



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:55 PM UTC

PDB ID : 8OFF / pdb_00008off
EMDB ID : EMD-16859
Title : Structure of BARD1 ARD-BRCTs in complex with H2AKc15ub nucleosomes (Map1)
Authors : Foglizzo, M.; Burdett, H.; Wilson, M.D.; Zeqiraj, E.
Deposited on : 2023-03-15
Resolution : 3.40 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

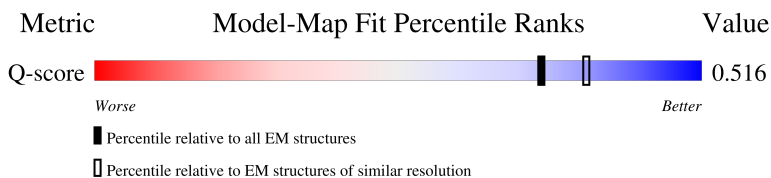
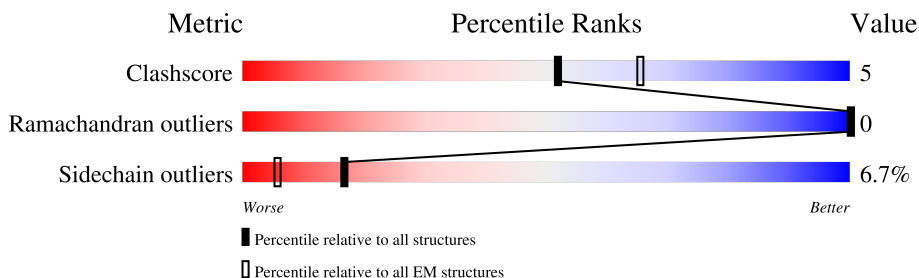
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



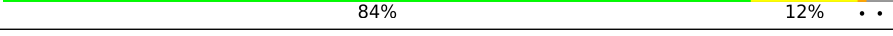
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	350	
1	J	350	
2	Ca	135	
2	Cb	135	

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Mol	Chain	Length	Quality of chain
3	Ba	126	
3	Bb	126	
4	Aa	130	
4	Ab	130	
5	Da	103	
5	Db	103	
6	Ea	773	
6	Eb	773	
7	Fa	76	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14424 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 DNA (142-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	144	Total	C	N	O	P	0	0
			2938	1395	534	865	144		
1	I	145	Total	C	N	O	P	0	0
			2988	1414	560	869	145		

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ca	96	Total	C	N	O	S	0	0
			779	493	150	132	4		
2	Cb	97	Total	C	N	O	S	0	0
			774	492	151	127	4		

- Molecule 3 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ba	92	Total	C	N	O	S	0	0
			701	442	126	131	2		
3	Bb	93	Total	C	N	O	S	0	0
			709	446	128	133	2		

- Molecule 4 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Aa	106	Total	C	N	O	0	0
			774	491	152	131		
4	Ab	107	Total	C	N	O	0	0
			778	495	150	133		

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Da	77	Total	C	N	O	S	0	0
			611	387	118	105	1		
5	Db	84	Total	C	N	O	S	0	0
			662	420	131	110	1		

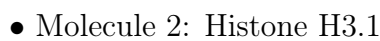
- Molecule 6 is a protein called BRCA1 associated RING domain 1.

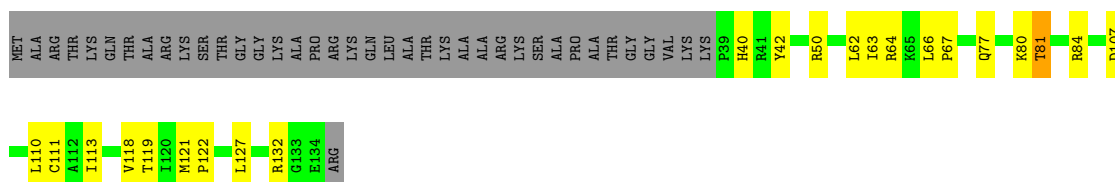
Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ea	121	Total	C	N	O	S	0	0
			822	516	158	147	1		
6	Eb	199	Total	C	N	O	S	1	0
			1363	875	241	242	5		

- Molecule 7 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Fa	74	Total	C	N	O	0	0
			525	338	92	95		

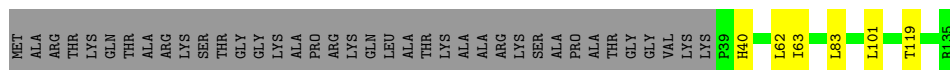
- Molecule 1: DNA (142-MER)





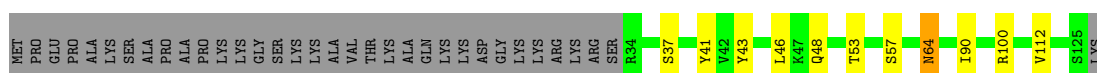
- Molecule 2: Histone H3.1

Chain Cb: 67% 0% 28%



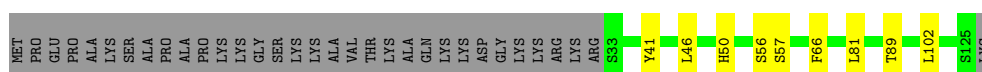
- Molecule 3: Histone H2B type 1-C/E/F/G/I

Chain Ba: 64% 8% 27%



- Molecule 3: Histone H2B type 1-C/E/F/G/I

Chain Bb: 67% 7% 26%



- Molecule 4: Histone H2A type 1

Chain Aa: 75% 7% 18%



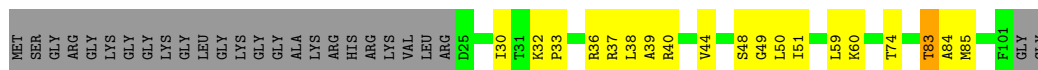
- Molecule 4: Histone H2A type 1

Chain Ab: 73% 9% 18%



- Molecule 5: Histone H4

Chain Da: 56% 17% 25%



- Molecule 5: Histone H4

MET	GLY	ARG	GLY	LYS	GLY	LYS	LEU	GLY	LYS	GLY	ALA	LYS	R18	H19	127	Q28	G29	130	T31	K32	P33	R36	R40	R46	I47	S48	Q49	E53	E54	V58	T81	D86	R93	R96	I97	F101	GLY	GLY
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MET	PRO	GLY	ASN	ARG	GLN	LEU	ARG	VAL	ARG	SER	GLY	ASN	GLU	PRO	PRO	ARG	ALA	ALA	ALA	ALA	HIS	SER	ARG	ALA	ALA	PHE	ASP	ARG	ARG	LEU	LEU	GLU	LYS	LEU	LEU	ARG	CYS	SER	ARG	CYS	THR	ASN	ILE	LEU	LEU	CYS	LEU	GLY	GLY
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CYS	GLU	HIS	ILE	PLE	CYS	SER	ASN	VAL	ASP	CYS	ILE	GLY	THR	GLY	CYS	PRO	THR	PRO	ALA	TRP	ILE	ILE	GLN	ASP	VAL	LYS	ILE	ILE	ASN	ARG	GLN	LEU	ASP	SER	MET	LEU	LEU	LEU	LEU	ASN	LYS	SER	LEU	ASP	LEU	LEU	LEU	LYS	GLU
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ASP	THR	SER	ARG	GLN	ASN	VAL	PHE	ASN	ASP	ALA	GLU	ASN	LYS	LYS	ASN	SER	THR	ILE	LYS	MET	TRP	PHE	PRO	PRO	ARG	SER	LYS	LYS	VAL	VAL	ARG	TYR	VAL	VAL	VAL	THR	THR	LYS	VAL	SER	SER	GLN	VAL	GLN	THR	THR	GLN	PRO	GLN	VAL	VAL	ILE	ASP	ILE	ASP	GLY	ALA	ALA	GLN	GLN	GLN	ALA	ALA	ALA	SER	VAL	TYR	LYS	PHE	VAL	VAL	SER
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THR	SER	PRO	PRO	THR	SER	VAL	PRO	GLU	ARG	ALA	LYS	LYS	ALA	SER	THR	ARG	ARG	SER	ARG	LYS	GLN	LYS	LYS	LYS	THR	LEU	ALA	ALA	GLU	ILE	ASN	GLN	GLU	TRP	TRP	ASN	PHE	GLU	ALA	GLU	LYS	GLU	ASP	GLY	GLY	PRO	ASP	SER	LYS	GLU	LYS	LYS	LEU	VAL	SER	PHE	SER	CYS	SER
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GLN	PRO	VAL	ILE	ALA	SER	GLN	THR	ASN	GLY	GLY	ILE	ASP	LEU	LEU	ALA	SER	ASP	SER	VAL	THR	THR	GLU	SER	GLU	CYS	SER	ARG	SER	LEU	THR	GLU	VAL	GLU	SER	LEU	PRO	LEU	ALA	ALA	GLN	GLN	ILE	GLU	SER	PRO	GLU	GLU	THR	GLY	SER	ASN	ARG	GLU	ASP	ALA	ALA	THR	PRO	GLU	LYS	ASN	ALA
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CYS	VAL	ASP	HIS	LEU	THR	SER	LYS	GLN	PRO	LEU	PRO	SER	GLY	HIS	ASN	GLY	ARG	PRO	GLY	ARG	ARG	SER	SER	SER	PRO	VAL	SER	LYS	ARG	CYS	ARG	SER	SER	SER	ILE	PRO	GLY	THR	SER	GLY	GLN	GLN	MET	LEU	LEU	LEU	PRO	LYS	GLY	SER	SER	PRO	PRO	PRO
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PRO	SER	LYS	ARG	LYS	VAL	GLY	ASP	THR	LEU	ARG	ARG	LYS	ASN	SER	ASN	ILE	SER	ASP	GLU	SER	MET	SER	LEU	SER	PRO	GLY	THR	PRO	PRO	SER	THR	LEU	ASN	SER	PRO	SER	SER	TYR	ARG	MET	MET	PHE	SER	PRO	SER	ALA	VAL	LYS	LEU	SER	PRO	GLY	SER	LEU	THR	ALA	V418	V421
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Amino Acid	Count
H422	1
R423	1
T426	1
L427	1
A431	1
D435	2
D436	2
L437	2
V440	1
L443	1
L444	1
P450	1
N451	1
V452	1
H455	1
H467	1
D468	2
H469	2
L475	1
S485	1
S492	1
G501	1
H502	1
L538	2
LEU	1
LEU	1
LEU	1
PRO	1
GLU	1
GLU	1
GLN	1
ASN	1
GLU	1
SER	1
SER	1
SER	1
THR	1
ARG	1
HIS	1
CYS	1
SER	1
VAL	1
THR	1
ASN	1
THR	1
GLY	1
GLN	1

ARG ASP GLY GLY PRO PRO LEU VAL LEU LEU ILE ILE GLY GLY GLY LEU LEU SER SER SER GLU GLU GLN GLN LYS LYS MET MET LEU LEU SER SER GLU GLU LEU LEU ALA ALA VAL VAL ILE ILE LEU LEU LYS LYS LYS LYS CYS CYS CYS CYS GLU GLU PHE PHE ASP ASP SER SER THR THR THR THR HIS HIS VAL VAL ILE ILE VAL VAL PRO PRO GLY GLY ASP ASP THR THR VAL VAL GLN GLN SER SER THR THR LEU LEU LYS LYS CYS CYS MET MET LEU LEU GLY GLY ILE ILE LEU LEU

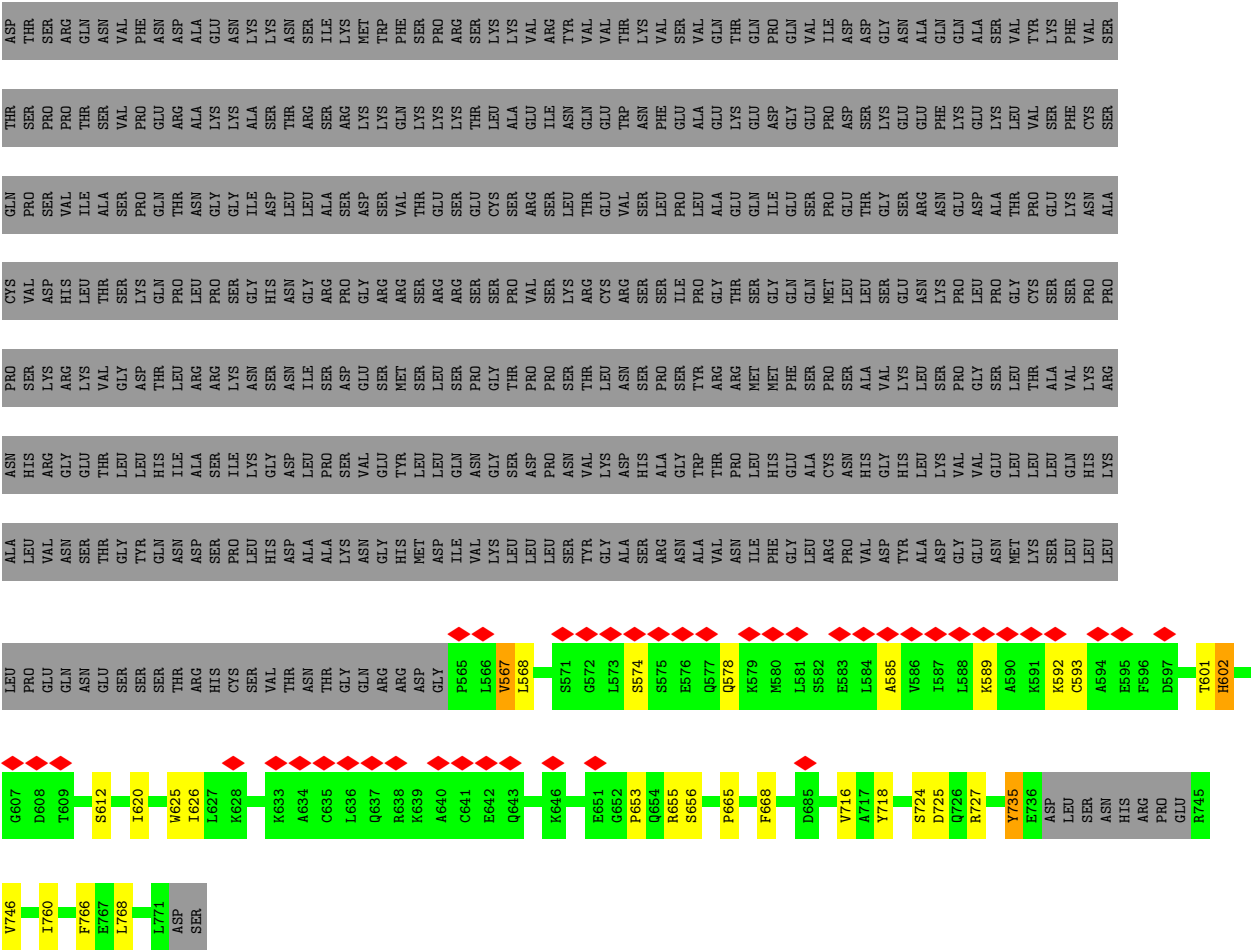
ASN	CYS	GLY	TRP	ILE	LEU	LYS	PHE	GLU	GLU	TRP	GLY	VAL	LYS	ALA	CYS	LEU	GLN	ARG	LYS	ALA	CYS	GLU	GLN	GLU	GLY	LYS	TYR	GLU	ILE	PRO	PRO	GLY	GLY	GLN	ARG	SER	ARG	ARG	LEU	ASN	LYS	LYS	GLU	GLN	LEU	LEU	PRO	PRO	LYS	PHE	PHE	TYR	TYR	GLY	ALA	ALA	PHE	LYS	THR
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HIS	PRO	PRO	LYS	ASP	ASN	LEU	VAL	LYS	LEU	VAL	THR	ALA	ALA	GLY	GLY	GLN	VAL	LEU	SER	ARG	LYS	PRO	PRO	LYS	ASP	SER	ASP	VAL	VAL	THR	THR	GLN	THR	ILE	ILE	ASN	THR	THR	VAL	ALA	ALA	TYR	HIS	ALA	LYS	ASP	ALA	ASP	ASP	GLN	SER	ASP	ARG	ARG	PHE	CYS	THR	GLN	TYR	ILE	ILE	TYR	GLU	ASP	LEU	SER	ASN	HIS
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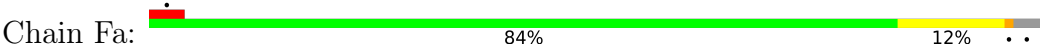
ARG PRO GLU ARG VAL ARG GLN GLY LYS VAL TRP MET ALA PRO SER SER TRP PHE ILE ASP CYS VAL MET SER PHE GLU LEU LEU PRO PRO LEU ASP SER

MET	PRO	GLY	ASN	ARG	GLN	LEU	ARG	VAL	ARG	GLY	SER	ASN	GLU	PRO	ARG	ALA	ALA	ALA	HIS	SER	ARG	ALA	PHE	ASP	LEU	GLU	LYS	LEU	LEU	ARG	CYS	SER	ARG	CYS	THR	ASN	ILE	VAL	CYS	LEU	GLY	TYR
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CYS	GLU	HIS	ILE	PHE	CYS	SER	ASN	CYS	VAL	ASP	SER	CYS	ILE	THR	GLY	CYS	PRO	VAL	CYS	TYR	THR	PRO	ALA	ILE	GLN	ASP	VAL	LYS	ILE	ASN	ARG	GLN	LEU	ASP	SER	MET	ILE	GLN	LEU	CYS	LYS	LEU	ARG	LEU	ASN	HIS	ASP	LYS	LEU	SER	ASP	LEU	LYS	THR
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● Molecule 7: Ubiquitin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	359954	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 ($e^-/\text{\AA}^2$)	36.37	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.258	Depositor
Minimum map value	-2.136	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.435	Depositor
Map size ($\text{\AA}$)	275.2, 275.2, 275.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.34	0/3355	0.40	0/5180
1	J	0.33	0/3292	0.39	0/5075
2	Ca	0.35	0/791	0.47	0/1063
2	Cb	0.34	0/786	0.43	0/1057
3	Ba	0.31	0/712	0.41	0/962
3	Bb	0.33	0/720	0.41	0/972
4	Aa	0.32	0/784	0.39	0/1067
4	Ab	0.31	0/788	0.40	0/1072
5	Da	0.35	0/618	0.44	0/830
5	Db	0.35	0/670	0.43	0/900
6	Ea	0.22	0/840	0.36	0/1156
6	Eb	0.26	0/1399	0.36	0/1918
7	Fa	0.20	0/531	0.32	0/724
All	All	0.32	0/15286	0.40	0/21976

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2988	0	1627	34	0
1	J	2938	0	1617	37	0
2	Ca	779	0	809	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Cb	774	0	803	5	0
3	Ba	701	0	696	5	0
3	Bb	709	0	712	4	0
4	Aa	774	0	797	6	0
4	Ab	778	0	802	8	0
5	Da	611	0	644	10	0
5	Db	662	0	697	9	0
6	Ea	822	0	712	8	0
6	Eb	1363	0	1149	16	0
7	Fa	525	0	516	5	0
All	All	14424	0	11581	140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (140) 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)
6:Eb:601:THR:O	6:Eb:602:HIS:ND1	2.11	0.81
1:J:-1:DG:H2''	1:J:0:DC:H5''	1.65	0.79
1:I:-31:DA:H2''	1:I:-30:DA:H5''	1.66	0.77
3:Ba:37:SER:HB2	3:Ba:64:ASN:HD21	1.61	0.62
5:Db:48:SER:OG	5:Db:49:GLY:N	2.30	0.62
1:I:9:DT:H2''	1:I:10:DG:C8	2.36	0.61
1:J:-54:DA:H2''	1:J:-53:DG:C8	2.36	0.61
1:I:11:DC:H2''	1:I:12:DG:C8	2.36	0.61
6:Eb:574:SER:O	6:Eb:578:GLN:N	2.34	0.60
6:Eb:716:VAL:HG23	6:Eb:727:ARG:HG3	1.82	0.60
3:Bb:46:LEU:HD13	4:Ab:64:LEU:HD13	1.86	0.58
1:J:-35:DA:H2''	1:J:-34:DG:C8	2.39	0.57
1:I:-54:DC:H2''	1:I:-53:DA:C8	2.39	0.57
1:I:0:DG:H2'	1:I:1:DC:C6	2.38	0.57
1:I:-43:DA:H2''	1:I:-42:DG:C8	2.40	0.56
3:Ba:41:TYR:CZ	4:Aa:27:PRO:HG3	2.41	0.56
6:Eb:592:LYS:HD3	6:Eb:593:CYS:H	1.71	0.56
6:Eb:585:ALA:O	6:Eb:589:LYS:N	2.38	0.55
6:Eb:655:ARG:NH1	6:Eb:766:PHE:O	2.38	0.55
1:J:-54:DA:H8	1:J:-54:DA:H5''	1.71	0.54
5:Da:83:THR:OG1	5:Da:84:ALA:N	2.40	0.54
1:J:49:DC:H2''	1:J:50:DA:C8	2.43	0.54
5:Da:48:SER:OG	5:Da:49:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:-70:DG:H2''	1:I:-69:DG:C8	2.43	0.53
3:Ba:100:ARG:HH21	3:Ba:112:VAL:HG21	1.73	0.53
6:Ea:431:ALA:HB1	6:Ea:440:VAL:HG22	1.91	0.53
6:Eb:724:SER:OG	6:Eb:725:ASP:N	2.42	0.53
1:J:24:DA:H2''	1:J:25:DG:C8	2.44	0.53
1:J:-68:DG:H22	1:I:69:DT:H3	1.56	0.53
5:Da:32:LYS:HB3	5:Da:33:PRO:HD3	1.91	0.53
1:J:67:DA:C2	1:I:-66:DG:N2	2.76	0.52
2:Ca:118:VAL:HG13	4:Aa:116:LEU:HD22	1.89	0.52
1:I:58:DC:H2''	1:I:59:DA:H8	1.73	0.52
6:Eb:665:PRO:HG2	6:Eb:718:TYR:HD2	1.75	0.52
1:J:48:DG:OP1	3:Bb:41:TYR:OH	2.28	0.51
1:I:-59:DT:H4'	1:I:-58:DC:OP1	2.10	0.51
1:I:-71:DA:H2''	1:I:-70:DG:C8	2.46	0.51
1:J:-51:DC:H2''	1:J:-50:DC:C5	2.46	0.51
1:J:-18:DC:H2''	1:J:-17:DT:C5	2.46	0.50
1:I:66:DT:H2''	1:I:67:DT:H71	1.92	0.50
1:I:49:DC:H2''	1:I:50:DG:H8	1.77	0.50
1:J:64:DT:H1'	1:J:65:DA:C8	2.47	0.49
1:J:-59:DT:H2''	1:J:-58:DG:H8	1.76	0.49
2:Ca:84:ARG:HG3	5:Db:81:THR:HG22	1.94	0.49
5:Da:59:LEU:HD13	2:Cb:101:LEU:HD11	1.94	0.49
3:Ba:46:LEU:HD13	4:Aa:64:LEU:HD13	1.95	0.49
6:Eb:620:ILE:HD12	6:Eb:653:PRO:HB3	1.95	0.49
2:Ca:40:HIS:HE1	2:Ca:42:TYR:CE2	2.31	0.48
7:Fa:45:PHE:HB2	7:Fa:67:LEU:HD22	1.95	0.48
1:J:-54:DA:H5''	1:J:-54:DA:C8	2.48	0.48
2:Ca:80:LYS:HG2	2:Ca:81:THR:H	1.78	0.48
1:J:-18:DC:H2''	1:J:-17:DT:C6	2.49	0.47
3:Bb:56:SER:OG	3:Bb:57:SER:N	2.46	0.47
6:Eb:625:TRP:O	6:Eb:626:ILE:HD13	2.13	0.47
1:I:2:DG:H5'	1:I:2:DG:H8	1.80	0.47
1:J:-23:DC:H2''	1:J:-22:DA:H8	1.80	0.47
5:Da:85:MET:HA	5:Da:85:MET:HE2	1.96	0.47
1:J:5:DC:H2''	1:J:6:DG:C8	2.50	0.47
6:Ea:421:ASN:OD1	6:Ea:422:HIS:N	2.37	0.47
1:I:-13:DA:H2''	1:I:-12:DA:C8	2.50	0.47
6:Eb:668:PHE:HE1	6:Eb:768:LEU:HD21	1.80	0.46
1:I:-59:DT:H2''	1:I:-58:DC:O5'	2.15	0.46
1:I:49:DC:H2''	1:I:50:DG:C8	2.51	0.46
1:I:-62:DA:C8	1:I:-61:DT:H72	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:DG:H5'	1:I:2:DG:C8	2.51	0.46
2:Ca:64:ARG:O	2:Ca:67:PRO:HD2	2.15	0.45
5:Db:86:ASP:N	5:Db:86:ASP:OD1	2.48	0.45
3:Bb:66:PHE:HE1	4:Ab:98:LEU:HD11	1.81	0.45
1:J:46:DA:N6	1:I:47:DC:H41	2.15	0.45
1:J:67:DA:N3	1:I:66:DG:N2	2.64	0.45
6:Eb:735:TYR:H	6:Eb:735:TYR:HD1	1.64	0.45
1:J:-49:DG:H1'	1:J:-48:DC:O4'	2.16	0.45
1:J:-4:DC:H2''	1:J:-3:DG:C8	2.52	0.45
6:Eb:760:ILE:HD12	6:Eb:760:ILE:HA	1.84	0.45
6:Eb:612:SER:O	6:Eb:612:SER:OG	2.28	0.45
1:I:-37:DG:H2''	1:I:-36:DG:C8	2.51	0.45
2:Ca:121:MET:HB3	2:Ca:122:PRO:HD2	1.98	0.45
6:Ea:467:HIS:HB3	6:Ea:469:HIS:HE1	1.82	0.45
7:Fa:43:LEU:O	7:Fa:44:ILE:HD13	2.17	0.45
6:Eb:567:VAL:HG12	6:Eb:568:LEU:H	1.82	0.45
5:Db:36:ARG:O	5:Db:40:ARG:HG2	2.18	0.44
5:Db:54:GLU:O	5:Db:58:VAL:HG23	2.17	0.44
1:J:-40:DG:H2'	1:J:-39:DT:C6	2.53	0.44
2:Ca:107:ASP:N	2:Ca:107:ASP:OD1	2.49	0.44
1:I:-63:DT:H2'	1:I:-62:DA:C8	2.52	0.44
1:I:-46:DT:H2''	1:I:-45:DG:C8	2.53	0.44
5:Da:33:PRO:O	5:Da:37:ARG:HG3	2.17	0.44
1:I:-37:DG:H2''	1:I:-36:DG:N7	2.33	0.44
7:Fa:50:LEU:HD22	7:Fa:59:TYR:CE1	2.53	0.43
1:J:-31:DA:H5''	1:J:-31:DA:H8	1.83	0.43
1:I:65:DA:H1'	1:I:66:DT:C2	2.53	0.43
6:Eb:665:PRO:HG2	6:Eb:718:TYR:CD2	2.53	0.43
1:I:-13:DA:H2''	1:I:-12:DA:H8	1.83	0.43
1:J:-49:DG:C8	1:J:-48:DC:C4	3.06	0.43
1:I:32:DG:H2''	1:I:33:DT:H5''	1.99	0.43
1:J:-54:DA:OP2	3:Ba:57:SER:HB3	2.19	0.42
1:J:-33:DA:H5'	1:J:-33:DA:C8	2.54	0.42
1:J:46:DA:H61	1:I:47:DC:H41	1.65	0.42
4:Ab:52:LEU:HD12	4:Ab:52:LEU:HA	1.83	0.42
7:Fa:21:ASP:OD2	7:Fa:21:ASP:N	2.51	0.42
1:I:58:DC:H2''	1:I:59:DA:C8	2.53	0.42
1:I:-28:DC:H2''	1:I:-27:DC:H6	1.82	0.42
5:Da:30:ILE:HD12	2:Cb:63:ILE:HD13	2.01	0.42
1:J:-15:DA:H2''	1:J:-14:DA:C8	2.54	0.42
2:Ca:110:LEU:HD23	2:Ca:110:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Aa:35:LEU:HD23	4:Aa:35:LEU:HA	1.92	0.42
4:Ab:35:LEU:HD23	4:Ab:35:LEU:HA	1.87	0.42
5:Db:32:LYS:HB3	5:Db:33:PRO:HD3	2.01	0.42
1:J:-59:DT:H2''	1:J:-58:DG:C8	2.53	0.42
4:Ab:64:LEU:HD23	4:Ab:64:LEU:HA	1.88	0.42
1:J:30:DT:H2'	1:J:31:DT:H71	2.01	0.42
1:J:-68:DG:N2	1:I:69:DT:H3	2.17	0.42
4:Ab:115:VAL:HG12	4:Ab:115:VAL:O	2.19	0.42
1:J:57:DA:H2''	1:J:58:DG:C8	2.55	0.42
2:Ca:50:ARG:HE	2:Ca:50:ARG:HB2	1.66	0.42
1:J:0:DC:H2'	1:J:1:DT:H71	2.02	0.41
1:J:2:DG:H2'	1:J:3:DT:H71	2.03	0.41
4:Aa:17:THR:HG23	4:Aa:20:SER:HB3	2.03	0.41
2:Cb:83:LEU:HD23	2:Cb:83:LEU:HA	1.82	0.41
5:Db:53:GLU:OE2	5:Db:53:GLU:N	2.53	0.41
4:Ab:32:HIS:HE2	4:Ab:36:ARG:NH1	2.19	0.41
1:J:-50:DC:H6	1:J:-50:DC:H2'	1.64	0.41
5:Da:39:ALA:HB1	5:Da:44:VAL:HG21	2.02	0.41
4:Ab:109:LEU:HD23	4:Ab:109:LEU:HA	1.96	0.41
2:Cb:101:LEU:HD23	2:Cb:101:LEU:HA	1.95	0.41
6:Ea:423:ARG:O	6:Ea:455:HIS:HD2	2.04	0.41
6:Ea:443:LEU:HD12	6:Ea:443:LEU:HA	1.91	0.41
5:Db:27:ILE:HD12	5:Db:27:ILE:HA	1.93	0.41
6:Ea:450:PRO:O	6:Ea:451:ASN:ND2	2.51	0.41
6:Ea:501:GLY:O	6:Ea:502:HIS:ND1	2.54	0.41
1:J:-52:DG:C5	1:J:-51:DC:C4	3.09	0.41
5:Da:36:ARG:O	5:Da:40:ARG:HG2	2.21	0.41
6:Ea:444:LEU:HD22	6:Ea:444:LEU:HA	1.95	0.41
1:I:61:DC:H2''	1:I:62:DG:C8	2.56	0.41
2:Ca:111:CYS:SG	2:Ca:127:LEU:HD23	2.61	0.40
4:Aa:64:LEU:HD23	4:Aa:64:LEU:HA	1.85	0.40
1:J:-43:DT:C2'	1:J:-42:DT:H71	2.51	0.40
7:Fa:56:LEU:HD12	7:Fa:56:LEU:HA	1.92	0.40
2:Ca:119:THR:HG22	5:Db:46:ARG:HD3	2.03	0.40
5:Da:38:LEU:HD23	2:Cb:62:LEU:HD12	2.01	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	
2	Ca	94/135 (70%)	87 (93%)	7 (7%)	0	100	100
2	Cb	95/135 (70%)	89 (94%)	6 (6%)	0	100	100
3	Ba	90/126 (71%)	83 (92%)	7 (8%)	0	100	100
3	Bb	91/126 (72%)	83 (91%)	8 (9%)	0	100	100
4	Aa	104/130 (80%)	95 (91%)	9 (9%)	0	100	100
4	Ab	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
5	Da	75/103 (73%)	66 (88%)	9 (12%)	0	100	100
5	Db	82/103 (80%)	75 (92%)	7 (8%)	0	100	100
6	Ea	119/773 (15%)	113 (95%)	6 (5%)	0	100	100
6	Eb	196/773 (25%)	169 (86%)	27 (14%)	0	100	100
7	Fa	72/76 (95%)	64 (89%)	8 (11%)	0	100	100
All	All	1123/2610 (43%)	1025 (91%)	98 (9%)	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	
2	Ca	81/111 (73%)	74 (91%)	7 (9%)	10	33
2	Cb	78/111 (70%)	76 (97%)	2 (3%)	40	61
3	Ba	73/106 (69%)	68 (93%)	5 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Bb	75/106 (71%)	71 (95%)	4 (5%)	20	47
4	Aa	72/99 (73%)	69 (96%)	3 (4%)	26	52
4	Ab	72/99 (73%)	68 (94%)	4 (6%)	19	46
5	Da	62/79 (78%)	57 (92%)	5 (8%)	11	36
5	Db	66/79 (84%)	57 (86%)	9 (14%)	3	15
6	Ea	68/685 (10%)	61 (90%)	7 (10%)	7	24
6	Eb	107/685 (16%)	102 (95%)	5 (5%)	23	50
7	Fa	50/68 (74%)	47 (94%)	3 (6%)	17	43
All	All	804/2228 (36%)	750 (93%)	54 (7%)	17	41

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Ca	62	LEU
2	Ca	63	ILE
2	Ca	66	LEU
2	Ca	77	GLN
2	Ca	81	THR
2	Ca	113	ILE
2	Ca	132	ARG
3	Ba	43	TYR
3	Ba	48	GLN
3	Ba	53	THR
3	Ba	64	ASN
3	Ba	90	ILE
4	Aa	50	VAL
4	Aa	63	ILE
4	Aa	66	LEU
3	Bb	50	HIS
3	Bb	81	LEU
3	Bb	89	THR
3	Bb	102	LEU
5	Da	50	LEU
5	Da	51	ILE
5	Da	60	LYS
5	Da	74	THR
5	Da	83	THR
4	Ab	60	THR
4	Ab	80	ILE

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Mol	Chain	Res	Type
4	Ab	94	LEU
4	Ab	103	ILE
2	Cb	40	HIS
2	Cb	119	THR
5	Db	19	HIS
5	Db	28	GLN
5	Db	30	ILE
5	Db	31	THR
5	Db	36	ARG
5	Db	86	ASP
5	Db	93	ARG
5	Db	96	ARG
5	Db	97	THR
6	Ea	426	THR
6	Ea	427	LEU
6	Ea	444	LEU
6	Ea	452	VAL
6	Ea	475	LEU
6	Ea	485	SER
6	Ea	492	SER
7	Fa	3	ILE
7	Fa	21	ASP
7	Fa	36	ILE
6	Eb	567	VAL
6	Eb	602	HIS
6	Eb	656	SER
6	Eb	735	TYR
6	Eb	746	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ca	40	HIS
2	Ca	114	HIS
3	Ba	64	ASN
4	Aa	39	ASN
4	Aa	85	GLN
6	Ea	455	HIS
6	Ea	462	HIS
6	Ea	469	HIS
6	Ea	484	ASN
6	Ea	500	ASN

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Mol	Chain	Res	Type
7	Fa	41	GLN
6	Eb	697	GLN
6	Eb	731	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

There are no ligands in this entry.

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.

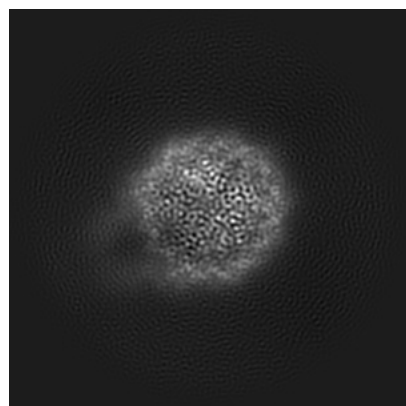
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16859. These allow visual inspection of the internal detail of the map and identification of artifacts.

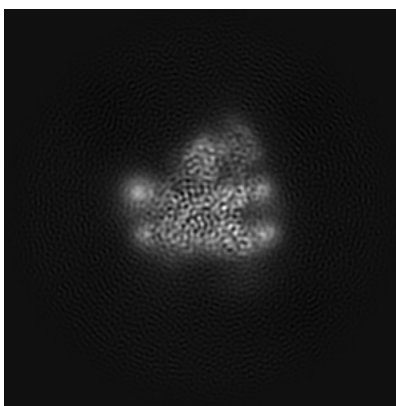
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

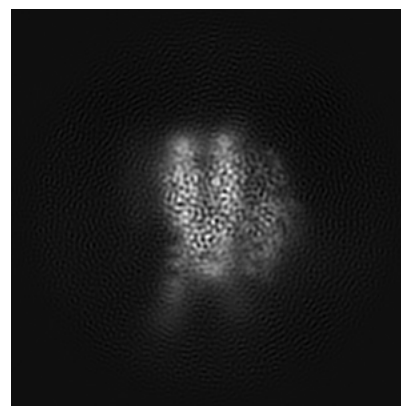
6.1.1 Primary map



X

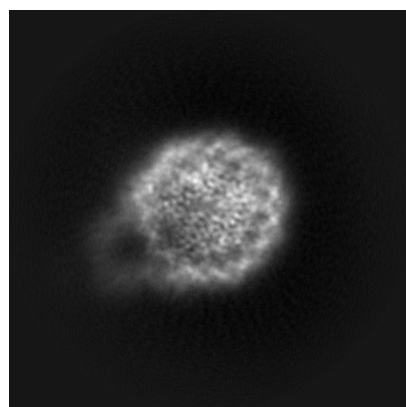


Y

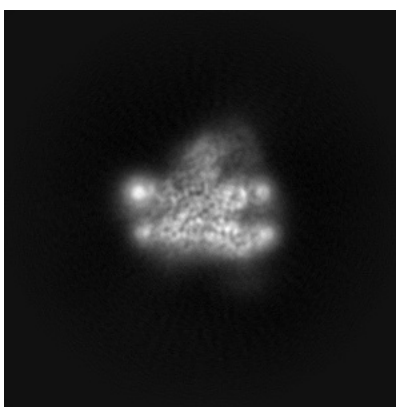


Z

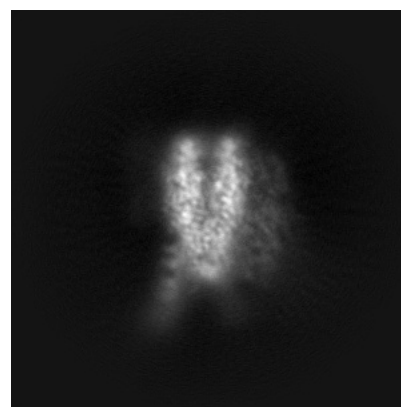
6.1.2 Raw map



X



Y

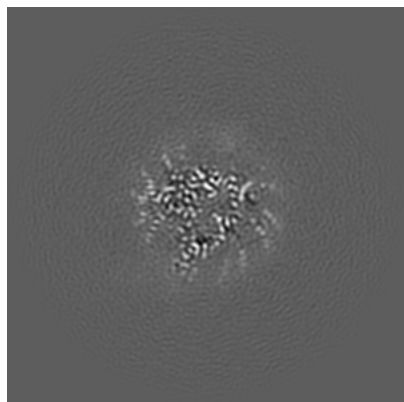


Z

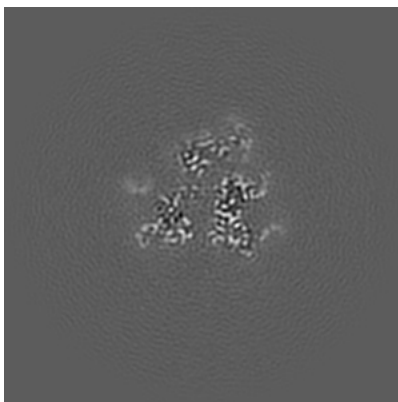
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

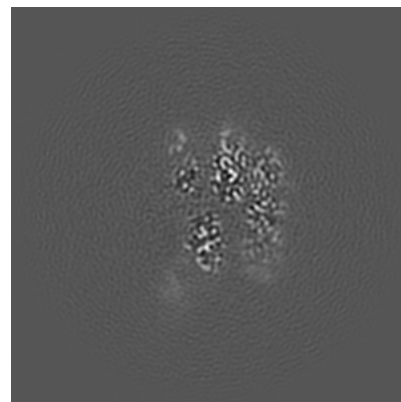
6.2.1 Primary map



X Index: 160

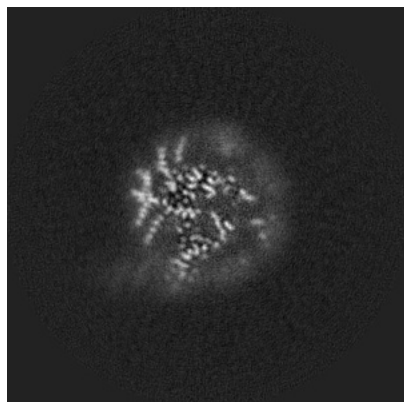


Y Index: 160

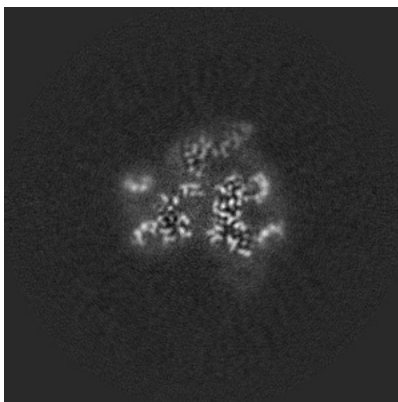


Z Index: 160

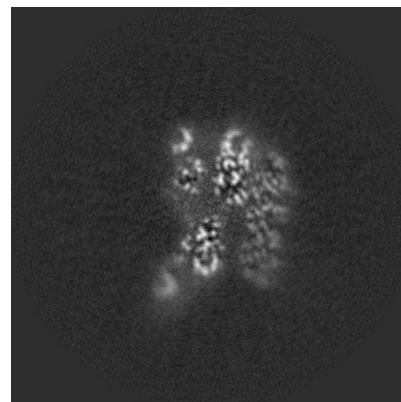
6.2.2 Raw map



X Index: 160



Y Index: 160

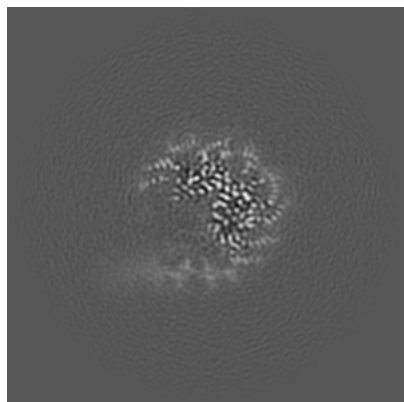


Z Index: 160

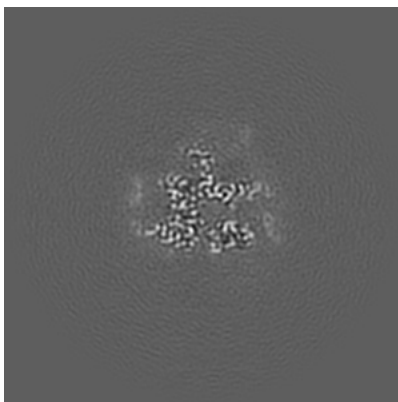
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

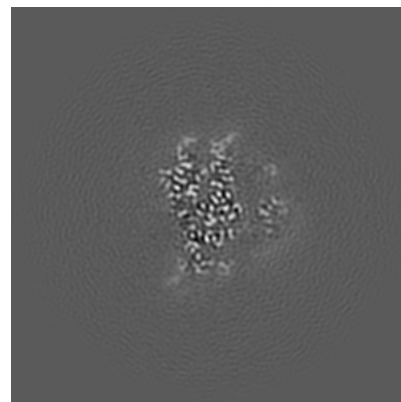
6.3.1 Primary map



X Index: 173

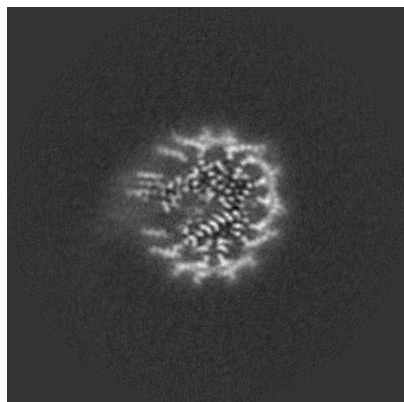


Y Index: 171

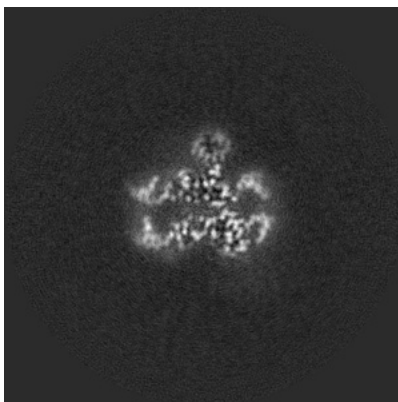


Z Index: 177

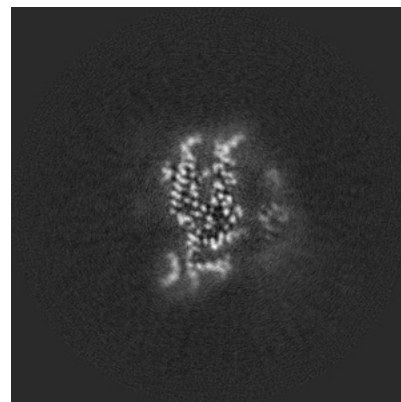
6.3.2 Raw map



X Index: 141



Y Index: 186

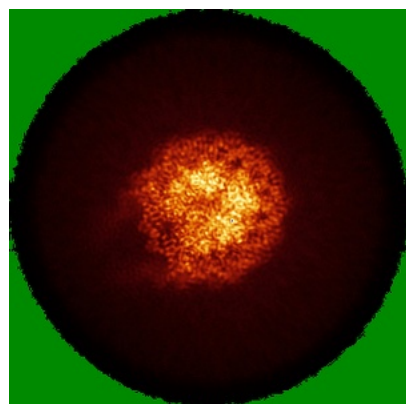


Z Index: 178

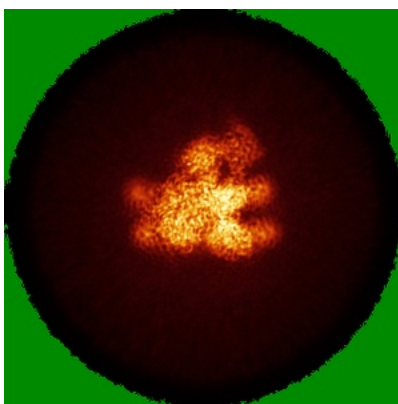
The images above show the largest variance slices of the map in three orthogonal directions.

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

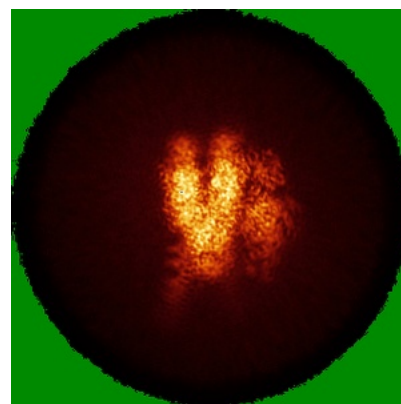
6.4.1 Primary map



X

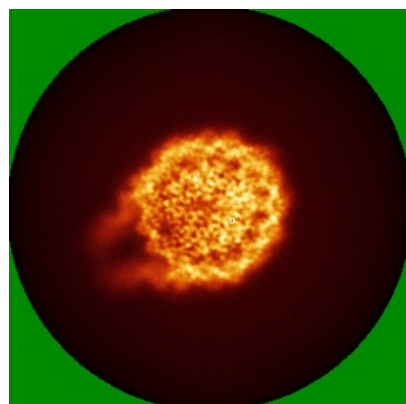


Y

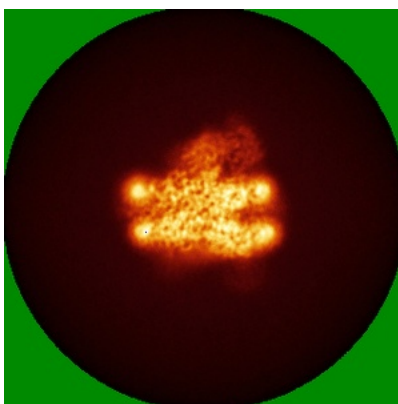


Z

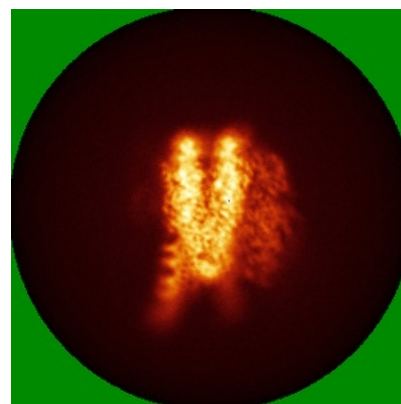
6.4.2 Raw map



X



Y

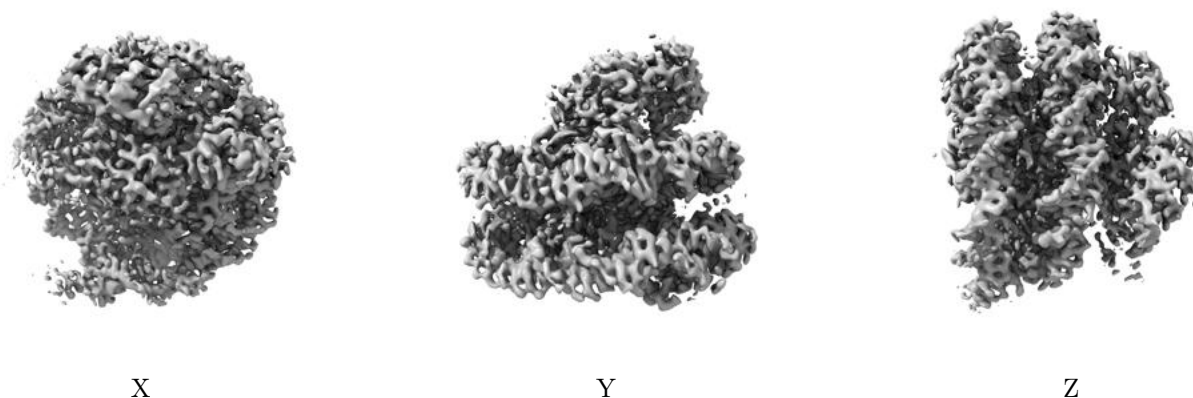


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.435. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

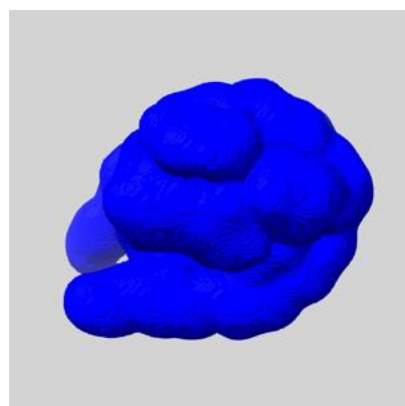
6.6 Mask visualisation [i](#)

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

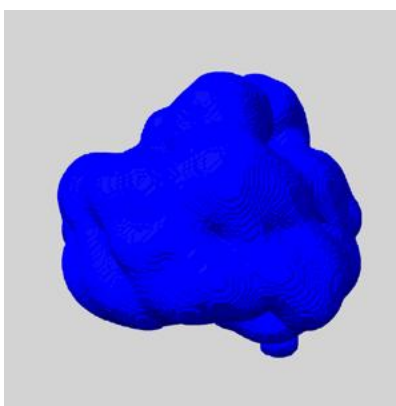
A mask typically either:

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

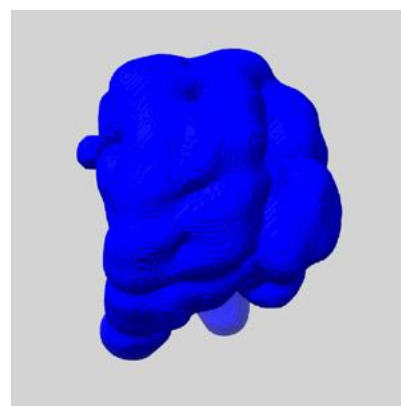
6.6.1 emd_16859_msk_1.map [i](#)



X



Y

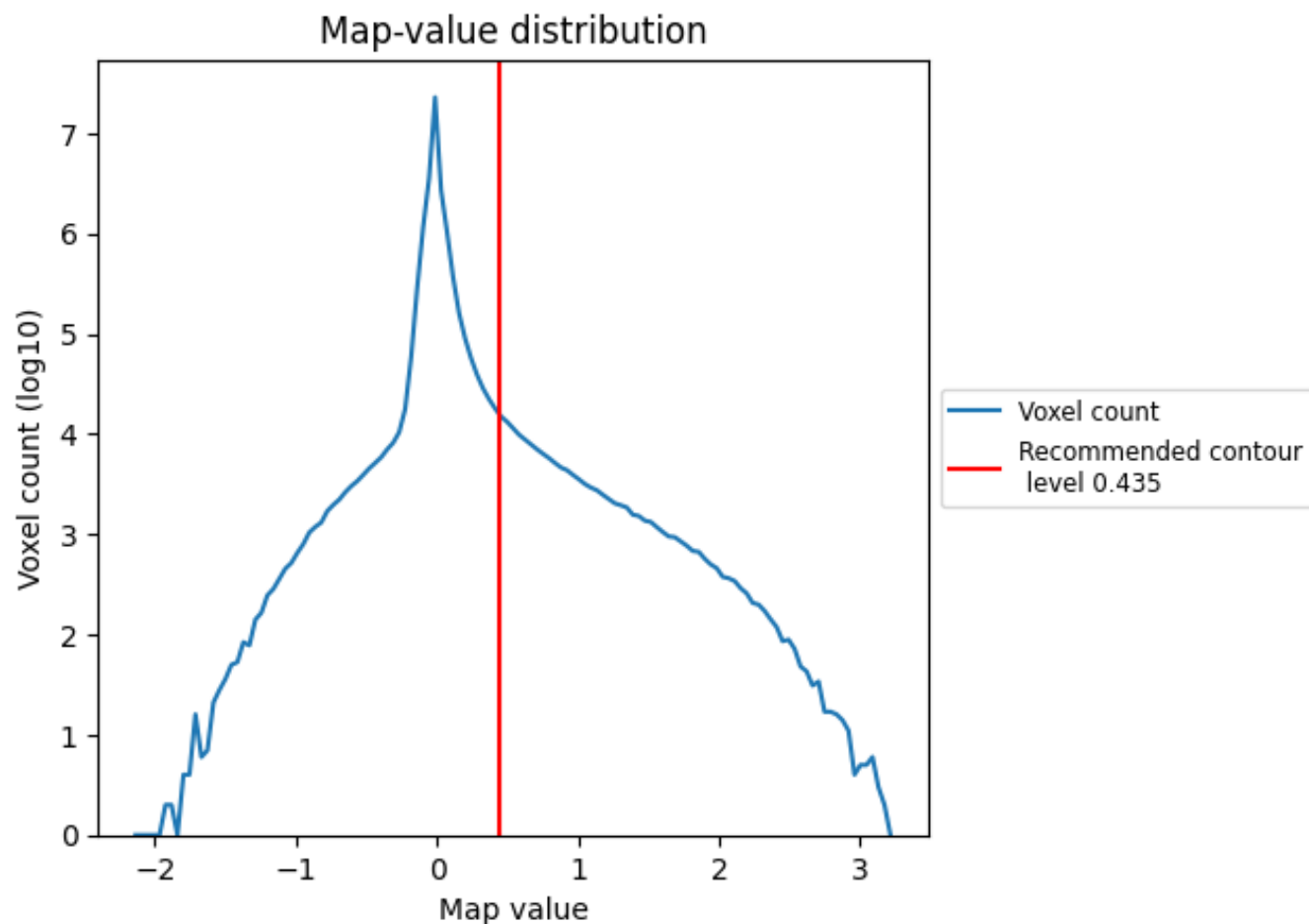


Z

7 Map analysis [i](#)

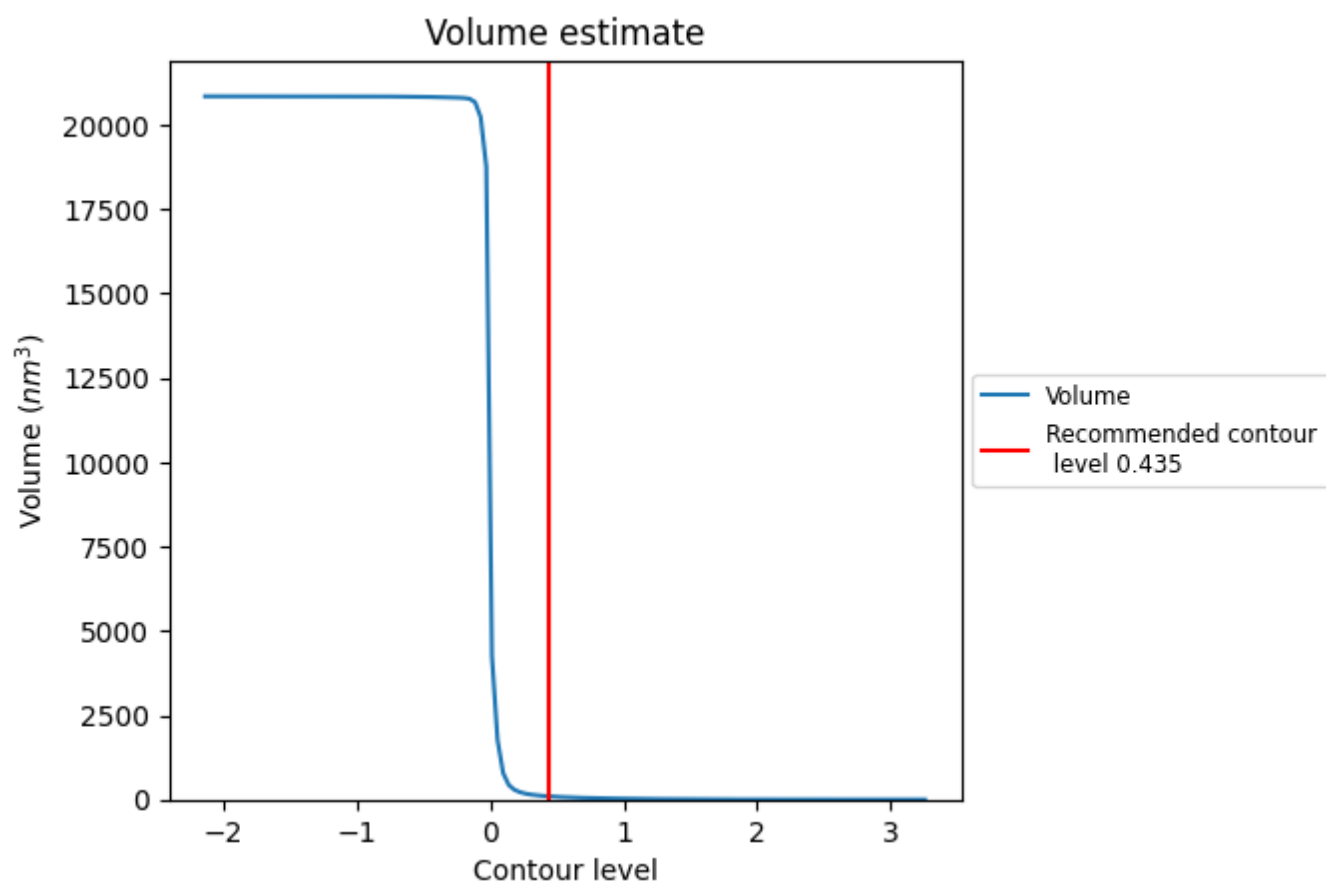
This section contains the results of statistical analysis of the map.

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.

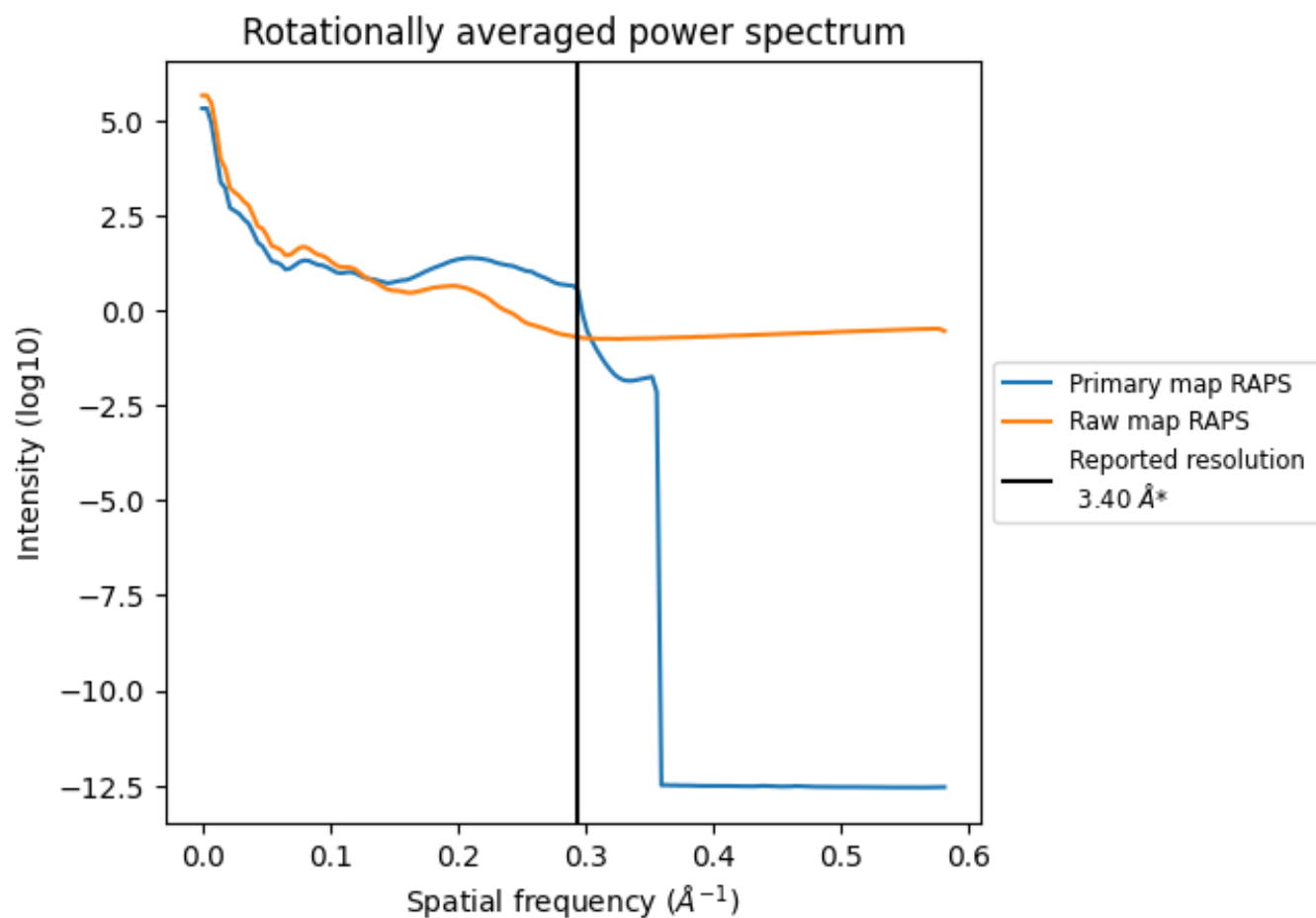
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm³; this corresponds to an approximate mass of 87 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 ⓘ

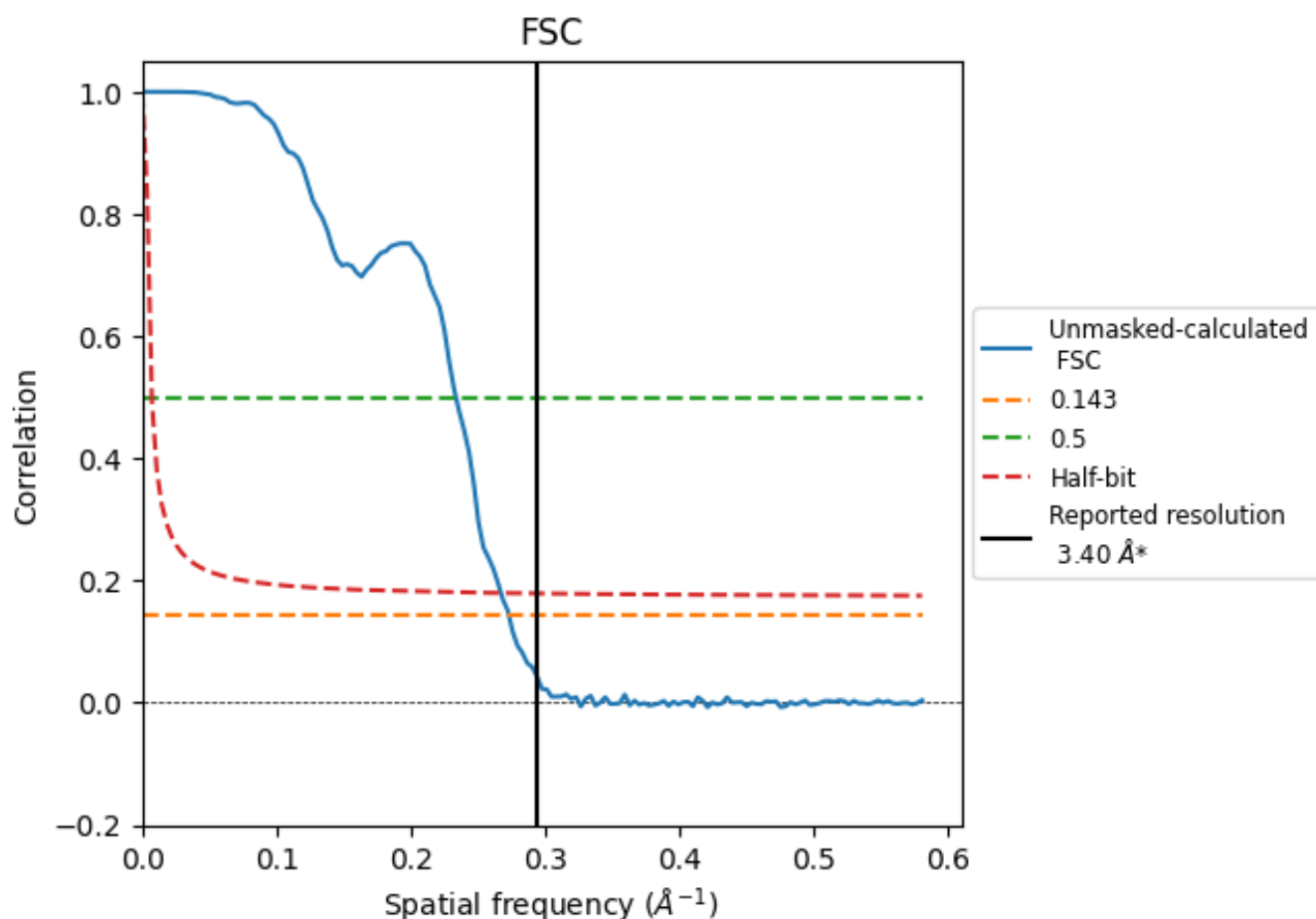


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

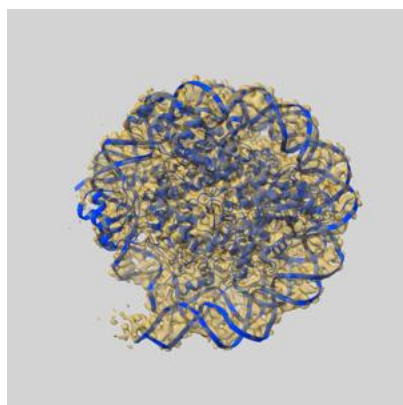
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.28	3.74

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

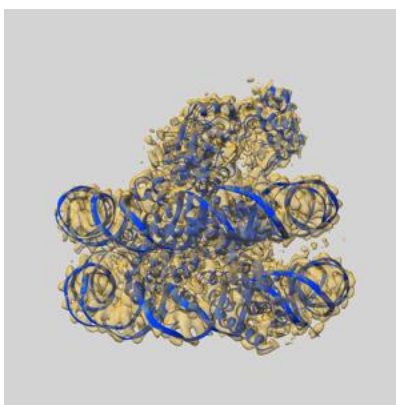
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16859 and PDB model 8OFF. Per-residue inclusion information can be found in section 3 on page 6.

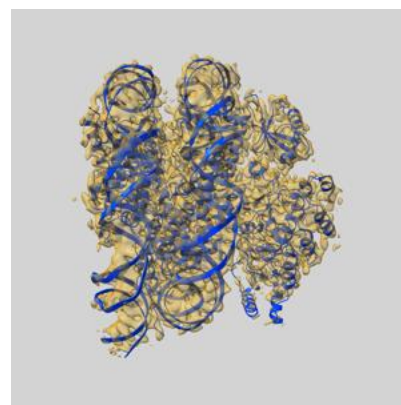
9.1 Map-model overlay [i](#)



X



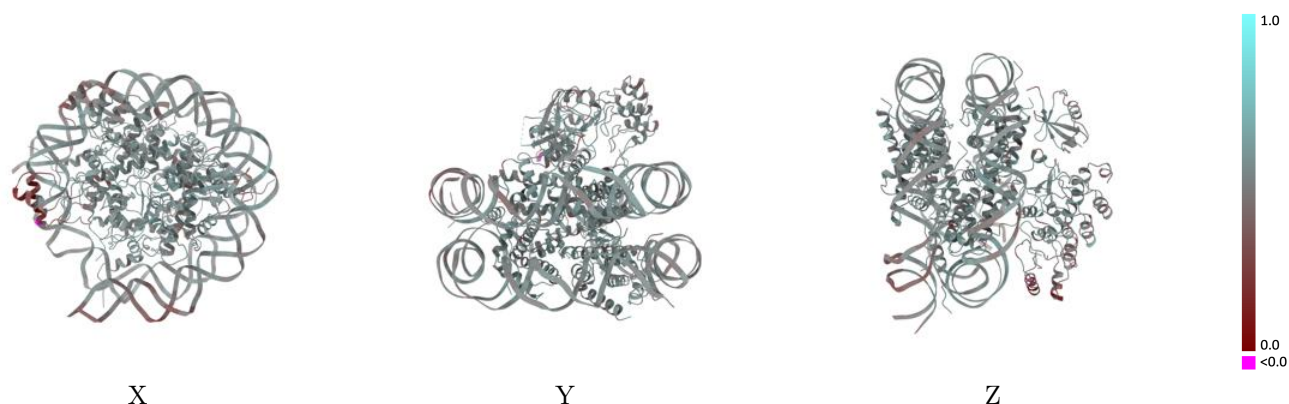
Y



Z

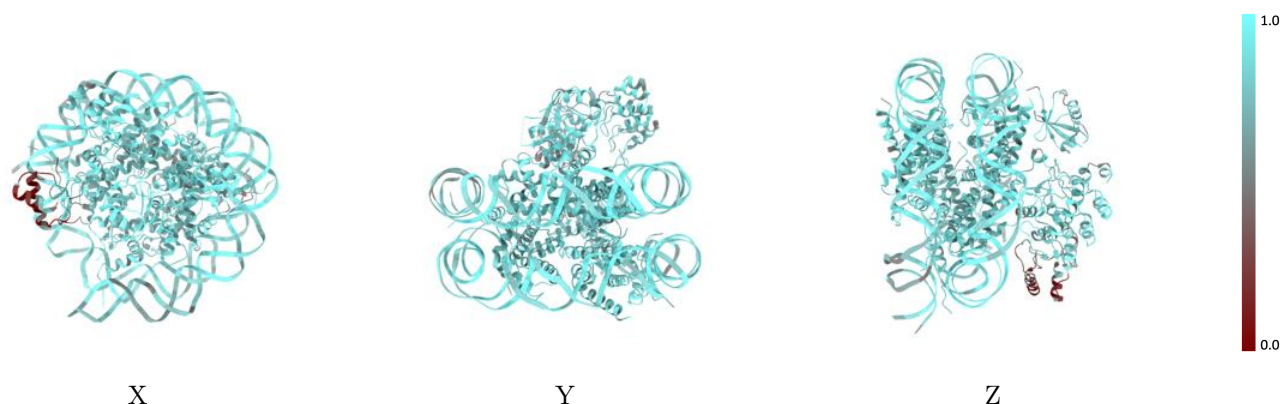
The images above show the 3D surface view of the map at the recommended contour level 0.435 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



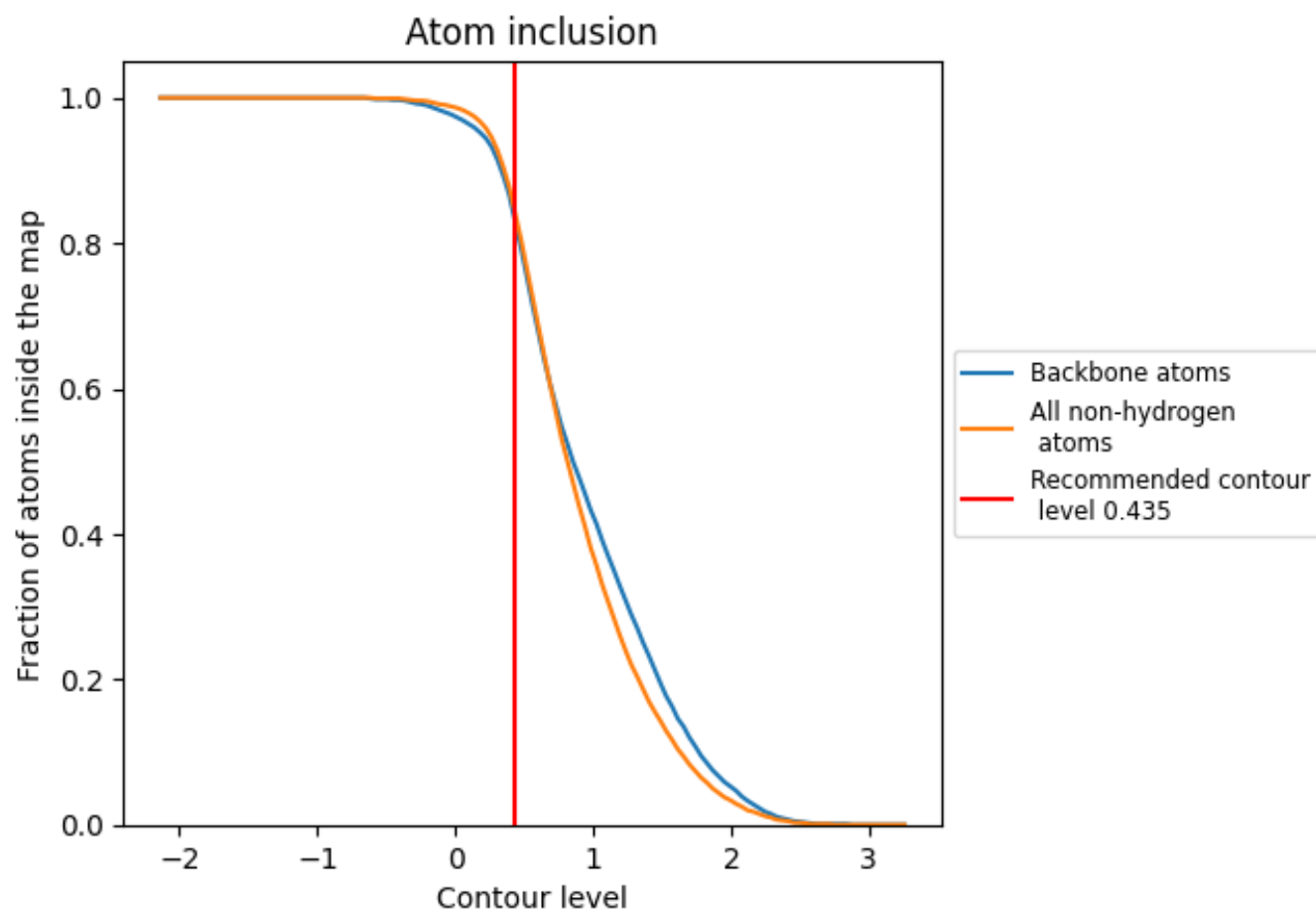
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.435).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.435) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.5160
Aa	 0.8850	 0.5500
Ab	 0.8800	 0.5520
Ba	 0.8610	 0.5260
Bb	 0.8790	 0.5350
Ca	 0.8750	 0.5370
Cb	 0.8790	 0.5400
Da	 0.8760	 0.5450
Db	 0.8850	 0.5530
Ea	 0.8350	 0.5070
Eb	 0.7240	 0.4930
Fa	 0.7830	 0.5090
I	 0.8410	 0.4970
J	 0.8390	 0.4990

