



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:13 PM UTC

PDB ID : 8HXB / pdb_00008hxb
EMDB ID : EMD-35075
Title : Cryo-EM structure of MPXV M2 hexamer in complex with human B7.2
Authors : Wang, Y.; Yang, S.; Zhao, H.; Deng, Z.
Deposited on : 2023-01-04
Resolution : 2.70 Å(reported)

This is a wwPDB EM Validation Summary 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:

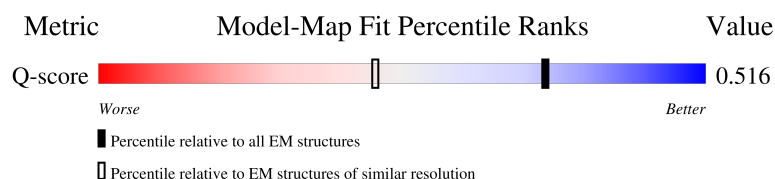
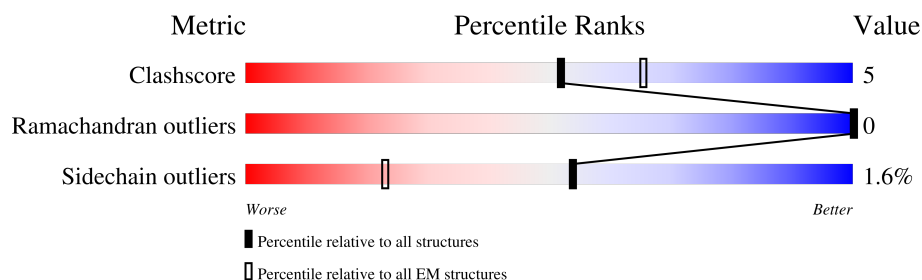
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.70 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	10327 (2.20 - 3.20)

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	A	203	
1	B	203	
1	C	203	
1	D	203	

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Mol	Chain	Length	Quality of chain
1	E	203	81%17%
1	F	203	84%14%
2	G	213	45%5%50%
2	H	213	45%5%50%
2	I	213	45%5%50%
2	J	213	45%5%50%
2	K	213	44%6%50%
2	L	213	44%6%50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14892 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 protein called NFkB inhibitor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	201	Total	C	N	O	S	0	0
			1610	1011	268	316	15		
1	B	201	Total	C	N	O	S	0	0
			1610	1011	268	316	15		
1	C	201	Total	C	N	O	S	0	0
			1610	1011	268	316	15		
1	D	201	Total	C	N	O	S	0	0
			1610	1011	268	316	15		
1	E	201	Total	C	N	O	S	0	0
			1610	1011	268	316	15		
1	F	201	Total	C	N	O	S	0	0
			1610	1011	268	316	15		

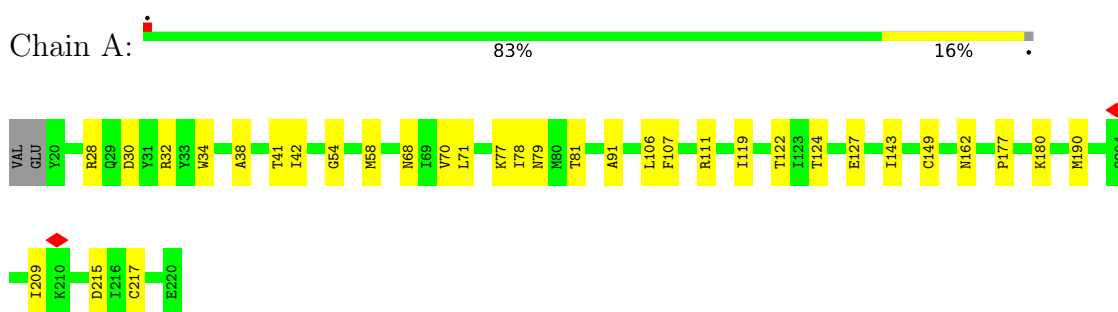
- Molecule 2 is a protein called T-lymphocyte activation antigen CD86.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	106	Total	C	N	O	S	0	0
			872	552	151	164	5		
2	H	106	Total	C	N	O	S	0	0
			872	552	151	164	5		
2	I	106	Total	C	N	O	S	0	0
			872	552	151	164	5		
2	J	106	Total	C	N	O	S	0	0
			872	552	151	164	5		
2	K	106	Total	C	N	O	S	0	0
			872	552	151	164	5		
2	L	106	Total	C	N	O	S	0	0
			872	552	151	164	5		

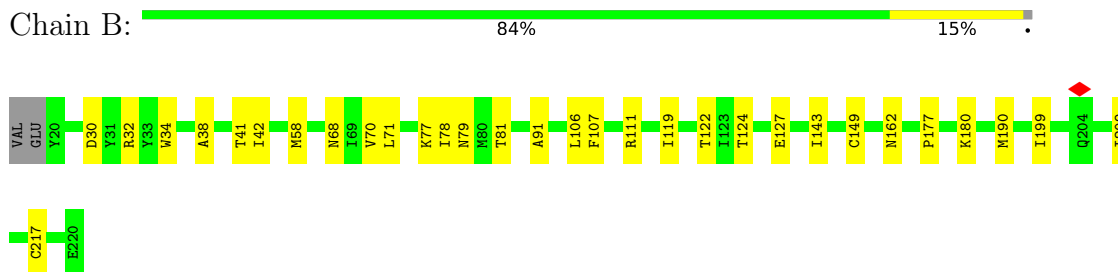
3 Residue-property plots

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

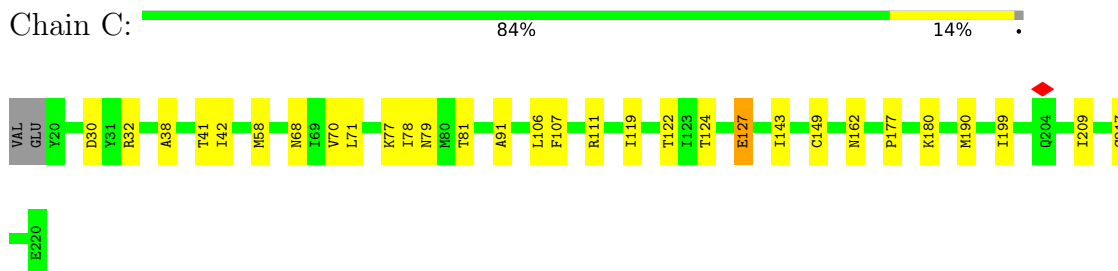
• Molecule 1: NFkB inhibitor



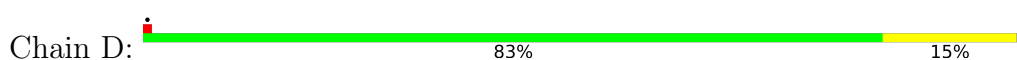
• Molecule 1: NFkB inhibitor

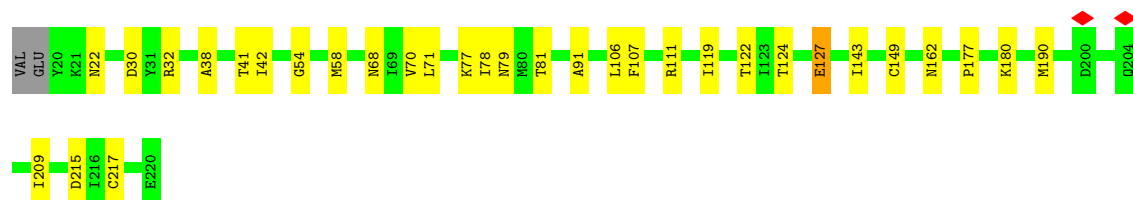


• Molecule 1: NFkB inhibitor

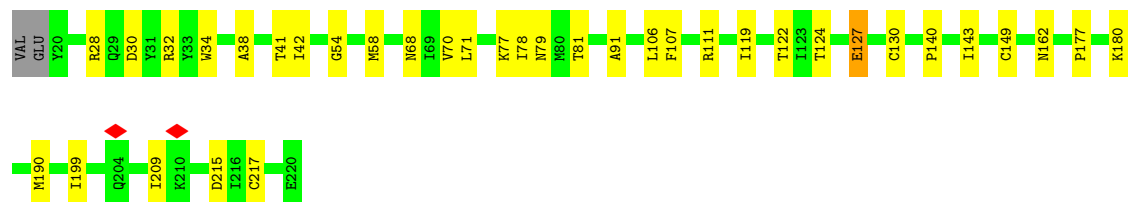
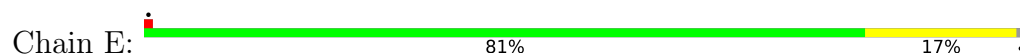


• Molecule 1: NFkB inhibitor

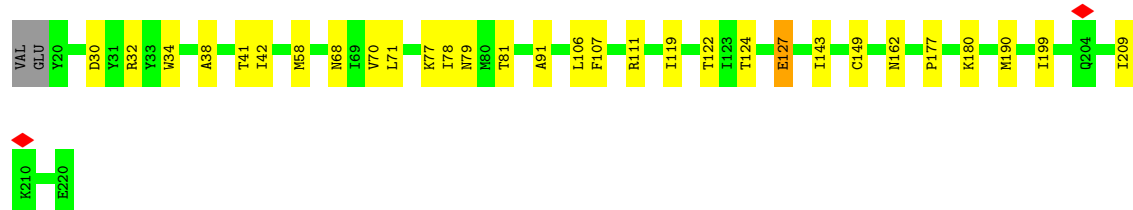
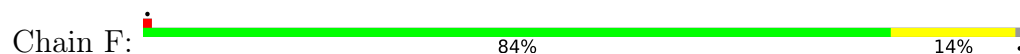




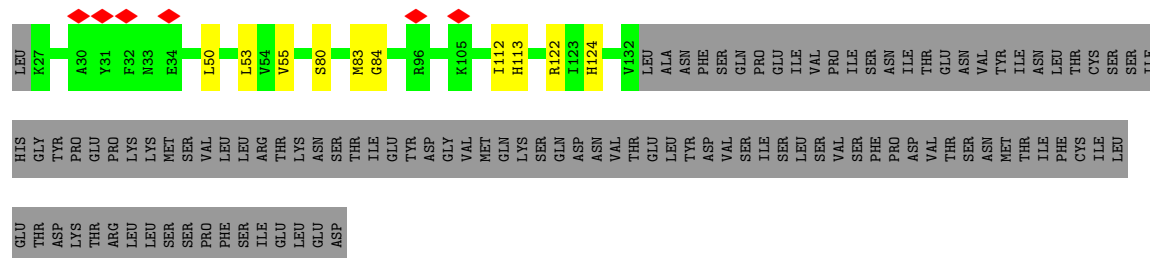
- Molecule 1: NFkB inhibitor



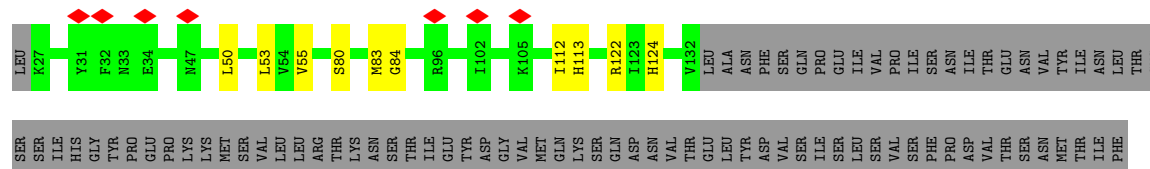
- Molecule 1: NFkB inhibitor



- Molecule 2: T-lymphocyte activation antigen CD86

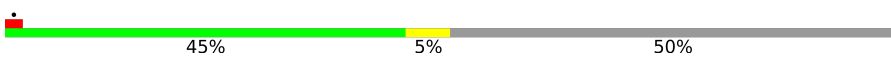


- Molecule 2: T-lymphocyte activation antigen CD86



CYS
ILE
LEU
GLU
THR
ASP
LYS
THR
ARG
LEU
LEU
SER
SER
PRO
PHE
SER
SER
ILE
GLU
LEU
GLU
ASP

- Molecule 2: T-lymphocyte activation antigen CD86

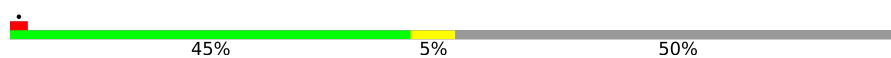
Chain I: 

LEU K27 Y31 F32 N33 E34 T35 L50 L53 V54 V55 S80 M83 G84 K105 I112 H113 R122 I123 H124 V132 LEU ALA ASN PHE SER GLN PRO GLU ILE VAL PRO ILE SER ASN ILE THR VAL ASN TYR MET ILE LEU THR CYS SER ILE HIS GLY

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

ASP
LYS
THR
ARG
LEU
LEU
SER
SER
PRO
PHE
LEU
GLU
ASP

- Molecule 2: T-lymphocyte activation antigen CD86

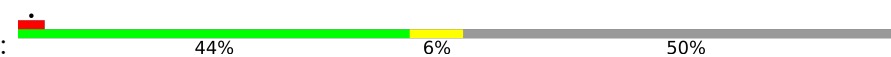
Chain J: 

LEU K27 Y31 F32 N33 E34 L50 L53 V54 V55 S80 M83 G84 K105 I112 H113 R122 I123 H124 V132 LEU ALA ASN PHE SER GLN PRO GLU ILE VAL PRO ILE SER ASN ILE THR VAL THR ASN VAL TYR MET ILE LEU THR CYS SER ILE LEU THR GLY TYR

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

LYS
THR
ARG
LEU
LEU
SER
SER
PRO
PHE
LEU
GLU
ASP

- Molecule 2: T-lymphocyte activation antigen CD86

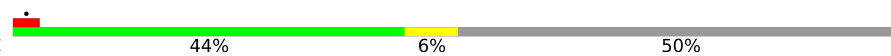
Chain K: 

LEU K27 A30 Y31 F32 N33 E34 M47 L50 L53 V54 V55 S80 M83 G84 R96 K105 I112 H113 R122 I123 H124 V132 LEU ALA ASN PHE SER GLN PRO GLU ILE VAL PRO ILE SER ASN ILE THR VAL THR ASN VAL TYR MET ILE LEU THR CYS SER

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

ILE
LEU
THR
GLU
ASP
LYS
THR
ARG
LEU
LEU
SER
SER
PRO
PHE
SER
SER
ILE
GLU
GLU
ASP

- Molecule 2: T-lymphocyte activation antigen CD86

Chain L: 

LEU K27 Y31 F32 N33 E34 L50 L53 V54 V55 D76 S80 M83 G84 R96 I102 K105 I112 H113 R122 I123 H124 V132 LEU ALA ASN PHE SER GLN PRO GLU ILE VAL PRO ILE SER ASN ILE THR VAL THR ASN VAL TYR MET ILE LEU THR CYS

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

CYS
ILE
LEU
GLU
THR
ASP
LYS
THR
ARG
LEU
LEU
SER
SER
PRO
PHE
SER
ILE
GLU
LEU
GLU
ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.131	Depositor
Minimum map value	-2.605	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	304.0, 304.0, 304.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.95, 0.95, 0.95	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	A	0.30	0/1643	0.62	0/2229
1	B	0.30	0/1643	0.62	0/2229
1	C	0.30	0/1643	0.62	0/2229
1	D	0.30	0/1643	0.62	0/2229
1	E	0.30	0/1643	0.62	0/2229
1	F	0.30	0/1643	0.62	0/2229
2	G	0.28	0/891	0.64	0/1201
2	H	0.28	0/891	0.64	0/1201
2	I	0.28	0/891	0.64	0/1201
2	J	0.28	0/891	0.64	0/1201
2	K	0.28	0/891	0.64	0/1201
2	L	0.28	0/891	0.64	0/1201
All	All	0.29	0/15204	0.63	0/20580

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	A	1610	0	1553	20	0
1	B	1610	0	1553	18	0
1	C	1610	0	1553	19	0
1	D	1610	0	1553	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1610	0	1553	25	0
1	F	1610	0	1553	18	0
2	G	872	0	847	6	0
2	H	872	0	847	6	0
2	I	872	0	847	7	0
2	J	872	0	847	8	0
2	K	872	0	847	9	0
2	L	872	0	847	8	0
All	All	14892	0	14400	151	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.

The worst 5 of 151 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:E:111:ARG:NH2	1:E:190:MET:SD	2.75	0.60
1:D:162:ASN:ND2	2:J:122:ARG:HH22	1.99	0.60
1:F:111:ARG:NH2	1:F:190:MET:SD	2.75	0.60
1:A:111:ARG:NH2	1:A:190:MET:SD	2.75	0.60
1:D:111:ARG:NH2	1:D:190:MET:SD	2.75	0.60

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/203 (98%)	188 (94%)	11 (6%)	0	100	100
1	B	199/203 (98%)	188 (94%)	11 (6%)	0	100	100
1	C	199/203 (98%)	188 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	199/203 (98%)	188 (94%)	11 (6%)	0	100	100
1	E	199/203 (98%)	188 (94%)	11 (6%)	0	100	100
1	F	199/203 (98%)	188 (94%)	11 (6%)	0	100	100
2	G	104/213 (49%)	95 (91%)	9 (9%)	0	100	100
2	H	104/213 (49%)	95 (91%)	9 (9%)	0	100	100
2	I	104/213 (49%)	95 (91%)	9 (9%)	0	100	100
2	J	104/213 (49%)	93 (89%)	11 (11%)	0	100	100
2	K	104/213 (49%)	94 (90%)	10 (10%)	0	100	100
2	L	104/213 (49%)	93 (89%)	11 (11%)	0	100	100
All	All	1818/2496 (73%)	1693 (93%)	125 (7%)	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	
1	A	186/188 (99%)	183 (98%)	3 (2%)	55	80
1	B	186/188 (99%)	182 (98%)	4 (2%)	45	74
1	C	186/188 (99%)	182 (98%)	4 (2%)	45	74
1	D	186/188 (99%)	183 (98%)	3 (2%)	55	80
1	E	186/188 (99%)	182 (98%)	4 (2%)	45	74
1	F	186/188 (99%)	182 (98%)	4 (2%)	45	74
2	G	99/203 (49%)	98 (99%)	1 (1%)	68	86
2	H	99/203 (49%)	98 (99%)	1 (1%)	68	86
2	I	99/203 (49%)	98 (99%)	1 (1%)	68	86
2	J	99/203 (49%)	98 (99%)	1 (1%)	68	86
2	K	99/203 (49%)	98 (99%)	1 (1%)	68	86
2	L	99/203 (49%)	98 (99%)	1 (1%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1710/2346 (73%)	1682 (98%)	28 (2%)	54 80

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	127	GLU
2	L	124	HIS
1	E	209	ILE
2	I	124	HIS
1	E	199	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	144	HIS
2	K	125	GLN
1	E	136	ASN
2	I	125	GLN
1	E	68	ASN

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

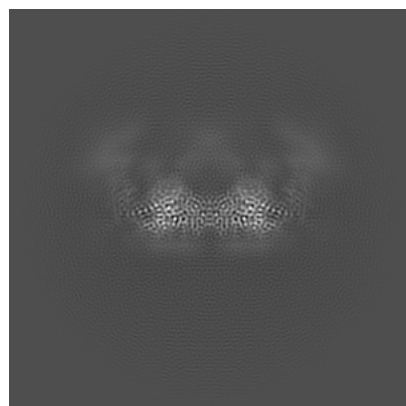
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35075. These allow visual inspection of the internal detail of the map and identification of artifacts.

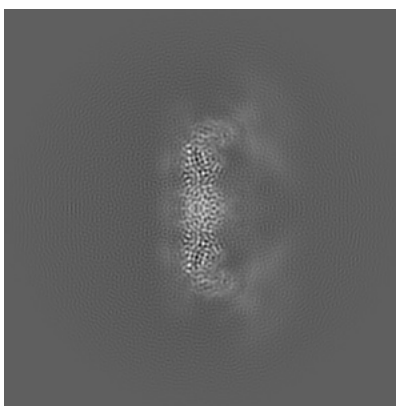
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

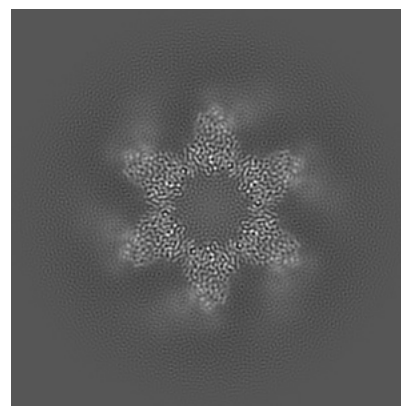
6.1.1 Primary map



X

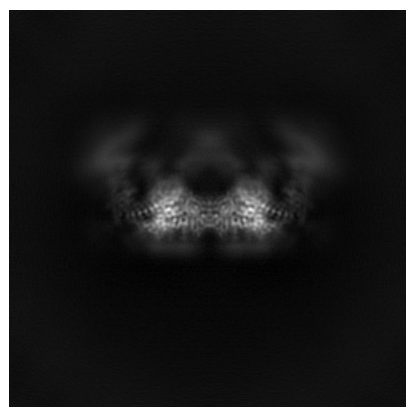


Y

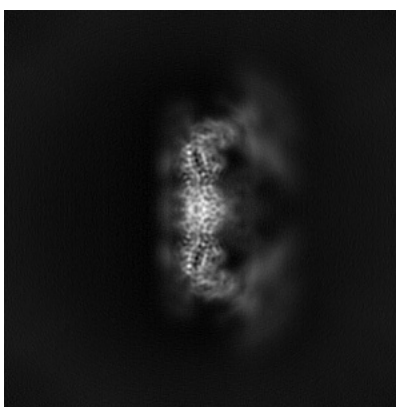


Z

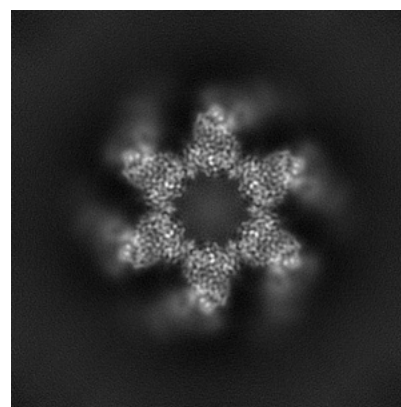
6.1.2 Raw map



X



Y

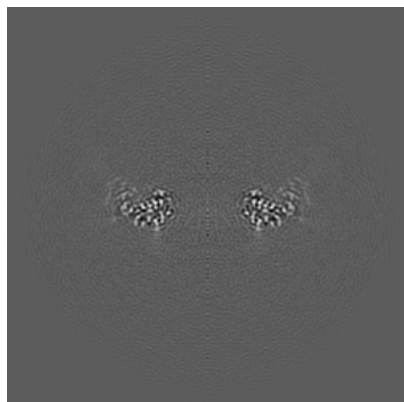


Z

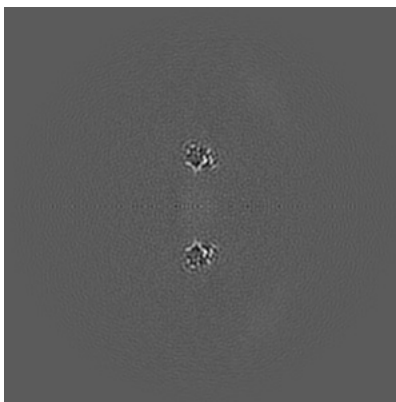
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

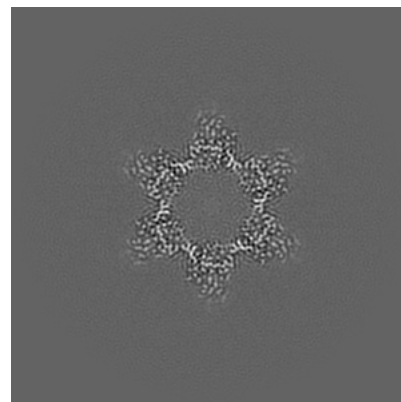
6.2.1 Primary map



X Index: 160

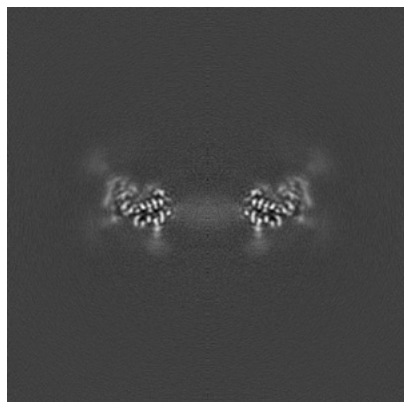


Y Index: 160

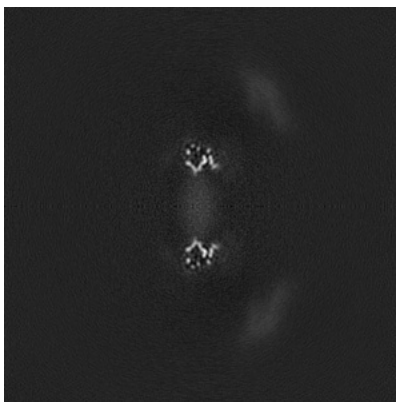


Z Index: 160

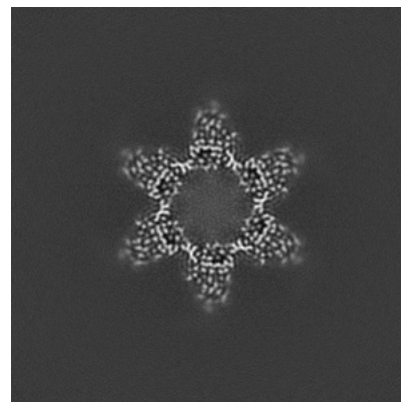
6.2.2 Raw map



X Index: 160



Y Index: 160

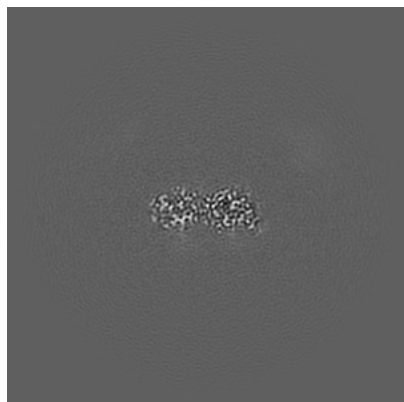


Z Index: 160

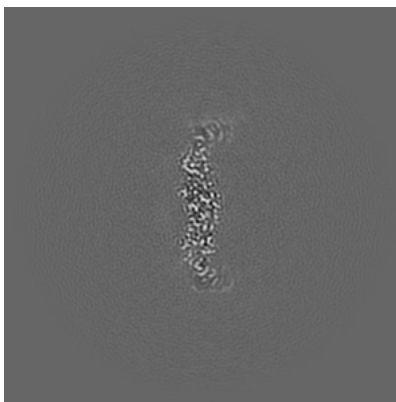
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

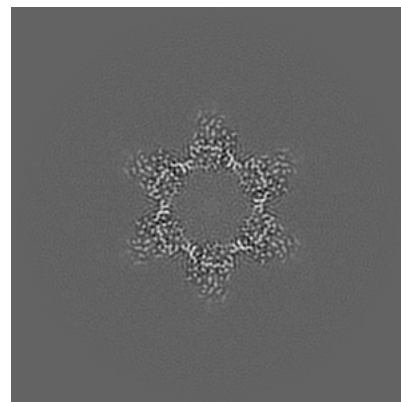
6.3.1 Primary map



X Index: 196

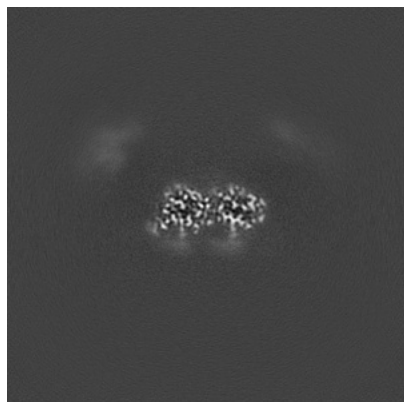


Y Index: 196

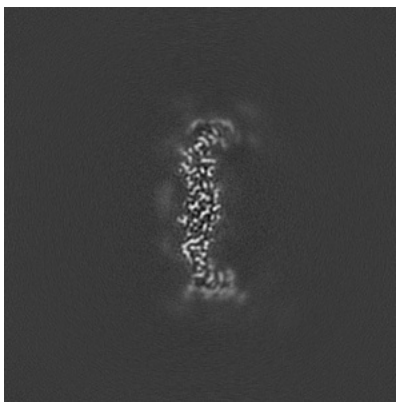


Z Index: 160

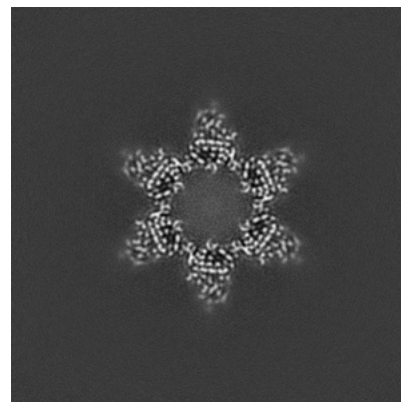
6.3.2 Raw map



X Index: 124



Y Index: 124

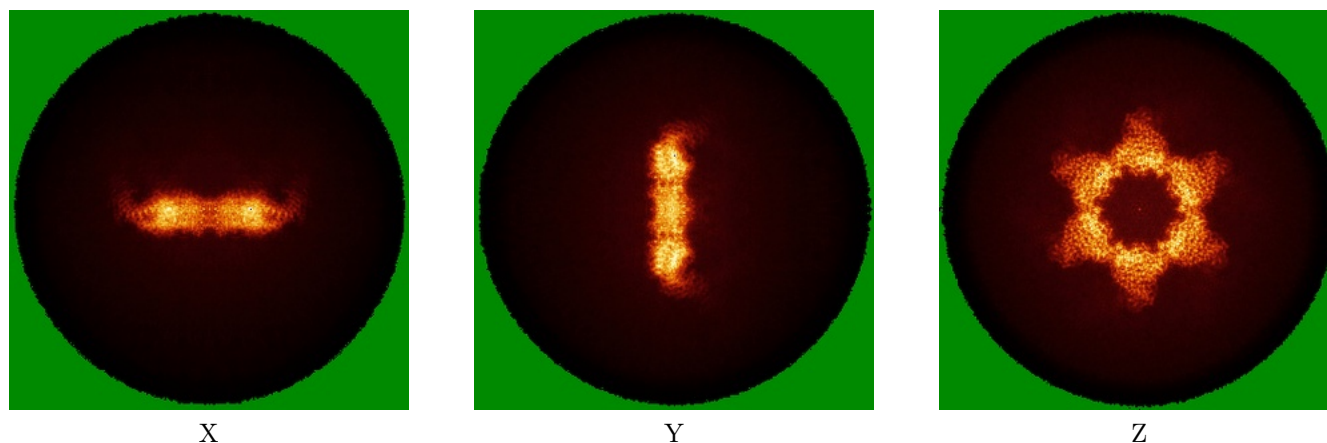


Z Index: 159

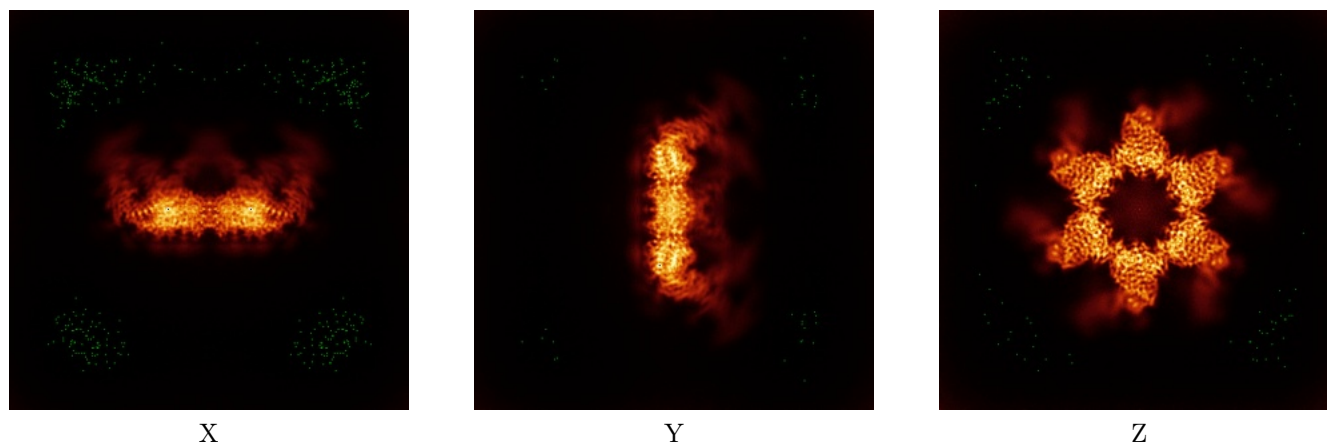
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

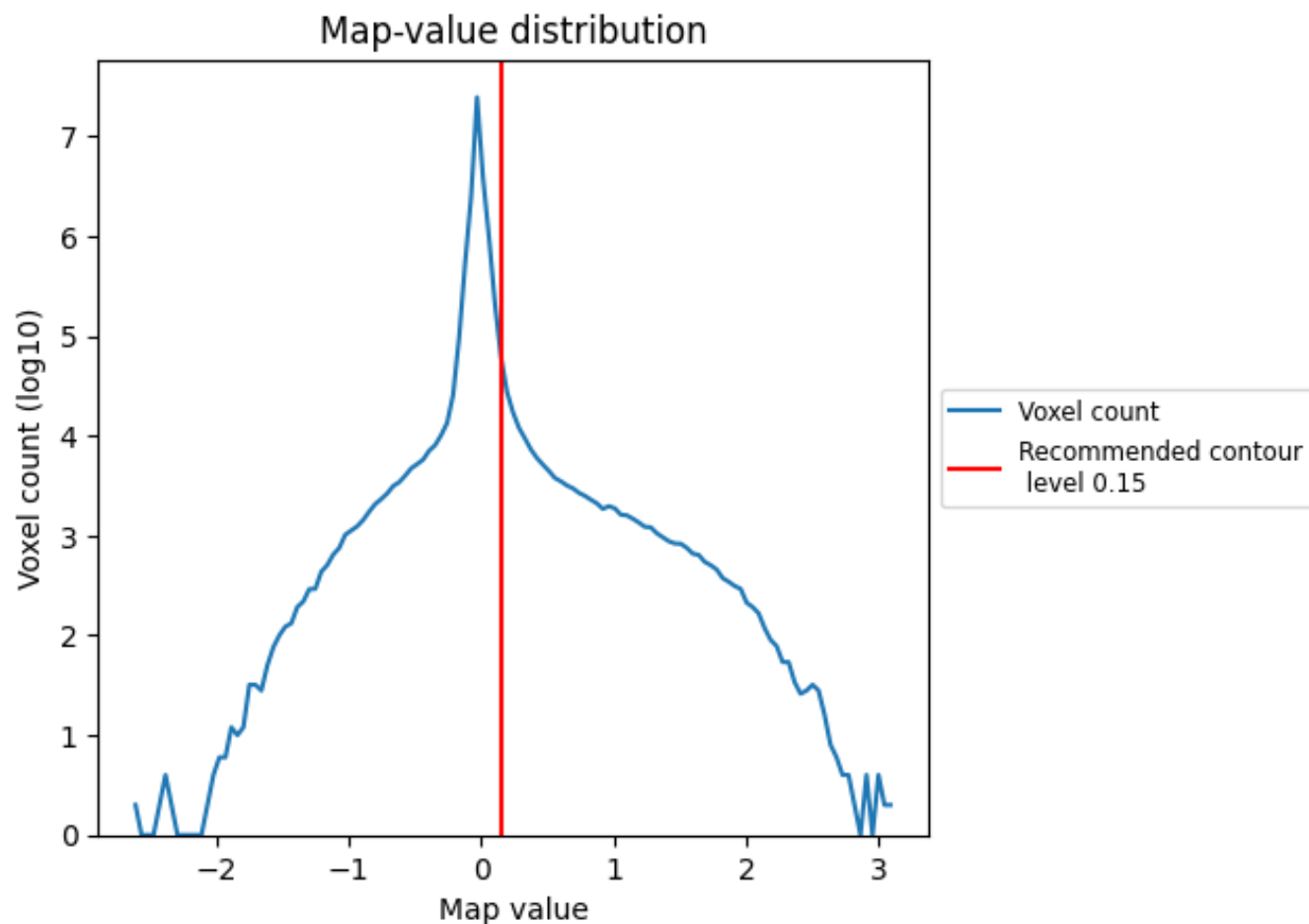
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

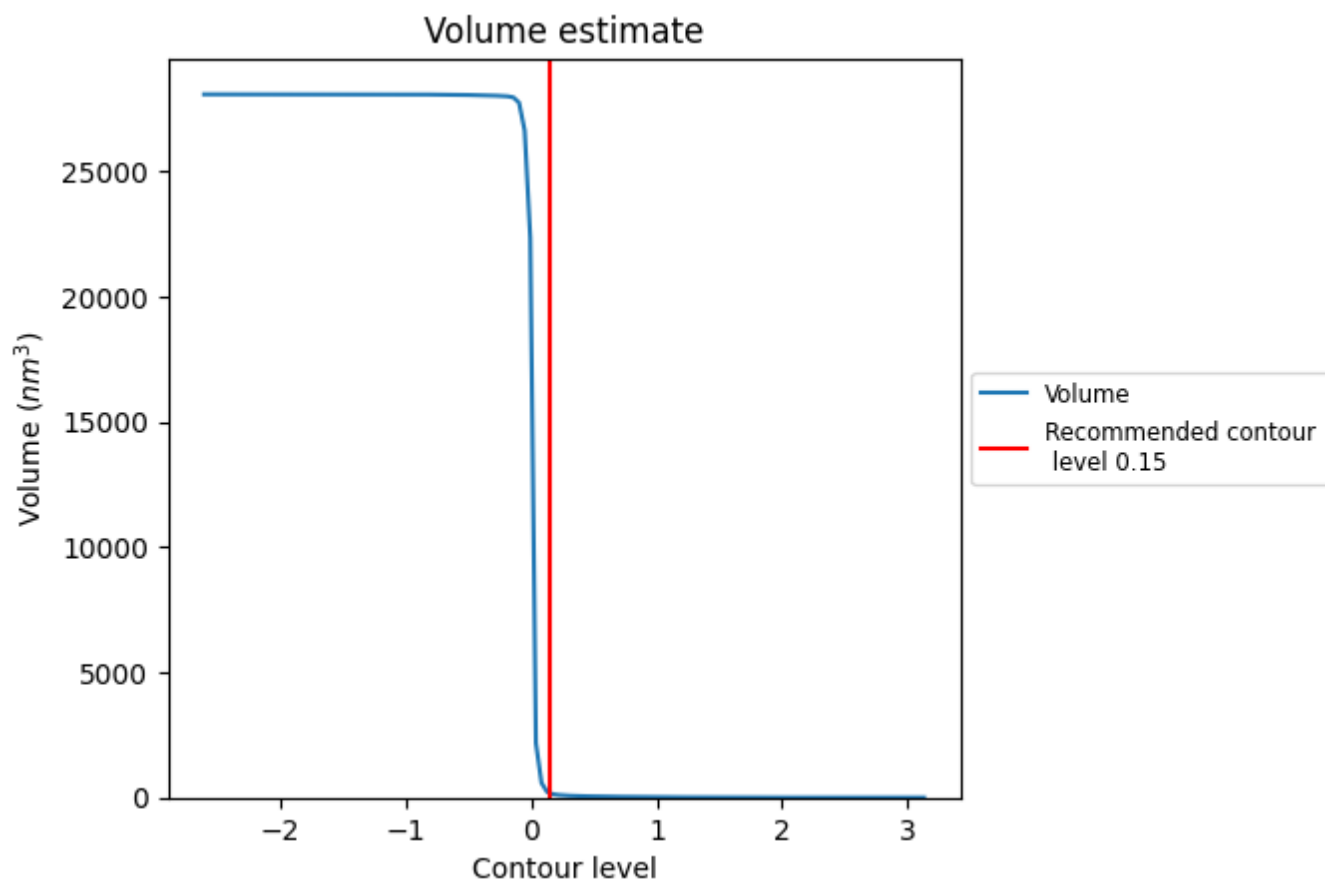
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

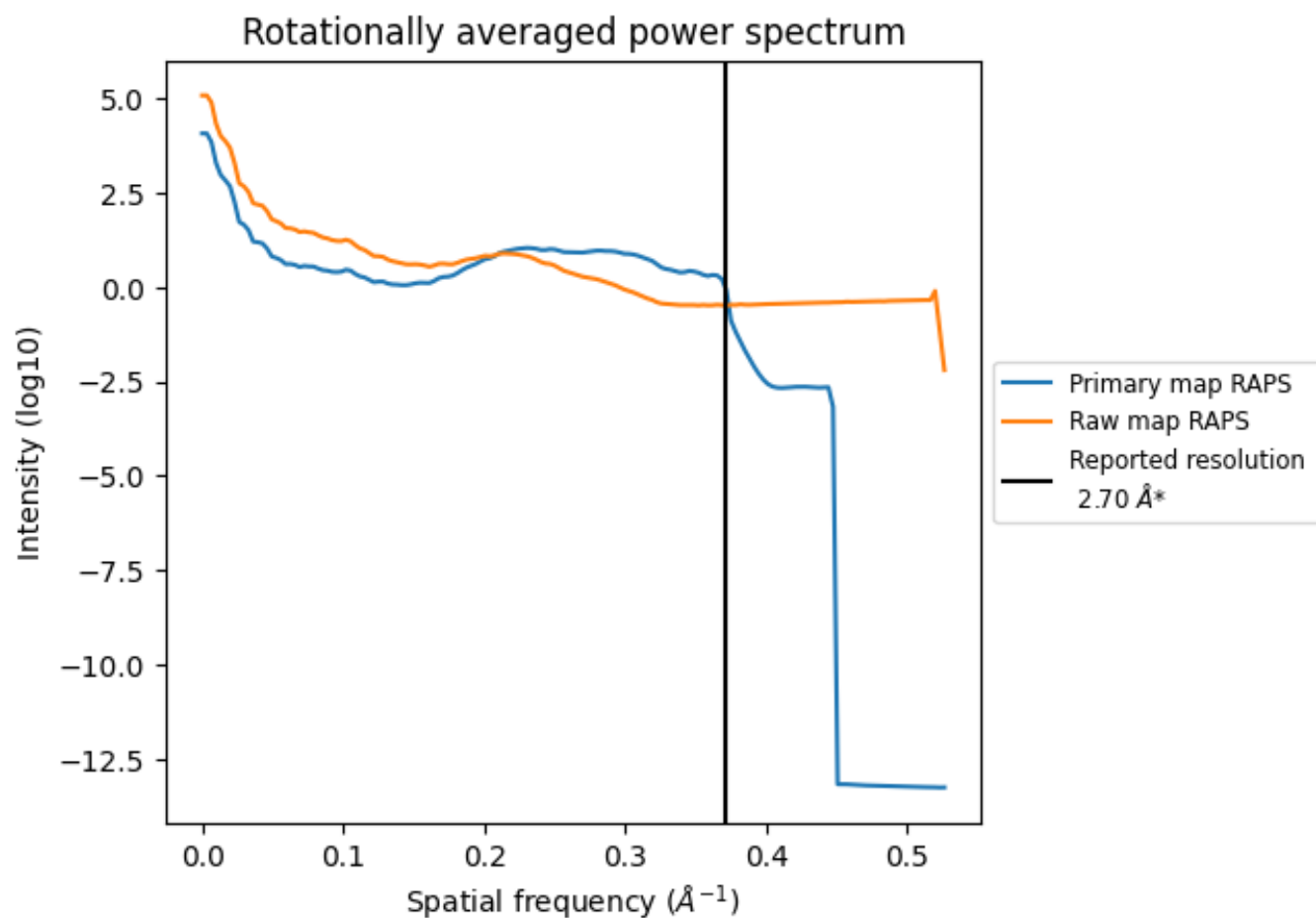
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm^3 ; this corresponds to an approximate mass of 163 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 ⓘ

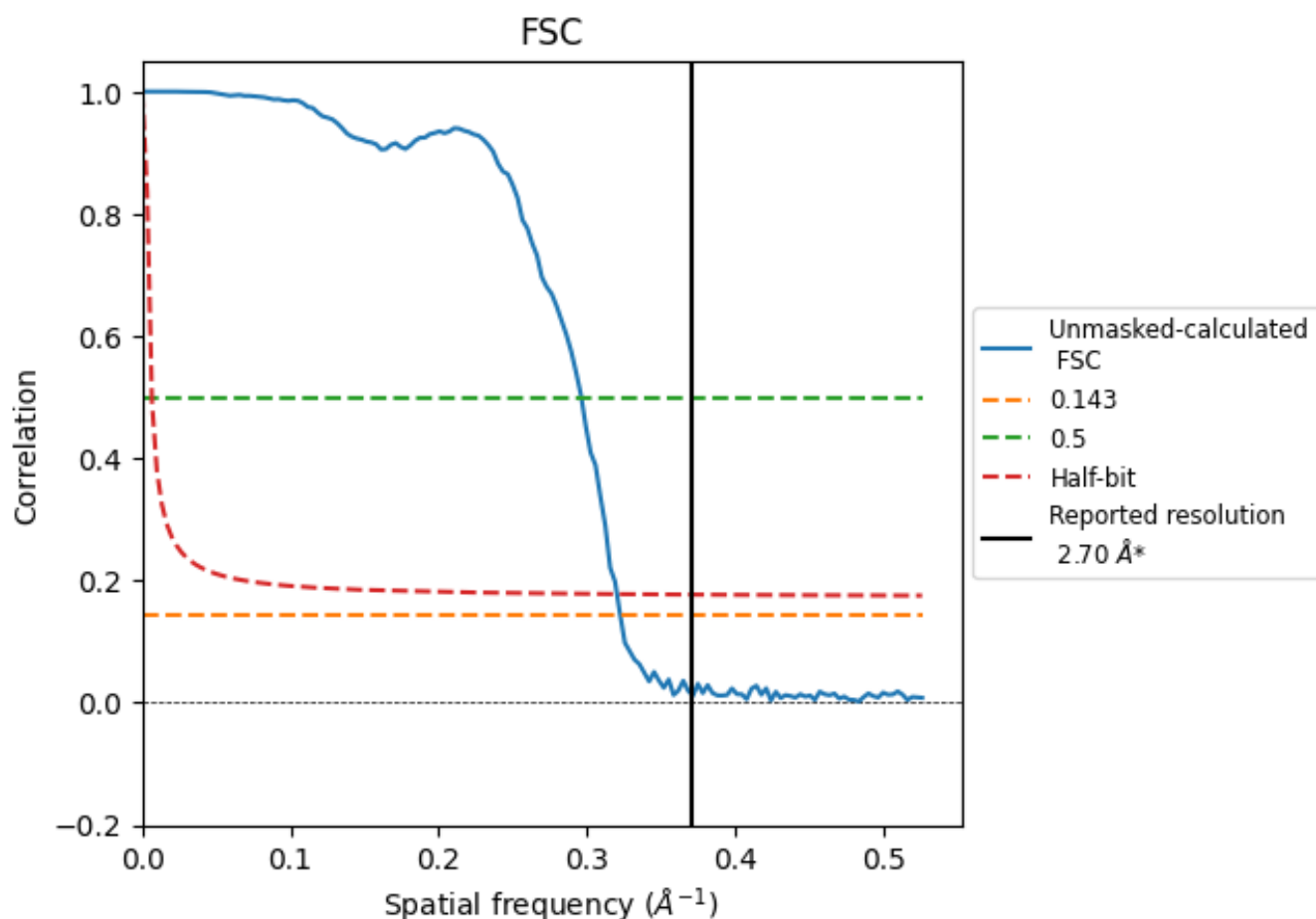


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.10	3.37	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.10 differs from the reported value 2.7 by more than 10 %

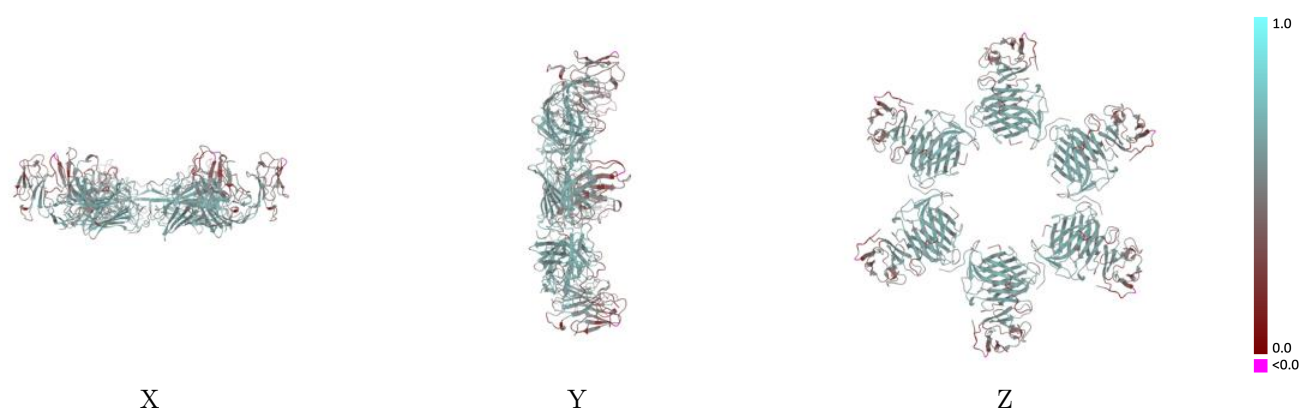
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35075 and PDB model 8HXB. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

This section was not generated.

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

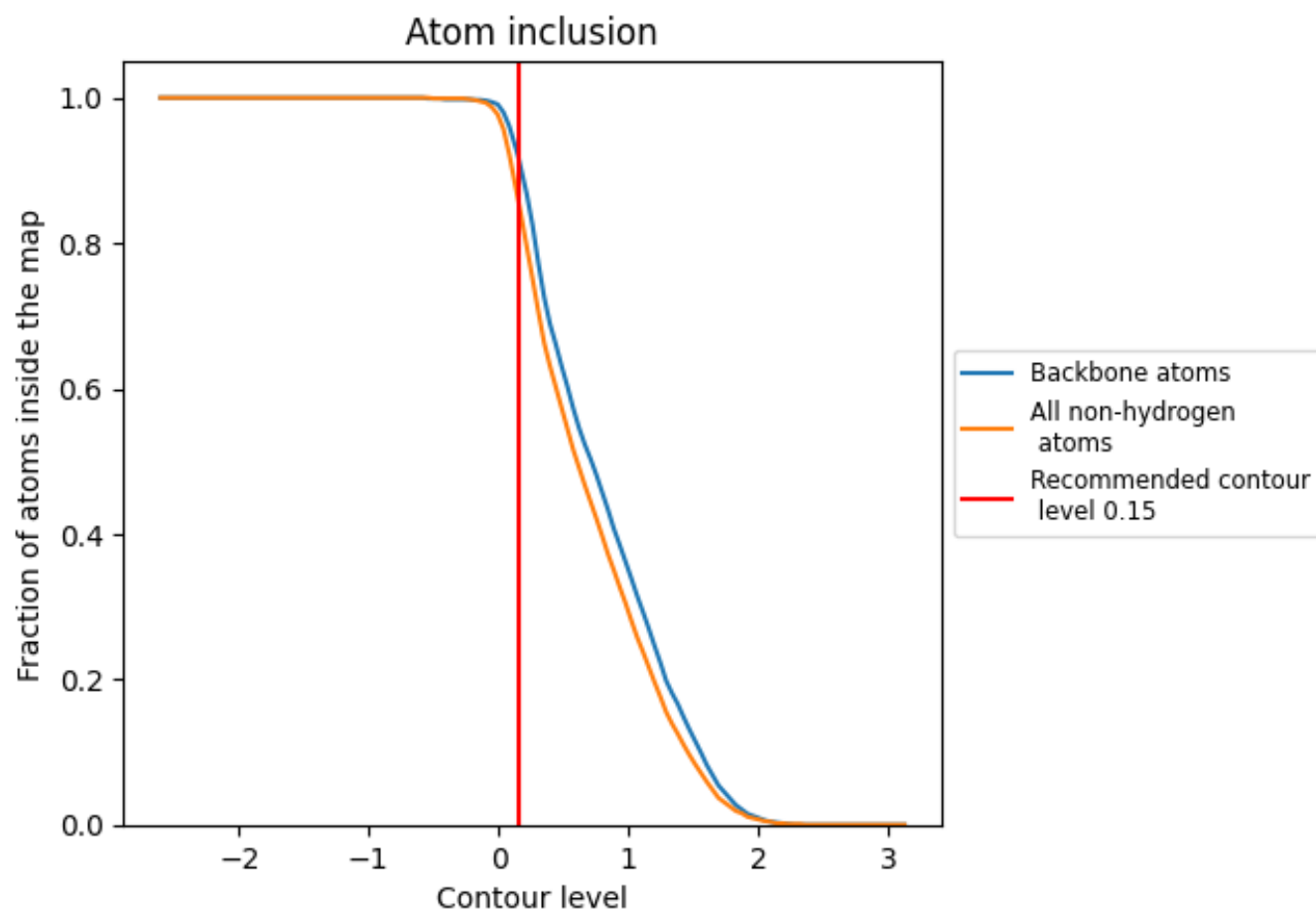


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.5160
A	0.9230	0.5660
B	0.9240	0.5670
C	0.9230	0.5660
D	0.9230	0.5650
E	0.9150	0.5590
F	0.9230	0.5640
G	0.7500	0.4310
H	0.7520	0.4280
I	0.7510	0.4190
J	0.7410	0.4190
K	0.7530	0.4320
L	0.7530	0.4290

1.0

0.0

<0.0