



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 01:04 AM UTC

PDB ID : 8DP5 / pdb_00008dp5
EMDB ID : EMD-27630
Title : Structure of the PEAK3/14-3-3 complex
Authors : Torosyan, H.; Paul, M.; Jura, N.; Verba, K.A.
Deposited on : 2022-07-14
Resolution : 3.10 Å(reported)

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

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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:

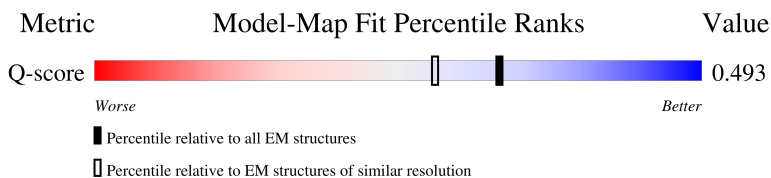
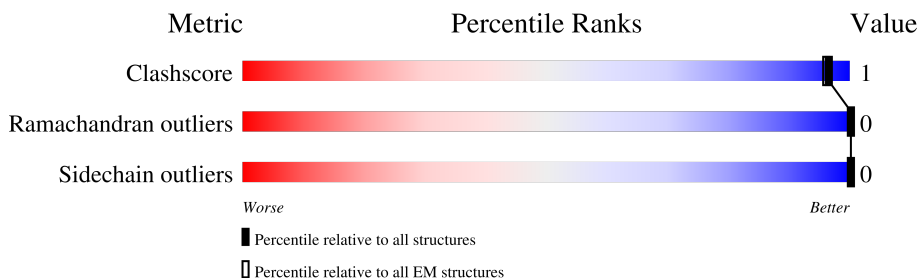
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.10 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.



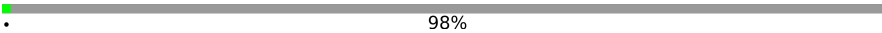
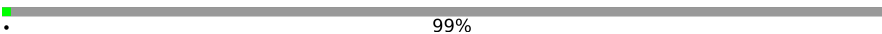
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	491	
1	B	491	
2	C	246	
3	D	255	

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Mol	Chain	Length	Quality of chain
4	E	491	 98%
4	P	491	 99%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17780 atoms, of which 8916 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 Protein PEAK3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0
			5051	1606	2544	453	438	10		
1	B	335	Total	C	H	N	O	S	0	0
			5084	1618	2563	456	437	10		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	LEU	-	expression tag	UNP Q6ZS72
A	475	GLU	-	expression tag	UNP Q6ZS72
A	476	GLY	-	expression tag	UNP Q6ZS72
A	477	GLY	-	expression tag	UNP Q6ZS72
A	478	GLY	-	expression tag	UNP Q6ZS72
A	479	GLY	-	expression tag	UNP Q6ZS72
A	480	ALA	-	expression tag	UNP Q6ZS72
A	481	ASP	-	expression tag	UNP Q6ZS72
A	482	TYR	-	expression tag	UNP Q6ZS72
A	483	LYS	-	expression tag	UNP Q6ZS72
A	484	ASP	-	expression tag	UNP Q6ZS72
A	485	ASP	-	expression tag	UNP Q6ZS72
A	486	ASP	-	expression tag	UNP Q6ZS72
A	487	ASP	-	expression tag	UNP Q6ZS72
A	488	LYS	-	expression tag	UNP Q6ZS72
A	489	GLY	-	expression tag	UNP Q6ZS72
A	490	PRO	-	expression tag	UNP Q6ZS72
A	491	VAL	-	expression tag	UNP Q6ZS72
B	474	LEU	-	expression tag	UNP Q6ZS72
B	475	GLU	-	expression tag	UNP Q6ZS72
B	476	GLY	-	expression tag	UNP Q6ZS72
B	477	GLY	-	expression tag	UNP Q6ZS72
B	478	GLY	-	expression tag	UNP Q6ZS72
B	479	GLY	-	expression tag	UNP Q6ZS72
B	480	ALA	-	expression tag	UNP Q6ZS72
B	481	ASP	-	expression tag	UNP Q6ZS72

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Chain	Residue	Modelled	Actual	Comment	Reference
B	482	TYR	-	expression tag	UNP Q6ZS72
B	483	LYS	-	expression tag	UNP Q6ZS72
B	484	ASP	-	expression tag	UNP Q6ZS72
B	485	ASP	-	expression tag	UNP Q6ZS72
B	486	ASP	-	expression tag	UNP Q6ZS72
B	487	ASP	-	expression tag	UNP Q6ZS72
B	488	LYS	-	expression tag	UNP Q6ZS72
B	489	GLY	-	expression tag	UNP Q6ZS72
B	490	PRO	-	expression tag	UNP Q6ZS72
B	491	VAL	-	expression tag	UNP Q6ZS72

- Molecule 2 is a protein called 14-3-3 protein beta/alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	230	Total	C	H	N	O	S	0	0
			3691	1161	1836	312	373	9		

- Molecule 3 is a protein called 14-3-3 protein epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	231	Total	C	H	N	O	S	0	0
			3698	1166	1846	312	363	11		

- Molecule 4 is a protein called Protein PEAK3 fragment.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	8	Total	C	H	N	O	P	0	0
			140	39	70	15	15	1		
4	P	7	Total	C	H	N	O	P	0	0
			116	33	57	11	14	1		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	474	LEU	-	expression tag	UNP Q6ZS72
E	475	GLU	-	expression tag	UNP Q6ZS72
E	476	GLY	-	expression tag	UNP Q6ZS72
E	477	GLY	-	expression tag	UNP Q6ZS72
E	478	GLY	-	expression tag	UNP Q6ZS72
E	479	GLY	-	expression tag	UNP Q6ZS72
E	480	ALA	-	expression tag	UNP Q6ZS72
E	481	ASP	-	expression tag	UNP Q6ZS72

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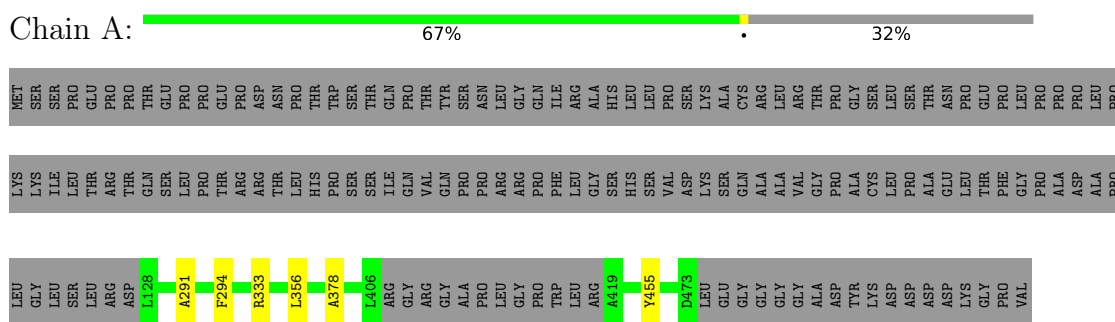
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Chain	Residue	Modelled	Actual	Comment	Reference
E	482	TYR	-	expression tag	UNP Q6ZS72
E	483	LYS	-	expression tag	UNP Q6ZS72
E	484	ASP	-	expression tag	UNP Q6ZS72
E	485	ASP	-	expression tag	UNP Q6ZS72
E	486	ASP	-	expression tag	UNP Q6ZS72
E	487	ASP	-	expression tag	UNP Q6ZS72
E	488	LYS	-	expression tag	UNP Q6ZS72
E	489	GLY	-	expression tag	UNP Q6ZS72
E	490	PRO	-	expression tag	UNP Q6ZS72
E	491	VAL	-	expression tag	UNP Q6ZS72
P	474	LEU	-	expression tag	UNP Q6ZS72
P	475	GLU	-	expression tag	UNP Q6ZS72
P	476	GLY	-	expression tag	UNP Q6ZS72
P	477	GLY	-	expression tag	UNP Q6ZS72
P	478	GLY	-	expression tag	UNP Q6ZS72
P	479	GLY	-	expression tag	UNP Q6ZS72
P	480	ALA	-	expression tag	UNP Q6ZS72
P	481	ASP	-	expression tag	UNP Q6ZS72
P	482	TYR	-	expression tag	UNP Q6ZS72
P	483	LYS	-	expression tag	UNP Q6ZS72
P	484	ASP	-	expression tag	UNP Q6ZS72
P	485	ASP	-	expression tag	UNP Q6ZS72
P	486	ASP	-	expression tag	UNP Q6ZS72
P	487	ASP	-	expression tag	UNP Q6ZS72
P	488	LYS	-	expression tag	UNP Q6ZS72
P	489	GLY	-	expression tag	UNP Q6ZS72
P	490	PRO	-	expression tag	UNP Q6ZS72
P	491	VAL	-	expression tag	UNP Q6ZS72

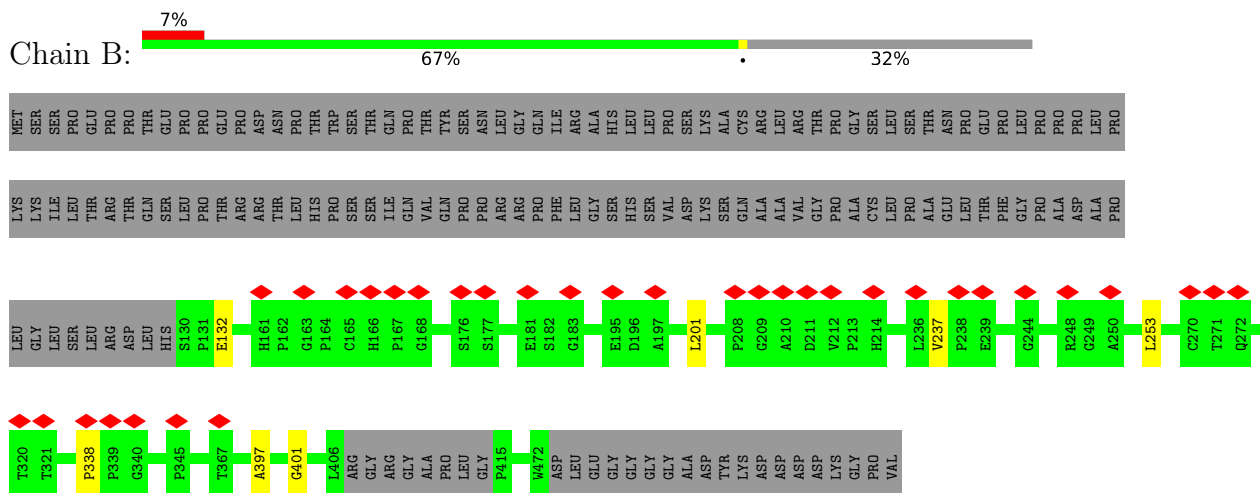
3 Residue-property plots [i](#)

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.

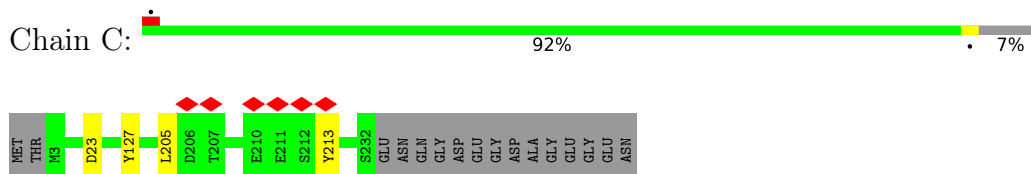
• Molecule 1: Protein PEA3



• Molecule 1: Protein PEA3



• Molecule 2: 14-3-3 protein beta/alpha



• Molecule 3: 14-3-3 protein epsilon

MET ASP D3 E76 L163 F177 S233 ASP MET GLN GLY ASP GLY GLU GLU GLN ASN LYS GLU ALA LEU GLN VAL GLU ASP GLU ASN GLN

Chain E: . 98%

ASP	LEU	ALA	GLU	GLY	ASP	SER	LYS	MET
ASP	ARG	PRO	LEU	LEU	ARG	LEU	LYS	SER
ASP	VAL	SER	ARG	PRO	PRO	LEU	ILE	SER
ASP	ARG	THR	GLU	TRP	ASP	TYR	THR	GLU
LYS	ARG	THR	GLU	ARG	TYR	THR	THR	PRO
GLY	GLY	PRO	ASN	GLY	ARG	HIS	R66	PRO
PRO	LEU	LEU	LEU	VAL	VAL	SER	S69	THR
VAL	LEU	ALA	LEU	ALA	ARG	GLU	S69	GLU
	VAL	ALA	LEU	ALA	ALA	ALA	R73	PRO
	ARG	LEU	VAL	VAL	ALA	VAL	ARG	PRO
	LEU	GLU	ALA	ALA	HIS	VAL	THR	GLU
	LEU	GLU	PRO	ALA	GLU	HIS	THR	PRO
	ALA	LEU	ARG	VAL	ASP	THR	LEU	GLU
	GLU	LEU	GLY	VAL	ALA	ALA	HIS	PRO
	ARG	LEU	CYS	PRO	TRP	LEU	ASP	ASN
	ALA	ALA	THR	GLU	THR	HIS	SER	PRO
	GLN	LEU	THR	ARG	ILE	ALA	SER	THR
	LEU	LEU	THR	THR	ARG	ARG	ILE	TRP
	GLY	THR	GLY	VAL	LEU	GLN	GLN	SER
	GLU	ARG	PRO	VAL	LEU	VAL	VAL	THR
	ALA	LEU	PRO	GLN	GLN	LYS	GLN	PRO
	PRO	ARG	ARG	TRP	VAL	PRO	PRO	THR
	SER	PRO	LEU	LEU	PRO	LEU	ARG	TYR
	LEU	SER	LEU	ALA	LYS	ARG	THR	SER
	GLU	ALA	LEU	GLU	PRO	THR	ARG	ASN
	ASP	SER	THR	ALA	GLY	ILE	PRO	LEU
	TRP	ARG	ASP	CYS	ALA	TYR	PHE	GLY
	LEU	THR	PHE	THR	ALA	ALA	LEU	GLN
	CYS	ARG	GLY	GLN	VAL	ARG	ASP	LEU
	CYS	GLY	ARG	PRO	PRO	LEU	LYS	LEU
	GLU	LEU	PRO	VAL	LEU	MET	SER	PRO
	ALA	LEU	PRO	TRP	GLU	GLY	SER	SER
	THR	TRP	GLY	ALA	LEU	GLY	GLN	ASN
	GLU	GLY	PRO	VAL	GLN	HIS	ALA	LYS
	SER	PRO	PRO	ALA	ALA	PRO	ALA	CYS
	SER	GLY	GLY	LEU	SER	GLY	VAL	ARG
	MET	PRO	SER	LEU	LEU	PRO	GLY	CYS
	GLY	GLU	PRO	LEU	SER	CYS	PRO	LEU
	GLN	LEU	GLY	LEU	HIS	HIS	ALA	ARG
	ALA	ARG	PRO	GLN	THR	PRO	ALA	THR
	LEU	GLY	HIS	LEU	GLY	GLY	LEU	PRO
	LEU	ARG	ALA	SER	ASN	HIS	PRO	GLY
	LEU	GLY	PRO	ALA	LEU	SER	ALA	SER
	LEU	ALA	GLN	ALA	GLN	PHE	GLU	LEU
	TRP	PRO	LEU	LEU	GLY	ARG	LEU	SER
	ASP	LEU	GLY	LYS	LEU	LEU	THR	LEU
	LEU	GLY	SER	PHE	CYS	LEU	PHE	ASN
	GLU	PRO	LEU	LEU	GLY	ASP	GLY	PRO
	GLY	TRP	LEU	GLU	LEU	SER	PRO	GLU
	GLY	LEU	ARG	ALA	VAL	SER	ALA	PRO
	GLY	ARG	ALA	TRP	PRO	PRO	ASP	LEU
	GLY	ALA	LEU	GLY	CYS	CYS	ALA	PRO
	ALA	LEU	LEU	ALA	GLY	ALA	PRO	PRO
	ASP	GLY	SER	ALA	THR	GLU	LEU	PRO
	TYR	TRP	LEU	ALA	PRO	SER	GLY	PRO

Chain P: 99%

[illegible]

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169563	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 ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.383	Depositor
Minimum map value	-1.276	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.268	Depositor
Map size (Å)	267.19998, 267.19998, 267.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8349999, 0.8349999, 0.8349999	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.83	1/2578 (0.0%)	1.33	3/3533 (0.1%)
1	B	0.87	1/2594 (0.0%)	1.34	2/3555 (0.1%)
2	C	0.71	0/1882	1.23	1/2533 (0.0%)
3	D	0.72	0/1880	1.24	3/2534 (0.1%)
4	E	0.97	0/59	1.57	0/77
4	P	0.99	0/48	1.55	0/63
All	All	0.80	2/9041 (0.0%)	1.30	9/12295 (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	A	0	1
2	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	GLU	C-O	-6.53	1.16	1.24
1	A	294	PHE	C-O	-5.25	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	PRO	N-CA-C	6.92	119.15	110.70
1	A	291	ALA	N-CA-C	-6.52	103.67	111.69
3	D	163	LEU	CA-C-N	6.00	124.04	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	163	LEU	C-N-CA	6.00	124.04	119.66
1	B	132	GLU	CA-C-O	-5.89	114.84	120.90
1	A	455	TYR	CA-C-O	-5.33	115.22	120.70
2	C	23	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	294	PHE	N-CA-C	-5.11	105.62	111.14
3	D	177	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	ARG	Sidechain
2	C	127	TYR	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	A	2507	2544	2542	1	0
1	B	2521	2563	2562	7	0
2	C	1855	1836	1835	6	0
3	D	1852	1846	1845	0	0
4	E	70	70	68	0	0
4	P	59	57	55	0	0
All	All	8864	8916	8907	14	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 1.

All (14) 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:C:205:LEU:HD11	2:C:213:TYR:CD1	1.88	1.06
1:B:201:LEU:HD22	1:B:253:LEU:HD13	1.56	0.88
2:C:205:LEU:HD21	2:C:213:TYR:CE1	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:HD22	1:B:253:LEU:CD1	2.08	0.81
2:C:205:LEU:HD11	2:C:213:TYR:HD1	1.41	0.81
1:A:356:LEU:HD22	1:A:378:ALA:HB2	1.62	0.81
1:B:201:LEU:CD2	1:B:253:LEU:HD13	2.18	0.74
1:B:237:VAL:HG23	1:B:253:LEU:HD23	1.85	0.57
2:C:205:LEU:CD1	2:C:213:TYR:HD1	2.15	0.56
1:B:201:LEU:CD2	1:B:253:LEU:CD1	2.80	0.55
2:C:205:LEU:CD1	2:C:213:TYR:CD1	2.77	0.54
1:B:397:ALA:HA	1:B:401:GLY:HA3	1.94	0.48
2:C:205:LEU:CD2	2:C:213:TYR:CE1	2.96	0.43
1:B:201:LEU:HD22	1:B:253:LEU:HD11	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/491 (67%)	330 (100%)	0	0	100	100
1	B	331/491 (67%)	325 (98%)	6 (2%)	0	100	100
2	C	228/246 (93%)	225 (99%)	3 (1%)	0	100	100
3	D	229/255 (90%)	226 (99%)	3 (1%)	0	100	100
4	E	5/491 (1%)	5 (100%)	0	0	100	100
4	P	4/491 (1%)	4 (100%)	0	0	100	100
All	All	1127/2465 (46%)	1115 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/387 (66%)	254 (100%)	0	100	100
1	B	255/387 (66%)	255 (100%)	0	100	100
2	C	204/215 (95%)	204 (100%)	0	100	100
3	D	199/220 (90%)	199 (100%)	0	100	100
4	E	7/386 (2%)	7 (100%)	0	100	100
4	P	6/386 (2%)	6 (100%)	0	100	100
All	All	925/1981 (47%)	925 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	ASN
1	B	221	GLN
1	B	309	ASN
1	B	351	GLN
3	D	129	HIS
3	D	147	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SEP	P	69	4	8,9,10	1.08	0	7,12,14	2.99	1 (14%)
4	SEP	E	69	4	8,9,10	1.14	0	7,12,14	2.17	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SEP	P	69	4	-	4/6/8/10	-
4	SEP	E	69	4	-	1/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	69	SEP	OG-CB-CA	7.48	115.42	108.14
4	E	69	SEP	OG-CB-CA	5.34	113.34	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	69	SEP	C-CA-CB-OG
4	P	69	SEP	CB-OG-P-O2P
4	P	69	SEP	CB-OG-P-O3P
4	P	69	SEP	CB-OG-P-O1P
4	P	69	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

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.

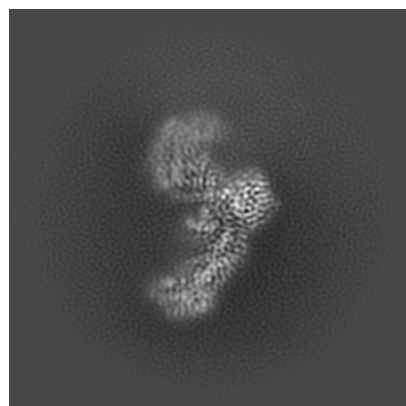
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27630. These allow visual inspection of the internal detail of the map and identification of artifacts.

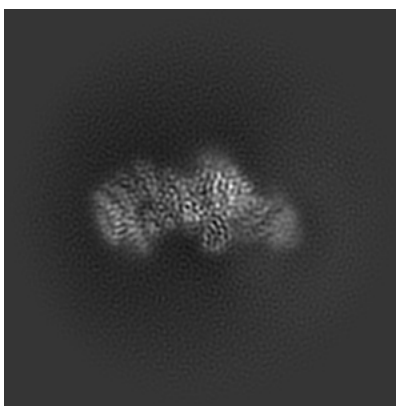
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

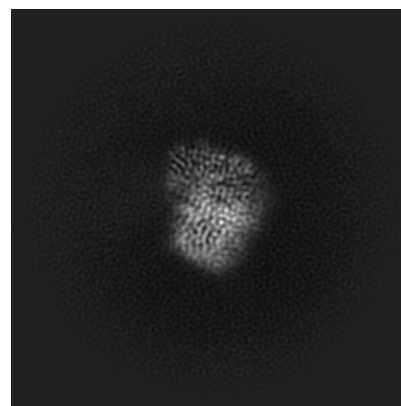
6.1.1 Primary map



X

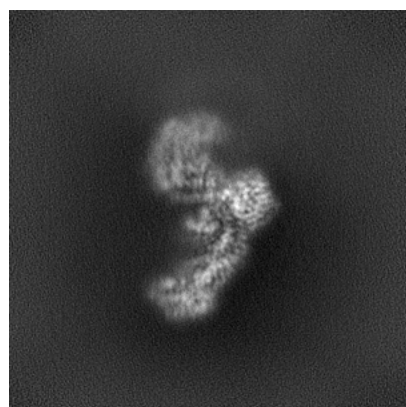


Y

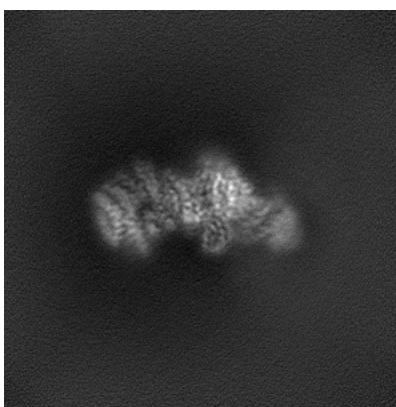


Z

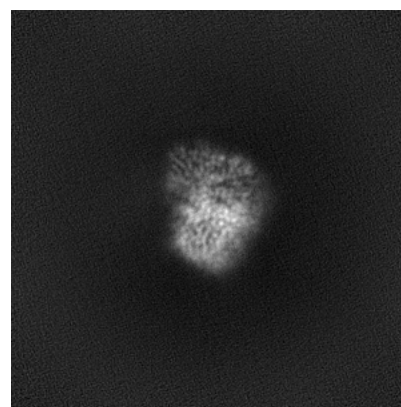
6.1.2 Raw map



X



Y

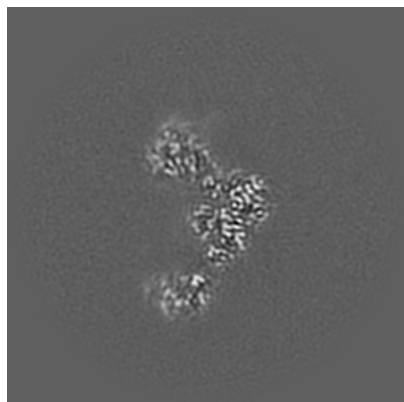


Z

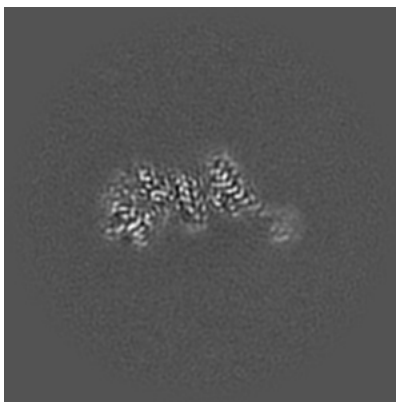
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

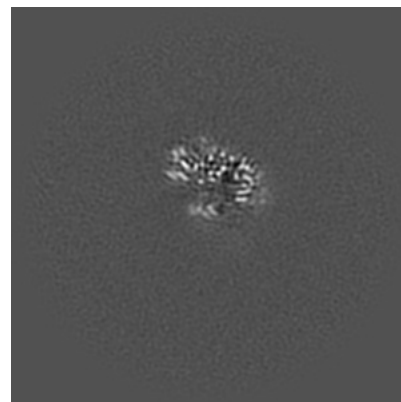
6.2.1 Primary map



X Index: 160

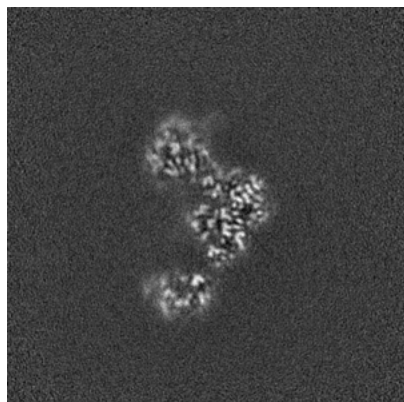


Y Index: 160

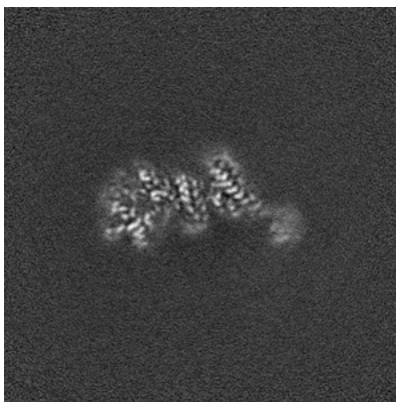


Z Index: 160

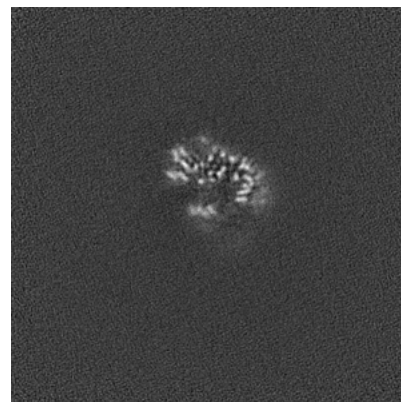
6.2.2 Raw map



X Index: 160



Y Index: 160

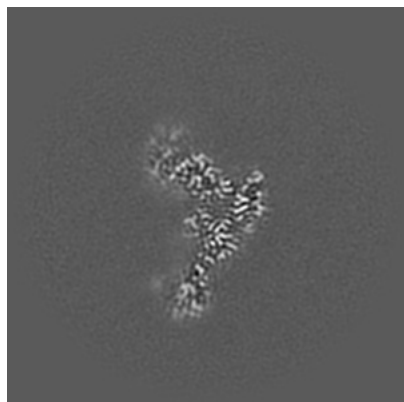


Z Index: 160

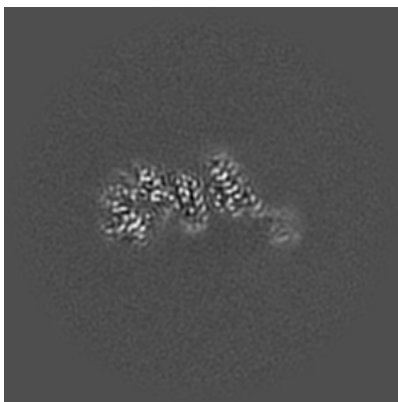
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

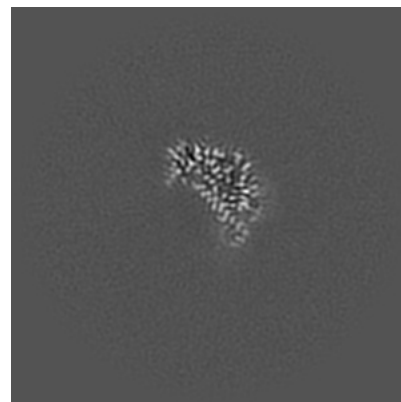
6.3.1 Primary map



X Index: 169

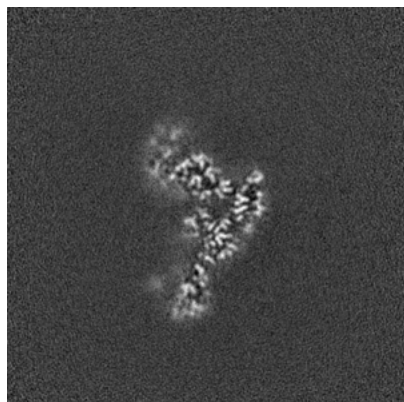


Y Index: 159

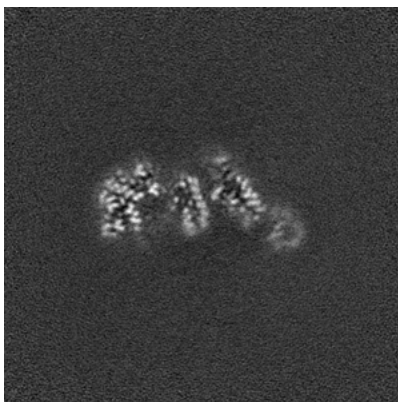


Z Index: 171

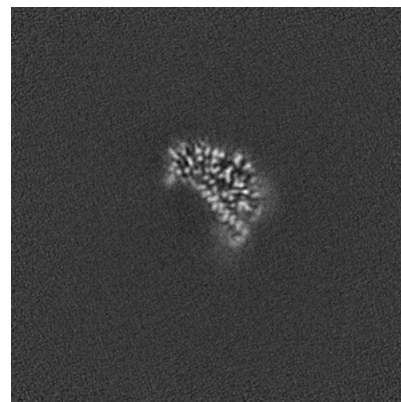
6.3.2 Raw map



X Index: 169



Y Index: 155

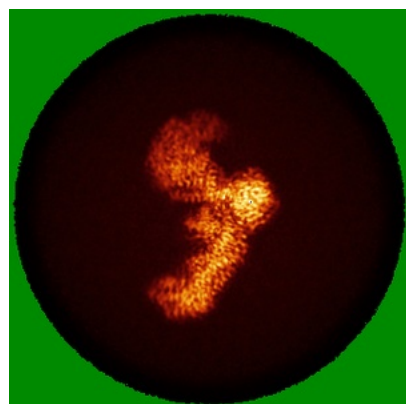


Z Index: 170

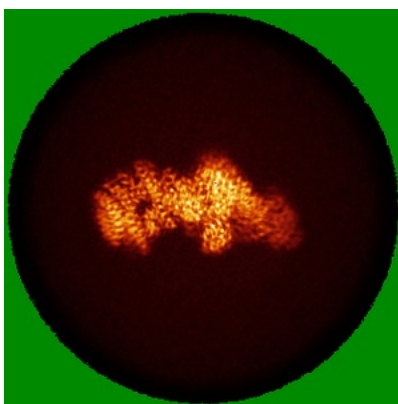
The images above show the largest variance slices of the map in three orthogonal directions.

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

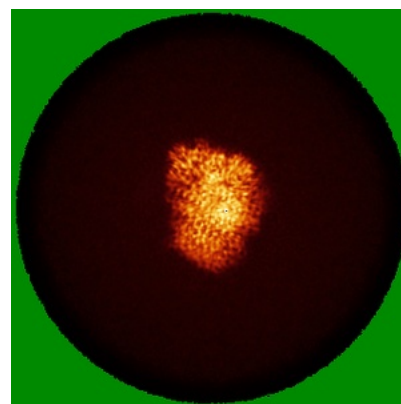
6.4.1 Primary map



X

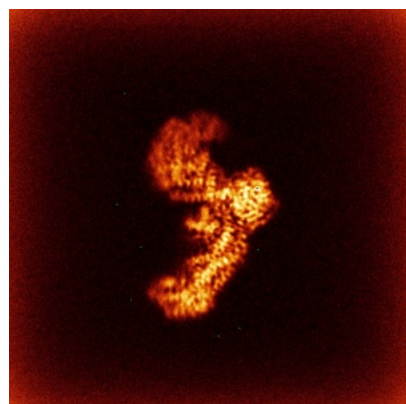


Y

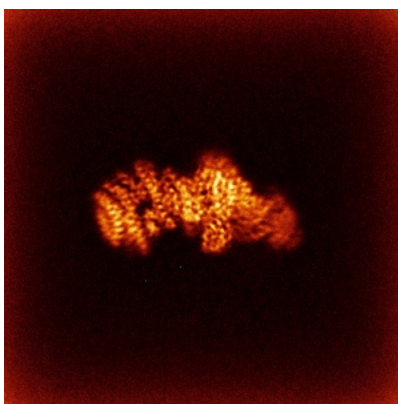


Z

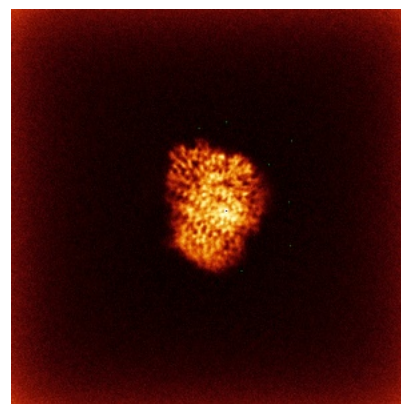
6.4.2 Raw map



X



Y

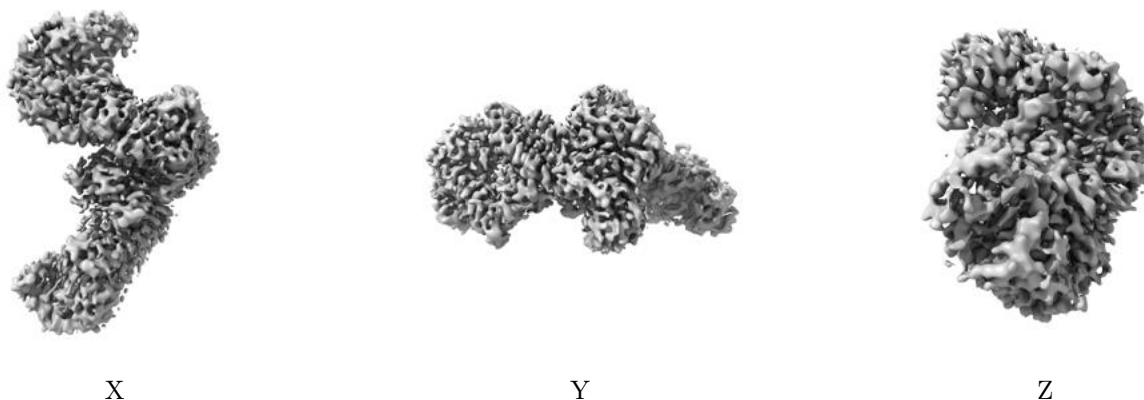


Z

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.

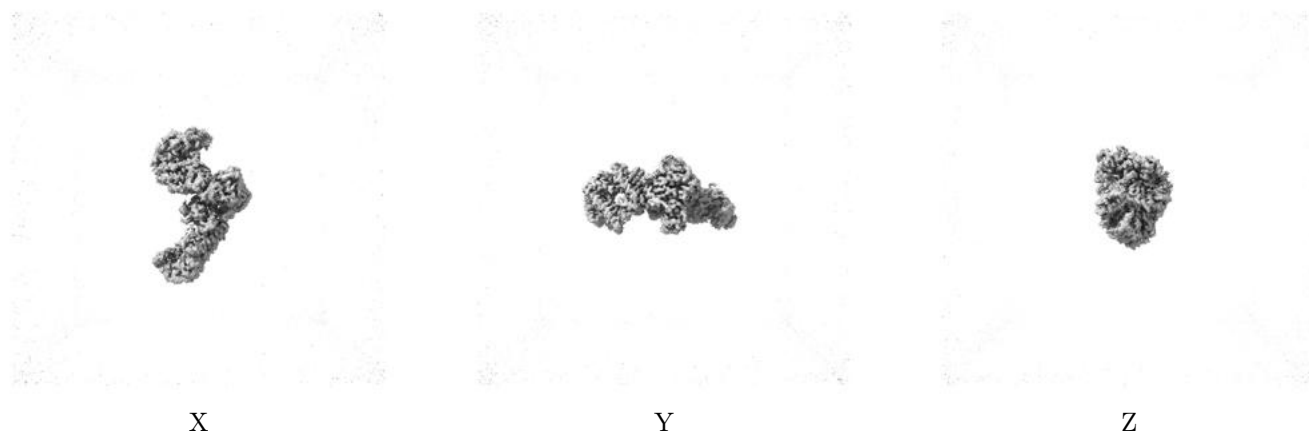
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.268. 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.

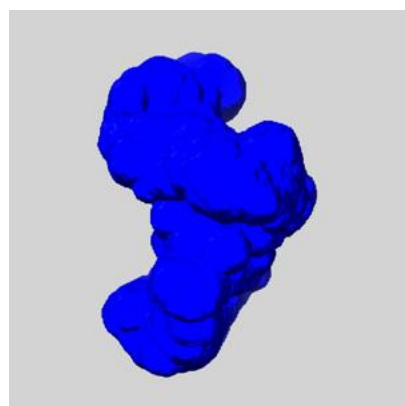
6.6 Mask visualisation [i](#)

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

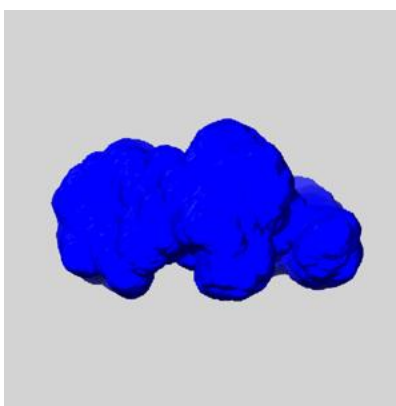
A mask typically either:

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

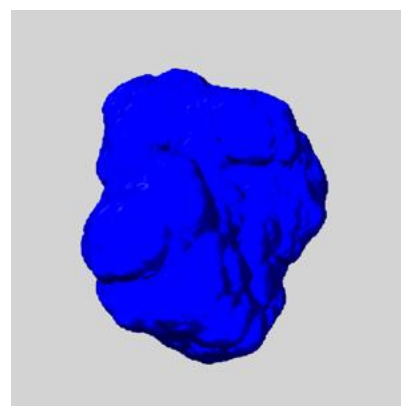
6.6.1 emd_27630_msk_1.map [i](#)



X



Y

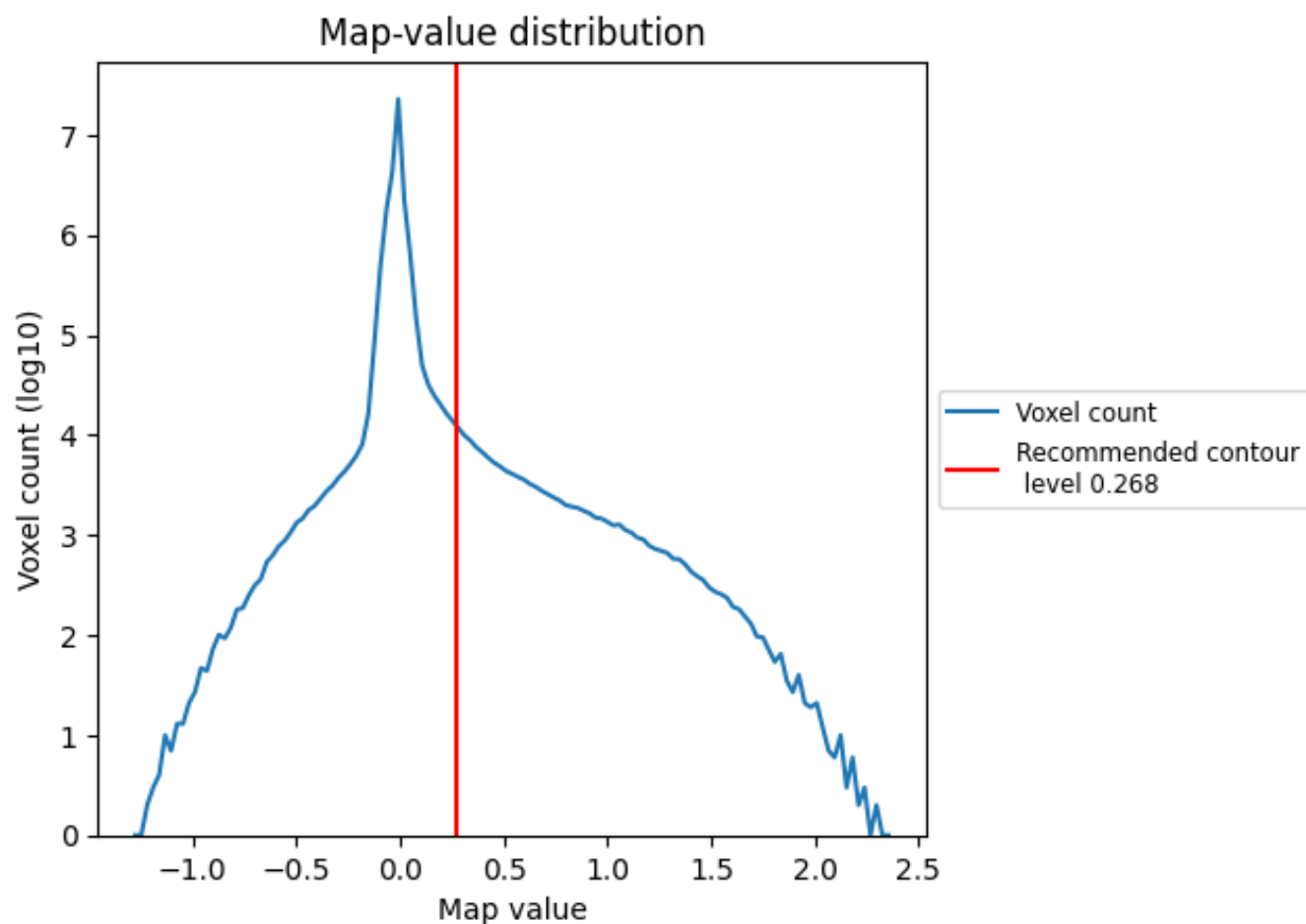


Z

7 Map analysis [i](#)

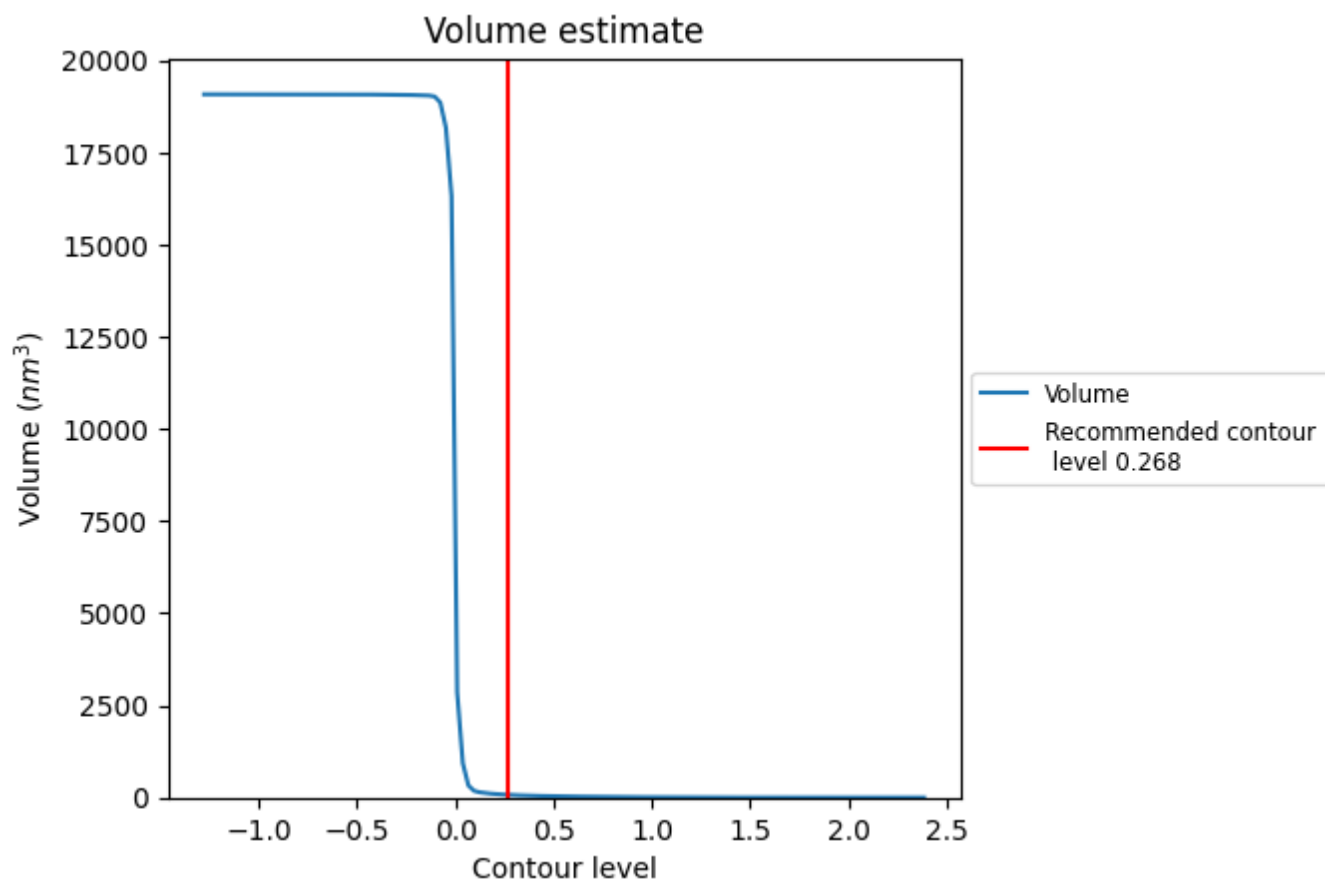
This section contains the results of statistical analysis of the map.

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.

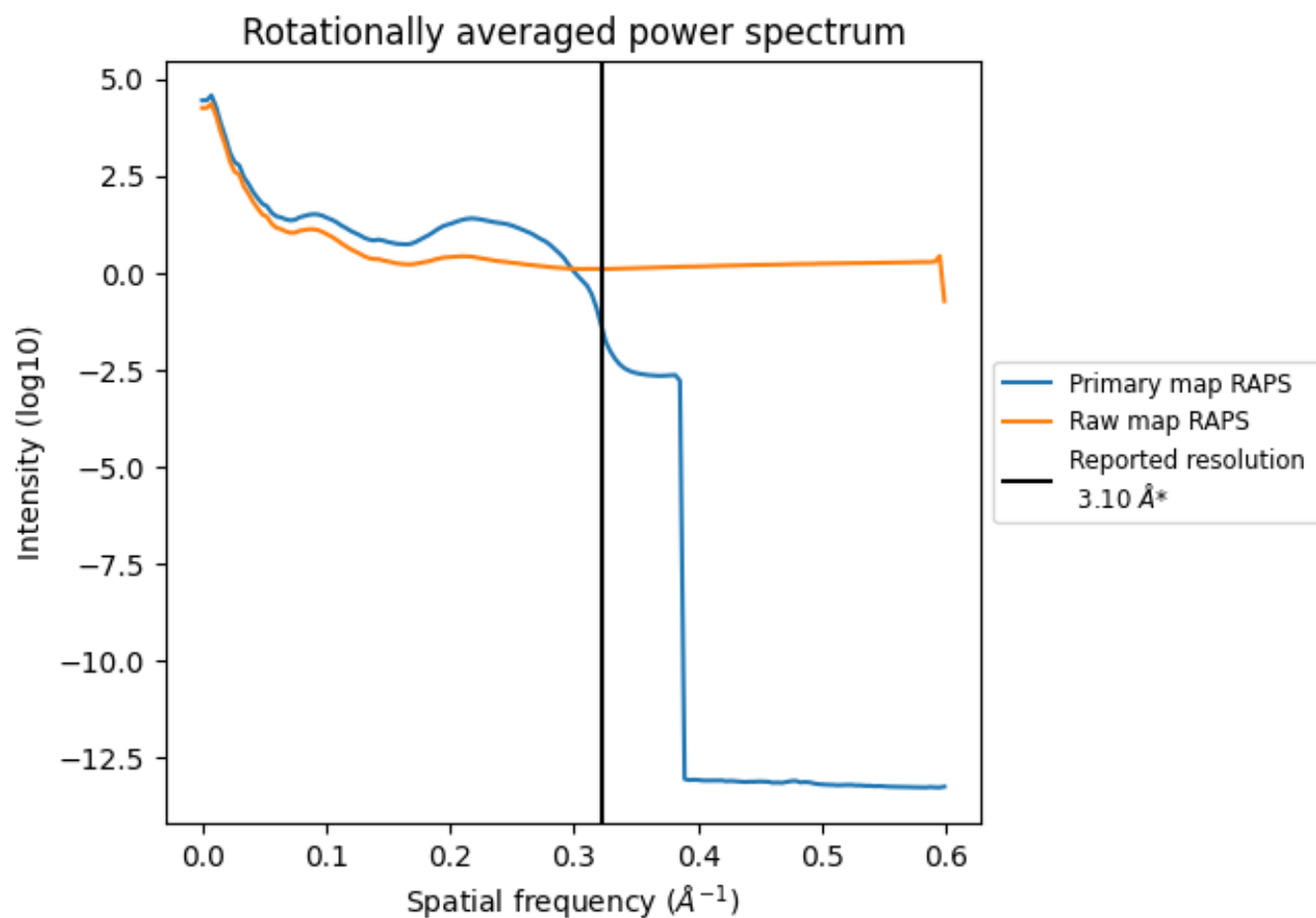
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 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 ⓘ

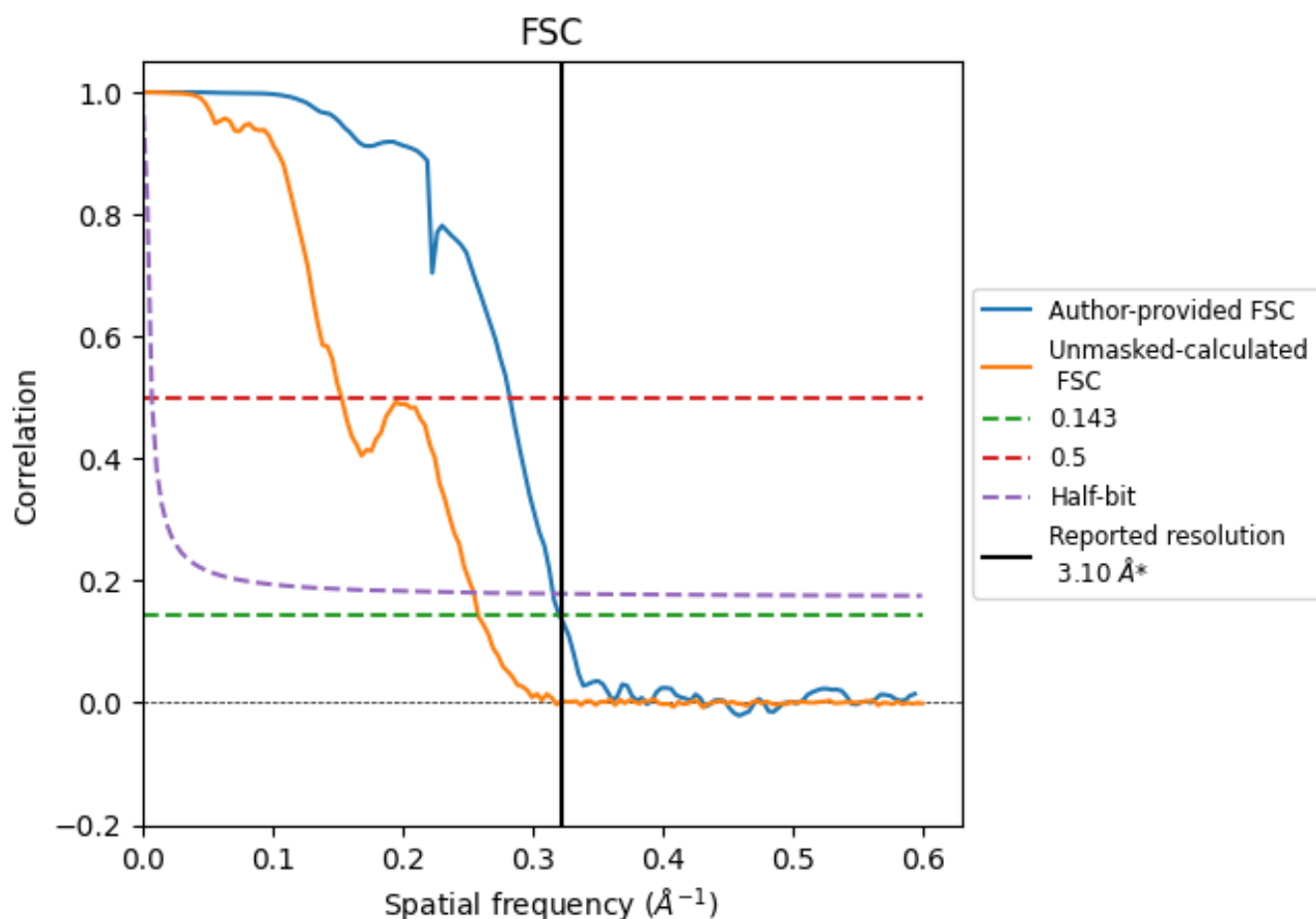


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

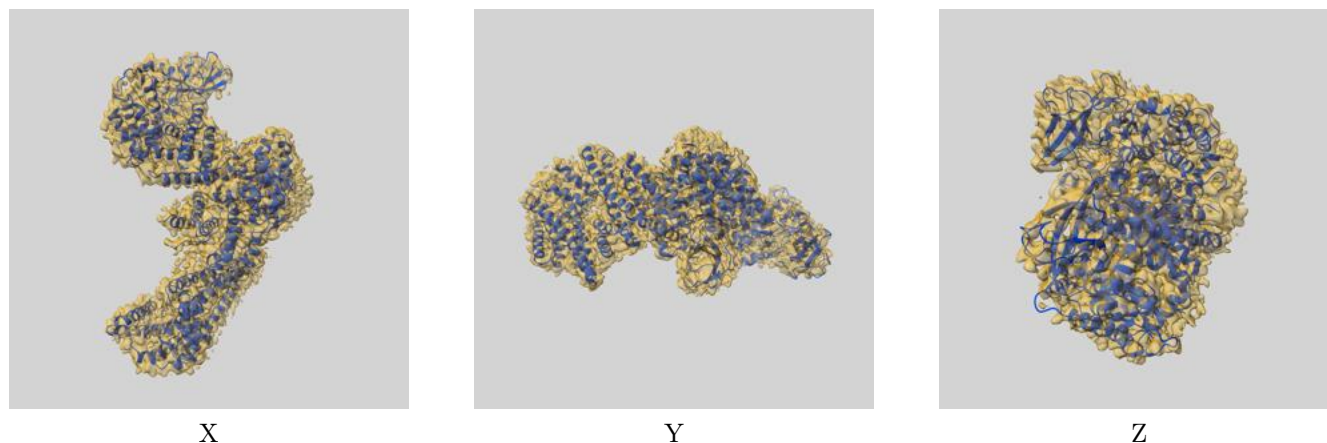
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.54	3.17
Unmasked-calculated*	3.88	6.54	3.93

*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 3.88 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

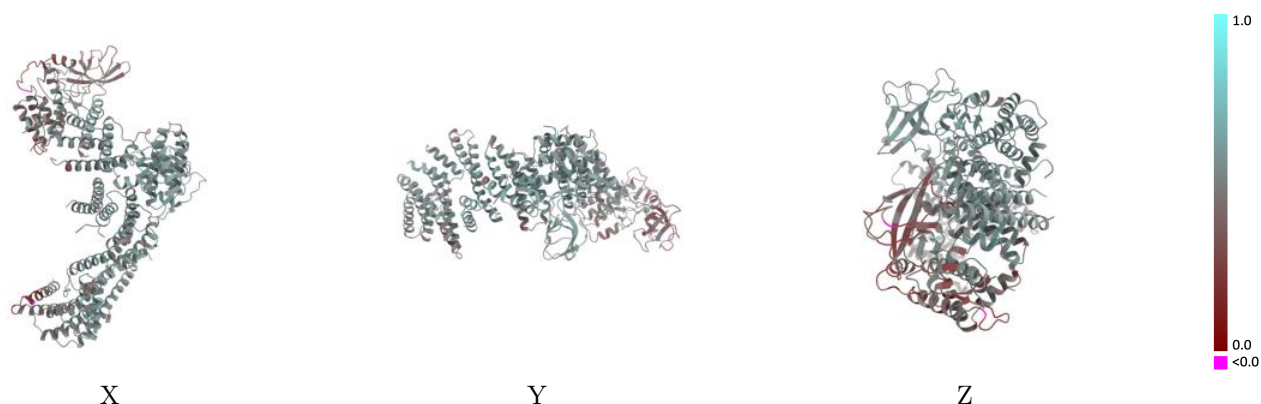
This section contains information regarding the fit between EMDB map EMD-27630 and PDB model 8DP5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



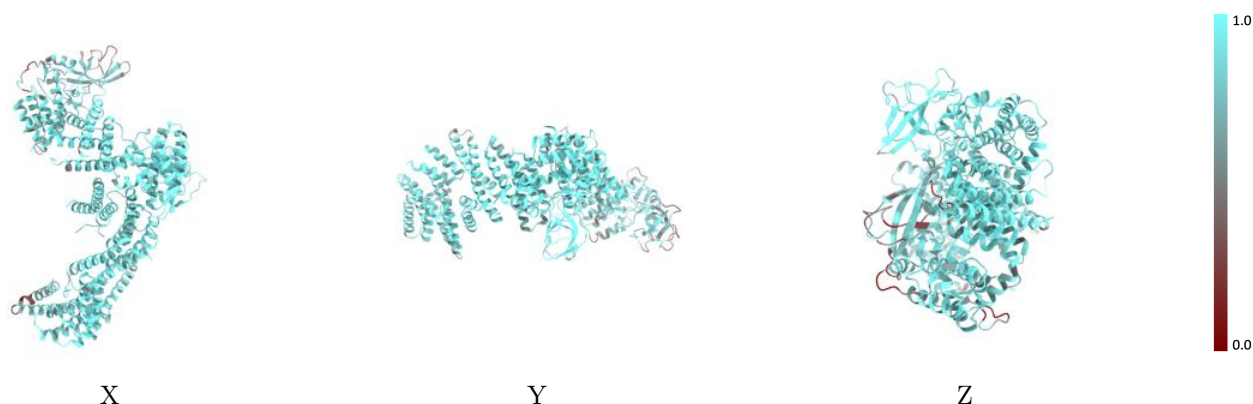
The images above show the 3D surface view of the map at the recommended contour level 0.268 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



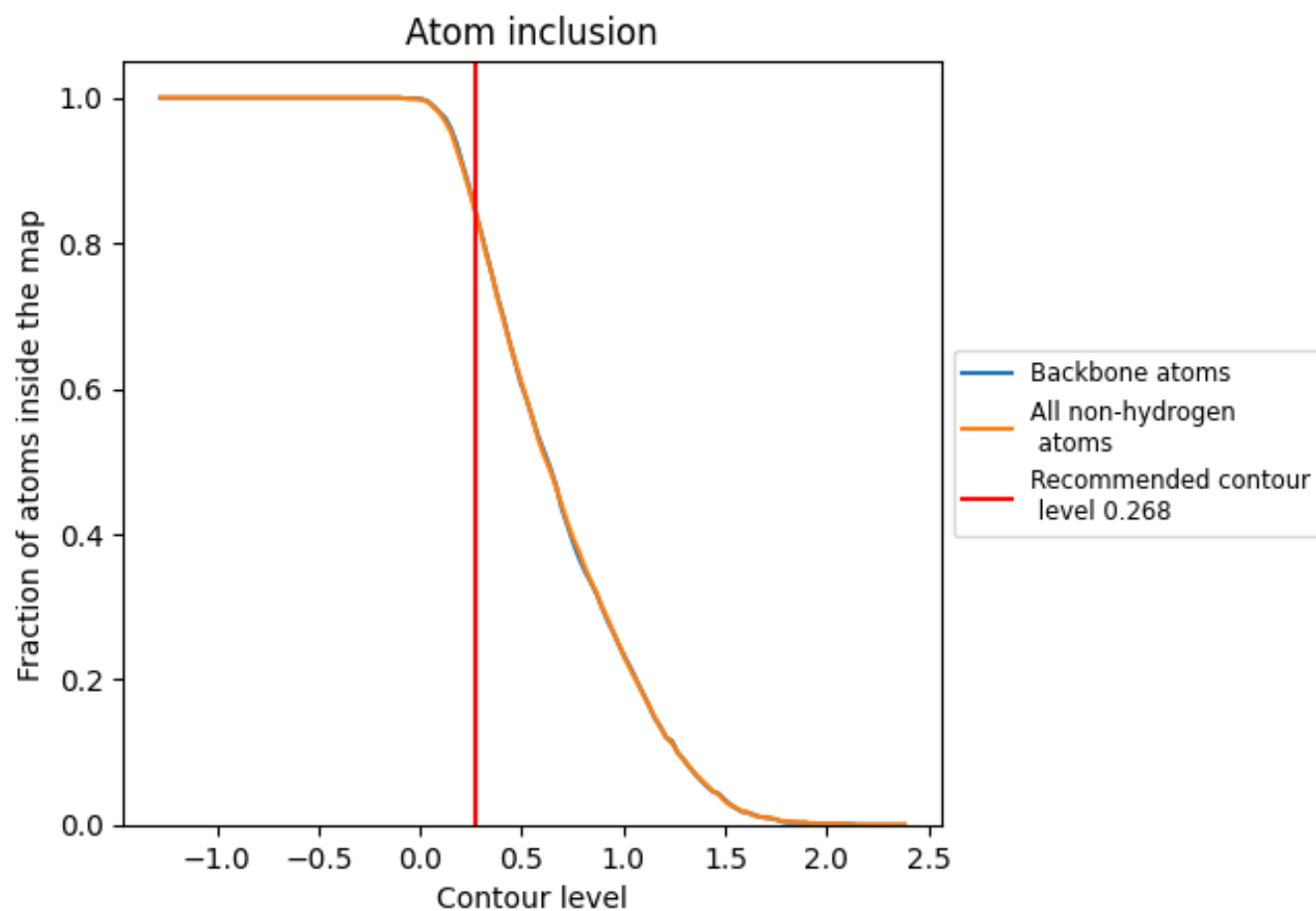
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.268).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.268) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.4930
A	0.9200	0.5420
B	0.7690	0.4180
C	0.8660	0.4840
D	0.8980	0.5390
E	0.8790	0.5000
P	0.8600	0.4730

1.0

0.0

<0.0