	3920	PSU	O4'-C1'-C2'	2.15	108.12	105.15
48	S2	966	PSU	C5-C6-N1	-2.14	119.17	122.14
48	S2	166	A2M	C2-N1-C6	-2.14	115.22	118.73
71	SX	62	HY3	O-C-CA	-2.14	119.21	124.86
48	S2	1842	4AC	C5-C4-N3	-2.14	119.26	122.60
2	L5	4571	A2M	C2-N1-C6	-2.13	115.23	118.73
2	L5	3639	PSU	O4'-C1'-C2'	2.13	108.10	105.15
48	S2	1643	PSU	O4'-C1'-C2'	2.13	108.10	105.15
2	L5	4636	PSU	O4'-C1'-C2'	2.13	108.10	105.15
2	L5	1744	PSU	C5-C6-N1	-2.13	119.19	122.14
2	L5	2351	OMC	O2-C2-N3	-2.13	118.98	122.33
48	S2	468	A2M	N3-C4-N9	2.13	130.78	127.17
48	S2	590	A2M	C5-C4-N3	-2.13	123.79	126.72
48	S2	159	A2M	C2-N1-C6	-2.12	115.24	118.73
48	S2	36	PSU	C5-C6-N1	-2.12	119.20	122.14
48	S2	484	A2M	N3-C4-N9	2.12	130.77	127.17
2	L5	4972	PSU	C5-C6-N1	-2.12	119.20	122.14
29	La	39	V5N	O2-CB-CG	-2.12	104.46	109.90
48	S2	210	PSU	C5-C6-N1	-2.12	119.20	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	1337	4AC	N4-C4-N3	2.12	117.30	113.87
48	S2	1081	PSU	C5-C6-N1	-2.11	119.21	122.14
2	L5	4456	OMC	O2-C2-N3	-2.11	119.00	122.33
2	L5	1340	OMC	O2-C2-N3	-2.11	119.00	122.33
2	L5	398	A2M	C2-N1-C6	-2.11	115.27	118.73
48	S2	218	PSU	O4'-C1'-C2'	2.11	108.07	105.15
48	S2	468	A2M	C2-N1-C6	-2.11	115.27	118.73
2	L5	4370	OMG	C5-C6-N1	2.10	118.61	113.25
48	S2	436	OMG	O6-C6-C5	-2.10	120.99	126.53
2	L5	4637	OMG	C5-C6-N1	2.10	118.60	113.25
2	L5	2363	A2M	N3-C2-N1	2.10	131.76	128.58
48	S2	1367	PSU	C5-C6-N1	-2.10	119.23	122.14
2	L5	3944	OMG	O6-C6-C5	-2.10	121.00	126.53
48	S2	1081	PSU	O4'-C1'-C2'	2.10	108.05	105.15
2	L5	4471	PSU	C5-C6-N1	-2.09	119.23	122.14
2	L5	2364	OMG	C5-C6-N1	2.09	118.58	113.25
48	S2	576	A2M	C2-N1-C6	-2.09	115.30	118.73
48	S2	121	OMU	O2-C2-N1	-2.09	120.08	122.80
48	S2	1004	PSU	C5-C6-N1	-2.09	119.24	122.14
2	L5	1522	OMG	C2'-C1'-N9	-2.09	110.28	114.24
48	S2	27	A2M	N3-C4-N9	2.08	130.71	127.17
2	L5	4689	PSU	C5-C6-N1	-2.08	119.25	122.14
2	L5	2363	A2M	C2-N1-C6	-2.08	115.31	118.73
2	L5	1881	OMC	O2-C2-N3	-2.08	119.05	122.33
2	L5	3762	PSU	C5-C6-N1	-2.08	119.25	122.14
48	S2	863	PSU	C5-C6-N1	-2.08	119.25	122.14
48	S2	159	A2M	N3-C4-N9	2.08	130.70	127.17
2	L5	1524	A2M	C2-N1-C6	-2.08	115.32	118.73
2	L5	2508	PSU	C5-C6-N1	-2.07	119.26	122.14
2	L5	4618	OMG	O6-C6-C5	-2.07	121.06	126.53
2	L5	3730	PSU	C5-C6-N1	-2.07	119.27	122.14
2	L5	3792	OMG	O6-C6-C5	-2.07	121.07	126.53
2	L5	3639	PSU	O2-C2-N3	-2.07	118.19	121.86
2	L5	3830	A2M	N3-C4-N9	2.07	130.68	127.17
48	S2	801	PSU	O2-C2-N3	-2.07	118.19	121.86
2	L5	1456	JMH	C6-N1-C2	-2.06	120.11	121.80
2	L5	1760	OMG	O6-C6-C5	-2.06	121.09	126.53
2	L5	1522	OMG	C8-N7-C5	2.06	107.93	104.26
2	L5	4299	PSU	C5-C6-N1	-2.06	119.28	122.14
48	S2	572	PSU	C5-C6-N1	-2.06	119.28	122.14
48	S2	1692	PSU	C5-C6-N1	-2.06	119.28	122.14
2	L5	2787	A2M	C2-N1-C6	-2.06	115.35	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	814	PSU	C5-C6-N1	-2.06	119.28	122.14
2	L5	4673	PSU	C5-C6-N1	-2.06	119.29	122.14
2	L5	1683	PSU	C5-C6-N1	-2.05	119.29	122.14
2	L5	398	A2M	C5-C4-N3	-2.05	123.89	126.72
2	L5	4457	PSU	O4'-C1'-C2'	2.05	107.99	105.15
48	S2	823	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	L5	3851	PSU	O2-C2-N3	-2.05	118.22	121.86
48	S2	34	PSU	C5-C6-N1	-2.05	119.30	122.14
2	L5	3695	PSU	O4'-C1'-C2'	2.04	107.98	105.15
2	L5	4499	OMG	C5-C6-N1	2.04	118.45	113.25
48	S2	1445	PSU	O4'-C1'-C2'	2.04	107.97	105.15
2	L5	4494	OMG	O6-C6-C5	-2.04	121.15	126.53
2	L5	3867	A2M	C2-N1-C6	-2.04	115.39	118.73
48	S2	1850	MA6	C10-N6-C9	-2.04	109.64	116.18
2	L5	4431	PSU	C5-C6-N1	-2.04	119.31	122.14
48	S2	918	PSU	C5-C6-N1	-2.03	119.32	122.14
48	S2	1850	MA6	N1-C6-N6	2.03	119.33	116.86
2	L5	4500	PSU	O4'-C1'-C2'	2.03	107.96	105.15
48	S2	683	OMG	C8-N7-C5	2.03	107.88	104.26
2	L5	4571	A2M	N3-C4-N9	2.03	130.62	127.17
2	L5	4228	OMG	C8-N7-C5	2.03	107.87	104.26
2	L5	4423	PSU	C5-C6-N1	-2.02	119.33	122.14
2	L5	2815	A2M	N3-C4-N9	2.02	130.61	127.17
2	L5	3825	A2M	C3'-C2'-C1'	-2.02	98.93	102.81
2	L5	1625	OMG	O6-C6-C5	-2.02	121.19	126.53
48	S2	1383	A2M	N3-C4-N9	2.02	130.60	127.17
48	S2	1328	OMG	O6-C6-C5	-2.02	121.21	126.53
2	L5	1862	PSU	C5-C6-N1	-2.02	119.34	122.14
48	S2	1046	PSU	O4'-C1'-C2'	2.02	107.94	105.15
2	L5	1860	PSU	C5-C6-N1	-2.01	119.34	122.14
2	L5	4196	OMG	C5-C6-N1	2.01	118.38	113.25
48	S2	99	A2M	C2-N1-C6	-2.01	115.42	118.73
2	L5	3760	A2M	C2-N1-C6	-2.01	115.43	118.73
48	S2	1288	OMU	O2-C2-N1	-2.01	120.18	122.80
48	S2	99	A2M	N3-C4-N9	2.01	130.58	127.17
48	S2	1383	A2M	C2-N1-C6	-2.01	115.43	118.73
2	L5	4521	PSU	O4'-C1'-C2'	2.00	107.92	105.15
2	L5	3818	UY1	O4'-C1'-C2'	2.00	108.06	104.56

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L5	3701	OMC	C2'-C1'-N1-C6
2	L5	3760	A2M	C1'-C2'-O2'-CM'
2	L5	4590	A2M	C4'-C5'-O5'-P
6	S4	18	OMG	C1'-C2'-O2'-CM2
6	S4	47	H2U	O4'-C4'-C5'-O5'
6	S4	47	H2U	C3'-C4'-C5'-O5'
48	S2	1248	B8N	O4'-C4'-C5'-O5'
48	S2	1383	A2M	C1'-C2'-O2'-CM'
48	S2	1678	A2M	C1'-C2'-O2'-CM'
48	S2	1832	6MZ	C5-C6-N6-C9
48	S2	1832	6MZ	N1-C6-N6-C9
48	S2	1851	MA6	C5-C6-N6-C10
2	L5	4636	PSU	C3'-C4'-C5'-O5'
2	L5	4870	OMG	O4'-C4'-C5'-O5'
6	S4	16	H2U	O4'-C4'-C5'-O5'
48	S2	576	A2M	C3'-C4'-C5'-O5'
2	L5	3701	OMC	C2'-C1'-N1-C2
2	L5	3760	A2M	O4'-C4'-C5'-O5'
2	L5	4500	PSU	O4'-C4'-C5'-O5'
2	L5	4636	PSU	O4'-C4'-C5'-O5'
2	L5	4870	OMG	C3'-C4'-C5'-O5'
48	S2	512	A2M	O4'-C4'-C5'-O5'
48	S2	576	A2M	O4'-C4'-C5'-O5'
48	S2	1639	7MG	C3'-C4'-C5'-O5'
48	S2	1851	MA6	N1-C6-N6-C10
2	L5	3760	A2M	C3'-C4'-C5'-O5'
2	L5	4500	PSU	C3'-C4'-C5'-O5'
48	S2	1248	B8N	C3'-C4'-C5'-O5'
2	L5	3851	PSU	C3'-C4'-C5'-O5'
6	S4	16	H2U	C3'-C4'-C5'-O5'
48	S2	668	A2M	O4'-C4'-C5'-O5'
48	S2	1639	7MG	O4'-C4'-C5'-O5'
48	S2	1248	B8N	N34-C33-C34-O36
48	S2	627	OMU	O4'-C4'-C5'-O5'
48	S2	668	A2M	C3'-C4'-C5'-O5'
48	S2	1850	MA6	C5-C6-N6-C9
2	L5	4447	5MC	C2'-C1'-N1-C6
6	S4	18	OMG	O4'-C4'-C5'-O5'
6	S4	20	H2U	O4'-C4'-C5'-O5'
33	Le	53	MLZ	CE-CD-CG-CB
2	L5	2787	A2M	C2'-C1'-N9-C8
48	S2	627	OMU	C3'-C4'-C5'-O5'
2	L5	1534	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
6	S4	58	1MA	O4'-C4'-C5'-O5'
48	S2	428	OMU	C2'-C1'-N1-C6
2	L5	2787	A2M	C2'-C1'-N9-C4
48	S2	1248	B8N	N34-C33-C34-O35
6	S4	20	H2U	C3'-C4'-C5'-O5'
48	S2	512	A2M	C3'-C4'-C5'-O5'
2	L5	3851	PSU	O4'-C4'-C5'-O5'
48	S2	590	A2M	C3'-C4'-C5'-O5'
2	L5	3818	UY1	C4'-C5'-O5'-P
2	L5	2364	OMG	O4'-C4'-C5'-O5'
30	Lb	5	MLZ	C-CA-CB-CG
2	L5	4447	5MC	O4'-C1'-N1-C6
30	Lb	5	MLZ	N-CA-CB-CG
63	SO	138	IAS	CA-CB-CG-OD1
2	L5	1326	A2M	C4'-C5'-O5'-P
48	S2	590	A2M	O4'-C4'-C5'-O5'
48	S2	799	OMU	C3'-C4'-C5'-O5'
48	S2	428	OMU	O4'-C1'-N1-C6
2	L5	3869	OMC	C3'-C2'-O2'-CM2
2	L5	4500	PSU	C4'-C5'-O5'-P
48	S2	644	OMG	C4'-C5'-O5'-P
2	L5	3701	OMC	O4'-C1'-N1-C2
2	L5	3701	OMC	O4'-C1'-N1-C6
6	S4	9	1MG	C4'-C5'-O5'-P
2	L5	3785	A2M	O4'-C4'-C5'-O5'
2	L5	4447	5MC	O4'-C1'-N1-C2
2	L5	4870	OMG	C4'-C5'-O5'-P
48	S2	1490	OMG	C4'-C5'-O5'-P
2	L5	4447	5MC	C2'-C1'-N1-C2
2	L5	2401	A2M	C3'-C2'-O2'-CM'
2	L5	3944	OMG	C3'-C2'-O2'-CM2
2	L5	4499	OMG	C3'-C2'-O2'-CM2
2	L5	1322	1MA	C2'-C1'-N9-C4
48	S2	1851	MA6	C4'-C5'-O5'-P
6	S4	58	1MA	C3'-C4'-C5'-O5'
48	S2	683	OMG	O4'-C4'-C5'-O5'
2	L5	1326	A2M	C3'-C4'-C5'-O5'
2	L5	2401	A2M	C3'-C4'-C5'-O5'
2	L5	1322	1MA	C2'-C1'-N9-C8
48	S2	174	OMC	C3'-C2'-O2'-CM2
2	L5	3760	A2M	C2'-C1'-N9-C8
48	S2	428	OMU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
48	S2	1081	PSU	C4'-C5'-O5'-P
2	L5	1524	A2M	C3'-C4'-C5'-O5'
2	L5	3944	OMG	C3'-C4'-C5'-O5'
48	S2	99	A2M	O4'-C4'-C5'-O5'
33	Le	53	MLZ	CG-CD-CE-NZ
48	S2	1851	MA6	C5-C6-N6-C9
2	L5	2351	OMC	O4'-C4'-C5'-O5'
2	L5	3867	A2M	C3'-C4'-C5'-O5'
2	L5	2787	A2M	O4'-C1'-N9-C8
2	L5	3844	PSU	C4'-C5'-O5'-P
6	S4	16	H2U	C4'-C5'-O5'-P
2	L5	1625	OMG	C3'-C2'-O2'-CM2
2	L5	2363	A2M	C3'-C2'-O2'-CM'
8	LD	216	V5N	O-C-CA-CB
48	S2	590	A2M	O4'-C1'-N9-C8
2	L5	3785	A2M	C2'-C1'-N9-C8
2	L5	3760	A2M	C4'-C5'-O5'-P
2	L5	2351	OMC	C2'-C1'-N1-C2
48	S2	428	OMU	C2'-C1'-N1-C2
2	L5	2787	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

64 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S2	1442	OMU	1	0
48	S2	116	OMU	2	0
2	L5	4420	PSU	1	0
6	S4	16	H2U	1	0
2	L5	1340	OMC	2	0
2	L5	4689	PSU	1	0
6	S4	54	5MU	1	0
48	S2	801	PSU	2	0
48	S2	1391	OMC	2	0
48	S2	99	A2M	1	0
2	L5	3944	OMG	1	0
48	S2	1850	MA6	1	0
48	S2	814	PSU	1	0
48	S2	1710	OMC	1	0
2	L5	3867	A2M	1	0
2	L5	4431	PSU	1	0
2	L5	4456	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	2632	PSU	1	0
2	L5	4457	PSU	1	0
2	L5	3818	UY1	1	0
2	L5	4521	PSU	1	0
2	L5	4618	OMG	1	0
48	S2	468	A2M	1	0
2	L5	3808	OMC	1	0
2	L5	4220	6MZ	1	0
2	L5	2050	OMG	1	0
2	L5	4536	OMC	1	0
48	S2	1643	PSU	1	0
2	L5	4579	PSU	2	0
48	S2	1232	PSU	2	0
2	L5	1871	A2M	1	0
2	L5	3637	PSU	1	0
6	S4	26	M2G	1	0
48	S2	1692	PSU	1	0
48	S2	1639	7MG	1	0
48	S2	436	OMG	1	0
48	S2	1678	A2M	2	0
1	L1	75	OMG	1	0
2	L5	398	A2M	1	0
2	L5	4870	OMG	1	0
2	L5	4620	OMU	2	0
2	L5	4872	2MG	1	0
48	S2	1851	MA6	1	0
2	L5	3785	A2M	1	0
2	L5	2351	OMC	1	0
2	L5	2876	OMG	2	0
2	L5	2424	OMG	2	0
48	S2	1328	OMG	1	0
2	L5	3718	A2M	3	0
6	S4	55	PSU	1	0
48	S2	159	A2M	1	0
2	L5	3792	OMG	1	0
2	L5	3734	PSU	1	0
48	S2	576	A2M	2	0
6	S4	47	H2U	3	0
48	S2	509	OMG	1	0
2	L5	2415	OMU	1	0
6	S4	18	OMG	2	0
48	S2	1804	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	2363	A2M	1	0
2	L5	4530	UR3	1	0
2	L5	4636	PSU	1	0
48	S2	1337	4AC	1	0
2	L5	2422	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 429 ligands modelled in this entry, 428 are monoatomic - leaving 1 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	$\# Z > 2$
86	B3P	L5	5129	-	18,18,18	0.72	0	23,23,23	0.97	1 (4%)

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
86	B3P	L5	5129	-	-	9/28/28/28	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	L5	5129	B3P	C11-C8-C10	-2.51	104.51	110.02

There are no chirality outliers.

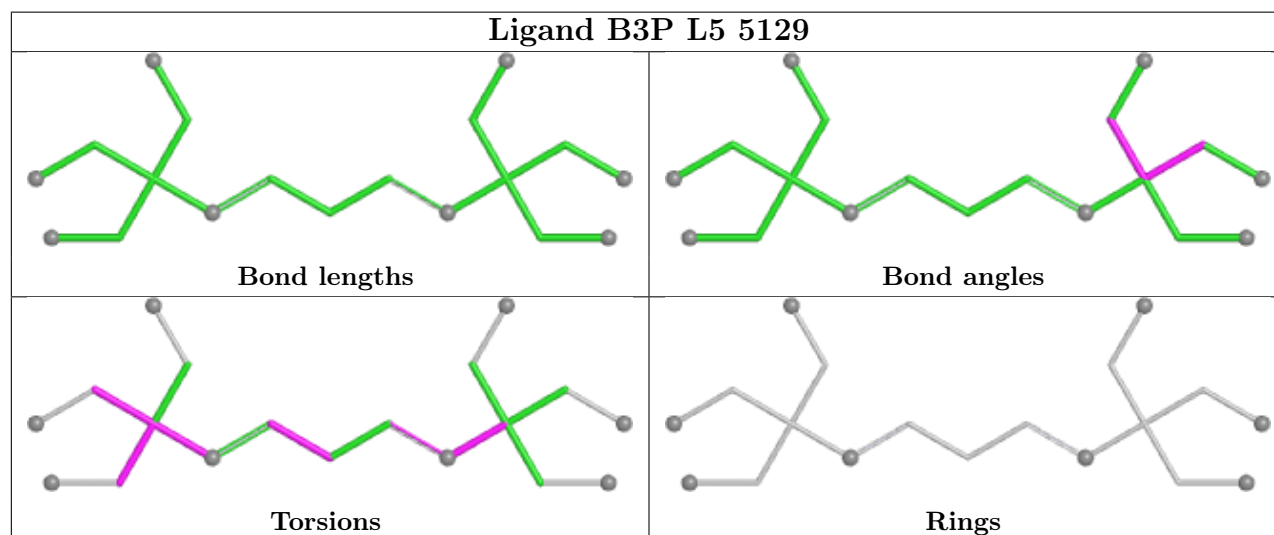
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	L5	5129	B3P	N1-C4-C7-O6
86	L5	5129	B3P	C1-C2-N2-C8
86	L5	5129	B3P	C5-C4-N1-C3
86	L5	5129	B3P	C7-C4-N1-C3
86	L5	5129	B3P	C10-C8-N2-C2
86	L5	5129	B3P	C11-C8-N2-C2
86	L5	5129	B3P	C2-C1-C3-N1
86	L5	5129	B3P	C6-C4-C7-O6
86	L5	5129	B3P	N1-C4-C6-O5

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

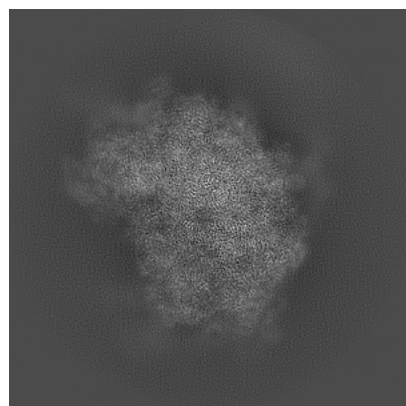
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45170. These allow visual inspection of the internal detail of the map and identification of artifacts.

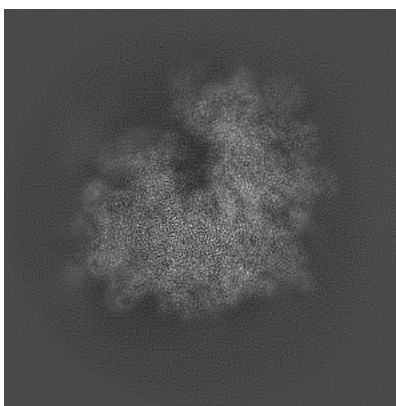
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

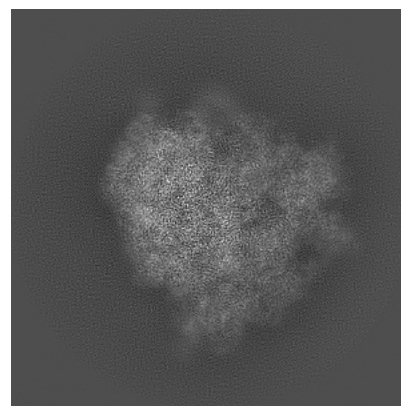
6.1.1 Primary map



X

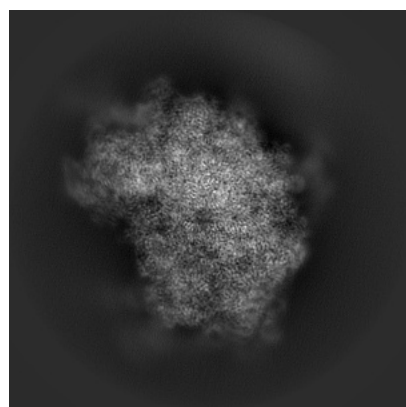


Y

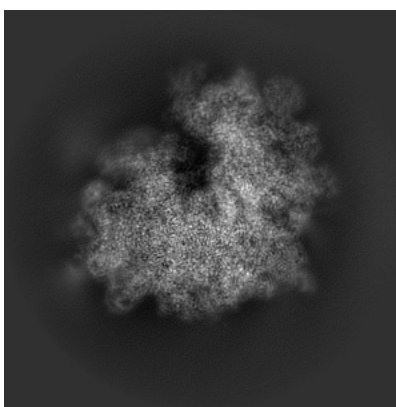


Z

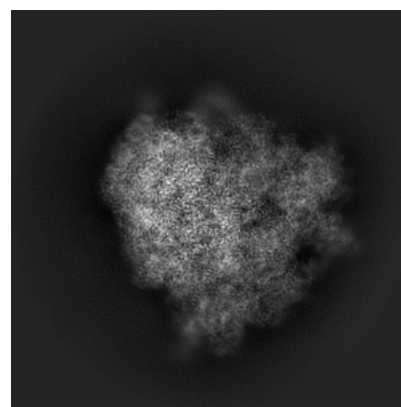
6.1.2 Raw map



X



Y

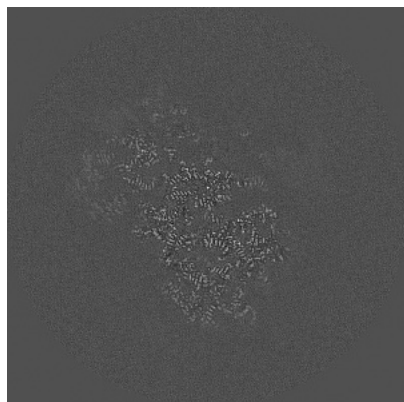


Z

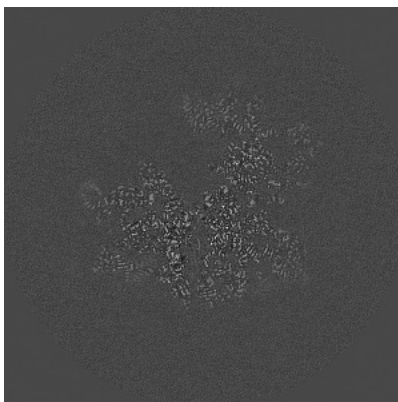
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

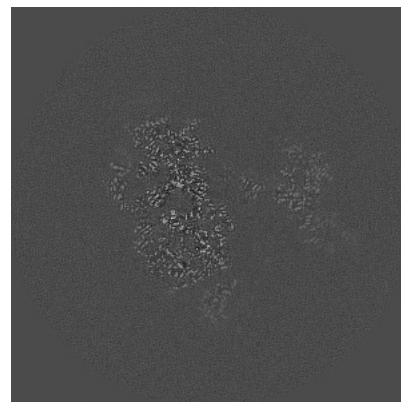
6.2.1 Primary map



X Index: 224

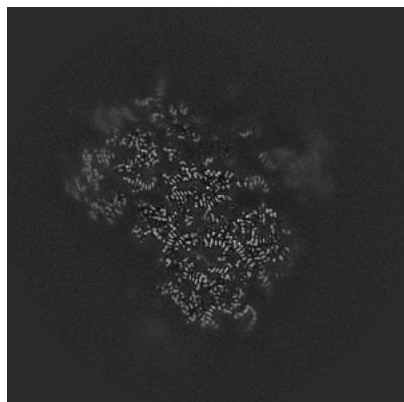


Y Index: 224

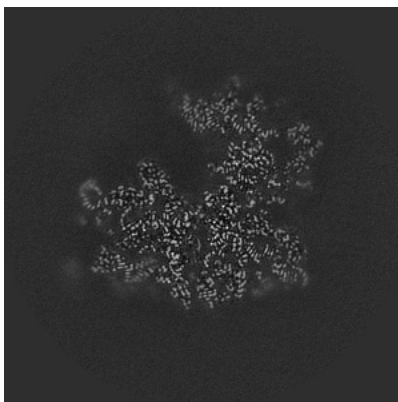


Z Index: 224

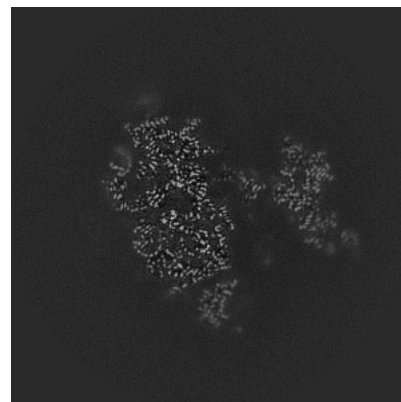
6.2.2 Raw map



X Index: 224



Y Index: 224

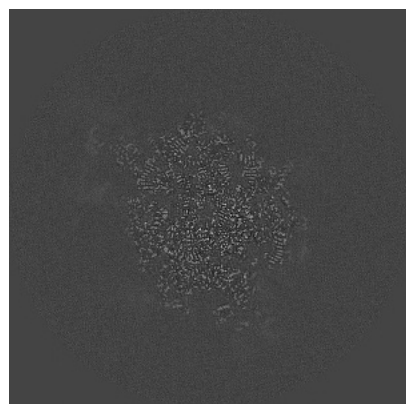


Z Index: 224

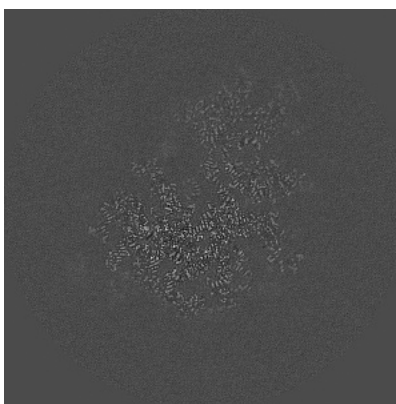
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

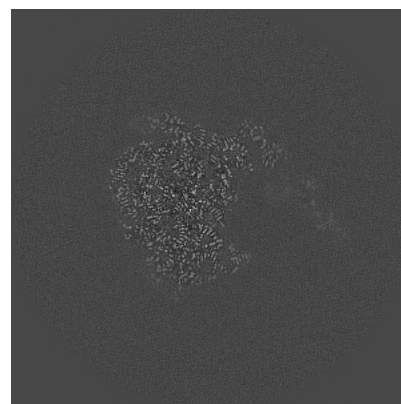
6.3.1 Primary map



X Index: 200

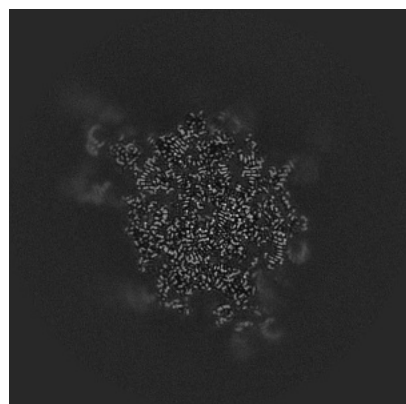


Y Index: 238

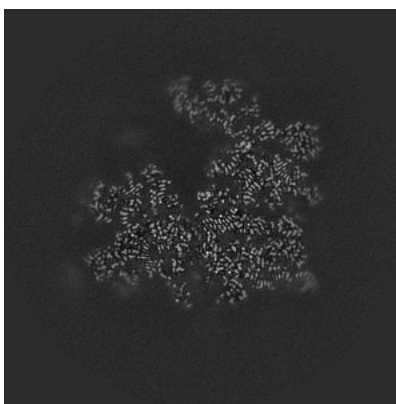


Z Index: 190

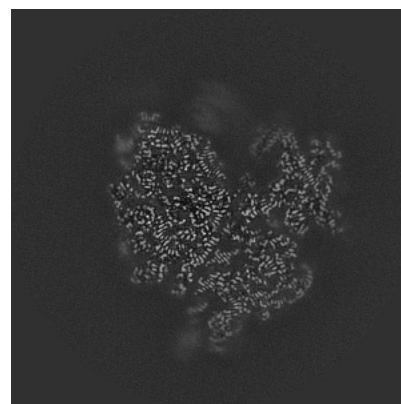
6.3.2 Raw map



X Index: 200



Y Index: 215

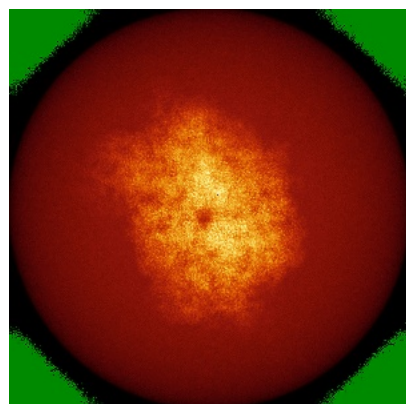


Z Index: 252

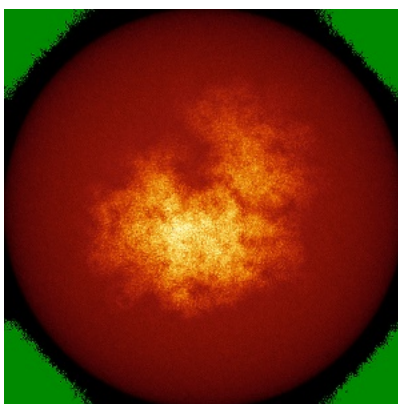
The images above show the largest variance slices of the map in three orthogonal directions.

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

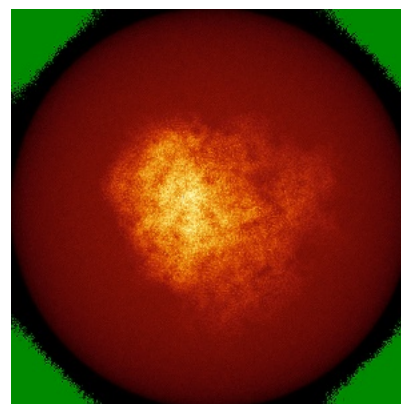
6.4.1 Primary map



X

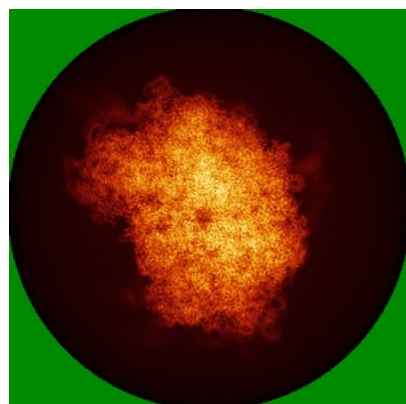


Y

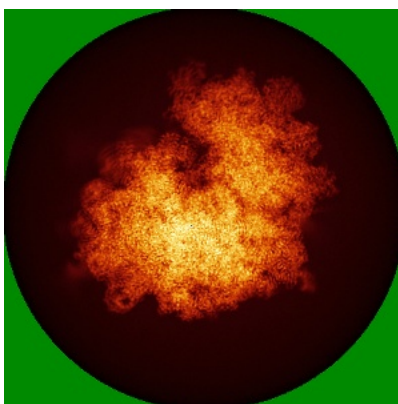


Z

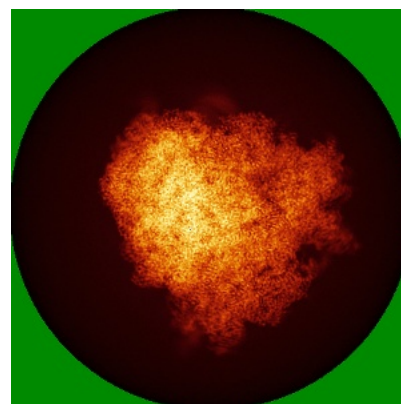
6.4.2 Raw map



X



Y

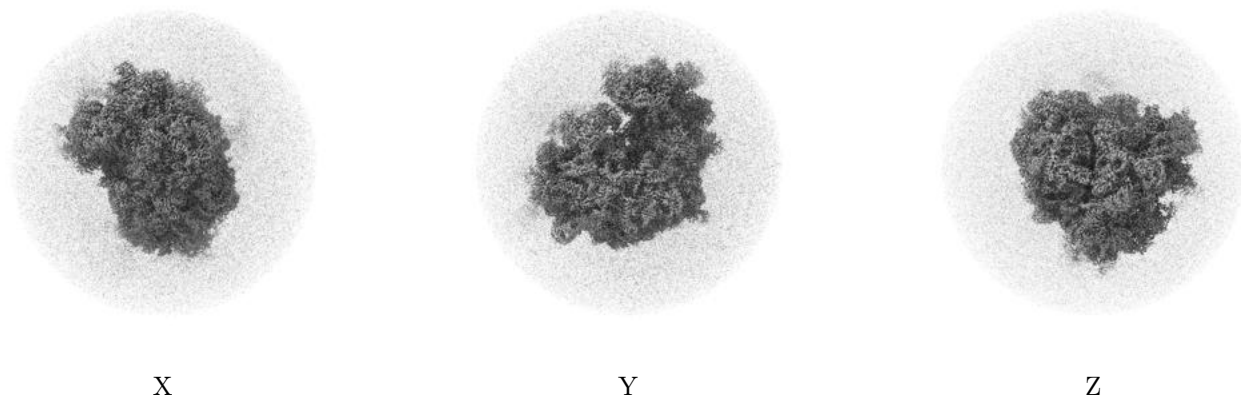


Z

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

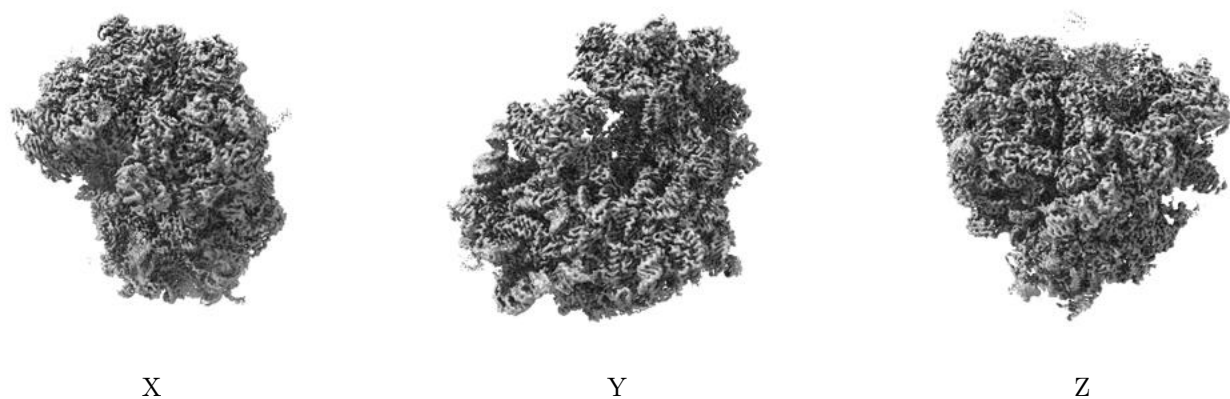
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

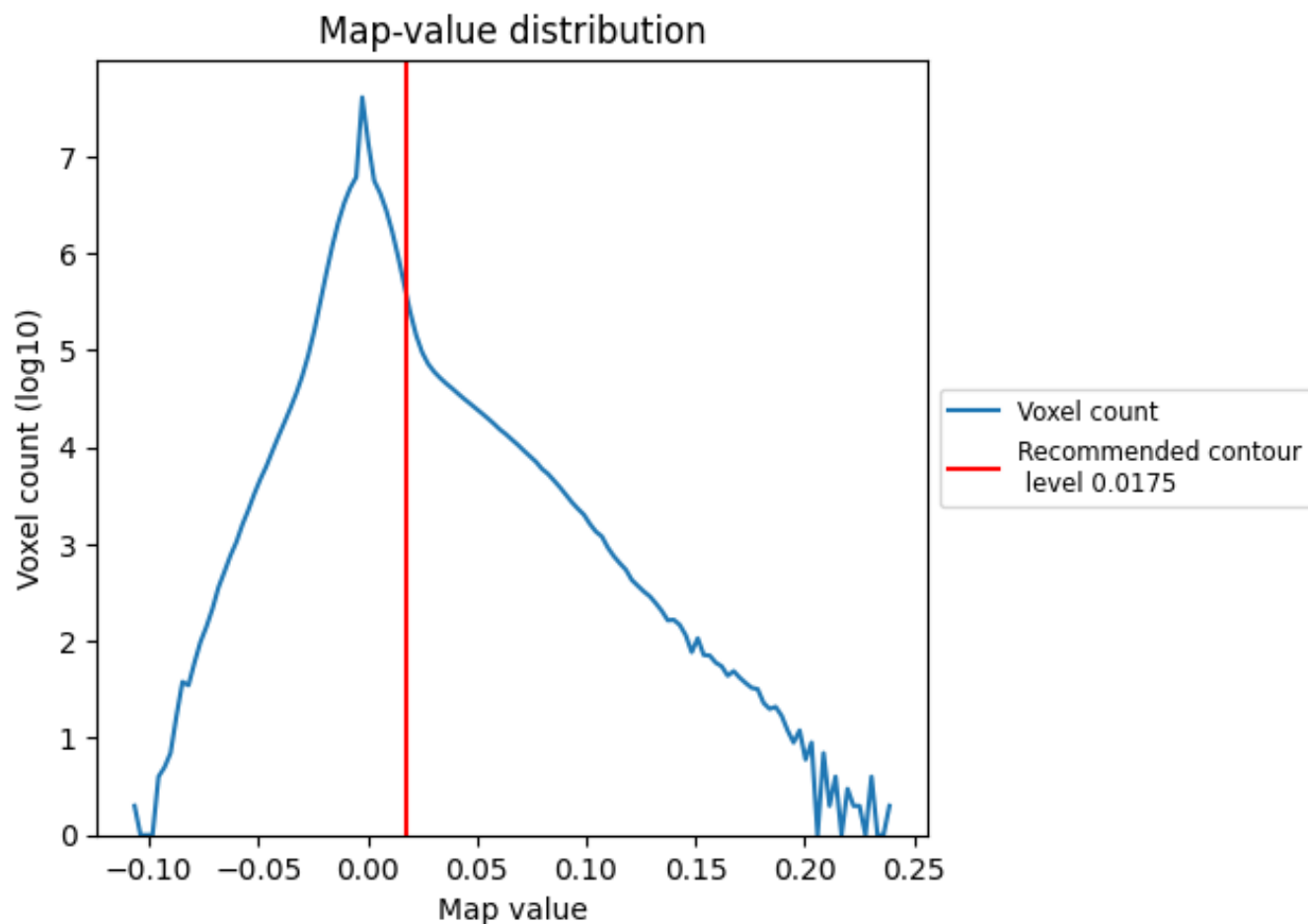
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

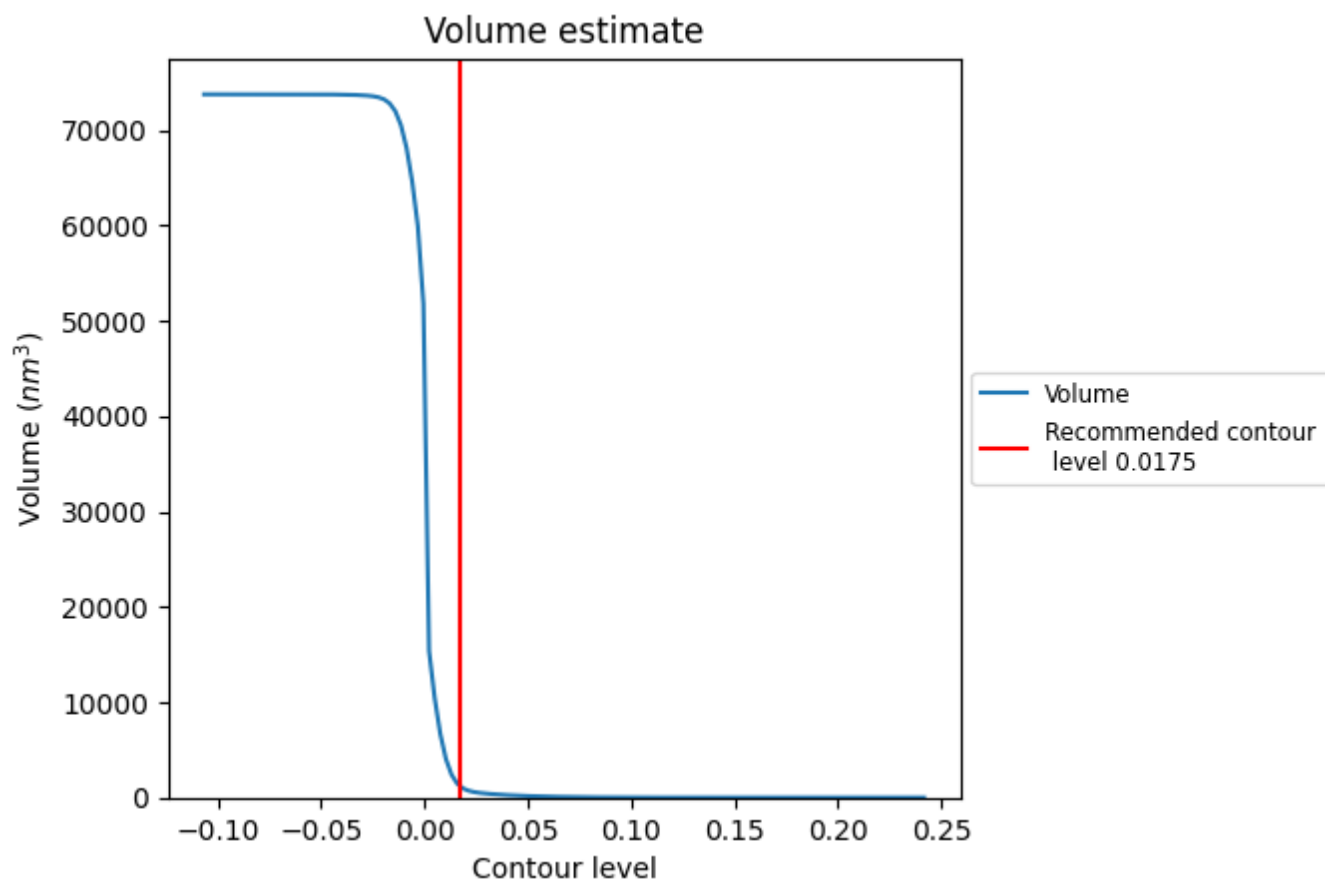
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

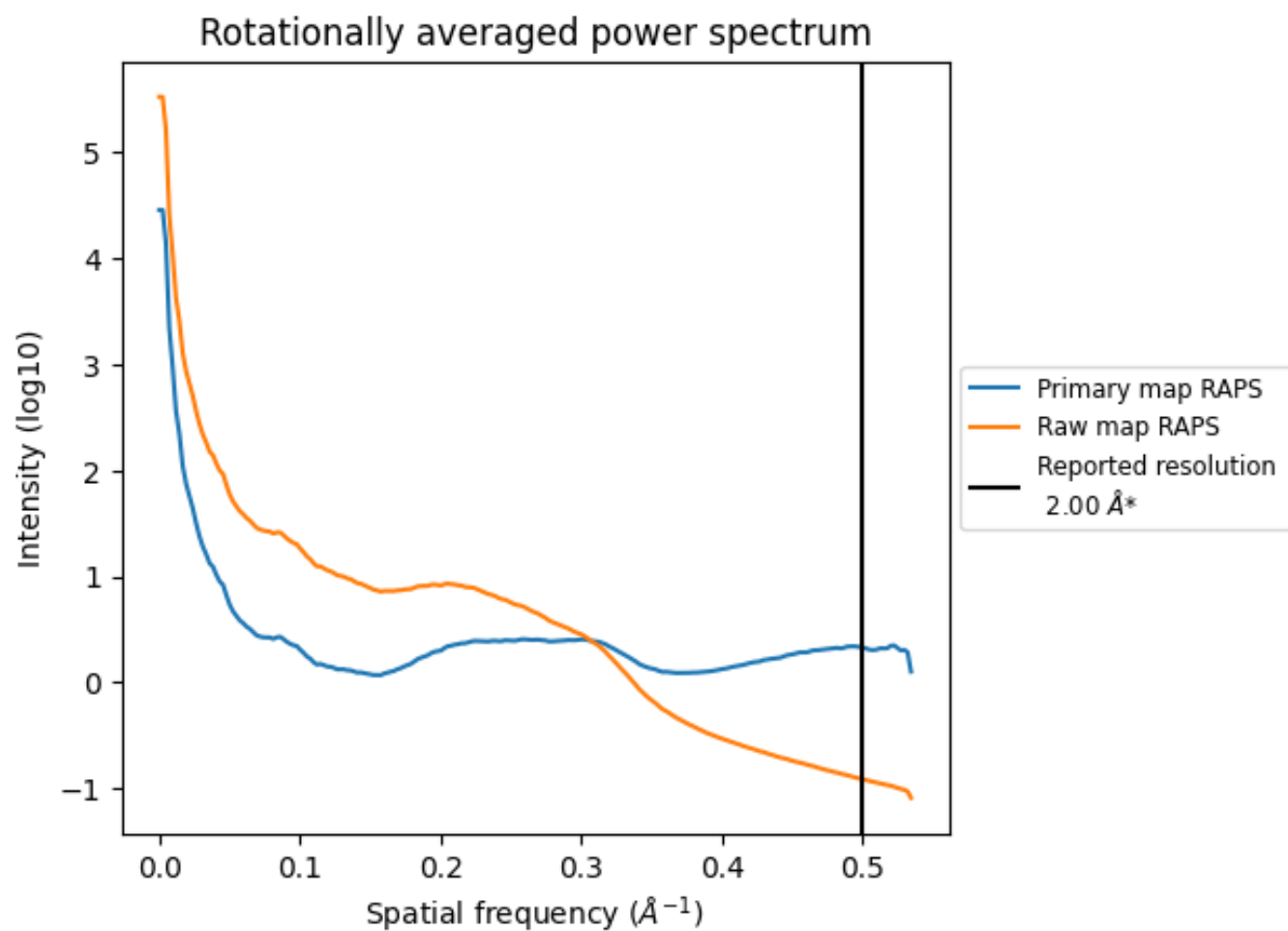
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1154 nm^3 ; this corresponds to an approximate mass of 1042 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 ⓘ

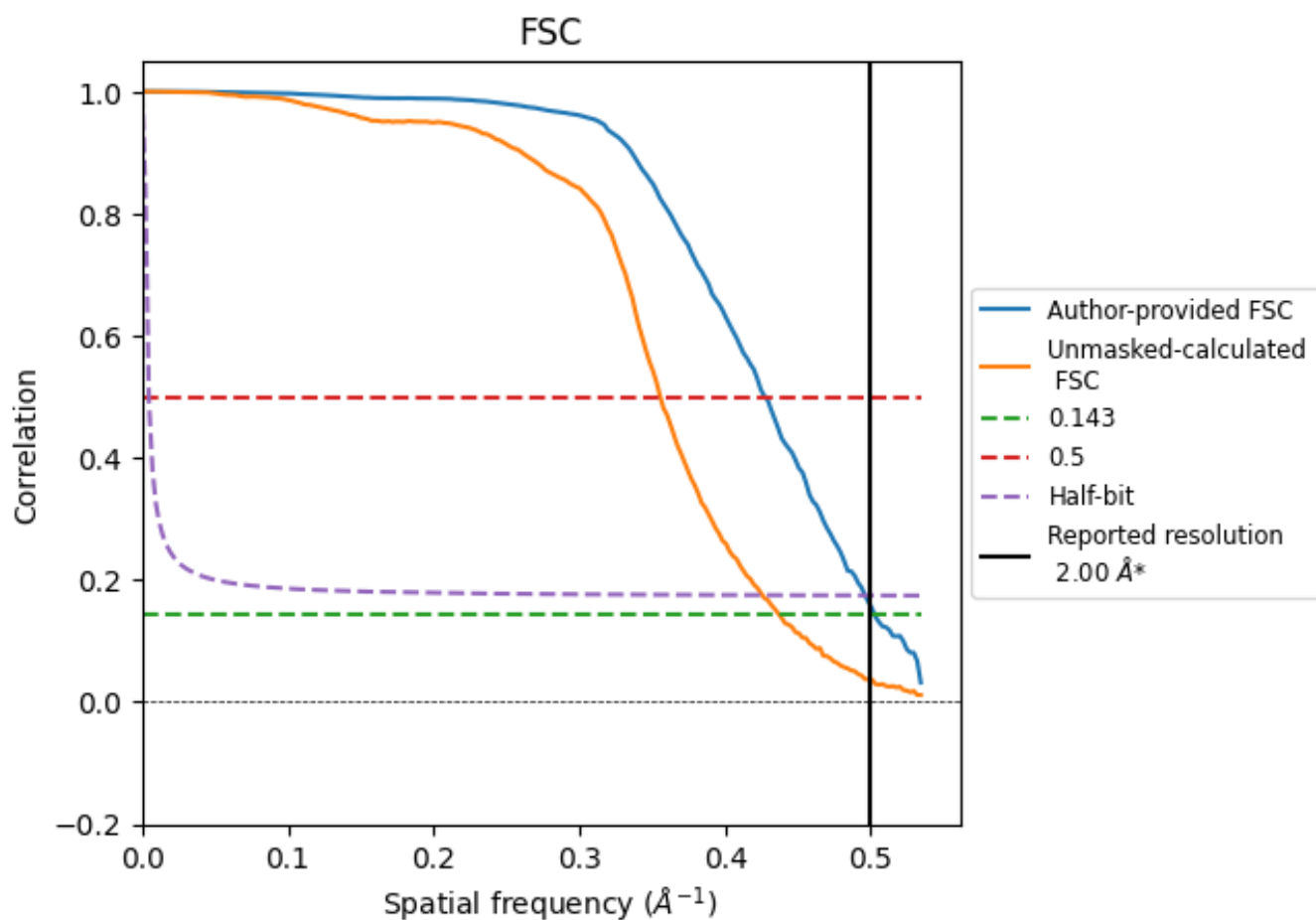


*Reported resolution corresponds to spatial frequency of 0.500 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

8.2 Resolution estimates [i](#)

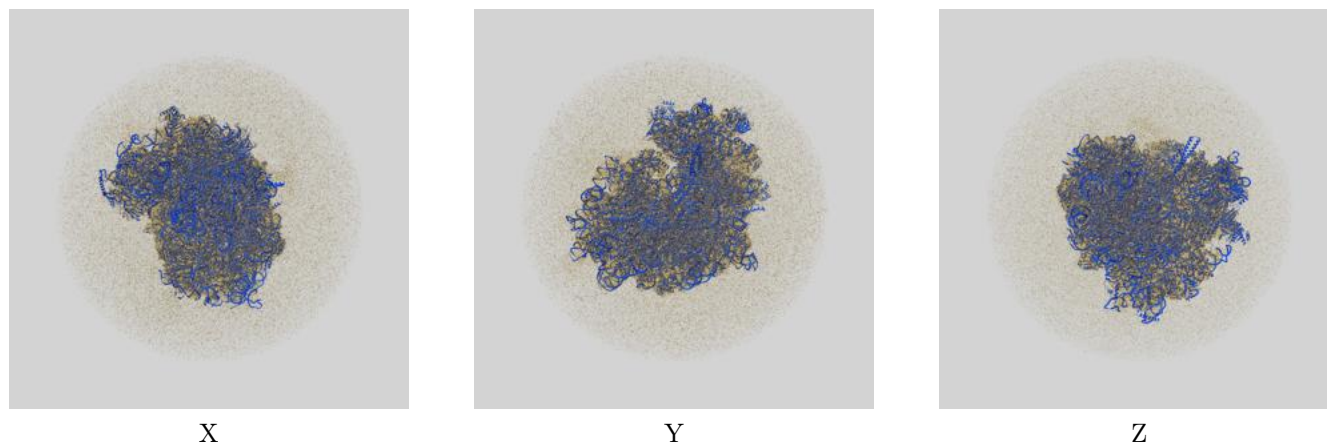
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	1.99	2.34	2.02
Unmasked-calculated*	2.29	2.81	2.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.29 differs from the reported value 2.0 by more than 10 %

9 Map-model fit [i](#)

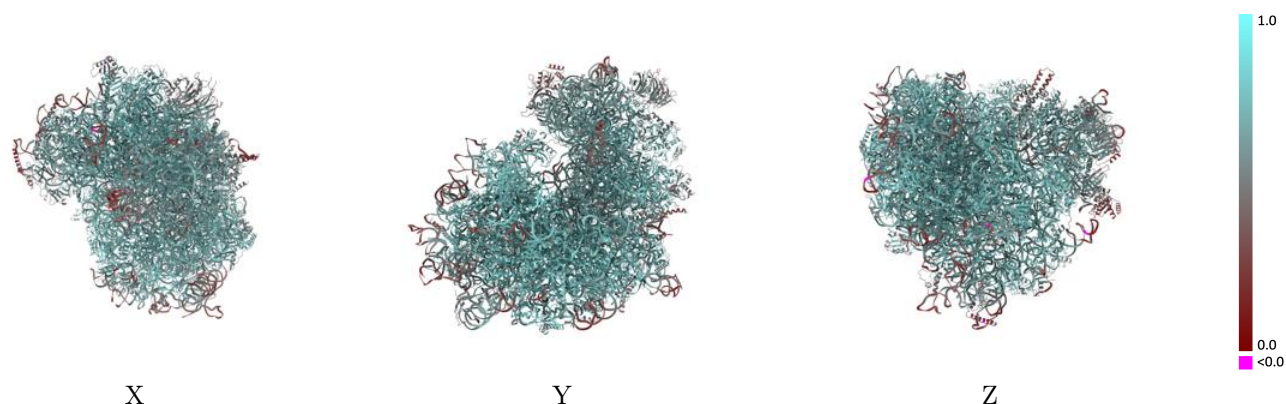
This section contains information regarding the fit between EMDB map EMD-45170 and PDB model 9C3H. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



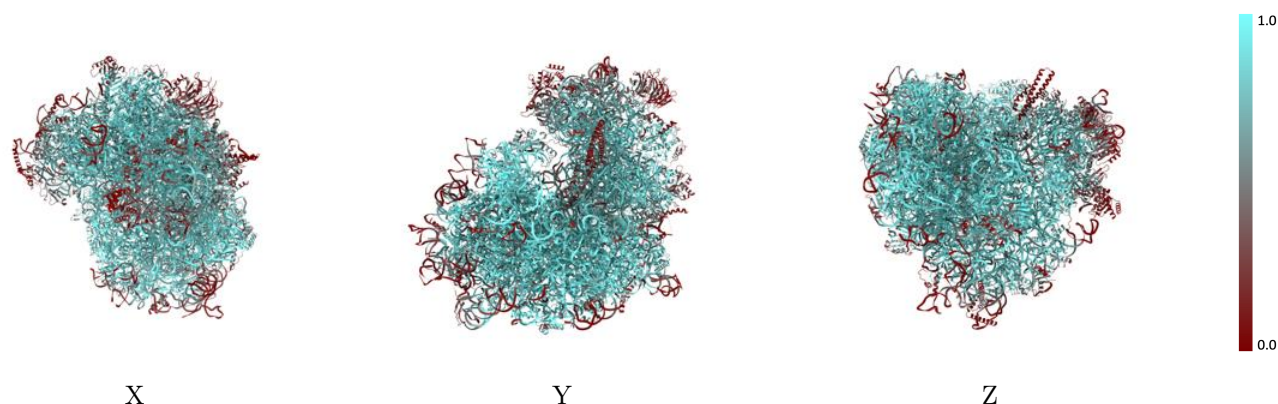
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



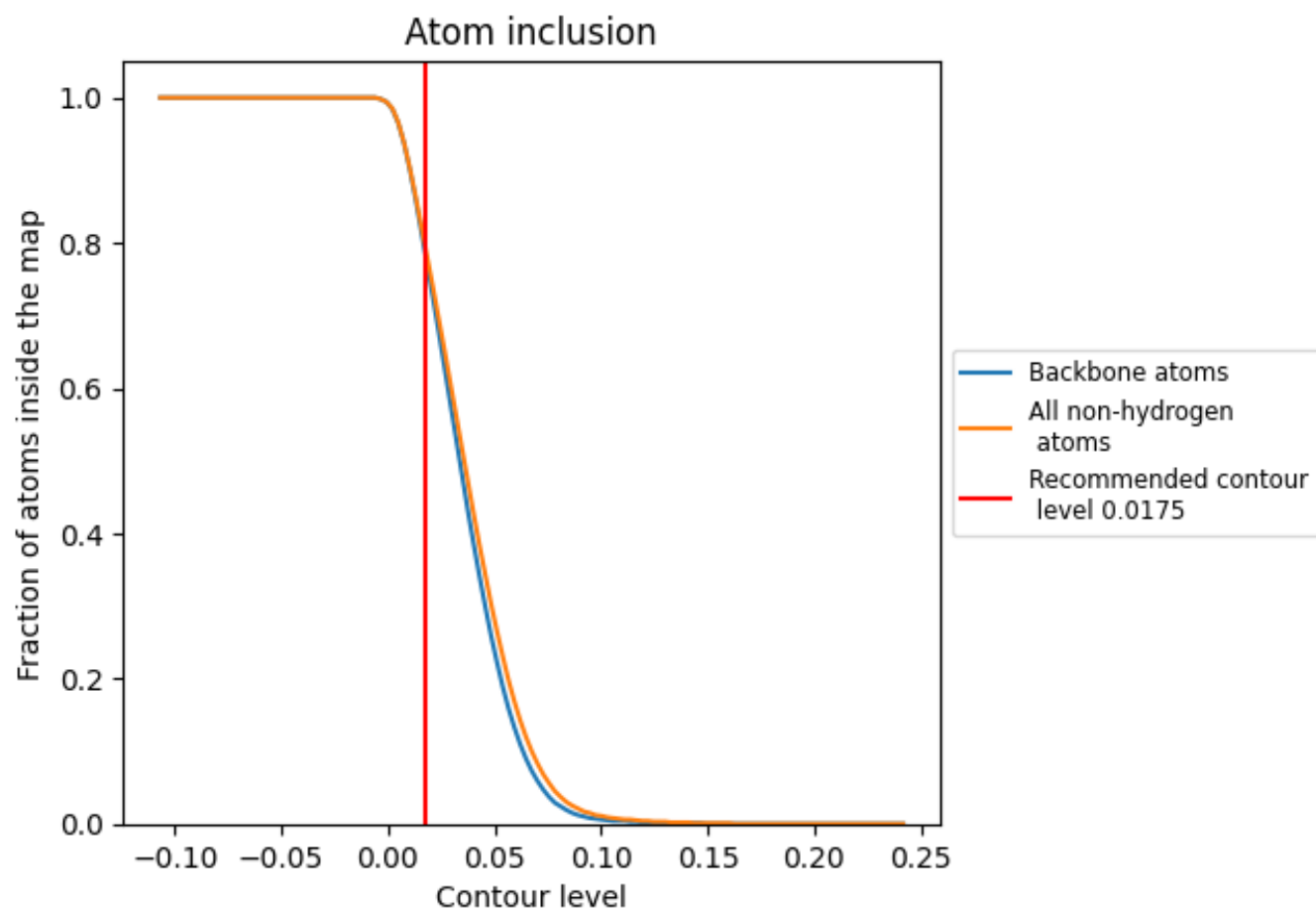
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0175).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 80% 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 (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.6840
L1	 0.9300	 0.7300
L5	 0.8260	 0.6900
L8	 0.8170	 0.6940
L9	 0.9590	 0.7290
LB	 0.9070	 0.7620
LC	 0.9150	 0.7580
LD	 0.9670	 0.7980
LE	 0.8660	 0.7310
LF	 0.9190	 0.7660
LG	 0.8140	 0.6910
LH	 0.8680	 0.7170
LI	 0.9440	 0.7780
LJ	 0.7340	 0.6530
LK	 0.7900	 0.6870
LM	 0.8760	 0.7220
LN	 0.9900	 0.7950
LO	 0.8420	 0.7120
LP	 0.9570	 0.7860
LQ	 0.8410	 0.7190
LR	 0.7860	 0.6910
LS	 0.9430	 0.7700
LT	 0.8500	 0.7320
LU	 0.9290	 0.7620
LV	 0.9450	 0.7820
LW	 0.5460	 0.5580
LY	 0.9220	 0.7670
LZ	 0.8460	 0.7070
La	 0.9480	 0.7810
Lb	 0.7250	 0.6580
Lc	 0.8530	 0.7260
Ld	 0.8530	 0.7320
Le	 0.8710	 0.7520
Lf	 0.9610	 0.7890
Lg	 0.8900	 0.7490



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Chain	Atom inclusion	Q-score
Lh	 0.8950	 0.7620
Li	 0.8220	 0.7050
Lj	 0.9580	 0.7850
Lk	 0.6380	 0.6390
Ll	 0.9330	 0.7610
Lm	 0.5580	 0.5820
Ln	 0.8940	 0.7330
Lo	 0.8970	 0.7570
Lp	 0.9380	 0.7800
Lz	 0.8890	 0.7440
NC	 0.7850	 0.7310
S1	 0.7900	 0.7010
S2	 0.8130	 0.6640
S4	 0.6970	 0.6070
S5	 0.6810	 0.6390
SA	 0.8100	 0.6880
SB	 0.1950	 0.4830
SC	 0.8710	 0.7160
SD	 0.7280	 0.6620
SE	 0.7310	 0.6680
SG	 0.4090	 0.5340
SH	 0.4950	 0.5730
SI	 0.7380	 0.6670
SJ	 0.7400	 0.6660
SK	 0.5540	 0.5990
SL	 0.8510	 0.7180
SM	 0.4130	 0.5430
SN	 0.8860	 0.7330
SO	 0.9000	 0.7400
SP	 0.4790	 0.5850
SQ	 0.6670	 0.6440
SS	 0.5800	 0.6090
ST	 0.5820	 0.6090
SU	 0.5910	 0.6100
SV	 0.8040	 0.6990
SW	 0.9320	 0.7530
SX	 0.9010	 0.7420
SY	 0.5650	 0.6070
SZ	 0.4730	 0.5500
Sa	 0.8770	 0.7360
Sb	 0.6980	 0.6580
Sc	 0.4800	 0.5800

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Chain	Atom inclusion	Q-score
Sd	 0.6380	 0.6400
Se	 0.6070	 0.6140
Sf	 0.7870	 0.6790
Sg	 0.2680	 0.5080
So	 0.8580	 0.7470
Sy	 0.0440	 0.2790
Sz	 0.0850	 0.3440