



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 6USJ / pdb_00006usj
EMDB ID : EMD-20864
Title : Structure of two nucleosomes bridged by human PARP2
Authors : Gaullier, G.; Bowerman, S.; Luger, K.
Deposited on : 2019-10-27
Resolution : 10.50 Å (reported)
Based on initial models : 6R1T, 6F5B, 5Y0C

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

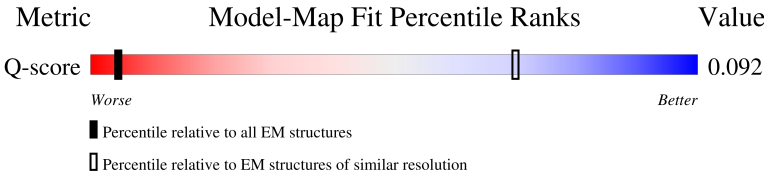
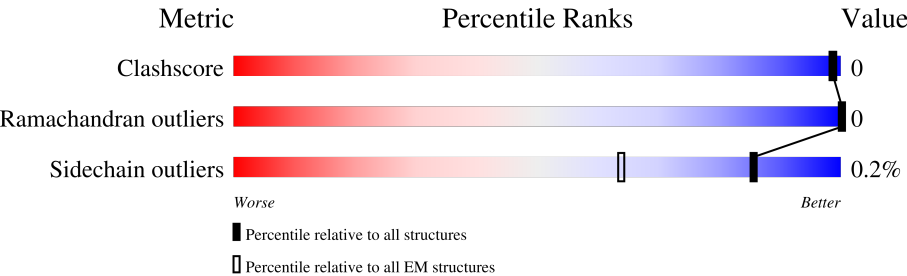
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.50 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.



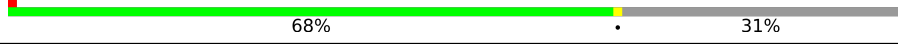
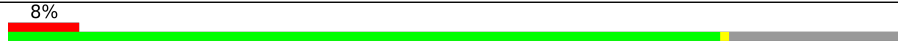
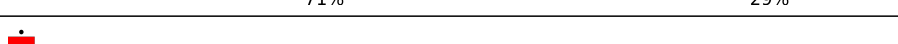
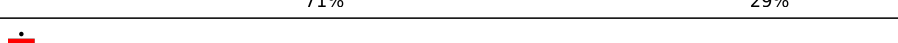
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	126 (10.00 - 11.00)

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	I	165	
1	S	165	
2	J	165	
2	T	165	

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Mol	Chain	Length	Quality of chain
3	A	139	
3	E	139	
3	K	139	
3	O	139	
4	B	106	
4	F	106	
4	L	106	
4	P	106	
5	C	133	
5	G	133	
5	M	133	
5	Q	133	
6	D	129	
6	H	129	
6	N	129	
6	R	129	
7	U	590	
7	V	590	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26939 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 DNA chain called Widom 601 DNA (160-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	160	Total	C	N	O	P	0	0
			3294	1558	617	959	160		
1	S	159	Total	C	N	O	P	0	0
			3279	1551	615	954	159		

- Molecule 2 is a DNA chain called Widom 601 DNA (160-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	160	Total	C	N	O	P	0	0
			3266	1549	596	961	160		
2	T	159	Total	C	N	O	P	0	0
			3241	1538	589	955	159		

- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	96	Total	C	N	O	S	0	0
			790	499	151	136	4		
3	E	99	Total	C	N	O	S	0	0
			819	517	159	139	4		
3	K	96	Total	C	N	O	S	0	0
			790	499	151	136	4		
3	O	99	Total	C	N	O	S	0	0
			819	517	159	139	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	HIS	-	expression tag	UNP P68431
K	-3	GLY	-	expression tag	UNP P68431
K	-2	SER	-	expression tag	UNP P68431
K	-1	HIS	-	expression tag	UNP P68431
O	-3	GLY	-	expression tag	UNP P68431
O	-2	SER	-	expression tag	UNP P68431
O	-1	HIS	-	expression tag	UNP P68431

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	77	Total	C	N	O	S	0	0
			614	389	119	105	1		
4	F	87	Total	C	N	O	S	0	0
			703	442	142	118	1		
4	L	77	Total	C	N	O	S	0	0
			614	389	119	105	1		
4	P	87	Total	C	N	O	S	0	0
			703	442	142	118	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
L	-3	GLY	-	expression tag	UNP P62805
L	-2	SER	-	expression tag	UNP P62805
L	-1	HIS	-	expression tag	UNP P62805
P	-3	GLY	-	expression tag	UNP P62805
P	-2	SER	-	expression tag	UNP P62805
P	-1	HIS	-	expression tag	UNP P62805

- Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	108	Total	C	N	O	0	0
			835	526	165	144		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	104	Total	C	N	O	0	0
			805	508	157	140		
5	M	108	Total	C	N	O	0	0
			835	526	165	144		
5	Q	104	Total	C	N	O	0	0
			805	508	157	140		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q08AJ9
C	-2	SER	-	expression tag	UNP Q08AJ9
C	-1	HIS	-	expression tag	UNP Q08AJ9
G	-3	GLY	-	expression tag	UNP Q08AJ9
G	-2	SER	-	expression tag	UNP Q08AJ9
G	-1	HIS	-	expression tag	UNP Q08AJ9
M	-3	GLY	-	expression tag	UNP Q08AJ9
M	-2	SER	-	expression tag	UNP Q08AJ9
M	-1	HIS	-	expression tag	UNP Q08AJ9
Q	-3	GLY	-	expression tag	UNP Q08AJ9
Q	-2	SER	-	expression tag	UNP Q08AJ9
Q	-1	HIS	-	expression tag	UNP Q08AJ9

- Molecule 6 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	92	Total	C	N	O	S	0	0
			720	453	129	136	2		
6	H	91	Total	C	N	O	S	0	0
			714	450	128	134	2		
6	N	92	Total	C	N	O	S	0	0
			720	453	129	136	2		
6	R	91	Total	C	N	O	S	0	0
			714	450	128	134	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899
N	-3	GLY	-	expression tag	UNP P06899
N	-2	SER	-	expression tag	UNP P06899
N	-1	HIS	-	expression tag	UNP P06899
R	-3	GLY	-	expression tag	UNP P06899
R	-2	SER	-	expression tag	UNP P06899
R	-1	HIS	-	expression tag	UNP P06899

- Molecule 7 is a protein called Poly [ADP-ribose] polymerase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	114	Total	C	N	O	S	0	0
			934	587	166	174	7		
7	V	113	Total	C	N	O	S	0	0
			925	582	164	172	7		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-19	MET	-	expression tag	UNP Q9UGN5
U	-18	GLY	-	expression tag	UNP Q9UGN5
U	-17	SER	-	expression tag	UNP Q9UGN5
U	-16	SER	-	expression tag	UNP Q9UGN5
U	-15	HIS	-	expression tag	UNP Q9UGN5
U	-14	HIS	-	expression tag	UNP Q9UGN5
U	-13	HIS	-	expression tag	UNP Q9UGN5
U	-12	HIS	-	expression tag	UNP Q9UGN5
U	-11	HIS	-	expression tag	UNP Q9UGN5
U	-10	HIS	-	expression tag	UNP Q9UGN5
U	-9	SER	-	expression tag	UNP Q9UGN5
U	-8	SER	-	expression tag	UNP Q9UGN5
U	-7	GLY	-	expression tag	UNP Q9UGN5
U	-6	LEU	-	expression tag	UNP Q9UGN5
U	-5	VAL	-	expression tag	UNP Q9UGN5
U	-4	PRO	-	expression tag	UNP Q9UGN5
U	-3	ARG	-	expression tag	UNP Q9UGN5
U	-2	GLY	-	expression tag	UNP Q9UGN5
U	-1	SER	-	expression tag	UNP Q9UGN5
U	0	HIS	-	expression tag	UNP Q9UGN5
U	112	ARG	GLN	engineered mutation	UNP Q9UGN5
U	113	ASP	PHE	engineered mutation	UNP Q9UGN5

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-19	MET	-	expression tag	UNP Q9UGN5
V	-18	GLY	-	expression tag	UNP Q9UGN5
V	-17	SER	-	expression tag	UNP Q9UGN5
V	-16	SER	-	expression tag	UNP Q9UGN5
V	-15	HIS	-	expression tag	UNP Q9UGN5
V	-14	HIS	-	expression tag	UNP Q9UGN5
V	-13	HIS	-	expression tag	UNP Q9UGN5
V	-12	HIS	-	expression tag	UNP Q9UGN5
V	-11	HIS	-	expression tag	UNP Q9UGN5
V	-10	HIS	-	expression tag	UNP Q9UGN5
V	-9	SER	-	expression tag	UNP Q9UGN5
V	-8	SER	-	expression tag	UNP Q9UGN5
V	-7	GLY	-	expression tag	UNP Q9UGN5
V	-6	LEU	-	expression tag	UNP Q9UGN5
V	-5	VAL	-	expression tag	UNP Q9UGN5
V	-4	PRO	-	expression tag	UNP Q9UGN5
V	-3	ARG	-	expression tag	UNP Q9UGN5
V	-2	GLY	-	expression tag	UNP Q9UGN5
V	-1	SER	-	expression tag	UNP Q9UGN5
V	0	HIS	-	expression tag	UNP Q9UGN5
V	112	ARG	GLN	engineered mutation	UNP Q9UGN5
V	113	ASP	PHE	engineered mutation	UNP Q9UGN5

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: Widom 601 DNA (160-MER)

Chain I: 



- Molecule 1: Widom 601 DNA (160-MER)

Chain S: 



- Molecule 2: Widom 601 DNA (160-MER)

Chain J: 



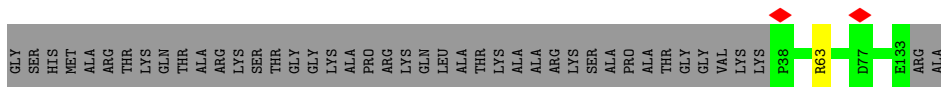
- Molecule 2: Widom 601 DNA (160-MER)

Chain T: 



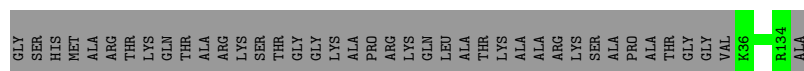
- Molecule 3: Histone H3.1

Chain A: 



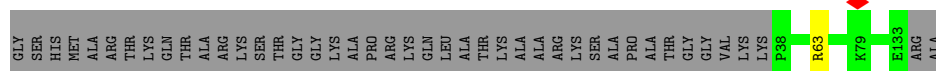
- Molecule 3: Histone H3.1

Chain E:  71% 29%



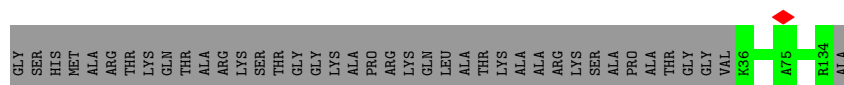
● Molecule 3: Histone H3.1

Chain K:  68% 31%



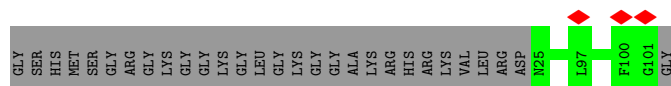
● Molecule 3: Histone H3.1

Chain O:  71% 29%



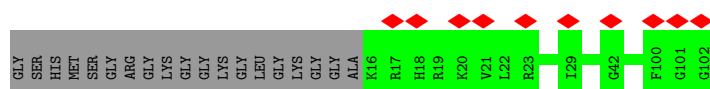
● Molecule 4: Histone H4

Chain B:  73% 27%



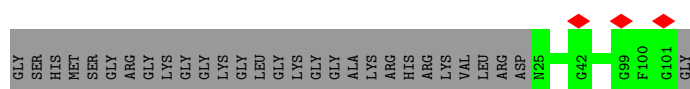
● Molecule 4: Histone H4

Chain F:  9% 82% 18%



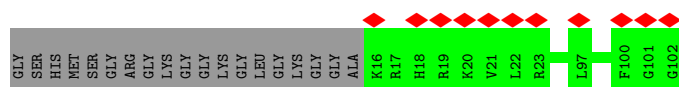
● Molecule 4: Histone H4

Chain L:  73% 27%

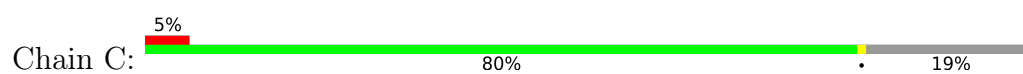


● Molecule 4: Histone H4

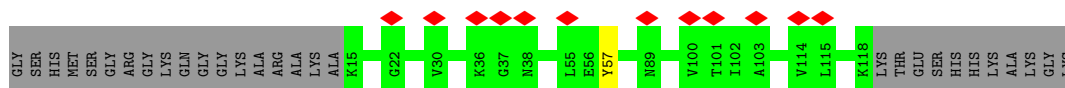
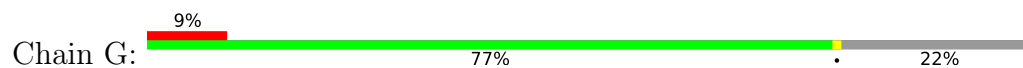
Chain P:  10% 82% 18%



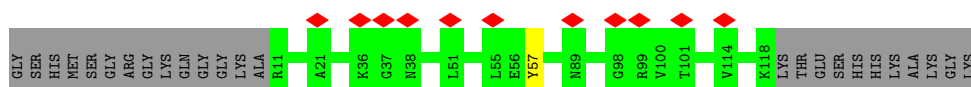
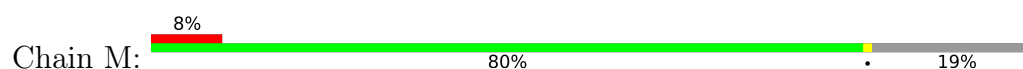
● Molecule 5: Histone H2A



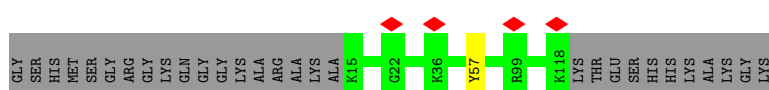
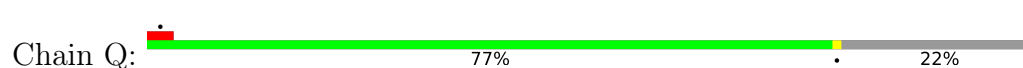
• Molecule 5: Histone H2A



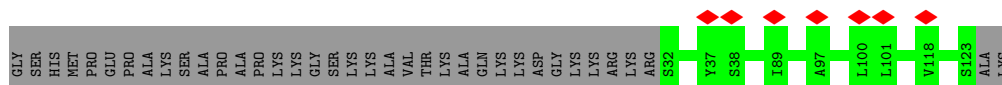
• Molecule 5: Histone H2A



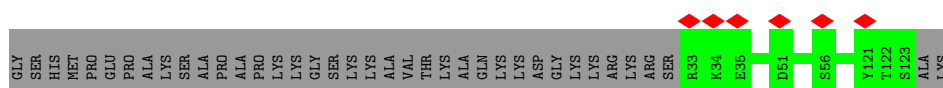
• Molecule 5: Histone H2A



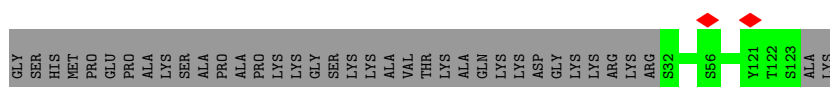
• Molecule 6: Histone H2B type 1-J



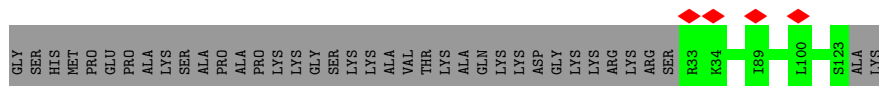
• Molecule 6: Histone H2B type 1-J



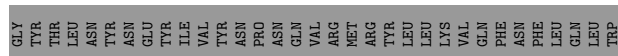
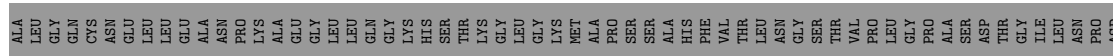
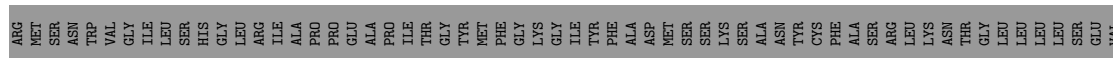
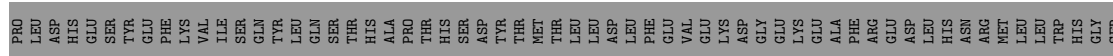
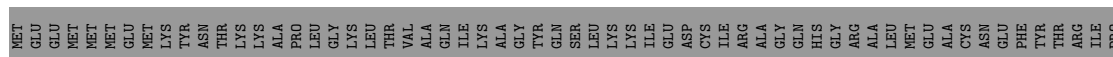
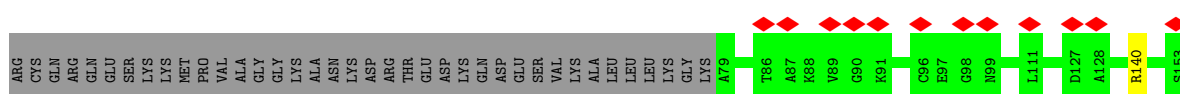
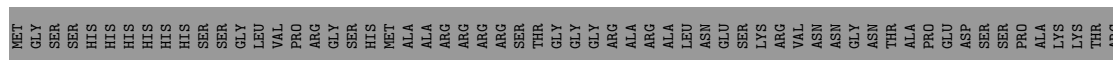
• Molecule 6: Histone H2B type 1-J



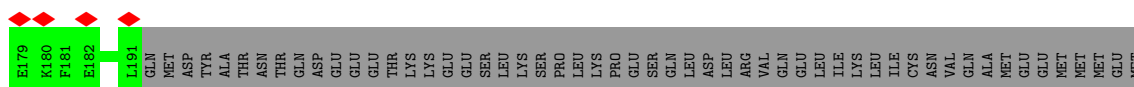
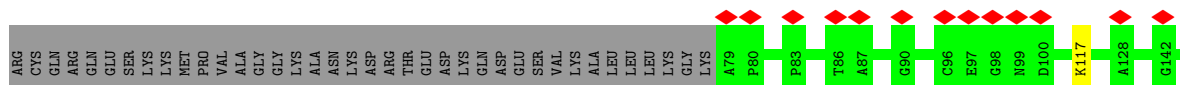
Chain R:



Chain U:



Chain V:



Tyr	Ile	Leu	Leu	Leu	Phe	Pro	Lys
	Val	Ala	Glu	Ser	Val	Leu	Tyr
	Tyr	Asn	Asn	Gly	Ile	Ile	Thr
	Asn	Pro	Lys	Leu	Ser	Thr	Lys
	Asn	Ala	Ile	Arg	Gln	Lys	Ala
	Gln	Glu	Ala	Ala	Tyr	Pro	Lys
	Val	Gly	Pro	Pro	Gln	Leu	Gly
	Arg	Gly	Pro	Ser	Ser	Ser	Lys
	Met	Leu	Glu	Ala	Thr	Glu	Lys
	Arg	Gln	Gln	Pro	Ala	Ile	Thr
Leu	Leu	Lys	Lys	Lys	Lys	Lys	Lys
	Leu	Lys	His	Ile	Pro	Gln	Val
	Leu	His	Thr	Thr	Thr	Leu	Ala
	Lys	Ser	Gly	Tyr	Ser	Gln	Lys
	Val	Thr	Thr	Met	Asp	Ile	Lys
	Val	Lys	Met	Phe	Tyr	Ala	Lys
	Gln	Gly	Leu	Gly	Thr	Gly	Gly
	Phe	Leu	Lys	Lys	Thr	Asp	Tyr
	Asn	Leu	Gly	Phe	Thr	Leu	Ser
	Thr	Lys	Met	Ile	Leu	Glu	Ser
Gln	Leu	Ala	Ala	Tyr	Leu	Ile	Leu
	Pro	Pro	Phe	Phe	Asp	Ala	Lys
	Ser	Ser	Ala	Leu	Ile	Lys	Lys
	Ser	Ala	Asp	Phe	Phe	Lys	Ile
	Ala	Ala	Met	Glu	Glu	Leu	Lys
	His	Ser	Ser	Val	Val	Leu	Asp
	Phe	Ser	Ser	Glu	Lys	Lys	Cys
	Val	Val	Lys	Lys	Thr	Thr	Ile
	Thr	Thr	Ser	Ser	Glu	Gly	Gly
	Thr	Val	Thr	Thr	Ala	Arg	Arg
Trp	Leu	Ser	Ser	Pro	Pro	Pro	Arg
	Leu	Asn	Asn	Leu	Leu	Leu	Leu
	Gln	Gly	Gly	Tyr	Ser	Met	Met
	Leu	Pro	Lys	Lys	Glu	Asn	Glu
	Leu	Ala	Ala	Leu	Leu	Leu	Leu
	Leu	Val	Val	Val	Val	Val	Val
	Leu	Thr	Thr	Thr	Thr	Thr	Thr
	Leu	Thr	Thr	Thr	Thr	Thr	Thr
	Leu	Thr	Thr	Thr	Thr	Thr	Thr
	Leu	Thr	Thr	Thr	Thr	Thr	Thr

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27889	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 ($e^-/\text{\AA}^2$)	56.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	325.376, 325.376, 325.376	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.271, 1.271, 1.271	Depositor

5 Model quality

5.1 Standard geometry

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	I	0.76	0/3698	1.38	10/5709 (0.2%)
1	S	0.76	0/3682	1.29	7/5686 (0.1%)
2	J	0.75	0/3660	1.30	6/5643 (0.1%)
2	T	0.78	1/3631 (0.0%)	1.33	8/5595 (0.1%)
3	A	0.90	0/802	1.33	0/1076
3	E	0.90	0/831	1.33	0/1113
3	K	0.90	0/802	1.34	0/1076
3	O	0.90	0/831	1.34	0/1113
4	B	0.94	0/621	1.31	0/832
4	F	0.95	0/711	1.33	0/948
4	L	0.94	0/621	1.31	0/832
4	P	0.95	0/711	1.33	0/948
5	C	0.91	0/845	1.36	0/1139
5	G	0.92	0/815	1.38	0/1100
5	M	0.91	0/845	1.36	0/1139
5	Q	0.92	0/815	1.38	0/1100
6	D	0.87	0/731	1.35	0/983
6	H	0.88	0/725	1.35	0/975
6	N	0.87	0/731	1.35	0/983
6	R	0.89	0/725	1.35	0/975
7	U	0.88	0/953	1.31	0/1281
7	V	0.86	0/944	1.29	0/1269
All	All	0.83	1/28730 (0.0%)	1.33	31/41515 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	16
1	S	0	19
2	J	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	12
5	C	0	1
5	G	0	1
5	M	0	1
5	Q	0	1
All	All	0	63

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	-81	DA	P-O5'	11.13	1.82	1.60

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	-81	DC	P-O5'-C5'	34.05	171.08	120.00
1	I	-81	DC	O5'-P-OP1	10.80	141.40	109.00
2	T	-81	DA	O5'-P-OP1	8.41	134.24	109.00
2	T	-81	DA	O5'-P-OP2	-8.02	83.95	108.00
1	S	78	DC	C4'-C3'-O3'	7.10	120.65	110.00
1	S	20	DG	C4'-C3'-O3'	6.31	119.47	110.00
1	I	20	DG	C4'-C3'-O3'	6.29	119.44	110.00
1	S	-57	DT	O5'-C5'-C4'	6.01	119.82	110.80
1	I	-57	DT	O5'-C5'-C4'	5.97	119.76	110.80
2	T	-58	DG	O5'-C5'-C4'	5.92	119.68	110.80
2	J	-58	DG	O5'-C5'-C4'	5.89	119.64	110.80
1	I	-81	DC	O5'-P-OP2	-5.89	90.34	108.00
1	S	70	DA	O5'-C5'-C4'	5.53	119.10	110.80
1	I	70	DA	O5'-C5'-C4'	5.52	119.08	110.80
2	T	-68	DA	O5'-C5'-C4'	5.48	119.02	110.80
2	J	-68	DA	O5'-C5'-C4'	5.42	118.93	110.80
2	J	-42	DT	O5'-C5'-C4'	5.35	118.82	110.80
2	T	-42	DT	O5'-C5'-C4'	5.34	118.80	110.80
1	I	-70	DG	O5'-C5'-C4'	5.28	118.72	110.80
2	J	49	DC	O5'-C5'-C4'	5.25	118.67	110.80
2	T	-20	DC	O5'-C5'-C4'	5.22	118.64	110.80
2	T	49	DC	O5'-C5'-C4'	5.21	118.61	110.80
2	T	63	DA	O5'-C5'-C4'	5.21	118.61	110.80
1	S	-70	DG	O5'-C5'-C4'	5.20	118.59	110.80
2	J	-20	DC	O5'-C5'-C4'	5.19	118.59	110.80
1	S	24	DC	O5'-C5'-C4'	5.17	118.56	110.80
1	I	24	DC	O5'-C5'-C4'	5.16	118.55	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	63	DA	O5'-C5'-C4'	5.14	118.51	110.80
1	S	20	DG	O5'-C5'-C4'	5.14	118.50	110.80
1	I	20	DG	O5'-C5'-C4'	5.13	118.49	110.80
1	I	-20	DC	O5'-C5'-C4'	5.02	118.33	110.80

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	57	TYR	Sidechain
5	G	57	TYR	Sidechain
1	I	-15	DA	Sidechain
1	I	-17	DT	Sidechain
1	I	-35	DG	Sidechain
1	I	-38	DA	Sidechain
1	I	-43	DA	Sidechain
1	I	-46	DT	Sidechain
1	I	-63	DT	Sidechain
1	I	-70	DG	Sidechain
1	I	-8	DG	Sidechain
1	I	-80	DC	Sidechain
1	I	25	DT	Sidechain
1	I	26	DA	Sidechain
1	I	36	DA	Sidechain
1	I	44	DT	Sidechain
1	I	52	DC	Sidechain
1	I	72	DG	Sidechain
2	J	-15	DA	Sidechain
2	J	-35	DA	Sidechain
2	J	-42	DT	Sidechain
2	J	-52	DG	Sidechain
2	J	-56	DC	Sidechain
2	J	-7	DG	Sidechain
2	J	-70	DT	Sidechain
2	J	-73	DG	Sidechain
2	J	26	DG	Sidechain
2	J	33	DC	Sidechain
2	J	36	DC	Sidechain
2	J	67	DA	Sidechain
5	M	57	TYR	Sidechain
5	Q	57	TYR	Sidechain
1	S	-15	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	S	-17	DT	Sidechain
1	S	-23	DT	Sidechain
1	S	-35	DG	Sidechain
1	S	-38	DA	Sidechain
1	S	-43	DA	Sidechain
1	S	-46	DT	Sidechain
1	S	-63	DT	Sidechain
1	S	-70	DG	Sidechain
1	S	-73	DC	Sidechain
1	S	-8	DG	Sidechain
1	S	25	DT	Sidechain
1	S	26	DA	Sidechain
1	S	36	DA	Sidechain
1	S	44	DT	Sidechain
1	S	52	DC	Sidechain
1	S	70	DA	Sidechain
1	S	79	DG	Sidechain
1	S	81	DT	Sidechain
2	T	-15	DA	Sidechain
2	T	-35	DA	Sidechain
2	T	-42	DT	Sidechain
2	T	-52	DG	Sidechain
2	T	-56	DC	Sidechain
2	T	-7	DG	Sidechain
2	T	-70	DT	Sidechain
2	T	-80	DT	Sidechain
2	T	26	DG	Sidechain
2	T	33	DC	Sidechain
2	T	36	DC	Sidechain
2	T	67	DA	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3294	0	1794	0	0
1	S	3279	0	1784	4	0
2	J	3266	0	1795	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	3241	0	1784	1	0
3	A	790	0	826	0	0
3	E	819	0	864	0	0
3	K	790	0	826	0	0
3	O	819	0	864	0	0
4	B	614	0	656	0	0
4	F	703	0	755	0	0
4	L	614	0	656	0	0
4	P	703	0	755	0	0
5	C	835	0	897	0	0
5	G	805	0	861	0	0
5	M	835	0	897	0	0
5	Q	805	0	861	0	0
6	D	720	0	740	0	0
6	H	714	0	735	0	0
6	N	720	0	740	0	0
6	R	714	0	735	0	0
7	U	934	0	911	2	0
7	V	925	0	903	1	0
All	All	26939	0	21639	7	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 0.

All (7) 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)
2:T:-81:DA:OP2	7:V:117:LYS:NZ	2.11	0.81
1:S:-77:DA:OP2	1:S:-77:DA:H4'	2.10	0.51
1:S:-77:DA:H1'	1:S:-76:DA:H5'	1.96	0.47
1:S:81:DT:OP1	7:U:140:ARG:NH1	2.45	0.47
1:S:81:DT:OP1	7:U:140:ARG:HD3	2.14	0.47
2:J:-78:DG:H1'	2:J:-77:DC:H5'	1.97	0.45
2:J:-78:DG:H5''	2:J:-78:DG:C8	2.56	0.41

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	
3	A	94/139 (68%)	94 (100%)	0	0	100	100
3	E	97/139 (70%)	97 (100%)	0	0	100	100
3	K	94/139 (68%)	94 (100%)	0	0	100	100
3	O	97/139 (70%)	97 (100%)	0	0	100	100
4	B	75/106 (71%)	74 (99%)	1 (1%)	0	100	100
4	F	85/106 (80%)	84 (99%)	1 (1%)	0	100	100
4	L	75/106 (71%)	74 (99%)	1 (1%)	0	100	100
4	P	85/106 (80%)	84 (99%)	1 (1%)	0	100	100
5	C	106/133 (80%)	104 (98%)	2 (2%)	0	100	100
5	G	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
5	M	106/133 (80%)	104 (98%)	2 (2%)	0	100	100
5	Q	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
6	D	90/129 (70%)	90 (100%)	0	0	100	100
6	H	89/129 (69%)	88 (99%)	1 (1%)	0	100	100
6	N	90/129 (70%)	90 (100%)	0	0	100	100
6	R	89/129 (69%)	88 (99%)	1 (1%)	0	100	100
7	U	112/590 (19%)	104 (93%)	8 (7%)	0	100	100
7	V	111/590 (19%)	106 (96%)	5 (4%)	0	100	100
All	All	1699/3208 (53%)	1672 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	84/113 (74%)	83 (99%)	1 (1%)	63	75
3	E	87/113 (77%)	87 (100%)	0	100	100
3	K	84/113 (74%)	83 (99%)	1 (1%)	63	75
3	O	87/113 (77%)	87 (100%)	0	100	100
4	B	63/81 (78%)	63 (100%)	0	100	100
4	F	72/81 (89%)	72 (100%)	0	100	100
4	L	63/81 (78%)	63 (100%)	0	100	100
4	P	72/81 (89%)	72 (100%)	0	100	100
5	C	85/102 (83%)	85 (100%)	0	100	100
5	G	83/102 (81%)	83 (100%)	0	100	100
5	M	85/102 (83%)	85 (100%)	0	100	100
5	Q	83/102 (81%)	83 (100%)	0	100	100
6	D	79/107 (74%)	79 (100%)	0	100	100
6	H	78/107 (73%)	78 (100%)	0	100	100
6	N	79/107 (74%)	79 (100%)	0	100	100
6	R	78/107 (73%)	78 (100%)	0	100	100
7	U	101/511 (20%)	100 (99%)	1 (1%)	68	78
7	V	100/511 (20%)	100 (100%)	0	100	100
All	All	1463/2634 (56%)	1460 (100%)	3 (0%)	85	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	63	ARG
3	K	63	ARG
7	U	172	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	GLN
3	A	93	GLN
4	B	25	ASN

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Mol	Chain	Res	Type
5	C	68	ASN
6	D	47	GLN
3	E	39	HIS
4	F	18	HIS
5	G	24	GLN
5	G	68	ASN
3	K	76	GLN
3	K	93	GLN
4	L	25	ASN
5	M	68	ASN
6	N	47	GLN
3	O	39	HIS
5	Q	24	GLN
5	Q	68	ASN
7	U	107	ASN
7	U	108	GLN
7	U	110	ASN
7	V	108	GLN
7	V	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

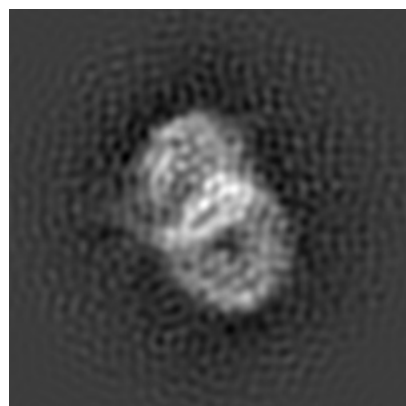
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20864. These allow visual inspection of the internal detail of the map and identification of artifacts.

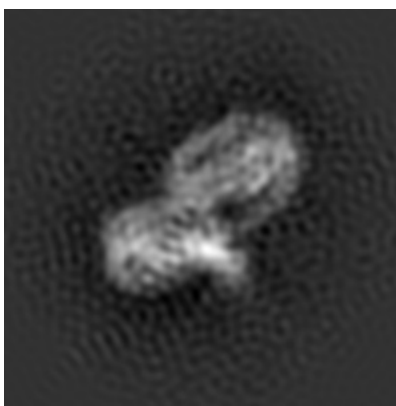
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

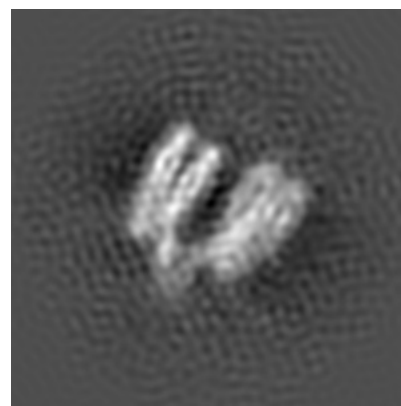
6.1.1 Primary map



X

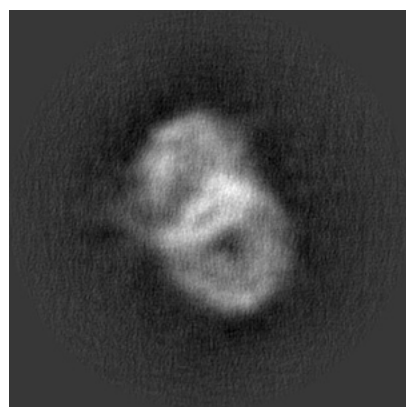


Y

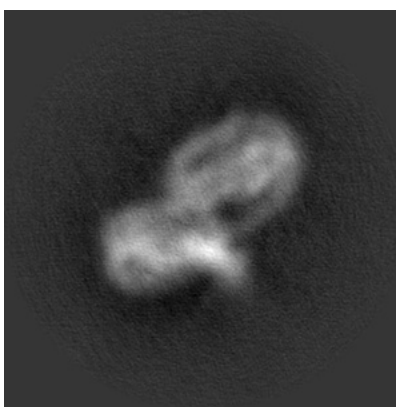


Z

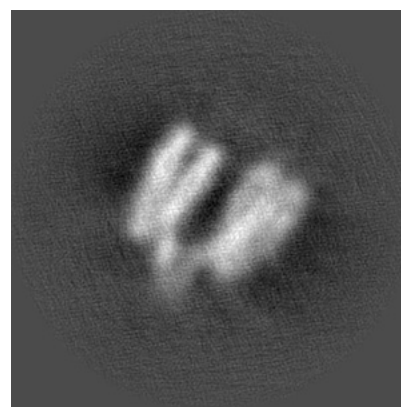
6.1.2 Raw map



X



Y

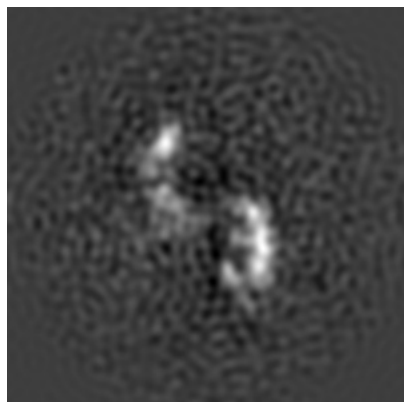


Z

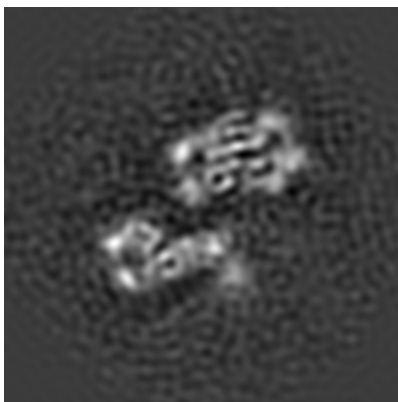
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

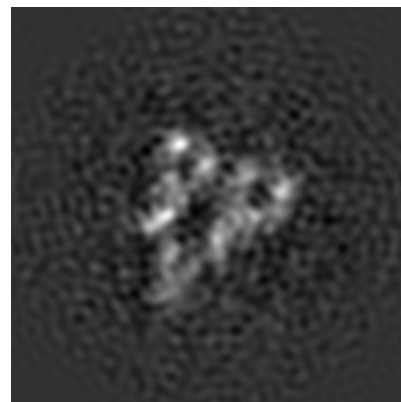
6.2.1 Primary map



X Index: 128

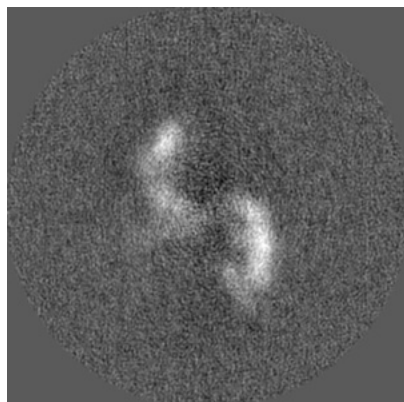


Y Index: 128

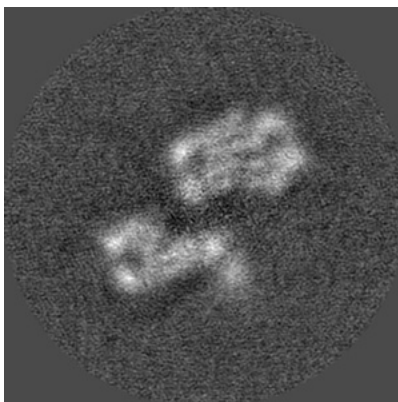


Z Index: 128

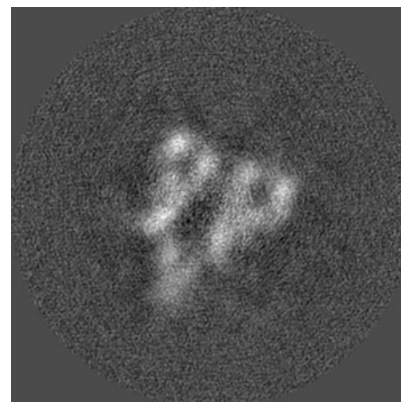
6.2.2 Raw map



X Index: 128



Y Index: 128

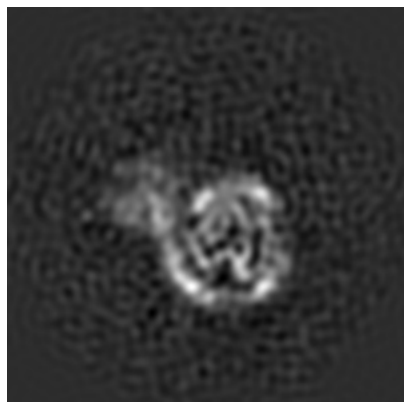


Z Index: 128

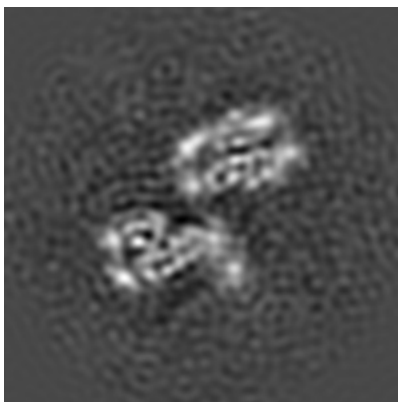
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

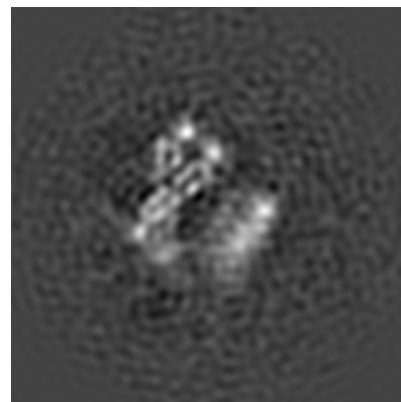
6.3.1 Primary map



X Index: 101

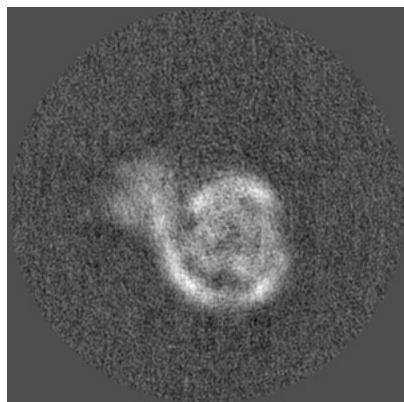


Y Index: 133

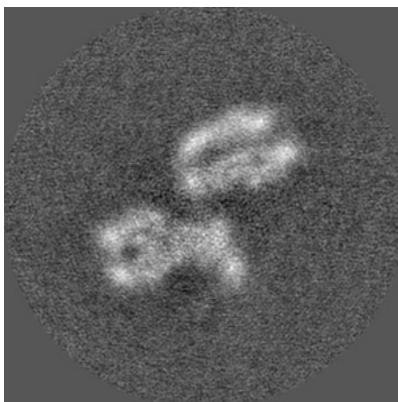


Z Index: 111

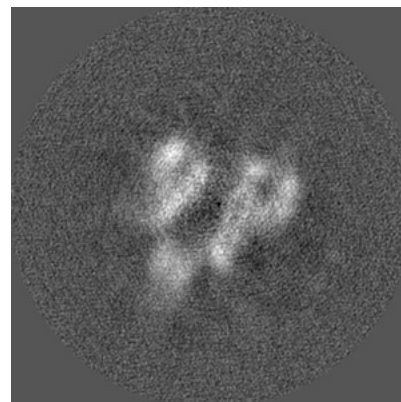
6.3.2 Raw map



X Index: 100



Y Index: 136

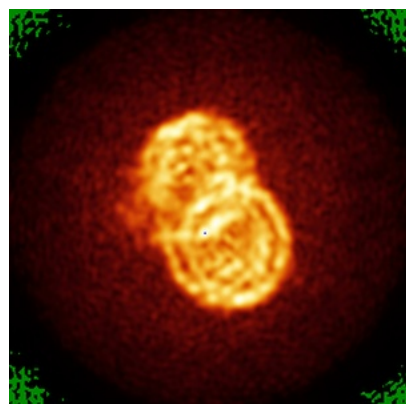


Z Index: 135

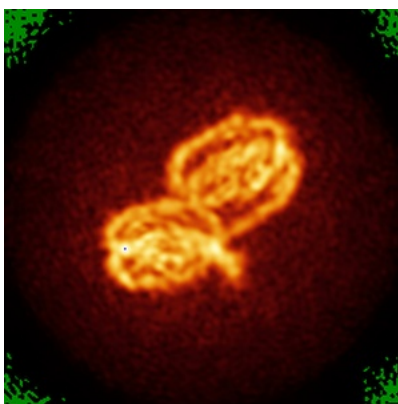
The images above show the largest variance slices of the map in three orthogonal directions.

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

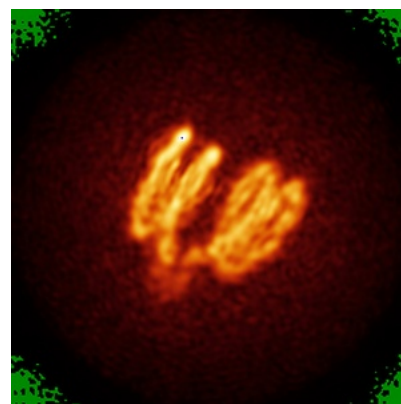
6.4.1 Primary map



X

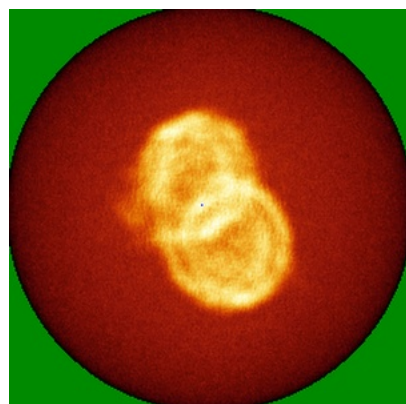


Y

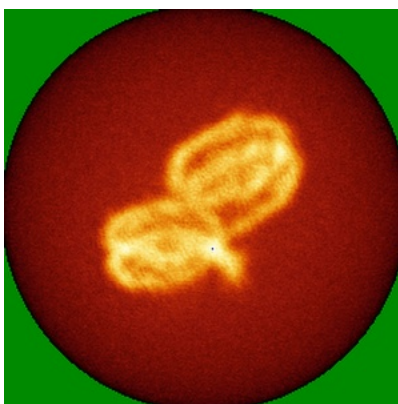


Z

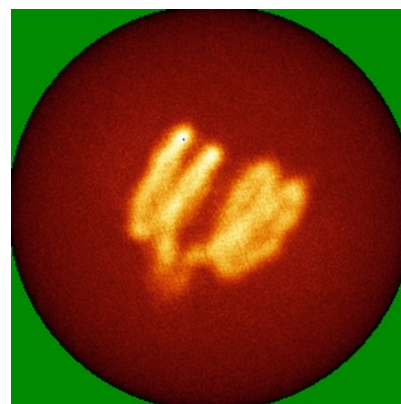
6.4.2 Raw map



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](#)

This section was not generated.

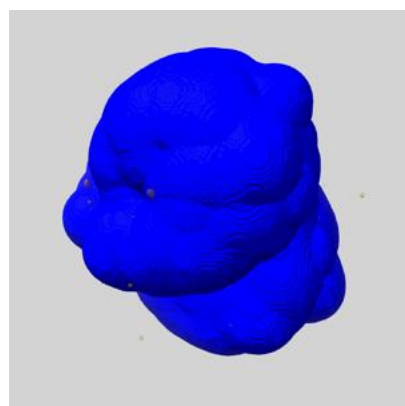
6.6 Mask visualisation [i](#)

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

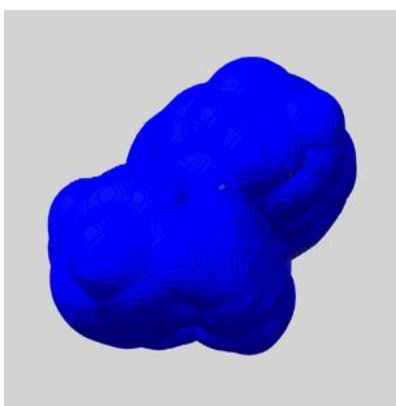
A mask typically either:

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

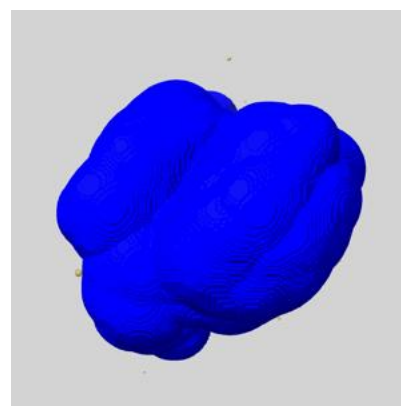
6.6.1 emd_20864_msk_1.map [i](#)



X



Y

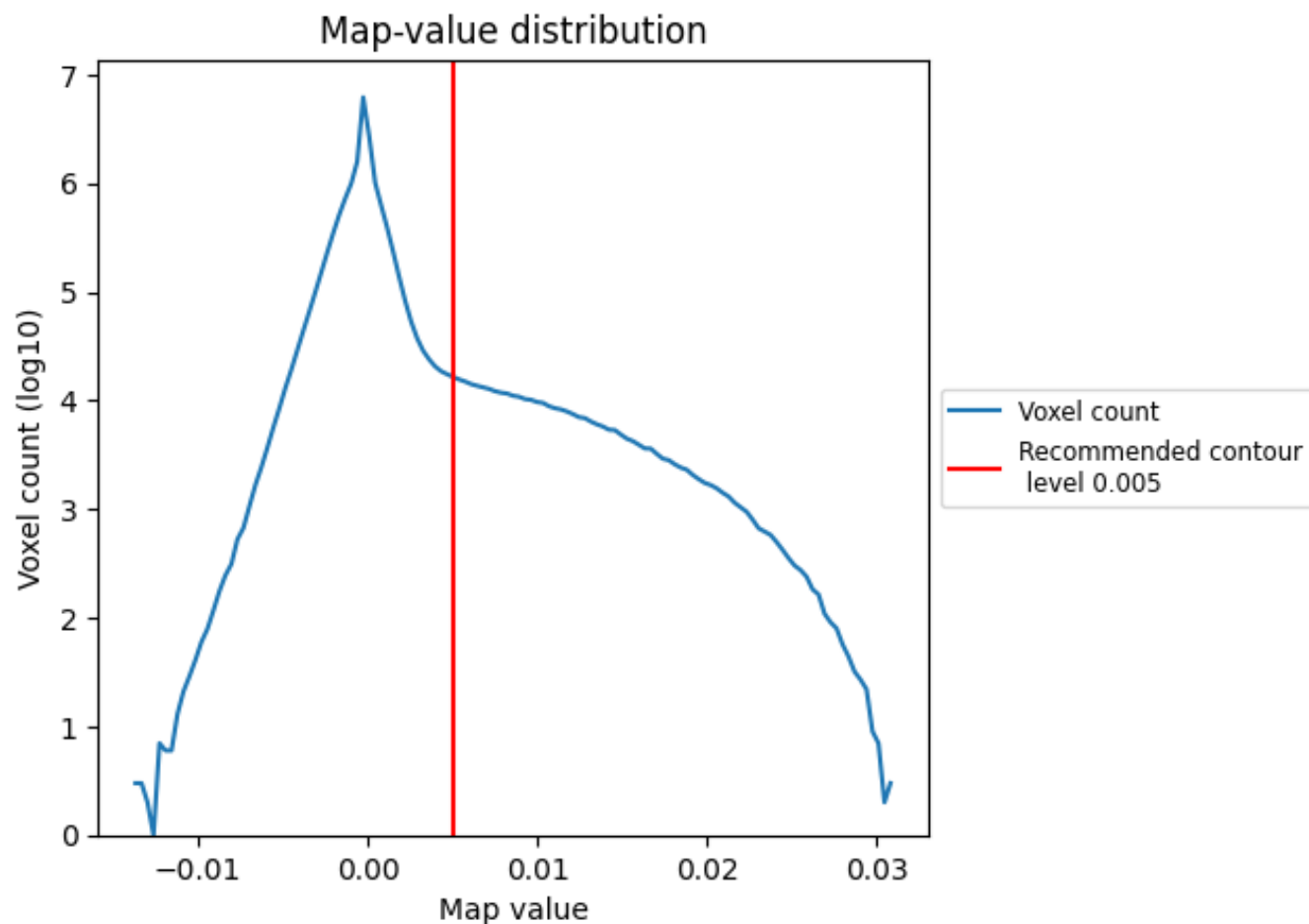


Z

7 Map analysis [i](#)

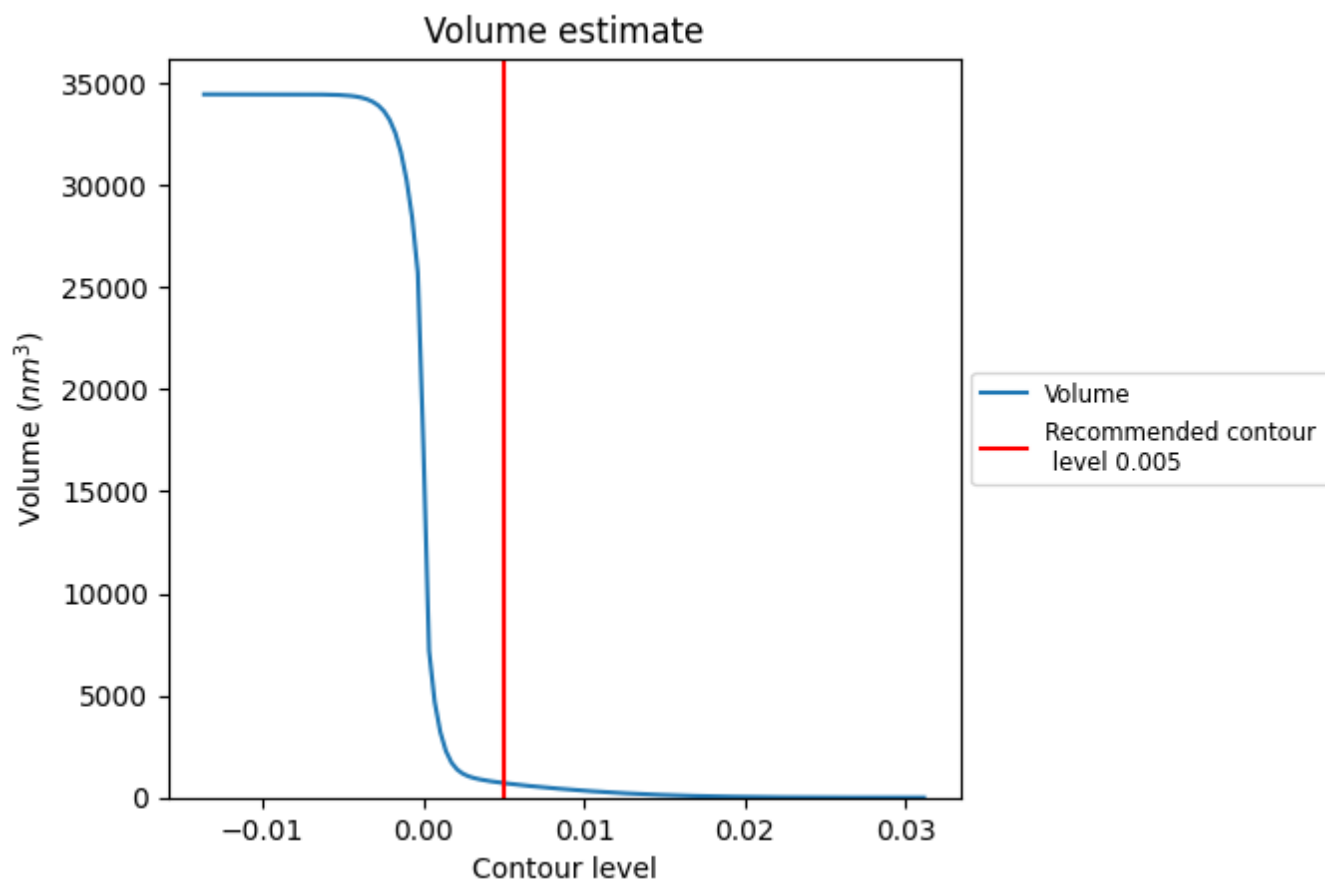
This section contains the results of statistical analysis of the map.

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.

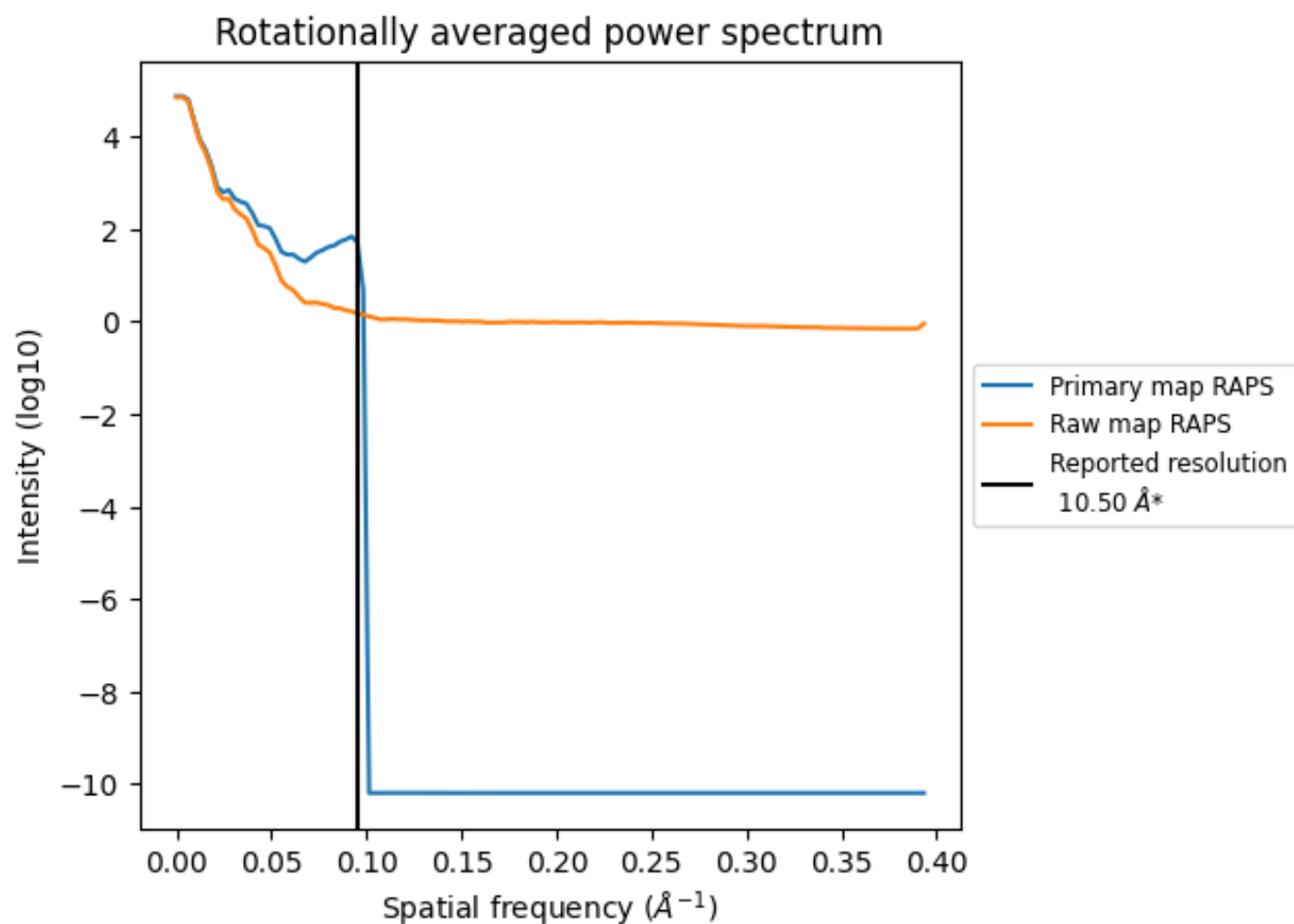
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 710 nm³; this corresponds to an approximate mass of 642 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 ⓘ

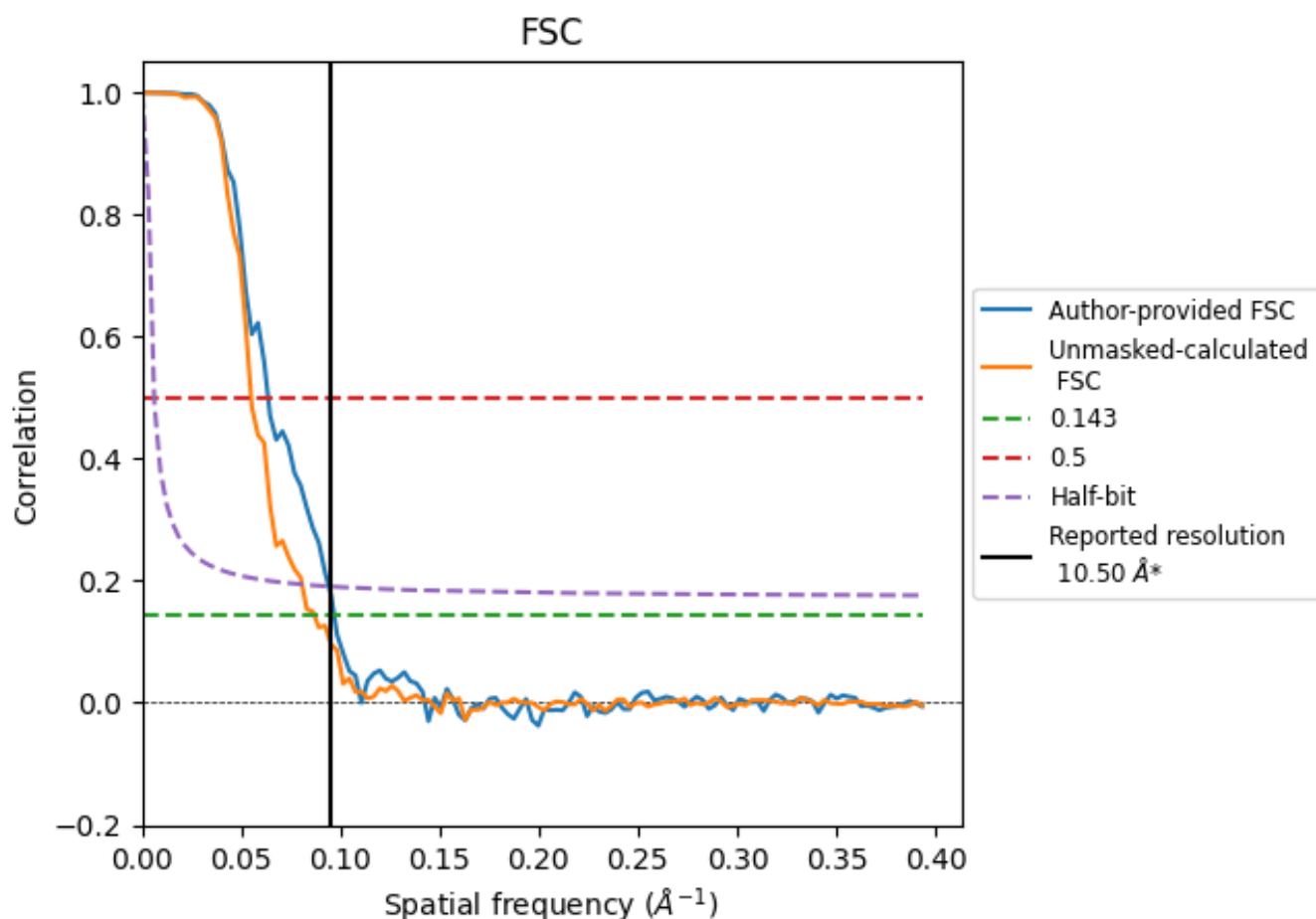


*Reported resolution corresponds to spatial frequency of 0.095 Å⁻¹

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 0.095 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.50	-	-
Author-provided FSC curve	10.32	15.75	10.63
Unmasked-calculated*	11.52	18.18	12.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20864 and PDB model 6USJ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

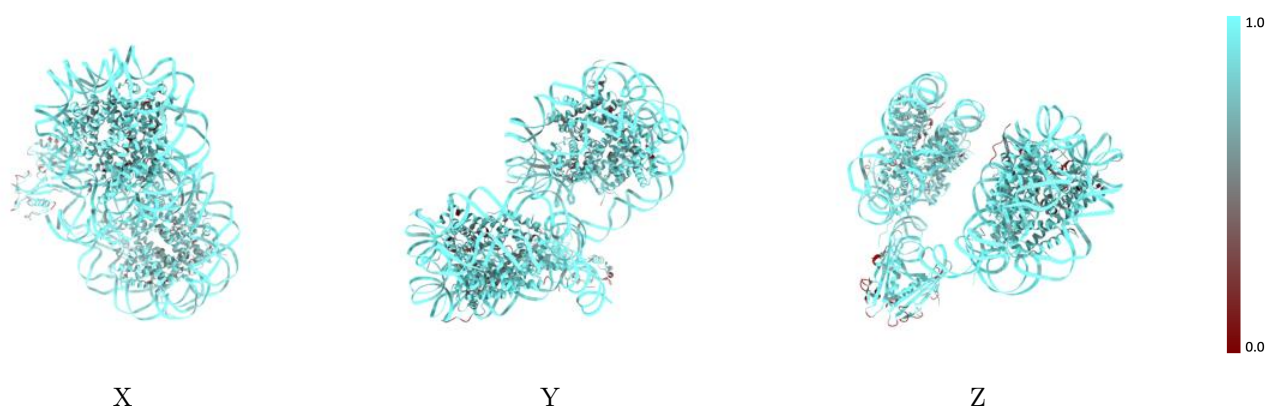
This section was not generated.

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



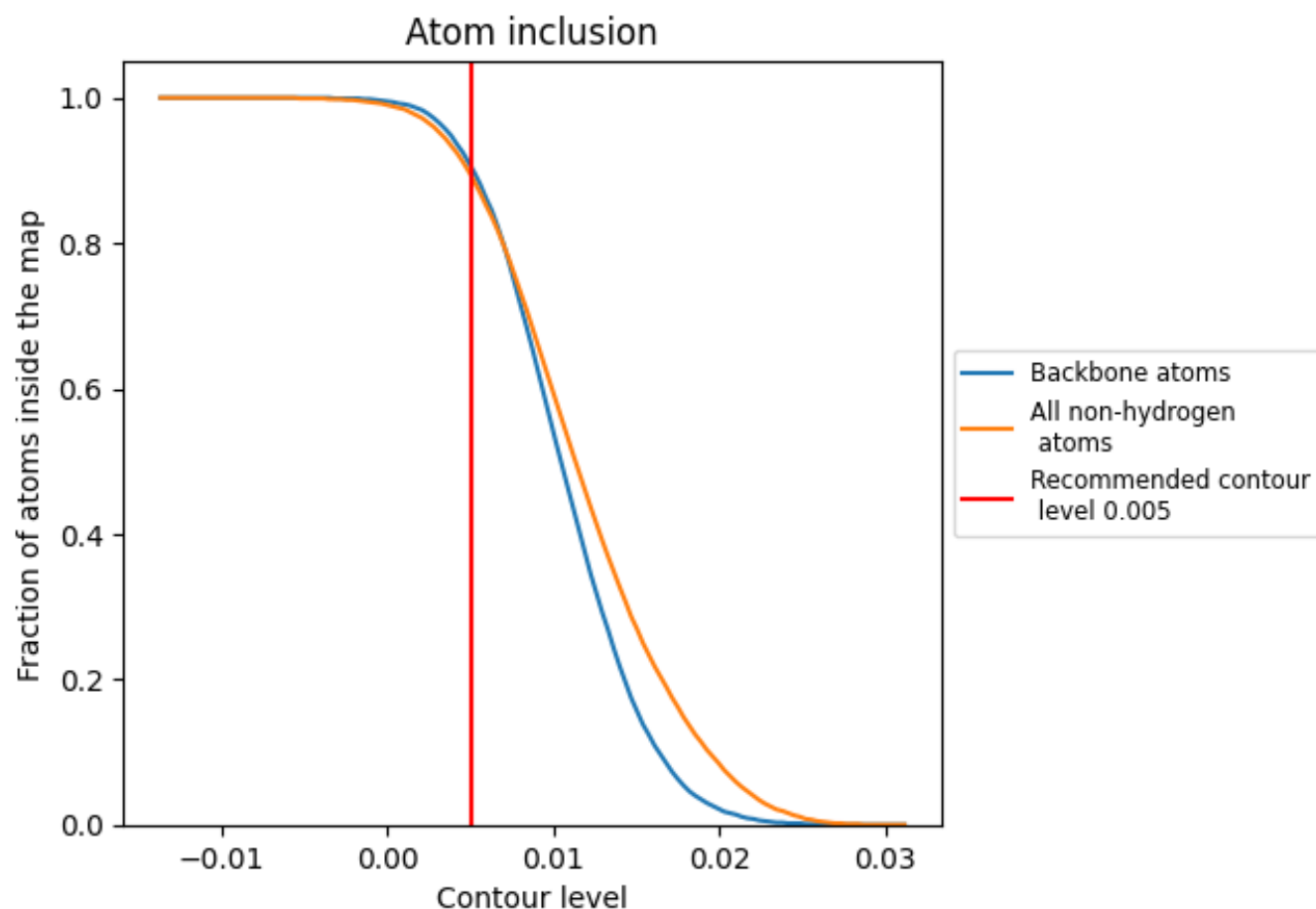
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.0920
A	 0.9120	 0.1080
B	 0.8370	 0.1030
C	 0.8590	 0.0960
D	 0.8250	 0.1000
E	 0.9190	 0.1160
F	 0.8050	 0.0670
G	 0.8190	 0.0760
H	 0.8620	 0.1090
I	 0.9440	 0.1000
J	 0.9400	 0.0970
K	 0.9180	 0.1170
L	 0.8830	 0.0760
M	 0.8020	 0.0390
N	 0.9000	 0.1030
O	 0.9020	 0.0960
P	 0.7730	 0.0750
Q	 0.8780	 0.0670
R	 0.8780	 0.1220
S	 0.9410	 0.0930
T	 0.9250	 0.0930
U	 0.8060	 0.0780
V	 0.7820	 0.0680

