



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:01 PM UTC

PDB ID : 8QFD / pdb_00008qfd
EMDB ID : EMD-18382
Title : UFL1 E3 ligase bound 60S ribosome
Authors : Makhlouf, L.; Kulathu, Y.; Zeqiraj, E.
Deposited on : 2023-09-04
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

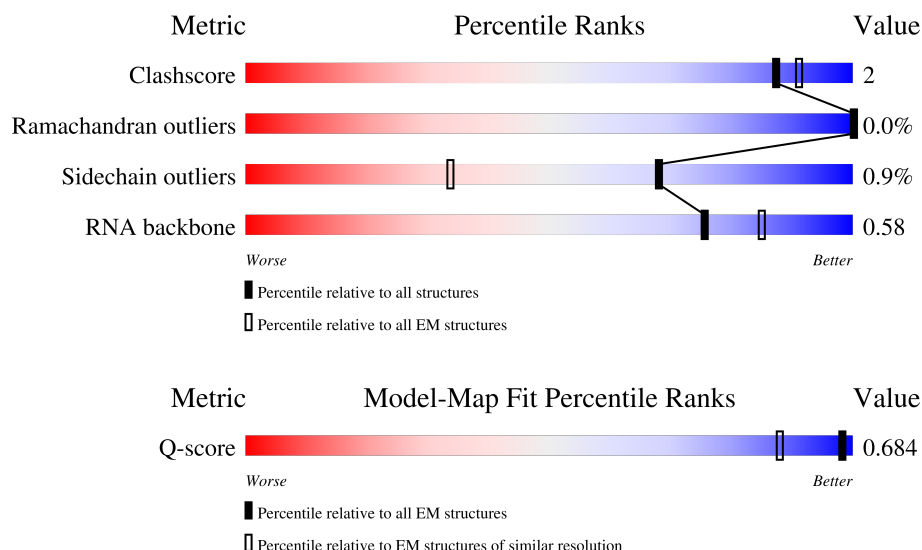
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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.



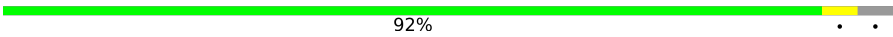
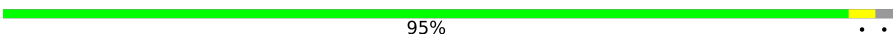
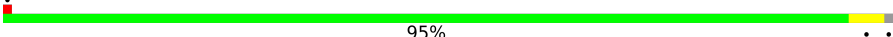
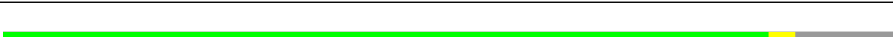
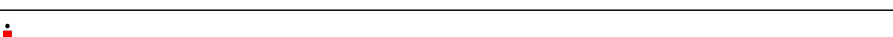
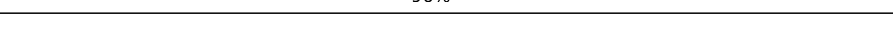
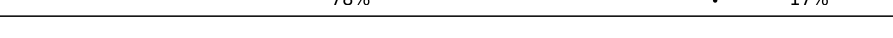
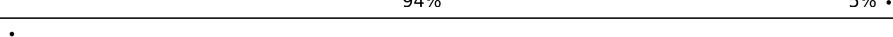
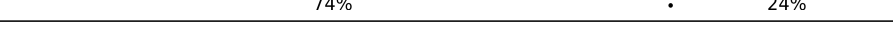
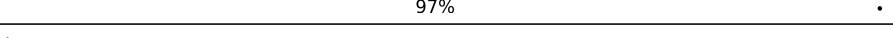
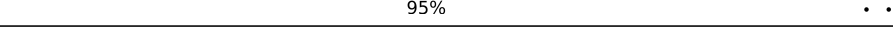
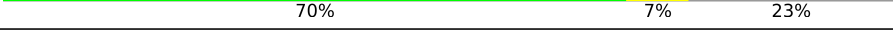
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	5	5070	
2	7	119	
3	8	157	

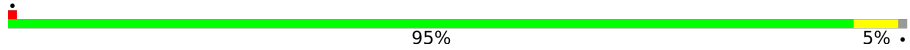
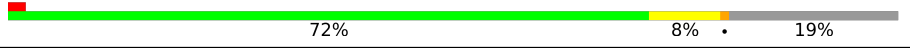
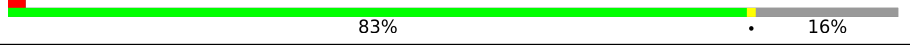
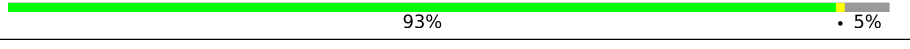
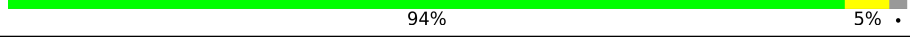
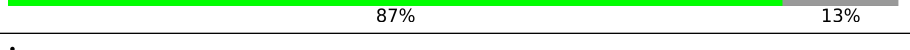
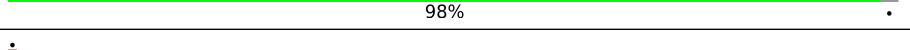
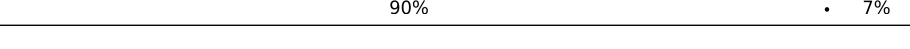
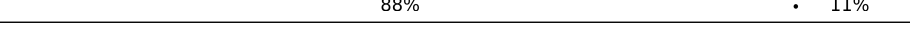
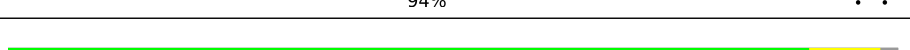
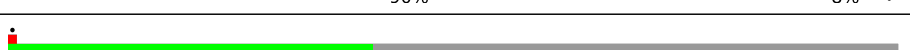
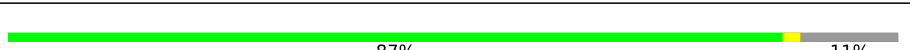
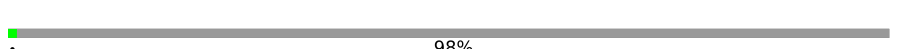
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Mol	Chain	Length	Quality of chain
4	A	257	 92%
5	B	403	 95%
6	C	427	 81% 17%
7	D	297	 95%
8	E	288	 67% 30%
9	F	248	 88% 11%
10	G	266	 77% 20%
11	H	192	 96%
12	I	214	 93% 6%
13	J	178	 90% 5%
14	L	211	 86% 11%
15	M	215	 62% 37%
16	N	204	 99%
17	O	203	 96%
18	P	184	 78% 17%
19	Q	188	 94% 5%
20	R	196	 74% 24%
21	S	176	 97%
22	T	160	 95%
23	U	128	 70% 7% 23%
24	V	140	 91% 7%
25	W	157	 39% 61%
26	X	156	 74% 24%
27	Y	145	 83% 5% 12%
28	Z	136	 97%

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Mol	Chain	Length	Quality of chain
29	a	148	
30	b	159	
31	c	115	
32	d	125	
33	e	135	
34	f	110	
35	g	117	
36	h	123	
37	i	105	
38	j	97	
39	k	70	
40	l	51	
41	m	128	
42	o	106	
43	p	92	
44	r	137	
45	s	809	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 125372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3130	Total	C	N	O	P	0	0
			67136	29909	12303	21794	3130		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1183	A	C	conflict	GB 86475748
5	4909	A	G	conflict	GB 86475748

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	144	Total	C	N	O	P	0	0
			3071	1369	548	1010	144		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	246	Total	C	N	O	S	0	0
			1881	1180	384	311	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	395	Total	C	N	O	S	0	0
			3176	2023	596	543	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	355	Total	C	N	O	S	0	0
			2832	1782	566	470	14		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	293	Total	C	N	O	S	0	0
			2351	1485	431	421	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	201	Total	C	N	O	S	0	0
			1632	1055	311	262	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	220	Total	C	N	O	S	0	0
			1798	1154	342	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	214	Total	C	N	O	S	0	0
			1722	1098	333	287	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	190	Total	C	N	O	S	0	0
			1506	947	281	272	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	201	Total	C	N	O	S	0	0
			1627	1033	314	268	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	170	Total	C	N	O	S	0	0
			1358	858	253	241	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	188	Total	C	N	O	S	0	0
			1500	937	310	249	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	136	Total	C	N	O	S	0	0
			1116	716	214	179	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	203	Total	C	N	O	S	0	0
			1695	1069	356	266	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	201	Total	C	N	O	S	0	0
			1644	1059	321	259	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	152	Total	C	N	O	S	0	0
			1225	765	238	213	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	187	Total	C	N	O	S	0	0
			1509	941	313	250	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	149	Total	C	N	O	S	0	0
			1229	765	264	191	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	176	Total	C	N	O	S	0	0
			1444	918	279	236	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	158	Total	C	N	O	S	0	0
			1276	808	247	215	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	98	Total	C	N	O	S	0	0
			791	507	137	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	130	Total	C	N	O	S	0	0
			973	615	183	170	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	62	Total	C	N	O	S	0	0
			515	329	100	83	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	118	Total	C	N	O	S	0	0
			950	606	176	167	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	128	Total	C	N	O	S	0	0
			1063	667	215	178	3		

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

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	147	Total	C	N	O	S	0	0
			1158	733	236	186	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	65	Total	C	N	O	S	0	0
			526	324	114	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	93	Total	C	N	O	S	0	0
			713	455	125	127	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	105	Total	C	N	O	S	0	0
			852	542	168	140	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	128	Total	C	N	O	S	0	0
			1039	658	211	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	108	Total	C	N	O	S	0	0
			863	546	172	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	102	Total	C	N	O	S	0	0
			814	508	169	131	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	120	Total	C	N	O	S	0	0
			993	627	201	164	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	98	Total	C	N	O	S	0	0
			776	485	161	125	5		

- Molecule 38 is a protein called Ribosomal protein L37.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	68	Total	C	N	O	S	0	0
			527	339	95	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	50	Total	C	N	O	S	0	0
			438	278	95	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	52	Total	C	N	O	S	0	0
			418	258	89	65	6		

- Molecule 42 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	102	Total	C	N	O	S	0	0
			810	507	162	135	6		

- Molecule 43 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	88	Total	C	N	O	S	0	0
			666	419	129	111	7		

- Molecule 44 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 45 is a protein called E3 UFM1-protein ligase 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	s	13	Total	C	N	O	0	0
			99	62	20	17		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	-14	MET	-	initiating methionine	UNP O94874
s	-13	GLY	-	expression tag	UNP O94874
s	-12	HIS	-	expression tag	UNP O94874
s	-11	HIS	-	expression tag	UNP O94874
s	-10	HIS	-	expression tag	UNP O94874
s	-9	HIS	-	expression tag	UNP O94874
s	-8	HIS	-	expression tag	UNP O94874
s	-7	HIS	-	expression tag	UNP O94874
s	-6	GLU	-	expression tag	UNP O94874
s	-5	ASN	-	expression tag	UNP O94874
s	-4	LEU	-	expression tag	UNP O94874
s	-3	TYR	-	expression tag	UNP O94874

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Chain	Residue	Modelled	Actual	Comment	Reference
s	-2	PHE	-	expression tag	UNP O94874
s	-1	GLN	-	expression tag	UNP O94874
s	0	GLY	-	expression tag	UNP O94874

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	5	151	Total 151	Mg 151	0
46	7	2	Total 2	Mg 2	0
46	8	2	Total 2	Mg 2	0
46	I	1	Total 1	Mg 1	0
46	N	1	Total 1	Mg 1	0
46	P	1	Total 1	Mg 1	0
46	Q	1	Total 1	Mg 1	0
46	V	1	Total 1	Mg 1	0
46	j	1	Total 1	Mg 1	0

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	g	1	Total 1	Zn 1	0
47	j	1	Total 1	Zn 1	0
47	m	1	Total 1	Zn 1	0
47	o	1	Total 1	Zn 1	0
47	p	1	Total 1	Zn 1	0

- Molecule 48 is water.

Mol	Chain	Residues	Atoms		AltConf
48	5	1643	Total 1643	O 1643	0
48	7	27	Total 27	O 27	0
48	8	47	Total 47	O 47	0
48	A	26	Total 26	O 26	0
48	B	40	Total 40	O 40	0
48	C	40	Total 40	O 40	0
48	D	8	Total 8	O 8	0
48	E	3	Total 3	O 3	0
48	F	15	Total 15	O 15	0
48	G	6	Total 6	O 6	0
48	H	4	Total 4	O 4	0
48	I	13	Total 13	O 13	0
48	L	18	Total 18	O 18	0
48	M	3	Total 3	O 3	0
48	N	41	Total 41	O 41	0
48	O	22	Total 22	O 22	0
48	P	11	Total 11	O 11	0
48	Q	20	Total 20	O 20	0
48	R	6	Total 6	O 6	0
48	S	15	Total 15	O 15	0
48	T	11	Total 11	O 11	0
48	V	7	Total 7	O 7	0

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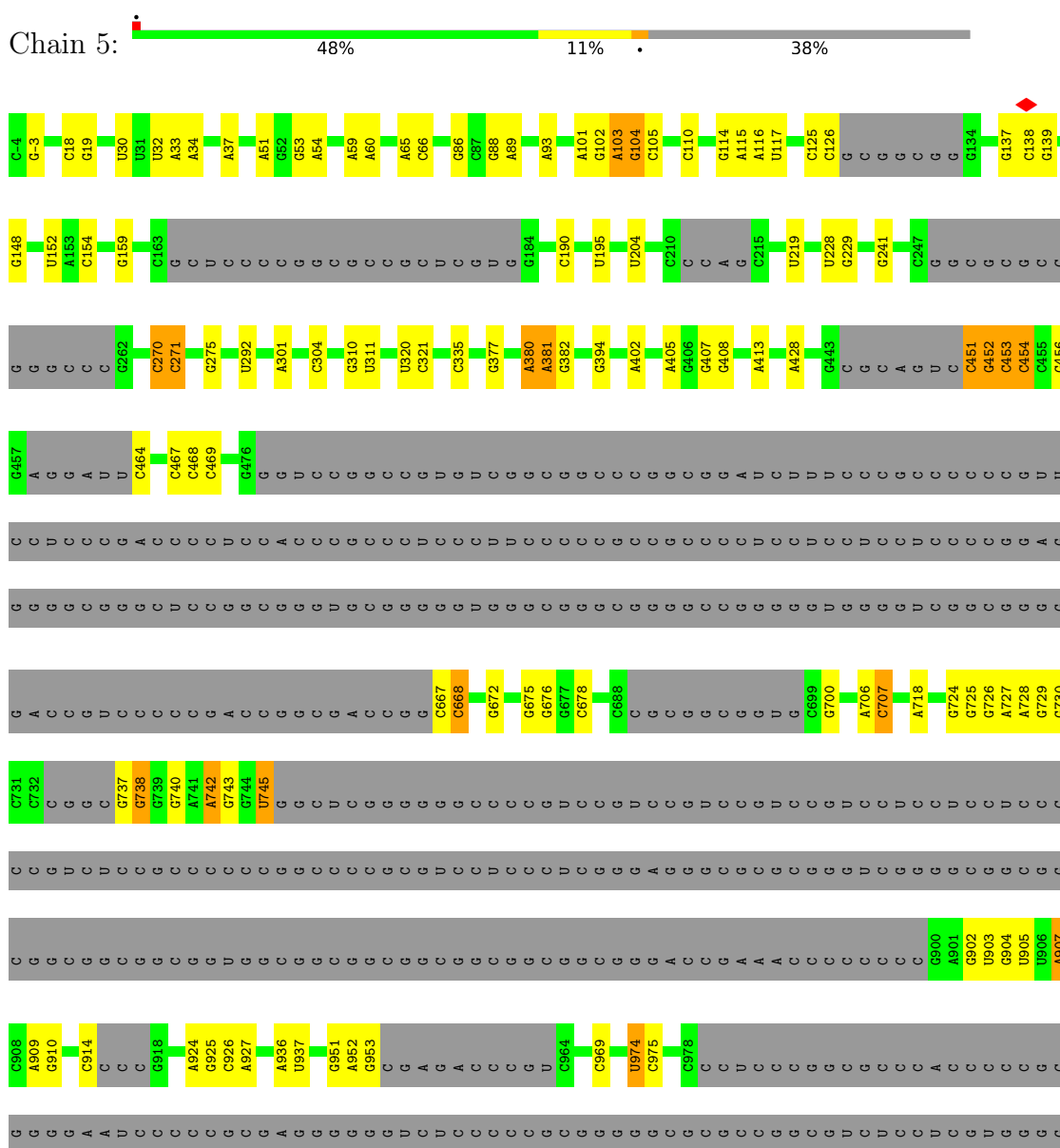
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Mol	Chain	Residues	Atoms		AltConf
48	X	3	Total 3	O 3	0
48	Y	9	Total 9	O 9	0
48	Z	2	Total 2	O 2	0
48	a	23	Total 23	O 23	0
48	b	4	Total 4	O 4	0
48	d	7	Total 7	O 7	0
48	e	23	Total 23	O 23	0
48	f	19	Total 19	O 19	0
48	g	7	Total 7	O 7	0
48	h	5	Total 5	O 5	0
48	i	1	Total 1	O 1	0
48	j	7	Total 7	O 7	0
48	l	3	Total 3	O 3	0
48	m	1	Total 1	O 1	0
48	o	7	Total 7	O 7	0
48	p	5	Total 5	O 5	0
48	r	12	Total 12	O 12	0

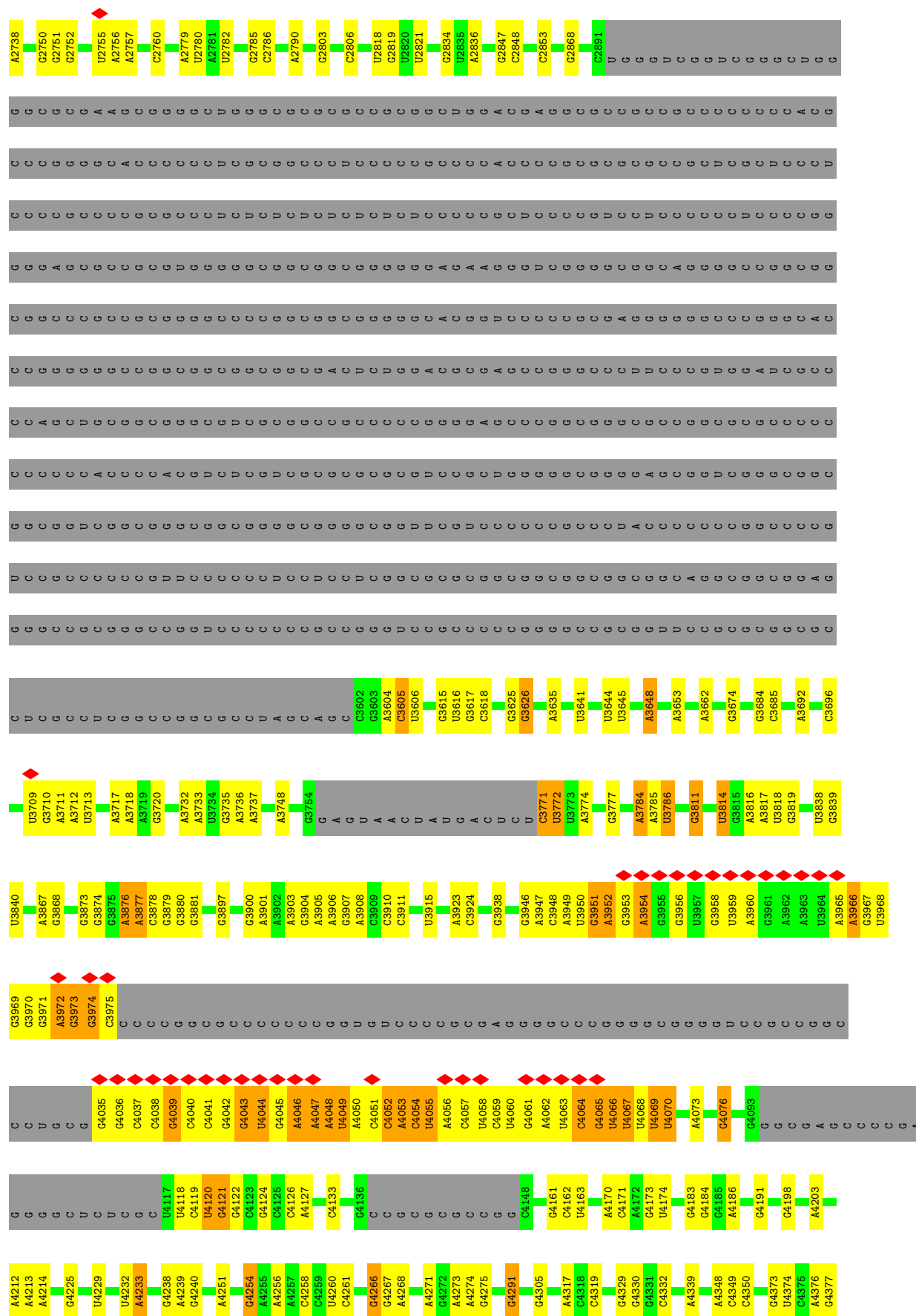
3 Residue-property plots [i](#)

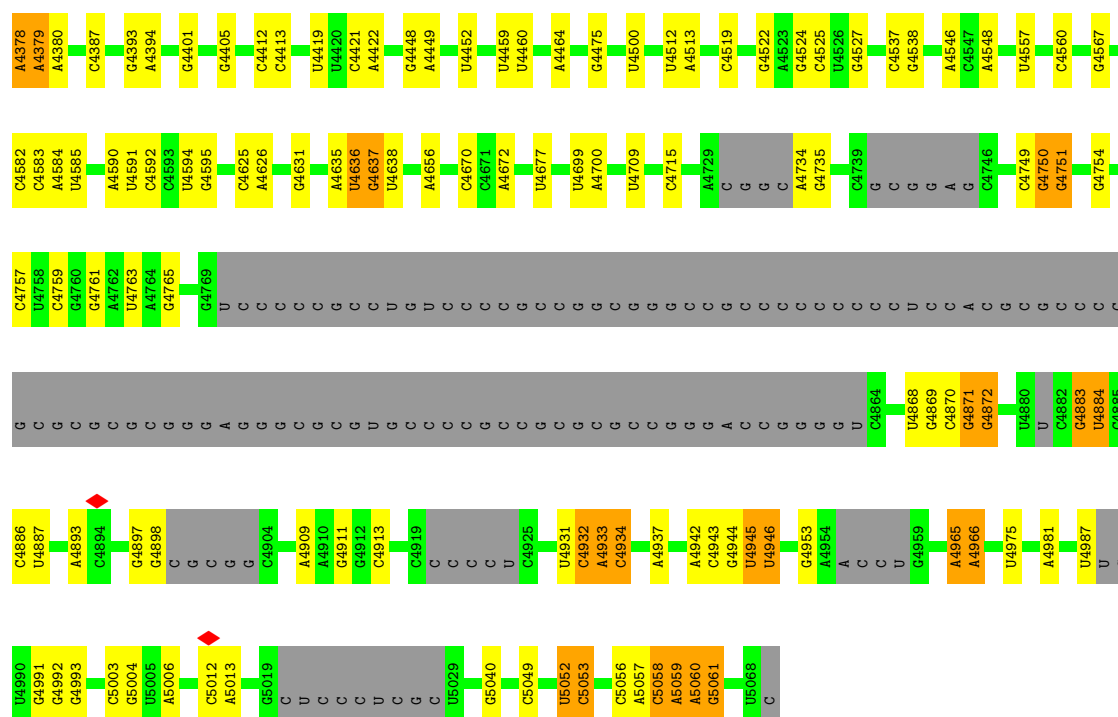
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 28S rRNA



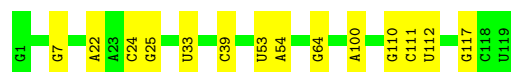






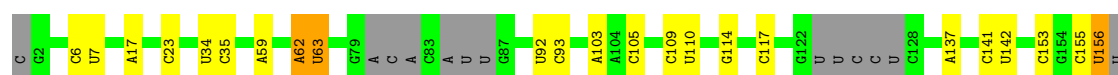
• Molecule 2: 5S rRNA

Chain 7: 88% 12%



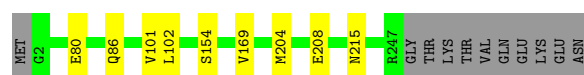
• Molecule 3: 5.8S rRNA

Chain 8: 77% 13% 8%



• Molecule 4: 60S ribosomal protein L8

Chain A: 92% 8%



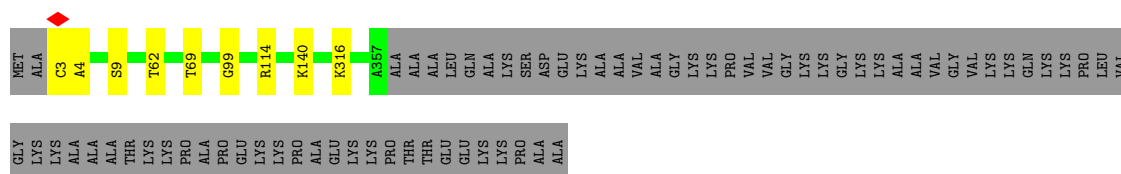
• Molecule 5: 60S ribosomal protein L3

Chain B: 95% 5%



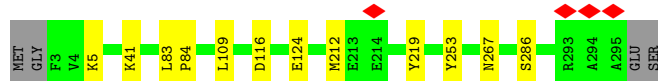
• Molecule 6: 60S ribosomal protein L4

Chain C:  81% 17%



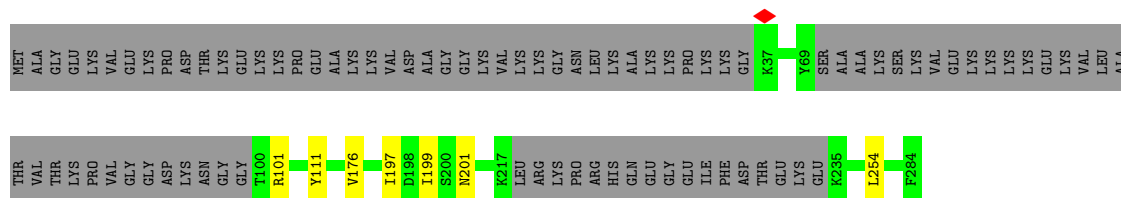
- Molecule 7: 60S ribosomal protein L5

Chain D:  95%



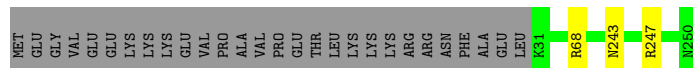
- Molecule 8: 60S ribosomal protein L6

Chain E:  67% 30%



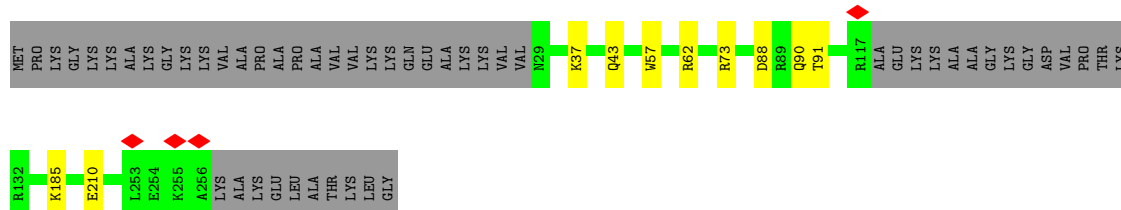
- Molecule 9: Large ribosomal subunit protein uL30

Chain F:  88% 11%



- Molecule 10: 60S ribosomal protein L7a

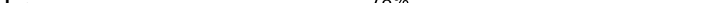
Chain G:  77% 20%

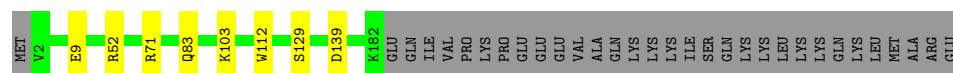


- Molecule 11: 60S ribosomal protein L9

Chain H:  96%

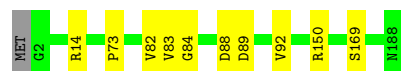
- Molecule 18: 60S ribosomal protein L17

Chain P:  78% . 17%



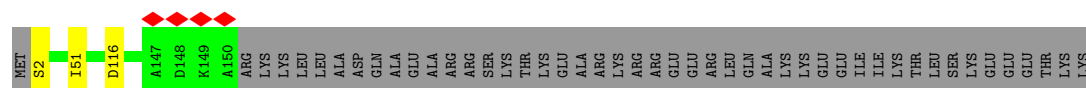
- Molecule 19: 60S ribosomal protein L18

Chain Q: 94% 5%



- Molecule 20: 60S ribosomal protein L19

Chain R:  74% 24%



- Molecule 21: 60S ribosomal protein L18a

Chain S: 97%



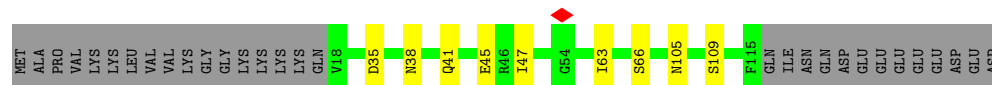
- Molecule 22: 60S ribosomal protein L21

Chain T: 95% ...

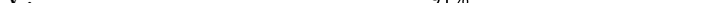


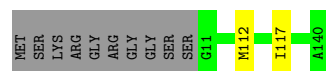
- Molecule 23: 60S ribosomal protein L22

Chain U:



- Molecule 24: 60S ribosomal protein L23

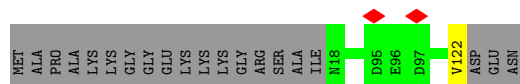
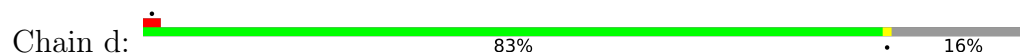
Chain V:  91% . 7%



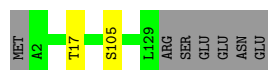
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31



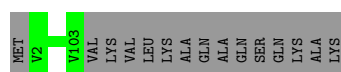
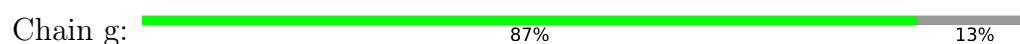
- Molecule 33: 60S ribosomal protein L32



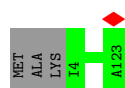
- Molecule 34: 60S ribosomal protein L35a



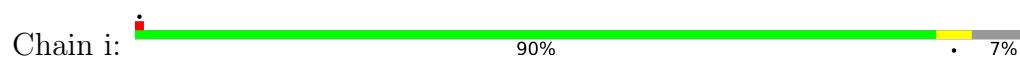
- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35

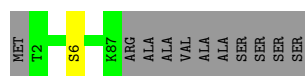


- Molecule 37: 60S ribosomal protein L36

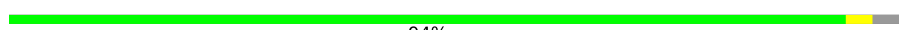


- Molecule 38: Ribosomal protein L37

Chain j:  88% 11%



- Molecule 39: 60S ribosomal protein L38

Chain k:  94%



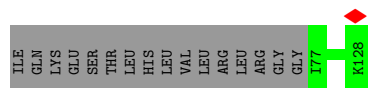
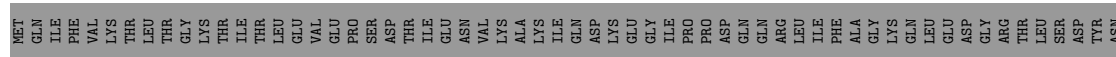
- Molecule 40: 60S ribosomal protein L39

Chain l:  90% 8%



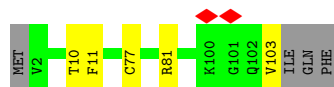
- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain m:  41% 59%

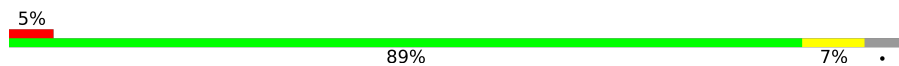


- Molecule 42: 60S ribosomal protein L36a

Chain o:  92% 5%



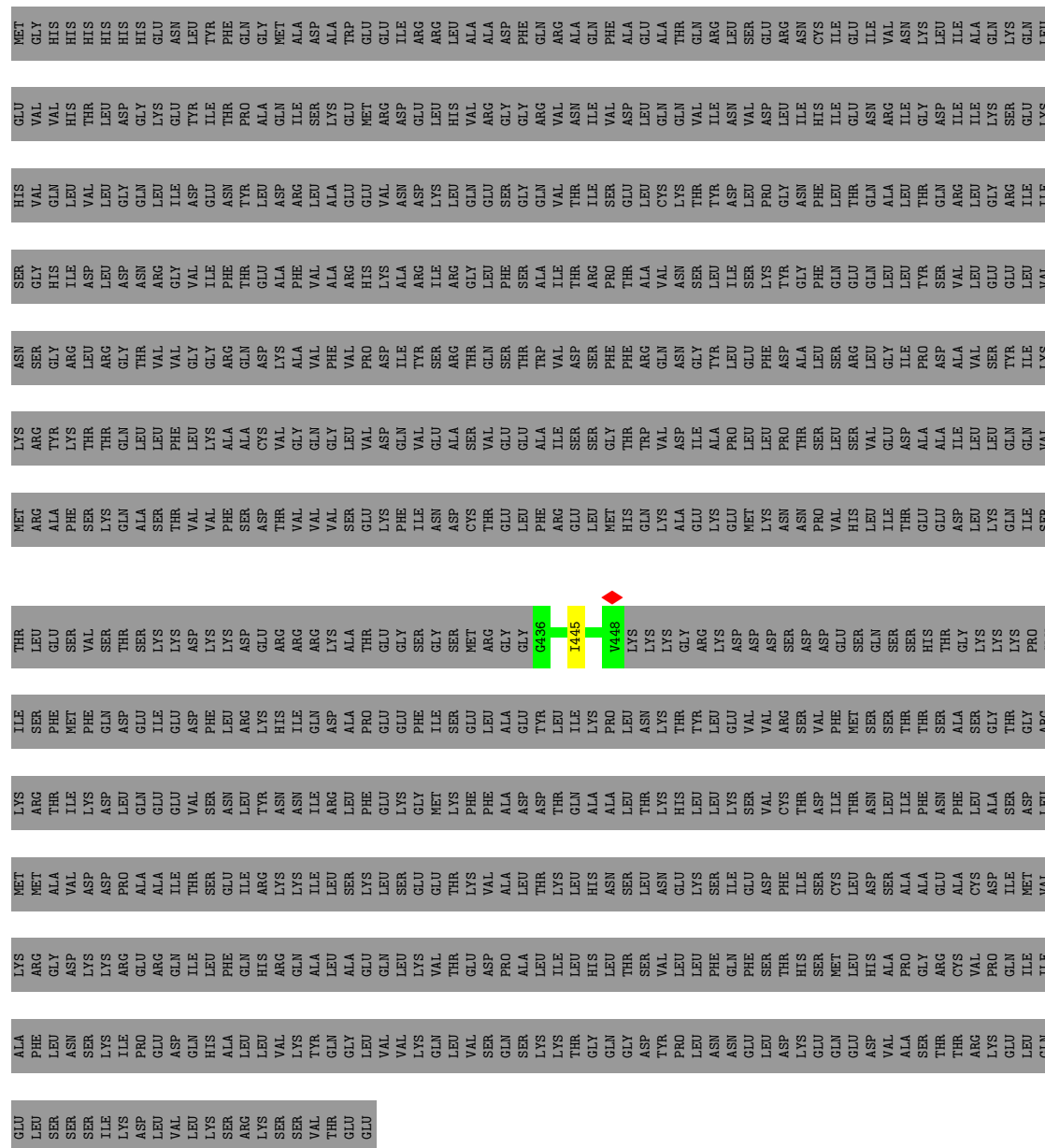
- Molecule 43: 60S ribosomal protein L37a

Chain p:  5% 89% 7%



- Molecule 44: 60S ribosomal protein L28

Chain r:  87% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33.4	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	39.734	Depositor
Minimum map value	-21.503	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.8	Depositor
Map size (Å)	435.12, 435.12, 435.12	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

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

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	5	0.21	0/75089	0.33	4/117047 (0.0%)
2	7	0.20	0/2836	0.29	0/4421
3	8	0.20	0/3428	0.30	0/5335
4	A	0.17	0/1919	0.35	0/2574
5	B	0.16	0/3244	0.33	0/4344
6	C	0.16	0/2886	0.32	0/3877
7	D	0.14	0/2396	0.29	0/3215
8	E	0.14	0/1665	0.28	0/2235
9	F	0.18	0/1832	0.35	0/2448
10	G	0.15	0/1753	0.31	0/2366
11	H	0.15	0/1525	0.31	0/2054
12	I	0.15	0/1665	0.30	0/2223
13	J	0.12	0/1381	0.30	0/1848
14	L	0.15	0/1530	0.30	0/2058
15	M	0.16	0/1138	0.33	0/1523
16	N	0.17	0/1740	0.33	0/2331
17	O	0.18	0/1676	0.33	0/2242
18	P	0.16	0/1251	0.34	0/1681
19	Q	0.18	0/1533	0.35	0/2048
20	R	0.14	0/1245	0.30	0/1653
21	S	0.17	0/1483	0.33	0/1993
22	T	0.15	0/1304	0.29	0/1747
23	U	0.12	0/805	0.33	0/1083
24	V	0.14	0/987	0.31	0/1324
25	W	0.15	0/528	0.30	0/704
26	X	0.14	0/967	0.29	0/1304
27	Y	0.16	0/1080	0.31	0/1441
28	Z	0.12	0/1130	0.24	0/1507
29	a	0.17	0/1187	0.33	0/1587
30	b	0.17	0/536	0.33	0/710
31	c	0.14	0/723	0.30	0/973
32	d	0.16	0/867	0.35	0/1170

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.16	0/1057	0.33	0/1414
34	f	0.16	0/882	0.32	0/1183
35	g	0.15	0/824	0.30	0/1098
36	h	0.15	0/1001	0.29	0/1324
37	i	0.13	0/787	0.31	0/1049
38	j	0.17	0/720	0.37	0/952
39	k	0.13	0/533	0.28	0/715
40	l	0.16	0/448	0.32	0/592
41	m	0.15	0/424	0.31	0/562
42	o	0.16	0/823	0.30	0/1091
43	p	0.15	0/676	0.32	0/902
44	r	0.16	0/994	0.32	0/1331
45	s	0.08	0/99	0.26	0/128
All	All	0.19	0/132597	0.33	4/195407 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1071	C	C1'-C2'-O2'	6.14	117.61	108.40
1	5	1071	C	C3'-C2'-O2'	5.62	119.13	110.70
1	5	1071	C	C4'-C3'-O3'	5.42	121.13	113.00
1	5	1071	C	C2'-C3'-O3'	5.35	121.72	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	67136	0	33910	340	0
2	7	2538	0	1286	4	0
3	8	3071	0	1558	7	0
4	A	1881	0	1972	5	0
5	B	3176	0	3303	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2832	0	2996	4	0
7	D	2351	0	2353	7	0
8	E	1632	0	1770	5	0
9	F	1798	0	1884	2	0
10	G	1722	0	1826	9	0
11	H	1506	0	1568	3	0
12	I	1627	0	1667	0	0
13	J	1358	0	1388	5	0
14	L	1500	0	1566	5	0
15	M	1116	0	1176	2	0
16	N	1695	0	1738	1	0
17	O	1644	0	1783	3	0
18	P	1225	0	1241	4	0
19	Q	1509	0	1617	7	0
20	R	1229	0	1333	1	0
21	S	1444	0	1464	3	0
22	T	1276	0	1317	3	0
23	U	791	0	801	5	0
24	V	973	0	1034	1	0
25	W	515	0	522	1	0
26	X	950	0	998	2	0
27	Y	1063	0	1132	4	0
28	Z	1107	0	1182	1	0
29	a	1158	0	1202	6	0
30	b	526	0	535	2	0
31	c	713	0	740	6	0
32	d	852	0	894	0	0
33	e	1039	0	1114	2	0
34	f	863	0	890	1	0
35	g	814	0	891	0	0
36	h	993	0	1115	0	0
37	i	776	0	812	1	0
38	j	705	0	737	0	0
39	k	527	0	555	1	0
40	l	438	0	472	2	0
41	m	418	0	441	0	0
42	o	810	0	846	3	0
43	p	666	0	696	4	0
44	r	980	0	1037	1	0
45	s	99	0	106	1	0
46	5	151	0	0	0	0
46	7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	8	2	0	0	0	0
46	I	1	0	0	0	0
46	N	1	0	0	0	0
46	P	1	0	0	0	0
46	Q	1	0	0	0	0
46	V	1	0	0	0	0
46	j	1	0	0	0	0
47	g	1	0	0	0	0
47	j	1	0	0	0	0
47	m	1	0	0	0	0
47	o	1	0	0	0	0
47	p	1	0	0	0	0
48	5	1643	0	0	7	0
48	7	27	0	0	0	0
48	8	47	0	0	0	0
48	A	26	0	0	1	0
48	B	40	0	0	0	0
48	C	40	0	0	1	0
48	D	8	0	0	0	0
48	E	3	0	0	0	0
48	F	15	0	0	0	0
48	G	6	0	0	0	0
48	H	4	0	0	0	0
48	I	13	0	0	0	0
48	L	18	0	0	0	0
48	M	3	0	0	0	0
48	N	41	0	0	0	0
48	O	22	0	0	0	0
48	P	11	0	0	0	0
48	Q	20	0	0	0	0
48	R	6	0	0	0	0
48	S	15	0	0	0	0
48	T	11	0	0	0	0
48	V	7	0	0	0	0
48	X	3	0	0	0	0
48	Y	9	0	0	0	0
48	Z	2	0	0	0	0
48	a	23	0	0	0	0
48	b	4	0	0	0	0
48	d	7	0	0	0	0
48	e	23	0	0	0	0
48	f	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	g	7	0	0	0	0
48	h	5	0	0	0	0
48	i	1	0	0	0	0
48	j	7	0	0	0	0
48	l	3	0	0	0	0
48	m	1	0	0	0	0
48	o	7	0	0	0	0
48	p	5	0	0	0	0
48	r	12	0	0	0	0
All	All	125372	0	89468	426	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 2.

All (426) 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)
1:5:451:C:O2'	1:5:452:G:OP1	1.83	0.97
1:5:1913:C:O2'	1:5:1914:G:OP1	1.90	0.90
1:5:4987:U:O2'	1:5:5060:A:N6	2.05	0.89
1:5:2494:G:O2'	1:5:2495:G:OP1	1.91	0.88
1:5:3946:G:H1	1:5:4067:U:H3	1.26	0.83
1:5:451:C:HO2'	1:5:452:G:P	2.02	0.82
10:G:88:ASP:OD1	10:G:91:THR:OG1	1.96	0.82
13:J:28:GLU:OE2	13:J:32:ARG:NH1	2.14	0.81
1:5:3973:G:N2	1:5:4039:G:O2'	2.14	0.81
1:5:4063:U:H2'	1:5:4064:C:H1'	1.61	0.80
1:5:1092:U:N3	1:5:1187:G:O6	2.14	0.80
1:5:1089:C:H2'	1:5:1090:G:C8	2.18	0.78
1:5:4065:G:H3'	1:5:4066:U:H5''	1.66	0.78
1:5:1190:G:H3'	1:5:1191:G:H5''	1.65	0.78
1:5:3735:G:N2	1:5:3735:G:OP2	2.15	0.76
1:5:4945:U:O2'	1:5:4946:U:OP1	2.03	0.76
1:5:4063:U:H2'	1:5:4064:C:C1'	2.15	0.76
1:5:4064:C:H2'	1:5:4065:G:C8	2.20	0.76
1:5:4065:G:C3'	1:5:4066:U:H5''	2.16	0.75
1:5:1089:C:H2'	1:5:1090:G:H8	1.51	0.74
1:5:4124:G:N2	10:G:43:GLN:O	2.20	0.74
1:5:110:C:O2'	1:5:271:C:OP1	2.05	0.74
1:5:453:C:O2'	1:5:454:C:OP1	2.04	0.74
21:S:99:ASP:OD2	21:S:108:GLN:NE2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4374:U:O2	48:5:5302:HOH:O	2.07	0.73
1:5:4291:G:OP2	42:o:10:THR:HG22	1.89	0.73
1:5:1481:G:OP1	29:a:131:ARG:NE	2.21	0.72
1:5:4065:G:H2'	1:5:4066:U:H5''	1.70	0.71
1:5:4065:G:C2'	1:5:4066:U:H5''	2.21	0.70
1:5:1293:C:H2'	33:e:17:THR:HG21	1.73	0.70
1:5:4715:C:OP2	48:5:5303:HOH:O	2.09	0.70
1:5:3973:G:H1	1:5:4039:G:H1'	1.57	0.70
1:5:4044:U:O2'	1:5:4045:G:H5'	1.93	0.69
14:L:174:LYS:O	29:a:138:LYS:NZ	2.26	0.68
10:G:210:GLU:N	10:G:210:GLU:OE1	2.25	0.68
1:5:2644:G:O2'	1:5:2645:C:OP1	2.09	0.68
1:5:1191:G:H4'	1:5:1192:G:O5'	1.91	0.68
1:5:5058:C:O2'	1:5:5059:A:O5'	2.12	0.67
1:5:3973:G:H2'	1:5:3974:G:N9	2.10	0.67
1:5:3956:G:N2	1:5:4057:C:O2	2.28	0.67
1:5:2561:G:O2'	1:5:2562:U:OP1	2.13	0.67
1:5:4054:C:H2'	1:5:4055:U:C6	2.30	0.67
5:B:139:ASP:OD1	5:B:141:ASP:N	2.28	0.67
1:5:4052:C:H5''	1:5:4053:A:OP2	1.94	0.66
1:5:4763:U:O2'	21:S:174:THR:OG1	2.03	0.66
1:5:3948:C:H2'	1:5:3949:A:C8	2.31	0.65
1:5:1069:C:OP1	1:5:1207:C:O2'	2.12	0.65
18:P:71:ARG:NH1	18:P:139:ASP:OD1	2.30	0.65
31:c:37:MET:HE2	31:c:37:MET:HA	1.78	0.65
1:5:4053:A:H2'	1:5:4054:C:C6	2.32	0.65
1:5:4060:U:H2'	1:5:4061:G:O4'	1.97	0.65
1:5:1266:A:O2'	1:5:1267:G:OP2	2.12	0.64
1:5:2254:G:OP2	44:r:98:ARG:NH1	2.25	0.64
1:5:4198:G:O2'	45:s:445:ILE:O	2.15	0.64
1:5:2562:U:O2'	1:5:2563:C:OP1	2.15	0.64
1:5:3967:G:H2'	1:5:3968:U:C6	2.32	0.63
1:5:4035:G:H2'	1:5:4036:G:C8	2.33	0.63
1:5:3972:A:C6	1:5:4040:C:H5''	2.34	0.63
1:5:4126:C:OP1	10:G:37:LYS:NZ	2.30	0.63
1:5:3973:G:N1	1:5:4039:G:H1'	2.13	0.62
1:5:4945:U:HO2'	1:5:4946:U:P	2.22	0.62
10:G:57:TRP:O	10:G:62:ARG:NH1	2.32	0.62
1:5:2751:G:O2'	1:5:2752:G:O4'	2.13	0.62
1:5:3811:G:O2'	1:5:3814:U:OP2	2.12	0.62
1:5:2593:A:N6	1:5:2736:A:OP2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3959:U:H2'	1:5:3960:A:O4'	2.00	0.61
1:5:3950:U:H2'	1:5:3951:G:C1'	2.30	0.61
14:L:167:ARG:NH2	14:L:173:GLU:OE2	2.31	0.61
1:5:3950:U:H2'	1:5:3951:G:C8	2.37	0.60
1:5:4405:G:OP1	48:5:5305:HOH:O	2.16	0.60
1:5:1425:A:N6	1:5:1443:G:O2'	2.32	0.60
1:5:718:A:OP1	1:5:926:C:N4	2.34	0.60
1:5:4076:G:OP1	10:G:73:ARG:NE	2.29	0.60
1:5:3948:C:H2'	1:5:3949:A:H8	1.66	0.60
1:5:453:C:HO2'	1:5:454:C:P	2.25	0.59
1:5:742:A:H62	1:5:907:A:H62	1.51	0.59
1:5:4059:C:H2'	1:5:4060:U:C6	2.37	0.59
1:5:1810:G:O2'	1:5:1812:C:OP2	2.19	0.59
18:P:9:GLU:OE1	18:P:9:GLU:N	2.35	0.59
1:5:4066:U:O2'	1:5:4067:U:OP1	2.12	0.58
1:5:3877:A:N3	1:5:4401:G:O2'	2.26	0.58
1:5:4059:C:O2'	1:5:4060:U:H5'	2.03	0.58
1:5:3973:G:H2'	1:5:3974:G:C1'	2.34	0.57
1:5:4046:A:H3'	1:5:4047:A:N3	2.19	0.57
1:5:1331:U:H2'	1:5:1332:C:C6	2.40	0.57
1:5:4040:C:O2'	1:5:4041:C:H5'	2.05	0.57
1:5:3973:G:H2'	1:5:3974:G:C8	2.39	0.57
1:5:1919:U:OP1	1:5:1941:U:O2'	2.19	0.56
1:5:4054:C:H2'	1:5:4055:U:H6	1.69	0.56
1:5:3876:A:H4'	1:5:3877:A:OP2	2.06	0.56
1:5:4883:G:O2'	1:5:4884:U:O5'	2.23	0.56
19:Q:83:VAL:HG12	19:Q:83:VAL:O	2.04	0.56
1:5:1088:C:O2'	1:5:1089:C:H5'	2.06	0.55
1:5:1191:G:H4'	1:5:1192:G:C5'	2.37	0.55
1:5:270:C:O2'	1:5:271:C:O5'	2.23	0.55
1:5:4064:C:H5'	1:5:4065:G:OP2	2.06	0.55
19:Q:82:VAL:HG22	19:Q:84:GLY:H	1.72	0.55
1:5:3974:G:H21	1:5:4050:A:H1'	1.71	0.55
1:5:3771:C:H2'	1:5:3772:U:C6	2.40	0.55
1:5:4522:G:O2'	1:5:4525:C:OP2	2.19	0.55
5:B:139:ASP:OD1	5:B:140:GLU:N	2.39	0.55
1:5:4050:A:H2'	1:5:4051:C:O4'	2.06	0.55
2:7:117:G:OP1	7:D:253:TYR:OH	2.21	0.55
11:H:128:MET:HE2	11:H:128:MET:HA	1.88	0.55
42:o:11:PHE:O	42:o:81:ARG:NH2	2.39	0.55
1:5:706:A:H2'	1:5:707:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4043:G:H5'	1:5:4044:U:OP2	2.07	0.55
1:5:1485:G:N7	48:5:5328:HOH:O	2.33	0.55
1:5:4048:A:H1'	1:5:4049:U:C6	2.43	0.55
1:5:4061:G:H2'	1:5:4062:A:C8	2.42	0.54
1:5:1174:C:H1'	1:5:1175:C:OP2	2.08	0.54
1:5:4054:C:H4'	1:5:4055:U:OP1	2.06	0.54
1:5:4065:G:H3'	1:5:4066:U:C5'	2.36	0.54
1:5:2561:G:HO2'	1:5:2562:U:P	2.30	0.54
1:5:3784:A:O2'	1:5:3786:U:OP2	2.16	0.54
8:E:197:ILE:HG13	8:E:199:ILE:HG23	1.89	0.54
1:5:4060:U:O2'	1:5:4061:G:H5'	2.07	0.54
1:5:3974:G:N2	1:5:4050:A:H1'	2.23	0.54
1:5:4378:A:O2'	1:5:4379:A:H2'	2.08	0.54
1:5:2580:C:OP1	1:5:2760:C:O2'	2.24	0.53
1:5:3717:A:H2'	1:5:3718:A:C8	2.44	0.53
1:5:4582:C:H2'	1:5:4583:C:O4'	2.09	0.53
1:5:1583:U:OP2	1:5:2848:C:O2'	2.23	0.53
1:5:3951:G:H8	1:5:3951:G:OP2	1.92	0.53
1:5:3952:A:H61	1:5:4060:U:H3	1.56	0.53
1:5:467:C:H2'	1:5:468:C:O2	2.08	0.53
1:5:903:U:H2'	1:5:904:G:O4'	2.09	0.53
1:5:3972:A:N6	1:5:4040:C:H5''	2.24	0.53
23:U:35:ASP:OD1	23:U:38:ASN:N	2.32	0.53
1:5:3971:G:H22	1:5:4049:U:P	2.32	0.53
1:5:5060:A:N3	1:5:5060:A:H2'	2.23	0.53
1:5:402:A:O2'	1:5:405:A:OP1	2.20	0.52
1:5:738:G:H22	1:5:910:G:H22	1.57	0.52
1:5:1274:G:OP2	6:C:316:LYS:NZ	2.41	0.52
2:7:111:C:H2'	2:7:112:U:O4'	2.09	0.52
1:5:4039:G:H2'	1:5:4040:C:H5'	1.92	0.52
1:5:2868:G:C8	43:p:16:THR:HG22	2.44	0.52
1:5:3946:G:H2'	1:5:3947:A:H8	1.74	0.52
1:5:3950:U:H2'	1:5:3951:G:O4'	2.09	0.52
7:D:116:ASP:OD1	7:D:116:ASP:N	2.43	0.52
22:T:88:ARG:NH2	30:b:30:GLU:OE2	2.43	0.52
1:5:2075:C:H4'	1:5:2076:C:OP2	2.08	0.52
1:5:4045:G:C2	1:5:4047:A:H5''	2.45	0.52
1:5:3771:C:O2'	1:5:3772:U:P	2.68	0.51
1:5:3947:A:O2'	1:5:3948:C:H5'	2.10	0.51
1:5:4039:G:H2'	1:5:4039:G:N3	2.25	0.51
1:5:5058:C:HO2'	1:5:5059:A:C5'	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:125:C:O2'	1:5:126:C:H5'	2.10	0.51
1:5:4042:G:H3'	1:5:4043:G:H8	1.75	0.51
1:5:1092:U:H2'	1:5:1092:U:O2	2.10	0.51
1:5:1625:G:H5'	1:5:1626:A:OP1	2.10	0.51
7:D:41:LYS:NZ	22:T:32:ARG:O	2.38	0.51
6:C:3:CYS:SG	6:C:4:ALA:N	2.81	0.51
1:5:4063:U:H3'	1:5:4063:U:H6	1.76	0.51
1:5:3946:G:H2'	1:5:3947:A:C8	2.46	0.51
1:5:3966:A:O2'	1:5:3967:G:H5'	2.10	0.51
1:5:2603:A:H5'	1:5:2680:G:H4'	1.93	0.50
1:5:4266:G:N3	1:5:4266:G:H2'	2.26	0.50
1:5:18:C:H2'	1:5:19:G:O4'	2.11	0.50
1:5:927:A:O2'	15:M:46:ARG:NH1	2.44	0.50
1:5:3974:G:H5''	1:5:3975:C:OP2	2.11	0.50
1:5:2075:C:OP2	19:Q:14:ARG:NH2	2.42	0.50
1:5:4040:C:H2'	1:5:4041:C:O4'	2.11	0.50
1:5:4050:A:C2'	1:5:4051:C:H5'	2.41	0.50
1:5:742:A:N6	1:5:907:A:H62	2.09	0.50
1:5:2803:G:N1	1:5:2806:C:OP2	2.34	0.50
1:5:4546:A:N7	4:A:215:ASN:ND2	2.57	0.50
11:H:44:GLU:OE2	15:M:2:VAL:N	2.45	0.50
29:a:131:ARG:HD2	29:a:135:GLU:OE2	2.11	0.50
1:5:1270:C:H2'	1:5:1271:A:O4'	2.12	0.50
1:5:2494:G:HO2'	1:5:2495:G:P	2.32	0.50
1:5:4527:G:OP1	5:B:243:LYS:NZ	2.44	0.50
1:5:4260:U:H2'	1:5:4261:C:C6	2.47	0.50
1:5:3720:G:OP1	37:i:75:LYS:NZ	2.45	0.49
1:5:1412:A:O2'	1:5:1493:C:OP2	2.30	0.49
1:5:4045:G:N3	1:5:4047:A:H5''	2.27	0.49
1:5:4120:U:H3'	1:5:4121:G:H5''	1.94	0.49
1:5:1370:C:O2	1:5:1370:C:O2'	2.29	0.49
1:5:1467:G:H22	1:5:1481:G:H1	1.58	0.49
1:5:2426:G:O2'	1:5:2519:A:N1	2.41	0.49
1:5:2562:U:O2'	1:5:2563:C:P	2.70	0.49
1:5:4348:A:O2'	1:5:4350:C:OP2	2.30	0.49
1:5:4591:U:H2'	1:5:4592:C:C6	2.47	0.49
1:5:1266:A:HO2'	1:5:1267:G:P	2.34	0.49
1:5:3771:C:O2'	1:5:3772:U:O5'	2.31	0.49
23:U:41:GLN:NE2	23:U:45:GLU:OE2	2.42	0.49
43:p:56:HIS:NE2	43:p:61:MET:HE3	2.27	0.49
1:5:3953:G:H3'	1:5:3954:A:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4883:G:O2'	1:5:4884:U:P	2.70	0.49
23:U:105:ASN:OD1	23:U:109:SER:OG	2.29	0.49
1:5:4987:U:H5	1:5:5059:A:HO2'	1.58	0.49
1:5:2562:U:HO2'	1:5:2563:C:P	2.36	0.49
1:5:3604:A:H2'	1:5:3605:C:O4'	2.11	0.49
1:5:4035:G:H2'	1:5:4036:G:H8	1.78	0.49
1:5:469:C:H5	1:5:675:G:H22	1.61	0.49
1:5:4055:U:H2'	1:5:4056:A:C8	2.48	0.49
1:5:4054:C:O2'	1:5:4055:U:P	2.70	0.48
8:E:201:ASN:OD1	8:E:201:ASN:C	2.56	0.48
1:5:4537:C:H2'	1:5:4538:G:C8	2.48	0.48
1:5:3910:C:H2'	1:5:3911:C:C6	2.48	0.48
1:5:737:G:H2'	1:5:738:G:O4'	2.13	0.48
1:5:1813:G:H21	1:5:1813:G:P	2.35	0.48
3:8:155:C:H2'	3:8:156:U:O4'	2.13	0.48
1:5:1266:A:O2'	1:5:1267:G:P	2.72	0.48
1:5:4933:A:O2'	1:5:4934:C:O5'	2.30	0.48
28:Z:92:ASP:OD2	28:Z:94:THR:OG1	2.26	0.48
1:5:1170:G:O2'	7:D:286:SER:OG	2.29	0.48
23:U:47:ILE:HD12	23:U:63:ILE:HD11	1.95	0.48
1:5:3771:C:HO2'	1:5:3772:U:P	2.37	0.48
1:5:4037:C:H2'	1:5:4038:C:N1	2.29	0.48
1:5:4052:C:H3'	1:5:4053:A:H5''	1.96	0.48
1:5:1582:C:H4'	1:5:1583:U:OP2	2.13	0.47
1:5:65:A:OP2	29:a:64:LYS:NZ	2.43	0.47
1:5:3959:U:H2'	1:5:3960:A:C8	2.49	0.47
40:l:24:PRO:HG2	40:l:27:ILE:HD13	1.95	0.47
1:5:1448:C:O2'	19:Q:73:PRO:O	2.30	0.47
1:5:3967:G:H2'	1:5:3968:U:H6	1.78	0.47
1:5:1796:A:O4'	1:5:1798:G:C8	2.68	0.47
1:5:4059:C:H2'	1:5:4060:U:H6	1.80	0.47
1:5:1300:C:H2'	1:5:1301:C:C6	2.50	0.47
1:5:3877:A:OP2	1:5:3877:A:H2'	2.14	0.47
1:5:4749:C:H2'	1:5:4750:G:O4'	2.14	0.47
1:5:1356:U:OP2	14:L:36:ARG:NH2	2.40	0.47
1:5:2457:C:H2'	1:5:2458:G:O4'	2.14	0.47
17:O:203:VAL:HG13	17:O:203:VAL:O	2.14	0.47
1:5:88:G:H2'	1:5:89:A:C8	2.50	0.47
1:5:104:G:OP2	14:L:74:ARG:NH2	2.41	0.47
1:5:453:C:O2'	1:5:454:C:P	2.73	0.47
1:5:464:C:N3	8:E:101:ARG:NH1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:169:VAL:O	48:A:301:HOH:O	2.20	0.47
5:B:384:GLU:OE2	25:W:14:TYR:OH	2.31	0.47
1:5:3873:G:H2'	1:5:3874:G:C8	2.50	0.46
1:5:4991:G:H2'	1:5:4992:G:C8	2.50	0.46
10:G:88:ASP:OD2	10:G:90:GLN:OE1	2.32	0.46
1:5:5056:C:H2'	1:5:5057:A:C8	2.50	0.46
1:5:4044:U:C2'	1:5:4045:G:H5'	2.45	0.46
1:5:4931:U:H2'	1:5:4932:C:O5'	2.16	0.46
31:c:14:ILE:HD12	31:c:18:LEU:HG	1.96	0.46
1:5:1654:C:H2'	1:5:1655:C:C6	2.50	0.46
2:7:39:C:N3	13:J:73:THR:HG22	2.30	0.46
1:5:914:C:O2	1:5:914:C:O4'	2.34	0.46
1:5:1293:C:C2'	33:e:17:THR:HG21	2.44	0.46
1:5:3736:A:H2'	1:5:3737:A:C8	2.51	0.46
1:5:4981:A:OP1	18:P:103:LYS:NZ	2.39	0.46
1:5:4037:C:O5'	1:5:4037:C:H6	1.99	0.46
3:8:153:C:OP1	10:G:185:LYS:NZ	2.48	0.46
1:5:468:C:O2	1:5:468:C:O4'	2.34	0.46
1:5:1318:A:H2'	1:5:1319:C:C6	2.51	0.46
1:5:320:U:H2'	1:5:321:C:C6	2.51	0.46
1:5:5058:C:O2'	1:5:5059:A:P	2.74	0.46
27:Y:91:ASN:OD1	27:Y:93:THR:HG23	2.16	0.46
1:5:2440:G:H2'	1:5:2441:A:C8	2.51	0.45
1:5:4040:C:H2'	1:5:4041:C:C5'	2.46	0.45
1:5:4734:A:H2'	1:5:4735:G:C8	2.51	0.45
1:5:4886:C:H2'	1:5:4887:U:O4'	2.16	0.45
1:5:380:A:H4'	1:5:381:A:OP1	2.17	0.45
1:5:1299:A:H2'	1:5:1300:C:C6	2.50	0.45
1:5:3968:U:H2'	1:5:3969:G:H8	1.80	0.45
1:5:4050:A:O2'	1:5:4051:C:H5'	2.16	0.45
4:A:80:GLU:OE2	43:p:76:ALA:HB2	2.15	0.45
17:O:185:VAL:O	17:O:189:ILE:HG12	2.16	0.45
1:5:4069:U:O2'	1:5:4070:U:P	2.74	0.45
1:5:4965:A:H2'	1:5:4966:A:O4'	2.16	0.45
10:G:90:GLN:H	10:G:90:GLN:CD	2.24	0.45
1:5:4945:U:O2'	1:5:4946:U:P	2.70	0.45
1:5:1596:G:H2'	1:5:1597:G:C8	2.51	0.45
22:T:118:GLU:C	22:T:118:GLU:OE1	2.60	0.45
1:5:148:G:OP1	16:N:56:LYS:NZ	2.44	0.45
1:5:1191:G:H4'	1:5:1192:G:H5''	1.99	0.45
1:5:2494:G:O2'	1:5:2495:G:P	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:4232:U:H4'	1:5:4233:A:O4'	2.16	0.45
26:X:155:ILE:O	26:X:156:ILE:CB	2.65	0.45
1:5:2750:G:O2'	1:5:2757:A:N3	2.43	0.45
1:5:3880:G:H2'	1:5:3881:G:C8	2.52	0.45
1:5:4186:A:N7	48:5:5346:HOH:O	2.36	0.45
1:5:4635:A:H3'	1:5:4636:U:H4'	1.99	0.45
4:A:101:VAL:C	4:A:102:LEU:HD12	2.42	0.45
1:5:1623:A:C2	4:A:204:MET:HG2	2.51	0.45
1:5:3641:U:C6	1:5:3645:U:C4	3.05	0.45
1:5:3923:A:H2'	1:5:3924:C:C6	2.52	0.45
5:B:139:ASP:OD1	5:B:139:ASP:C	2.59	0.44
6:C:99:GLY:O	48:C:501:HOH:O	2.21	0.44
1:5:2561:G:O2'	1:5:2562:U:P	2.74	0.44
1:5:5060:A:H4'	1:5:5061:G:OP2	2.16	0.44
1:5:4055:U:H2'	1:5:4056:A:H8	1.82	0.44
19:Q:88:ASP:OD1	19:Q:89:ASP:N	2.51	0.44
27:Y:37:GLU:H	27:Y:37:GLU:CD	2.24	0.44
1:5:2836:A:O2'	1:5:4631:G:H4'	2.17	0.44
1:5:4058:U:H2'	1:5:4059:C:C6	2.53	0.44
1:5:4459:U:H2'	1:5:4460:U:C6	2.53	0.44
5:B:92:TYR:HB2	5:B:159:VAL:HB	1.99	0.44
1:5:377:G:N1	1:5:380:A:OP2	2.48	0.44
1:5:469:C:O2	1:5:469:C:O4'	2.35	0.44
1:5:4039:G:OP1	1:5:4049:U:O2'	2.22	0.44
1:5:4051:C:H2'	1:5:4052:C:O4'	2.17	0.44
1:5:4274:A:H2'	1:5:4275:G:C8	2.53	0.44
1:5:2716:G:O2'	1:5:2718:G:OP2	2.28	0.44
1:5:4054:C:HO2'	1:5:4055:U:P	2.41	0.44
1:5:468:C:H41	1:5:676:G:H1	1.65	0.43
1:5:3952:A:N6	1:5:4061:G:N3	2.65	0.43
1:5:3653:A:C2	1:5:3692:A:O4'	2.71	0.43
1:5:3952:A:N6	1:5:4061:G:C2	2.86	0.43
1:5:413:A:C2	3:8:17:A:H1'	2.53	0.43
1:5:468:C:H5	1:5:676:G:H22	1.65	0.43
1:5:1073:C:C2'	1:5:1074:C:H5'	2.49	0.43
1:5:4066:U:H4'	1:5:4066:U:OP1	2.18	0.43
7:D:83:LEU:N	7:D:84:PRO:HD2	2.34	0.43
1:5:3972:A:N6	1:5:4040:C:O3'	2.50	0.43
1:5:4931:U:C2'	1:5:4932:C:O5'	2.67	0.43
1:5:667:C:C2	1:5:668:C:C5	3.07	0.43
1:5:1490:G:OP1	19:Q:150:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:82:THR:HG22	26:X:155:ILE:HG23	2.01	0.43
1:5:1337:A:H2'	1:5:1338:C:C6	2.54	0.43
1:5:2057:G:H2'	1:5:2058:C:O4'	2.19	0.43
1:5:4871:G:H1'	1:5:4872:G:OP2	2.18	0.43
1:5:5052:U:H3'	1:5:5053:C:C6	2.53	0.43
1:5:5058:C:HO2'	1:5:5059:A:P	2.40	0.43
3:8:62:A:H4'	3:8:63:U:O5'	2.18	0.43
18:P:83:GLN:HA	18:P:112:TRP:CD1	2.54	0.43
34:f:106:TYR:HA	34:f:107:PRO:C	2.44	0.43
1:5:1778:A:H2'	1:5:1781:C:C5	2.54	0.42
1:5:2737:A:H2'	1:5:2738:A:C8	2.54	0.42
1:5:4065:G:H2'	1:5:4066:U:C5'	2.46	0.42
39:k:8:ILE:HG23	39:k:56:LEU:HD11	2.01	0.42
43:p:52:VAL:O	43:p:52:VAL:HG13	2.19	0.42
1:5:1845:G:OP1	48:5:5306:HOH:O	2.21	0.42
7:D:212:MET:HE3	7:D:219:TYR:CZ	2.54	0.42
1:5:2399:G:O6	40:l:2:SER:N	2.53	0.42
1:5:3967:G:O2'	1:5:3968:U:H5'	2.20	0.42
1:5:3968:U:H2'	1:5:3969:G:C8	2.53	0.42
5:B:258:HIS:HA	5:B:259:PRO:C	2.44	0.42
31:c:99:PRO:HG3	31:c:105:ILE:HD12	2.00	0.42
1:5:103:A:H4'	1:5:104:G:OP1	2.19	0.42
1:5:110:C:O2	1:5:110:C:O4'	2.38	0.42
1:5:2531:C:H2'	1:5:2532:C:C6	2.55	0.42
1:5:2699:U:O2	1:5:2699:U:O4'	2.38	0.42
24:V:112:MET:HE1	24:V:117:ILE:HG13	2.02	0.42
1:5:1324:C:H2'	1:5:1325:A:H8	1.84	0.42
1:5:1609:G:H1'	1:5:2505:A:N6	2.34	0.42
1:5:4040:C:C2'	1:5:4041:C:H5'	2.49	0.42
1:5:4412:C:H2'	1:5:4413:C:O2	2.20	0.42
1:5:5003:C:H2'	1:5:5004:G:O4'	2.19	0.42
29:a:39:HIS:O	29:a:40:HIS:CG	2.73	0.42
1:5:729:G:C2	1:5:730:G:C8	3.08	0.42
2:7:24:C:H2'	2:7:25:G:O4'	2.20	0.42
1:5:1569:G:O2'	1:5:1604:G:H4'	2.20	0.42
1:5:3816:A:OP1	1:5:3818:U:H5	2.02	0.42
1:5:3959:U:H6	1:5:3959:U:O5'	2.03	0.42
31:c:47:ILE:HD12	31:c:94:LEU:HD11	2.00	0.42
1:5:1847:G:OP1	30:b:4:SER:HB2	2.19	0.42
1:5:3972:A:H2	1:5:4050:A:N6	2.17	0.42
1:5:4594:U:H2'	1:5:4595:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:141:C:H2'	3:8:142:U:C6	2.55	0.42
11:H:137:SER:HB3	11:H:143:GLU:HB3	2.02	0.42
21:S:160:ARG:NE	21:S:160:ARG:HA	2.35	0.42
1:5:1293:C:O2	1:5:1293:C:O4'	2.37	0.42
1:5:745:U:H3	1:5:902:G:H1	1.68	0.41
1:5:4046:A:H4'	1:5:4047:A:OP2	2.19	0.41
1:5:4065:G:C3'	1:5:4066:U:C5'	2.92	0.41
1:5:32:U:H2'	1:5:33:A:O4'	2.21	0.41
1:5:1814:U:O2	1:5:1814:U:O4'	2.38	0.41
1:5:2075:C:P	19:Q:14:ARG:HH22	2.43	0.41
1:5:2785:G:H5''	1:5:2786:C:H5''	2.02	0.41
1:5:3648:A:H1'	1:5:3785:A:N6	2.35	0.41
1:5:2603:A:H2'	1:5:2604:G:C8	2.56	0.41
1:5:3868:G:H22	1:5:3900:G:H1'	1.84	0.41
7:D:267:ASN:OD1	7:D:267:ASN:N	2.53	0.41
13:J:64:ARG:O	42:o:103:VAL:HG22	2.20	0.41
13:J:24:ILE:HG12	13:J:128:LEU:HB3	2.01	0.41
1:5:1074:C:H2'	1:5:1075:U:O4'	2.21	0.41
1:5:2335:G:O2'	48:5:5304:HOH:O	2.15	0.41
1:5:2736:A:H2'	1:5:2737:A:C8	2.55	0.41
1:5:4051:C:H6	1:5:4051:C:O5'	2.03	0.41
1:5:5058:C:H4'	1:5:5059:A:OP1	2.21	0.41
13:J:95:ARG:HG3	13:J:95:ARG:HH11	1.85	0.41
1:5:116:A:H5'	1:5:117:U:OP2	2.21	0.41
1:5:2624:U:H2'	1:5:2625:U:C6	2.55	0.41
1:5:2632:G:H2'	1:5:2633:A:C8	2.55	0.41
9:F:243:ASN:O	9:F:247:ARG:HG2	2.21	0.41
23:U:66:SER:O	23:U:66:SER:OG	2.36	0.41
1:5:428:A:C2	1:5:3867:A:H4'	2.56	0.41
1:5:2630:G:O2'	1:5:2631:U:H5'	2.21	0.41
1:5:2654:G:H2'	1:5:2655:G:O4'	2.21	0.41
1:5:3711:A:O2'	1:5:3712:A:H5'	2.21	0.41
1:5:4254:G:N3	1:5:4254:G:H2'	2.34	0.41
29:a:39:HIS:O	29:a:40:HIS:ND1	2.54	0.41
31:c:34:THR:HG23	31:c:95:ALA:HB2	2.01	0.41
1:5:727:A:H2'	1:5:728:A:O4'	2.21	0.41
1:5:1480:G:OP1	14:L:183:ARG:HD3	2.21	0.41
1:5:1838:G:H2'	1:5:1839:C:C6	2.56	0.41
1:5:2520:G:H2'	1:5:2521:A:O4'	2.21	0.41
1:5:2853:C:N3	1:5:3626:G:OP2	2.53	0.41
1:5:3732:A:H2'	1:5:3733:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3903:A:O2'	1:5:3904:G:H5'	2.20	0.41
1:5:4069:U:H2'	1:5:4070:U:C6	2.56	0.41
8:E:176:VAL:HG11	8:E:254:LEU:HD11	2.02	0.41
31:c:19:GLN:OE1	31:c:19:GLN:HA	2.20	0.41
1:5:190:C:O2'	27:Y:125:SER:HB2	2.21	0.41
1:5:2268:A:H2'	1:5:2269:C:O4'	2.21	0.41
1:5:2663:C:H2'	1:5:2664:C:C6	2.56	0.41
3:8:6:C:H2'	3:8:7:U:H6	1.85	0.41
3:8:92:U:H2'	3:8:93:C:O4'	2.21	0.41
1:5:101:A:H2'	1:5:102:G:O4'	2.21	0.40
1:5:452:G:OP1	8:E:111:TYR:HD2	2.05	0.40
1:5:1351:G:OP1	6:C:114:ARG:HD2	2.22	0.40
1:5:3684:G:H2'	1:5:3685:C:C6	2.56	0.40
1:5:4212:A:H4'	1:5:4213:A:O5'	2.21	0.40
1:5:4238:G:H2'	1:5:4239:A:C8	2.56	0.40
1:5:4239:A:H2'	1:5:4240:G:C8	2.57	0.40
1:5:4584:A:H2'	1:5:4585:U:O4'	2.21	0.40
20:R:116:ASP:OD2	20:R:116:ASP:C	2.63	0.40
1:5:451:C:H2'	1:5:452:G:H8	1.85	0.40
1:5:1423:C:H2'	1:5:1424:G:O4'	2.22	0.40
1:5:3967:G:H2'	1:5:3968:U:C5	2.57	0.40
1:5:4637:G:H2'	1:5:4638:U:C6	2.56	0.40
1:5:1731:G:H2'	1:5:1732:C:C6	2.56	0.40
1:5:4625:C:O2'	1:5:4626:A:H5'	2.20	0.40
5:B:80:GLU:OE1	5:B:323:TYR:OH	2.34	0.40
17:O:61:ARG:HA	17:O:70:PRO:HD2	2.03	0.40
1:5:974:U:H2'	1:5:975:C:C6	2.57	0.40
1:5:3974:G:C6	1:5:4037:C:N4	2.89	0.40
1:5:4173:G:H2'	1:5:4174:U:C6	2.57	0.40
1:5:1202:C:H42	9:F:68:ARG:CZ	2.34	0.40
1:5:1874:U:C4	1:5:2271:A:C2	3.10	0.40
1:5:4750:G:H2'	1:5:4751:G:C8	2.57	0.40
27:Y:51:LYS:O	27:Y:52:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	244/257 (95%)	234 (96%)	10 (4%)	0	100	100
5	B	393/403 (98%)	388 (99%)	5 (1%)	0	100	100
6	C	353/427 (83%)	349 (99%)	4 (1%)	0	100	100
7	D	291/297 (98%)	288 (99%)	3 (1%)	0	100	100
8	E	195/288 (68%)	191 (98%)	4 (2%)	0	100	100
9	F	218/248 (88%)	211 (97%)	7 (3%)	0	100	100
10	G	210/266 (79%)	206 (98%)	4 (2%)	0	100	100
11	H	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
12	I	197/214 (92%)	196 (100%)	1 (0%)	0	100	100
13	J	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
14	L	186/211 (88%)	183 (98%)	3 (2%)	0	100	100
15	M	134/215 (62%)	130 (97%)	4 (3%)	0	100	100
16	N	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	O	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
18	P	150/184 (82%)	148 (99%)	2 (1%)	0	100	100
19	Q	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
20	R	147/196 (75%)	147 (100%)	0	0	100	100
21	S	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
22	T	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
23	U	96/128 (75%)	95 (99%)	1 (1%)	0	100	100
24	V	128/140 (91%)	127 (99%)	1 (1%)	0	100	100
25	W	60/157 (38%)	60 (100%)	0	0	100	100
26	X	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	Y	126/145 (87%)	124 (98%)	2 (2%)	0	100	100
28	Z	133/136 (98%)	133 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	a	145/148 (98%)	139 (96%)	5 (3%)	1 (1%)	18	19
30	b	63/159 (40%)	61 (97%)	2 (3%)	0	100	100
31	c	91/115 (79%)	90 (99%)	1 (1%)	0	100	100
32	d	103/125 (82%)	102 (99%)	1 (1%)	0	100	100
33	e	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
34	f	106/110 (96%)	106 (100%)	0	0	100	100
35	g	100/117 (86%)	100 (100%)	0	0	100	100
36	h	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
37	i	96/105 (91%)	93 (97%)	3 (3%)	0	100	100
38	j	84/97 (87%)	84 (100%)	0	0	100	100
39	k	66/70 (94%)	66 (100%)	0	0	100	100
40	l	48/51 (94%)	48 (100%)	0	0	100	100
41	m	50/128 (39%)	50 (100%)	0	0	100	100
42	o	100/106 (94%)	99 (99%)	1 (1%)	0	100	100
43	p	86/92 (94%)	80 (93%)	6 (7%)	0	100	100
44	r	118/137 (86%)	117 (99%)	1 (1%)	0	100	100
45	s	11/809 (1%)	11 (100%)	0	0	100	100
All	All	6159/7996 (77%)	6062 (98%)	96 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	a	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	188/199 (94%)	185 (98%)	3 (2%)	55	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	341/349 (98%)	339 (99%)	2 (1%)	78	89
6	C	297/348 (85%)	293 (99%)	4 (1%)	61	76
7	D	238/250 (95%)	235 (99%)	3 (1%)	61	76
8	E	179/252 (71%)	179 (100%)	0	100	100
9	F	183/215 (85%)	183 (100%)	0	100	100
10	G	182/223 (82%)	182 (100%)	0	100	100
11	H	166/171 (97%)	164 (99%)	2 (1%)	63	78
12	I	170/181 (94%)	169 (99%)	1 (1%)	78	89
13	J	142/149 (95%)	140 (99%)	2 (1%)	59	75
14	L	154/177 (87%)	153 (99%)	1 (1%)	78	89
15	M	115/161 (71%)	114 (99%)	1 (1%)	70	84
16	N	170/172 (99%)	170 (100%)	0	100	100
17	O	171/174 (98%)	169 (99%)	2 (1%)	63	78
18	P	131/163 (80%)	129 (98%)	2 (2%)	57	73
19	Q	163/165 (99%)	161 (99%)	2 (1%)	63	78
20	R	129/175 (74%)	127 (98%)	2 (2%)	55	71
21	S	153/157 (98%)	151 (99%)	2 (1%)	61	76
22	T	135/140 (96%)	132 (98%)	3 (2%)	45	61
23	U	86/115 (75%)	86 (100%)	0	100	100
24	V	100/107 (94%)	100 (100%)	0	100	100
25	W	53/126 (42%)	53 (100%)	0	100	100
26	X	102/133 (77%)	102 (100%)	0	100	100
27	Y	118/135 (87%)	117 (99%)	1 (1%)	73	85
28	Z	117/118 (99%)	116 (99%)	1 (1%)	70	84
29	a	119/121 (98%)	119 (100%)	0	100	100
30	b	53/126 (42%)	52 (98%)	1 (2%)	50	66
31	c	75/97 (77%)	74 (99%)	1 (1%)	61	76
32	d	90/110 (82%)	89 (99%)	1 (1%)	65	79
33	e	111/121 (92%)	110 (99%)	1 (1%)	70	84
34	f	86/89 (97%)	83 (96%)	3 (4%)	32	43
35	g	88/100 (88%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	106/110 (96%)	106 (100%)	0	100	100
37	i	78/89 (88%)	75 (96%)	3 (4%)	29	40
38	j	73/80 (91%)	72 (99%)	1 (1%)	59	75
39	k	55/65 (85%)	55 (100%)	0	100	100
40	l	46/48 (96%)	45 (98%)	1 (2%)	45	61
41	m	45/116 (39%)	45 (100%)	0	100	100
42	o	85/94 (90%)	84 (99%)	1 (1%)	63	78
43	p	67/75 (89%)	66 (98%)	1 (2%)	57	73
44	r	106/121 (88%)	104 (98%)	2 (2%)	50	66
45	s	9/717 (1%)	9 (100%)	0	100	100
All	All	5275/6834 (77%)	5225 (99%)	50 (1%)	68	84

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	86	GLN
4	A	154	SER
4	A	208	GLU
5	B	74	GLU
5	B	152	SER
6	C	9	SER
6	C	62	THR
6	C	69	THR
6	C	140	LYS
7	D	5	LYS
7	D	109	LEU
7	D	124	GLU
11	H	106	GLN
11	H	121	LYS
12	I	195	CYS
13	J	51	SER
13	J	171	ASP
14	L	129	ARG
15	M	16	SER
17	O	61	ARG
17	O	148	LYS
18	P	52	ARG
18	P	129	SER

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Mol	Chain	Res	Type
19	Q	92	VAL
19	Q	169	SER
20	R	2	SER
20	R	51	ILE
21	S	24	THR
21	S	161	ARG
22	T	76	VAL
22	T	102	ARG
22	T	126	VAL
27	Y	94	THR
28	Z	124	THR
30	b	9	THR
31	c	14	ILE
32	d	122	VAL
33	e	105	SER
34	f	47	CYS
34	f	57	THR
34	f	59	THR
37	i	18	THR
37	i	21	VAL
37	i	81	ILE
38	j	6	SER
40	l	31	THR
42	o	77	CYS
43	p	26	VAL
44	r	5	LEU
44	r	26	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	38	HIS
5	B	145	GLN
5	B	245	HIS
5	B	376	HIS
6	C	21	ASN
6	C	89	GLN
7	D	131	ASN
7	D	282	GLN
8	E	39	HIS
8	E	187	GLN
8	E	241	GLN

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Mol	Chain	Res	Type
9	F	194	HIS
9	F	241	GLN
9	F	250	ASN
10	G	38	ASN
10	G	66	GLN
11	H	42	ASN
11	H	98	HIS
12	I	143	GLN
15	M	48	GLN
16	N	37	HIS
16	N	201	HIS
17	O	96	GLN
18	P	50	ASN
18	P	57	ASN
20	R	40	GLN
20	R	141	HIS
21	S	36	ASN
21	S	125	GLN
23	U	94	ASN
27	Y	14	ASN
27	Y	18	HIS
29	a	39	HIS
29	a	60	HIS
32	d	34	HIS
36	h	98	HIS
38	j	48	ASN
41	m	109	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3088/5070 (60%)	406 (13%)	30 (0%)
2	7	118/119 (99%)	8 (6%)	0
3	8	140/157 (89%)	14 (10%)	0
All	All	3346/5346 (62%)	428 (12%)	30 (0%)

All (428) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	-3	G
1	5	30	U

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Mol	Chain	Res	Type
1	5	34	A
1	5	37	A
1	5	51	A
1	5	53	G
1	5	54	A
1	5	59	A
1	5	60	A
1	5	66	C
1	5	86	G
1	5	93	A
1	5	103	A
1	5	104	G
1	5	105	C
1	5	114	G
1	5	115	A
1	5	138	C
1	5	139	G
1	5	152	U
1	5	154	C
1	5	159	G
1	5	195	U
1	5	204	U
1	5	219	U
1	5	228	U
1	5	229	G
1	5	241	G
1	5	271	C
1	5	275	G
1	5	292	U
1	5	301	A
1	5	304	C
1	5	310	G
1	5	311	U
1	5	335	C
1	5	381	A
1	5	382	G
1	5	394	G
1	5	407	G
1	5	408	G
1	5	452	G
1	5	453	C
1	5	454	C

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Mol	Chain	Res	Type
1	5	456	G
1	5	668	C
1	5	672	G
1	5	678	C
1	5	700	G
1	5	707	C
1	5	724	G
1	5	725	G
1	5	726	G
1	5	738	G
1	5	740	G
1	5	742	A
1	5	743	G
1	5	745	U
1	5	905	U
1	5	907	A
1	5	909	A
1	5	924	A
1	5	925	G
1	5	936	A
1	5	937	U
1	5	951	G
1	5	952	A
1	5	953	G
1	5	969	C
1	5	974	U
1	5	1064	C
1	5	1070	A
1	5	1074	C
1	5	1162	G
1	5	1167	A
1	5	1173	C
1	5	1175	C
1	5	1178	U
1	5	1179	G
1	5	1187	G
1	5	1191	G
1	5	1192	G
1	5	1203	G
1	5	1211	G
1	5	1267	G
1	5	1271	A

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Mol	Chain	Res	Type
1	5	1272	C
1	5	1274	G
1	5	1276	G
1	5	1277	U
1	5	1279	G
1	5	1281	C
1	5	1293	C
1	5	1296	C
1	5	1305	C
1	5	1318	A
1	5	1329	A
1	5	1346	A
1	5	1351	G
1	5	1369	G
1	5	1371	C
1	5	1379	A
1	5	1386	G
1	5	1389	A
1	5	1448	C
1	5	1449	G
1	5	1457	G
1	5	1481	G
1	5	1490	G
1	5	1494	G
1	5	1515	A
1	5	1526	A
1	5	1539	A
1	5	1570	U
1	5	1574	U
1	5	1583	U
1	5	1588	U
1	5	1594	U
1	5	1605	A
1	5	1616	G
1	5	1617	G
1	5	1623	A
1	5	1625	G
1	5	1626	A
1	5	1632	C
1	5	1633	G
1	5	1634	A
1	5	1646	G

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Mol	Chain	Res	Type
1	5	1653	C
1	5	1668	C
1	5	1669	U
1	5	1713	G
1	5	1718	U
1	5	1726	G
1	5	1727	U
1	5	1733	G
1	5	1734	A
1	5	1742	G
1	5	1779	A
1	5	1796	A
1	5	1797	A
1	5	1813	G
1	5	1826	U
1	5	1828	G
1	5	1829	A
1	5	1834	G
1	5	1847	G
1	5	1861	G
1	5	1889	A
1	5	1910	U
1	5	1912	C
1	5	1914	G
1	5	1924	A
1	5	1937	G
1	5	1940	G
1	5	1943	G
1	5	2038	G
1	5	2040	U
1	5	2044	G
1	5	2047	G
1	5	2048	G
1	5	2049	A
1	5	2061	A
1	5	2076	C
1	5	2077	G
1	5	2259	U
1	5	2271	A
1	5	2281	C
1	5	2292	A
1	5	2293	G

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Mol	Chain	Res	Type
1	5	2305	A
1	5	2306	G
1	5	2325	G
1	5	2340	G
1	5	2343	C
1	5	2352	A
1	5	2387	A
1	5	2414	C
1	5	2417	U
1	5	2442	G
1	5	2462	C
1	5	2495	G
1	5	2504	A
1	5	2505	A
1	5	2522	U
1	5	2546	U
1	5	2562	U
1	5	2563	C
1	5	2579	A
1	5	2581	C
1	5	2593	A
1	5	2619	C
1	5	2630	G
1	5	2644	G
1	5	2645	C
1	5	2654	G
1	5	2661	C
1	5	2665	G
1	5	2679	U
1	5	2687	A
1	5	2688	A
1	5	2699	U
1	5	2700	U
1	5	2702	C
1	5	2703	G
1	5	2706	G
1	5	2708	C
1	5	2716	G
1	5	2718	G
1	5	2732	U
1	5	2735	A
1	5	2755	U

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Mol	Chain	Res	Type
1	5	2756	A
1	5	2779	A
1	5	2780	U
1	5	2782	U
1	5	2790	A
1	5	2818	U
1	5	2819	G
1	5	2821	U
1	5	2834	G
1	5	2847	G
1	5	3605	C
1	5	3606	U
1	5	3615	G
1	5	3616	U
1	5	3617	G
1	5	3618	C
1	5	3625	G
1	5	3626	G
1	5	3635	A
1	5	3644	U
1	5	3648	A
1	5	3662	A
1	5	3674	G
1	5	3696	C
1	5	3709	U
1	5	3710	G
1	5	3713	U
1	5	3748	A
1	5	3772	U
1	5	3774	A
1	5	3777	G
1	5	3784	A
1	5	3786	U
1	5	3811	G
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3838	U
1	5	3839	G
1	5	3840	U
1	5	3877	A
1	5	3878	C

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Mol	Chain	Res	Type
1	5	3879	G
1	5	3897	G
1	5	3901	A
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3938	G
1	5	3951	G
1	5	3952	A
1	5	3954	A
1	5	3958	G
1	5	3965	A
1	5	3966	A
1	5	3970	G
1	5	3972	A
1	5	3973	G
1	5	3974	G
1	5	4039	G
1	5	4043	G
1	5	4044	U
1	5	4046	A
1	5	4047	A
1	5	4048	A
1	5	4049	U
1	5	4052	C
1	5	4053	A
1	5	4054	C
1	5	4055	U
1	5	4064	C
1	5	4065	G
1	5	4066	U
1	5	4067	U
1	5	4068	U
1	5	4070	U
1	5	4073	A
1	5	4076	G
1	5	4118	U
1	5	4119	C
1	5	4120	U
1	5	4121	G

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Mol	Chain	Res	Type
1	5	4122	G
1	5	4127	A
1	5	4133	C
1	5	4161	G
1	5	4162	C
1	5	4163	U
1	5	4170	A
1	5	4171	C
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4203	A
1	5	4214	A
1	5	4225	G
1	5	4229	U
1	5	4233	A
1	5	4251	A
1	5	4254	G
1	5	4256	A
1	5	4258	C
1	5	4266	G
1	5	4267	G
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4291	G
1	5	4305	G
1	5	4317	A
1	5	4319	C
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4339	A
1	5	4349	C
1	5	4373	G
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4379	A
1	5	4380	A
1	5	4387	C
1	5	4393	G

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Mol	Chain	Res	Type
1	5	4394	A
1	5	4419	U
1	5	4421	C
1	5	4422	A
1	5	4448	G
1	5	4449	A
1	5	4452	U
1	5	4464	A
1	5	4475	G
1	5	4500	U
1	5	4512	U
1	5	4513	A
1	5	4519	C
1	5	4524	G
1	5	4548	A
1	5	4557	U
1	5	4560	C
1	5	4567	G
1	5	4590	A
1	5	4636	U
1	5	4637	G
1	5	4656	A
1	5	4670	C
1	5	4672	A
1	5	4677	U
1	5	4700	A
1	5	4709	U
1	5	4750	G
1	5	4751	G
1	5	4754	G
1	5	4757	C
1	5	4759	C
1	5	4761	G
1	5	4765	G
1	5	4868	U
1	5	4869	G
1	5	4870	C
1	5	4872	G
1	5	4884	U
1	5	4893	A
1	5	4897	G
1	5	4898	G

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Mol	Chain	Res	Type
1	5	4909	A
1	5	4911	G
1	5	4913	C
1	5	4932	C
1	5	4933	A
1	5	4934	C
1	5	4937	A
1	5	4942	A
1	5	4943	C
1	5	4944	G
1	5	4946	U
1	5	4953	G
1	5	4965	A
1	5	4966	A
1	5	4975	U
1	5	4993	G
1	5	5006	A
1	5	5012	C
1	5	5013	A
1	5	5040	G
1	5	5049	C
1	5	5052	U
1	5	5053	C
1	5	5059	A
1	5	5060	A
1	5	5061	G
2	7	7	G
2	7	22	A
2	7	33	U
2	7	53	U
2	7	54	A
2	7	64	G
2	7	100	A
2	7	110	G
3	8	23	C
3	8	34	U
3	8	35	C
3	8	59	A
3	8	62	A
3	8	63	U
3	8	103	A
3	8	105	C

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Mol	Chain	Res	Type
3	8	109	C
3	8	110	U
3	8	114	G
3	8	117	C
3	8	137	A
3	8	156	U

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	137	G
1	5	270	C
1	5	380	A
1	5	451	C
1	5	453	C
1	5	1174	C
1	5	1191	G
1	5	1582	C
1	5	1605	A
1	5	1625	G
1	5	1796	A
1	5	1913	C
1	5	2075	C
1	5	2494	G
1	5	2561	G
1	5	2562	U
1	5	2755	U
1	5	3771	C
1	5	3876	A
1	5	4054	C
1	5	4066	U
1	5	4069	U
1	5	4378	A
1	5	4448	G
1	5	4699	U
1	5	4871	G
1	5	4883	G
1	5	4945	U
1	5	5058	C
1	5	5060	A

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 166 ligands modelled in this entry, 166 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18382. These allow visual inspection of the internal detail of the map and identification of artifacts.

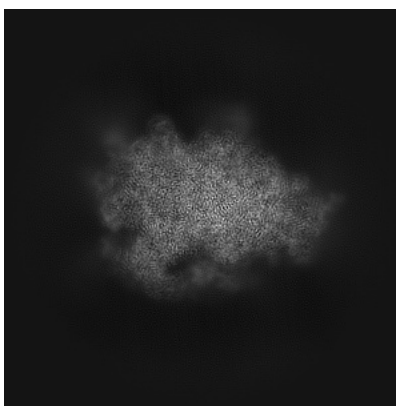
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

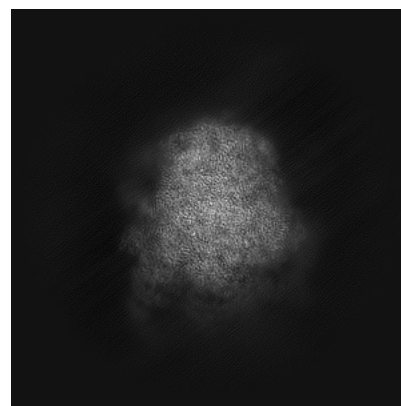
6.1.1 Primary map



X

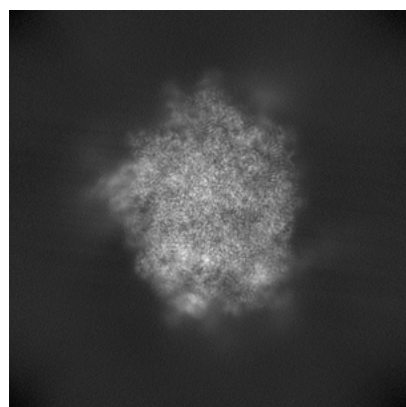


Y

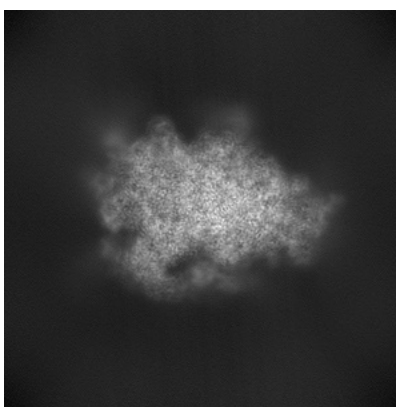


Z

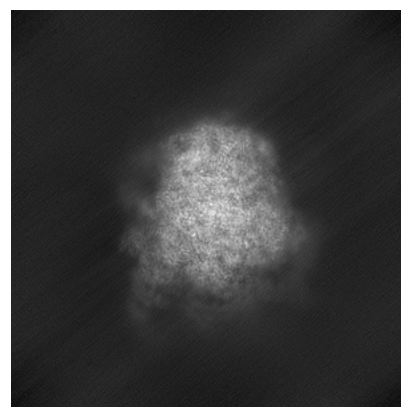
6.1.2 Raw map



X



Y

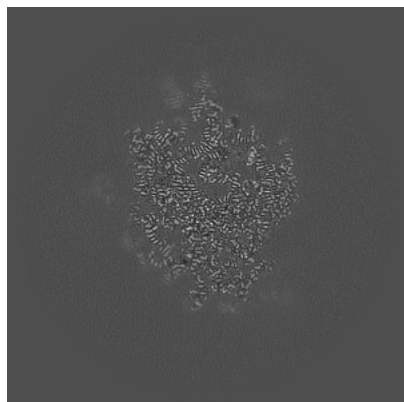


Z

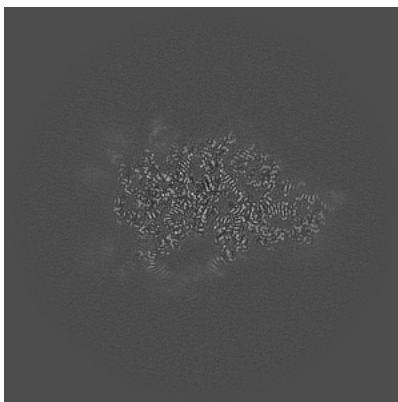
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

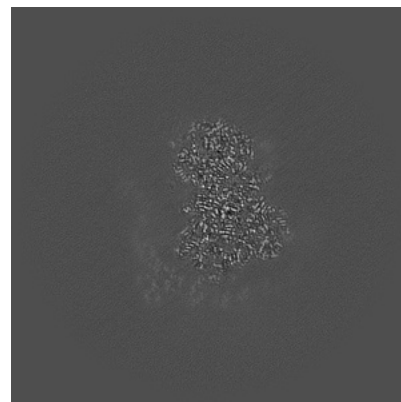
6.2.1 Primary map



X Index: 294

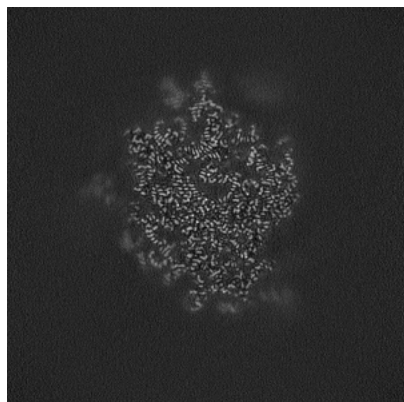


Y Index: 294

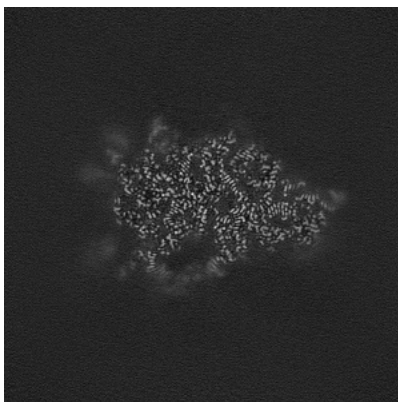


Z Index: 294

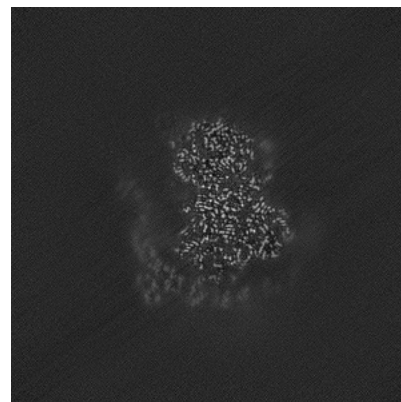
6.2.2 Raw map



X Index: 294



Y Index: 294

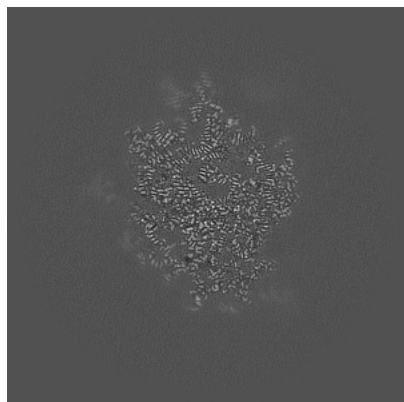


Z Index: 294

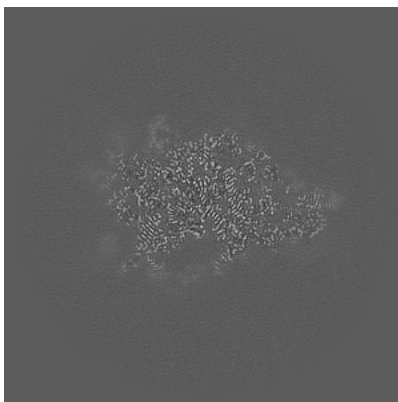
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

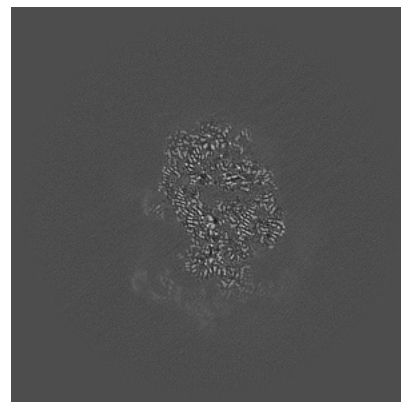
6.3.1 Primary map



X Index: 293

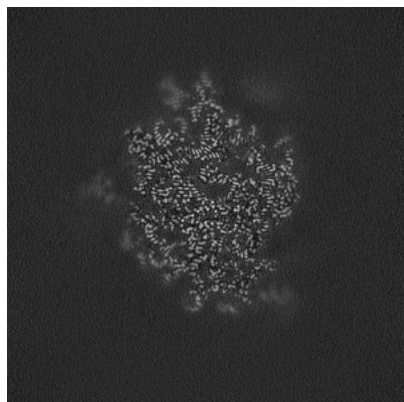


Y Index: 288

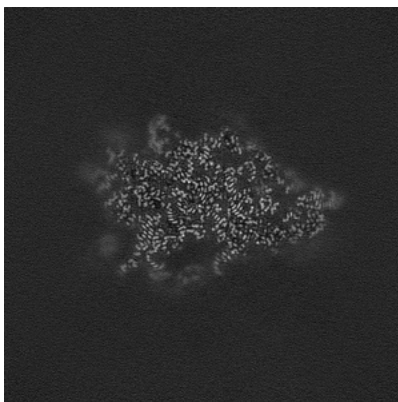


Z Index: 315

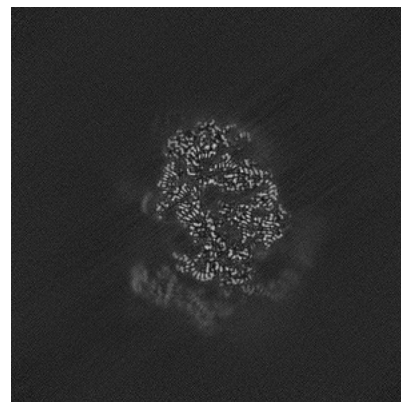
6.3.2 Raw map



X Index: 293



Y Index: 287

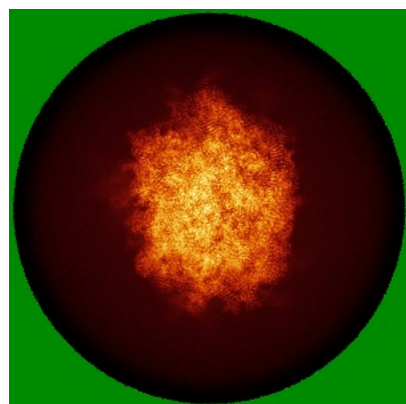


Z Index: 319

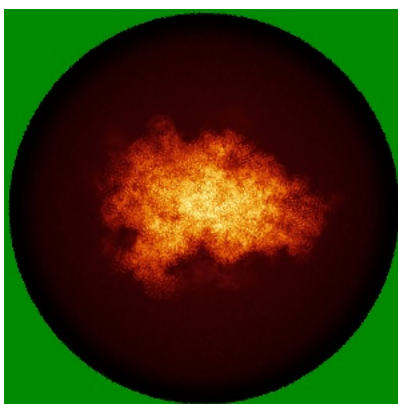
The images above show the largest variance slices of the map in three orthogonal directions.

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

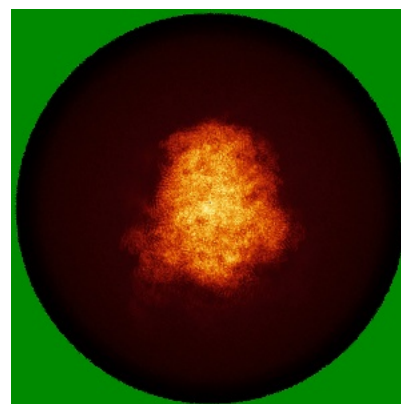
6.4.1 Primary map



X

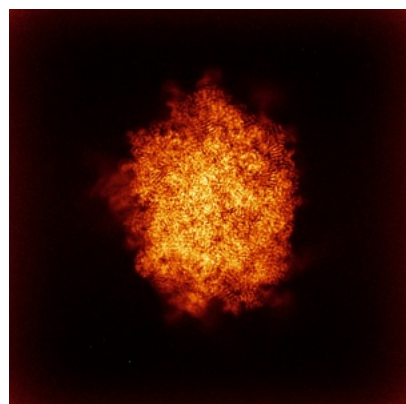


Y

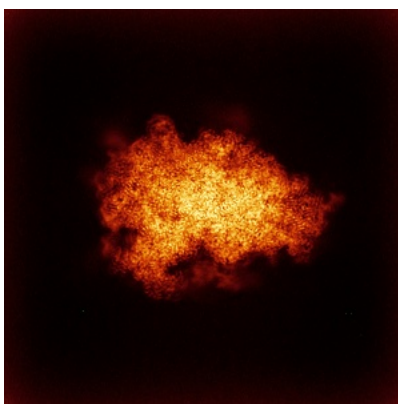


Z

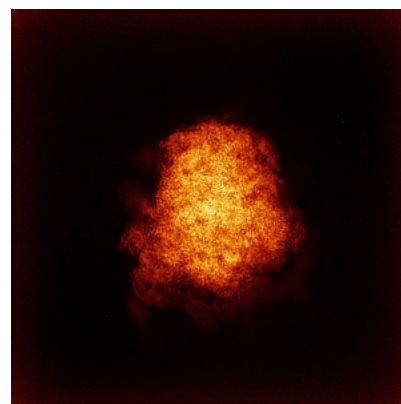
6.4.2 Raw map



X



Y



Z

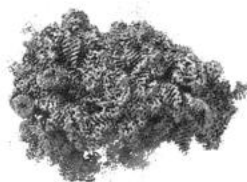
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

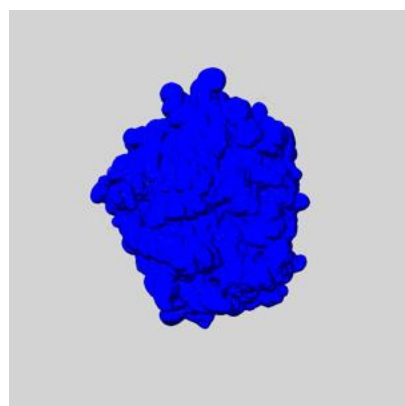
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

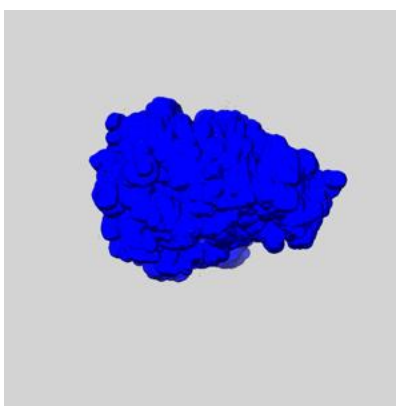
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

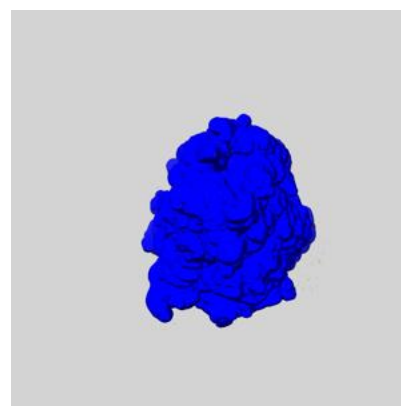
6.6.1 emd_18382_msk_1.map [i](#)



X



Y

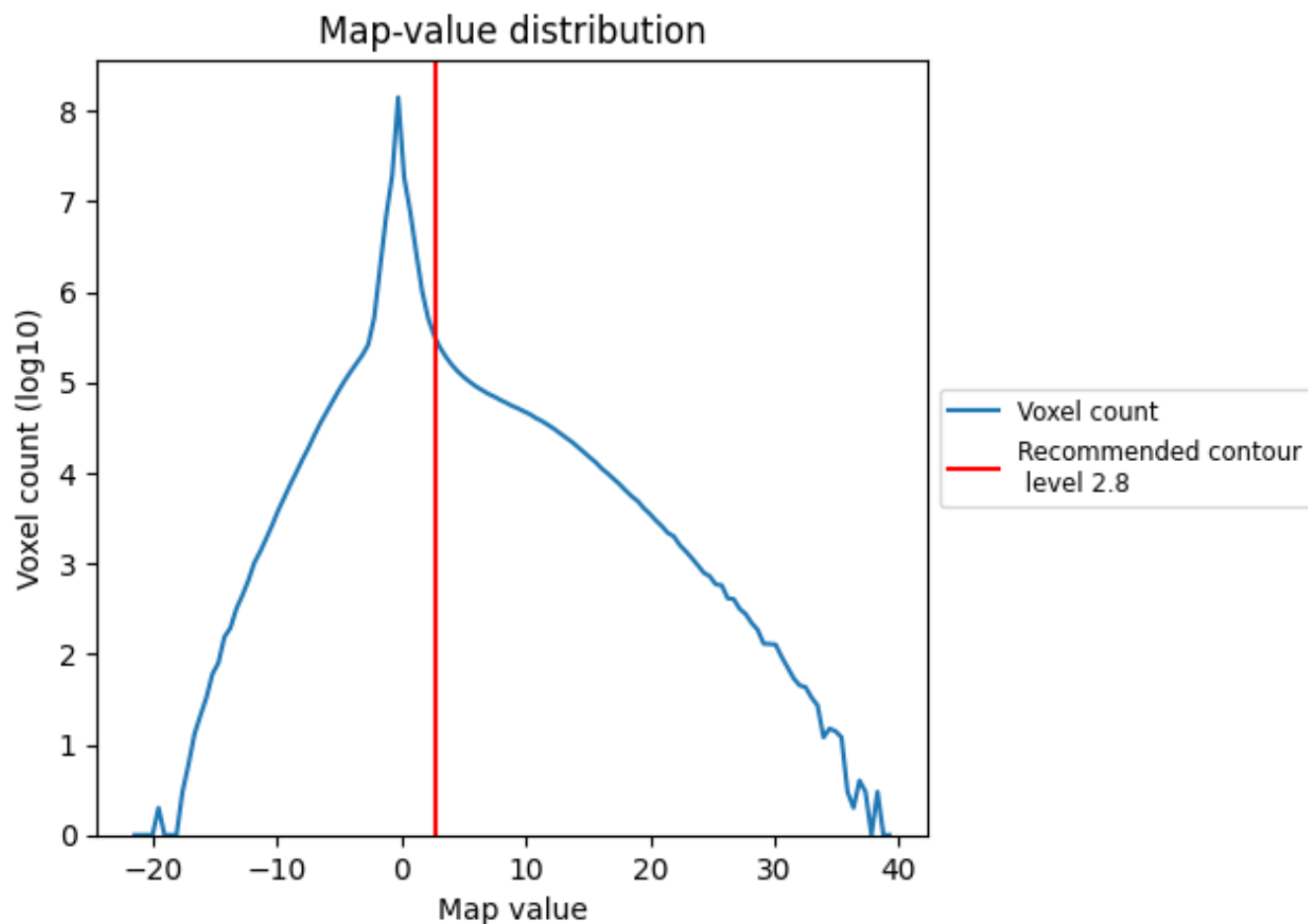


Z

7 Map analysis [i](#)

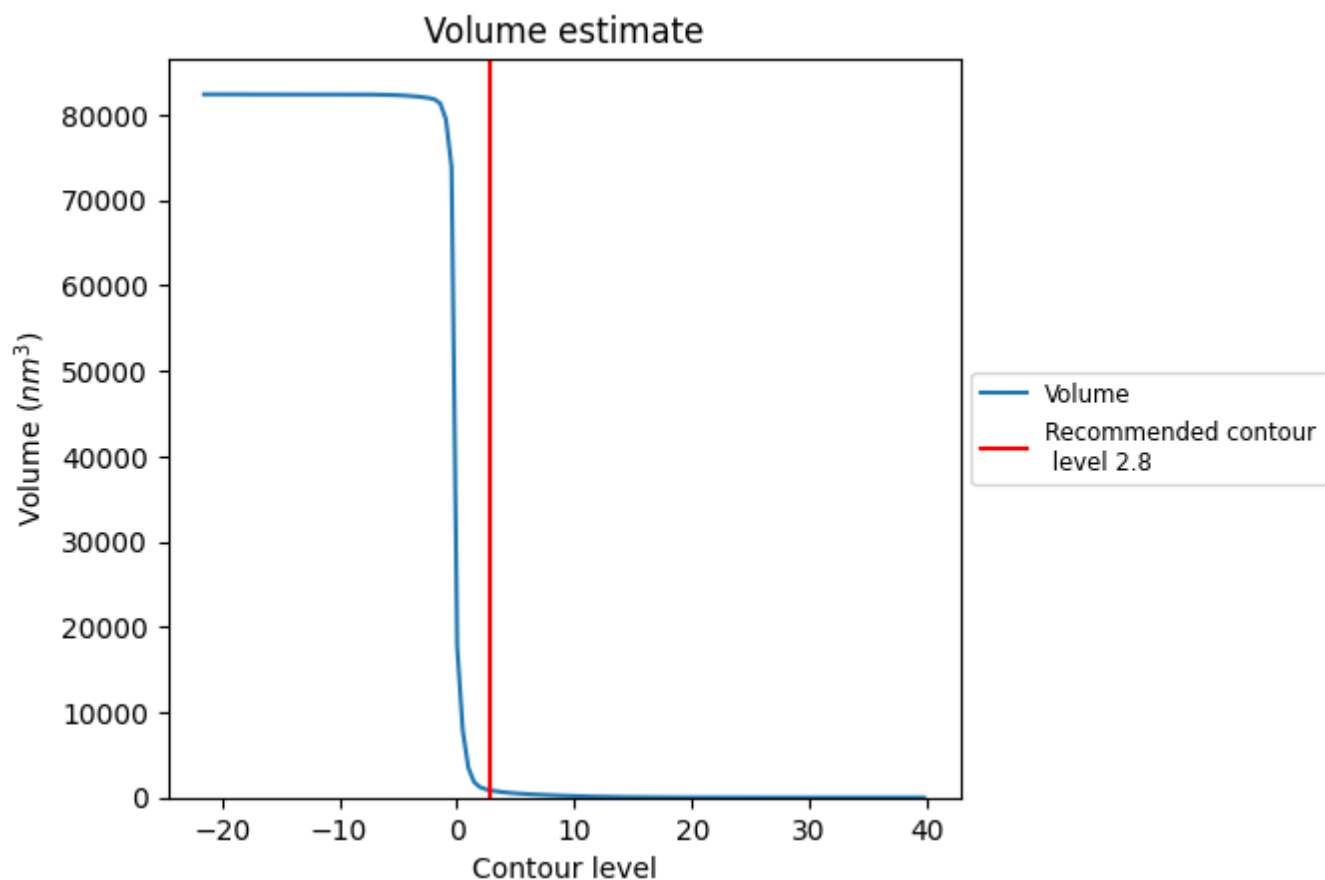
This section contains the results of statistical analysis of the map.

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.

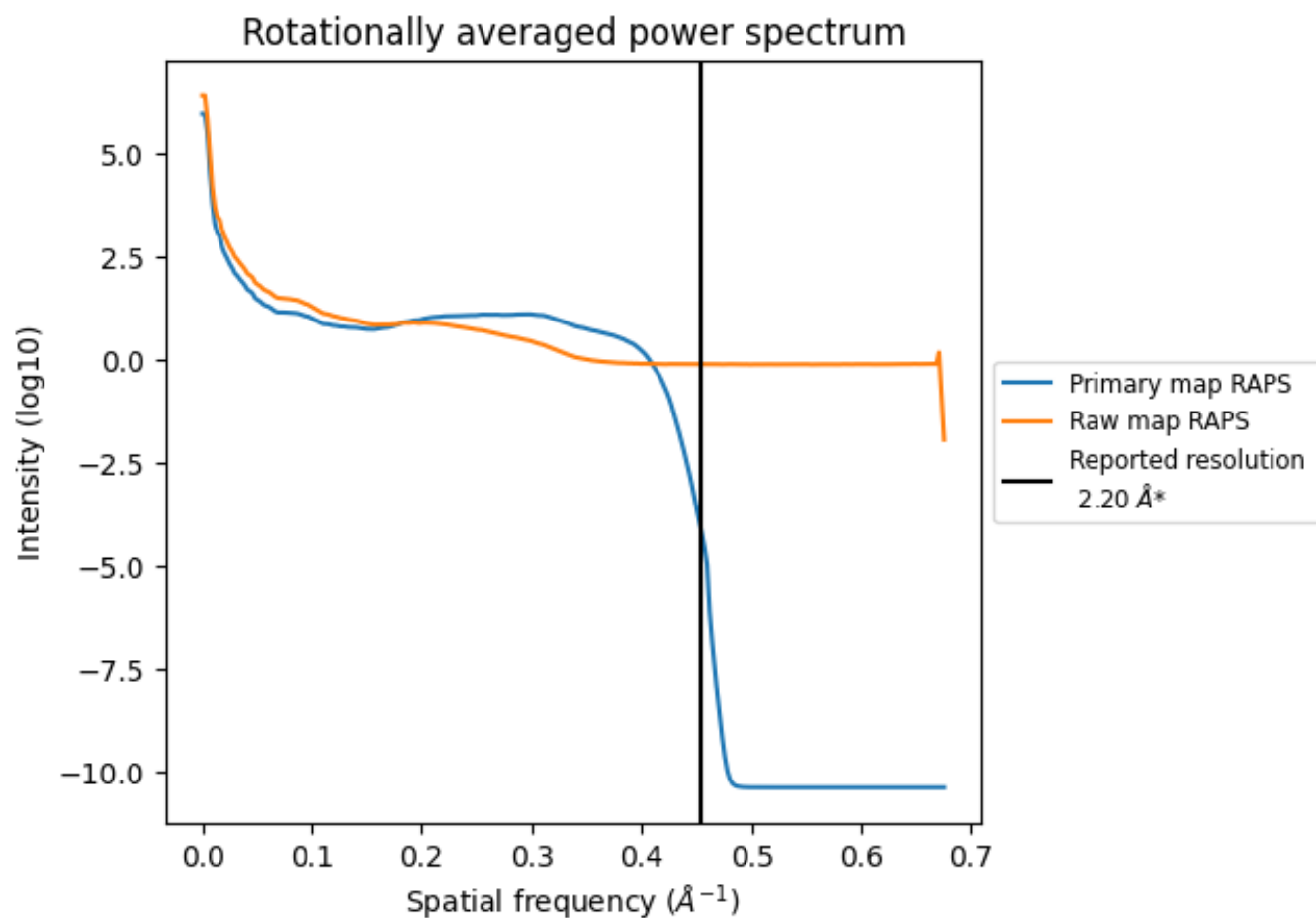
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 862 nm^3 ; this corresponds to an approximate mass of 779 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

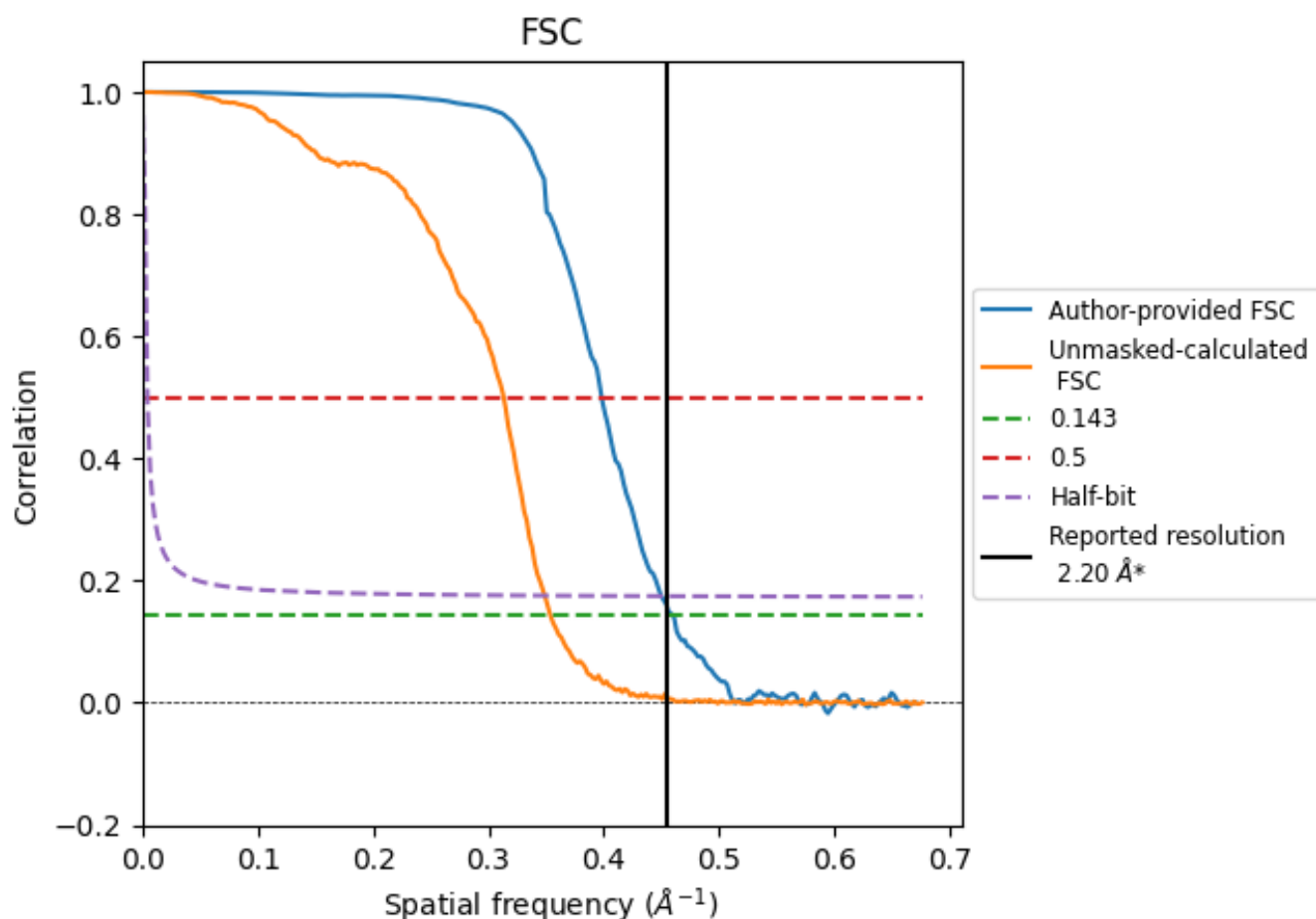


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

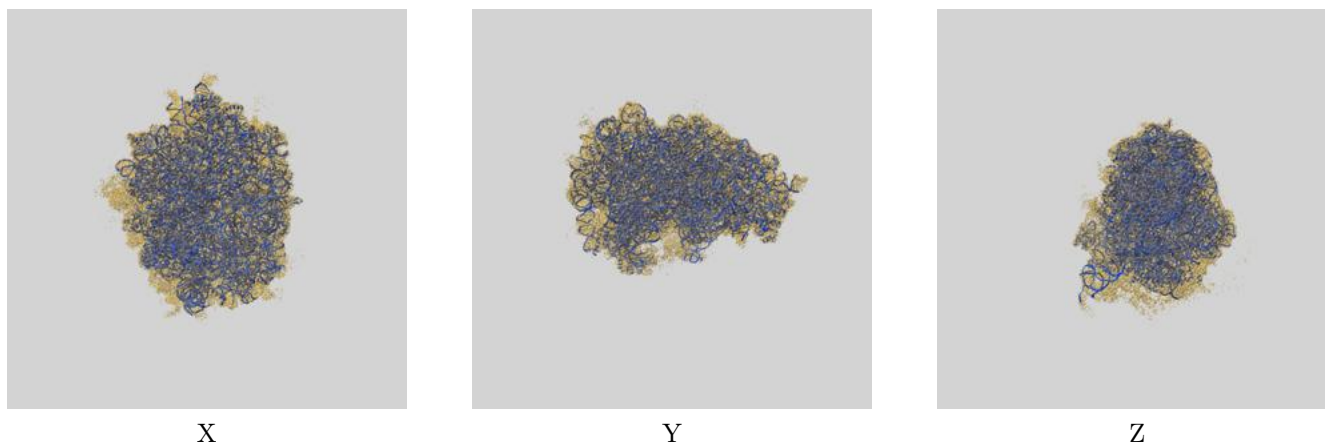
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.18	2.51	2.22
Unmasked-calculated*	2.83	3.19	2.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.83 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

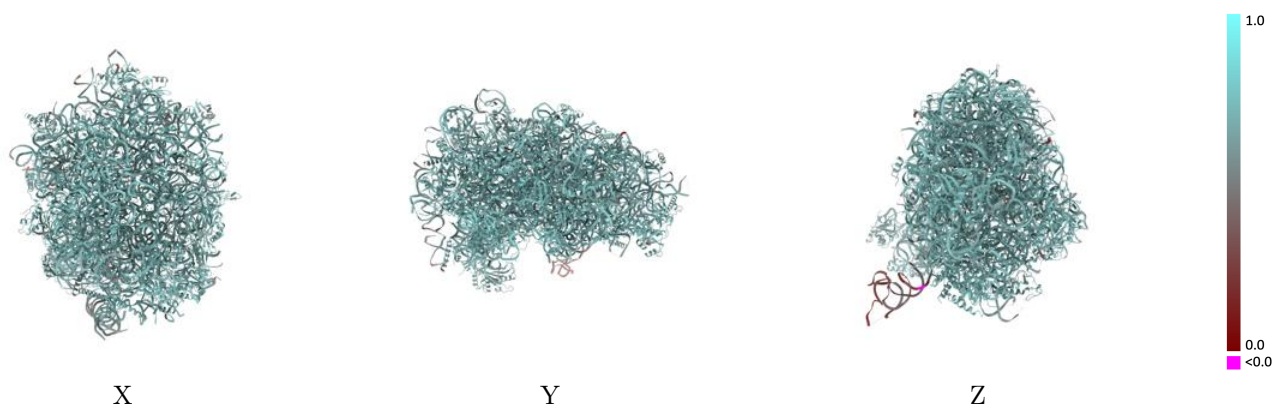
This section contains information regarding the fit between EMDB map EMD-18382 and PDB model 8QFD. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



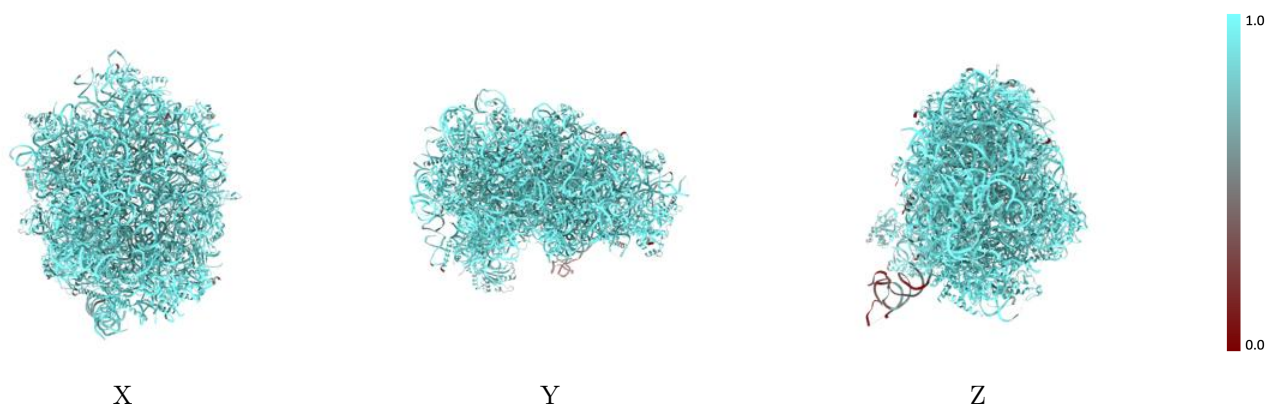
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



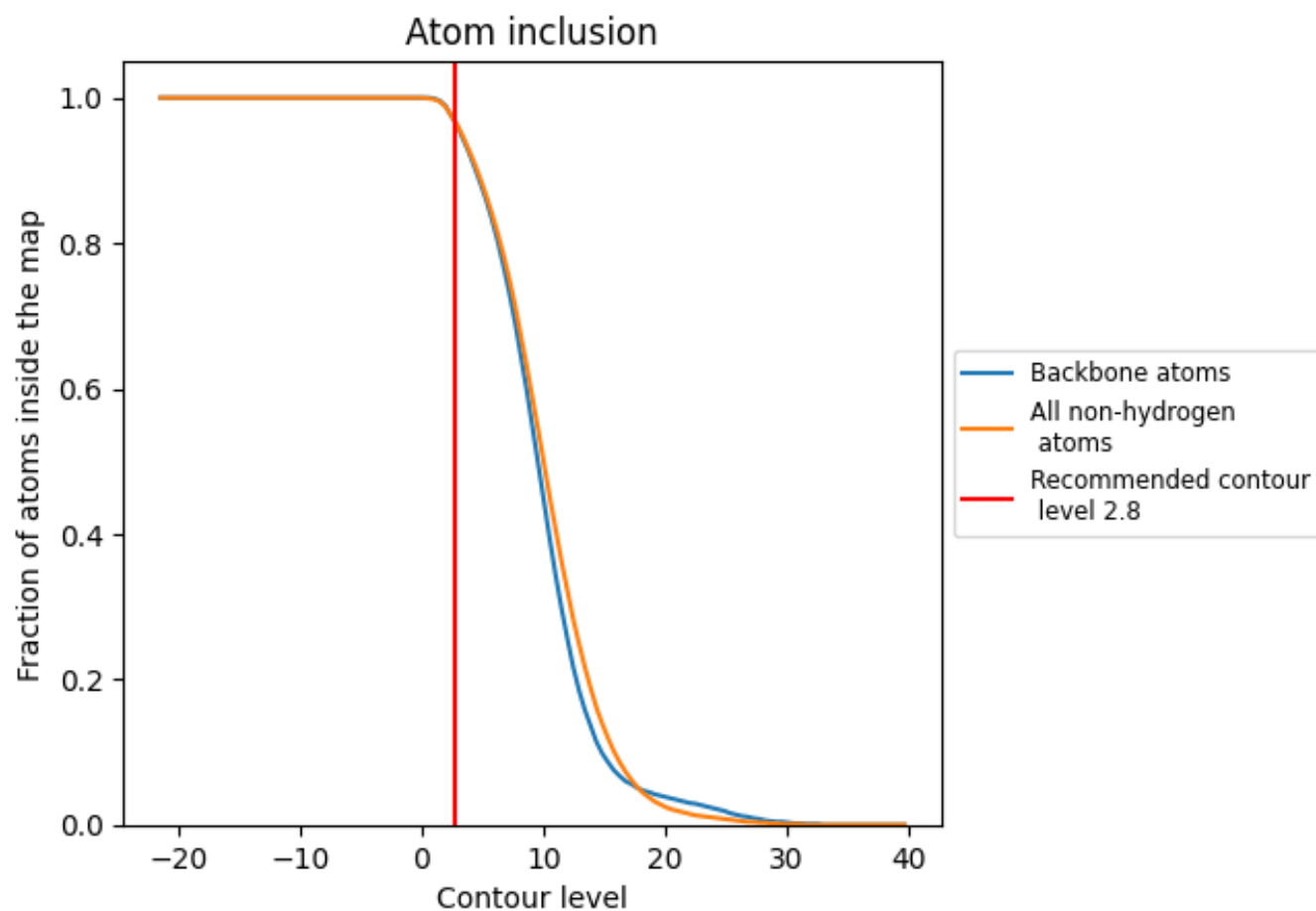
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.6840
5	 0.9650	 0.6710
7	 0.9980	 0.6910
8	 0.9870	 0.6830
A	 0.9920	 0.7190
B	 0.9770	 0.7120
C	 0.9830	 0.7130
D	 0.9510	 0.6890
E	 0.9610	 0.6910
F	 0.9860	 0.7160
G	 0.9340	 0.6830
H	 0.9680	 0.7020
I	 0.9780	 0.7060
J	 0.8500	 0.6370
L	 0.9590	 0.7000
M	 0.9660	 0.6930
N	 0.9980	 0.7240
O	 0.9760	 0.7120
P	 0.9850	 0.7130
Q	 0.9900	 0.7170
R	 0.9630	 0.6940
S	 0.9910	 0.7140
T	 0.9500	 0.6920
U	 0.8690	 0.6380
V	 0.9750	 0.7070
W	 0.9460	 0.7000
X	 0.9740	 0.7030
Y	 0.9720	 0.7040
Z	 0.9430	 0.6840
a	 0.9740	 0.7110
b	 0.9570	 0.6890
c	 0.9150	 0.6760
d	 0.9660	 0.6960
e	 0.9890	 0.7170
f	 0.9980	 0.7230



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Chain	Atom inclusion	Q-score
g	 0.9760	 0.7030
h	 0.9520	 0.6960
i	 0.9540	 0.6870
j	 0.9960	 0.7170
k	 0.9050	 0.6600
l	 0.9760	 0.7050
m	 0.9730	 0.7100
o	 0.9540	 0.6990
p	 0.9130	 0.6930
r	 0.9870	 0.7120
s	 0.7500	 0.6590