



Full wwPDB EM Validation Report ⓘ

Jul 2, 2026 – 02:42 PM JST

PDB ID : 9L98 / pdb_00009198
EMDB ID : EMD-62897
Title : State C of archaeal pre-50S ribosome
Authors : Li, Z.Q.; Yang, X.Y.
Deposited on : 2024-12-29
Resolution : 2.76 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:

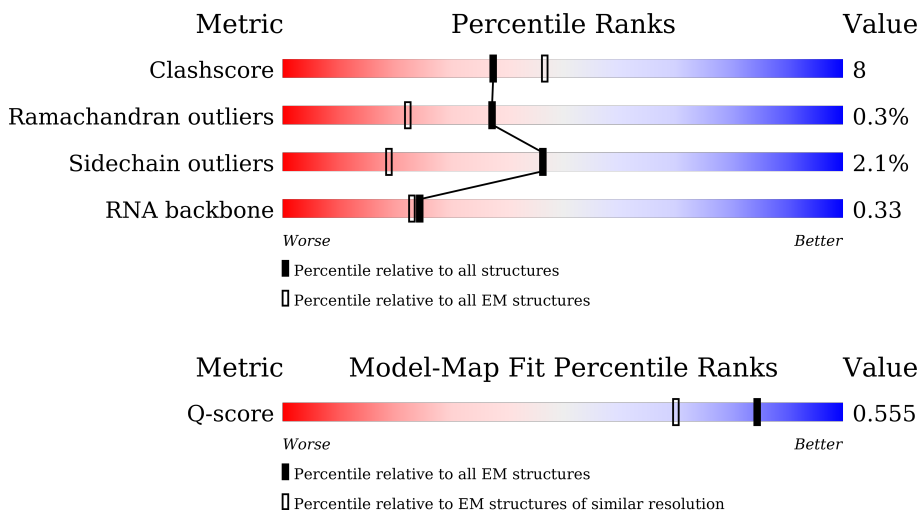
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.76 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	10642 (2.26 - 3.26)

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	0	2916	
2	9	122	
3	A	50	


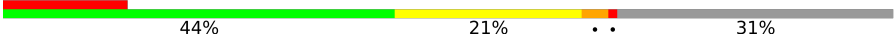
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Mol	Chain	Length	Quality of chain
4	E	120	82% 17%
5	F	176	78% 20%
6	G	196	87% 12%
7	H	116	83% 16%
8	I	184	83% 15%
9	J	151	78% 21%
10	K	96	81% 18%
11	L	153	84% 14%
12	M	67	64% 22% 13%
13	N	118	75% 22%
14	O	154	77% 23%
15	P	92	9% 76% 21%
16	Q	234	48% 12% 39%
17	R	89	65% 22% 10%
18	S	58	83% 16%
19	T	93	78% 22%
20	U	241	79% 18%
21	V	338	85% 14%
22	W	248	85% 15%
23	X	172	17% 65% 32%
24	Y	178	80% 17%
25	b	145	89% 10%
26	c	83	5% 72% 28%
27	d	70	14% 59% 40%
28	e	58	10% 81% 19%

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Mol	Chain	Length	Quality of chain
29	f	132	 89% 11%
30	a	406	 14% 44% 21% 31%

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 95799 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 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	0	2826	60579	27039	11153	19561	2826	0	0

- Molecule 2 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	9	120	2551	1138	453	840	120	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	31	252	159	51	40	2	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	119	880	546	141	192	1	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	174	1372	852	251	261	8	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	194	1579	963	338	276	2	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	H	115	887	544	167	176	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	183	1417	880	258	278	1	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	150	1205	728	247	229	1	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	95	736	451	150	133	2	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	151	1174	730	214	226	4	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	58	466	287	83	94	2	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	N	114	903	545	171	187	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	154	Total	C	N	O	S	0	0
			1200	731	220	245	4		

- Molecule 15 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	89	Total	C	N	O	S	0	0
			726	448	138	139	1		

- Molecule 16 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	142	Total	C	N	O	S	0	0
			1146	698	231	216	1		

- Molecule 17 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	80	Total	C	N	O	S	0	0
			617	374	125	117	1		

- Molecule 18 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	57	Total	C	N	O	S	0	0
			439	265	90	80	4		

- Molecule 19 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	93	Total	C	N	O	S	0	0
			746	457	152	129	8		

- Molecule 20 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	238	Total	C	N	O	S	0	0
			1783	1099	353	326	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	337	2619	1623	484	502	10	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	248	1898	1164	354	377	3	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	169	1245	762	225	255	3	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	174	1346	832	228	283	3	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	144	1127	701	201	220	5	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	83	659	408	113	134	4	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	69	529	324	89	115	1	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	58	443	274	77	91	1	0	0

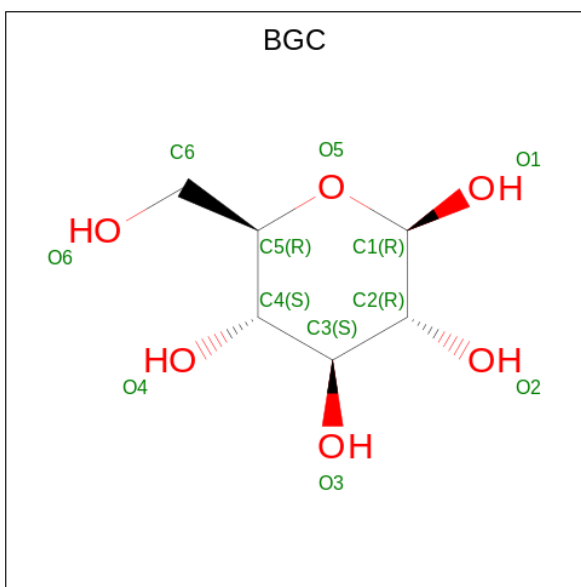
- Molecule 29 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	f	132	996	612	188	191	5	0	0

- Molecule 30 is a protein called CBS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	a	281	2123	1326	361	432	4	0	0

- Molecule 31 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	0	1	12	6	6	0

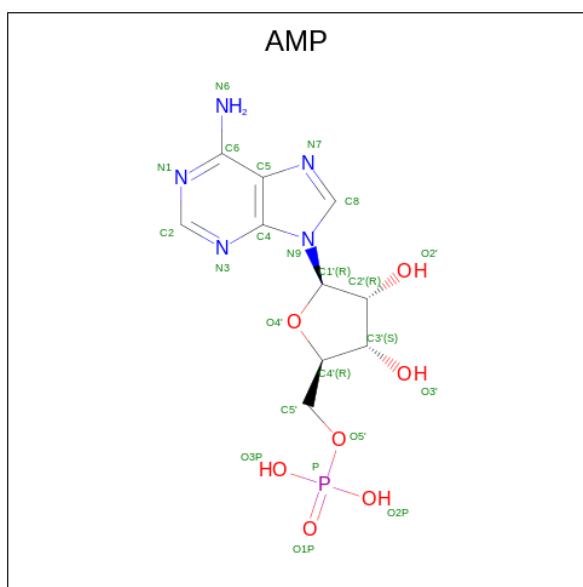
- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
32	0	183	Total 183	Mg 183	0
32	A	1	Total 1	Mg 1	0
32	F	2	Total 2	Mg 2	0
32	G	1	Total 1	Mg 1	0
32	L	1	Total 1	Mg 1	0
32	N	1	Total 1	Mg 1	0
32	O	1	Total 1	Mg 1	0
32	Q	1	Total 1	Mg 1	0
32	U	1	Total 1	Mg 1	0
32	V	2	Total 2	Mg 2	0
32	f	1	Total 1	Mg 1	0

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
33	S	1	Total 1	Zn 1	0
33	T	1	Total 1	Zn 1	0

- Molecule 34 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	a	1	Total	C	N	O	P	0
			23	10	5	7	1	
34	a	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	0	1567	Total	O	0
			1567	1567	
35	9	33	Total	O	0
			33	33	
35	A	2	Total	O	0
			2	2	
35	E	3	Total	O	0
			3	3	
35	F	14	Total	O	0
			14	14	
35	G	24	Total	O	0
			24	24	
35	H	8	Total	O	0
			8	8	
35	I	2	Total	O	0
			2	2	
35	J	10	Total	O	0
			10	10	
35	K	19	Total	O	0
			19	19	

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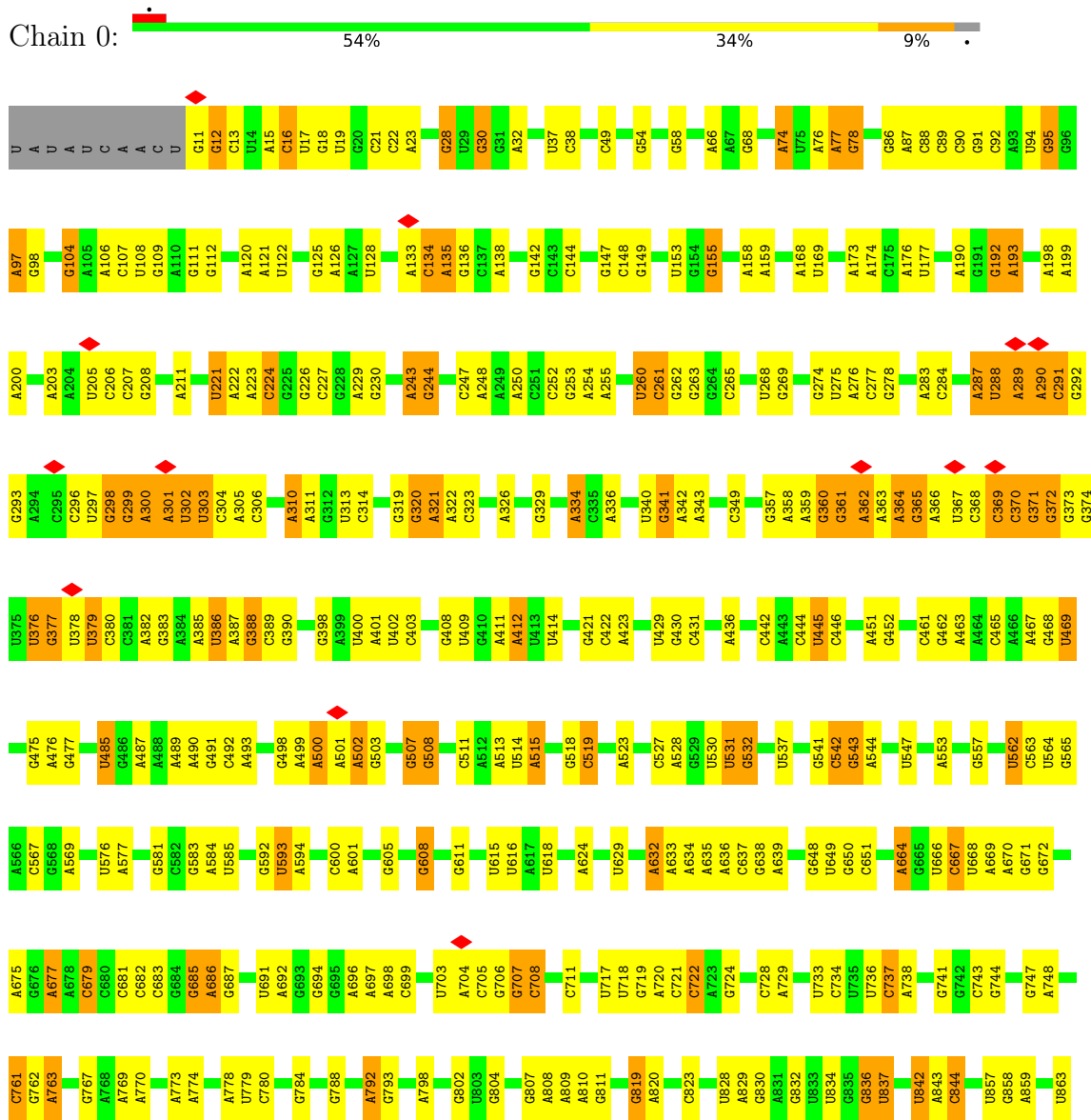
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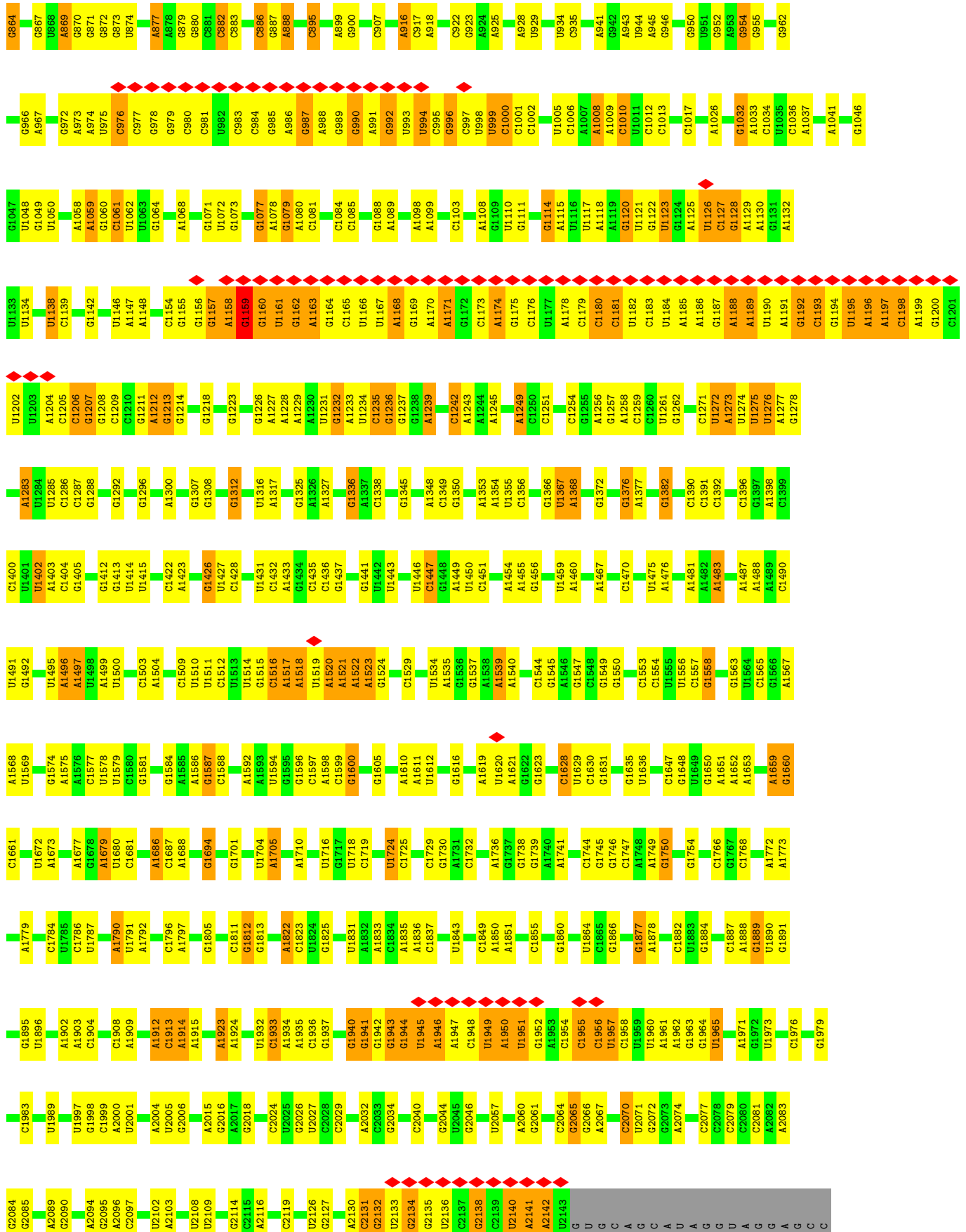
Mol	Chain	Residues	Atoms		AltConf
35	L	19	Total 19	O 19	0
35	M	5	Total 5	O 5	0
35	N	10	Total 10	O 10	0
35	O	20	Total 20	O 20	0
35	P	10	Total 10	O 10	0
35	Q	27	Total 27	O 27	0
35	R	2	Total 2	O 2	0
35	S	13	Total 13	O 13	0
35	T	12	Total 12	O 12	0
35	U	25	Total 25	O 25	0
35	V	29	Total 29	O 29	0
35	W	19	Total 19	O 19	0
35	X	1	Total 1	O 1	0
35	Y	3	Total 3	O 3	0
35	b	13	Total 13	O 13	0
35	c	1	Total 1	O 1	0
35	f	6	Total 6	O 6	0
35	a	4	Total 4	O 4	0

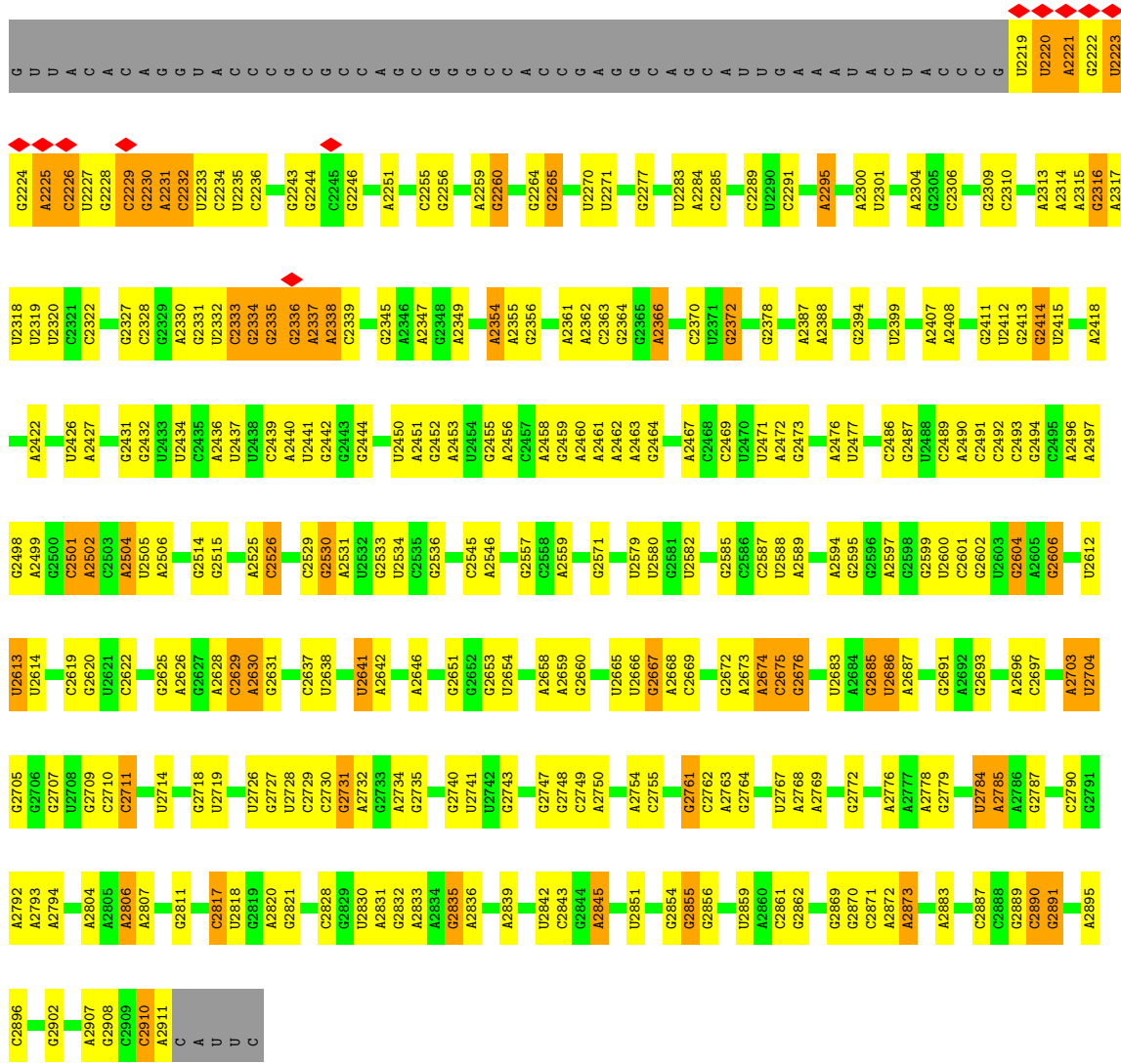
3 Residue-property plots

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.

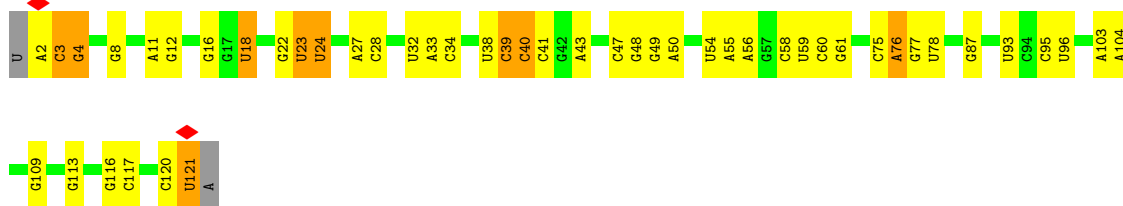
• Molecule 1: 23S RNA



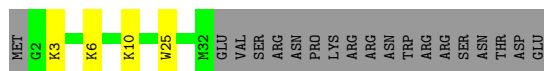




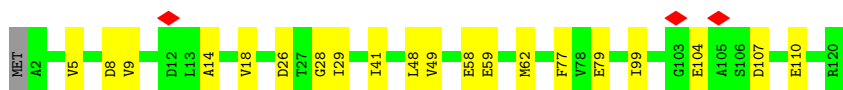
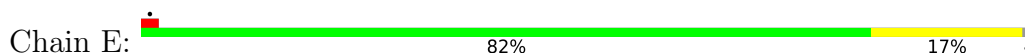
• Molecule 2: 5S RNA



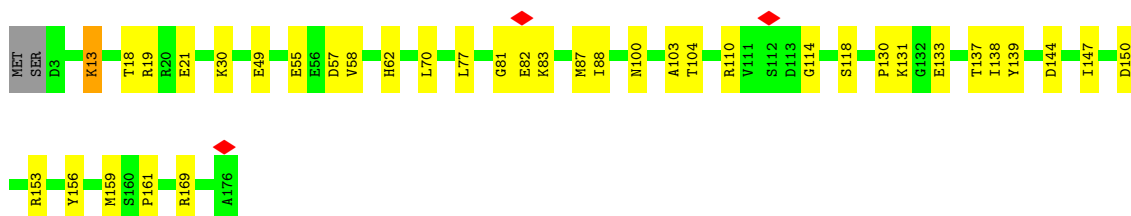
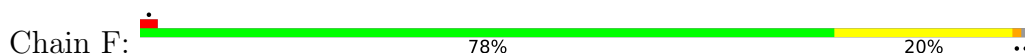
• Molecule 3: Large ribosomal subunit protein eL39



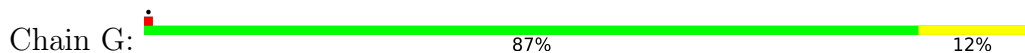
• Molecule 4: Large ribosomal subunit protein eL8



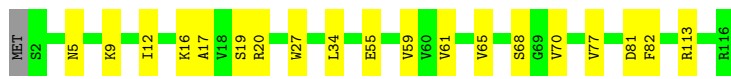
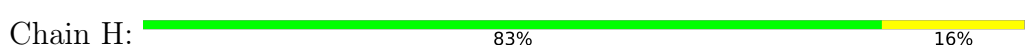
• Molecule 5: Large ribosomal subunit protein uL16



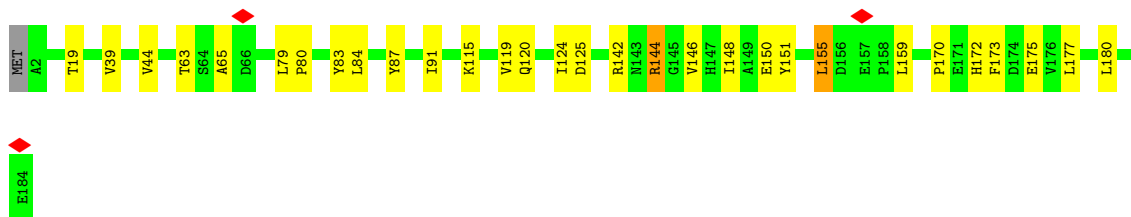
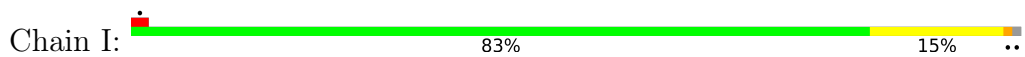
• Molecule 6: Large ribosomal subunit protein eL15



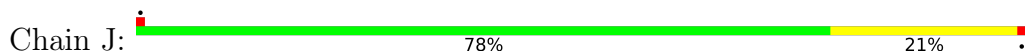
• Molecule 7: Large ribosomal subunit protein eL18

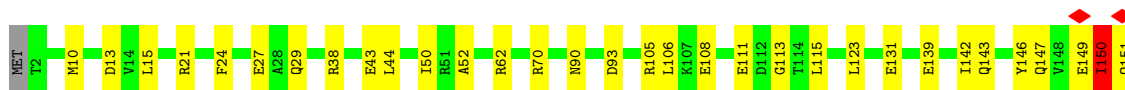


• Molecule 8: Large ribosomal subunit protein uL18

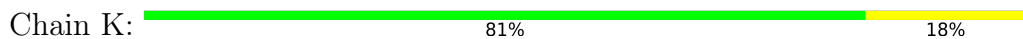


• Molecule 9: Large ribosomal subunit protein eL19

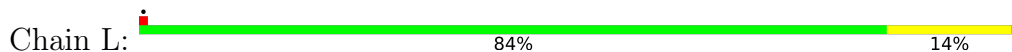




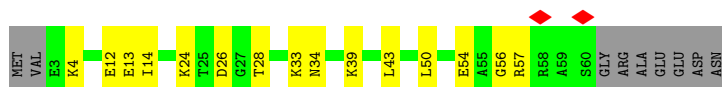
- Molecule 10: Large ribosomal subunit protein eL21



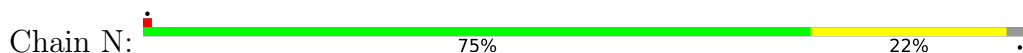
- Molecule 11: Large ribosomal subunit protein uL22



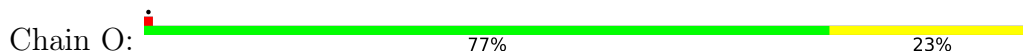
- Molecule 12: Large ribosomal subunit protein eL24



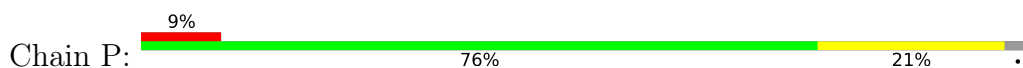
- Molecule 13: Large ribosomal subunit protein uL24

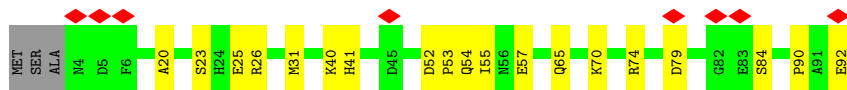


- Molecule 14: Large ribosomal subunit protein uL30

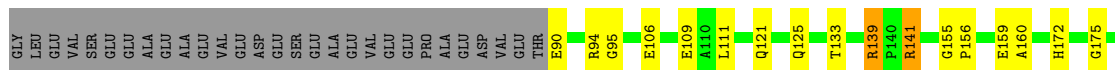


- Molecule 15: Large ribosomal subunit protein eL31

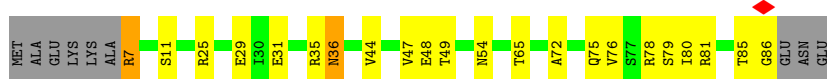




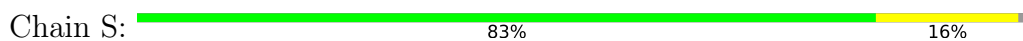
• Molecule 16: Large ribosomal subunit protein eL32



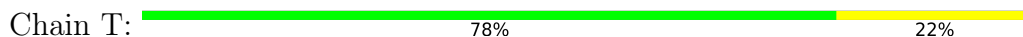
• Molecule 17: Large ribosomal subunit protein eL43



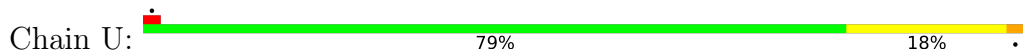
• Molecule 18: Large ribosomal subunit protein eL37



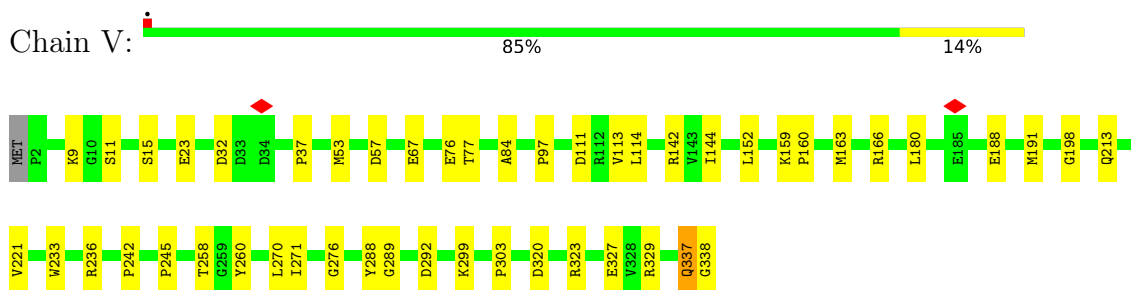
• Molecule 19: Large ribosomal subunit protein eL42



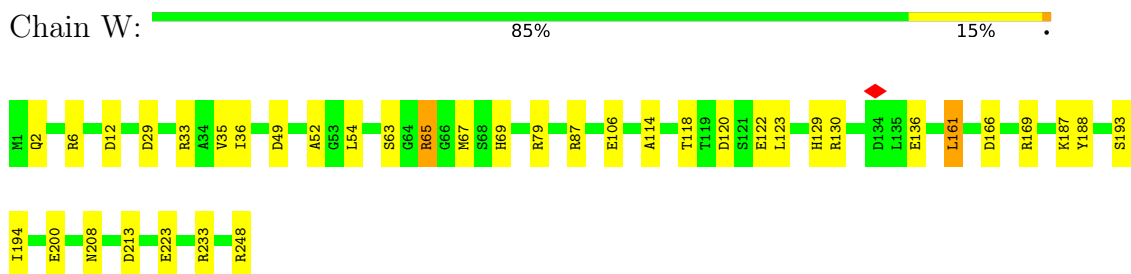
• Molecule 20: Large ribosomal subunit protein uL2



• Molecule 21: Large ribosomal subunit protein uL3



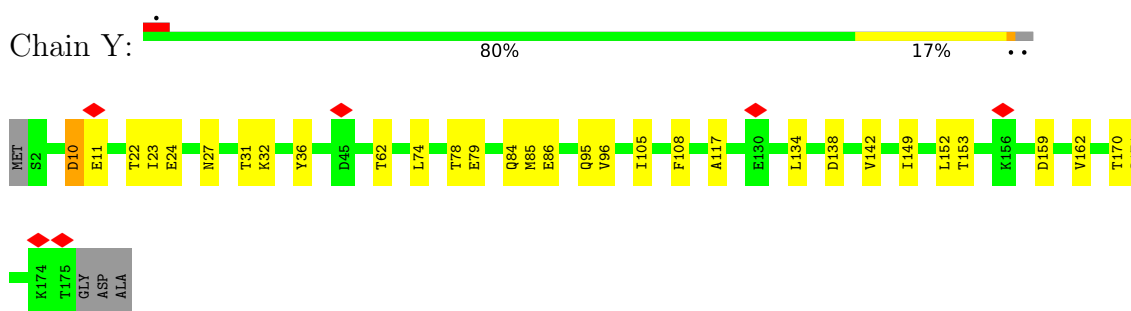
• Molecule 22: Large ribosomal subunit protein uL4



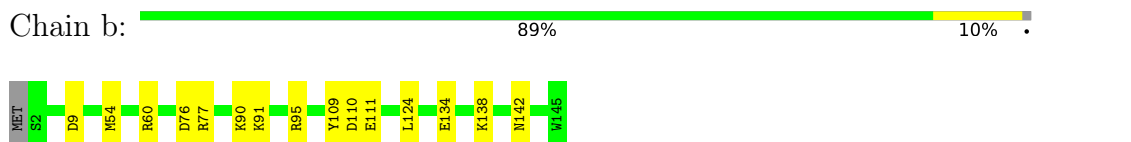
• Molecule 23: Large ribosomal subunit protein uL5



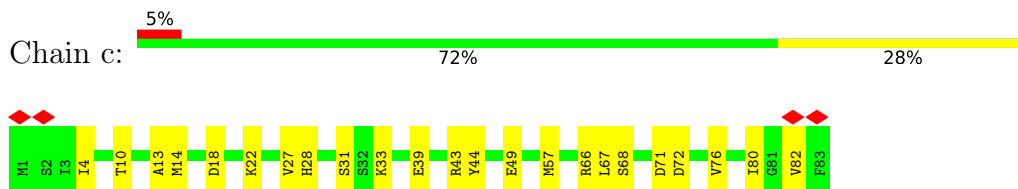
• Molecule 24: Large ribosomal subunit protein uL6



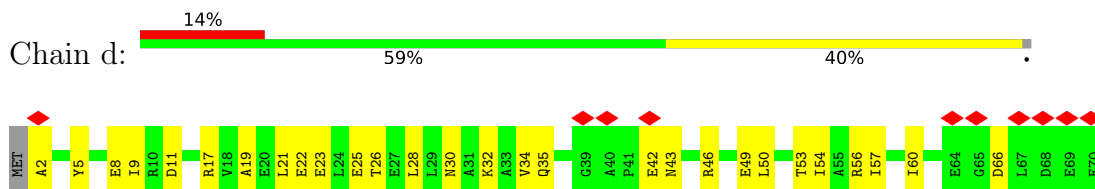
• Molecule 25: Large ribosomal subunit protein uL13



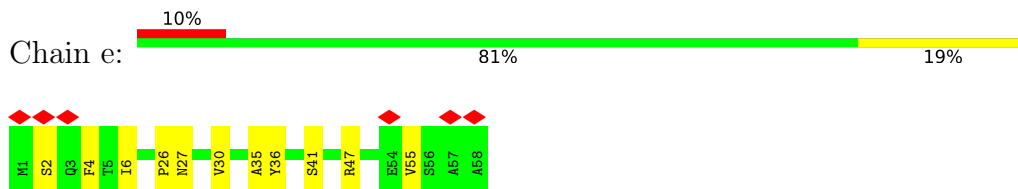
• Molecule 26: Large ribosomal subunit protein uL23



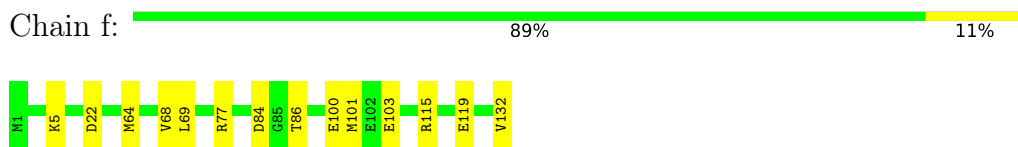
• Molecule 27: Large ribosomal subunit protein uL29



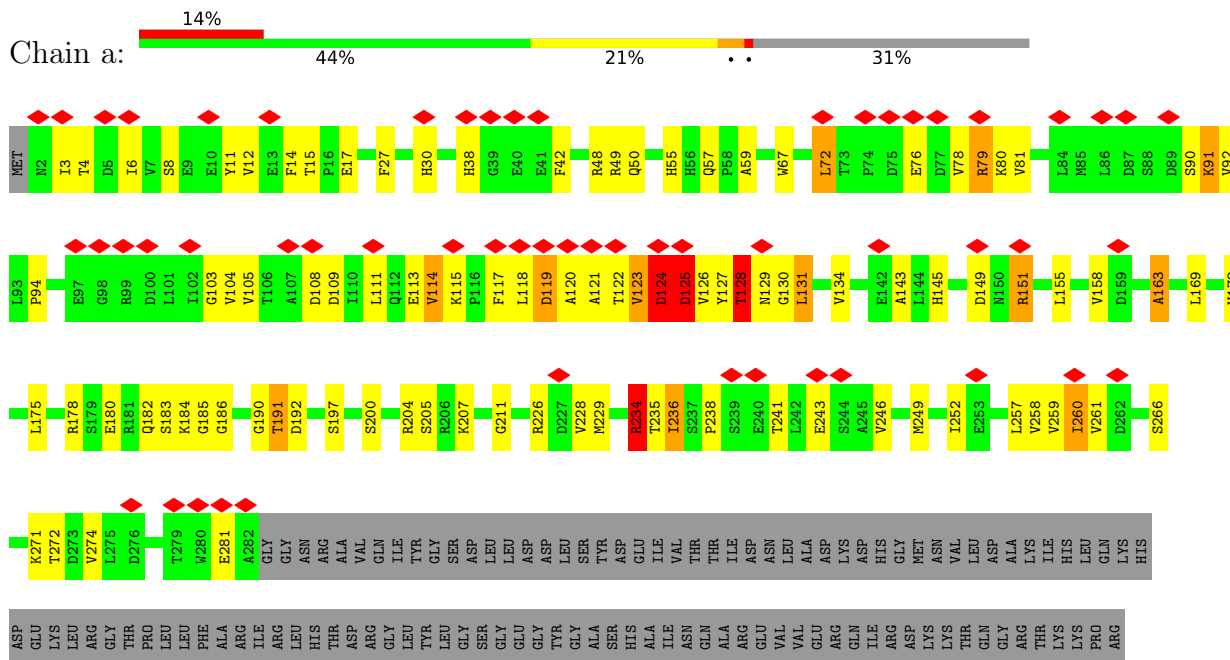
• Molecule 28: Large ribosomal subunit protein eL20



• Molecule 29: Large ribosomal subunit protein uL14



• Molecule 30: CBS domain-containing protein



ASP
ALA
GLU
TYR
TRP
GLU
LYS
ARG
PHE
GLY
TRP
MET
LEU
GLU
GLY
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	918876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.744	Depositor
Minimum map value	-0.406	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	427.52, 427.52, 427.52	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.668, 0.668, 0.668	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AMP, BGC, ZN

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	0	0.69	0/67834	0.85	1/105799 (0.0%)
2	9	0.25	0/2848	0.32	0/4436
3	A	0.26	0/254	0.46	0/333
4	E	0.27	0/889	0.44	0/1209
5	F	0.28	0/1395	0.44	0/1875
6	G	0.34	0/1606	0.41	0/2145
7	H	0.27	0/895	0.45	0/1210
8	I	0.23	0/1447	0.40	0/1969
9	J	0.36	0/1217	0.49	1/1622 (0.1%)
10	K	0.28	0/750	0.37	0/1001
11	L	0.28	0/1199	0.45	0/1619
12	M	0.31	0/474	0.52	0/634
13	N	0.29	0/911	0.42	0/1232
14	O	0.30	0/1218	0.44	0/1651
15	P	0.31	0/741	0.49	0/998
16	Q	0.29	0/1165	0.42	0/1561
17	R	0.33	0/624	0.47	0/835
18	S	0.29	0/446	0.37	0/586
19	T	0.26	0/764	0.38	0/1015
20	U	0.35	0/1817	0.55	0/2441
21	V	0.29	0/2677	0.41	0/3617
22	W	0.29	0/1925	0.43	0/2598
23	X	0.24	0/1263	0.57	2/1709 (0.1%)
24	Y	0.23	0/1368	0.42	0/1859
25	b	0.32	0/1144	0.40	0/1541
26	c	0.26	0/665	0.55	0/891
27	d	0.25	0/532	0.54	0/716
28	e	0.24	0/449	0.45	0/604
29	f	0.27	0/1004	0.47	0/1347
30	a	0.64	0/2158	0.84	2/2937 (0.1%)
All	All	0.59	0/101679	0.75	6/151990 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	1
8	I	0	1
16	Q	0	2
17	R	0	1
20	U	0	2
22	W	0	1
30	a	0	4
All	All	0	12

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1159	G	C2'-C3'-O3'	6.81	119.72	109.50
30	a	186	GLY	CA-C-O	-6.53	116.81	122.16
23	X	10	ARG	CA-C-N	6.30	131.38	121.17
23	X	10	ARG	C-N-CA	6.30	131.38	121.17
30	a	125	ASP	N-CA-C	-5.85	105.72	112.92
9	J	150	ILE	N-CA-C	-5.05	107.91	112.96

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	194	ARG	Sidechain
8	I	144	ARG	Sidechain
16	Q	139	ARG	Sidechain
16	Q	141	ARG	Sidechain
17	R	7	ARG	Sidechain
20	U	232	ARG	Sidechain
20	U	235	ARG	Sidechain
22	W	65	ARG	Sidechain
30	a	151	ARG	Sidechain
30	a	204	ARG	Sidechain
30	a	234	ARG	Sidechain
30	a	79	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	0	60579	0	30550	638	0
2	9	2551	0	1298	25	0
3	A	252	0	287	3	0
4	E	880	0	852	13	0
5	F	1372	0	1371	26	0
6	G	1579	0	1606	16	0
7	H	887	0	907	12	0
8	I	1417	0	1365	22	0
9	J	1205	0	1208	28	0
10	K	736	0	745	14	0
11	L	1174	0	1146	15	0
12	M	466	0	443	13	0
13	N	903	0	886	18	0
14	O	1200	0	1159	23	0
15	P	726	0	703	13	0
16	Q	1146	0	1146	23	0
17	R	617	0	618	12	0
18	S	439	0	445	6	0
19	T	746	0	736	13	0
20	U	1783	0	1818	39	0
21	V	2619	0	2572	38	0
22	W	1898	0	1895	28	0
23	X	1245	0	1149	38	0
24	Y	1346	0	1292	21	0
25	b	1127	0	1118	10	0
26	c	659	0	664	16	0
27	d	529	0	525	20	0
28	e	443	0	438	9	0
29	f	996	0	1046	11	0
30	a	2123	0	2104	58	0
31	0	12	0	12	1	0
32	0	183	0	0	0	0
32	A	1	0	0	0	0
32	F	2	0	0	0	0
32	G	1	0	0	0	0
32	L	1	0	0	0	0
32	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	O	1	0	0	0	0
32	Q	1	0	0	0	0
32	U	1	0	0	0	0
32	V	2	0	0	0	0
32	f	1	0	0	0	0
33	S	1	0	0	0	0
33	T	1	0	0	0	0
34	a	46	0	24	0	0
35	0	1567	0	0	116	0
35	9	33	0	0	1	0
35	A	2	0	0	0	0
35	E	3	0	0	1	0
35	F	14	0	0	2	0
35	G	24	0	0	1	0
35	H	8	0	0	1	0
35	I	2	0	0	0	0
35	J	10	0	0	0	0
35	K	19	0	0	3	0
35	L	19	0	0	4	0
35	M	5	0	0	1	0
35	N	10	0	0	1	0
35	O	20	0	0	2	0
35	P	10	0	0	1	0
35	Q	27	0	0	9	0
35	R	2	0	0	0	0
35	S	13	0	0	1	0
35	T	12	0	0	0	0
35	U	25	0	0	7	0
35	V	29	0	0	7	0
35	W	19	0	0	3	0
35	X	1	0	0	0	0
35	Y	3	0	0	0	0
35	a	4	0	0	1	0
35	b	13	0	0	0	0
35	c	1	0	0	0	0
35	f	6	0	0	0	0
All	All	95799	0	62128	1161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:999:U:H2'	1:0:1000:C:C5	1.22	1.66
1:0:999:U:H2'	1:0:1000:C:C4	1.43	1.49
1:0:999:U:C2'	1:0:1000:C:C5	2.06	1.39
20:U:211:GLN:NE2	35:U:401:HOH:O	1.60	1.30
1:0:1000:C:OP1	1:0:1000:C:C6	1.86	1.28
1:0:287:A:N3	1:0:372:G:N7	1.84	1.23
1:0:1276:U:OP2	1:0:1276:U:H3'	1.40	1.22
1:0:2887:C:H5''	35:0:3666:HOH:O	1.15	1.21
1:0:873:G:OP2	35:0:3204:HOH:O	1.55	1.21
1:0:1773:A:O2'	35:0:3205:HOH:O	1.61	1.19
11:L:34:ARG:HD3	35:L:310:HOH:O	1.41	1.17
21:V:338:GLY:O	35:V:501:HOH:O	1.59	1.17
1:0:1000:C:C5	1:0:1000:C:OP1	1.97	1.16
9:J:123:LEU:HD11	9:J:146:TYR:HE2	1.01	1.15
1:0:1275:U:H4'	1:0:1276:U:H5'	1.25	1.14
1:0:2887:C:C5'	35:0:3666:HOH:O	1.67	1.14
9:J:123:LEU:HD11	9:J:146:TYR:CE2	1.86	1.11
35:0:3474:HOH:O	5:F:18:THR:HG21	0.95	1.10
1:0:1694:G:H5''	35:0:3554:HOH:O	1.52	1.09
1:0:1659:A:H4'	1:0:1660:G:OP2	1.35	1.09
1:0:842:U:OP1	35:0:3206:HOH:O	1.69	1.09
1:0:2079:C:OP2	35:0:3207:HOH:O	1.71	1.08
1:0:1650:G:OP2	35:0:3208:HOH:O	1.72	1.07
1:0:1000:C:C6	1:0:1000:C:P	2.48	1.06
1:0:1000:C:P	1:0:1000:C:H6	1.79	1.06
1:0:999:U:C2'	1:0:1000:C:C4	2.33	1.05
1:0:1050:U:O4	35:0:3209:HOH:O	1.73	1.03
9:J:123:LEU:CD1	9:J:146:TYR:HE2	1.73	1.01
1:0:1891:G:N2	35:0:3215:HOH:O	1.87	1.00
15:P:65:GLN:NE2	35:P:101:HOH:O	1.72	1.00
1:0:977:C:H2'	1:0:978:G:C8	1.96	1.00
1:0:1159:G:O6	1:0:1181:C:N4	1.96	0.98
1:0:1158:A:N6	1:0:1188:A:OP1	1.95	0.98
1:0:297:U:O2	1:0:362:A:N1	1.96	0.98
1:0:1940:G:H2'	1:0:1941:G:C8	1.98	0.98
1:0:601:A:OP1	35:0:3211:HOH:O	1.82	0.98
1:0:1423:A:N7	35:0:3233:HOH:O	1.98	0.96
1:0:2317:A:N3	35:0:3228:HOH:O	1.97	0.96
1:0:773:A:N3	35:0:3235:HOH:O	2.00	0.95
16:Q:218:ARG:HD3	35:Q:419:HOH:O	1.66	0.95
1:0:287:A:C2	1:0:372:G:N7	2.36	0.93
1:0:1275:U:H4'	1:0:1276:U:C5'	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2718:G:O6	35:0:3212:HOH:O	1.85	0.92
1:0:326:A:OP2	35:0:3216:HOH:O	1.87	0.92
1:0:608:G:O6	35:0:3214:HOH:O	1.86	0.91
1:0:1812:G:H4'	1:0:1812:G:OP1	1.69	0.91
21:V:37:PRO:O	35:V:502:HOH:O	1.89	0.91
1:0:2862:G:O6	35:0:3219:HOH:O	1.89	0.90
1:0:223:A:OP2	35:0:3220:HOH:O	1.90	0.90
1:0:1679:A:H2'	35:0:3213:HOH:O	1.71	0.90
35:9:227:HOH:O	5:F:13:LYS:HG2	1.70	0.90
1:0:1998:G:OP2	35:0:3218:HOH:O	1.88	0.89
22:W:79:ARG:NH1	35:W:301:HOH:O	2.01	0.89
11:L:73:ILE:O	35:L:301:HOH:O	1.90	0.89
1:0:2335:G:O2'	1:0:2336:G:H4'	1.74	0.88
1:0:2672:G:OP2	35:0:3221:HOH:O	1.91	0.88
1:0:1679:A:C2'	35:0:3213:HOH:O	2.19	0.88
14:O:11:VAL:O	35:O:301:HOH:O	1.90	0.88
2:9:3:C:H3'	2:9:4:G:H5'	1.54	0.87
1:0:1877:G:O6	35:0:3223:HOH:O	1.92	0.87
1:0:388:G:O2'	35:0:3217:HOH:O	1.88	0.86
1:0:300:A:H3'	1:0:301:A:H5''	1.54	0.86
1:0:696:A:N7	35:0:3246:HOH:O	2.06	0.86
1:0:722:C:O2'	35:0:3224:HOH:O	1.94	0.86
1:0:1679:A:O2'	35:0:3213:HOH:O	1.86	0.85
20:U:127:GLN:HB2	35:U:417:HOH:O	1.76	0.85
1:0:1033:A:H4'	35:0:3617:HOH:O	1.77	0.84
1:0:1171:A:H5'	1:0:1173:C:OP2	1.76	0.84
1:0:1167:U:O2	1:0:1169:G:H3'	1.78	0.84
16:Q:184:THR:HG22	35:Q:416:HOH:O	1.77	0.84
1:0:2856:G:O6	35:0:3227:HOH:O	1.96	0.83
1:0:412:A:OP2	35:0:3225:HOH:O	1.95	0.83
1:0:192:G:H4'	1:0:193:A:OP1	1.76	0.83
1:0:1122:G:C2'	1:0:1123:U:H5'	2.09	0.82
1:0:1168:A:H3'	1:0:1169:G:C8	2.14	0.82
1:0:227:C:O2	35:0:3226:HOH:O	1.95	0.82
1:0:1864:U:O2'	35:0:3229:HOH:O	1.97	0.82
1:0:1949:U:H4'	1:0:1950:A:N7	1.95	0.82
1:0:774:A:OP2	35:0:3230:HOH:O	1.97	0.82
11:L:126:ARG:NH1	35:L:302:HOH:O	2.11	0.82
1:0:2851:U:O2	35:0:3231:HOH:O	1.98	0.81
1:0:1196:A:H3'	1:0:1197:A:C8	2.13	0.81
1:0:2090:G:OP2	35:0:3232:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:38:U:O2'	2:9:43:A:N6	2.13	0.81
1:0:836:G:H4'	1:0:837:U:OP2	1.80	0.81
1:0:1168:A:H3'	1:0:1169:G:H8	1.46	0.81
1:0:1000:C:OP1	1:0:1000:C:H6	1.39	0.80
1:0:1000:C:C6	1:0:1000:C:O5'	2.35	0.80
1:0:1495:U:OP2	35:0:3234:HOH:O	1.99	0.80
1:0:999:U:C2	1:0:1000:C:N3	2.47	0.80
1:0:1537:G:OP2	35:0:3236:HOH:O	2.00	0.80
1:0:2587:C:O2'	1:0:2588:U:H5'	1.81	0.80
1:0:2230:G:O4'	1:0:2230:G:OP1	1.99	0.79
5:F:110:ARG:NH1	30:a:180:GLU:OE1	2.13	0.79
1:0:2345:G:OP2	35:0:3237:HOH:O	2.01	0.78
1:0:1276:U:OP2	1:0:1276:U:C3'	2.28	0.78
1:0:1000:C:OP1	1:0:1000:C:H5	1.67	0.78
1:0:886:C:OP2	35:0:3241:HOH:O	2.02	0.77
30:a:175:LEU:O	30:a:178:ARG:NH1	2.18	0.77
1:0:999:U:C2'	1:0:1000:C:H5	1.96	0.77
5:F:114:GLY:O	35:F:301:HOH:O	2.03	0.77
1:0:537:U:C5	1:0:2077:C:H5'	2.20	0.76
30:a:236:ILE:HG22	30:a:259:VAL:HG12	1.67	0.76
12:M:12:GLU:OE1	12:M:13:GLU:N	2.18	0.76
1:0:1659:A:C4'	1:0:1660:G:OP2	2.27	0.76
1:0:86:G:H22	1:0:104:G:H1'	1.51	0.76
1:0:2628:A:C2'	1:0:2629:C:H5'	2.15	0.76
16:Q:125:GLN:OE1	35:Q:401:HOH:O	2.02	0.76
1:0:1058:A:H2'	1:0:1059:A:C8	2.21	0.75
1:0:2134:G:H1	1:0:2226:C:H1'	1.52	0.75
1:0:2418:A:OP1	35:0:3243:HOH:O	2.03	0.75
1:0:74:A:N6	35:0:3238:HOH:O	2.02	0.75
1:0:668:U:O4	1:0:685:G:H5'	1.87	0.75
1:0:1745:G:OP2	35:0:3242:HOH:O	2.03	0.74
1:0:1196:A:H3'	1:0:1197:A:H8	1.49	0.74
1:0:1741:A:C8	35:0:3318:HOH:O	2.39	0.74
20:U:205:GLY:O	35:U:402:HOH:O	2.05	0.74
1:0:1000:C:H6	1:0:1000:C:O5'	1.68	0.74
1:0:2628:A:O2'	1:0:2629:C:H5'	1.87	0.74
35:0:3256:HOH:O	14:O:31:HIS:HD2	1.69	0.74
1:0:1949:U:H4'	1:0:1950:A:C8	2.23	0.74
13:N:5:PRO:HD2	35:W:306:HOH:O	1.88	0.74
14:O:2:GLN:NE2	14:O:37:GLU:OE2	2.21	0.73
1:0:1483:A:H5'	35:0:3973:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:667:C:C5	35:0:3513:HOH:O	2.41	0.73
1:0:2887:C:H5'	35:0:3666:HOH:O	1.56	0.73
30:a:235:THR:HB	30:a:260:ILE:HD11	1.68	0.73
30:a:15:THR:HG23	30:a:17:GLU:H	1.52	0.72
1:0:1940:G:H2'	1:0:1941:G:H8	1.50	0.72
1:0:672:G:N7	35:0:3274:HOH:O	2.22	0.72
1:0:1171:A:C5'	1:0:1173:C:OP2	2.37	0.72
16:Q:203:VAL:O	35:Q:402:HOH:O	2.07	0.72
1:0:1744:C:OP2	35:0:3248:HOH:O	2.07	0.72
1:0:2685:G:O2'	1:0:2686:U:P	2.46	0.71
30:a:158:VAL:HG22	30:a:163:ALA:HA	1.72	0.71
13:N:50:GLU:HB3	13:N:60:GLU:HG2	1.72	0.71
1:0:999:U:H2'	1:0:1000:C:N4	2.03	0.71
10:K:72:PHE:HE1	10:K:89:PRO:HG3	1.56	0.71
1:0:1790:A:OP1	35:0:3249:HOH:O	2.08	0.71
1:0:537:U:C6	1:0:2077:C:H5'	2.26	0.71
1:0:1275:U:C4'	1:0:1276:U:H5'	2.14	0.71
1:0:2134:G:H3'	1:0:2135:G:H8	1.56	0.71
1:0:2499:A:OP2	35:0:3247:HOH:O	2.07	0.71
1:0:1157:G:H2'	1:0:1204:A:H61	1.56	0.70
1:0:1156:G:H3'	1:0:1157:G:H8	1.54	0.70
1:0:2140:U:H4'	1:0:2222:G:H1	1.56	0.70
1:0:2571:G:OP2	35:0:3250:HOH:O	2.08	0.70
1:0:1235:C:C6	1:0:1237:G:OP2	2.45	0.70
30:a:243:GLU:N	30:a:243:GLU:OE1	2.24	0.70
1:0:319:G:OP1	35:0:3251:HOH:O	2.09	0.70
1:0:369:C:H1'	1:0:370:C:H5''	1.74	0.70
1:0:1812:G:OP1	1:0:1812:G:C4'	2.40	0.70
35:0:3408:HOH:O	19:T:46:THR:HG22	1.91	0.70
9:J:27:GLU:OE1	9:J:27:GLU:N	2.24	0.70
15:P:25:GLU:N	15:P:25:GLU:OE2	2.25	0.70
1:0:2335:G:H5''	1:0:2336:G:H21	1.56	0.70
1:0:1276:U:H3'	1:0:1276:U:P	2.30	0.70
22:W:194:ILE:HD12	22:W:194:ILE:H	1.57	0.70
1:0:2501:C:O2'	1:0:2502:A:H5'	1.92	0.69
1:0:250:A:H61	1:0:274:G:H1'	1.56	0.69
23:X:102:PHE:HB2	23:X:126:VAL:HB	1.73	0.69
1:0:2587:C:C2'	1:0:2588:U:H5'	2.22	0.69
5:F:87:MET:HG3	5:F:138:ILE:HG12	1.73	0.69
1:0:667:C:H5	35:0:3513:HOH:O	1.75	0.69
1:0:999:U:C2'	1:0:1000:C:N4	2.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:608:G:OP2	35:0:3255:HOH:O	2.11	0.68
1:0:978:G:H1	1:0:994:U:H1'	1.58	0.68
9:J:123:LEU:HG	9:J:146:TYR:OH	1.93	0.68
1:0:1488:A:H1'	1:0:1509:C:H1'	1.74	0.68
6:G:114:ARG:NH1	6:G:151:ILE:O	2.27	0.68
1:0:737:C:H3'	1:0:738:A:H8	1.58	0.68
1:0:1122:G:O2'	1:0:1123:U:H5'	1.93	0.68
1:0:1681:C:OP1	35:0:3254:HOH:O	2.11	0.68
30:a:78:VAL:C	30:a:80:LYS:H	2.02	0.68
35:0:3284:HOH:O	24:Y:32:LYS:NZ	2.27	0.67
21:V:188:GLU:HB2	35:V:518:HOH:O	1.94	0.67
23:X:33:SER:HA	23:X:36:ILE:HD12	1.76	0.67
11:L:26:LEU:HD22	11:L:119:LYS:HB2	1.74	0.67
23:X:105:GLU:HA	23:X:123:GLY:HA2	1.75	0.67
1:0:2387:A:H4'	1:0:2388:A:OP1	1.94	0.67
1:0:769:A:OP1	35:0:3258:HOH:O	2.12	0.67
35:0:3780:HOH:O	19:T:1:MET:HG3	1.95	0.67
1:0:2525:A:OP1	35:0:3259:HOH:O	2.12	0.67
24:Y:27:ASN:ND2	24:Y:79:GLU:O	2.28	0.67
1:0:341:G:N1	13:N:55:ASP:OD1	2.28	0.66
6:G:16:PRO:HA	6:G:21:LEU:HD23	1.76	0.66
23:X:19:VAL:HG13	23:X:126:VAL:HG22	1.76	0.66
6:G:103:GLU:HG2	6:G:115:VAL:HG11	1.75	0.66
1:0:1168:A:C3'	1:0:1169:G:H8	2.08	0.66
14:O:6:GLN:NE2	14:O:8:ARG:O	2.24	0.66
1:0:977:C:C2'	1:0:978:G:C8	2.77	0.66
1:0:2676:G:N7	35:0:3302:HOH:O	2.30	0.66
1:0:1232:G:OP2	35:0:3262:HOH:O	2.14	0.65
1:0:1184:U:H1'	1:0:1187:G:H22	1.61	0.65
1:0:436:A:N3	35:0:3298:HOH:O	2.28	0.65
1:0:134:C:H2'	1:0:135:A:H8	1.62	0.65
13:N:48:THR:HB	13:N:101:GLU:HB2	1.79	0.65
1:0:508:G:OP1	35:0:3261:HOH:O	2.13	0.65
29:f:103:GLU:OE2	29:f:103:GLU:N	2.30	0.65
30:a:128:THR:HG22	30:a:130:GLY:H	1.62	0.65
1:0:297:U:O2	1:0:362:A:C2	2.49	0.65
1:0:1520:A:N3	1:0:1520:A:H2'	2.11	0.65
12:M:54:GLU:OE1	12:M:57:ARG:NH2	2.30	0.65
1:0:300:A:H2'	1:0:301:A:C8	2.32	0.64
35:0:3474:HOH:O	5:F:18:THR:CG2	1.78	0.64
1:0:977:C:H2'	1:0:978:G:N7	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:990:G:H2'	1:0:991:A:C8	2.31	0.64
1:0:1206:C:H4'	1:0:1206:C:OP1	1.96	0.64
30:a:123:VAL:HG23	30:a:241:THR:H	1.61	0.64
21:V:271:ILE:HD11	21:V:299:LYS:HB2	1.78	0.64
29:f:100:GLU:OE1	29:f:100:GLU:N	2.24	0.64
1:0:2703:A:H2'	1:0:2704:U:C6	2.33	0.64
11:L:18:MET:HE3	11:L:145:GLU:HB3	1.79	0.64
17:R:44:VAL:HG12	17:R:54:ASN:HA	1.78	0.64
22:W:33:ARG:NH1	22:W:106:GLU:OE2	2.31	0.64
1:0:1549:G:O6	35:0:3260:HOH:O	2.13	0.64
14:O:105:THR:OG1	14:O:110:GLN:NE2	2.29	0.64
1:0:999:U:C3'	1:0:1000:C:C5	2.81	0.63
1:0:21:C:H2'	1:0:22:C:C6	2.33	0.63
1:0:2134:G:H3'	1:0:2135:G:C8	2.33	0.63
30:a:57:GLN:O	30:a:59:ALA:N	2.25	0.63
1:0:260:U:H5''	1:0:261:C:C5	2.34	0.63
1:0:2750:A:O2'	35:0:3239:HOH:O	2.02	0.63
9:J:123:LEU:CG	9:J:146:TYR:HE2	2.11	0.63
1:0:1951:U:H2'	1:0:1952:G:C8	2.33	0.63
21:V:67:GLU:OE2	21:V:329:ARG:NH1	2.32	0.63
1:0:2784:U:H1'	1:0:2785:A:H5''	1.80	0.63
7:H:55:GLU:N	7:H:55:GLU:OE2	2.31	0.63
4:E:5:VAL:HA	4:E:77:PHE:HE2	1.62	0.63
1:0:1158:A:H62	1:0:1188:A:P	2.22	0.62
1:0:2219:U:O2'	1:0:2220:U:O5'	2.12	0.62
4:E:8:ASP:OD1	4:E:9:VAL:N	2.31	0.62
22:W:12:ASP:OD1	22:W:12:ASP:N	2.33	0.62
13:N:84:ASP:OD1	13:N:85:GLY:N	2.32	0.62
6:G:166:ASN:OD1	6:G:167:ALA:N	2.33	0.62
1:0:1660:G:O2'	1:0:1661:C:H5'	2.00	0.62
8:I:170:PRO:O	8:I:173:PHE:HB3	2.00	0.62
22:W:200:GLU:OE2	22:W:200:GLU:N	2.32	0.62
25:b:134:GLU:O	25:b:138:LYS:HG3	1.99	0.62
1:0:946:G:H21	14:O:44:MET:HE2	1.64	0.62
16:Q:109:GLU:HB3	35:Q:414:HOH:O	2.00	0.62
1:0:493:A:H61	1:0:507:G:C2'	2.12	0.62
1:0:737:C:H3'	1:0:738:A:C8	2.35	0.62
1:0:1171:A:H2'	1:0:1198:C:H4'	1.81	0.62
1:0:2667:G:H1'	1:0:2806:A:N6	2.14	0.62
6:G:153:ASN:OD1	6:G:154:ASP:N	2.33	0.62
23:X:99:ASN:ND2	23:X:129:ASN:OD1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:67:LEU:HD21	26:c:71:ASP:HB2	1.81	0.62
1:0:2910:C:H3'	1:0:2911:A:H8	1.65	0.61
8:I:120:GLN:O	8:I:124:ILE:HG13	2.00	0.61
30:a:123:VAL:O	30:a:124:ASP:C	2.42	0.61
1:0:2221:A:H1'	1:0:2222:G:C4	2.35	0.61
21:V:23:GLU:OE1	21:V:260:TYR:OH	2.18	0.61
21:V:233:TRP:HD1	21:V:236:ARG:HD2	1.64	0.61
1:0:299:G:C5	1:0:300:A:H1'	2.36	0.61
1:0:698:A:O5'	1:0:698:A:H8	1.84	0.61
28:e:6:ILE:HG23	28:e:55:VAL:HG22	1.83	0.61
1:0:485:U:H4'	1:0:519:C:H2'	1.83	0.61
1:0:999:U:O2'	1:0:1000:C:C5	2.53	0.61
21:V:320:ASP:OD1	21:V:320:ASP:N	2.34	0.61
1:0:1198:C:H3'	1:0:1199:A:H8	1.63	0.60
35:0:3663:HOH:O	13:N:3:ARG:HD3	2.00	0.60
1:0:1168:A:H2'	1:0:1169:G:C8	2.37	0.60
1:0:1943:G:H3'	1:0:1944:G:H8	1.66	0.60
27:d:30:ASN:O	27:d:34:VAL:HG23	2.02	0.60
30:a:123:VAL:HA	30:a:241:THR:HA	1.83	0.60
20:U:212:PRO:O	20:U:213:LYS:HB2	2.00	0.60
24:Y:78:THR:OG1	24:Y:79:GLU:OE2	2.18	0.60
27:d:56:ARG:O	27:d:60:ILE:HD12	2.02	0.60
9:J:105:ARG:NH1	9:J:108:GLU:OE2	2.29	0.60
16:Q:207:LYS:NZ	35:Q:403:HOH:O	2.14	0.60
30:a:27:PHE:O	30:a:48:ARG:NH2	2.35	0.60
1:0:773:A:C2	35:0:3235:HOH:O	2.49	0.60
1:0:2817:C:O2	1:0:2817:C:O4'	2.19	0.60
30:a:191:THR:HA	30:a:197:SER:HA	1.84	0.60
1:0:153:U:O4	35:0:3264:HOH:O	2.14	0.60
2:9:95:C:H2'	2:9:96:U:C6	2.37	0.60
9:J:44:LEU:HB3	9:J:50:ILE:HD12	1.84	0.60
1:0:1199:A:H3'	1:0:1200:G:H8	1.67	0.60
22:W:193:SER:OG	22:W:194:ILE:HD12	2.02	0.60
22:W:213:ASP:OD1	22:W:233:ARG:NH2	2.23	0.60
1:0:1168:A:C3'	1:0:1169:G:C8	2.84	0.59
27:d:2:ALA:N	27:d:49:GLU:OE2	2.35	0.59
8:I:63:THR:HG22	8:I:65:ALA:H	1.65	0.59
1:0:1945:U:H2'	1:0:1946:A:C5	2.37	0.59
4:E:79:GLU:HB3	35:E:202:HOH:O	2.02	0.59
20:U:36:LYS:HZ3	20:U:37:ASP:H	1.51	0.59
26:c:14:MET:HE3	26:c:14:MET:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1396:C:H4'	15:P:57:GLU:HG3	1.85	0.59
1:0:2768:A:H2'	1:0:2769:A:C8	2.38	0.59
17:R:75:GLN:HA	17:R:78:ARG:HD3	1.84	0.59
22:W:136:GLU:N	22:W:136:GLU:OE1	2.31	0.59
27:d:19:ALA:O	27:d:23:GLU:HG2	2.03	0.59
30:a:38:HIS:HA	30:a:42:PHE:HA	1.83	0.59
1:0:1000:C:C5	1:0:1000:C:P	2.87	0.59
1:0:2729:C:OP1	35:0:3267:HOH:O	2.16	0.59
20:U:211:GLN:CD	20:U:211:GLN:H	2.11	0.59
21:V:113:VAL:HG13	21:V:114:LEU:HD12	1.84	0.59
26:c:57:MET:HE3	26:c:57:MET:O	2.03	0.59
30:a:128:THR:C	30:a:130:GLY:H	2.11	0.59
35:0:3651:HOH:O	25:b:90:LYS:HE2	2.02	0.59
2:9:103:A:H2'	2:9:104:A:H8	1.68	0.59
7:H:81:ASP:OD1	7:H:82:PHE:N	2.36	0.59
23:X:132:ARG:NH1	23:X:152:ARG:O	2.36	0.59
1:0:1170:A:H1'	1:0:1197:A:H4'	1.84	0.58
1:0:1372:G:H5'	1:0:1376:G:C6	2.38	0.58
1:0:1741:A:N7	35:0:3318:HOH:O	2.35	0.58
26:c:43:ARG:HG2	26:c:44:TYR:CD1	2.38	0.58
1:0:1196:A:N3	1:0:1196:A:H2'	2.17	0.58
24:Y:85:MET:HE2	24:Y:134:LEU:HD11	1.83	0.58
1:0:2318:U:H2'	1:0:2319:U:C6	2.38	0.58
1:0:2338:A:H4'	23:X:54:SER:HA	1.84	0.58
27:d:9:ILE:HD12	27:d:57:ILE:HD13	1.86	0.58
1:0:1522:A:H1'	1:0:1523:A:C8	2.39	0.58
2:9:8:G:H5''	10:K:28:GLN:HG3	1.86	0.58
21:V:76:GLU:OE2	21:V:288:TYR:OH	2.16	0.58
23:X:107:HIS:HE1	23:X:122:TYR:HB2	1.66	0.58
1:0:2835:G:H2'	1:0:2836:A:H5'	1.84	0.58
1:0:1272:U:H3'	1:0:1273:A:N3	2.19	0.58
2:9:23:U:H3'	2:9:24:U:O2	2.03	0.58
1:0:288:U:H1'	1:0:289:A:C2	2.39	0.57
1:0:1283:A:H1'	35:0:3256:HOH:O	2.04	0.57
23:X:151:HIS:O	23:X:151:HIS:ND1	2.37	0.57
1:0:2277:G:C8	35:0:3507:HOH:O	2.53	0.57
1:0:2619:C:H2'	1:0:2620:G:C8	2.39	0.57
1:0:1635:G:O6	35:0:3266:HOH:O	2.16	0.57
1:0:1122:G:H2'	1:0:1123:U:H5'	1.85	0.57
1:0:1156:G:H3'	1:0:1157:G:C8	2.39	0.57
1:0:1161:U:H1'	1:0:1162:G:H3'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1487:A:H2'	1:0:1488:A:C8	2.39	0.57
7:H:17:ALA:HA	7:H:20:ARG:NH1	2.20	0.57
15:P:74:ARG:NH2	15:P:92:GLU:OE1	2.30	0.57
24:Y:108:PHE:CZ	24:Y:153:THR:HB	2.40	0.57
30:a:78:VAL:C	30:a:80:LYS:N	2.63	0.57
1:0:2032:A:H1'	35:0:3891:HOH:O	2.05	0.57
1:0:1199:A:H3'	1:0:1200:G:C8	2.40	0.57
28:e:36:TYR:CD1	28:e:47:ARG:HG2	2.39	0.57
1:0:869:A:N1	1:0:882:C:O2'	2.33	0.57
1:0:1534:U:H2'	1:0:1535:A:H8	1.70	0.57
1:0:2855:G:H4'	21:V:338:GLY:HA2	1.86	0.57
10:K:4:SER:OG	35:K:102:HOH:O	2.18	0.57
1:0:984:C:H2'	1:0:985:G:C8	2.40	0.56
1:0:1120:G:N2	1:0:1243:A:N7	2.53	0.56
1:0:1249:A:H4'	28:e:47:ARG:NE	2.20	0.56
29:f:64:MET:HE3	29:f:64:MET:HA	1.87	0.56
1:0:1402:U:H1'	35:0:3447:HOH:O	2.04	0.56
1:0:2579:U:H3	1:0:2585:G:H1	1.53	0.56
1:0:1520:A:O2'	1:0:1521:A:H2'	2.05	0.56
1:0:1567:A:H2'	1:0:1568:A:C8	2.40	0.56
9:J:123:LEU:CG	9:J:146:TYR:CE2	2.89	0.56
30:a:14:PHE:O	30:a:15:THR:HG22	2.05	0.56
30:a:281:GLU:OE1	30:a:281:GLU:N	2.38	0.56
1:0:978:G:O5'	1:0:978:G:H8	1.87	0.56
1:0:1174:A:H3'	1:0:1175:G:H8	1.68	0.56
1:0:1235:C:C6	1:0:1237:G:P	2.98	0.56
1:0:1729:C:H2'	1:0:1730:G:H8	1.70	0.56
1:0:2831:A:H2'	1:0:2832:G:C8	2.40	0.56
6:G:155:ASP:O	6:G:162:ARG:NH2	2.39	0.56
1:0:1588:C:N4	35:0:3222:HOH:O	1.91	0.56
20:U:224:LYS:HD2	20:U:228:ILE:HG23	1.88	0.56
23:X:78:GLU:O	23:X:82:THR:HG22	2.06	0.56
23:X:78:GLU:HA	23:X:81:GLU:HG3	1.88	0.56
10:K:77:ASN:ND2	10:K:82:GLU:OE2	2.31	0.56
17:R:75:GLN:OE1	17:R:79:SER:OG	2.23	0.56
9:J:123:LEU:CD1	9:J:146:TYR:CE2	2.64	0.56
1:0:2265:G:H5'	20:U:223:ARG:HB2	1.88	0.55
1:0:2587:C:H2'	1:0:2588:U:H5'	1.88	0.55
9:J:15:LEU:HD13	9:J:52:ALA:HB2	1.88	0.55
1:0:1791:U:H3'	1:0:1792:A:H8	1.71	0.55
1:0:2354:A:H2'	1:0:2355:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2604:G:N3	1:0:2604:G:H2'	2.20	0.55
1:0:290:A:H3'	1:0:291:C:H5''	1.87	0.55
1:0:1068:A:H5'	14:O:14:SER:HA	1.88	0.55
1:0:386:U:H2'	1:0:387:A:H8	1.70	0.55
1:0:1943:G:H3'	1:0:1944:G:C8	2.41	0.55
1:0:2685:G:HO2'	1:0:2686:U:P	2.28	0.55
1:0:77:A:H4'	1:0:78:G:O5'	2.07	0.55
8:I:87:TYR:O	8:I:91:ILE:HG13	2.06	0.55
13:N:42:ARG:NH1	13:N:43:VAL:O	2.39	0.55
27:d:28:LEU:O	27:d:32:LYS:HG3	2.06	0.55
1:0:2667:G:H1'	1:0:2806:A:H61	1.72	0.55
4:E:14:ALA:O	4:E:18:VAL:HG23	2.07	0.55
21:V:327:GLU:OE1	21:V:327:GLU:N	2.37	0.55
1:0:451:A:OP2	13:N:4:GLN:HG3	2.07	0.55
1:0:376:U:H2'	1:0:377:G:C8	2.42	0.55
1:0:1276:U:C3'	1:0:1276:U:P	2.94	0.55
17:R:76:VAL:O	17:R:80:ILE:HG22	2.06	0.55
1:0:409:U:O4	35:O:3268:HOH:O	2.18	0.55
5:F:21:GLU:OE2	5:F:21:GLU:N	2.33	0.55
23:X:107:HIS:HB3	23:X:113:GLN:HG2	1.88	0.55
1:0:1944:G:H21	1:0:1955:C:H5	1.55	0.54
4:E:58:GLU:HB2	6:G:24:LEU:HD11	1.90	0.54
5:F:88:ILE:HB	5:F:137:THR:HG22	1.88	0.54
14:O:41:TYR:O	14:O:45:ILE:HG13	2.07	0.54
1:0:1544:C:H2'	1:0:1545:G:H8	1.72	0.54
1:0:2910:C:H3'	1:0:2911:A:C8	2.42	0.54
17:R:85:THR:OG1	17:R:86:GLY:N	2.39	0.54
23:X:36:ILE:HG22	23:X:40:ILE:HD12	1.89	0.54
1:0:422:C:H2'	1:0:423:A:H8	1.73	0.54
5:F:144:ASP:O	5:F:147:ILE:HG22	2.07	0.54
7:H:61:VAL:HG21	7:H:65:VAL:HG23	1.89	0.54
14:O:16:ASP:OD1	14:O:17:VAL:N	2.40	0.54
21:V:233:TRP:CD1	21:V:236:ARG:HD2	2.42	0.54
1:0:2628:A:H2'	1:0:2629:C:H5'	1.88	0.54
1:0:836:G:C4'	1:0:837:U:OP2	2.54	0.54
1:0:863:U:H2'	1:0:864:G:C8	2.43	0.54
1:0:2426:U:H2'	1:0:2427:A:C8	2.43	0.54
24:Y:138:ASP:O	24:Y:142:VAL:HG23	2.07	0.54
1:0:877:A:OP1	35:O:3269:HOH:O	2.18	0.54
1:0:2135:G:H2'	1:0:2136:U:C6	2.42	0.54
2:9:75:C:H3'	2:9:76:A:H5''	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:6:ARG:HD3	22:W:161:LEU:HD11	1.90	0.54
26:c:28:HIS:HB3	26:c:31:SER:OG	2.08	0.54
27:d:43:ASN:ND2	27:d:46:ARG:HB2	2.23	0.54
1:0:1822:A:H5'	35:0:3875:HOH:O	2.07	0.54
23:X:37:LEU:O	23:X:41:THR:OG1	2.21	0.54
1:0:1724:U:C2	15:P:20:ALA:HB2	2.43	0.54
1:0:1950:A:H3'	1:0:1950:A:N3	2.23	0.54
2:9:28:C:OP1	23:X:136:ARG:NH1	2.39	0.54
4:E:41:ILE:HD11	4:E:49:VAL:HG21	1.90	0.54
28:e:26:PRO:HD2	28:e:30:VAL:HG11	1.88	0.54
1:0:2084:G:H22	1:0:2646:A:H2	1.56	0.53
5:F:130:PRO:HD2	5:F:133:GLU:OE2	2.07	0.53
22:W:49:ASP:HB3	22:W:52:ALA:HB2	1.90	0.53
25:b:124:LEU:HD12	25:b:124:LEU:H	1.72	0.53
11:L:3:ILE:HG13	11:L:18:MET:HE1	1.90	0.53
1:0:493:A:H61	1:0:507:G:H2'	1.72	0.53
1:0:1098:A:H2'	1:0:1099:A:C8	2.44	0.53
1:0:1902:A:H2'	1:0:1903:A:C8	2.43	0.53
1:0:155:G:H5''	18:S:45:LYS:HG2	1.90	0.53
1:0:707:G:O2'	1:0:708:C:H5'	2.08	0.53
1:0:1212:A:N3	1:0:1213:G:H1'	2.24	0.53
10:K:72:PHE:CE1	10:K:89:PRO:HG3	2.39	0.53
17:R:11:SER:HB3	17:R:35:ARG:HH22	1.74	0.53
21:V:9:LYS:HD2	21:V:221:VAL:HA	1.90	0.53
30:a:11:TYR:HE2	30:a:103:GLY:HA2	1.73	0.53
1:0:934:U:H2'	1:0:935:C:C6	2.44	0.53
9:J:13:ASP:OD2	9:J:38:ARG:NH2	2.33	0.53
1:0:999:U:O2'	1:0:1000:C:H5	1.91	0.53
1:0:1786:C:H2'	1:0:1787:U:C6	2.44	0.53
1:0:2628:A:O2'	1:0:2629:C:C5'	2.56	0.53
26:c:49:GLU:HG2	26:c:68:SER:HA	1.91	0.53
1:0:2536:G:OP2	35:0:3270:HOH:O	2.19	0.53
20:U:175:LYS:HD2	20:U:179:MET:HE2	1.91	0.53
26:c:10:THR:H	26:c:13:ALA:HB3	1.74	0.53
5:F:88:ILE:HD12	5:F:139:TYR:HE1	1.74	0.53
1:0:600:C:H2'	1:0:601:A:C8	2.44	0.52
1:0:928:A:H2'	1:0:929:U:C6	2.45	0.52
4:E:107:ASP:O	4:E:110:GLU:HB2	2.08	0.52
1:0:1914:A:H3'	1:0:1915:A:H8	1.74	0.52
35:0:3256:HOH:O	14:O:31:HIS:CD2	2.53	0.52
1:0:1129:A:N6	1:0:1226:G:H2'	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:287:A:N3	1:0:372:G:C5	2.73	0.52
1:0:1940:G:C2'	1:0:1941:G:C8	2.84	0.52
1:0:2525:A:H1'	1:0:2526:C:H5	1.74	0.52
3:A:6:LYS:O	3:A:10:LYS:HG3	2.10	0.52
21:V:338:GLY:C	35:V:501:HOH:O	2.30	0.52
1:0:247:C:H2'	1:0:247:C:O2	2.08	0.52
1:0:260:U:H5''	1:0:261:C:H5	1.72	0.52
1:0:493:A:N6	1:0:507:G:H2'	2.24	0.52
1:0:1945:U:H2'	1:0:1946:A:C4	2.44	0.52
6:G:185:ARG:O	35:G:301:HOH:O	2.19	0.52
22:W:130:ARG:HG2	22:W:130:ARG:HH11	1.75	0.52
1:0:68:G:H1	1:0:92:C:H5	1.56	0.52
1:0:986:A:H2'	1:0:987:G:O4'	2.10	0.52
24:Y:22:THR:HG22	24:Y:31:THR:OG1	2.10	0.52
24:Y:24:GLU:OE2	24:Y:24:GLU:N	2.42	0.52
1:0:377:G:C6	1:0:379:U:O4	2.62	0.52
1:0:649:U:H2'	1:0:650:G:C8	2.45	0.52
1:0:974:A:H2	1:0:998:U:H3	1.58	0.52
1:0:1170:A:H5''	1:0:1171:A:OP1	2.09	0.52
1:0:1535:A:N3	35:0:3312:HOH:O	2.34	0.52
1:0:2407:A:H2'	1:0:2408:A:C8	2.44	0.52
1:0:2845:A:H2'	35:0:4442:HOH:O	2.10	0.52
17:R:25:ARG:O	17:R:29:GLU:HG3	2.10	0.52
24:Y:86:GLU:HB2	24:Y:170:THR:HG21	1.91	0.52
1:0:697:A:H2'	1:0:698:A:C8	2.45	0.52
1:0:1197:A:H8	1:0:1197:A:OP2	1.93	0.52
22:W:187:LYS:HD3	22:W:188:TYR:CZ	2.45	0.52
2:9:3:C:C3'	2:9:4:G:H5'	2.34	0.52
23:X:123:GLY:O	23:X:124:LEU:HD23	2.09	0.52
25:b:54:MET:HE3	25:b:54:MET:HA	1.92	0.52
1:0:2734:A:N6	35:0:3289:HOH:O	2.27	0.51
20:U:114:ASP:OD1	20:U:115:GLY:N	2.42	0.51
1:0:2439:C:H2'	1:0:2440:A:C8	2.45	0.51
7:H:19:SER:HB2	7:H:27:TRP:HB2	1.92	0.51
12:M:24:LYS:HB2	12:M:28:THR:HB	1.92	0.51
1:0:632:A:H5'	1:0:2064:C:H5	1.73	0.51
1:0:916:A:H62	1:0:1071:G:H21	1.58	0.51
1:0:1949:U:C4'	1:0:1950:A:N7	2.70	0.51
1:0:1010:C:H5''	5:F:19:ARG:HH12	1.76	0.51
1:0:1412:G:H1'	1:0:1681:C:H5'	1.91	0.51
23:X:137:VAL:HA	23:X:140:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:888:A:H1'	35:0:3439:HOH:O	2.10	0.51
2:9:18:U:H3	2:9:61:G:H1	1.59	0.51
1:0:954:G:N3	1:0:2295:A:H2'	2.26	0.51
1:0:1623:G:H1	1:0:1628:C:H42	1.59	0.51
23:X:165:THR:HG23	23:X:170:VAL:HG22	1.93	0.51
1:0:1490:C:H2'	1:0:1491:U:C6	2.45	0.51
25:b:142:ASN:OD1	25:b:142:ASN:N	2.41	0.51
1:0:1161:U:C2	1:0:1163:A:H5''	2.46	0.51
1:0:1750:G:H21	1:0:2024:C:H1'	1.74	0.51
1:0:1912:A:H3'	1:0:1913:C:H6	1.75	0.51
21:V:245:PRO:HD3	35:V:526:HOH:O	2.10	0.51
1:0:543:G:H2'	1:0:544:A:C8	2.46	0.51
11:L:57:SER:OG	11:L:72:ASP:OD1	2.28	0.51
22:W:130:ARG:HG3	22:W:169:ARG:HD3	1.93	0.51
1:0:672:G:O2'	35:0:3252:HOH:O	2.09	0.50
1:0:1195:U:H1'	1:0:1198:C:H5	1.75	0.50
1:0:1496:A:H2'	1:0:1497:A:C8	2.46	0.50
4:E:59:GLU:HA	4:E:62:MET:HE3	1.91	0.50
20:U:127:GLN:CB	35:U:417:HOH:O	2.45	0.50
21:V:57:ASP:O	21:V:323:ARG:NH1	2.44	0.50
24:Y:74:LEU:O	24:Y:78:THR:HG23	2.11	0.50
27:d:46:ARG:O	27:d:50:LEU:HD13	2.12	0.50
1:0:2243:G:H3'	1:0:2244:G:H8	1.76	0.50
27:d:21:LEU:O	27:d:25:GLU:HG3	2.10	0.50
27:d:32:LYS:HA	27:d:35:GLN:HG2	1.93	0.50
5:F:100:ASN:ND2	35:F:302:HOH:O	2.43	0.50
22:W:122:GLU:N	22:W:122:GLU:OE1	2.43	0.50
1:0:1168:A:C2'	1:0:1169:G:C8	2.94	0.50
1:0:1510:U:H2'	1:0:1511:U:C6	2.46	0.50
1:0:2685:G:H1'	1:0:2686:U:H5	1.76	0.50
9:J:105:ARG:NH2	9:J:139:GLU:OE2	2.42	0.50
26:c:80:ILE:HG13	26:c:82:VAL:HG23	1.92	0.50
29:f:22:ASP:OD1	29:f:22:ASP:N	2.43	0.50
1:0:68:G:N7	35:0:3315:HOH:O	2.35	0.50
1:0:248:A:C2	1:0:382:A:H4'	2.46	0.50
1:0:1195:U:H2'	1:0:1197:A:N7	2.27	0.50
1:0:1382:G:H21	9:J:29:GLN:HE22	1.60	0.50
1:0:2316:G:H5''	1:0:2414:G:H1'	1.94	0.50
1:0:2319:U:H2'	1:0:2320:U:C6	2.46	0.50
13:N:106:ASP:N	13:N:106:ASP:OD1	2.45	0.50
16:Q:106:GLU:H	16:Q:106:GLU:CD	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:47:VAL:HG12	17:R:48:GLU:HG3	1.94	0.50
21:V:142:ARG:HG2	21:V:166:ARG:HA	1.94	0.50
1:0:974:A:H61	1:0:997:C:H42	1.59	0.50
1:0:2108:U:H2'	1:0:2109:U:C6	2.46	0.50
22:W:120:ASP:HB3	22:W:123:LEU:HB2	1.93	0.50
30:a:271:LYS:O	30:a:274:VAL:HG22	2.12	0.50
1:0:500:A:H2'	1:0:502:A:C8	2.46	0.50
1:0:1902:A:H2'	1:0:1903:A:H8	1.75	0.50
1:0:2138:G:N1	1:0:2225:A:N6	2.59	0.50
1:0:2230:G:OP1	1:0:2230:G:C4'	2.59	0.50
19:T:4:PRO:HG2	19:T:7:PHE:HD2	1.76	0.50
24:Y:10:ASP:OD1	24:Y:11:GLU:N	2.31	0.50
27:d:5:TYR:CE1	27:d:8:GLU:HG3	2.47	0.50
27:d:11:ASP:OD1	27:d:11:ASP:N	2.43	0.50
1:0:1198:C:H3'	1:0:1199:A:C8	2.45	0.50
1:0:1944:G:H2'	1:0:1945:U:O4'	2.11	0.50
19:T:1:MET:HE1	19:T:84:TRP:HZ2	1.77	0.50
19:T:52:ARG:HA	19:T:55:LYS:HD3	1.94	0.50
27:d:17:ARG:NH1	27:d:66:ASP:OD2	2.45	0.50
1:0:1167:U:C2	1:0:1169:G:H3'	2.45	0.49
6:G:124:ASP:OD1	6:G:126:SER:N	2.33	0.49
16:Q:204:GLY:O	16:Q:208:ARG:HB2	2.12	0.49
1:0:979:G:N7	1:0:992:G:N2	2.60	0.49
1:0:1791:U:H3'	1:0:1792:A:C8	2.46	0.49
1:0:2081:C:O2'	35:0:3271:HOH:O	2.20	0.49
27:d:49:GLU:O	27:d:53:THR:HG22	2.12	0.49
35:0:3780:HOH:O	19:T:1:MET:CG	2.57	0.49
24:Y:85:MET:HE1	24:Y:149:ILE:HB	1.94	0.49
30:a:11:TYR:CE2	30:a:103:GLY:HA2	2.46	0.49
2:9:34:C:H2'	8:I:142:ARG:HH12	1.78	0.49
14:O:67:ARG:HH21	14:O:93:VAL:HB	1.77	0.49
19:T:45:SER:O	19:T:45:SER:OG	2.29	0.49
1:0:1084:C:H2'	1:0:1085:C:C6	2.47	0.49
1:0:1160:G:O6	1:0:1180:C:N3	2.45	0.49
1:0:1366:G:HO2'	1:0:1367:U:P	2.35	0.49
1:0:2612:U:H2'	1:0:2613:U:C6	2.48	0.49
24:Y:96:VAL:HG22	24:Y:105:ILE:HG12	1.93	0.49
1:0:299:G:C4	1:0:300:A:H1'	2.47	0.49
1:0:600:C:H2'	1:0:601:A:H8	1.77	0.49
6:G:72:GLY:O	6:G:74:ARG:NH1	2.42	0.49
6:G:100:ARG:HD3	6:G:168:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:123:LEU:HD21	9:J:146:TYR:CE2	2.48	0.49
11:L:124:PRO:HA	11:L:138:ASN:OD1	2.11	0.49
16:Q:90:GLU:OE1	16:Q:90:GLU:N	2.46	0.49
16:Q:224:ASN:OD1	16:Q:224:ASN:N	2.46	0.49
20:U:134:GLU:N	20:U:134:GLU:OE1	2.45	0.49
30:a:90:SER:OG	30:a:92:VAL:O	2.30	0.49
1:0:1520:A:H4'	1:0:1521:A:OP1	2.12	0.49
1:0:1908:C:H2'	1:0:1909:A:C8	2.48	0.49
24:Y:36:TYR:CG	24:Y:62:THR:HG21	2.48	0.49
24:Y:117:ALA:HB2	24:Y:152:LEU:HD22	1.94	0.49
1:0:1557:C:H3'	1:0:1558:G:C8	2.48	0.49
1:0:1914:A:H3'	1:0:1915:A:C8	2.47	0.49
12:M:4:LYS:HB3	12:M:14:ILE:O	2.13	0.49
17:R:49:THR:HG23	17:R:65:THR:HG23	1.94	0.49
1:0:445:U:H1'	1:0:446:C:H5	1.77	0.49
1:0:1908:C:H2'	1:0:1909:A:H8	1.78	0.49
1:0:2499:A:N6	1:0:2504:A:O2'	2.46	0.49
1:0:707:G:C2'	1:0:708:C:H5'	2.42	0.49
4:E:48:LEU:HB3	4:E:99:ILE:HD12	1.94	0.49
13:N:29:SER:OG	13:N:30:ALA:N	2.46	0.49
22:W:129:HIS:ND1	22:W:166:ASP:OD2	2.46	0.49
1:0:637:C:H5''	1:0:2530:G:H2'	1.94	0.48
1:0:808:A:H3'	1:0:809:A:H8	1.77	0.48
1:0:1167:U:N3	1:0:1169:G:O5'	2.46	0.48
1:0:675:A:H2	1:0:679:C:H41	1.61	0.48
1:0:1353:A:H2'	35:0:3354:HOH:O	2.12	0.48
1:0:1694:G:C5'	35:0:3554:HOH:O	2.34	0.48
22:W:193:SER:OG	22:W:194:ILE:N	2.46	0.48
1:0:1129:A:H61	1:0:1226:G:H2'	1.78	0.48
1:0:1165:C:H3'	1:0:1166:U:C6	2.48	0.48
1:0:1520:A:HO2'	1:0:1521:A:H2'	1.78	0.48
12:M:50:LEU:O	12:M:56:GLY:HA3	2.13	0.48
19:T:3:MET:HE2	19:T:89:LEU:HD11	1.94	0.48
19:T:23:GLU:OE2	19:T:26:ARG:NH2	2.46	0.48
30:a:234:ARG:HG2	30:a:252:ILE:HG12	1.94	0.48
1:0:983:C:H2'	1:0:984:C:C2	2.47	0.48
1:0:1108:A:H1'	1:0:1254:C:H1'	1.95	0.48
1:0:1534:U:H2'	1:0:1535:A:C8	2.48	0.48
1:0:1587:G:H2'	1:0:1588:C:C6	2.49	0.48
2:9:103:A:H2'	2:9:104:A:C8	2.46	0.48
8:I:172:HIS:HA	8:I:175:GLU:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1796:C:H2'	1:0:1797:A:C8	2.48	0.48
9:J:131:GLU:OE2	9:J:131:GLU:N	2.47	0.48
15:P:40:LYS:HG2	15:P:41:HIS:CD2	2.49	0.48
15:P:79:ASP:OD1	15:P:84:SER:HB3	2.14	0.48
1:0:297:U:C2	1:0:362:A:N1	2.78	0.48
1:0:320:G:H2'	1:0:321:A:C8	2.49	0.48
1:0:1193:C:H3'	1:0:1194:G:H8	1.78	0.48
1:0:2140:U:H4'	1:0:2222:G:N1	2.26	0.48
1:0:2683:U:H2'	1:0:2696:A:N6	2.28	0.48
20:U:62:GLU:CD	20:U:62:GLU:H	2.21	0.48
30:a:271:LYS:O	30:a:272:THR:C	2.57	0.48
1:0:682:C:H5	35:0:4443:HOH:O	1.95	0.48
23:X:32:LYS:HA	23:X:35:ASP:OD2	2.13	0.48
1:0:1128:G:N2	1:0:2515:G:O2'	2.46	0.48
1:0:1426:G:H1'	1:0:1686:A:N6	2.29	0.48
1:0:1961:A:H2'	1:0:1962:A:C8	2.48	0.48
4:E:26:ASP:OD1	4:E:26:ASP:N	2.46	0.48
26:c:72:ASP:O	26:c:76:VAL:HG23	2.13	0.48
27:d:9:ILE:HG23	27:d:57:ILE:HD12	1.95	0.48
1:0:946:G:C4	14:O:23:MET:HE1	2.49	0.48
1:0:994:U:H2'	1:0:995:C:C6	2.48	0.48
1:0:2131:C:H2'	1:0:2132:G:C8	2.48	0.48
24:Y:159:ASP:OD2	24:Y:162:VAL:HG12	2.14	0.48
1:0:985:G:H2'	1:0:986:A:N9	2.29	0.48
23:X:71:LEU:HD12	23:X:76:ALA:HA	1.96	0.48
1:0:429:U:H2'	1:0:430:G:C8	2.48	0.47
1:0:2300:A:H2'	1:0:2301:U:C6	2.49	0.47
22:W:114:ALA:O	22:W:118:THR:HG23	2.13	0.47
1:0:2040:C:H5'	35:0:3603:HOH:O	2.12	0.47
12:M:54:GLU:OE1	12:M:54:GLU:HA	2.14	0.47
23:X:5:GLU:HG2	23:X:6:PHE:O	2.15	0.47
1:0:1079:G:H2'	1:0:1080:A:C8	2.49	0.47
1:0:1239:A:OP2	25:b:60:ARG:NH2	2.47	0.47
1:0:2083:A:H2'	1:0:2084:G:C8	2.49	0.47
1:0:247:C:O2	1:0:247:C:C2'	2.62	0.47
1:0:1249:A:H4'	28:e:47:ARG:HE	1.80	0.47
1:0:2016:G:N7	35:0:3319:HOH:O	2.35	0.47
20:U:208:HIS:HB3	35:U:419:HOH:O	2.14	0.47
27:d:54:ILE:O	27:d:57:ILE:HG22	2.15	0.47
1:0:980:C:N4	1:0:992:G:N3	2.62	0.47
1:0:1503:C:H2'	1:0:1504:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1517:A:H1'	1:0:1518:A:H5'	1.96	0.47
2:9:49:G:H2'	2:9:50:A:C8	2.48	0.47
14:O:68:THR:HG22	14:O:69:ARG:HD2	1.96	0.47
19:T:11:CYS:HB2	19:T:20:HIS:CE1	2.50	0.47
1:0:11:G:H1'	1:0:12:G:H5'	1.95	0.47
1:0:1447:C:OP2	1:0:1447:C:H3'	2.14	0.47
2:9:39:C:H5'	2:9:40:C:H5'	1.95	0.47
2:9:116:G:H2'	2:9:117:C:H6	1.80	0.47
5:F:30:LYS:HG3	5:F:62:HIS:ND1	2.29	0.47
18:S:45:LYS:NZ	35:S:201:HOH:O	2.44	0.47
21:V:15:SER:CB	35:V:503:HOH:O	2.53	0.47
23:X:55:GLN:CG	23:X:56:ASP:H	2.28	0.47
1:0:869:A:C2	1:0:882:C:O2'	2.64	0.47
1:0:972:G:H2'	1:0:973:A:C8	2.50	0.47
1:0:1889:G:O5'	1:0:1889:G:H8	1.97	0.47
1:0:2223:U:O2'	1:0:2225:A:N6	2.48	0.47
20:U:30:HIS:NE2	20:U:107:ASN:OD1	2.48	0.47
1:0:576:U:H2'	1:0:577:A:C8	2.50	0.47
16:Q:106:GLU:OE1	16:Q:106:GLU:N	2.30	0.47
16:Q:207:LYS:HB2	16:Q:207:LYS:HE3	1.71	0.47
1:0:97:A:H3'	1:0:98:G:H8	1.80	0.47
1:0:1170:A:H5'	1:0:1171:A:H8	1.78	0.47
7:H:59:VAL:HG22	7:H:77:VAL:HA	1.97	0.47
15:P:70:LYS:HB3	15:P:70:LYS:HE3	1.73	0.47
20:U:84:VAL:HG23	20:U:98:GLU:HG3	1.97	0.47
29:f:5:LYS:NZ	29:f:119:GLU:OE1	2.31	0.47
1:0:360:G:H4'	1:0:361:G:OP1	2.14	0.47
1:0:1206:C:H2'	1:0:1207:G:C8	2.50	0.47
1:0:1600:G:H2'	35:0:3440:HOH:O	2.15	0.47
10:K:49:ARG:HG3	35:K:109:HOH:O	2.14	0.47
14:O:71:GLU:OE2	35:O:302:HOH:O	2.20	0.47
17:R:36:ASN:O	17:R:36:ASN:ND2	2.44	0.47
1:0:2641:U:C4	35:0:3349:HOH:O	2.56	0.46
25:b:76:ASP:OD1	25:b:77:ARG:N	2.48	0.46
1:0:2489:C:H2'	1:0:2490:A:C8	2.49	0.46
2:9:12:G:OP2	10:K:20:ARG:NH2	2.48	0.46
5:F:62:HIS:H	5:F:62:HIS:CD2	2.32	0.46
27:d:19:ALA:O	27:d:22:GLU:HG2	2.15	0.46
1:0:1496:A:H5''	9:J:10:MET:SD	2.55	0.46
1:0:1557:C:H3'	1:0:1558:G:H8	1.80	0.46
1:0:1951:U:H2'	1:0:1952:G:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:34:ARG:CD	35:L:310:HOH:O	2.25	0.46
20:U:52:ARG:NH1	20:U:120:ARG:O	2.48	0.46
23:X:80:LEU:O	23:X:84:LEU:HD12	2.15	0.46
1:0:1163:A:H2'	1:0:1164:G:C8	2.51	0.46
1:0:1165:C:H3'	1:0:1166:U:H6	1.79	0.46
1:0:2471:U:H2'	1:0:2472:A:C8	2.51	0.46
5:F:49:GLU:HB3	5:F:169:ARG:HB3	1.97	0.46
7:H:70:VAL:HG23	35:H:204:HOH:O	2.14	0.46
17:R:72:ALA:O	17:R:76:VAL:HG23	2.15	0.46
21:V:32:ASP:N	21:V:32:ASP:OD1	2.45	0.46
28:e:6:ILE:HD12	28:e:35:ALA:HB2	1.97	0.46
1:0:808:A:H3'	1:0:809:A:C8	2.51	0.46
1:0:917:C:H2'	1:0:918:A:H8	1.81	0.46
1:0:1544:C:H2'	1:0:1545:G:C8	2.50	0.46
5:F:55:GLU:C	5:F:131:LYS:HG3	2.40	0.46
10:K:24:THR:OG1	35:K:101:HOH:O	1.86	0.46
15:P:23:SER:HA	15:P:26:ARG:HG3	1.98	0.46
30:a:78:VAL:O	30:a:80:LYS:N	2.45	0.46
1:0:2135:G:N2	1:0:2226:C:O2	2.48	0.46
8:I:83:TYR:OH	8:I:125:ASP:OD2	2.25	0.46
26:c:67:LEU:HD23	26:c:68:SER:N	2.31	0.46
30:a:128:THR:C	30:a:130:GLY:N	2.74	0.46
1:0:1459:U:H2'	1:0:1460:A:C8	2.51	0.46
24:Y:84:GLN:HB2	24:Y:171:GLN:HB3	1.98	0.46
30:a:131:LEU:HB2	30:a:266:SER:O	2.16	0.46
1:0:975:U:H2'	1:0:976:C:C6	2.51	0.46
1:0:1173:C:H2'	1:0:1194:G:O6	2.15	0.46
1:0:1933:C:H5'	20:U:233:THR:HG23	1.98	0.46
8:I:80:PRO:HB3	8:I:173:PHE:HD2	1.81	0.46
30:a:11:TYR:CD2	30:a:104:VAL:HG13	2.50	0.46
30:a:114:VAL:HA	30:a:117:PHE:CD2	2.51	0.46
1:0:530:U:H2'	1:0:531:U:C6	2.50	0.46
1:0:638:G:H2'	1:0:639:A:C8	2.51	0.46
1:0:1178:A:H2	1:0:1189:A:H8	1.64	0.46
1:0:1235:C:C5	1:0:1237:G:P	3.08	0.46
1:0:1648:G:N7	20:U:174:LYS:NZ	2.60	0.46
1:0:2366:A:H1'	35:0:3514:HOH:O	2.14	0.46
14:O:142:ASP:OD1	14:O:145:GLN:HG3	2.15	0.46
18:S:5:GLY:O	18:S:9:GLN:HG2	2.16	0.46
25:b:91:LYS:O	25:b:95:ARG:HG3	2.16	0.46
29:f:115:ARG:N	29:f:132:VAL:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1936:C:H4'	20:U:212:PRO:HA	1.98	0.46
30:a:49:ARG:HG3	30:a:49:ARG:HH11	1.79	0.46
30:a:123:VAL:O	30:a:125:ASP:N	2.49	0.46
1:0:991:A:H2'	1:0:992:G:O4'	2.16	0.45
1:0:1154:C:H2'	1:0:1155:G:C8	2.51	0.45
5:F:58:VAL:HG21	5:F:161:PRO:HD3	1.98	0.45
5:F:70:LEU:HD12	5:F:70:LEU:HA	1.76	0.45
20:U:238:LYS:HA	20:U:238:LYS:HD2	1.33	0.45
30:a:50:GLN:HE21	30:a:67:TRP:HB2	1.80	0.45
1:0:303:U:H2'	1:0:304:C:O4'	2.16	0.45
1:0:738:A:C2	1:0:2399:U:H1'	2.51	0.45
1:0:836:G:H5''	1:0:837:U:O5'	2.16	0.45
1:0:1171:A:H5''	1:0:1173:C:OP2	2.16	0.45
1:0:1183:C:H3'	1:0:1184:U:C6	2.51	0.45
1:0:1796:C:H2'	1:0:1797:A:H8	1.81	0.45
1:0:2141:A:H2'	1:0:2142:A:C8	2.51	0.45
1:0:2728:U:H2'	1:0:2729:C:C6	2.51	0.45
4:E:59:GLU:HG3	4:E:62:MET:HE3	1.99	0.45
16:Q:183:ASN:HA	16:Q:211:ILE:HD11	1.99	0.45
23:X:39:GLU:OE1	23:X:113:GLN:NE2	2.42	0.45
30:a:72:LEU:HD21	30:a:81:VAL:HG23	1.98	0.45
1:0:229:A:C5	1:0:230:G:H1'	2.50	0.45
1:0:668:U:O4	1:0:685:G:C5'	2.62	0.45
1:0:1475:U:H2'	1:0:1476:A:C8	2.52	0.45
15:P:31:MET:HE1	15:P:55:ILE:HG22	1.97	0.45
20:U:31:LYS:O	20:U:153:ARG:NH2	2.45	0.45
1:0:15:A:H3'	1:0:16:C:C6	2.51	0.45
1:0:169:U:H1'	1:0:895:C:H41	1.81	0.45
1:0:1509:C:H2'	1:0:1510:U:C6	2.52	0.45
2:9:4:G:H8	2:9:4:G:OP2	1.99	0.45
2:9:59:U:H2'	2:9:60:C:C6	2.51	0.45
11:L:21:ASP:HA	11:L:141:ILE:HG23	1.98	0.45
1:0:694:G:H1'	1:0:733:U:H1'	1.99	0.45
1:0:1117:U:H2'	1:0:1118:A:H8	1.82	0.45
2:9:47:C:OP1	8:I:115:LYS:HG3	2.15	0.45
12:M:34:ASN:HA	35:M:104:HOH:O	2.17	0.45
1:0:468:G:H1'	1:0:469:U:H5	1.81	0.45
1:0:1367:U:H2'	1:0:1368:A:H8	1.81	0.45
1:0:1932:U:HO2'	20:U:233:THR:H	1.64	0.45
1:0:2138:G:C6	1:0:2225:A:N6	2.85	0.45
1:0:2289:C:P	10:K:6:GLY:HA3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:80:PRO:HB3	8:I:173:PHE:CD2	2.52	0.45
16:Q:94:ARG:HD3	16:Q:212:GLU:OE1	2.17	0.45
16:Q:159:GLU:HG3	16:Q:160:ALA:N	2.32	0.45
20:U:93:THR:HA	20:U:154:ALA:O	2.17	0.45
1:0:583:G:H2'	1:0:584:A:C8	2.51	0.45
1:0:997:C:H2'	1:0:998:U:C6	2.51	0.45
1:0:1193:C:H2'	1:0:1194:G:O4'	2.17	0.45
1:0:1236:G:H1'	1:0:2072:G:H4'	1.98	0.45
1:0:1884:G:H1'	1:0:1965:U:H1'	1.99	0.45
15:P:54:GLN:HB3	15:P:90:PRO:HG3	1.98	0.45
1:0:475:G:H2'	1:0:476:A:C8	2.51	0.45
1:0:2710:C:H5'	21:V:303:PRO:HA	1.99	0.45
7:H:12:ILE:O	7:H:16:LYS:HG3	2.17	0.45
8:I:146:VAL:O	8:I:150:GLU:HG2	2.17	0.45
22:W:79:ARG:HG2	22:W:79:ARG:O	2.17	0.45
26:c:22:LYS:HG2	26:c:66:ARG:HA	1.97	0.45
30:a:131:LEU:HD12	30:a:131:LEU:HA	1.82	0.45
1:0:1084:C:H2'	1:0:1085:C:H6	1.82	0.45
1:0:1652:A:H2'	1:0:1653:A:C8	2.51	0.45
12:M:26:ASP:OD1	12:M:26:ASP:N	2.47	0.45
30:a:238:PRO:HG3	30:a:261:VAL:HG12	1.99	0.45
1:0:1138:U:H2'	1:0:1139:C:C6	2.52	0.45
1:0:1950:A:OP1	1:0:1950:A:O4'	2.35	0.45
23:X:17:VAL:HG13	23:X:128:VAL:HG12	1.98	0.45
30:a:190:GLY:O	30:a:191:THR:C	2.59	0.45
1:0:89:C:H2'	1:0:90:C:C6	2.52	0.44
1:0:302:U:H2'	1:0:303:U:C6	2.51	0.44
1:0:1366:G:O2'	1:0:1367:U:OP2	2.35	0.44
1:0:2372:G:H1'	1:0:2412:U:H5'	1.98	0.44
30:a:120:ALA:O	30:a:121:ALA:C	2.60	0.44
1:0:1008:A:N1	1:0:2304:A:H1'	2.32	0.44
1:0:1008:A:H2'	1:0:1009:A:C8	2.51	0.44
1:0:1610:A:H2'	1:0:1611:A:C8	2.52	0.44
6:G:124:ASP:OD1	6:G:124:ASP:C	2.60	0.44
21:V:53:MET:HE3	21:V:53:MET:HB3	1.78	0.44
1:0:1114:G:N2	28:e:41:SER:HB2	2.32	0.44
1:0:2355:A:H2'	1:0:2356:G:C8	2.53	0.44
1:0:2872:A:H2'	1:0:2873:A:C8	2.52	0.44
8:I:79:LEU:HD22	8:I:142:ARG:HG2	1.99	0.44
30:a:119:ASP:HA	30:a:243:GLU:HB3	1.99	0.44
1:0:1170:A:H4'	1:0:1171:A:H5''	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2665:U:H1'	1:0:2811:G:N2	2.32	0.44
1:0:2811:G:N3	21:V:97:PRO:HG2	2.32	0.44
30:a:235:THR:HA	30:a:258:VAL:O	2.16	0.44
1:0:287:A:N3	1:0:372:G:C8	2.75	0.44
1:0:310:A:H2'	1:0:311:A:C8	2.52	0.44
1:0:844:C:N4	35:0:3278:HOH:O	2.24	0.44
1:0:991:A:H3'	1:0:992:G:H8	1.81	0.44
1:0:1048:U:H2'	1:0:1049:G:C8	2.52	0.44
1:0:1261:U:H2'	1:0:1262:G:C8	2.52	0.44
1:0:1516:C:H2'	1:0:1517:A:C8	2.53	0.44
23:X:46:VAL:HG22	23:X:68:LYS:O	2.17	0.44
1:0:941:A:N6	1:0:1032:G:H1'	2.33	0.44
8:I:80:PRO:O	8:I:84:LEU:HD22	2.18	0.44
9:J:106:LEU:HA	9:J:106:LEU:HD23	1.74	0.44
16:Q:133:THR:O	35:Q:404:HOH:O	2.21	0.44
29:f:84:ASP:OD1	29:f:86:THR:HG23	2.18	0.44
30:a:143:ALA:C	30:a:145:HIS:H	2.25	0.44
1:0:95:G:C2	3:A:25:TRP:HB2	2.52	0.44
1:0:694:G:H5''	1:0:743:C:O2'	2.18	0.44
1:0:792:A:H2'	1:0:793:G:O4'	2.17	0.44
1:0:1193:C:H3'	1:0:1194:G:C8	2.53	0.44
1:0:1739:G:H4'	35:0:3318:HOH:O	2.17	0.44
1:0:2335:G:OP1	1:0:2335:G:O4'	2.35	0.44
2:9:76:A:H8	2:9:76:A:OP1	2.00	0.44
13:N:30:ALA:O	13:N:34:GLU:HG2	2.17	0.44
23:X:55:GLN:C	23:X:57:PHE:H	2.25	0.44
1:0:943:A:H4'	1:0:1034:C:H4'	1.99	0.44
1:0:1197:A:C8	1:0:1197:A:OP2	2.71	0.44
1:0:1261:U:H2'	1:0:1262:G:H8	1.82	0.44
1:0:2333:C:H5'	23:X:22:GLY:O	2.18	0.44
1:0:2630:A:H5''	30:a:182:GLN:HG2	1.99	0.44
1:0:2707:G:H4'	21:V:11:SER:HB2	2.00	0.44
1:0:2762:C:H2'	1:0:2763:A:O4'	2.18	0.44
1:0:2871:C:H2'	1:0:2872:A:O4'	2.18	0.44
5:F:104:THR:OG1	30:a:226:ARG:NH1	2.50	0.44
22:W:136:GLU:H	22:W:136:GLU:CD	2.24	0.44
23:X:105:GLU:OE1	23:X:105:GLU:N	2.51	0.44
26:c:18:ASP:OD1	26:c:18:ASP:C	2.61	0.44
1:0:761:C:H2'	1:0:763:A:H62	1.81	0.44
2:9:95:C:H2'	2:9:96:U:H6	1.82	0.44
14:O:122:ARG:NH1	14:O:152:ALA:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:562:U:H2'	1:0:563:C:C6	2.52	0.43
1:0:733:U:H2'	1:0:734:C:C6	2.53	0.43
1:0:809:A:H2'	1:0:810:A:C8	2.53	0.43
1:0:2835:G:C2'	1:0:2836:A:H5'	2.48	0.43
6:G:124:ASP:OD1	6:G:125:GLY:N	2.51	0.43
9:J:90:ASN:ND2	9:J:93:ASP:OD2	2.48	0.43
27:d:42:GLU:CD	27:d:42:GLU:H	2.26	0.43
30:a:91:LYS:HA	30:a:91:LYS:HD3	1.39	0.43
1:0:1187:G:O2'	1:0:1188:A:N7	2.51	0.43
1:0:1950:A:H2'	1:0:1951:U:O4'	2.18	0.43
1:0:2747:G:OP1	12:M:39:LYS:HD2	2.18	0.43
1:0:1366:G:O2'	1:0:1367:U:P	2.77	0.43
20:U:186:TRP:CG	20:U:187:PRO:HA	2.53	0.43
25:b:109:TYR:HB3	25:b:111:GLU:OE1	2.18	0.43
26:c:44:TYR:HE2	26:c:80:ILE:HD13	1.83	0.43
1:0:934:U:H1'	1:0:1292:G:H1'	2.00	0.43
1:0:2604:G:N3	1:0:2604:G:C2'	2.80	0.43
1:0:2731:G:H2'	1:0:2732:A:H8	1.84	0.43
10:K:8:MET:O	10:K:11:THR:OG1	2.31	0.43
16:Q:172:HIS:CD2	16:Q:223:LEU:HD13	2.53	0.43
21:V:15:SER:HB3	35:V:503:HOH:O	2.17	0.43
21:V:84:ALA:HB3	21:V:144:ILE:HB	2.00	0.43
1:0:18:G:H3'	1:0:19:U:H6	1.83	0.43
1:0:224:C:H4'	1:0:398:G:H5'	2.00	0.43
1:0:1167:U:C2	1:0:1169:G:O5'	2.71	0.43
1:0:1578:U:H2'	1:0:1579:U:C6	2.54	0.43
15:P:52:ASP:OD1	15:P:53:PRO:HD2	2.18	0.43
29:f:84:ASP:OD1	29:f:84:ASP:C	2.61	0.43
30:a:191:THR:OG1	30:a:192:ASP:N	2.52	0.43
1:0:28:G:H4'	11:L:3:ILE:HG22	2.00	0.43
1:0:340:U:O3'	13:N:93:GLN:NE2	2.52	0.43
1:0:1432:C:H2'	1:0:1433:A:C8	2.54	0.43
1:0:1441:G:H21	1:0:1673:A:H1'	1.83	0.43
1:0:2441:U:H2'	1:0:2442:G:C8	2.53	0.43
1:0:2453:A:C6	31:0:3001:BGC:H1	2.54	0.43
14:O:130:HIS:ND1	14:O:134:GLU:OE2	2.52	0.43
20:U:36:LYS:HZ3	20:U:38:THR:H	1.67	0.43
21:V:198:GLY:N	21:V:270:LEU:O	2.45	0.43
30:a:11:TYR:HB3	30:a:104:VAL:HG11	1.99	0.43
1:0:370:C:H2'	1:0:371:G:C4	2.52	0.43
1:0:1192:G:H2'	1:0:1193:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1454:A:H2'	1:0:1455:A:C8	2.54	0.43
1:0:2749:C:H2'	1:0:2750:A:C8	2.54	0.43
2:9:120:C:H2'	2:9:121:U:O4'	2.19	0.43
9:J:113:GLY:C	9:J:115:LEU:H	2.26	0.43
30:a:72:LEU:HB2	30:a:94:PRO:O	2.18	0.43
1:0:15:A:N3	1:0:15:A:H2'	2.32	0.43
1:0:721:C:O2'	7:H:113:ARG:NH2	2.52	0.43
1:0:1183:C:H3'	1:0:1184:U:H6	1.84	0.43
1:0:1242:C:H5''	1:0:1243:A:H2	1.83	0.43
1:0:1275:U:O3'	1:0:1276:U:H2'	2.19	0.43
1:0:2891:G:H4'	21:V:289:GLY:HA2	2.01	0.43
14:O:58:SER:O	14:O:62:VAL:HG23	2.18	0.43
15:P:92:GLU:H	15:P:92:GLU:CD	2.26	0.43
16:Q:95:GLY:HA2	16:Q:216:GLU:HG2	2.00	0.43
19:T:14:CYS:HB3	19:T:75:CYS:HB3	2.01	0.43
9:J:143:GLN:HB3	9:J:150:ILE:HB	1.99	0.43
11:L:96:VAL:HG12	11:L:148:ILE:HD13	2.01	0.43
13:N:52:LEU:HD11	13:N:98:ARG:HB2	2.00	0.43
20:U:179:MET:SD	20:U:184:ILE:HG21	2.59	0.43
30:a:134:VAL:HG13	30:a:155:LEU:HD22	2.00	0.43
1:0:593:U:H2'	1:0:594:A:H8	1.83	0.43
1:0:2230:G:H3'	1:0:2231:A:H8	1.83	0.43
9:J:24:PHE:CD1	9:J:50:ILE:HG12	2.54	0.43
10:K:15:LEU:HD23	10:K:15:LEU:HA	1.74	0.43
1:0:364:A:H1'	1:0:365:G:C4	2.54	0.42
1:0:567:C:H5	35:0:3517:HOH:O	2.01	0.42
1:0:650:G:H2'	1:0:651:C:C6	2.54	0.42
1:0:669:A:H2'	1:0:670:A:C8	2.54	0.42
1:0:934:U:H2'	1:0:935:C:H6	1.84	0.42
1:0:1449:A:H3'	1:0:1450:U:H6	1.84	0.42
8:I:115:LYS:O	8:I:119:VAL:HG23	2.18	0.42
18:S:30:VAL:O	18:S:33:LYS:NZ	2.36	0.42
28:e:2:SER:HB2	28:e:4:PHE:CE2	2.54	0.42
1:0:527:C:H2'	1:0:528:A:H8	1.84	0.42
21:V:163:MET:HE2	21:V:163:MET:HB3	1.87	0.42
22:W:29:ASP:OD1	22:W:29:ASP:N	2.52	0.42
23:X:21:MET:HE2	23:X:37:LEU:CD2	2.49	0.42
23:X:21:MET:HE2	23:X:37:LEU:HD21	2.00	0.42
23:X:156:GLU:HB2	23:X:160:ALA:HB3	2.01	0.42
1:0:462:G:H2'	1:0:463:A:C8	2.54	0.42
1:0:649:U:H2'	1:0:650:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:863:U:H1'	1:0:1483:A:N6	2.35	0.42
1:0:1129:A:H2'	1:0:1130:A:C8	2.54	0.42
1:0:1436:C:H2'	1:0:1437:G:C8	2.54	0.42
1:0:1539:A:H3'	1:0:1540:A:H8	1.85	0.42
1:0:1647:C:N4	20:U:167:LYS:O	2.53	0.42
9:J:111:GLU:C	9:J:111:GLU:CD	2.87	0.42
1:0:23:A:C6	1:0:532:G:C6	3.07	0.42
1:0:319:G:N2	1:0:321:A:H3'	2.33	0.42
1:0:542:C:H5''	1:0:543:G:C8	2.54	0.42
1:0:1242:C:H5''	1:0:1243:A:C2	2.54	0.42
1:0:1701:G:H1'	1:0:1705:A:N6	2.35	0.42
1:0:2232:C:H2'	1:0:2233:U:C6	2.54	0.42
1:0:2451:A:H2'	1:0:2452:G:C8	2.54	0.42
7:H:5:ASN:O	7:H:9:LYS:HG3	2.18	0.42
8:I:39:VAL:HG12	8:I:44:VAL:HG22	2.01	0.42
10:K:27:PRO:O	10:K:31:ILE:HG23	2.20	0.42
12:M:33:LYS:HB3	12:M:34:ASN:OD1	2.18	0.42
20:U:89:LYS:HG2	20:U:92:ASN:OD1	2.20	0.42
30:a:119:ASP:HB3	30:a:120:ALA:H	1.61	0.42
1:0:168:A:H2'	1:0:169:U:C6	2.54	0.42
1:0:1036:C:H2'	1:0:1037:A:C8	2.55	0.42
1:0:1596:G:H2'	1:0:1597:C:C6	2.55	0.42
1:0:2070:C:H2'	1:0:2071:U:C6	2.54	0.42
1:0:2492:C:C2	1:0:2515:G:C2	3.08	0.42
12:M:12:GLU:OE1	12:M:12:GLU:C	2.62	0.42
14:O:3:ALA:O	14:O:54:HIS:HA	2.19	0.42
19:T:9:THR:HB	19:T:81:ARG:HH22	1.83	0.42
21:V:77:THR:HG21	21:V:191:MET:SD	2.59	0.42
21:V:180:LEU:HD23	21:V:180:LEU:HA	1.91	0.42
23:X:38:GLU:OE2	23:X:44:GLU:HA	2.20	0.42
29:f:101:MET:HE3	29:f:101:MET:HB3	1.92	0.42
30:a:249:MET:HG3	30:a:257:LEU:HD11	2.00	0.42
1:0:1738:G:OP1	29:f:77:ARG:NH1	2.53	0.42
6:G:135:VAL:HG11	6:G:151:ILE:HD13	2.02	0.42
9:J:150:ILE:HD13	9:J:150:ILE:HA	1.83	0.42
11:L:77:ASP:OD1	11:L:78:ALA:N	2.51	0.42
12:M:43:LEU:HD12	12:M:43:LEU:HA	1.82	0.42
13:N:14:ASP:HB2	35:N:307:HOH:O	2.18	0.42
24:Y:95:GLN:HA	24:Y:95:GLN:OE1	2.19	0.42
1:0:298:G:N2	1:0:362:A:H5'	2.35	0.42
1:0:369:C:H4'	1:0:370:C:OP1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:698:A:O5'	1:0:698:A:C8	2.69	0.42
1:0:728:C:H2'	1:0:728:C:O2	2.18	0.42
1:0:863:U:H2'	1:0:864:G:H8	1.85	0.42
1:0:1400:C:OP2	35:0:3273:HOH:O	2.22	0.42
1:0:1843:U:H5''	20:U:235:ARG:HH22	1.85	0.42
1:0:2234:C:H2'	1:0:2235:U:C6	2.54	0.42
5:F:82:GLU:HG3	5:F:83:LYS:HG2	2.01	0.42
9:J:44:LEU:HD23	9:J:44:LEU:HA	1.85	0.42
16:Q:121:GLN:CB	35:Q:426:HOH:O	2.68	0.42
18:S:14:LYS:H	18:S:14:LYS:HG2	1.65	0.42
22:W:63:SER:HG	22:W:69:HIS:CE1	2.38	0.42
22:W:248:ARG:NH1	35:W:303:HOH:O	2.48	0.42
30:a:169:LEU:HA	30:a:172:VAL:HG12	2.02	0.42
1:0:675:A:H3'	1:0:677:A:H62	1.84	0.42
6:G:153:ASN:OD1	6:G:153:ASN:C	2.62	0.42
17:R:81:ARG:O	17:R:85:THR:HG22	2.19	0.42
20:U:5:ILE:HG12	20:U:8:GLN:HG3	2.02	0.42
24:Y:78:THR:OG1	24:Y:79:GLU:N	2.53	0.42
29:f:68:VAL:C	29:f:69:LEU:HD22	2.44	0.42
1:0:828:U:H2'	1:0:829:A:O4'	2.20	0.42
1:0:2090:G:P	35:0:3232:HOH:O	2.71	0.42
35:0:3533:HOH:O	9:J:21:ARG:CG	2.68	0.42
2:9:58:C:H2'	2:9:59:U:C6	2.54	0.42
16:Q:111:LEU:HD11	16:Q:175:GLY:HA2	2.02	0.42
24:Y:22:THR:C	24:Y:23:ILE:HD13	2.45	0.42
27:d:23:GLU:O	27:d:26:THR:HB	2.19	0.42
1:0:498:G:O2'	35:0:3240:HOH:O	2.02	0.42
1:0:978:G:C8	1:0:978:G:O5'	2.71	0.42
1:0:1312:G:H1'	1:0:1336:G:H22	1.84	0.42
1:0:2685:G:O2'	1:0:2686:U:OP2	2.29	0.42
8:I:159:LEU:HD23	8:I:159:LEU:HA	1.76	0.42
12:M:34:ASN:OD1	12:M:34:ASN:N	2.51	0.42
14:O:1:MET:SD	14:O:34:PHE:HB3	2.60	0.42
20:U:125:SER:HB3	20:U:158:VAL:HG22	2.01	0.42
30:a:246:VAL:HA	30:a:249:MET:HE3	2.02	0.42
1:0:513:A:H4'	1:0:515:A:H5'	2.01	0.41
1:0:691:U:H5'	35:0:4149:HOH:O	2.20	0.41
1:0:1940:G:C2'	1:0:1941:G:H8	2.24	0.41
2:9:48:G:H5'	8:I:148:ILE:HD11	2.01	0.41
5:F:57:ASP:OD1	5:F:131:LYS:N	2.52	0.41
19:T:40:GLN:HG2	19:T:53:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:127:GLN:HG2	35:U:417:HOH:O	2.19	0.41
22:W:2:GLN:N	22:W:2:GLN:OE1	2.53	0.41
22:W:35:VAL:HG13	22:W:223:GLU:HG3	2.01	0.41
26:c:33:LYS:HE3	26:c:33:LYS:HB2	1.81	0.41
30:a:185:GLY:HA2	30:a:211:GLY:HA3	2.02	0.41
1:0:11:G:O2'	1:0:12:G:H8	2.03	0.41
1:0:302:U:H2'	1:0:302:U:O2	2.19	0.41
1:0:798:A:N6	1:0:819:G:H1'	2.35	0.41
1:0:1534:U:O2'	1:0:1535:A:H5'	2.20	0.41
1:0:1855:C:OP1	20:U:8:GLN:NE2	2.52	0.41
1:0:2259:A:H2'	1:0:2260:G:C8	2.55	0.41
9:J:123:LEU:HD13	9:J:142:ILE:HD11	2.01	0.41
22:W:54:LEU:HD21	22:W:87:ARG:HD3	2.02	0.41
1:0:2467:A:N6	30:a:183:SER:O	2.53	0.41
1:0:2471:U:H2'	1:0:2472:A:H8	1.85	0.41
20:U:34:GLU:OE1	20:U:34:GLU:N	2.45	0.41
26:c:4:ILE:HG23	26:c:39:GLU:HG2	2.02	0.41
30:a:81:VAL:HG21	30:a:105:VAL:HG11	2.02	0.41
1:0:498:G:N2	1:0:500:A:H3'	2.35	0.41
1:0:1157:G:H2'	1:0:1204:A:N6	2.29	0.41
1:0:1514:U:H2'	1:0:1515:G:C8	2.55	0.41
1:0:1956:C:H1'	1:0:1957:U:C2	2.56	0.41
1:0:2138:G:H1	1:0:2225:A:H62	1.63	0.41
1:0:2361:A:N6	8:I:19:THR:O	2.53	0.41
1:0:2487:G:N2	5:F:103:ALA:O	2.53	0.41
1:0:2588:U:H2'	1:0:2589:A:C8	2.55	0.41
5:F:156:TYR:HA	5:F:159:MET:HE3	2.02	0.41
14:O:150:LEU:HD23	14:O:150:LEU:HA	1.90	0.41
20:U:175:LYS:HD2	20:U:179:MET:CE	2.50	0.41
1:0:334:A:OP2	22:W:208:ASN:HB2	2.20	0.41
1:0:946:G:H1'	14:O:23:MET:HE1	2.00	0.41
1:0:981:C:H41	1:0:991:A:H2	1.69	0.41
1:0:1923:A:H2'	1:0:1924:A:C8	2.56	0.41
1:0:1945:U:O2'	1:0:1955:C:N4	2.54	0.41
1:0:2335:G:HO2'	1:0:2336:G:H4'	1.80	0.41
1:0:2336:G:H1'	1:0:2337:A:C8	2.56	0.41
1:0:2625:G:H2'	1:0:2626:A:C8	2.56	0.41
20:U:34:GLU:HG2	20:U:36:LYS:HG2	2.02	0.41
28:e:27:ASN:OD1	28:e:27:ASN:C	2.63	0.41
1:0:341:G:C6	13:N:55:ASP:OD1	2.74	0.41
1:0:2710:C:O2'	1:0:2711:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2761:G:N7	35:0:3327:HOH:O	2.37	0.41
6:G:166:ASN:OD1	6:G:166:ASN:C	2.62	0.41
13:N:13:ARG:O	13:N:20:ARG:NH2	2.52	0.41
16:Q:109:GLU:CD	16:Q:109:GLU:H	2.29	0.41
23:X:10:ARG:NH2	23:X:150:SER:O	2.53	0.41
30:a:109:ASP:O	30:a:113:GLU:HG2	2.20	0.41
1:0:867:G:O2'	35:0:3244:HOH:O	2.04	0.41
1:0:1008:A:N3	1:0:2291:C:O2'	2.52	0.41
1:0:2854:G:N3	21:V:337:GLN:NE2	2.69	0.41
3:A:3:LYS:HB2	3:A:3:LYS:HE2	1.83	0.41
10:K:8:MET:HE3	10:K:8:MET:HB3	1.98	0.41
13:N:90:ARG:NH1	13:N:91:PRO:O	2.51	0.41
21:V:213:GLN:HB2	21:V:258:THR:OG1	2.21	0.41
23:X:55:GLN:OE1	23:X:55:GLN:HA	2.20	0.41
23:X:139:LYS:HE3	23:X:139:LYS:HB2	1.77	0.41
25:b:110:ASP:OD1	25:b:110:ASP:C	2.64	0.41
30:a:207:LYS:HB2	35:a:602:HOH:O	2.20	0.41
1:0:106:A:H3'	1:0:107:C:H6	1.84	0.41
1:0:681:C:H5''	22:W:248:ARG:NH2	2.36	0.41
1:0:1126:U:H6	1:0:1126:U:H2'	1.69	0.41
1:0:1126:U:H3'	1:0:1127:C:H6	1.86	0.41
1:0:1235:C:H6	1:0:1237:G:OP1	2.03	0.41
1:0:243:A:H4'	1:0:244:G:OP1	2.21	0.41
1:0:1077:G:OP1	35:0:3272:HOH:O	2.21	0.41
1:0:2065:G:C6	1:0:2526:C:H1'	2.55	0.41
1:0:2334:G:H5''	1:0:2335:G:N7	2.36	0.41
1:0:2504:A:H2'	1:0:2505:U:C6	2.55	0.41
1:0:2587:C:C2'	1:0:2588:U:C5'	2.97	0.41
1:0:2683:U:H2'	1:0:2696:A:H61	1.85	0.41
1:0:2890:C:OP1	35:0:3239:HOH:O	2.22	0.41
8:I:177:LEU:O	8:I:180:LEU:HB2	2.21	0.41
13:N:29:SER:O	13:N:33:ARG:HB2	2.20	0.41
21:V:159:LYS:HA	21:V:160:PRO:HD3	1.97	0.41
26:c:4:ILE:HA	26:c:27:VAL:HG12	2.02	0.41
1:0:221:U:H2'	1:0:222:A:H8	1.85	0.41
1:0:386:U:H2'	1:0:387:A:C8	2.51	0.41
1:0:389:C:H2'	1:0:390:G:H8	1.87	0.41
1:0:422:C:H2'	1:0:423:A:C8	2.55	0.41
1:0:1166:U:N3	1:0:1170:A:OP2	2.52	0.41
1:0:2134:G:H22	1:0:2226:C:H1'	1.86	0.41
1:0:2599:G:N2	21:V:242:PRO:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2604:G:H5'	1:0:2606:G:C8	2.56	0.41
1:0:2651:G:H4'	1:0:2835:G:C8	2.55	0.41
2:9:33:A:C2	8:I:151:TYR:HB2	2.55	0.41
4:E:104:GLU:H	4:E:104:GLU:CD	2.29	0.41
16:Q:121:GLN:HB3	35:Q:426:HOH:O	2.20	0.41
20:U:188:ARG:HH11	20:U:188:ARG:HB2	1.85	0.41
24:Y:22:THR:O	24:Y:23:ILE:HD13	2.21	0.41
1:0:30:G:N2	1:0:523:A:N7	2.69	0.40
1:0:1511:U:H2'	1:0:1512:C:C6	2.56	0.40
1:0:2372:G:N3	1:0:2411:G:H2'	2.36	0.40
1:0:2493:C:H2'	1:0:2494:G:H8	1.86	0.40
1:0:2686:U:H2'	1:0:2687:A:H8	1.86	0.40
1:0:2730:C:OP2	9:J:62:ARG:NH2	2.48	0.40
5:F:77:LEU:HD12	5:F:81:GLY:O	2.22	0.40
8:I:180:LEU:HD23	8:I:180:LEU:HA	1.92	0.40
16:Q:155:GLY:HA2	16:Q:156:PRO:HD3	1.96	0.40
21:V:111:ASP:OD1	21:V:111:ASP:C	2.64	0.40
23:X:34:GLU:O	23:X:38:GLU:HG2	2.21	0.40
1:0:108:U:H2'	1:0:109:G:C8	2.56	0.40
1:0:2135:G:N2	1:0:2225:A:O2'	2.54	0.40
5:F:150:ASP:O	5:F:153:ARG:HB3	2.21	0.40
18:S:32:LYS:HB2	18:S:32:LYS:HE3	1.96	0.40
23:X:155:VAL:O	23:X:158:ALA:N	2.54	0.40
1:0:135:A:H1'	1:0:136:G:C4	2.56	0.40
1:0:664:A:H5''	7:H:68:SER:HB3	2.02	0.40
1:0:668:U:N3	1:0:686:A:N7	2.69	0.40
1:0:1061:C:H2'	1:0:1062:U:C6	2.57	0.40
1:0:1170:A:H5''	1:0:1171:A:P	2.61	0.40
1:0:2132:G:H1	1:0:2229:C:H5''	1.85	0.40
1:0:2674:A:H4'	1:0:2675:C:OP1	2.20	0.40
8:I:151:TYR:O	8:I:155:LEU:HB2	2.22	0.40
20:U:127:GLN:CG	35:U:417:HOH:O	2.70	0.40
1:0:733:U:H2'	1:0:734:C:H6	1.86	0.40
1:0:1166:U:H2'	1:0:1167:U:C6	2.57	0.40
1:0:1459:U:H2'	1:0:1460:A:H8	1.86	0.40
1:0:2255:C:H2'	1:0:2256:G:H8	1.87	0.40
4:E:28:GLY:O	4:E:29:ILE:HD13	2.21	0.40
7:H:34:LEU:HD23	7:H:34:LEU:HA	1.85	0.40
11:L:110:MET:HE2	11:L:150:GLU:N	2.36	0.40
1:0:291:C:H4'	1:0:291:C:OP1	2.20	0.40
1:0:444:C:H2'	1:0:445:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:615:U:H2'	1:0:616:U:C6	2.57	0.40
1:0:618:U:OP1	35:0:3275:HOH:O	2.22	0.40
1:0:985:G:H2'	1:0:986:A:C8	2.57	0.40
1:0:995:C:H2'	1:0:996:G:C8	2.57	0.40
1:0:1283:A:C4	14:O:115:VAL:HG11	2.56	0.40
1:0:1503:C:H2'	1:0:1504:A:H8	1.87	0.40
1:0:2726:U:H2'	1:0:2727:G:C8	2.57	0.40
10:K:11:THR:HG22	10:K:14:LYS:HD2	2.02	0.40
11:L:22:ARG:HA	11:L:23:PRO:HD3	1.96	0.40
21:V:152:LEU:HD23	21:V:152:LEU:HA	1.87	0.40
21:V:276:GLY:O	21:V:292:ASP:HA	2.21	0.40
27:d:9:ILE:HD13	27:d:9:ILE:HA	1.79	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	A	29/50 (58%)	29 (100%)	0	0	100	100
4	E	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
5	F	172/176 (98%)	167 (97%)	5 (3%)	0	100	100
6	G	192/196 (98%)	190 (99%)	2 (1%)	0	100	100
7	H	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
8	I	181/184 (98%)	175 (97%)	6 (3%)	0	100	100
9	J	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
10	K	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
11	L	149/153 (97%)	144 (97%)	5 (3%)	0	100	100
12	M	56/67 (84%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
14	O	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
15	P	87/92 (95%)	83 (95%)	4 (5%)	0	100	100
16	Q	140/234 (60%)	135 (96%)	5 (4%)	0	100	100
17	R	78/89 (88%)	73 (94%)	5 (6%)	0	100	100
18	S	55/58 (95%)	52 (94%)	3 (6%)	0	100	100
19	T	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
20	U	236/241 (98%)	215 (91%)	19 (8%)	2 (1%)	16	30
21	V	335/338 (99%)	324 (97%)	11 (3%)	0	100	100
22	W	246/248 (99%)	233 (95%)	13 (5%)	0	100	100
23	X	167/172 (97%)	150 (90%)	16 (10%)	1 (1%)	21	38
24	Y	172/178 (97%)	165 (96%)	6 (4%)	1 (1%)	21	38
25	b	142/145 (98%)	134 (94%)	8 (6%)	0	100	100
26	c	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
27	d	67/70 (96%)	67 (100%)	0	0	100	100
28	e	56/58 (97%)	56 (100%)	0	0	100	100
29	f	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
30	a	279/406 (69%)	223 (80%)	50 (18%)	6 (2%)	5	10
All	All	3876/4218 (92%)	3672 (95%)	194 (5%)	10 (0%)	37	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	U	213	LYS
30	a	124	ASP
30	a	163	ALA
30	a	191	THR
20	U	237	GLY
24	Y	10	ASP
30	a	128	THR
30	a	131	LEU
23	X	99	ASN
30	a	129	ASN

5.3.2 Protein sidechains [i](#)

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	A	27/46 (59%)	27 (100%)	0	100	100
4	E	93/94 (99%)	93 (100%)	0	100	100
5	F	145/147 (99%)	143 (99%)	2 (1%)	59	75
6	G	161/163 (99%)	160 (99%)	1 (1%)	78	88
7	H	98/99 (99%)	98 (100%)	0	100	100
8	I	144/145 (99%)	142 (99%)	2 (1%)	59	75
9	J	120/121 (99%)	114 (95%)	6 (5%)	22	42
10	K	77/78 (99%)	76 (99%)	1 (1%)	61	76
11	L	122/124 (98%)	122 (100%)	0	100	100
12	M	48/55 (87%)	48 (100%)	0	100	100
13	N	98/102 (96%)	97 (99%)	1 (1%)	68	81
14	O	132/132 (100%)	131 (99%)	1 (1%)	73	84
15	P	78/80 (98%)	78 (100%)	0	100	100
16	Q	120/191 (63%)	118 (98%)	2 (2%)	53	71
17	R	61/68 (90%)	58 (95%)	3 (5%)	22	43
18	S	48/49 (98%)	46 (96%)	2 (4%)	26	49
19	T	77/77 (100%)	77 (100%)	0	100	100
20	U	184/186 (99%)	178 (97%)	6 (3%)	33	57
21	V	277/278 (100%)	276 (100%)	1 (0%)	84	91
22	W	198/198 (100%)	194 (98%)	4 (2%)	48	69
23	X	125/147 (85%)	124 (99%)	1 (1%)	73	84
24	Y	149/151 (99%)	149 (100%)	0	100	100
25	b	122/123 (99%)	121 (99%)	1 (1%)	73	84
26	c	76/76 (100%)	76 (100%)	0	100	100
27	d	55/56 (98%)	55 (100%)	0	100	100
28	e	49/49 (100%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	f	106/106 (100%)	106 (100%)	0	100	100
30	a	240/344 (70%)	206 (86%)	34 (14%)	3	6
All	All	3230/3485 (93%)	3162 (98%)	68 (2%)	46	67

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	13	LYS
5	F	118	SER
6	G	174	LEU
8	I	144	ARG
8	I	155	LEU
9	J	43	GLU
9	J	70	ARG
9	J	147	GLN
9	J	149	GLU
9	J	150	ILE
9	J	151	GLN
10	K	96	GLN
13	N	31	ASP
14	O	73	GLU
16	Q	139	ARG
16	Q	141	ARG
17	R	7	ARG
17	R	31	GLU
17	R	36	ASN
18	S	15	THR
18	S	55	SER
20	U	36	LYS
20	U	47	GLU
20	U	82	ILE
20	U	232	ARG
20	U	235	ARG
20	U	238	LYS
21	V	337	GLN
22	W	36	ILE
22	W	65	ARG
22	W	67	MET
22	W	161	LEU
23	X	18	VAL
25	b	9	ASP

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Mol	Chain	Res	Type
30	a	3	ILE
30	a	4	THR
30	a	6	ILE
30	a	8	SER
30	a	12	VAL
30	a	30	HIS
30	a	55	HIS
30	a	72	LEU
30	a	76	GLU
30	a	79	ARG
30	a	91	LYS
30	a	108	ASP
30	a	111	LEU
30	a	114	VAL
30	a	115	LYS
30	a	118	LEU
30	a	119	ASP
30	a	122	THR
30	a	123	VAL
30	a	124	ASP
30	a	125	ASP
30	a	126	VAL
30	a	127	TYR
30	a	128	THR
30	a	149	ASP
30	a	151	ARG
30	a	184	LYS
30	a	200	SER
30	a	205	SER
30	a	228	VAL
30	a	229	MET
30	a	234	ARG
30	a	236	ILE
30	a	260	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	19	ASN
5	F	62	HIS
5	F	100	ASN
5	F	157	ASN

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Mol	Chain	Res	Type
6	G	130	GLN
7	H	28	GLN
7	H	111	ASN
8	I	143	ASN
9	J	143	GLN
9	J	147	GLN
10	K	68	GLN
11	L	103	GLN
13	N	4	GLN
14	O	27	HIS
14	O	31	HIS
14	O	49	ASN
14	O	54	HIS
14	O	110	GLN
15	P	37	HIS
16	Q	125	GLN
19	T	67	HIS
20	U	81	GLN
20	U	127	GLN
21	V	3	GLN
21	V	239	ASN
21	V	306	ASN
22	W	9	ASN
23	X	107	HIS
24	Y	27	ASN
25	b	28	GLN
25	b	40	ASN
26	c	20	GLN
26	c	52	ASN
30	a	30	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2824/2916 (96%)	838 (29%)	74 (2%)
2	9	120/122 (98%)	23 (19%)	2 (1%)
All	All	2944/3038 (96%)	861 (29%)	76 (2%)

All (861) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	12	G
1	0	13	C
1	0	16	C
1	0	17	U
1	0	28	G
1	0	30	G
1	0	32	A
1	0	37	U
1	0	38	C
1	0	49	C
1	0	54	G
1	0	58	G
1	0	66	A
1	0	74	A
1	0	76	A
1	0	77	A
1	0	78	G
1	0	87	A
1	0	88	C
1	0	91	G
1	0	94	U
1	0	95	G
1	0	97	A
1	0	104	G
1	0	111	G
1	0	112	G
1	0	120	A
1	0	121	A
1	0	122	U
1	0	125	G
1	0	126	A
1	0	128	U
1	0	133	A
1	0	134	C
1	0	135	A
1	0	138	A
1	0	142	G
1	0	144	C
1	0	147	G
1	0	148	C
1	0	149	G
1	0	155	G
1	0	158	A

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Mol	Chain	Res	Type
1	0	159	A
1	0	173	A
1	0	174	A
1	0	176	A
1	0	177	U
1	0	190	A
1	0	192	G
1	0	193	A
1	0	198	A
1	0	199	A
1	0	200	A
1	0	203	A
1	0	205	U
1	0	206	C
1	0	207	C
1	0	208	G
1	0	211	A
1	0	221	U
1	0	224	C
1	0	226	G
1	0	243	A
1	0	244	G
1	0	252	C
1	0	253	G
1	0	254	A
1	0	255	A
1	0	260	U
1	0	261	C
1	0	262	G
1	0	263	G
1	0	265	C
1	0	268	U
1	0	269	G
1	0	275	U
1	0	276	A
1	0	277	C
1	0	278	G
1	0	283	A
1	0	284	C
1	0	287	A
1	0	288	U
1	0	289	A

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Mol	Chain	Res	Type
1	0	290	A
1	0	291	C
1	0	292	G
1	0	293	G
1	0	296	C
1	0	298	G
1	0	299	G
1	0	300	A
1	0	301	A
1	0	302	U
1	0	303	U
1	0	305	A
1	0	306	C
1	0	310	A
1	0	313	U
1	0	314	C
1	0	320	G
1	0	321	A
1	0	322	A
1	0	323	C
1	0	329	G
1	0	334	A
1	0	336	A
1	0	341	G
1	0	342	A
1	0	343	A
1	0	349	C
1	0	357	G
1	0	358	A
1	0	359	A
1	0	360	G
1	0	361	G
1	0	362	A
1	0	363	A
1	0	364	A
1	0	365	G
1	0	366	A
1	0	367	U
1	0	368	C
1	0	369	C
1	0	370	C
1	0	371	G

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Mol	Chain	Res	Type
1	0	372	G
1	0	373	G
1	0	374	G
1	0	376	U
1	0	377	G
1	0	378	U
1	0	379	U
1	0	380	C
1	0	383	G
1	0	385	A
1	0	386	U
1	0	388	G
1	0	400	U
1	0	401	A
1	0	402	U
1	0	403	C
1	0	408	G
1	0	411	A
1	0	412	A
1	0	414	U
1	0	421	G
1	0	431	C
1	0	442	C
1	0	445	U
1	0	452	G
1	0	461	C
1	0	465	C
1	0	467	A
1	0	469	U
1	0	477	G
1	0	485	U
1	0	487	A
1	0	489	A
1	0	490	A
1	0	491	G
1	0	492	C
1	0	499	A
1	0	500	A
1	0	501	A
1	0	502	A
1	0	503	G
1	0	507	G

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Mol	Chain	Res	Type
1	0	508	G
1	0	511	C
1	0	514	U
1	0	515	A
1	0	518	G
1	0	519	C
1	0	531	U
1	0	532	G
1	0	541	G
1	0	542	C
1	0	543	G
1	0	547	U
1	0	553	A
1	0	557	G
1	0	562	U
1	0	564	U
1	0	565	G
1	0	569	A
1	0	581	G
1	0	585	U
1	0	592	G
1	0	593	U
1	0	605	G
1	0	608	G
1	0	611	G
1	0	624	A
1	0	629	U
1	0	632	A
1	0	633	A
1	0	634	A
1	0	635	A
1	0	636	A
1	0	648	G
1	0	664	A
1	0	666	U
1	0	667	C
1	0	671	G
1	0	677	A
1	0	679	C
1	0	683	C
1	0	685	G
1	0	686	A

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Mol	Chain	Res	Type
1	0	687	G
1	0	692	A
1	0	699	C
1	0	703	U
1	0	704	A
1	0	705	C
1	0	706	G
1	0	707	G
1	0	708	C
1	0	711	C
1	0	717	U
1	0	718	U
1	0	719	G
1	0	720	A
1	0	722	C
1	0	724	G
1	0	729	A
1	0	736	U
1	0	737	C
1	0	741	G
1	0	744	G
1	0	747	G
1	0	748	A
1	0	761	C
1	0	762	G
1	0	763	A
1	0	767	G
1	0	770	A
1	0	778	A
1	0	779	U
1	0	780	C
1	0	784	G
1	0	788	G
1	0	792	A
1	0	802	G
1	0	804	G
1	0	807	G
1	0	811	G
1	0	819	G
1	0	820	A
1	0	823	C
1	0	830	G

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Mol	Chain	Res	Type
1	0	832	G
1	0	834	U
1	0	837	U
1	0	842	U
1	0	843	A
1	0	844	C
1	0	857	U
1	0	858	G
1	0	859	A
1	0	864	G
1	0	870	G
1	0	871	G
1	0	872	G
1	0	874	U
1	0	877	A
1	0	879	G
1	0	880	G
1	0	882	C
1	0	883	C
1	0	886	C
1	0	887	G
1	0	888	A
1	0	895	C
1	0	899	A
1	0	900	G
1	0	907	C
1	0	916	A
1	0	922	C
1	0	923	G
1	0	925	A
1	0	944	U
1	0	945	A
1	0	950	G
1	0	952	G
1	0	954	G
1	0	955	G
1	0	962	G
1	0	966	G
1	0	967	A
1	0	976	C
1	0	987	G
1	0	988	A

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Mol	Chain	Res	Type
1	0	989	G
1	0	990	G
1	0	992	G
1	0	993	U
1	0	994	U
1	0	996	G
1	0	999	U
1	0	1001	C
1	0	1002	C
1	0	1005	U
1	0	1006	C
1	0	1008	A
1	0	1010	C
1	0	1012	C
1	0	1013	C
1	0	1017	C
1	0	1026	A
1	0	1032	G
1	0	1041	A
1	0	1046	G
1	0	1059	A
1	0	1060	G
1	0	1061	C
1	0	1064	G
1	0	1072	U
1	0	1073	G
1	0	1077	G
1	0	1078	A
1	0	1079	G
1	0	1081	C
1	0	1088	G
1	0	1089	A
1	0	1103	C
1	0	1110	U
1	0	1111	G
1	0	1114	G
1	0	1115	A
1	0	1120	G
1	0	1121	U
1	0	1123	U
1	0	1125	A
1	0	1126	U

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Mol	Chain	Res	Type
1	0	1127	C
1	0	1128	G
1	0	1132	A
1	0	1134	U
1	0	1138	U
1	0	1142	G
1	0	1146	U
1	0	1147	A
1	0	1148	A
1	0	1157	G
1	0	1158	A
1	0	1159	G
1	0	1160	G
1	0	1161	U
1	0	1162	G
1	0	1163	A
1	0	1168	A
1	0	1171	A
1	0	1174	A
1	0	1176	C
1	0	1179	C
1	0	1180	C
1	0	1181	C
1	0	1182	U
1	0	1185	A
1	0	1186	A
1	0	1188	A
1	0	1189	A
1	0	1190	U
1	0	1191	A
1	0	1192	G
1	0	1193	C
1	0	1195	U
1	0	1196	A
1	0	1197	A
1	0	1198	C
1	0	1202	U
1	0	1205	C
1	0	1206	C
1	0	1207	G
1	0	1208	G
1	0	1209	C

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Mol	Chain	Res	Type
1	0	1211	G
1	0	1212	A
1	0	1213	G
1	0	1214	G
1	0	1218	G
1	0	1223	G
1	0	1227	A
1	0	1228	A
1	0	1229	A
1	0	1231	U
1	0	1232	G
1	0	1233	A
1	0	1234	U
1	0	1235	C
1	0	1236	G
1	0	1239	A
1	0	1242	C
1	0	1245	A
1	0	1249	A
1	0	1251	C
1	0	1256	A
1	0	1257	G
1	0	1258	A
1	0	1259	C
1	0	1271	C
1	0	1272	U
1	0	1273	A
1	0	1274	U
1	0	1275	U
1	0	1276	U
1	0	1277	A
1	0	1278	G
1	0	1283	A
1	0	1285	U
1	0	1286	C
1	0	1287	C
1	0	1288	G
1	0	1296	G
1	0	1300	A
1	0	1307	G
1	0	1308	G
1	0	1312	G

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Mol	Chain	Res	Type
1	0	1316	U
1	0	1317	A
1	0	1325	G
1	0	1327	A
1	0	1336	G
1	0	1338	C
1	0	1345	G
1	0	1348	A
1	0	1349	C
1	0	1350	G
1	0	1354	A
1	0	1355	U
1	0	1356	C
1	0	1367	U
1	0	1368	A
1	0	1376	G
1	0	1377	A
1	0	1382	G
1	0	1390	C
1	0	1391	C
1	0	1392	C
1	0	1398	A
1	0	1402	U
1	0	1403	A
1	0	1404	C
1	0	1405	G
1	0	1414	U
1	0	1415	U
1	0	1422	C
1	0	1426	G
1	0	1427	U
1	0	1428	C
1	0	1431	U
1	0	1435	C
1	0	1443	U
1	0	1447	C
1	0	1451	C
1	0	1456	G
1	0	1467	A
1	0	1470	C
1	0	1481	A
1	0	1483	A

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Mol	Chain	Res	Type
1	0	1492	G
1	0	1496	A
1	0	1497	A
1	0	1499	A
1	0	1500	U
1	0	1516	C
1	0	1517	A
1	0	1518	A
1	0	1519	U
1	0	1520	A
1	0	1521	A
1	0	1522	A
1	0	1523	A
1	0	1524	G
1	0	1529	C
1	0	1539	A
1	0	1547	G
1	0	1550	G
1	0	1553	C
1	0	1554	C
1	0	1556	U
1	0	1558	G
1	0	1563	G
1	0	1565	C
1	0	1569	U
1	0	1574	G
1	0	1575	A
1	0	1577	C
1	0	1581	G
1	0	1584	G
1	0	1586	A
1	0	1587	G
1	0	1592	A
1	0	1594	U
1	0	1598	A
1	0	1599	C
1	0	1600	G
1	0	1605	G
1	0	1612	U
1	0	1616	G
1	0	1619	A
1	0	1620	U

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Mol	Chain	Res	Type
1	0	1621	A
1	0	1628	C
1	0	1629	U
1	0	1630	C
1	0	1631	G
1	0	1636	U
1	0	1651	A
1	0	1659	A
1	0	1660	G
1	0	1677	A
1	0	1679	A
1	0	1680	U
1	0	1686	A
1	0	1687	C
1	0	1688	A
1	0	1694	G
1	0	1704	U
1	0	1705	A
1	0	1710	A
1	0	1716	U
1	0	1718	U
1	0	1719	C
1	0	1724	U
1	0	1725	C
1	0	1732	C
1	0	1736	A
1	0	1746	G
1	0	1747	C
1	0	1749	A
1	0	1750	G
1	0	1754	G
1	0	1766	C
1	0	1768	C
1	0	1772	A
1	0	1779	A
1	0	1784	C
1	0	1790	A
1	0	1805	G
1	0	1811	C
1	0	1812	G
1	0	1813	G
1	0	1822	A

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Mol	Chain	Res	Type
1	0	1823	C
1	0	1825	G
1	0	1831	U
1	0	1833	A
1	0	1835	A
1	0	1836	A
1	0	1837	C
1	0	1849	C
1	0	1850	A
1	0	1851	A
1	0	1860	G
1	0	1866	G
1	0	1877	G
1	0	1878	A
1	0	1882	C
1	0	1887	C
1	0	1888	A
1	0	1889	G
1	0	1890	U
1	0	1895	G
1	0	1896	U
1	0	1904	C
1	0	1912	A
1	0	1913	C
1	0	1914	A
1	0	1923	A
1	0	1933	C
1	0	1934	A
1	0	1935	A
1	0	1937	G
1	0	1940	G
1	0	1942	G
1	0	1943	G
1	0	1944	G
1	0	1945	U
1	0	1946	A
1	0	1947	A
1	0	1948	C
1	0	1949	U
1	0	1950	A
1	0	1951	U
1	0	1954	C

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Mol	Chain	Res	Type
1	0	1955	C
1	0	1956	C
1	0	1957	U
1	0	1958	C
1	0	1960	U
1	0	1963	G
1	0	1964	G
1	0	1965	U
1	0	1971	A
1	0	1973	U
1	0	1976	C
1	0	1979	G
1	0	1983	C
1	0	1989	U
1	0	1997	U
1	0	1999	C
1	0	2000	A
1	0	2001	U
1	0	2004	A
1	0	2005	U
1	0	2006	G
1	0	2015	A
1	0	2018	G
1	0	2026	G
1	0	2027	U
1	0	2029	C
1	0	2034	G
1	0	2044	G
1	0	2046	G
1	0	2057	U
1	0	2060	A
1	0	2061	G
1	0	2065	G
1	0	2066	G
1	0	2067	A
1	0	2070	C
1	0	2074	A
1	0	2085	G
1	0	2089	A
1	0	2094	A
1	0	2095	G
1	0	2096	A

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Mol	Chain	Res	Type
1	0	2097	C
1	0	2102	U
1	0	2103	A
1	0	2114	G
1	0	2116	A
1	0	2119	C
1	0	2127	G
1	0	2130	A
1	0	2131	C
1	0	2132	G
1	0	2133	U
1	0	2134	G
1	0	2138	G
1	0	2140	U
1	0	2141	A
1	0	2142	A
1	0	2220	U
1	0	2221	A
1	0	2223	U
1	0	2224	G
1	0	2225	A
1	0	2226	C
1	0	2227	U
1	0	2228	G
1	0	2229	C
1	0	2230	G
1	0	2231	A
1	0	2232	C
1	0	2236	C
1	0	2246	G
1	0	2251	A
1	0	2260	G
1	0	2264	G
1	0	2265	G
1	0	2270	U
1	0	2271	U
1	0	2283	U
1	0	2284	A
1	0	2285	C
1	0	2295	A
1	0	2306	C
1	0	2309	G

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Mol	Chain	Res	Type
1	0	2310	C
1	0	2313	A
1	0	2314	A
1	0	2315	A
1	0	2316	G
1	0	2322	C
1	0	2327	G
1	0	2328	C
1	0	2330	A
1	0	2331	G
1	0	2332	U
1	0	2333	C
1	0	2334	G
1	0	2335	G
1	0	2336	G
1	0	2337	A
1	0	2338	A
1	0	2339	C
1	0	2347	A
1	0	2349	A
1	0	2354	A
1	0	2362	A
1	0	2363	C
1	0	2364	G
1	0	2366	A
1	0	2370	C
1	0	2372	G
1	0	2378	G
1	0	2394	G
1	0	2413	G
1	0	2414	G
1	0	2415	U
1	0	2422	A
1	0	2431	G
1	0	2432	G
1	0	2434	U
1	0	2436	A
1	0	2437	U
1	0	2444	G
1	0	2450	U
1	0	2455	G
1	0	2456	A

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Mol	Chain	Res	Type
1	0	2458	A
1	0	2459	G
1	0	2460	A
1	0	2461	A
1	0	2462	A
1	0	2463	A
1	0	2464	G
1	0	2469	C
1	0	2473	G
1	0	2476	A
1	0	2477	U
1	0	2491	C
1	0	2496	A
1	0	2497	A
1	0	2498	G
1	0	2501	C
1	0	2502	A
1	0	2504	A
1	0	2506	A
1	0	2514	G
1	0	2526	C
1	0	2529	C
1	0	2530	G
1	0	2531	A
1	0	2533	G
1	0	2534	U
1	0	2545	C
1	0	2546	A
1	0	2557	G
1	0	2559	A
1	0	2580	U
1	0	2582	U
1	0	2594	A
1	0	2595	G
1	0	2597	A
1	0	2600	U
1	0	2601	C
1	0	2602	G
1	0	2604	G
1	0	2606	G
1	0	2613	U
1	0	2614	U

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Mol	Chain	Res	Type
1	0	2622	C
1	0	2629	C
1	0	2630	A
1	0	2631	G
1	0	2637	C
1	0	2638	U
1	0	2641	U
1	0	2642	A
1	0	2653	G
1	0	2654	U
1	0	2658	A
1	0	2659	A
1	0	2660	G
1	0	2666	U
1	0	2668	A
1	0	2669	C
1	0	2673	A
1	0	2674	A
1	0	2675	C
1	0	2676	G
1	0	2686	U
1	0	2691	G
1	0	2693	G
1	0	2697	C
1	0	2703	A
1	0	2704	U
1	0	2705	G
1	0	2709	G
1	0	2714	U
1	0	2719	U
1	0	2731	G
1	0	2735	G
1	0	2740	G
1	0	2741	U
1	0	2743	G
1	0	2748	G
1	0	2754	A
1	0	2755	C
1	0	2761	G
1	0	2764	G
1	0	2767	U
1	0	2772	G

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Mol	Chain	Res	Type
1	0	2776	A
1	0	2778	A
1	0	2779	G
1	0	2785	A
1	0	2787	G
1	0	2790	C
1	0	2792	A
1	0	2793	A
1	0	2794	A
1	0	2804	A
1	0	2806	A
1	0	2807	A
1	0	2817	C
1	0	2818	U
1	0	2820	A
1	0	2821	G
1	0	2828	C
1	0	2830	U
1	0	2833	A
1	0	2835	G
1	0	2839	A
1	0	2843	C
1	0	2845	A
1	0	2855	G
1	0	2859	U
1	0	2861	C
1	0	2869	G
1	0	2870	G
1	0	2873	A
1	0	2883	A
1	0	2889	G
1	0	2890	C
1	0	2891	G
1	0	2895	A
1	0	2896	C
1	0	2902	G
1	0	2907	A
1	0	2908	G
1	0	2910	C
2	9	3	C
2	9	4	G
2	9	11	A

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Mol	Chain	Res	Type
2	9	16	G
2	9	18	U
2	9	23	U
2	9	24	U
2	9	27	A
2	9	32	U
2	9	39	C
2	9	40	C
2	9	41	C
2	9	54	U
2	9	55	A
2	9	56	A
2	9	76	A
2	9	77	G
2	9	78	U
2	9	87	G
2	9	93	U
2	9	109	G
2	9	113	G
2	9	121	U

All (76) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	16	C
1	0	37	U
1	0	147	G
1	0	173	A
1	0	176	A
1	0	192	G
1	0	206	C
1	0	243	A
1	0	253	G
1	0	254	A
1	0	261	C
1	0	275	U
1	0	300	A
1	0	313	U
1	0	360	G
1	0	366	A
1	0	369	C
1	0	370	C

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Mol	Chain	Res	Type
1	0	378	U
1	0	499	A
1	0	703	U
1	0	819	G
1	0	836	G
1	0	843	A
1	0	857	U
1	0	859	A
1	0	869	A
1	0	879	G
1	0	887	G
1	0	944	U
1	0	954	G
1	0	988	A
1	0	992	G
1	0	1000	C
1	0	1032	G
1	0	1072	U
1	0	1159	G
1	0	1171	A
1	0	1190	U
1	0	1258	A
1	0	1272	U
1	0	1286	C
1	0	1390	C
1	0	1413	G
1	0	1426	G
1	0	1446	U
1	0	1499	A
1	0	1519	U
1	0	1520	A
1	0	1521	A
1	0	1586	A
1	0	1659	A
1	0	1672	U
1	0	1725	C
1	0	1849	C
1	0	1941	G
1	0	1955	C
1	0	2126	U
1	0	2283	U
1	0	2309	G

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Mol	Chain	Res	Type
1	0	2337	A
1	0	2414	G
1	0	2460	A
1	0	2461	A
1	0	2486	C
1	0	2496	A
1	0	2501	C
1	0	2529	C
1	0	2545	C
1	0	2667	G
1	0	2685	G
1	0	2711	C
1	0	2784	U
1	0	2842	U
2	9	2	A
2	9	22	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 200 ligands modelled in this entry, 197 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	AMP	a	502	-	25,25,25	0.35	0	38,38,38	0.46	0
34	AMP	a	501	-	25,25,25	0.32	0	38,38,38	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BGC	0	3001	-	12,12,12	0.42	0	17,17,17	0.79	1 (5%)

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
34	AMP	a	502	-	-	6/10/26/26	0/3/3/3
34	AMP	a	501	-	-	2/10/26/26	0/3/3/3
31	BGC	0	3001	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	0	3001	BGC	C1-O5-C5	2.19	117.80	113.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	501	AMP	O4'-C4'-C5'-O5'
34	a	502	AMP	C5'-O5'-P-O1P
34	a	502	AMP	C5'-O5'-P-O2P
34	a	502	AMP	C5'-O5'-P-O3P
34	a	502	AMP	O4'-C4'-C5'-O5'
34	a	501	AMP	C3'-C4'-C5'-O5'
34	a	502	AMP	C3'-C4'-C5'-O5'
31	0	3001	BGC	O5-C5-C6-O6
34	a	502	AMP	C4'-C5'-O5'-P

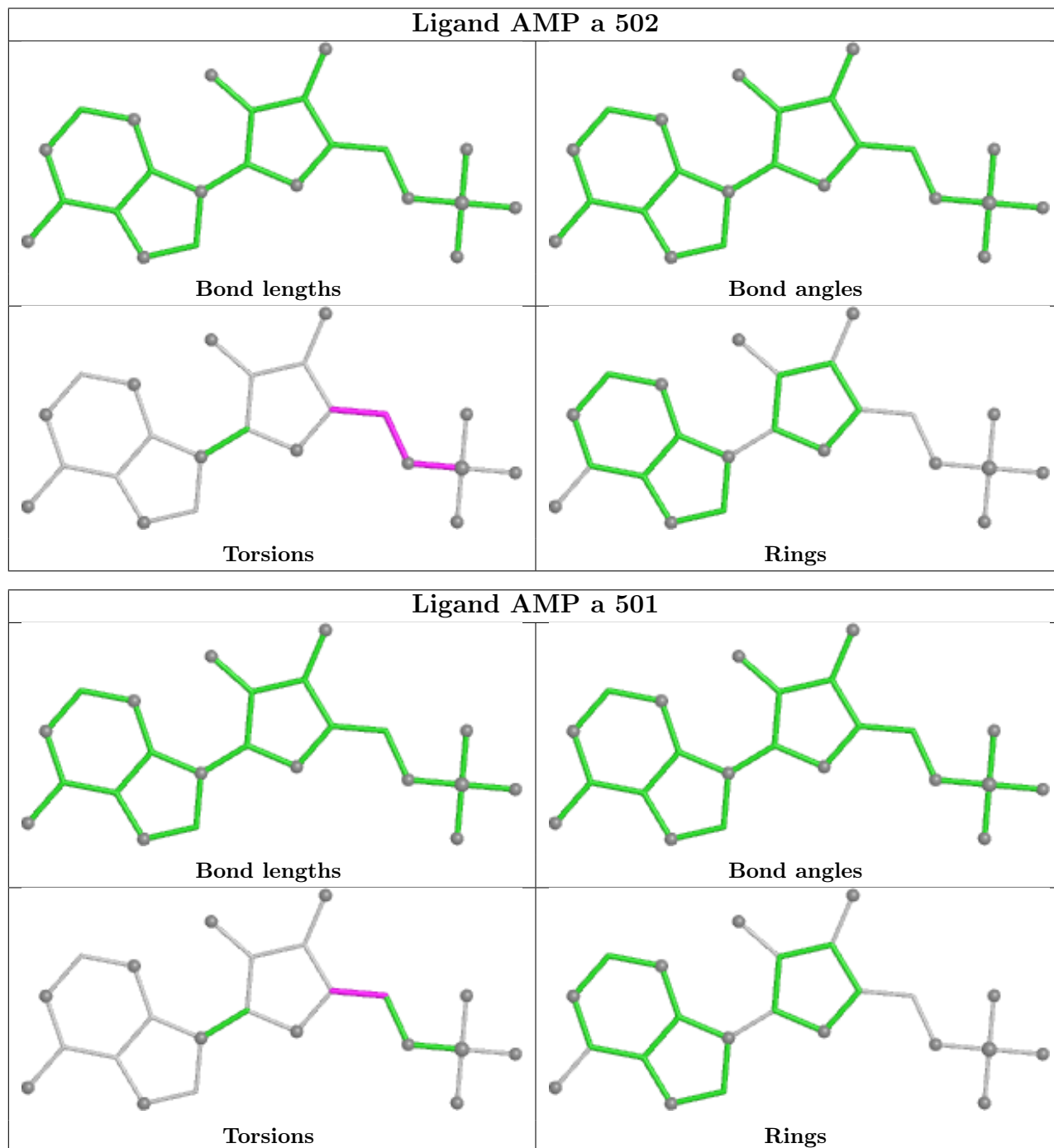
There are no ring outliers.

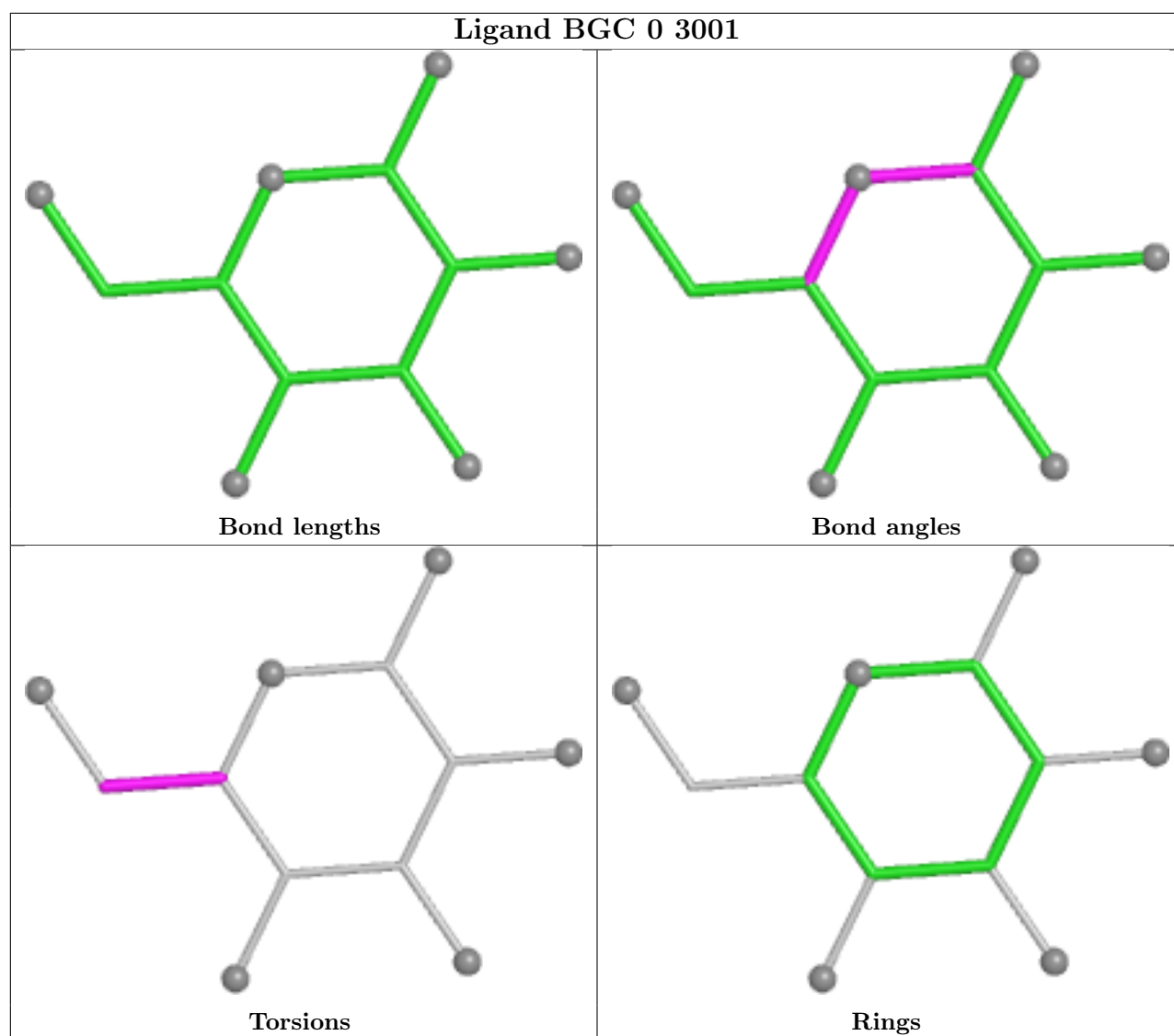
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	3001	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

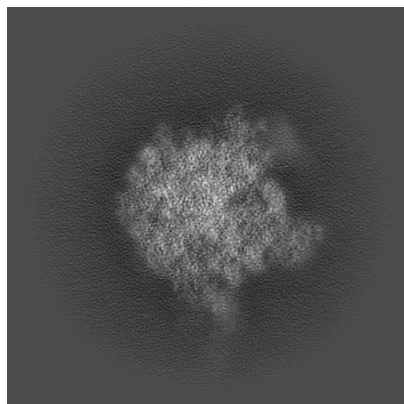
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62897. These allow visual inspection of the internal detail of the map and identification of artifacts.

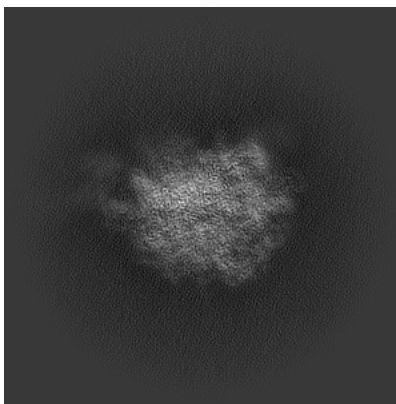
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

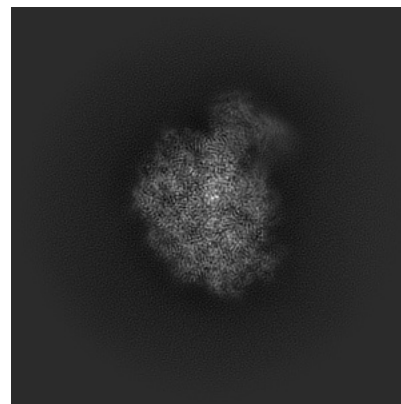
6.1.1 Primary map



X

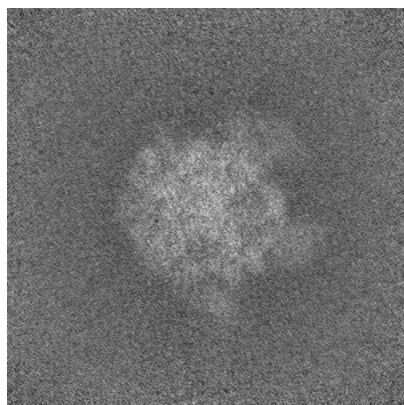


Y

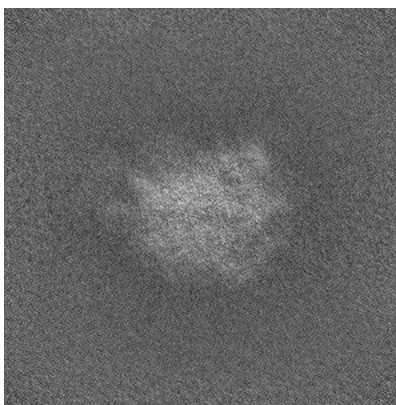


Z

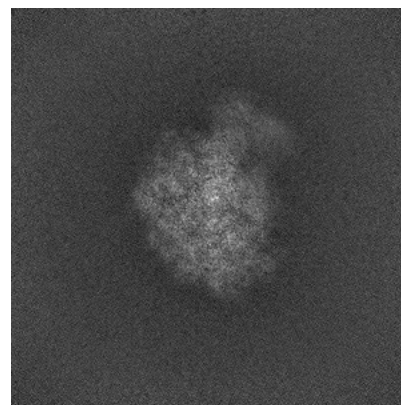
6.1.2 Raw map



X



Y

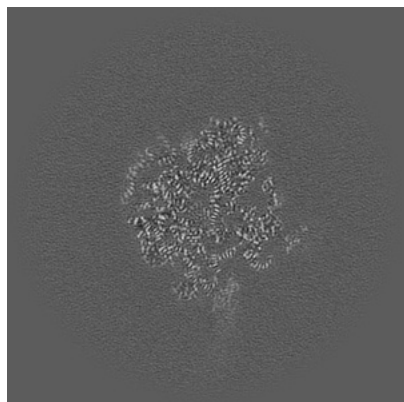


Z

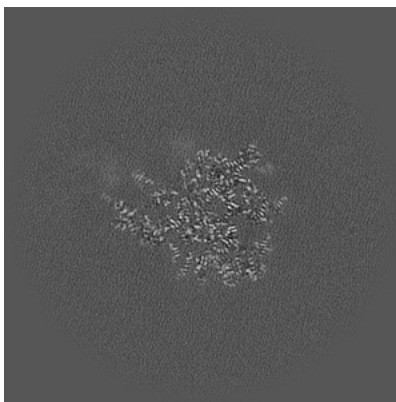
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

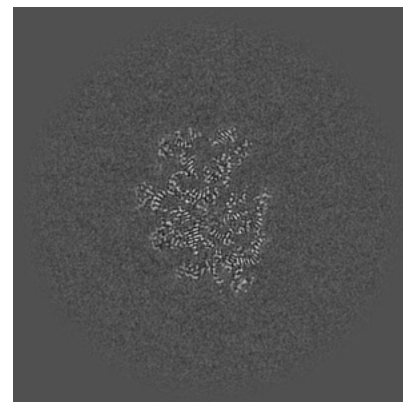
6.2.1 Primary map



X Index: 320

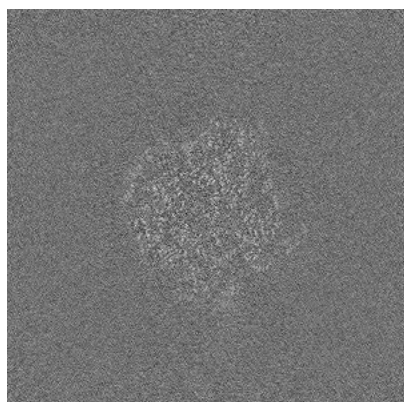


Y Index: 320

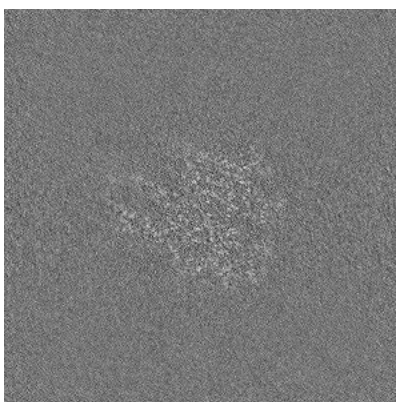


Z Index: 320

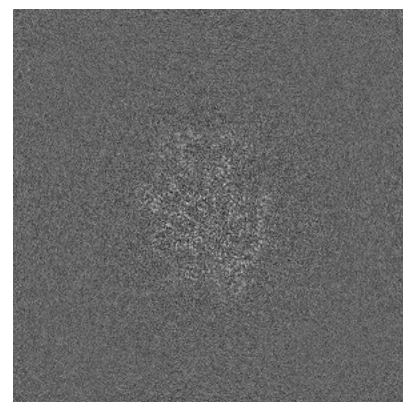
6.2.2 Raw map



X Index: 320



Y Index: 320

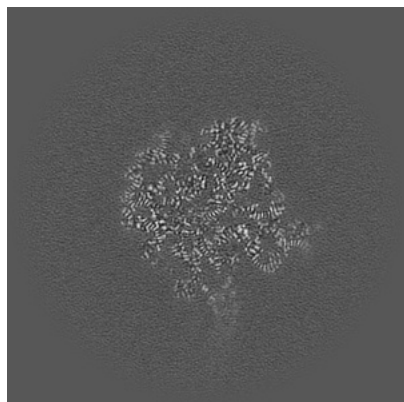


Z Index: 320

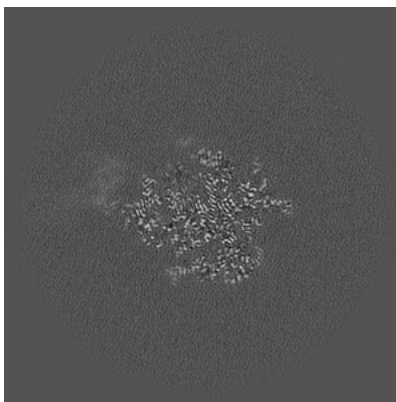
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

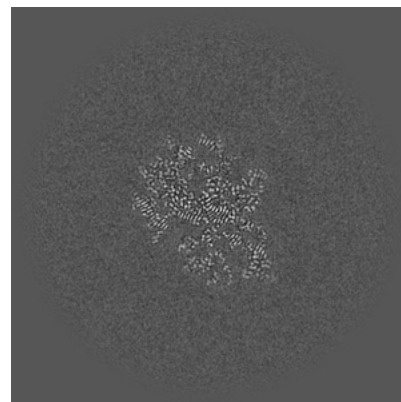
6.3.1 Primary map



X Index: 328

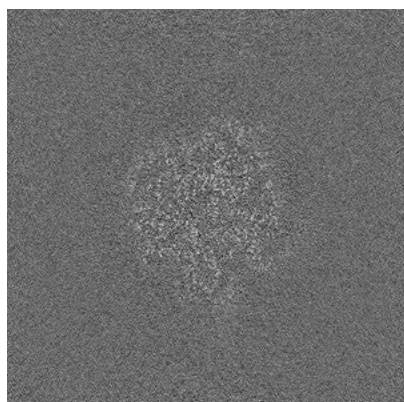


Y Index: 335

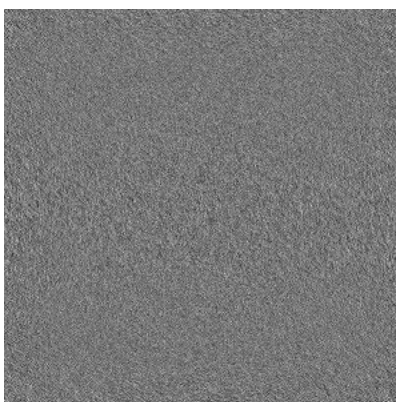


Z Index: 359

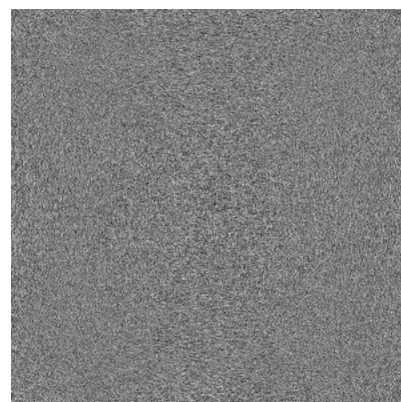
6.3.2 Raw map



X Index: 322



Y Index: 0

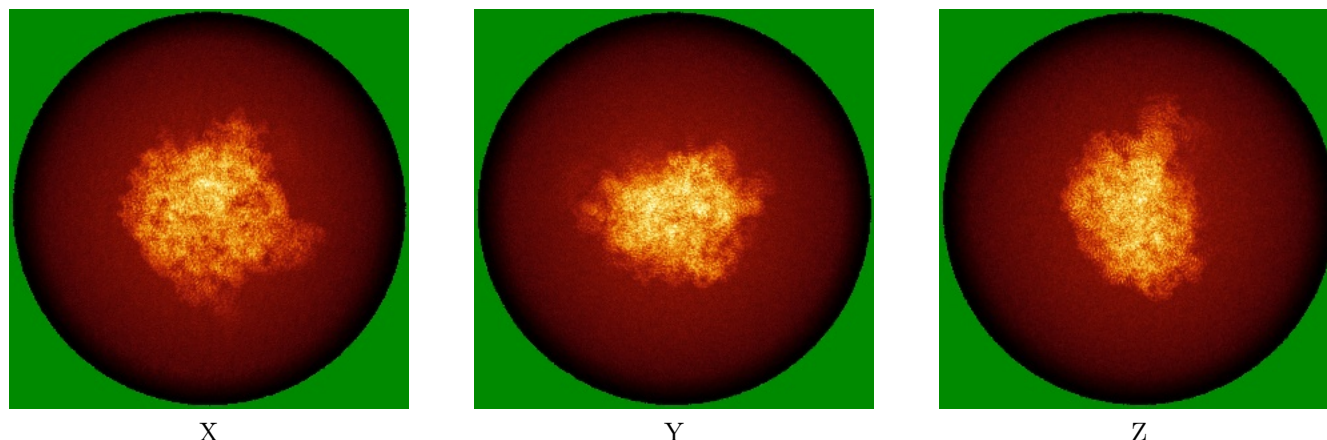


Z Index: 0

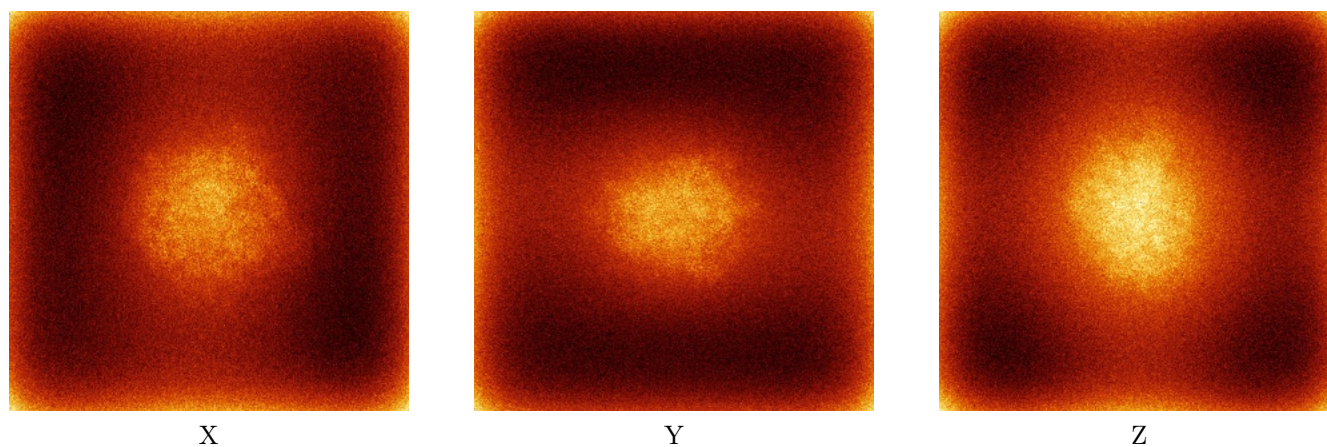
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



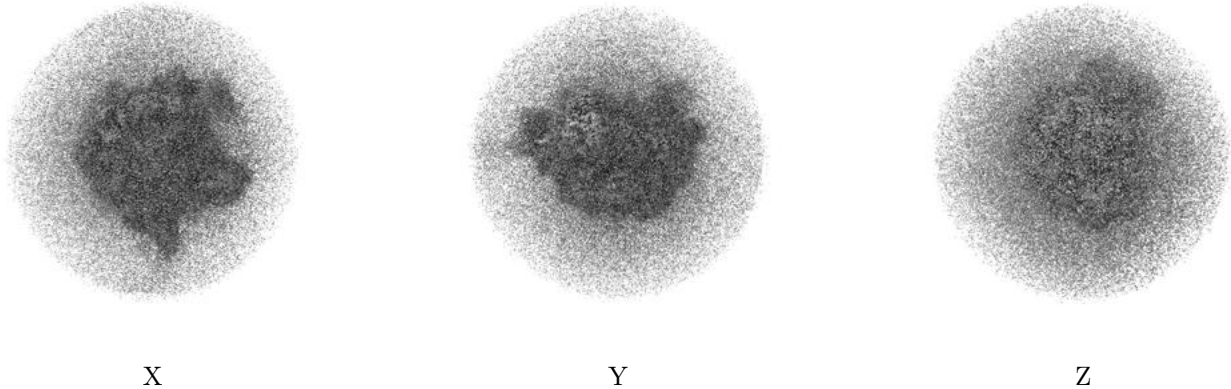
6.4.2 Raw map



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.

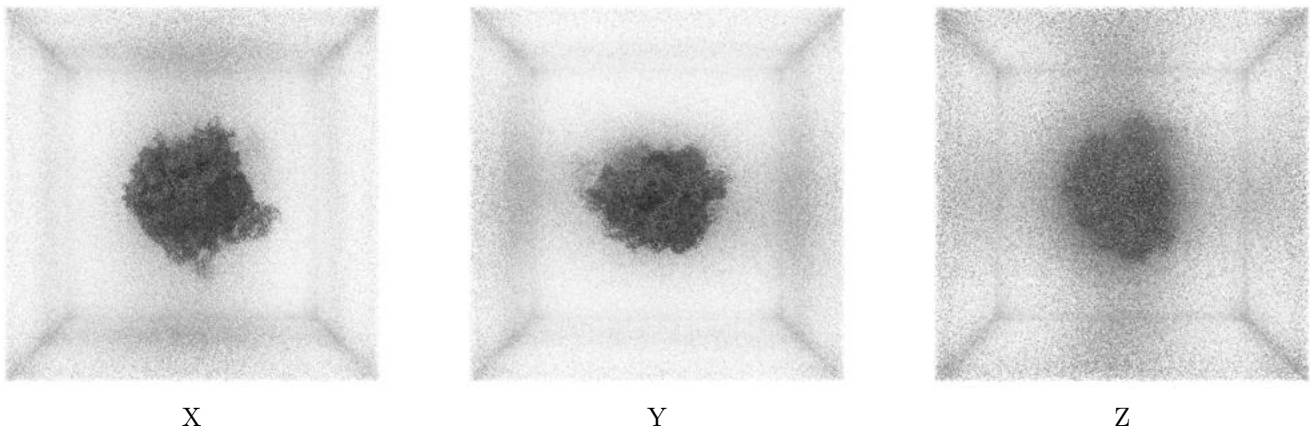
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

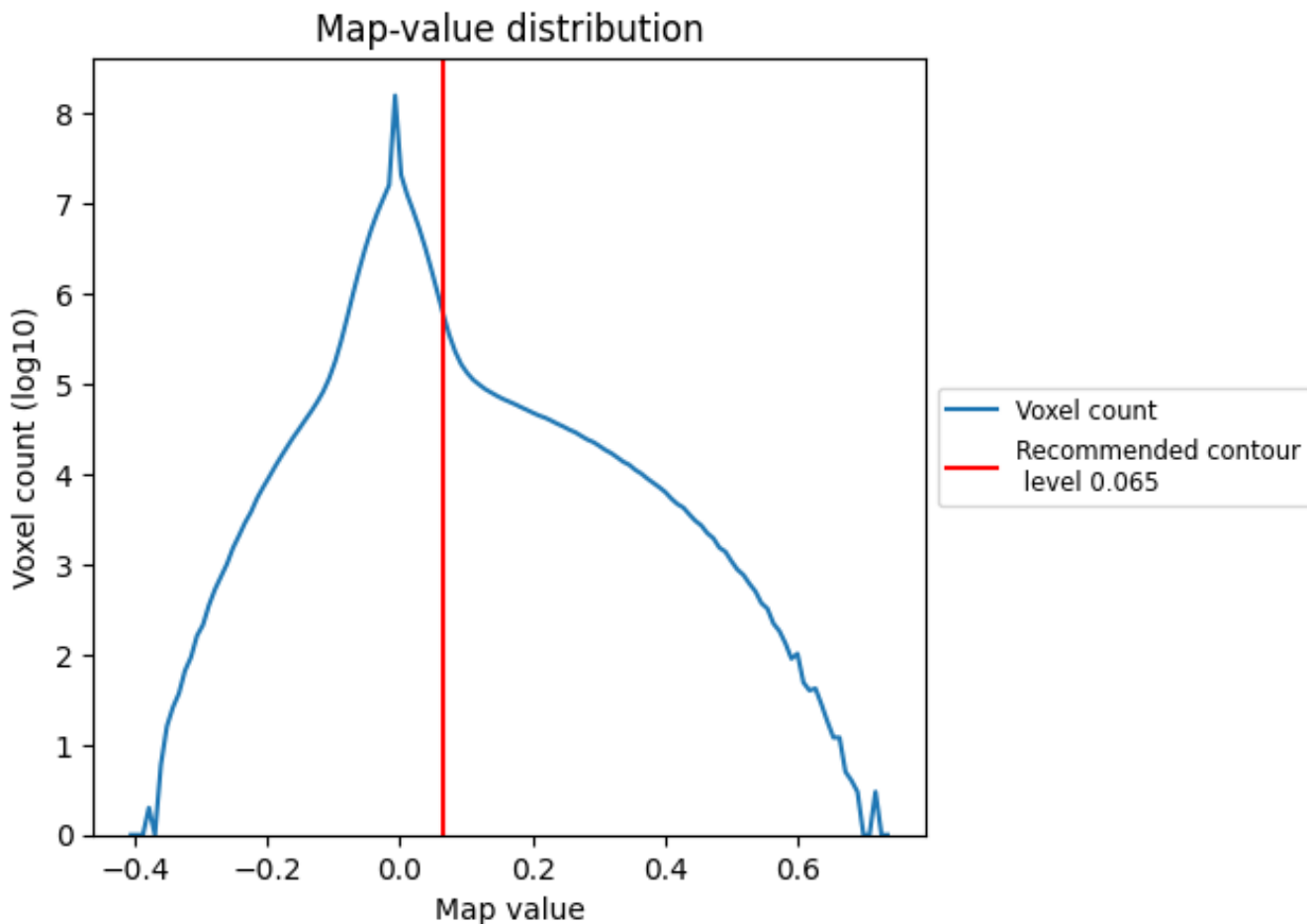
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

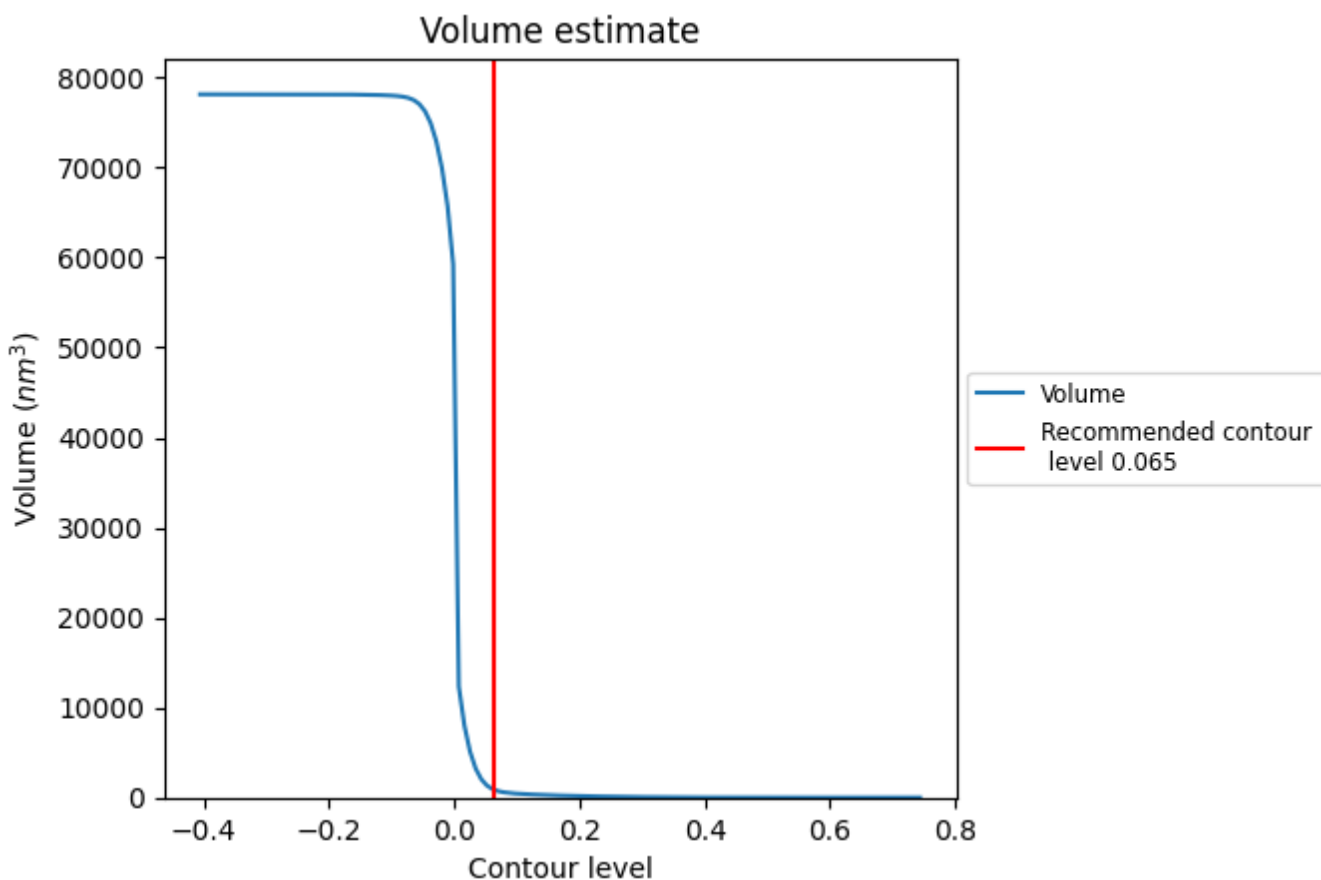
This section contains the results of statistical analysis of the map.

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.

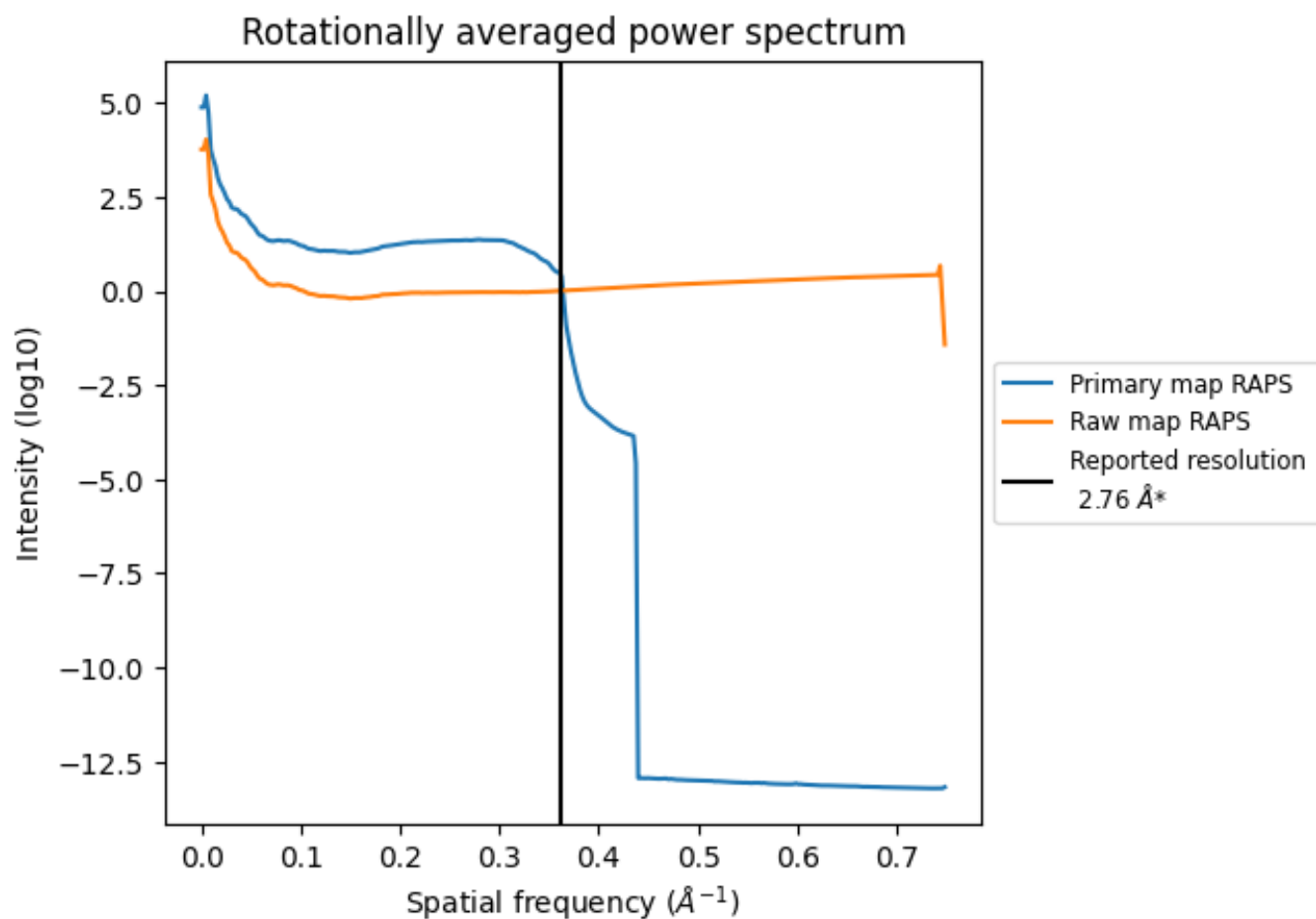
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 848 nm³; this corresponds to an approximate mass of 766 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

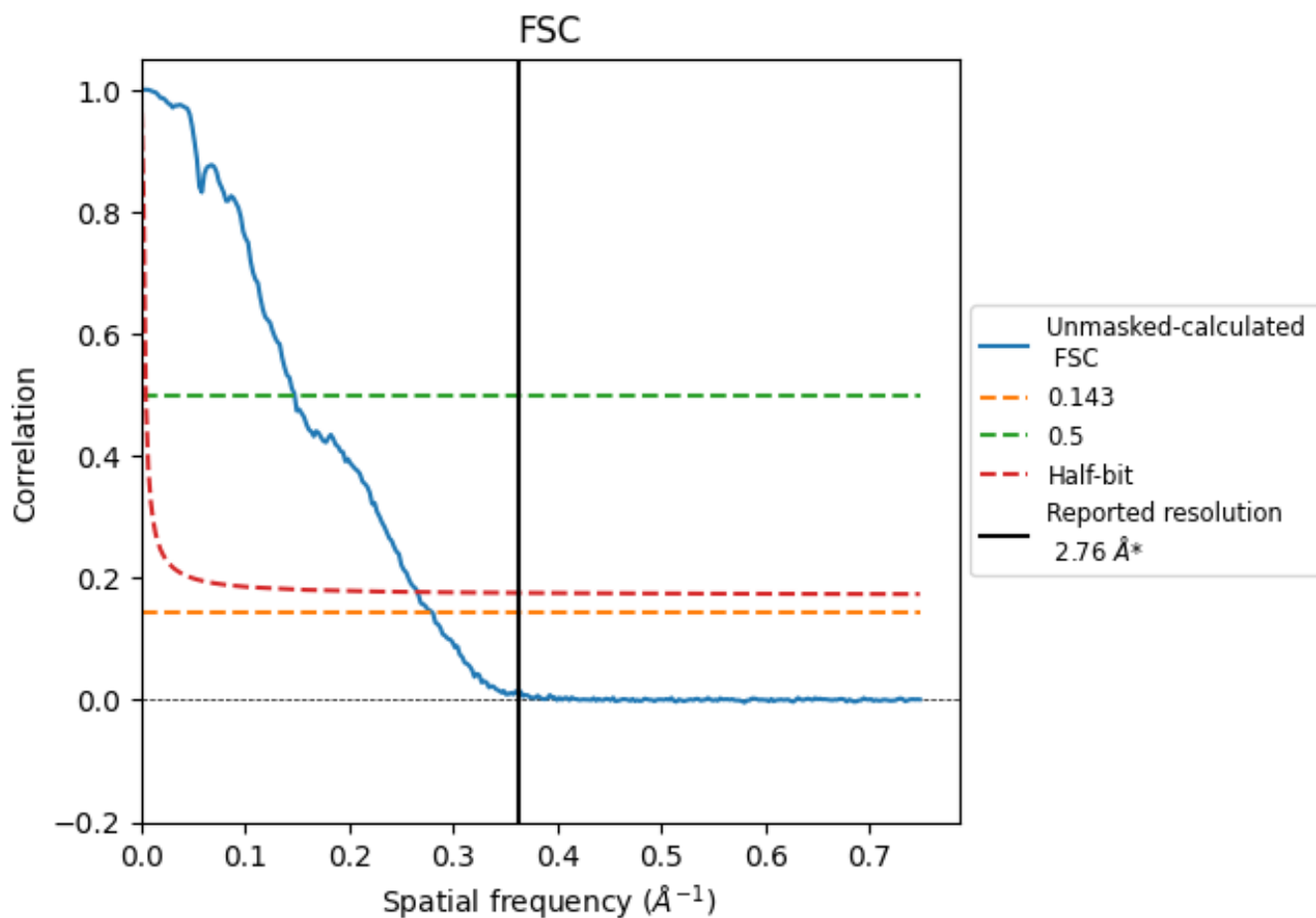


*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.362 Å⁻¹

8.2 Resolution estimates [i](#)

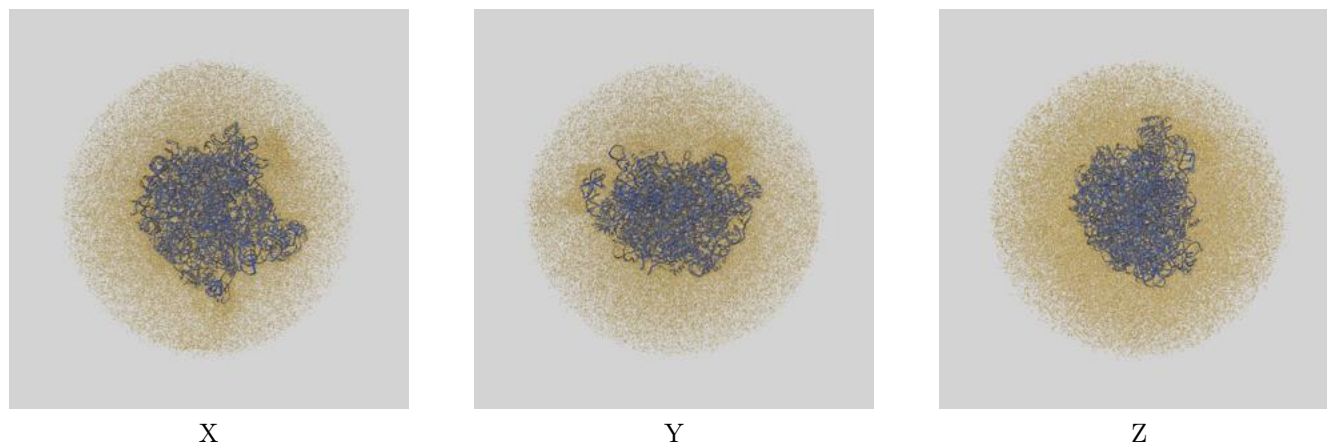
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	6.78	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

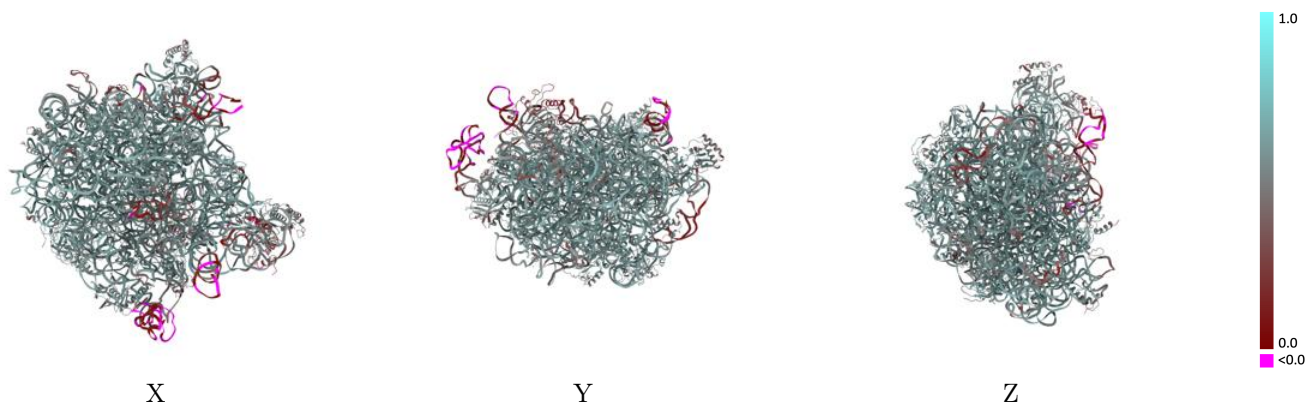
This section contains information regarding the fit between EMDB map EMD-62897 and PDB model 9L98. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



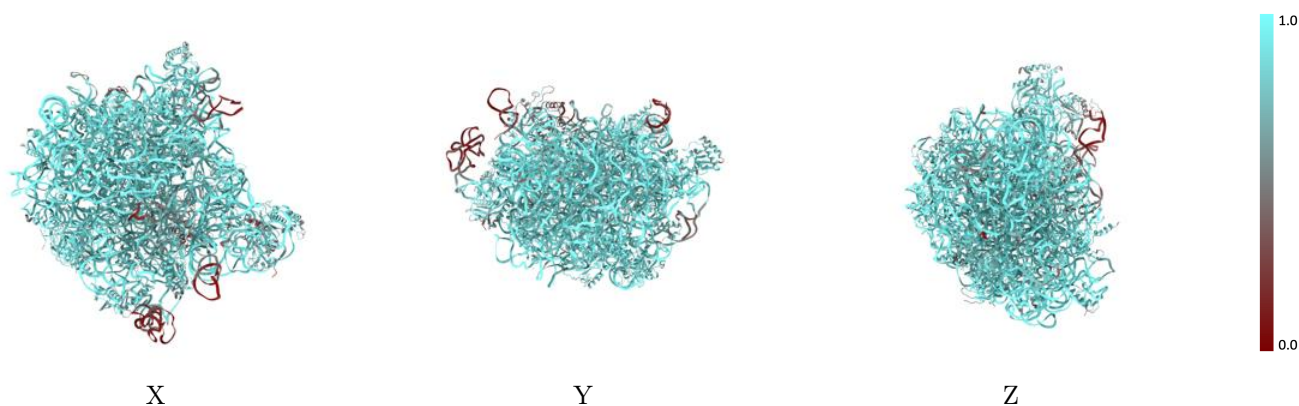
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



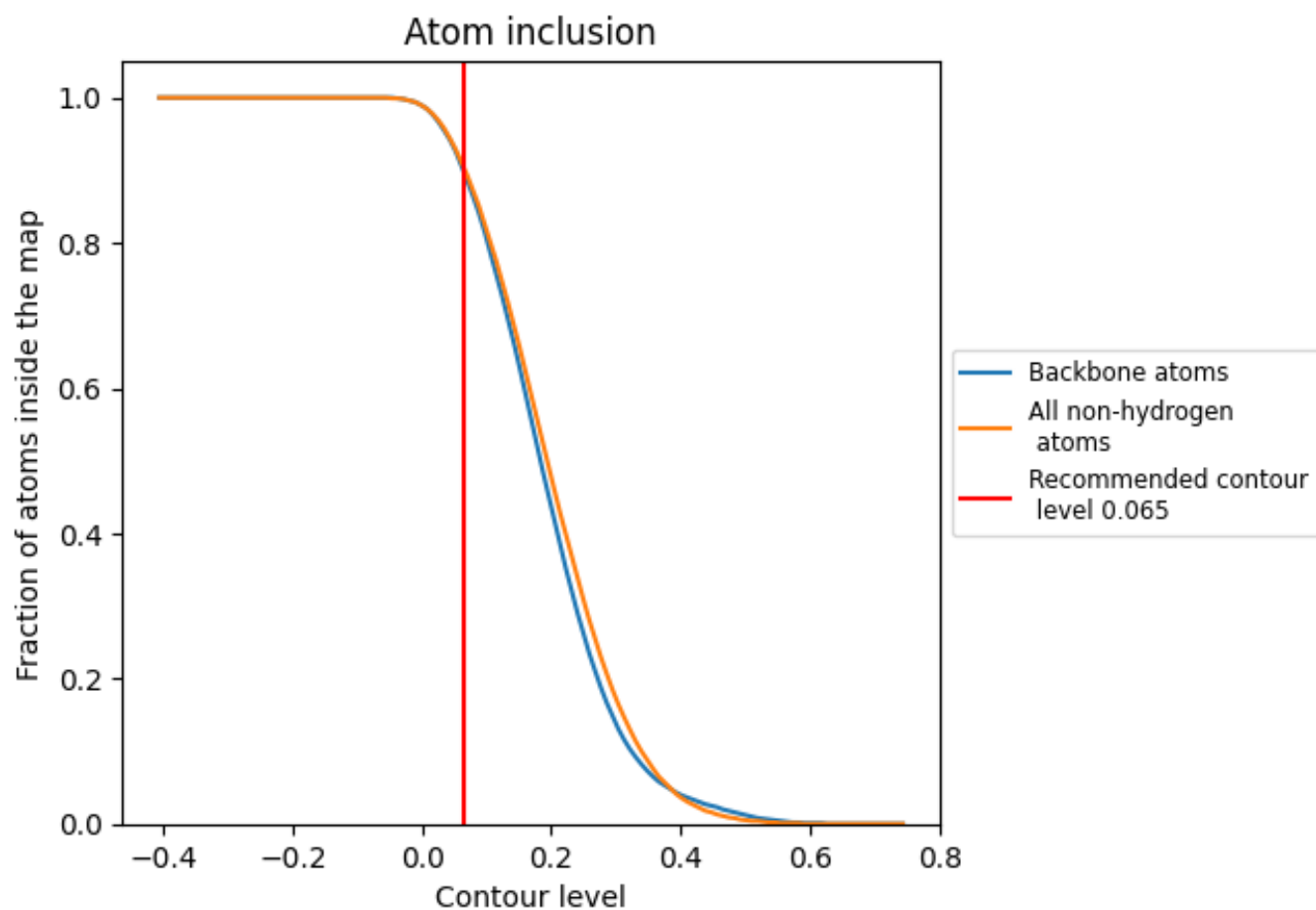
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.5550
0	 0.9250	 0.5580
9	 0.9380	 0.5550
A	 0.9190	 0.5660
E	 0.8200	 0.5210
F	 0.8760	 0.5680
G	 0.9560	 0.6160
H	 0.8950	 0.5640
I	 0.8480	 0.5170
J	 0.8960	 0.5650
K	 0.9390	 0.6000
L	 0.9230	 0.5970
M	 0.8720	 0.5400
N	 0.9040	 0.5810
O	 0.9170	 0.5840
P	 0.8530	 0.5420
Q	 0.8970	 0.5750
R	 0.8700	 0.5500
S	 0.9580	 0.6180
T	 0.9270	 0.5860
U	 0.9030	 0.5740
V	 0.9280	 0.5970
W	 0.9020	 0.5840
X	 0.6390	 0.3640
Y	 0.8210	 0.5250
a	 0.6180	 0.4520
b	 0.9180	 0.5730
c	 0.7850	 0.5030
d	 0.6860	 0.4310
e	 0.7130	 0.4980
f	 0.8950	 0.5630

