



Full wwPDB EM Validation Report ⓘ

Jul 2, 2026 – 03:01 PM JST

PDB ID : 9L9K / pdb_0000919k
EMDB ID : EMD-62908
Title : State E of archaeal pre-50S ribosome
Authors : Li, Z.Q.; Yang, X.Y.
Deposited on : 2024-12-30
Resolution : 2.36 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:

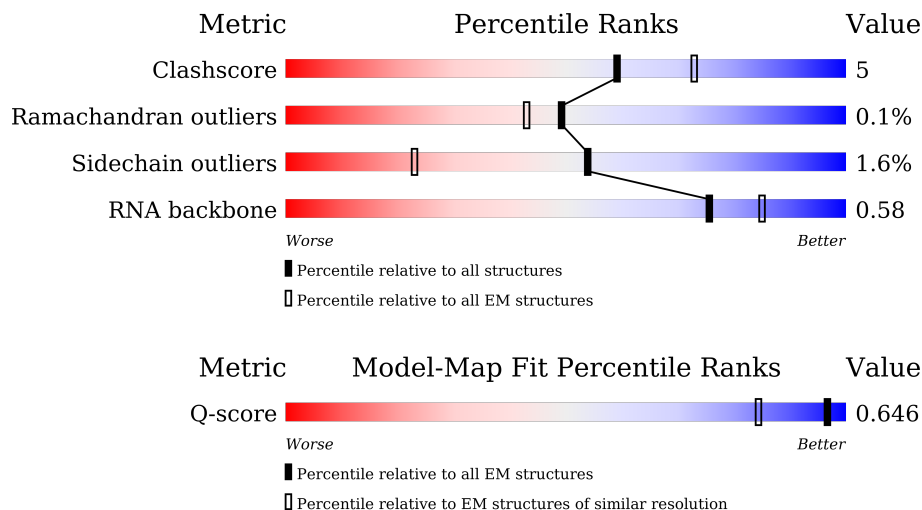
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

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

The reported resolution of this entry is 2.36 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.









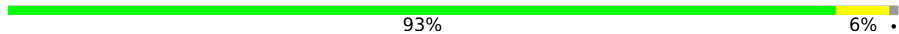



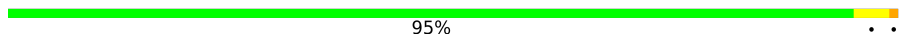




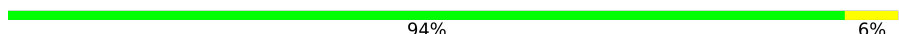

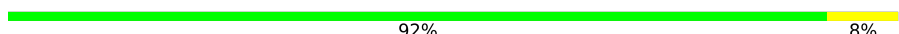
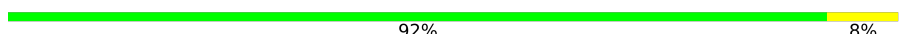






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4686 (1.86 - 2.86)

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	1	122	
3	i	168	

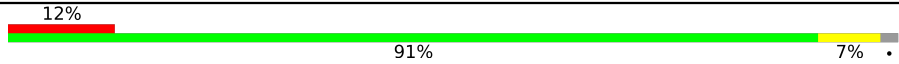

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Mol	Chain	Length	Quality of chain
4	E	120	 83% 13% ..
5	F	176	 84% 9% • 6%
6	G	196	 87% 11% •
7	H	116	 89% 9% ..
8	I	184	 87% 12% •
9	J	151	 83% 13% ..
10	K	96	 93% 6% •
11	L	153	 87% 11% ..
12	M	67	 70% 15% • 13%
13	N	118	 85% 12% •
14	O	154	 95% ..
15	P	92	 7% 84% 13% •
16	Q	234	 56% • 39%
17	R	89	 82% 7% • 10%
18	S	58	 90% 7% ..
19	T	93	 94% 6%
20	U	241	 86% 9% 5%
21	V	338	 92% 8%
22	W	248	 92% 8%
23	X	172	 16% 65% 33% ..
24	Y	178	 83% 15% ..
25	b	145	 88% 11% •
26	c	83	 5% 87% 12% •
27	d	70	 11% 73% 23% ..
28	f	132	 82% 17% •

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Mol	Chain	Length	Quality of chain
29	e	58	
30	A	50	

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 94687 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	2633	56457	25198	10407	18219	2633	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	120	2551	1138	453	840	120	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	i	154	1166	699	231	236	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	165	1316	820	239	249	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	192	1564	955	333	274	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	147	1179	712	243	223	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	230	Total	C	N	O	S	0	0
			1729	1069	338	317	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	1308	808	229	268	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	68	519	319	88	111	1	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein uL14.

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

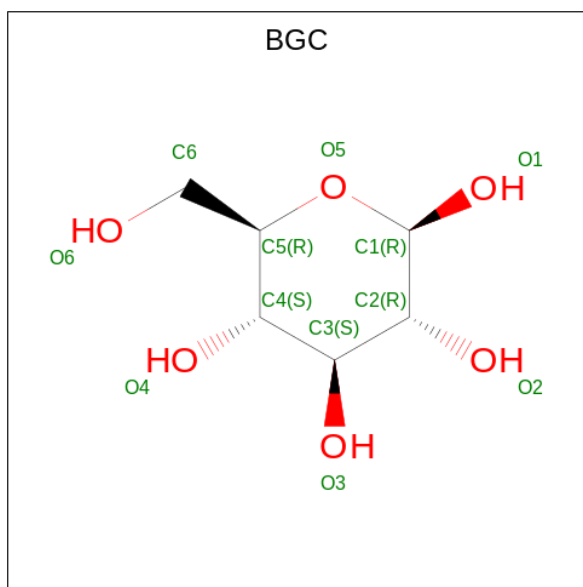
- Molecule 29 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	e	57	435	269	76	90	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	A	49	414	252	89	71	2	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	376	Total Mg 376 376	0
32	1	4	Total Mg 4 4	0
32	F	2	Total Mg 2 2	0
32	G	5	Total Mg 5 5	0
32	I	2	Total Mg 2 2	0
32	K	1	Total Mg 1 1	0
32	L	1	Total Mg 1 1	0
32	O	2	Total Mg 2 2	0
32	Q	1	Total Mg 1 1	0
32	T	1	Total Mg 1 1	0
32	U	2	Total Mg 2 2	0
32	V	3	Total Mg 3 3	0
32	W	1	Total Mg 1 1	0
32	b	1	Total Mg 1 1	0
32	f	1	Total Mg 1 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 Zn 1 1	0
33	T	1	Total Zn 1 1	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	0	4733	Total 4733	O 4733	0
34	1	72	Total 72	O 72	0
34	i	38	Total 38	O 38	0
34	E	5	Total 5	O 5	0
34	F	35	Total 35	O 35	0
34	G	79	Total 79	O 79	0
34	H	12	Total 12	O 12	0
34	I	7	Total 7	O 7	0
34	J	33	Total 33	O 33	0
34	K	32	Total 32	O 32	0
34	L	40	Total 40	O 40	0
34	M	7	Total 7	O 7	0
34	N	23	Total 23	O 23	0
34	O	49	Total 49	O 49	0
34	P	16	Total 16	O 16	0
34	Q	47	Total 47	O 47	0
34	R	14	Total 14	O 14	0
34	S	36	Total 36	O 36	0
34	T	28	Total 28	O 28	0
34	U	58	Total 58	O 58	0
34	V	108	Total 108	O 108	0
34	W	80	Total 80	O 80	0

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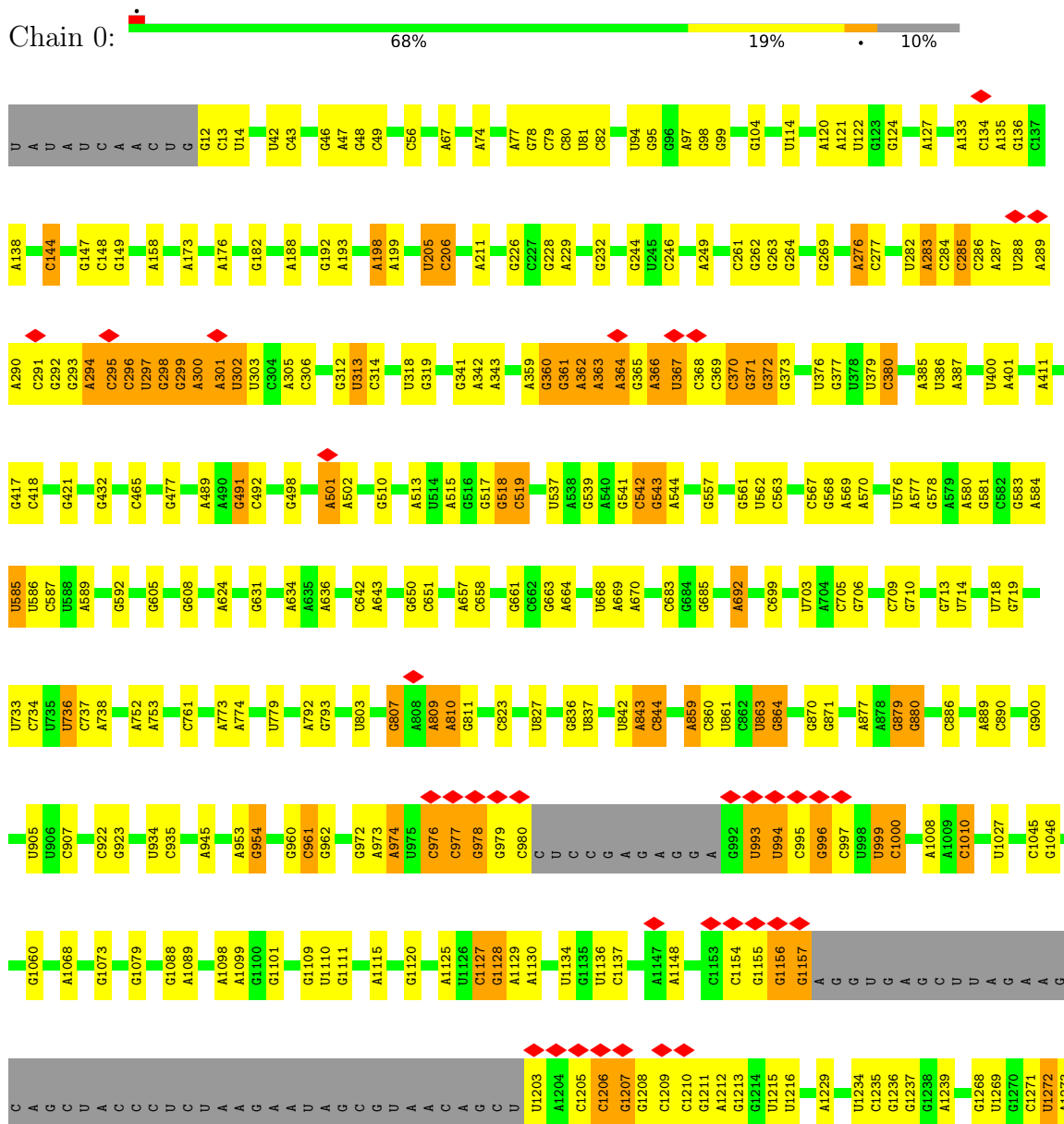
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Mol	Chain	Residues	Atoms		AltConf
34	Y	13	Total 13	O 13	0
34	b	29	Total 29	O 29	0
34	c	11	Total 11	O 11	0
34	d	1	Total 1	O 1	0
34	f	25	Total 25	O 25	0
34	e	3	Total 3	O 3	0
34	A	16	Total 16	O 16	0

3 Residue-property plots [i](#)

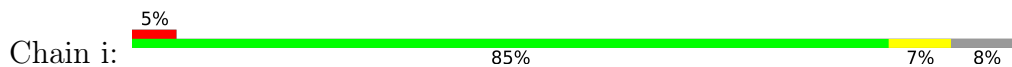
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 23S RNA

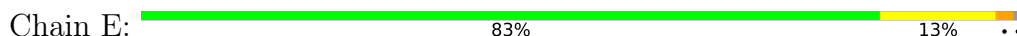




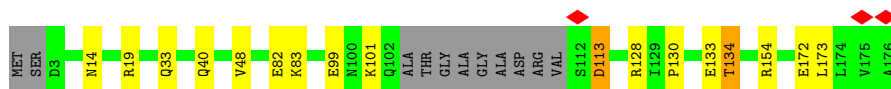
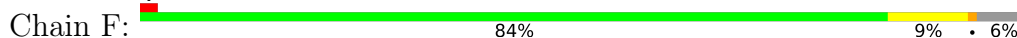
- Molecule 3: Large ribosomal subunit protein uL15



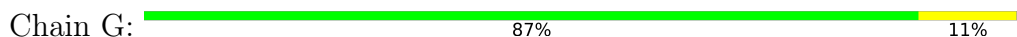
- Molecule 4: Large ribosomal subunit protein eL8



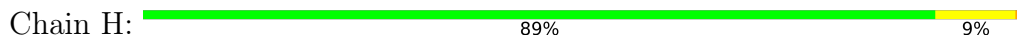
- Molecule 5: Large ribosomal subunit protein uL16



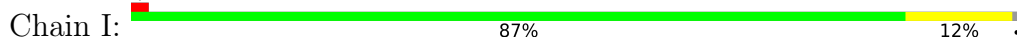
- Molecule 6: Large ribosomal subunit protein eL15




- Molecule 7: Large ribosomal subunit protein eL18



- Molecule 8: Large ribosomal subunit protein uL18



- Molecule 9: Large ribosomal subunit protein eL19

Chain J:  83% 13% ..




- Molecule 10: Large ribosomal subunit protein eL21

Chain K:  93% 6% ..



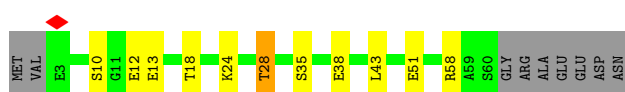
- Molecule 11: Large ribosomal subunit protein uL22

Chain L:  87% 11% ..




- Molecule 12: Large ribosomal subunit protein eL24

Chain M:  70% 15% 13%



- Molecule 13: Large ribosomal subunit protein uL24

Chain N:  85% 12% .




- Molecule 14: Large ribosomal subunit protein uL30

Chain O:  95% ..

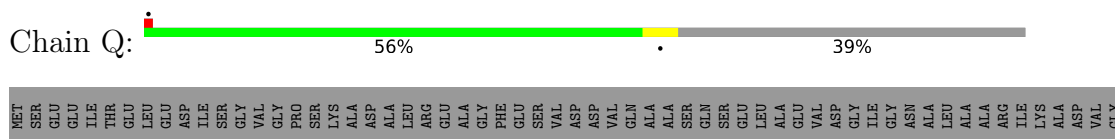


- Molecule 15: Large ribosomal subunit protein eL31

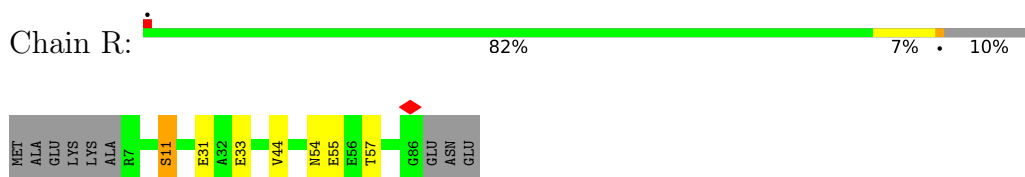
Chain P:  7% 84% 13% .



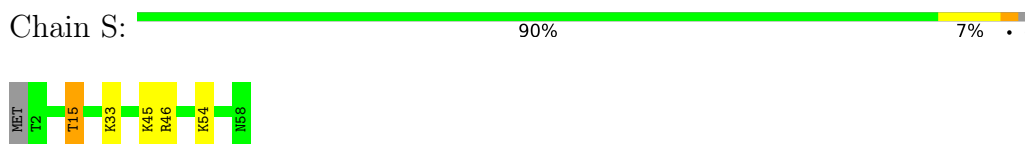
- Molecule 16: Large ribosomal subunit protein eL32



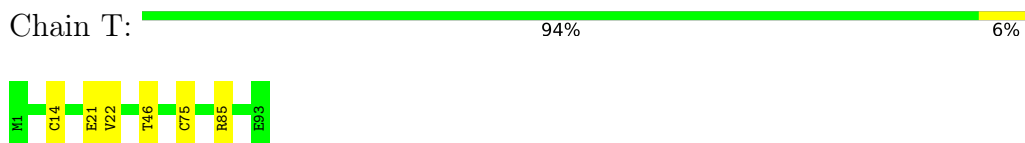
• Molecule 17: Large ribosomal subunit protein eL43



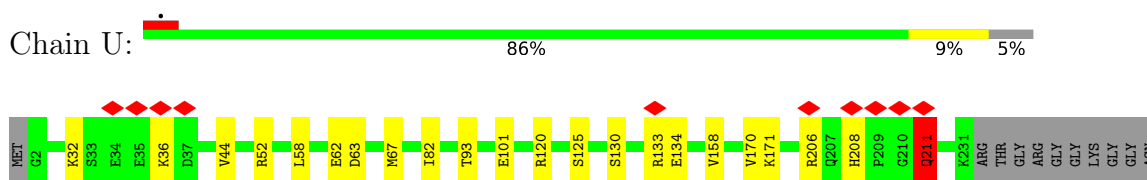
• Molecule 18: Large ribosomal subunit protein eL37



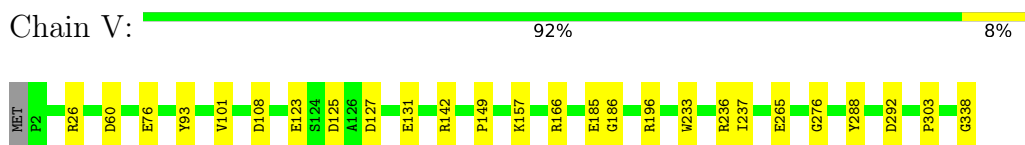
• Molecule 19: Large ribosomal subunit protein eL42



• Molecule 20: Large ribosomal subunit protein uL2



• Molecule 21: Large ribosomal subunit protein uL3

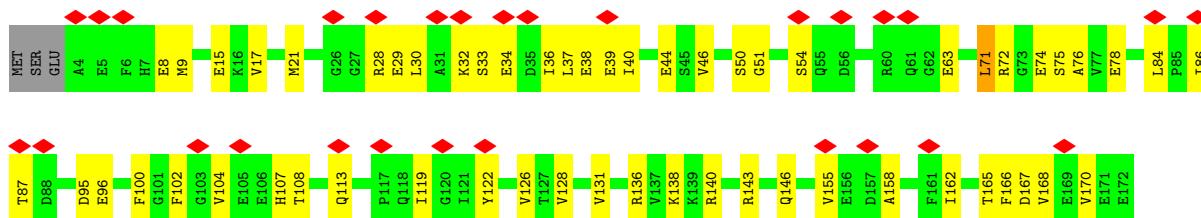


• Molecule 22: Large ribosomal subunit protein uL4

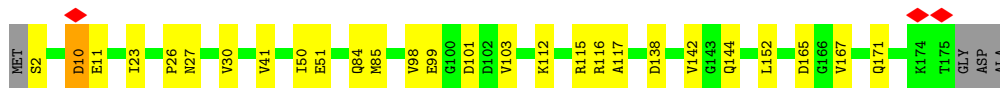
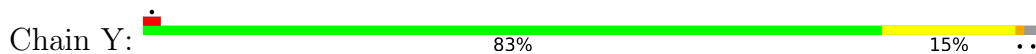




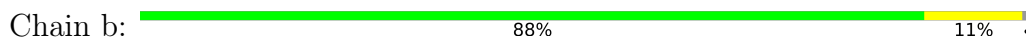
- Molecule 23: Large ribosomal subunit protein uL5



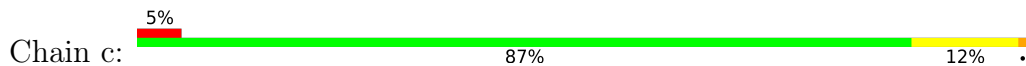
- Molecule 24: Large ribosomal subunit protein uL6



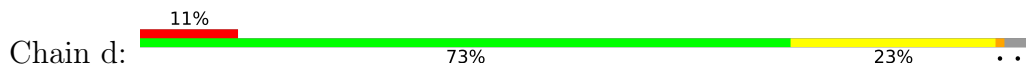
- Molecule 25: Large ribosomal subunit protein uL13



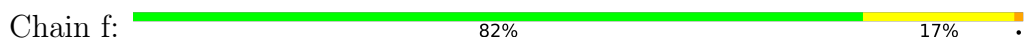
- Molecule 26: Large ribosomal subunit protein uL23



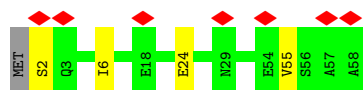
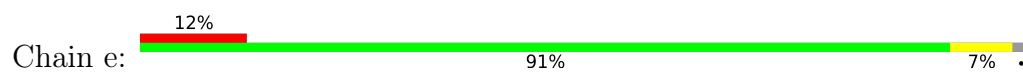
- Molecule 27: Large ribosomal subunit protein uL29



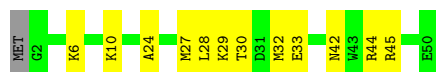
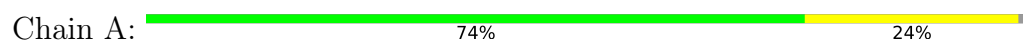
- Molecule 28: Large ribosomal subunit protein uL14



- Molecule 29: Large ribosomal subunit protein eL20



- Molecule 30: Large ribosomal subunit protein eL39



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	4.268	Depositor
Minimum map value	-1.882	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.28	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, 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	0.37	0/63219	0.33	3/98597 (0.0%)
2	1	0.31	0/2848	0.28	0/4436
3	i	0.24	0/1181	0.32	0/1584
4	E	0.26	0/889	0.37	0/1209
5	F	0.29	0/1338	0.39	0/1796
6	G	0.32	0/1591	0.31	0/2126
7	H	0.28	0/895	0.34	0/1210
8	I	0.25	0/1447	0.33	0/1969
9	J	0.29	0/1191	0.34	0/1587
10	K	0.31	0/750	0.33	0/1001
11	L	0.31	0/1199	0.37	0/1619
12	M	0.29	0/474	0.34	0/634
13	N	0.30	0/911	0.38	0/1232
14	O	0.30	0/1218	0.35	0/1651
15	P	0.29	0/741	0.38	0/998
16	Q	0.33	0/1165	0.35	0/1561
17	R	0.28	0/624	0.36	0/835
18	S	0.34	0/446	0.31	0/586
19	T	0.30	0/764	0.30	0/1015
20	U	0.29	0/1763	0.35	0/2372
21	V	0.33	0/2677	0.37	0/3617
22	W	0.30	0/1925	0.35	0/2598
23	X	0.24	0/1329	0.51	0/1793
24	Y	0.26	0/1368	0.33	0/1859
25	b	0.30	0/1144	0.32	0/1541
26	c	0.24	0/665	0.32	0/891
27	d	0.19	0/522	0.42	0/704
28	f	0.28	0/1004	0.37	0/1347
29	e	0.15	0/441	0.28	0/594
30	A	0.26	0/419	0.49	0/553
All	All	0.35	0/96148	0.34	3/143515 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	736	U	C4'-C3'-O3'	-5.84	100.63	109.40
1	0	863	U	C4'-C3'-O3'	-5.74	104.39	113.00
1	0	1519	U	C4'-C3'-O3'	-5.20	105.20	113.00

There are no chirality outliers.

There are no planarity outliers.

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	56457	0	28469	356	0
2	1	2551	0	1298	19	0
3	i	1166	0	1113	8	0
4	E	880	0	852	15	0
5	F	1316	0	1316	11	0
6	G	1564	0	1590	16	0
7	H	887	0	907	9	0
8	I	1417	0	1365	18	0
9	J	1179	0	1183	17	0
10	K	736	0	745	4	0
11	L	1174	0	1146	13	0
12	M	466	0	443	7	0
13	N	903	0	886	9	0
14	O	1200	0	1159	7	0
15	P	726	0	703	10	0
16	Q	1146	0	1146	11	0
17	R	617	0	618	3	0
18	S	439	0	445	5	0
19	T	746	0	736	5	0
20	U	1729	0	1760	16	0
21	V	2619	0	2572	19	0
22	W	1898	0	1895	12	0
23	X	1308	0	1251	45	0
24	Y	1346	0	1292	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	b	1127	0	1118	12	0
26	c	659	0	664	7	0
27	d	519	0	519	20	0
28	f	996	0	1046	18	0
29	e	435	0	426	2	0
30	A	414	0	442	8	0
31	0	12	0	12	5	0
32	0	376	0	0	3	0
32	1	4	0	0	0	0
32	F	2	0	0	0	0
32	G	5	0	0	0	0
32	I	2	0	0	0	0
32	K	1	0	0	0	0
32	L	1	0	0	0	0
32	O	2	0	0	0	0
32	Q	1	0	0	0	0
32	T	1	0	0	0	0
32	U	2	0	0	0	0
32	V	3	0	0	0	0
32	W	1	0	0	0	0
32	b	1	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	0	4733	0	0	41	0
34	1	72	0	0	0	0
34	A	16	0	0	0	0
34	E	5	0	0	1	0
34	F	35	0	0	2	0
34	G	79	0	0	2	0
34	H	12	0	0	1	0
34	I	7	0	0	0	0
34	J	33	0	0	0	0
34	K	32	0	0	0	0
34	L	40	0	0	3	0
34	M	7	0	0	0	0
34	N	23	0	0	0	0
34	O	49	0	0	2	0
34	P	16	0	0	2	0
34	Q	47	0	0	4	0
34	R	14	0	0	0	0
34	S	36	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	T	28	0	0	2	0
34	U	58	0	0	0	0
34	V	108	0	0	4	0
34	W	80	0	0	3	0
34	Y	13	0	0	0	0
34	b	29	0	0	0	0
34	c	11	0	0	1	0
34	d	1	0	0	0	0
34	e	3	0	0	0	0
34	f	25	0	0	1	0
34	i	38	0	0	1	0
All	All	94687	0	59117	673	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 5.

All (673) 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)
19:T:46:THR:HG22	34:T:219:HOH:O	1.18	1.31
18:S:33:LYS:HD3	34:S:228:HOH:O	1.33	1.21
1:0:1514:U:N3	1:0:1662:A:N6	2.01	1.07
19:T:14:CYS:SG	19:T:75:CYS:HB3	1.94	1.06
1:0:300:A:C5	1:0:360:G:N2	2.26	1.02
1:0:1519:U:H3	1:0:1521:A:H5'	1.23	1.01
1:0:300:A:N7	1:0:360:G:C2	2.29	1.00
1:0:1453:U:HO2'	1:0:1652:A:H8	1.05	0.99
11:L:34:ARG:HD2	34:L:315:HOH:O	1.61	0.98
22:W:224:ASP:OD1	34:W:401:HOH:O	1.82	0.96
1:0:1514:U:H3	1:0:1662:A:N6	1.64	0.94
1:0:580:A:N1	1:0:585:U:C5	2.37	0.92
1:0:580:A:N1	1:0:585:U:H5	1.69	0.91
1:0:79:C:OP1	34:0:3405:HOH:O	1.88	0.90
1:0:1517:A:HO2'	1:0:1518:A:H8	0.95	0.90
3:i:59:GLN:O	34:i:201:HOH:O	1.89	0.90
1:0:2663:A:N1	1:0:2812:U:C5	2.40	0.89
1:0:580:A:C2	1:0:585:U:H5	1.92	0.88
1:0:1285:U:H2'	34:0:3404:HOH:O	1.75	0.87
1:0:2761:G:H1'	34:0:4348:HOH:O	1.76	0.85
16:Q:133:THR:CB	34:Q:443:HOH:O	2.23	0.85
1:0:299:G:H1	1:0:361:G:H8	1.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:300:A:C5	1:0:360:G:C2	2.64	0.84
1:0:300:A:C8	1:0:360:G:N2	2.45	0.84
1:0:188:A:OP1	34:0:3408:HOH:O	1.97	0.83
1:0:1285:U:C2'	34:0:3404:HOH:O	2.24	0.83
1:0:2453:A:C6	31:0:3001:BGC:H1	2.15	0.82
1:0:2663:A:N1	1:0:2812:U:H5	1.76	0.82
1:0:2709:G:OP1	34:0:3407:HOH:O	1.96	0.82
16:Q:133:THR:HB	34:Q:443:HOH:O	1.79	0.82
1:0:2663:A:C2	1:0:2812:U:H5	1.99	0.81
34:0:7630:HOH:O	3:i:69:LYS:HD3	1.78	0.81
1:0:492:C:O2'	34:0:3409:HOH:O	1.98	0.81
16:Q:133:THR:HG22	34:Q:443:HOH:O	1.80	0.81
23:X:74:GLU:OE2	23:X:74:GLU:N	2.13	0.79
1:0:1529:C:H42	1:0:1652:A:H2	1.28	0.79
1:0:295:C:OP1	1:0:296:C:N4	2.15	0.79
1:0:300:A:C4	1:0:360:G:N2	2.51	0.79
1:0:300:A:N7	1:0:360:G:N2	2.28	0.78
4:E:66:GLU:OE2	4:E:66:GLU:N	2.16	0.78
16:Q:133:THR:CG2	34:Q:443:HOH:O	2.31	0.78
1:0:973:A:H2	1:0:1000:C:H42	1.31	0.77
15:P:7:GLU:N	15:P:7:GLU:OE1	2.19	0.76
1:0:2805:A:O2'	34:0:3406:HOH:O	1.90	0.75
22:W:136:GLU:N	22:W:136:GLU:OE1	2.19	0.75
1:0:12:G:N1	1:0:2910:C:N3	2.34	0.75
1:0:360:G:H1'	1:0:361:G:H5'	1.69	0.75
1:0:2730:C:OP2	9:J:62:ARG:NH2	2.19	0.74
1:0:1519:U:N3	1:0:1521:A:H5'	2.01	0.74
1:0:1520:A:H1'	1:0:1521:A:O5'	1.87	0.74
1:0:710:G:OP2	34:0:3414:HOH:O	2.06	0.74
1:0:827:U:O4	34:0:3412:HOH:O	2.03	0.74
1:0:1469:U:OP2	34:0:3413:HOH:O	2.05	0.73
28:f:63:GLU:OE1	28:f:63:GLU:N	2.19	0.73
28:f:116:GLU:N	28:f:116:GLU:OE2	2.21	0.73
1:0:2502:A:OP2	34:0:3415:HOH:O	2.06	0.72
1:0:1285:U:O2'	34:0:3404:HOH:O	1.82	0.72
28:f:2:GLU:OE1	28:f:2:GLU:N	2.22	0.72
20:U:208:HIS:HB3	20:U:211:GLN:HB2	1.71	0.72
1:0:2452:G:C5	31:0:3001:BGC:H2	2.25	0.71
20:U:62:GLU:OE2	20:U:62:GLU:N	2.16	0.71
1:0:498:G:N2	1:0:501:A:OP2	2.24	0.71
5:F:82:GLU:HG2	5:F:83:LYS:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:973:A:H2'	1:0:974:A:C8	2.26	0.70
1:0:2134:G:H21	1:0:2228:G:H2'	1.56	0.70
1:0:2713:C:O2	28:f:87:ARG:NH2	2.24	0.70
27:d:41:PRO:O	27:d:43:ASN:N	2.25	0.70
32:0:3099:MG:MG	34:0:3935:HOH:O	1.34	0.70
18:S:45:LYS:NZ	34:S:201:HOH:O	2.24	0.70
5:F:113:ASP:OD1	5:F:113:ASP:N	2.25	0.69
1:0:580:A:N1	1:0:585:U:C4	2.61	0.69
1:0:2083:A:H2'	1:0:2084:G:C8	2.28	0.69
2:1:41:C:O2	23:X:72:ARG:NH1	2.25	0.69
23:X:102:PHE:HB2	23:X:126:VAL:HB	1.75	0.68
1:0:1268:G:N7	34:0:3429:HOH:O	2.27	0.68
1:0:387:A:OP2	34:0:3416:HOH:O	2.11	0.68
28:f:100:GLU:N	28:f:100:GLU:OE1	2.27	0.68
5:F:40:GLN:N	5:F:40:GLN:OE1	2.27	0.68
34:0:5423:HOH:O	25:b:3:PHE:CE1	2.46	0.67
1:0:976:C:N4	1:0:996:G:O6	2.15	0.67
23:X:36:ILE:O	23:X:40:ILE:HG22	1.95	0.67
1:0:2134:G:N2	1:0:2228:G:H2'	2.10	0.66
1:0:2497:A:OP1	5:F:154:ARG:NH1	2.28	0.66
23:X:17:VAL:HG22	23:X:128:VAL:HG12	1.78	0.66
23:X:32:LYS:O	23:X:36:ILE:HD12	1.96	0.65
1:0:362:A:O2'	1:0:363:A:O4'	2.15	0.65
1:0:362:A:H1'	1:0:363:A:O5'	1.97	0.65
1:0:2663:A:N1	1:0:2812:U:C4	2.63	0.65
32:0:3034:MG:MG	34:0:5318:HOH:O	1.39	0.65
1:0:232:G:OP1	34:0:3417:HOH:O	2.15	0.65
5:F:99:GLU:HG2	5:F:101:LYS:HG2	1.77	0.65
28:f:60:GLY:O	28:f:65:ARG:NH1	2.30	0.65
7:H:40:THR:O	7:H:116:ARG:NH2	2.29	0.65
19:T:46:THR:CG2	34:T:219:HOH:O	1.99	0.65
1:0:297:U:O2	1:0:365:G:N1	2.30	0.64
20:U:101:GLU:HG2	20:U:130:SER:HA	1.79	0.64
1:0:1276:U:H1'	1:0:1277:A:C8	2.33	0.64
23:X:95:ASP:OD1	23:X:96:GLU:N	2.31	0.64
1:0:2062:U:OP2	34:0:3418:HOH:O	2.15	0.64
4:E:12:ASP:OD1	4:E:12:ASP:N	2.29	0.64
1:0:365:G:H1'	1:0:366:A:H62	1.62	0.63
8:I:105:ILE:O	8:I:108:ASN:ND2	2.30	0.63
1:0:370:C:H3'	1:0:371:G:C8	2.34	0.63
23:X:32:LYS:HD2	23:X:36:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:138:LYS:HD2	23:X:146:GLN:HE22	1.64	0.62
14:O:75:GLY:HA3	34:O:312:HOH:O	1.99	0.62
34:O:4078:HOH:O	21:V:157:LYS:HE2	1.98	0.62
15:P:83:GLU:OE2	15:P:83:GLU:N	2.26	0.62
1:O:2719:U:H5	34:O:5629:HOH:O	1.81	0.62
20:U:82:ILE:HG23	20:U:93:THR:HB	1.82	0.62
24:Y:27:ASN:O	24:Y:27:ASN:ND2	2.22	0.62
1:O:980:C:H42	1:O:993:U:H1'	1.65	0.62
26:c:49:GLU:HB2	26:c:66:ARG:HG2	1.79	0.62
32:O:3039:MG:MG	34:O:4616:HOH:O	1.42	0.62
21:V:26:ARG:HD3	34:V:516:HOH:O	1.99	0.62
21:V:108:ASP:OD1	21:V:108:ASP:N	2.32	0.62
1:O:246:C:H3'	34:O:4540:HOH:O	2.00	0.61
1:O:661:G:OP2	7:H:38:ARG:NH2	2.33	0.61
9:J:113:GLY:O	9:J:115:LEU:N	2.34	0.61
5:F:33:GLN:HB2	34:F:323:HOH:O	2.01	0.61
23:X:36:ILE:HA	23:X:39:GLU:HG2	1.82	0.61
1:O:360:G:O2'	1:O:361:G:N3	2.27	0.61
1:O:359:A:H3'	1:O:360:G:H5''	1.81	0.61
25:b:64:GLY:HA2	25:b:69:PRO:HD2	1.83	0.61
5:F:130:PRO:HD2	5:F:133:GLU:HG3	1.83	0.61
3:i:88:ASP:OD1	3:i:88:ASP:N	2.33	0.61
30:A:32:MET:HE3	30:A:32:MET:HA	1.82	0.60
1:O:1514:U:C4	1:O:1662:A:N6	2.69	0.60
27:d:42:GLU:OE1	27:d:43:ASN:HB2	2.00	0.60
3:i:61:THR:OG1	3:i:105:ASP:OD1	2.16	0.60
12:M:24:LYS:HD3	12:M:28:THR:HG23	1.84	0.60
1:O:973:A:H2'	1:O:974:A:H8	1.65	0.59
30:A:30:THR:HB	30:A:33:GLU:HB2	1.85	0.59
1:O:543:G:H2'	1:O:544:A:C8	2.37	0.59
1:O:807:G:N2	1:O:809:A:H8	2.01	0.59
21:V:149:PRO:HD2	34:V:562:HOH:O	2.01	0.59
1:O:99:G:H5'	27:d:43:ASN:HD21	1.65	0.59
1:O:376:U:H2'	1:O:377:G:C8	2.38	0.59
20:U:58:LEU:HD13	20:U:67:MET:HE2	1.84	0.59
26:c:9:VAL:HA	26:c:14:MET:HE3	1.85	0.59
6:G:153:ASN:OD1	6:G:154:ASP:N	2.35	0.59
15:P:72:ARG:NH1	34:P:101:HOH:O	2.36	0.59
7:H:41:HIS:ND1	34:H:201:HOH:O	2.32	0.59
5:F:134:THR:HG22	34:F:326:HOH:O	2.02	0.58
1:O:2098:C:H2'	1:O:2099:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2238:C:OP1	6:G:33:ARG:NH1	2.36	0.58
30:A:24:ALA:HA	30:A:27:MET:HE3	1.86	0.58
4:E:70:GLU:N	4:E:70:GLU:OE1	2.36	0.58
6:G:193:ARG:HD3	34:G:327:HOH:O	2.04	0.58
1:0:205:U:O2'	1:0:206:C:O5'	2.16	0.58
4:E:32:LYS:NZ	34:E:201:HOH:O	2.35	0.58
5:F:14:ASN:O	5:F:128:ARG:NH2	2.36	0.58
1:0:80:C:OP1	27:d:56:ARG:NH1	2.36	0.58
8:I:87:TYR:O	8:I:91:ILE:HD12	2.04	0.58
24:Y:101:ASP:OD1	24:Y:101:ASP:N	2.34	0.58
1:0:1802:G:N2	1:0:1805:G:OP2	2.33	0.58
1:0:1567:A:H2'	1:0:1568:A:C8	2.39	0.57
23:X:71:LEU:HD13	23:X:76:ALA:HA	1.85	0.57
29:e:6:ILE:HD12	29:e:55:VAL:HG22	1.86	0.57
23:X:15:GLU:HB2	23:X:131:VAL:HG22	1.86	0.57
1:0:2619:C:OP2	20:U:206:ARG:NH1	2.36	0.57
1:0:1276:U:H1'	1:0:1277:A:N7	2.20	0.57
29:e:2:SER:N	29:e:24:GLU:OE2	2.37	0.57
9:J:39:GLU:OE1	9:J:42:ARG:NH2	2.29	0.57
21:V:276:GLY:O	21:V:292:ASP:HA	2.05	0.57
1:0:809:A:O2'	1:0:810:A:O4'	2.23	0.57
1:0:2319:U:H2'	1:0:2320:U:C6	2.40	0.57
1:0:2355:A:H2'	1:0:2356:G:C8	2.40	0.57
1:0:1129:A:H2'	1:0:1130:A:C8	2.39	0.56
3:i:145:GLU:N	3:i:145:GLU:OE2	2.37	0.56
3:i:149:GLU:OE2	3:i:149:GLU:N	2.38	0.56
1:0:56:C:O2	18:S:46:ARG:NH1	2.38	0.56
1:0:365:G:H1'	1:0:366:A:N7	2.20	0.56
27:d:12:MET:O	27:d:17:ARG:NH1	2.39	0.56
1:0:1209:C:H2'	1:0:1210:C:C6	2.40	0.56
1:0:510:G:N1	1:0:513:A:OP2	2.38	0.56
1:0:1276:U:O2	1:0:1276:U:O4'	2.21	0.56
22:W:213:ASP:OD2	34:W:402:HOH:O	2.17	0.56
27:d:7:GLU:N	27:d:7:GLU:OE1	2.38	0.56
1:0:1239:A:OP2	25:b:60:ARG:NH2	2.29	0.56
6:G:65:ARG:HD2	34:G:310:HOH:O	2.05	0.56
1:0:2772:G:H21	24:Y:144:GLN:HE22	1.54	0.56
23:X:162:ILE:HG23	23:X:166:PHE:CE2	2.41	0.56
1:0:293:G:H2'	1:0:294:A:C8	2.41	0.56
27:d:16:GLU:OE2	27:d:16:GLU:N	2.21	0.56
1:0:293:G:N1	1:0:295:C:OP2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:97:A:N6	34:0:3448:HOH:O	2.32	0.55
1:0:1510:U:H2'	1:0:1511:U:C6	2.41	0.55
1:0:1702:A:O2'	34:0:3411:HOH:O	2.02	0.55
1:0:2336:G:H1'	1:0:2337:A:C8	2.41	0.55
1:0:1517:A:H1'	1:0:1518:A:H5'	1.88	0.55
4:E:104:GLU:OE2	4:E:104:GLU:N	2.38	0.55
1:0:1157:G:O2'	1:0:1203:U:O4	2.15	0.55
1:0:380:C:H4'	6:G:2:ALA:HB3	1.87	0.55
16:Q:102:GLN:HA	16:Q:102:GLN:OE1	2.07	0.55
22:W:247:GLU:N	22:W:247:GLU:OE2	2.39	0.55
27:d:12:MET:HE3	27:d:16:GLU:HG2	1.87	0.55
13:N:104:LEU:HD13	13:N:110:GLU:HG3	1.89	0.55
27:d:12:MET:HB3	27:d:16:GLU:HG2	1.88	0.55
1:0:1534:U:H2'	1:0:1535:A:C8	2.42	0.55
1:0:843:A:O2'	1:0:844:C:OP1	2.25	0.55
24:Y:84:GLN:HB2	24:Y:171:GLN:HB3	1.89	0.55
15:P:24:HIS:CD2	34:P:111:HOH:O	2.59	0.54
24:Y:11:GLU:OE2	24:Y:26:PRO:HD3	2.07	0.54
17:R:11:SER:OG	17:R:31:GLU:OE1	2.18	0.54
1:0:1534:U:H2'	1:0:1535:A:H8	1.72	0.54
1:0:1828:U:H5	1:0:1833:A:N7	2.05	0.54
15:P:5:ASP:N	15:P:5:ASP:OD1	2.38	0.54
1:0:299:G:N1	1:0:361:G:H8	2.01	0.54
1:0:2098:C:H2'	1:0:2099:C:H6	1.73	0.54
12:M:10:SER:OG	12:M:12:GLU:HG3	2.07	0.54
23:X:140:ARG:NH2	23:X:143:ARG:O	2.39	0.54
1:0:198:A:OP1	6:G:177:ARG:NH2	2.41	0.54
1:0:300:A:H5''	1:0:302:U:C6	2.43	0.54
1:0:583:G:H2'	1:0:584:A:C8	2.42	0.54
1:0:803:U:O2'	9:J:131:GLU:OE1	2.26	0.54
1:0:2318:U:H2'	1:0:2319:U:C6	2.43	0.54
1:0:1127:C:H4'	1:0:1128:G:O5'	2.08	0.53
1:0:2663:A:C2	1:0:2812:U:C5	2.87	0.53
4:E:15:ASP:O	4:E:19:GLU:HG2	2.08	0.53
1:0:286:C:O2	1:0:372:G:N1	2.35	0.53
1:0:1520:A:N3	1:0:1520:A:H2'	2.24	0.53
1:0:1634:G:H2'	1:0:1635:G:O4'	2.09	0.53
1:0:1679:A:H1'	30:A:44:ARG:HH22	1.73	0.53
13:N:13:ARG:O	13:N:20:ARG:NH2	2.41	0.53
1:0:284:C:H2'	1:0:285:C:C5	2.43	0.53
1:0:360:G:O2'	1:0:361:G:H2'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:863:U:O2'	1:0:864:G:C8	2.62	0.53
1:0:994:U:O2'	1:0:995:C:O4'	2.21	0.53
1:0:1098:A:H2'	1:0:1099:A:C8	2.44	0.53
21:V:265:GLU:OE1	21:V:303:PRO:HD3	2.09	0.53
1:0:2361:A:N6	8:I:19:THR:O	2.42	0.53
1:0:2453:A:C5	31:0:3001:BGC:H1	2.44	0.53
2:1:75:C:H3'	2:1:76:A:H5''	1.91	0.53
25:b:51:GLU:CD	25:b:51:GLU:H	2.16	0.53
1:0:581:G:N2	1:0:584:A:OP2	2.32	0.53
23:X:107:HIS:HE1	23:X:113:GLN:HE21	1.57	0.53
1:0:2099:C:H2'	1:0:2100:U:C6	2.45	0.52
1:0:960:G:H2'	1:0:961:C:C6	2.44	0.52
1:0:1156:G:C6	1:0:1206:C:C4	2.97	0.52
1:0:1587:G:O2'	1:0:1588:C:O4'	2.24	0.52
6:G:16:PRO:HA	6:G:21:LEU:HD23	1.90	0.52
1:0:1664:G:O2'	34:0:3403:HOH:O	1.60	0.52
1:0:2244:G:O6	20:U:32:LYS:NZ	2.36	0.52
23:X:28:ARG:NH2	23:X:29:GLU:HA	2.23	0.52
1:0:954:G:N3	1:0:2295:A:H2'	2.25	0.52
1:0:1454:A:H2'	1:0:1455:A:C8	2.44	0.52
1:0:1372:G:H5'	1:0:1376:G:C6	2.45	0.52
8:I:144:ARG:HA	8:I:173:PHE:CD2	2.45	0.52
28:f:44:HIS:HD2	34:f:312:HOH:O	1.93	0.52
23:X:39:GLU:OE2	23:X:113:GLN:NE2	2.33	0.52
4:E:108:ASP:O	4:E:112:ILE:HG13	2.10	0.52
23:X:51:GLY:N	23:X:54:SER:OG	2.37	0.52
15:P:47:GLU:OE2	15:P:47:GLU:N	2.34	0.52
1:0:2740:G:H5'	34:0:5590:HOH:O	2.10	0.51
21:V:157:LYS:NZ	34:V:505:HOH:O	2.44	0.51
8:I:39:VAL:HG12	8:I:44:VAL:HG22	1.91	0.51
8:I:179:ASN:O	8:I:182:GLU:HG3	2.11	0.51
1:0:1010:C:OP1	5:F:19:ARG:NH1	2.40	0.51
1:0:293:G:H22	1:0:295:C:H5	1.58	0.51
30:A:6:LYS:O	30:A:10:LYS:HG3	2.10	0.51
17:R:55:GLU:OE2	17:R:55:GLU:HA	2.11	0.51
2:1:23:U:H3'	2:1:24:U:O2	2.10	0.51
23:X:84:LEU:HD23	23:X:102:PHE:HZ	1.75	0.51
1:0:1510:U:H2'	1:0:1511:U:H6	1.75	0.51
11:L:77:ASP:OD1	11:L:77:ASP:N	2.37	0.51
1:0:1271:C:O2'	1:0:1272:U:H5'	2.11	0.51
1:0:1511:U:H2'	1:0:1512:C:H6	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:42:U:H2'	1:0:43:C:C6	2.45	0.51
1:0:362:A:N3	1:0:363:A:H4'	2.26	0.51
24:Y:117:ALA:HB2	24:Y:152:LEU:HD22	1.93	0.51
27:d:12:MET:HE2	27:d:17:ARG:HG2	1.93	0.51
7:H:55:GLU:N	7:H:55:GLU:OE2	2.44	0.51
21:V:76:GLU:OE2	21:V:288:TYR:OH	2.27	0.51
23:X:30:LEU:O	23:X:34:GLU:HG3	2.11	0.51
27:d:8:GLU:O	27:d:12:MET:HG3	2.11	0.51
1:0:300:A:H2'	1:0:302:U:O4'	2.11	0.50
9:J:43:GLU:O	9:J:47:GLU:HG3	2.11	0.50
24:Y:115:ARG:NH1	24:Y:152:LEU:O	2.44	0.50
26:c:75:GLU:CD	26:c:79:ARG:HH21	2.19	0.50
1:0:543:G:H2'	1:0:544:A:H8	1.75	0.50
1:0:1453:U:O2'	1:0:1652:A:H8	1.83	0.50
1:0:2108:U:H2'	1:0:2109:U:C6	2.46	0.50
1:0:977:C:N4	1:0:996:G:H1	2.09	0.50
1:0:2408:A:O2'	8:I:30:SER:HB3	2.11	0.50
27:d:5:TYR:O	27:d:8:GLU:HG2	2.11	0.50
1:0:300:A:C8	1:0:360:G:C2	2.94	0.50
1:0:2677:U:H2'	1:0:2678:U:C6	2.46	0.50
1:0:2354:A:H2'	1:0:2355:A:C8	2.47	0.50
23:X:155:VAL:HB	23:X:158:ALA:HB3	1.92	0.50
26:c:14:MET:HE2	26:c:14:MET:HA	1.93	0.50
1:0:2580:U:H2'	1:0:2582:U:H5	1.77	0.50
8:I:170:PRO:O	8:I:173:PHE:HB3	2.11	0.50
6:G:100:ARG:HD3	6:G:168:GLY:HA2	1.93	0.50
20:U:63:ASP:OD1	20:U:63:ASP:N	2.44	0.50
25:b:76:ASP:N	25:b:76:ASP:OD1	2.45	0.50
1:0:301:A:N6	1:0:303:U:H5'	2.26	0.49
1:0:2850:C:H2'	1:0:2851:U:C6	2.47	0.49
24:Y:99:GLU:OE1	24:Y:116:ARG:NH2	2.31	0.49
1:0:537:U:O2	25:b:95:ARG:NH2	2.45	0.49
1:0:569:A:H2'	1:0:570:A:C8	2.47	0.49
1:0:1511:U:H2'	1:0:1512:C:C6	2.47	0.49
1:0:542:C:H5''	1:0:543:G:C8	2.48	0.49
12:M:38:GLU:OE2	28:f:89:LYS:NZ	2.45	0.49
17:R:44:VAL:HG12	17:R:54:ASN:HA	1.94	0.49
25:b:126:ASN:HD22	25:b:127:ILE:N	2.09	0.49
1:0:305:A:H2'	1:0:306:C:C6	2.48	0.49
23:X:167:ASP:OD1	23:X:168:VAL:HG22	2.13	0.49
1:0:13:C:H2'	1:0:14:U:C6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:642:C:H2'	1:0:643:A:C8	2.47	0.49
21:V:185:GLU:HG3	21:V:186:GLY:H	1.77	0.49
22:W:33:ARG:NH1	22:W:106:GLU:OE2	2.45	0.49
1:0:95:G:N7	30:A:29:LYS:HD2	2.28	0.49
1:0:999:U:H2'	1:0:1000:C:C6	2.48	0.49
1:0:1882:C:HO2'	1:0:1883:U:C5'	2.25	0.49
9:J:109:LEU:HB3	9:J:115:LEU:HD12	1.95	0.49
1:0:1277:A:HO2'	1:0:1278:G:H8	1.59	0.49
1:0:2269:U:H2'	1:0:2270:U:C6	2.48	0.49
1:0:1519:U:C4	1:0:1520:A:H8	2.31	0.49
1:0:2134:G:O5'	1:0:2134:G:H8	1.96	0.49
13:N:110:GLU:O	13:N:114:LYS:HG3	2.12	0.49
1:0:297:U:O2'	1:0:362:A:N6	2.45	0.49
4:E:32:LYS:HD3	4:E:88:ALA:HB1	1.94	0.49
15:P:84:SER:C	15:P:85:ILE:HD13	2.37	0.49
24:Y:27:ASN:HD22	24:Y:27:ASN:C	2.11	0.49
1:0:300:A:N7	1:0:360:G:N1	2.60	0.49
1:0:2230:G:H2'	1:0:2230:G:N3	2.28	0.49
9:J:112:ASP:OD1	9:J:114:THR:OG1	2.31	0.49
15:P:55:ILE:HG13	15:P:90:PRO:HD3	1.95	0.49
20:U:52:ARG:NH1	20:U:120:ARG:O	2.46	0.49
1:0:364:A:H1'	1:0:365:G:C2	2.48	0.48
1:0:752:A:H2'	1:0:753:A:C8	2.48	0.48
1:0:1459:U:H2'	1:0:1460:A:H8	1.78	0.48
2:1:38:U:O2'	2:1:43:A:N6	2.45	0.48
1:0:2313:A:H4'	1:0:2314:A:O4'	2.14	0.48
15:P:72:ARG:HH11	15:P:72:ARG:HG2	1.78	0.48
22:W:29:ASP:OD1	22:W:29:ASP:N	2.41	0.48
28:f:22:ASP:OD1	28:f:24:THR:HG23	2.13	0.48
1:0:98:G:O2'	27:d:43:ASN:ND2	2.46	0.48
1:0:1418:U:H2'	1:0:1419:C:C6	2.48	0.48
1:0:2099:C:H2'	1:0:2100:U:H6	1.78	0.48
1:0:144:C:OP1	1:0:264:G:O2'	2.31	0.48
1:0:1366:G:OP1	11:L:65:SER:HB3	2.13	0.48
14:O:27:HIS:HE1	34:O:329:HOH:O	1.95	0.48
1:0:114:U:O2'	34:O:3410:HOH:O	2.00	0.48
1:0:807:G:H21	1:0:809:A:H8	1.60	0.48
1:0:733:U:H2'	1:0:734:C:C6	2.49	0.48
1:0:879:G:H5'	1:0:880:G:OP1	2.13	0.48
1:0:2244:G:H2'	1:0:2245:C:C6	2.48	0.48
1:0:2813:U:H2'	1:0:2814:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:93:ASP:OD1	9:J:93:ASP:N	2.45	0.48
1:0:669:A:H2'	1:0:670:A:C8	2.49	0.48
1:0:2426:U:H2'	1:0:2427:A:C8	2.49	0.48
1:0:302:U:H2'	1:0:303:U:C6	2.49	0.48
1:0:1520:A:C1'	1:0:1521:A:O5'	2.60	0.48
1:0:1522:A:H1'	1:0:1523:A:C8	2.49	0.48
1:0:1701:G:N1	1:0:1704:U:OP2	2.47	0.47
1:0:288:U:C2	1:0:371:G:C2	3.02	0.47
1:0:1210:C:H2'	1:0:1211:G:O4'	2.14	0.47
1:0:2319:U:H2'	1:0:2320:U:H6	1.78	0.47
1:0:1457:U:H2'	1:0:1458:C:C6	2.50	0.47
1:0:1839:U:H2'	1:0:1840:A:C8	2.49	0.47
16:Q:90:GLU:N	16:Q:229:GLU:OE2	2.47	0.47
22:W:79:ARG:HG2	22:W:79:ARG:O	2.13	0.47
6:G:42:GLU:OE1	6:G:42:GLU:HA	2.14	0.47
20:U:125:SER:HB2	20:U:158:VAL:HG12	1.96	0.47
21:V:123:GLU:H	21:V:123:GLU:CD	2.23	0.47
1:0:1653:A:H2'	1:0:1654:A:C8	2.49	0.47
1:0:1739:G:O2'	1:0:2025:U:O4	2.27	0.47
20:U:44:VAL:HG23	20:U:58:LEU:HD23	1.95	0.47
28:f:32:ILE:HD11	28:f:56:SER:HB3	1.96	0.47
1:0:863:U:H2'	1:0:864:G:N7	2.29	0.47
1:0:1207:G:C2	1:0:1208:G:C8	3.02	0.47
7:H:5:ASN:C	7:H:5:ASN:HD22	2.22	0.47
1:0:312:G:OP2	13:N:39:ARG:NH2	2.47	0.47
1:0:580:A:C2	1:0:585:U:C5	2.84	0.47
1:0:580:A:H2	1:0:585:U:H5	1.57	0.47
1:0:642:C:H2'	1:0:643:A:H8	1.78	0.47
1:0:2046:G:OP1	11:L:139:THR:HB	2.15	0.47
13:N:62:GLU:H	13:N:76:GLU:HG2	1.79	0.47
1:0:1206:C:C4	1:0:1207:G:N7	2.83	0.47
1:0:1607:A:H2'	1:0:1608:A:C8	2.49	0.47
14:O:82:GLU:O	14:O:86:GLU:HG2	2.14	0.47
1:0:2658:A:O3'	1:0:2659:A:H3'	2.14	0.47
23:X:100:PHE:CE1	23:X:128:VAL:HG21	2.49	0.47
24:Y:85:MET:HE2	24:Y:167:VAL:HG12	1.97	0.47
1:0:650:G:H2'	1:0:651:C:C6	2.50	0.47
11:L:74:GLU:OE1	11:L:74:GLU:HA	2.15	0.47
23:X:32:LYS:NZ	23:X:119:ILE:HG23	2.30	0.46
1:0:364:A:N3	1:0:364:A:H2'	2.31	0.46
1:0:561:G:H2'	1:0:562:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:113:G:H2'	2:1:114:C:C6	2.50	0.46
23:X:100:PHE:CZ	23:X:128:VAL:HG21	2.50	0.46
24:Y:138:ASP:O	24:Y:142:VAL:HG23	2.16	0.46
6:G:104:GLU:HG2	6:G:161:PHE:CD1	2.50	0.46
23:X:28:ARG:HH12	23:X:32:LYS:HG2	1.81	0.46
24:Y:10:ASP:CG	24:Y:11:GLU:H	2.23	0.46
23:X:29:GLU:O	23:X:33:SER:OG	2.23	0.46
1:0:1416:C:OP2	34:0:3421:HOH:O	2.21	0.46
1:0:300:A:N9	1:0:360:G:N2	2.64	0.46
6:G:157:ASP:O	6:G:162:ARG:NH1	2.49	0.46
1:0:2407:A:H2'	1:0:2408:A:C8	2.51	0.46
1:0:2859:U:H4'	1:0:2860:A:H5'	1.98	0.46
2:1:27:A:H2'	2:1:28:C:C6	2.51	0.46
23:X:38:GLU:HG2	23:X:44:GLU:HA	1.97	0.46
26:c:72:ASP:OD1	26:c:75:GLU:N	2.33	0.46
1:0:104:G:N2	13:N:106:ASP:OD2	2.36	0.46
1:0:282:U:H3	1:0:376:U:H3	1.63	0.46
1:0:228:G:H2'	1:0:229:A:C8	2.51	0.45
1:0:713:G:H2'	1:0:714:U:C6	2.51	0.45
1:0:2452:G:C2	31:0:3001:BGC:H4	2.51	0.45
1:0:2678:U:H2'	1:0:2679:C:C6	2.50	0.45
11:L:133:ARG:NH2	34:L:304:HOH:O	2.49	0.45
28:f:1:MET:HE2	28:f:1:MET:HB3	1.82	0.45
1:0:668:U:C5	1:0:685:G:C5	3.04	0.45
1:0:2629:C:H3'	1:0:2630:A:H5''	1.99	0.45
1:0:2893:G:H2'	1:0:2894:C:O4'	2.16	0.45
11:L:34:ARG:CD	34:L:315:HOH:O	2.37	0.45
21:V:101:VAL:HG22	21:V:125:ASP:HB3	1.98	0.45
23:X:37:LEU:HD23	23:X:37:LEU:HA	1.77	0.45
1:0:188:A:O3'	6:G:108:ARG:NH2	2.49	0.45
1:0:1268:G:H2'	1:0:1269:U:C6	2.50	0.45
16:Q:96:HIS:CD2	16:Q:219:GLU:HA	2.52	0.45
23:X:86:ILE:HG22	23:X:87:THR:HG23	1.97	0.45
28:f:105:ARG:HE	28:f:105:ARG:HB3	1.60	0.45
1:0:2748:G:OP1	12:M:35:SER:OG	2.33	0.45
22:W:78:ARG:HD2	34:W:414:HOH:O	2.15	0.45
1:0:276:A:O2'	1:0:432:G:H5''	2.16	0.45
20:U:206:ARG:H	20:U:206:ARG:HG2	1.54	0.45
1:0:586:U:H2'	1:0:587:C:H6	1.81	0.45
1:0:2784:U:H1'	1:0:2785:A:H5''	1.99	0.45
2:1:31:G:C6	2:1:48:G:C6	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1735:U:O2'	1:0:2716:G:H4'	2.16	0.45
7:H:19:SER:HB2	7:H:27:TRP:HB2	1.98	0.45
9:J:31:ASP:OD1	9:J:31:ASP:N	2.48	0.45
1:0:2338:A:H4'	23:X:54:SER:HA	1.99	0.45
1:0:1457:U:H2'	1:0:1458:C:H6	1.81	0.45
26:c:15:ASN:HB2	34:c:109:HOH:O	2.17	0.45
28:f:63:GLU:H	28:f:63:GLU:CD	2.16	0.45
30:A:42:ASN:HB3	30:A:45:ARG:HG2	1.99	0.45
1:0:953:A:H2'	1:0:954:G:H5''	1.99	0.44
9:J:137:ARG:HG2	9:J:137:ARG:NH1	2.32	0.44
11:L:96:VAL:HG21	11:L:146:LEU:HD23	1.98	0.44
1:0:283:A:N6	1:0:376:U:O4	2.51	0.44
1:0:809:A:O2'	1:0:810:A:O5'	2.33	0.44
2:1:38:U:H1'	2:1:43:A:H61	1.82	0.44
13:N:13:ARG:HG3	13:N:13:ARG:HH11	1.82	0.44
21:V:233:TRP:HD1	21:V:236:ARG:HD2	1.81	0.44
26:c:35:ASP:OD1	26:c:35:ASP:N	2.49	0.44
1:0:296:C:OP2	1:0:296:C:H3'	2.17	0.44
1:0:2842:U:C4	1:0:2844:G:N2	2.85	0.44
4:E:15:ASP:N	4:E:15:ASP:OD1	2.48	0.44
9:J:137:ARG:HG2	9:J:137:ARG:HH11	1.82	0.44
16:Q:224:ASN:OD1	16:Q:224:ASN:N	2.51	0.44
1:0:298:G:O2'	1:0:299:G:OP2	2.32	0.44
1:0:792:A:H2'	1:0:793:G:O4'	2.17	0.44
1:0:2240:C:HO2'	1:0:2241:C:P	2.41	0.44
28:f:127:THR:O	28:f:127:THR:OG1	2.35	0.44
1:0:365:G:C1'	1:0:366:A:H62	2.28	0.44
2:1:30:C:C2	2:1:49:G:N2	2.86	0.44
1:0:577:A:H2'	1:0:578:G:H8	1.83	0.44
1:0:580:A:N1	1:0:585:U:O4	2.51	0.44
1:0:2647:U:H2'	1:0:2648:U:C6	2.53	0.44
23:X:36:ILE:HG21	23:X:107:HIS:CE1	2.52	0.44
25:b:30:VAL:HG11	25:b:101:VAL:HB	2.00	0.44
1:0:709:C:H2'	1:0:710:G:O4'	2.18	0.44
18:S:54:LYS:HA	18:S:54:LYS:HD2	1.87	0.44
27:d:13:THR:OG1	27:d:16:GLU:OE2	2.28	0.44
1:0:249:A:OP1	6:G:51:ARG:NH1	2.51	0.43
1:0:301:A:C6	1:0:303:U:H5'	2.53	0.43
1:0:1154:C:H2'	1:0:1155:G:H8	1.82	0.43
11:L:22:ARG:HA	11:L:23:PRO:HD3	1.89	0.43
1:0:1587:G:O2'	1:0:1588:C:O5'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2425:C:H2'	1:0:2426:U:C6	2.54	0.43
24:Y:41:VAL:HG22	24:Y:50:ILE:HG12	2.00	0.43
1:0:296:C:H2'	1:0:297:U:O2	2.18	0.43
1:0:301:A:N7	1:0:302:U:O2'	2.49	0.43
1:0:562:U:H2'	1:0:563:C:C6	2.53	0.43
25:b:59:LYS:HA	25:b:59:LYS:HD3	1.83	0.43
1:0:124:G:OP2	34:0:3420:HOH:O	2.21	0.43
1:0:269:G:N1	4:E:36:GLU:OE1	2.44	0.43
1:0:313:U:H2'	13:N:52:LEU:HD13	1.99	0.43
1:0:972:G:N1	1:0:973:A:N6	2.65	0.43
1:0:1352:A:H5''	34:0:3735:HOH:O	2.19	0.43
1:0:2762:C:H2'	1:0:2763:A:O4'	2.18	0.43
1:0:318:U:H2'	1:0:319:G:O4'	2.18	0.43
1:0:1467:A:H2'	1:0:1468:U:C6	2.54	0.43
11:L:82:PRO:O	11:L:86:SER:OG	2.35	0.43
1:0:859:A:H2'	34:0:5826:HOH:O	2.19	0.43
1:0:1459:U:H2'	1:0:1460:A:C8	2.53	0.43
2:1:95:C:H2'	2:1:96:U:H6	1.83	0.43
13:N:82:LYS:HB3	13:N:82:LYS:HE3	1.65	0.43
16:Q:98:ASP:OD1	16:Q:98:ASP:N	2.48	0.43
23:X:9:MET:HE3	23:X:9:MET:HA	2.01	0.43
1:0:1271:C:C2'	1:0:1272:U:H5'	2.48	0.43
1:0:1749:A:H2'	1:0:1750:G:O4'	2.18	0.43
1:0:2289:C:OP2	10:K:4:SER:OG	2.30	0.43
34:0:3884:HOH:O	28:f:38:SER:HB3	2.18	0.43
27:d:25:GLU:HG3	27:d:26:THR:N	2.34	0.43
1:0:1317:A:H2'	1:0:1318:C:C6	2.54	0.43
1:0:1589:C:OP2	9:J:121:ARG:HD2	2.19	0.43
1:0:2320:U:H2'	1:0:2321:C:C6	2.53	0.43
1:0:663:G:N7	7:H:64:LYS:NZ	2.60	0.43
1:0:999:U:H2'	1:0:1000:C:C5	2.54	0.43
1:0:1662:A:N6	1:0:1663:A:C6	2.87	0.43
2:1:47:C:OP1	8:I:115:LYS:HG3	2.19	0.43
4:E:106:SER:O	4:E:110:GLU:HG2	2.19	0.43
2:1:49:G:OP1	8:I:78:ASN:ND2	2.50	0.43
2:1:76:A:H8	2:1:76:A:OP1	2.01	0.43
11:L:5:TYR:CZ	11:L:16:LYS:HD3	2.54	0.43
14:O:89:ASP:OD1	14:O:89:ASP:N	2.52	0.43
23:X:75:SER:O	23:X:78:GLU:HG3	2.19	0.43
1:0:367:U:O2	1:0:367:U:H2'	2.18	0.42
1:0:2677:U:H2'	1:0:2678:U:H6	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2824:C:C2	1:0:2825:A:C8	3.06	0.42
4:E:58:GLU:O	4:E:62:MET:HG3	2.18	0.42
14:O:82:GLU:CD	14:O:82:GLU:H	2.27	0.42
23:X:155:VAL:O	23:X:158:ALA:N	2.49	0.42
1:0:1509:C:H2'	1:0:1510:U:H6	1.84	0.42
1:0:2713:C:H4'	12:M:18:THR:HG22	2.01	0.42
1:0:2820:A:H2'	1:0:2821:G:O4'	2.19	0.42
4:E:67:LEU:HD23	4:E:67:LEU:HA	1.80	0.42
8:I:84:LEU:HD21	8:I:173:PHE:HE1	1.84	0.42
10:K:72:PHE:HE2	10:K:89:PRO:HG3	1.84	0.42
12:M:58:ARG:HH11	12:M:58:ARG:HG2	1.84	0.42
28:f:17:LEU:HD22	28:f:28:GLU:OE2	2.19	0.42
1:0:1509:C:H2'	1:0:1510:U:C6	2.54	0.42
1:0:2006:G:O2'	1:0:2007:G:O4'	2.36	0.42
8:I:144:ARG:HA	8:I:173:PHE:CE2	2.54	0.42
19:T:21:GLU:HG3	19:T:22:VAL:N	2.34	0.42
21:V:233:TRP:CD1	21:V:236:ARG:HD2	2.54	0.42
22:W:133:ASP:OD1	22:W:133:ASP:N	2.53	0.42
1:0:491:G:O2'	1:0:517:G:O6	2.27	0.42
1:0:2259:A:H2'	1:0:2260:G:C8	2.55	0.42
27:d:43:ASN:HD22	27:d:43:ASN:HA	1.66	0.42
1:0:978:G:H1	1:0:995:C:H42	1.68	0.42
1:0:2804:A:H4'	1:0:2805:A:H5'	2.01	0.42
1:0:417:G:H2'	1:0:418:C:C6	2.55	0.42
1:0:1520:A:O2'	1:0:1521:A:C8	2.69	0.42
1:0:2426:U:H2'	1:0:2427:A:H8	1.84	0.42
4:E:35:ASN:O	4:E:39:LYS:HG2	2.19	0.42
7:H:5:ASN:HD22	7:H:6:PRO:N	2.18	0.42
20:U:133:ARG:HE	20:U:133:ARG:HB3	1.58	0.42
23:X:166:PHE:CD1	23:X:166:PHE:N	2.87	0.42
27:d:22:GLU:HA	27:d:25:GLU:HG2	2.00	0.42
1:0:773:A:H2'	1:0:774:A:C8	2.54	0.42
1:0:905:U:OP2	3:i:12:ARG:NH1	2.43	0.42
1:0:2133:U:H3'	1:0:2134:G:C8	2.55	0.42
1:0:2758:A:H2'	1:0:2759:C:C6	2.54	0.42
11:L:64:ASN:OD1	11:L:64:ASN:N	2.48	0.42
1:0:2678:U:H2'	1:0:2679:C:H6	1.84	0.42
23:X:50:SER:OG	23:X:63:GLU:N	2.44	0.42
1:0:863:U:O2'	1:0:864:G:H8	2.01	0.42
1:0:889:A:H2'	1:0:890:C:C6	2.55	0.42
1:0:1154:C:H2'	1:0:1155:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:126:ASN:ND2	25:b:128:LYS:H	2.17	0.42
1:0:1045:C:H5	34:0:3585:HOH:O	2.02	0.42
1:0:1372:G:H5'	1:0:1376:G:O6	2.20	0.42
1:0:1789:G:OP1	9:J:104:ARG:NH1	2.53	0.42
1:0:2005:U:H2'	1:0:2006:G:O4'	2.20	0.42
1:0:2401:A:N6	34:0:3628:HOH:O	2.47	0.42
1:0:2538:U:H2'	1:0:2539:U:C6	2.55	0.42
1:0:2625:G:H2'	1:0:2626:A:C8	2.55	0.42
1:0:2864:G:H2'	1:0:2865:U:C6	2.54	0.42
28:f:68:VAL:O	28:f:69:LEU:HD23	2.19	0.42
1:0:42:U:H2'	1:0:43:C:H6	1.85	0.41
1:0:300:A:H2'	1:0:302:U:C1'	2.49	0.41
1:0:692:A:N7	3:i:66:LYS:NZ	2.67	0.41
1:0:2855:G:H4'	21:V:338:GLY:HA2	2.02	0.41
8:I:78:ASN:O	8:I:81:SER:OG	2.36	0.41
20:U:134:GLU:N	20:U:134:GLU:OE1	2.53	0.41
21:V:196:ARG:HE	21:V:196:ARG:HB3	1.61	0.41
23:X:32:LYS:HE3	23:X:122:TYR:HE2	1.85	0.41
1:0:1790:A:H2'	1:0:1791:U:C6	2.55	0.41
1:0:2336:G:C2	1:0:2337:A:C6	3.08	0.41
8:I:87:TYR:CD1	8:I:91:ILE:HD11	2.54	0.41
8:I:168:ASN:N	8:I:168:ASN:OD1	2.51	0.41
10:K:77:ASN:ND2	10:K:82:GLU:OE2	2.41	0.41
24:Y:98:VAL:HG12	24:Y:103:VAL:HG22	2.02	0.41
1:0:934:U:H2'	1:0:935:C:C6	2.55	0.41
1:0:1129:A:H2'	1:0:1130:A:H8	1.82	0.41
2:1:118:C:N3	2:1:119:C:C5	2.89	0.41
9:J:13:ASP:OD2	9:J:38:ARG:NH2	2.52	0.41
12:M:43:LEU:HD23	12:M:43:LEU:HA	1.89	0.41
20:U:36:LYS:HB3	20:U:36:LYS:HE3	1.84	0.41
24:Y:165:ASP:OD1	24:Y:165:ASP:N	2.53	0.41
27:d:5:TYR:O	27:d:9:ILE:HG13	2.20	0.41
1:0:827:U:H4'	34:0:3452:HOH:O	2.20	0.41
1:0:2452:G:C6	31:0:3001:BGC:H2	2.55	0.41
23:X:8:GLU:OE1	23:X:8:GLU:N	2.35	0.41
1:0:300:A:H5'	1:0:302:U:OP2	2.20	0.41
1:0:631:G:H2'	1:0:2064:C:C5	2.56	0.41
1:0:860:C:H2'	1:0:861:U:C6	2.55	0.41
1:0:1882:C:O2'	1:0:1883:U:O5'	2.33	0.41
2:1:38:U:H1'	2:1:43:A:N6	2.35	0.41
22:W:144:ASP:OD1	22:W:144:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:112:LYS:HA	24:Y:112:LYS:HD3	1.87	0.41
28:f:122:GLY:O	28:f:126:SER:OG	2.39	0.41
1:0:1136:U:H2'	1:0:1137:C:C6	2.55	0.41
1:0:1234:U:O2'	1:0:1237:G:OP1	2.27	0.41
1:0:2394:G:H2'	1:0:2395:U:C6	2.55	0.41
5:F:172:GLU:HG2	5:F:173:LEU:HD12	2.02	0.41
6:G:24:LEU:HA	6:G:24:LEU:HD23	1.77	0.41
1:0:567:C:H2'	1:0:568:G:O4'	2.21	0.41
1:0:2658:A:N3	1:0:2658:A:H2'	2.36	0.41
2:1:95:C:H2'	2:1:96:U:C6	2.55	0.41
23:X:165:THR:HB	23:X:170:VAL:HG13	2.02	0.41
24:Y:23:ILE:HB	24:Y:30:VAL:HG23	2.03	0.41
27:d:21:LEU:HG	27:d:57:ILE:HG21	2.03	0.41
1:0:860:C:H2'	1:0:861:U:H6	1.86	0.41
1:0:2373:A:H3'	1:0:2374:C:H5''	2.01	0.41
2:1:91:G:H2'	2:1:92:A:C8	2.56	0.41
1:0:81:U:H2'	1:0:82:C:C6	2.56	0.41
1:0:489:A:N3	1:0:491:G:H5''	2.36	0.41
1:0:518:G:H4'	1:0:519:C:O5'	2.20	0.41
1:0:713:G:H2'	1:0:714:U:H6	1.84	0.41
1:0:1870:G:O2'	1:0:1871:G:H5'	2.21	0.41
1:0:2243:G:H2'	1:0:2244:G:C8	2.56	0.41
1:0:2812:U:H2'	1:0:2813:U:C6	2.56	0.41
2:1:39:C:H5'	2:1:40:C:H5''	2.03	0.41
8:I:157:GLU:OE1	8:I:157:GLU:N	2.46	0.41
11:L:17:GLY:HA3	11:L:96:VAL:HG22	2.02	0.41
20:U:170:VAL:HG12	20:U:171:LYS:HG3	2.03	0.41
22:W:142:SER:OG	22:W:144:ASP:OD1	2.28	0.41
1:0:1215:U:H2'	1:0:1216:U:C6	2.56	0.41
1:0:1667:G:H5''	1:0:1668:C:H5'	2.03	0.41
1:0:1752:U:N3	1:0:1813:G:OP2	2.53	0.41
1:0:2318:U:H2'	1:0:2319:U:H6	1.84	0.41
34:0:7244:HOH:O	18:S:15:THR:HG22	2.21	0.41
7:H:59:VAL:HG13	7:H:77:VAL:HA	2.02	0.41
9:J:81:ARG:HG2	9:J:88:ARG:CZ	2.50	0.41
16:Q:166:LYS:HE3	16:Q:166:LYS:HB2	1.88	0.41
21:V:237:ILE:O	34:V:501:HOH:O	2.22	0.41
23:X:15:GLU:C	23:X:15:GLU:OE1	2.63	0.41
23:X:21:MET:CE	23:X:33:SER:HB3	2.51	0.41
23:X:107:HIS:CE1	23:X:113:GLN:HE21	2.37	0.41
23:X:165:THR:O	23:X:170:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:945:A:O2'	14:O:19:ASP:OD2	2.30	0.40
1:0:2320:U:H2'	1:0:2321:C:H6	1.86	0.40
8:I:179:ASN:OD1	8:I:179:ASN:N	2.51	0.40
9:J:99:ILE:HD12	9:J:99:ILE:HA	1.90	0.40
23:X:136:ARG:O	23:X:140:ARG:HG3	2.21	0.40
1:0:47:A:H2'	1:0:48:G:C8	2.57	0.40
1:0:361:G:N3	1:0:361:G:H2'	2.36	0.40
1:0:1027:U:OP1	14:O:108:ARG:NH1	2.54	0.40
1:0:1779:A:H61	1:0:1800:U:H3	1.68	0.40
34:0:6555:HOH:O	6:G:84:THR:HG23	2.21	0.40
2:1:2:A:H2	2:1:23:U:H3	1.69	0.40
15:P:38:LEU:HD23	15:P:38:LEU:HA	1.89	0.40
21:V:93:TYR:CZ	25:b:3:PHE:HD2	2.39	0.40
1:0:577:A:H2'	1:0:578:G:C8	2.57	0.40
1:0:657:A:H2'	1:0:658:C:C6	2.56	0.40
1:0:1471:G:H2'	1:0:1472:A:C8	2.57	0.40
1:0:1746:G:H2'	34:0:7275:HOH:O	2.22	0.40
16:Q:210:ARG:HB3	16:Q:210:ARG:CZ	2.51	0.40
24:Y:2:SER:O	24:Y:51:GLU:HA	2.22	0.40
1:0:295:C:H3'	1:0:296:C:C5	2.57	0.40
1:0:561:G:H2'	1:0:562:U:H6	1.86	0.40
1:0:1376:G:H5'	1:0:1717:G:C5	2.55	0.40
1:0:2421:G:OP2	19:T:85:ARG:NH2	2.54	0.40
1:0:2729:C:OP2	9:J:62:ARG:NH1	2.54	0.40
8:I:172:HIS:HA	8:I:175:GLU:CD	2.46	0.40
10:K:9:LYS:HE3	10:K:9:LYS:HB3	1.89	0.40
21:V:127:ASP:O	21:V:131:GLU:HG2	2.21	0.40
22:W:120:ASP:HB3	22:W:123:LEU:HB2	2.04	0.40
30:A:28:LEU:HD23	30:A:28:LEU:HA	1.88	0.40
1:0:182:G:H2'	6:G:192:ARG:HD2	2.03	0.40
1:0:300:A:C6	1:0:360:G:N3	2.90	0.40
1:0:2318:U:OP1	1:0:2410:C:O2'	2.35	0.40
4:E:71:LYS:HA	4:E:71:LYS:HD2	1.90	0.40
21:V:142:ARG:HG2	21:V:166:ARG:HA	2.04	0.40
25:b:9:ASP:OD1	25:b:9:ASP:N	2.55	0.40
27:d:21:LEU:HD23	27:d:21:LEU:HA	1.85	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	i	152/168 (90%)	149 (98%)	3 (2%)	0	100	100
4	E	117/120 (98%)	117 (100%)	0	0	100	100
5	F	161/176 (92%)	159 (99%)	2 (1%)	0	100	100
6	G	190/196 (97%)	186 (98%)	4 (2%)	0	100	100
7	H	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
8	I	181/184 (98%)	179 (99%)	2 (1%)	0	100	100
9	J	145/151 (96%)	141 (97%)	4 (3%)	0	100	100
10	K	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
11	L	149/153 (97%)	148 (99%)	1 (1%)	0	100	100
12	M	56/67 (84%)	54 (96%)	2 (4%)	0	100	100
13	N	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
14	O	152/154 (99%)	151 (99%)	1 (1%)	0	100	100
15	P	87/92 (95%)	86 (99%)	1 (1%)	0	100	100
16	Q	140/234 (60%)	138 (99%)	2 (1%)	0	100	100
17	R	78/89 (88%)	75 (96%)	3 (4%)	0	100	100
18	S	55/58 (95%)	53 (96%)	2 (4%)	0	100	100
19	T	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
20	U	228/241 (95%)	212 (93%)	15 (7%)	1 (0%)	30	34
21	V	335/338 (99%)	329 (98%)	6 (2%)	0	100	100
22	W	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
23	X	167/172 (97%)	155 (93%)	12 (7%)	0	100	100
24	Y	172/178 (97%)	168 (98%)	3 (2%)	1 (1%)	21	24
25	b	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
26	c	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
27	d	66/70 (94%)	62 (94%)	3 (4%)	1 (2%)	8	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	f	130/132 (98%)	129 (99%)	1 (1%)	0	100	100
29	e	55/58 (95%)	55 (100%)	0	0	100	100
30	A	47/50 (94%)	43 (92%)	4 (8%)	0	100	100
All	All	3741/3980 (94%)	3642 (97%)	96 (3%)	3 (0%)	49	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	d	42	GLU
20	U	211	GLN
24	Y	10	ASP

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	i	112/123 (91%)	110 (98%)	2 (2%)	51	66
4	E	93/94 (99%)	90 (97%)	3 (3%)	34	46
5	F	141/147 (96%)	138 (98%)	3 (2%)	47	61
6	G	160/163 (98%)	159 (99%)	1 (1%)	78	87
7	H	98/99 (99%)	97 (99%)	1 (1%)	68	81
8	I	144/145 (99%)	142 (99%)	2 (1%)	59	73
9	J	117/121 (97%)	114 (97%)	3 (3%)	40	54
10	K	77/78 (99%)	77 (100%)	0	100	100
11	L	122/124 (98%)	119 (98%)	3 (2%)	42	55
12	M	48/55 (87%)	45 (94%)	3 (6%)	16	19
13	N	98/102 (96%)	95 (97%)	3 (3%)	35	47
14	O	132/132 (100%)	131 (99%)	1 (1%)	73	84
15	P	78/80 (98%)	77 (99%)	1 (1%)	61	76
16	Q	120/191 (63%)	118 (98%)	2 (2%)	53	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	61/68 (90%)	58 (95%)	3 (5%)	22	28
18	S	48/49 (98%)	47 (98%)	1 (2%)	47	61
19	T	77/77 (100%)	77 (100%)	0	100	100
20	U	180/186 (97%)	179 (99%)	1 (1%)	78	87
21	V	277/278 (100%)	276 (100%)	1 (0%)	84	91
22	W	198/198 (100%)	192 (97%)	6 (3%)	36	48
23	X	141/147 (96%)	137 (97%)	4 (3%)	38	51
24	Y	149/151 (99%)	149 (100%)	0	100	100
25	b	122/123 (99%)	120 (98%)	2 (2%)	55	70
26	c	76/76 (100%)	73 (96%)	3 (4%)	28	39
27	d	54/56 (96%)	54 (100%)	0	100	100
28	f	106/106 (100%)	104 (98%)	2 (2%)	50	65
29	e	48/49 (98%)	48 (100%)	0	100	100
30	A	45/46 (98%)	45 (100%)	0	100	100
All	All	3122/3264 (96%)	3071 (98%)	51 (2%)	54	70

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	i	19	HIS
3	i	57	SER
4	E	12	ASP
4	E	15	ASP
4	E	106	SER
5	F	48	VAL
5	F	113	ASP
5	F	134	THR
6	G	67	SER
7	H	59	VAL
8	I	156	ASP
8	I	163	ASP
9	J	31	ASP
9	J	36	ILE
9	J	114	THR
11	L	6	SER
11	L	139	THR
11	L	151	VAL

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Mol	Chain	Res	Type
12	M	13	GLU
12	M	28	THR
12	M	51	GLU
13	N	36	TYR
13	N	41	VAL
13	N	79	THR
14	O	89	ASP
15	P	17	ASP
16	Q	106	GLU
16	Q	133	THR
17	R	11	SER
17	R	33	GLU
17	R	57	THR
18	S	15	THR
20	U	211	GLN
21	V	60	ASP
22	W	11	ASP
22	W	118	THR
22	W	193	SER
22	W	212	VAL
22	W	243	GLU
22	W	245	VAL
23	X	46	VAL
23	X	71	LEU
23	X	104	VAL
23	X	108	THR
25	b	49	SER
25	b	125	SER
26	c	31	SER
26	c	35	ASP
26	c	82	VAL
28	f	64	MET
28	f	127	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
3	i	19	HIS
3	i	39	HIS
3	i	43	HIS
4	E	47	GLN
5	F	79	ASN

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Mol	Chain	Res	Type
6	G	8	HIS
6	G	30	GLN
6	G	76	GLN
6	G	78	HIS
6	G	143	GLN
7	H	5	ASN
7	H	28	GLN
7	H	54	GLN
7	H	101	GLN
8	I	23	GLN
8	I	43	HIS
8	I	120	GLN
8	I	143	ASN
9	J	144	ASN
10	K	68	GLN
11	L	95	ASN
11	L	103	GLN
11	L	114	HIS
14	O	6	GLN
14	O	12	ASN
14	O	27	HIS
14	O	87	ASN
14	O	98	GLN
15	P	24	HIS
15	P	37	HIS
15	P	48	ASN
15	P	54	GLN
15	P	56	ASN
15	P	62	HIS
15	P	65	GLN
17	R	36	ASN
17	R	43	ASN
18	S	58	ASN
19	T	2	GLN
19	T	8	ASN
19	T	20	HIS
19	T	92	GLN
20	U	111	GLN
21	V	231	GLN
22	W	39	GLN
22	W	159	GLN
22	W	208	ASN

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Mol	Chain	Res	Type
23	X	107	HIS
23	X	129	ASN
23	X	146	GLN
24	Y	144	GLN
25	b	67	GLN
25	b	126	ASN
26	c	24	GLN
27	d	43	ASN
28	f	44	HIS
30	A	18	GLN
30	A	37	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2628/2916 (90%)	360 (13%)	18 (0%)
2	1	119/122 (97%)	16 (13%)	0
All	All	2747/3038 (90%)	376 (13%)	18 (0%)

All (376) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	46	G
1	0	49	C
1	0	67	A
1	0	74	A
1	0	77	A
1	0	78	G
1	0	94	U
1	0	120	A
1	0	121	A
1	0	122	U
1	0	127	A
1	0	133	A
1	0	134	C
1	0	135	A
1	0	136	G
1	0	138	A
1	0	144	C
1	0	147	G
1	0	148	C

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Mol	Chain	Res	Type
1	0	149	G
1	0	158	A
1	0	173	A
1	0	176	A
1	0	192	G
1	0	193	A
1	0	198	A
1	0	199	A
1	0	205	U
1	0	206	C
1	0	211	A
1	0	226	G
1	0	244	G
1	0	261	C
1	0	262	G
1	0	263	G
1	0	276	A
1	0	277	C
1	0	283	A
1	0	285	C
1	0	287	A
1	0	289	A
1	0	290	A
1	0	291	C
1	0	292	G
1	0	294	A
1	0	295	C
1	0	296	C
1	0	297	U
1	0	298	G
1	0	299	G
1	0	300	A
1	0	301	A
1	0	302	U
1	0	313	U
1	0	314	C
1	0	341	G
1	0	342	A
1	0	343	A
1	0	360	G
1	0	361	G
1	0	362	A

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Mol	Chain	Res	Type
1	0	363	A
1	0	364	A
1	0	366	A
1	0	367	U
1	0	368	C
1	0	369	C
1	0	370	C
1	0	371	G
1	0	372	G
1	0	373	G
1	0	379	U
1	0	380	C
1	0	385	A
1	0	386	U
1	0	400	U
1	0	401	A
1	0	411	A
1	0	421	G
1	0	465	C
1	0	477	G
1	0	491	G
1	0	501	A
1	0	502	A
1	0	515	A
1	0	518	G
1	0	519	C
1	0	539	G
1	0	541	G
1	0	542	C
1	0	543	G
1	0	557	G
1	0	576	U
1	0	585	U
1	0	589	A
1	0	592	G
1	0	605	G
1	0	608	G
1	0	624	A
1	0	634	A
1	0	636	A
1	0	664	A
1	0	683	C

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Mol	Chain	Res	Type
1	0	692	A
1	0	699	C
1	0	703	U
1	0	705	C
1	0	706	G
1	0	718	U
1	0	719	G
1	0	736	U
1	0	737	C
1	0	738	A
1	0	761	C
1	0	779	U
1	0	807	G
1	0	809	A
1	0	810	A
1	0	811	G
1	0	823	C
1	0	837	U
1	0	842	U
1	0	843	A
1	0	844	C
1	0	859	A
1	0	864	G
1	0	870	G
1	0	871	G
1	0	877	A
1	0	879	G
1	0	880	G
1	0	886	C
1	0	900	G
1	0	907	C
1	0	922	C
1	0	923	G
1	0	954	G
1	0	962	G
1	0	974	A
1	0	976	C
1	0	977	C
1	0	978	G
1	0	979	G
1	0	993	U
1	0	994	U

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Mol	Chain	Res	Type
1	0	996	G
1	0	997	C
1	0	999	U
1	0	1000	C
1	0	1008	A
1	0	1010	C
1	0	1046	G
1	0	1053	G
1	0	1060	G
1	0	1068	A
1	0	1073	G
1	0	1079	G
1	0	1088	G
1	0	1089	A
1	0	1101	G
1	0	1109	G
1	0	1110	U
1	0	1111	G
1	0	1115	A
1	0	1120	G
1	0	1125	A
1	0	1128	G
1	0	1134	U
1	0	1148	A
1	0	1156	G
1	0	1157	G
1	0	1205	C
1	0	1206	C
1	0	1207	G
1	0	1212	A
1	0	1213	G
1	0	1229	A
1	0	1235	C
1	0	1236	G
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	1285	U

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Mol	Chain	Res	Type
1	0	1286	C
1	0	1288	G
1	0	1327	A
1	0	1338	C
1	0	1350	G
1	0	1356	C
1	0	1376	G
1	0	1377	A
1	0	1382	G
1	0	1402	U
1	0	1403	A
1	0	1408	C
1	0	1437	G
1	0	1447	C
1	0	1453	U
1	0	1456	G
1	0	1481	A
1	0	1483	A
1	0	1499	A
1	0	1500	U
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	1529	C
1	0	1539	A
1	0	1575	A
1	0	1584	G
1	0	1587	G
1	0	1595	G
1	0	1600	G
1	0	1621	A
1	0	1630	C
1	0	1631	G
1	0	1636	U
1	0	1651	A
1	0	1660	G
1	0	1662	A
1	0	1668	C

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Mol	Chain	Res	Type
1	0	1677	A
1	0	1679	A
1	0	1680	U
1	0	1687	C
1	0	1688	A
1	0	1704	U
1	0	1705	A
1	0	1717	G
1	0	1718	U
1	0	1719	C
1	0	1724	U
1	0	1725	C
1	0	1746	G
1	0	1747	C
1	0	1772	A
1	0	1812	G
1	0	1813	G
1	0	1822	A
1	0	1825	G
1	0	1844	G
1	0	1849	C
1	0	1866	G
1	0	1872	U
1	0	1878	A
1	0	1883	U
1	0	2006	G
1	0	2007	G
1	0	2020	G
1	0	2025	U
1	0	2027	U
1	0	2057	U
1	0	2065	G
1	0	2066	G
1	0	2067	A
1	0	2089	A
1	0	2094	A
1	0	2095	G
1	0	2096	A
1	0	2103	A
1	0	2117	G
1	0	2127	G
1	0	2128	A

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Mol	Chain	Res	Type
1	0	2130	A
1	0	2131	C
1	0	2132	G
1	0	2133	U
1	0	2229	C
1	0	2230	G
1	0	2231	A
1	0	2233	U
1	0	2236	C
1	0	2241	C
1	0	2246	G
1	0	2249	G
1	0	2251	A
1	0	2264	G
1	0	2265	G
1	0	2277	G
1	0	2284	A
1	0	2306	C
1	0	2310	C
1	0	2314	A
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	2347	A
1	0	2349	A
1	0	2362	A
1	0	2374	C
1	0	2378	G
1	0	2413	G
1	0	2415	U
1	0	2455	G
1	0	2460	A
1	0	2461	A
1	0	2462	A
1	0	2469	C
1	0	2473	G
1	0	2476	A
1	0	2496	A
1	0	2502	A

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Mol	Chain	Res	Type
1	0	2530	G
1	0	2531	A
1	0	2546	A
1	0	2548	C
1	0	2557	G
1	0	2583	U
1	0	2584	C
1	0	2585	G
1	0	2594	A
1	0	2595	G
1	0	2601	C
1	0	2606	G
1	0	2630	A
1	0	2642	A
1	0	2643	U
1	0	2659	A
1	0	2660	G
1	0	2665	U
1	0	2674	A
1	0	2675	C
1	0	2676	G
1	0	2691	G
1	0	2693	G
1	0	2709	G
1	0	2740	G
1	0	2741	U
1	0	2743	G
1	0	2754	A
1	0	2755	C
1	0	2761	G
1	0	2776	A
1	0	2785	A
1	0	2793	A
1	0	2794	A
1	0	2804	A
1	0	2805	A
1	0	2818	U
1	0	2830	U
1	0	2843	C
1	0	2869	G
1	0	2881	U
1	0	2883	A

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Mol	Chain	Res	Type
1	0	2889	G
1	0	2895	A
1	0	2896	C
1	0	2902	G
1	0	2907	A
2	1	3	C
2	1	4	G
2	1	7	G
2	1	10	C
2	1	23	U
2	1	33	A
2	1	39	C
2	1	54	U
2	1	55	A
2	1	56	A
2	1	65	G
2	1	76	A
2	1	77	G
2	1	87	G
2	1	109	G
2	1	113	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	205	U
1	0	261	C
1	0	360	G
1	0	362	A
1	0	366	A
1	0	518	G
1	0	809	A
1	0	836	G
1	0	843	A
1	0	879	G
1	0	961	C
1	0	1127	C
1	0	1275	U
1	0	1520	A
1	0	2240	C
1	0	2529	C
1	0	2784	U

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Mol	Chain	Res	Type
1	0	2842	U

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 406 ligands modelled in this entry, 405 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BGC	0	3001	-	12,12,12	0.47	0	17,17,17	1.71	2 (11%)

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
31	BGC	0	3001	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	0	3001	BGC	C4-C3-C2	-4.81	102.43	110.82
31	0	3001	BGC	C3-C4-C5	-3.46	104.06	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

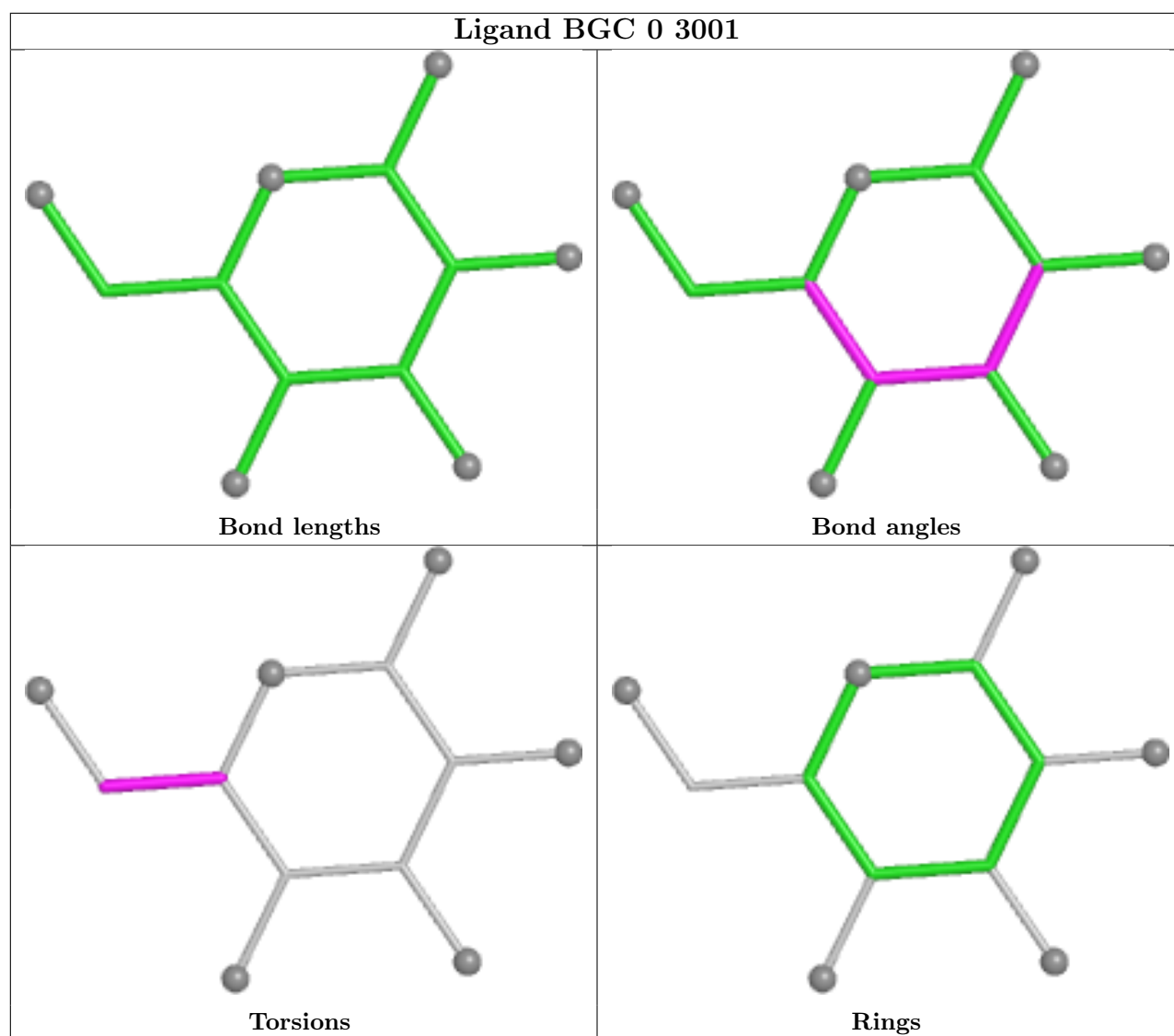
Mol	Chain	Res	Type	Atoms
31	0	3001	BGC	O5-C5-C6-O6
31	0	3001	BGC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	3001	BGC	5	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.

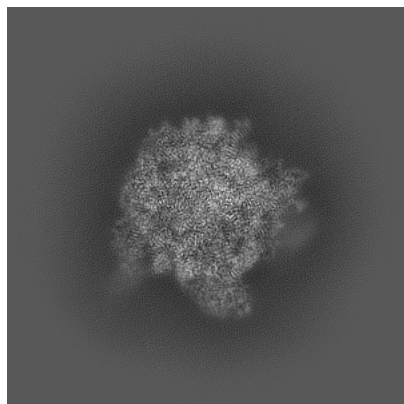
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62908. These allow visual inspection of the internal detail of the map and identification of artifacts.

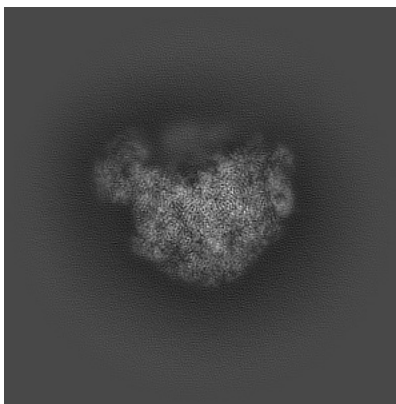
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

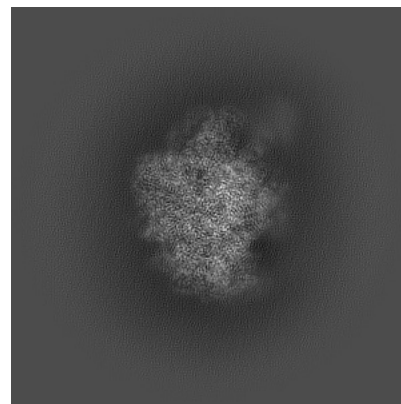
6.1.1 Primary map



X

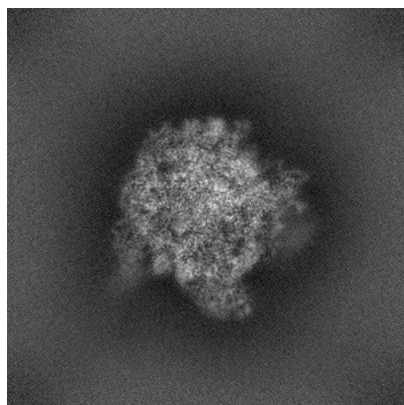


Y

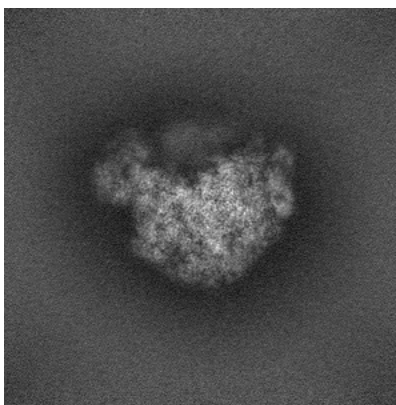


Z

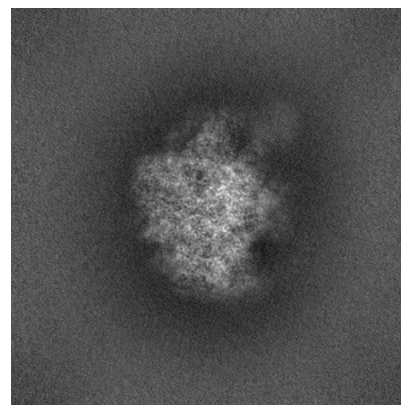
6.1.2 Raw map



X



Y

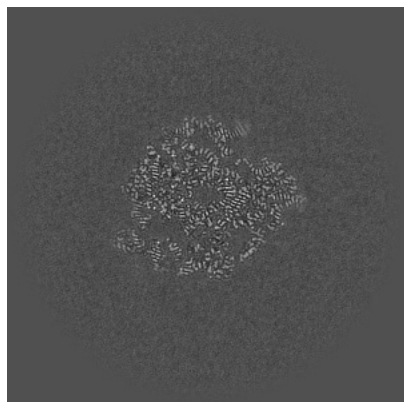


Z

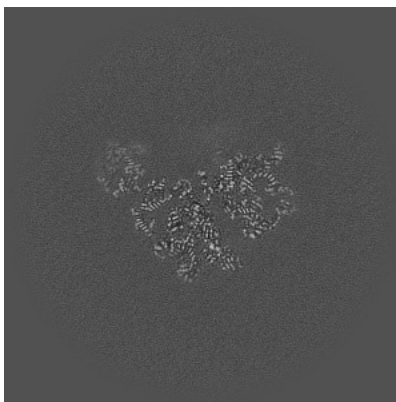
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

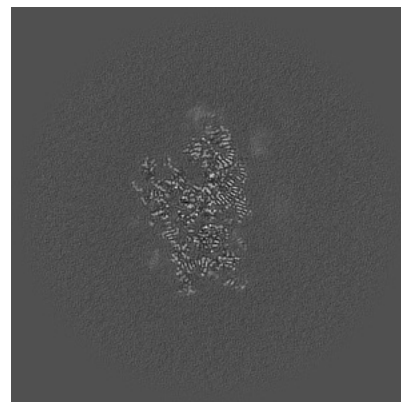
6.2.1 Primary map



X Index: 320

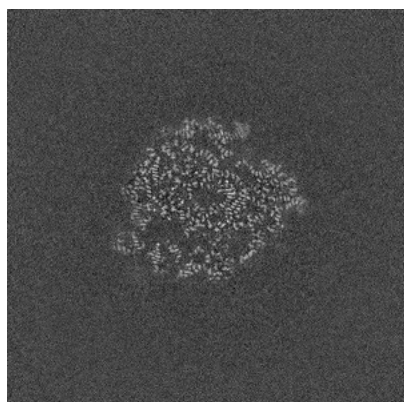


Y Index: 320

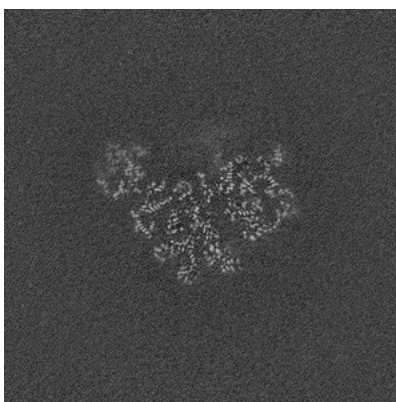


Z Index: 320

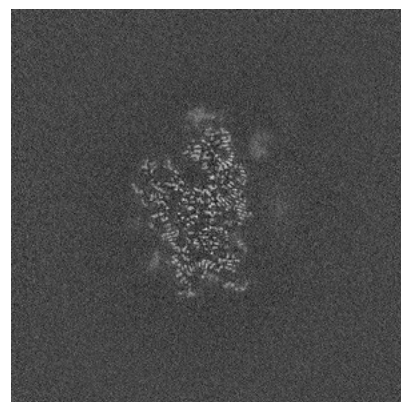
6.2.2 Raw map



X Index: 320



Y Index: 320

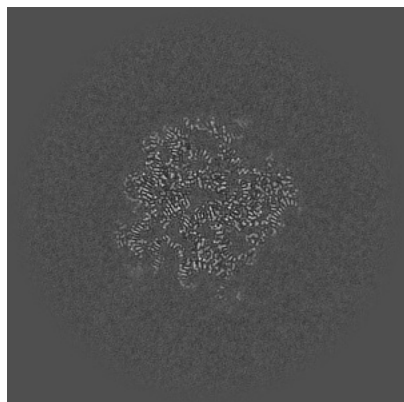


Z Index: 320

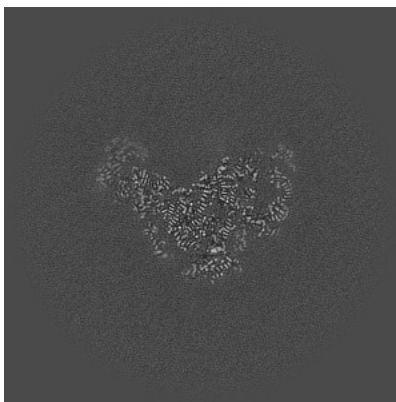
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

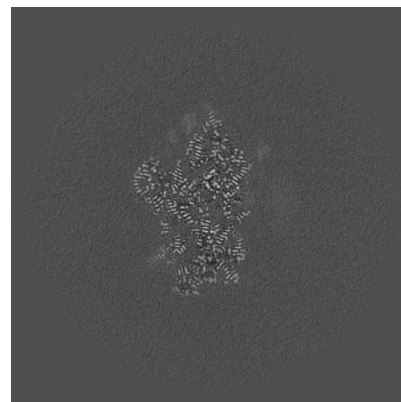
6.3.1 Primary map



X Index: 327

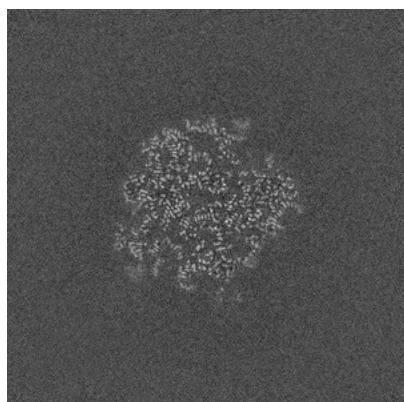


Y Index: 335

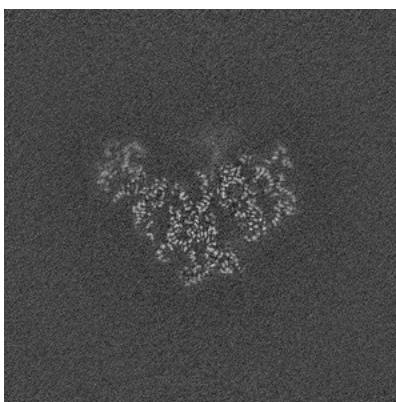


Z Index: 330

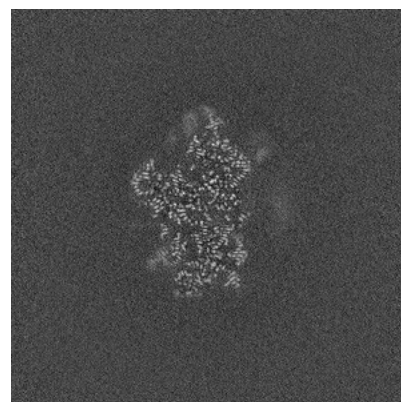
6.3.2 Raw map



X Index: 326



Y Index: 325

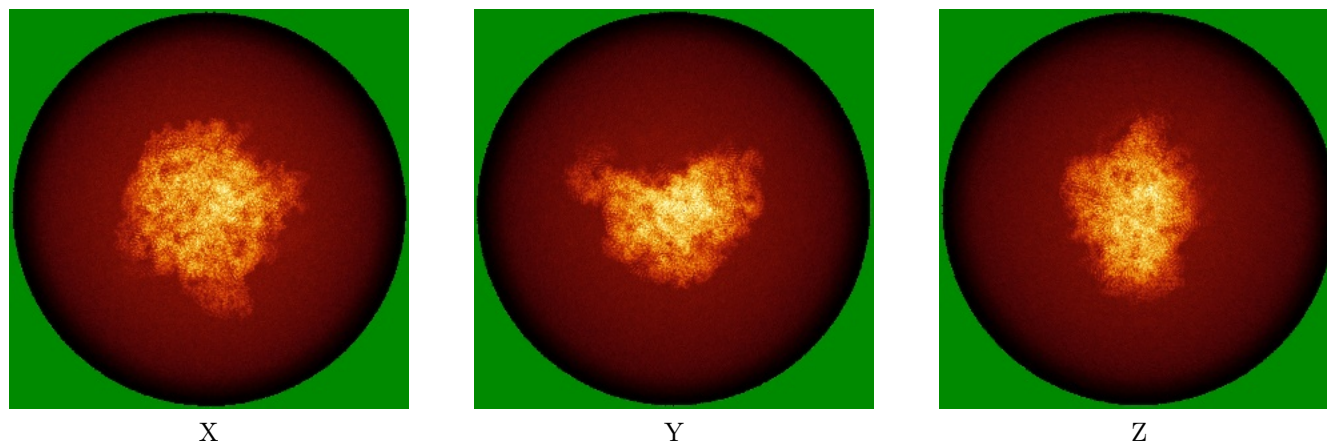


Z Index: 328

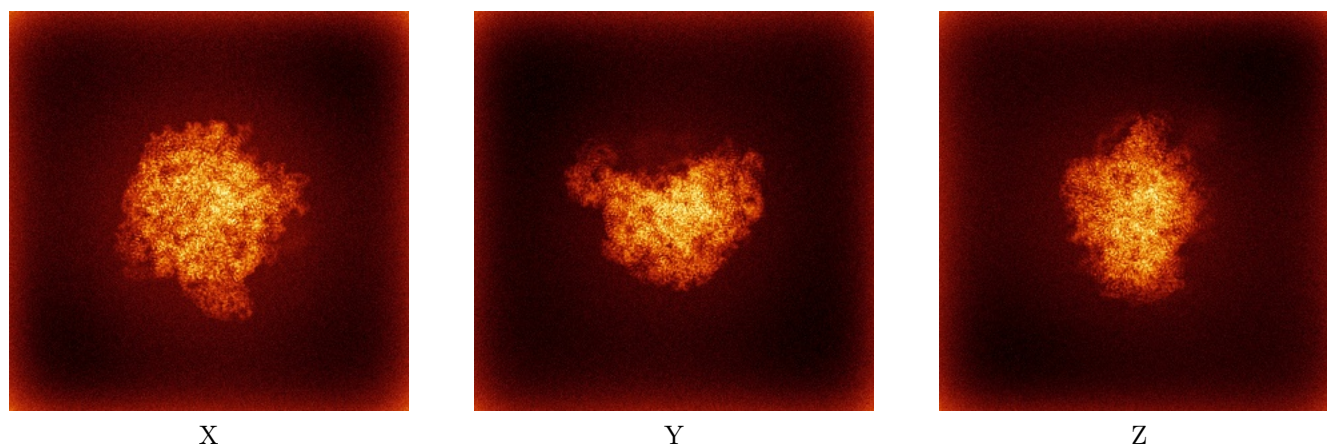
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



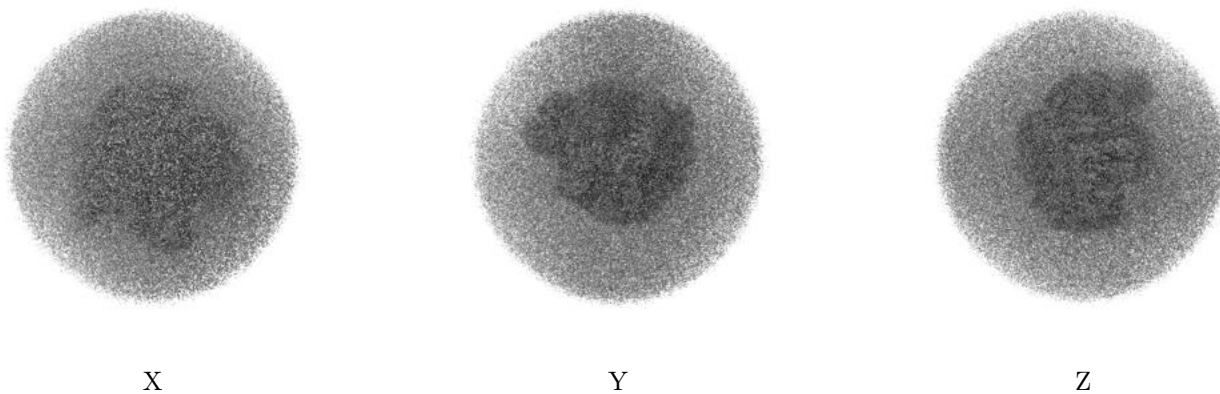
6.4.2 Raw map



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.

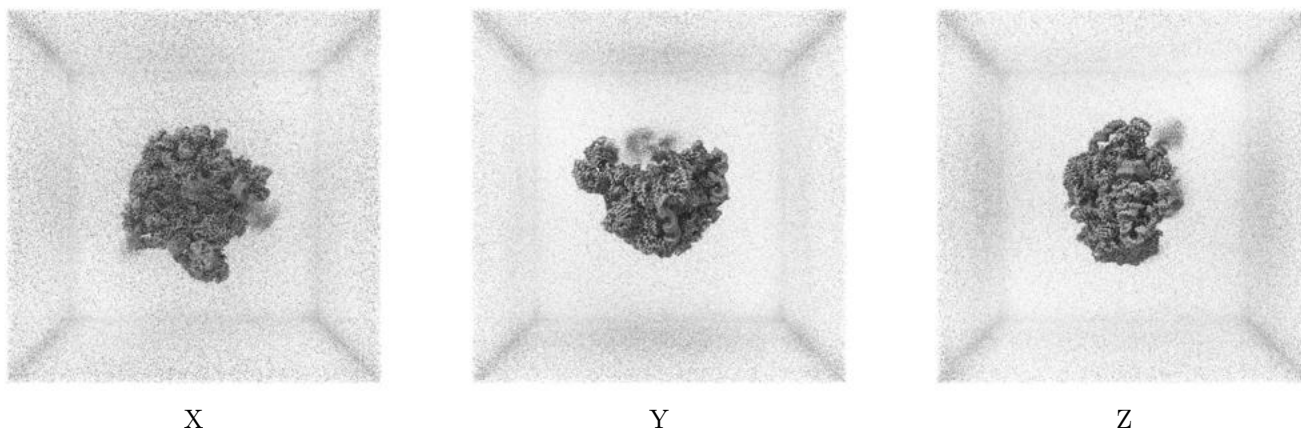
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. 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.

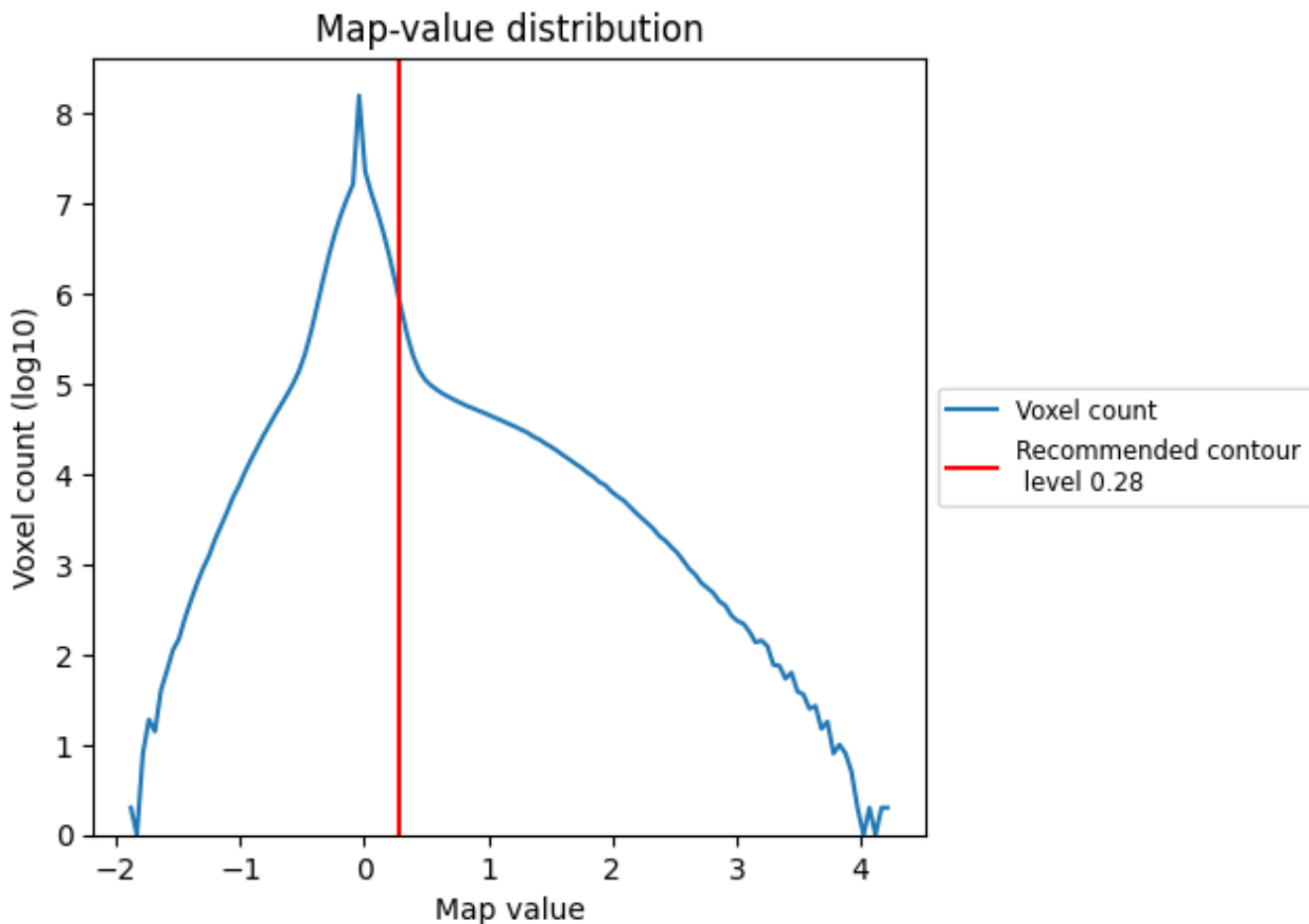
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

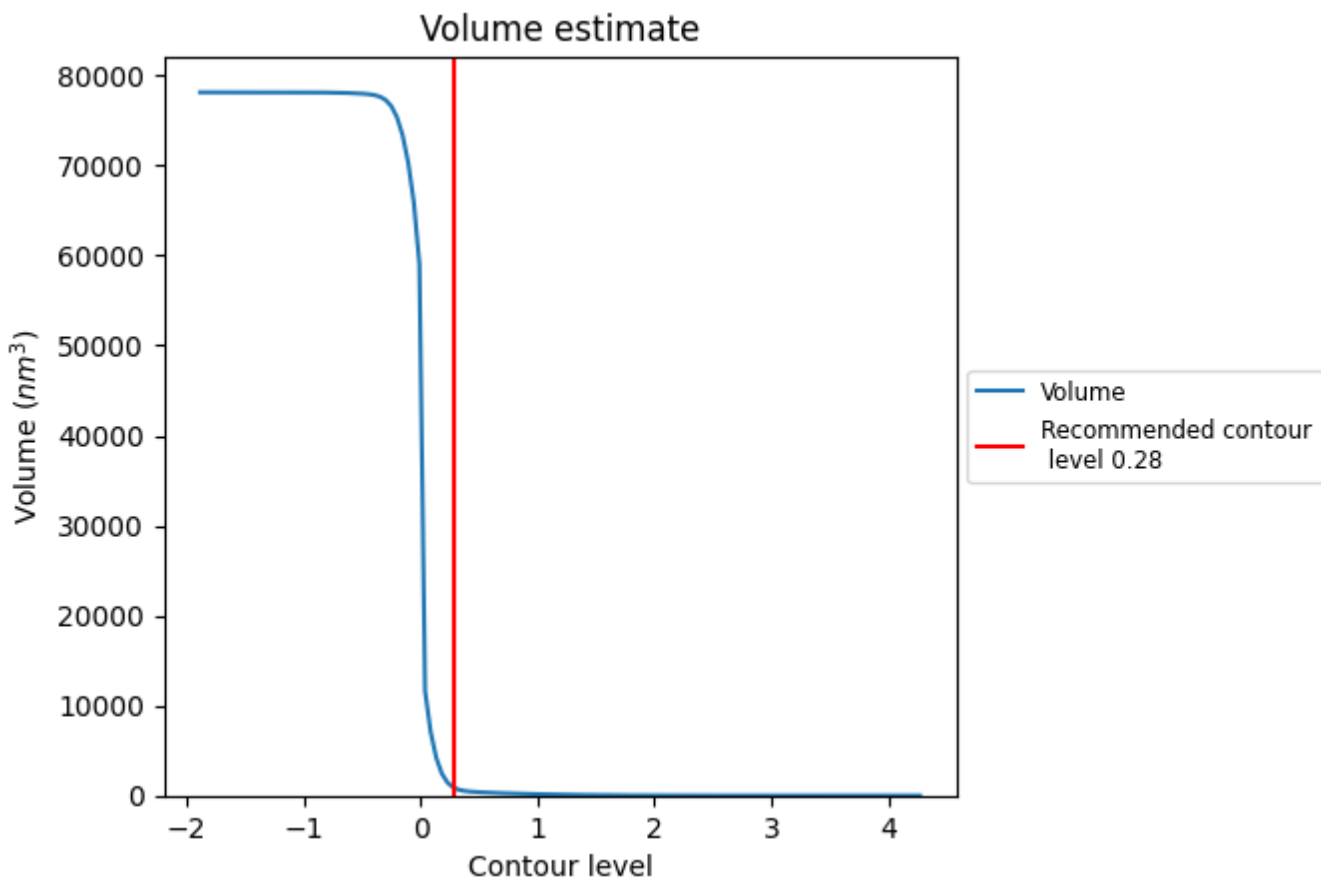
This section contains the results of statistical analysis of the map.

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.

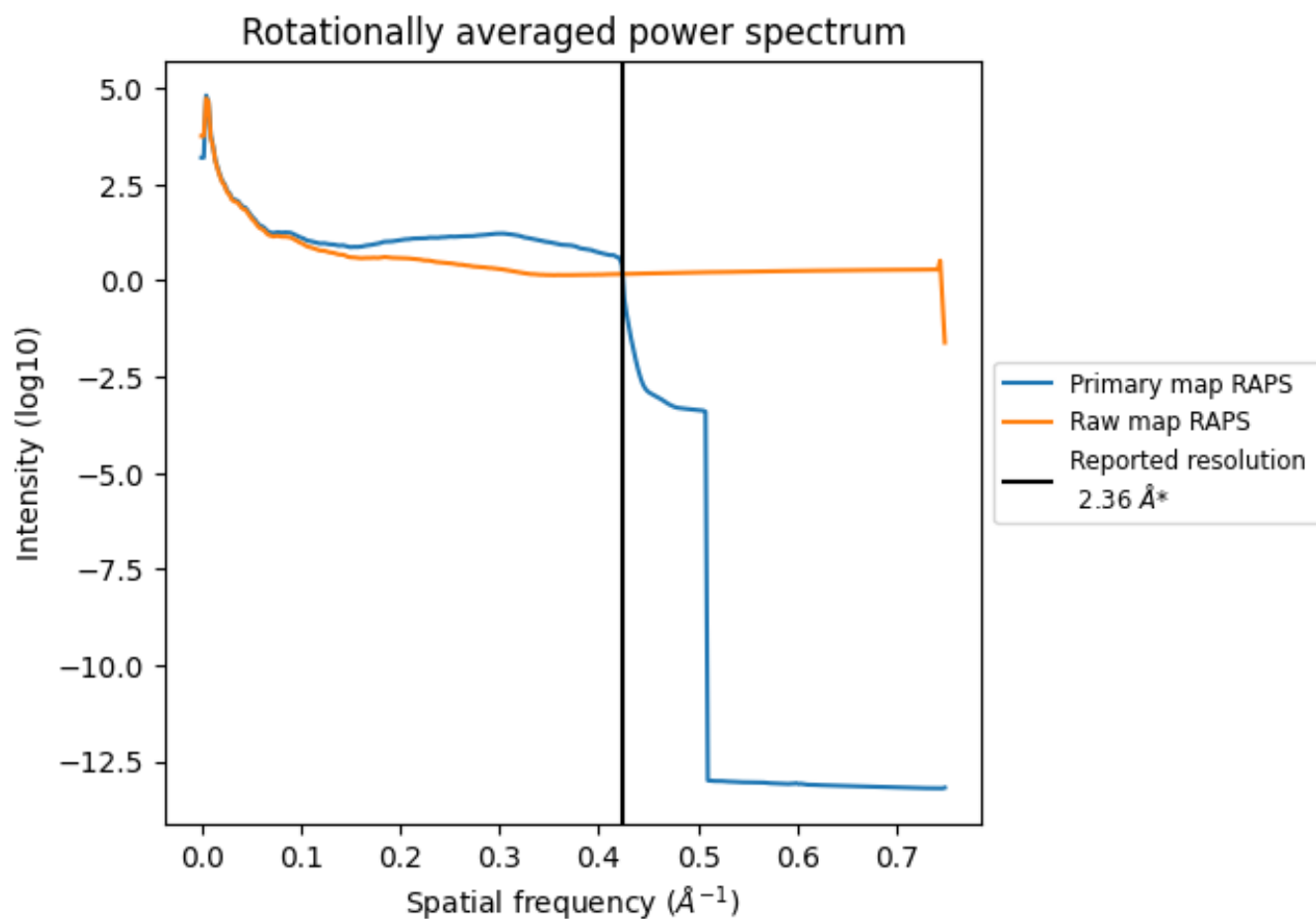
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 911 nm³; this corresponds to an approximate mass of 823 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](#)

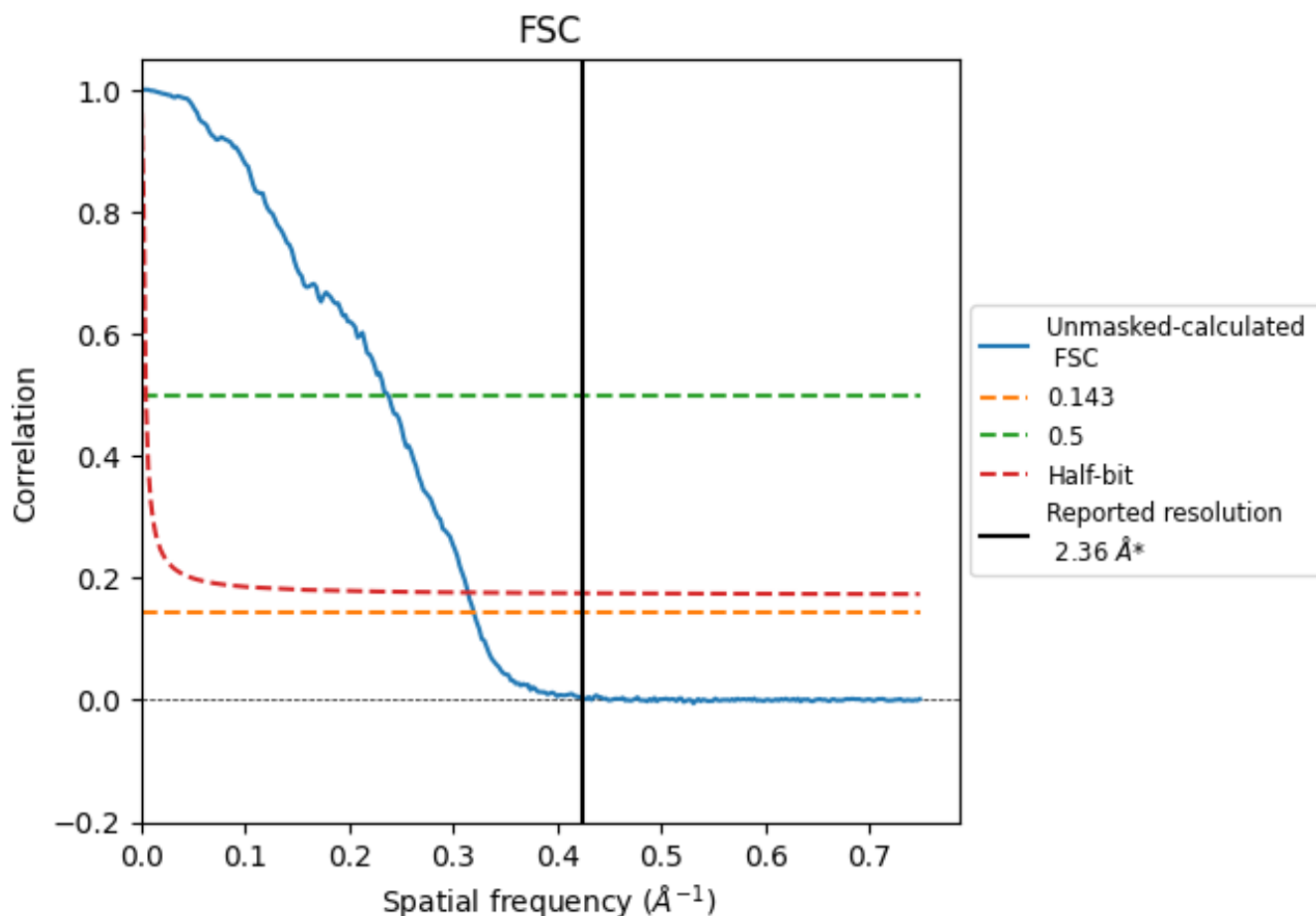


*Reported resolution corresponds to spatial frequency of 0.424 Å⁻¹

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 0.424 Å⁻¹

8.2 Resolution estimates [i](#)

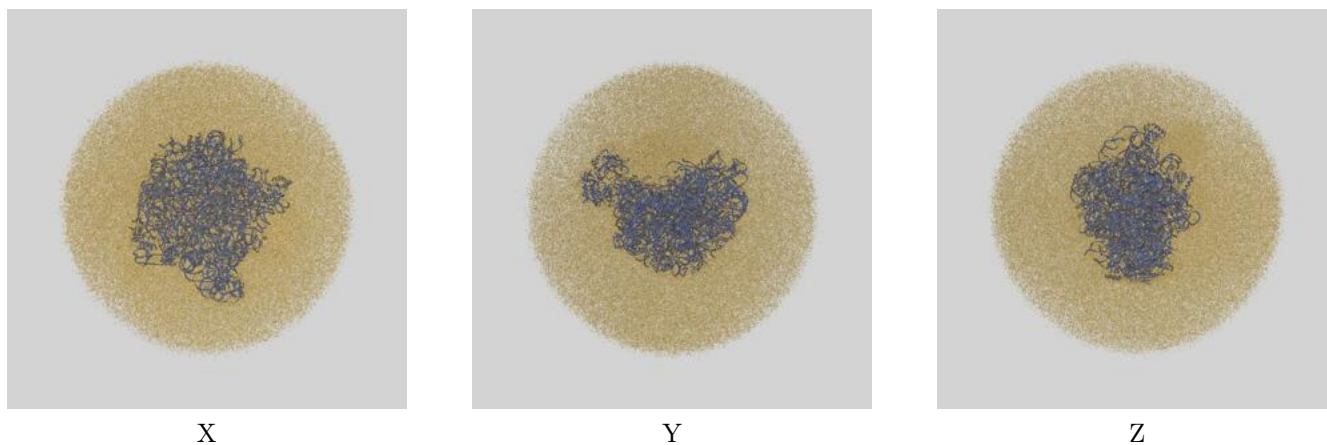
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	4.22	3.18

*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 3.13 differs from the reported value 2.36 by more than 10 %

9 Map-model fit [i](#)

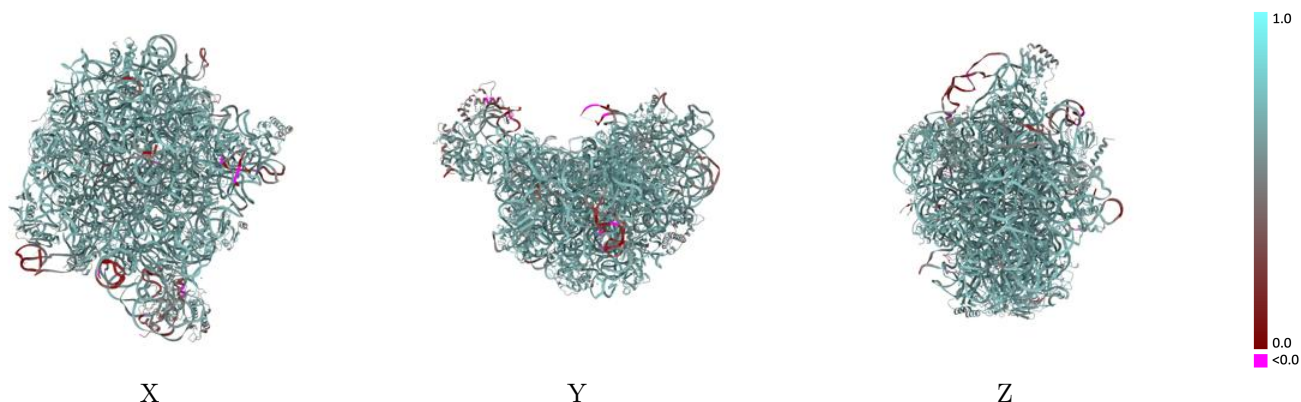
This section contains information regarding the fit between EMDB map EMD-62908 and PDB model 9L9K. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



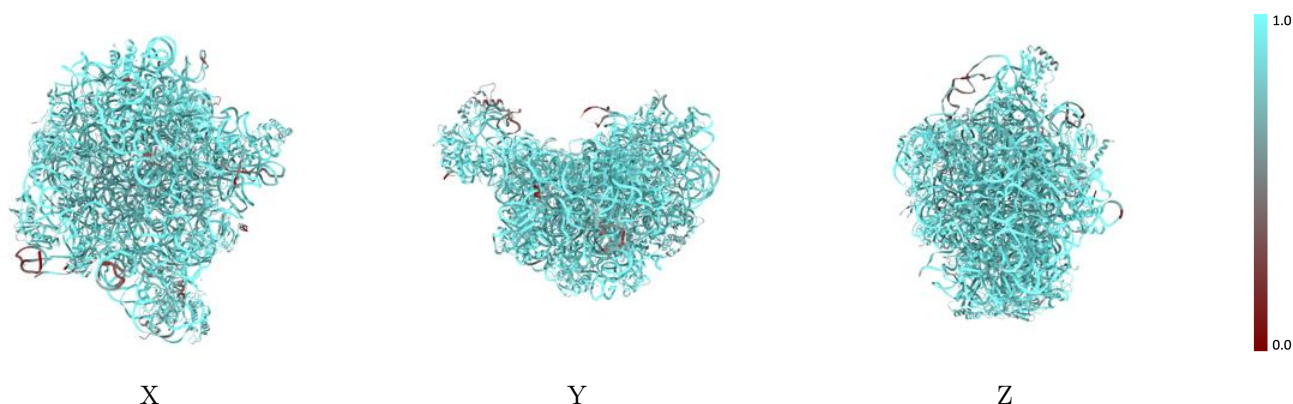
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



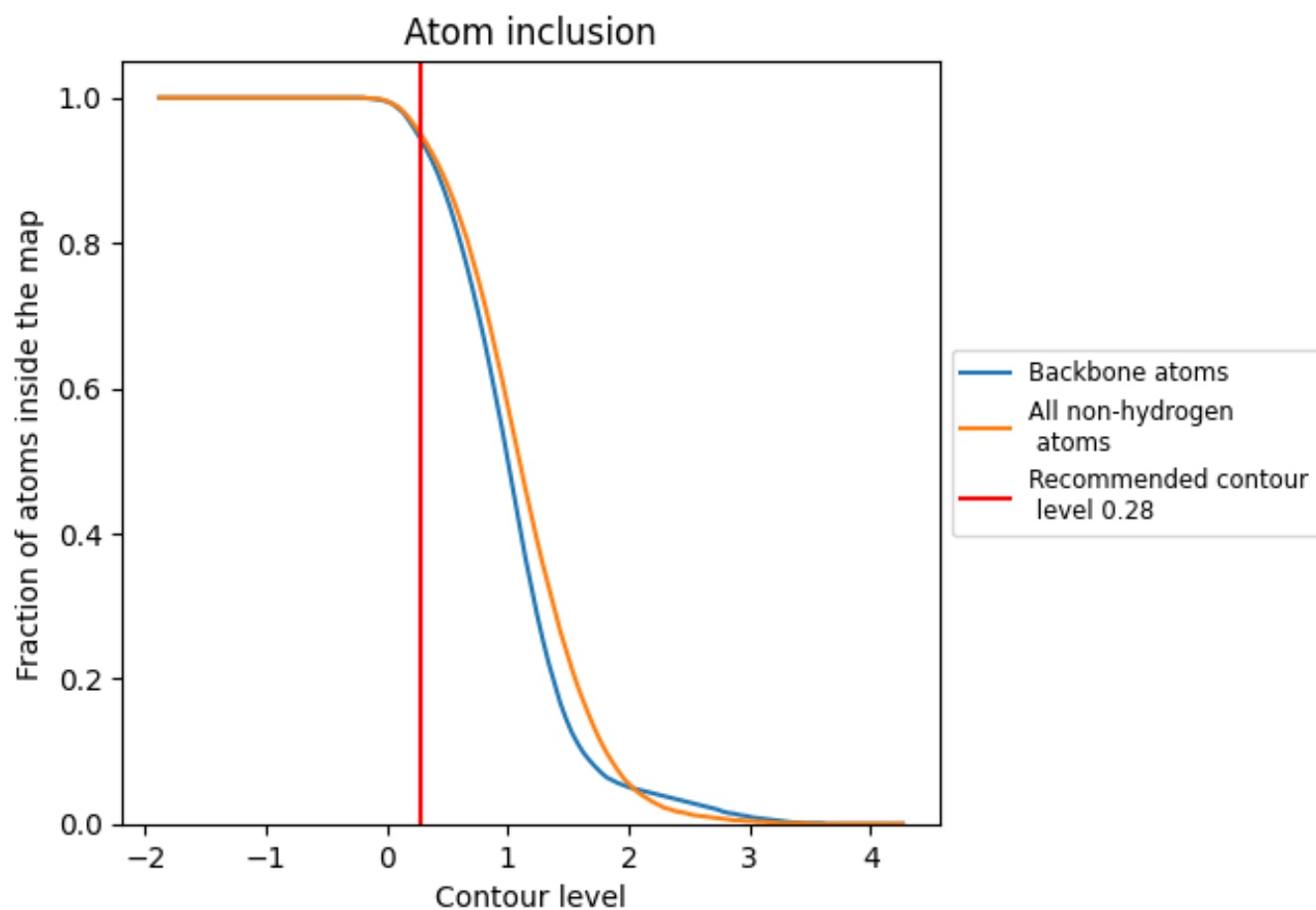
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.6460
0	 0.9670	 0.6520
1	 0.9620	 0.6200
A	 0.8940	 0.6340
E	 0.8920	 0.6020
F	 0.9360	 0.6550
G	 0.9830	 0.7010
H	 0.9480	 0.6540
I	 0.9170	 0.6060
J	 0.9490	 0.6550
K	 0.9640	 0.6770
L	 0.9530	 0.6740
M	 0.9050	 0.6130
N	 0.9320	 0.6510
O	 0.9620	 0.6770
P	 0.8740	 0.6010
Q	 0.9370	 0.6570
R	 0.9020	 0.6260
S	 0.9720	 0.6900
T	 0.9530	 0.6640
U	 0.9260	 0.6450
V	 0.9620	 0.6790
W	 0.9440	 0.6650
X	 0.6710	 0.4260
Y	 0.8970	 0.6040
b	 0.9540	 0.6710
c	 0.8470	 0.5840
d	 0.7450	 0.5170
e	 0.6870	 0.5530
f	 0.9460	 0.6540
i	 0.8770	 0.6230

