



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:43 AM EST

PDB ID : 7MYN
EMDB ID : EMD-24081
Title : Cryo-EM Structure of p110alpha in complex with p85alpha
Authors : Liu, X.; Yang, S.; Hart, J.R.; Xu, Y.; Zou, X.; Zhang, H.; Zhou, Q.; Xia, T.;
Zhang, Y.; Yang, D.; Wang, M.-W.; Vogt, P.K.
Deposited on : 2021-05-21
Resolution : 2.79 Å (reported)
Based on initial models : 6VO7, 2IUG, 4JPS, 2V1Y

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

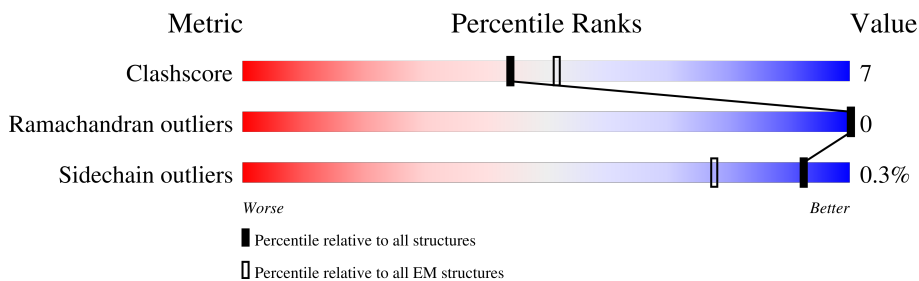
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1096	
2	B	723	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10426 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	977	8072	5164	1381	1461	66	11	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336
A	-1	GLY	-	expression tag	UNP P42336

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	276	2346	1469	419	451	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP P27986

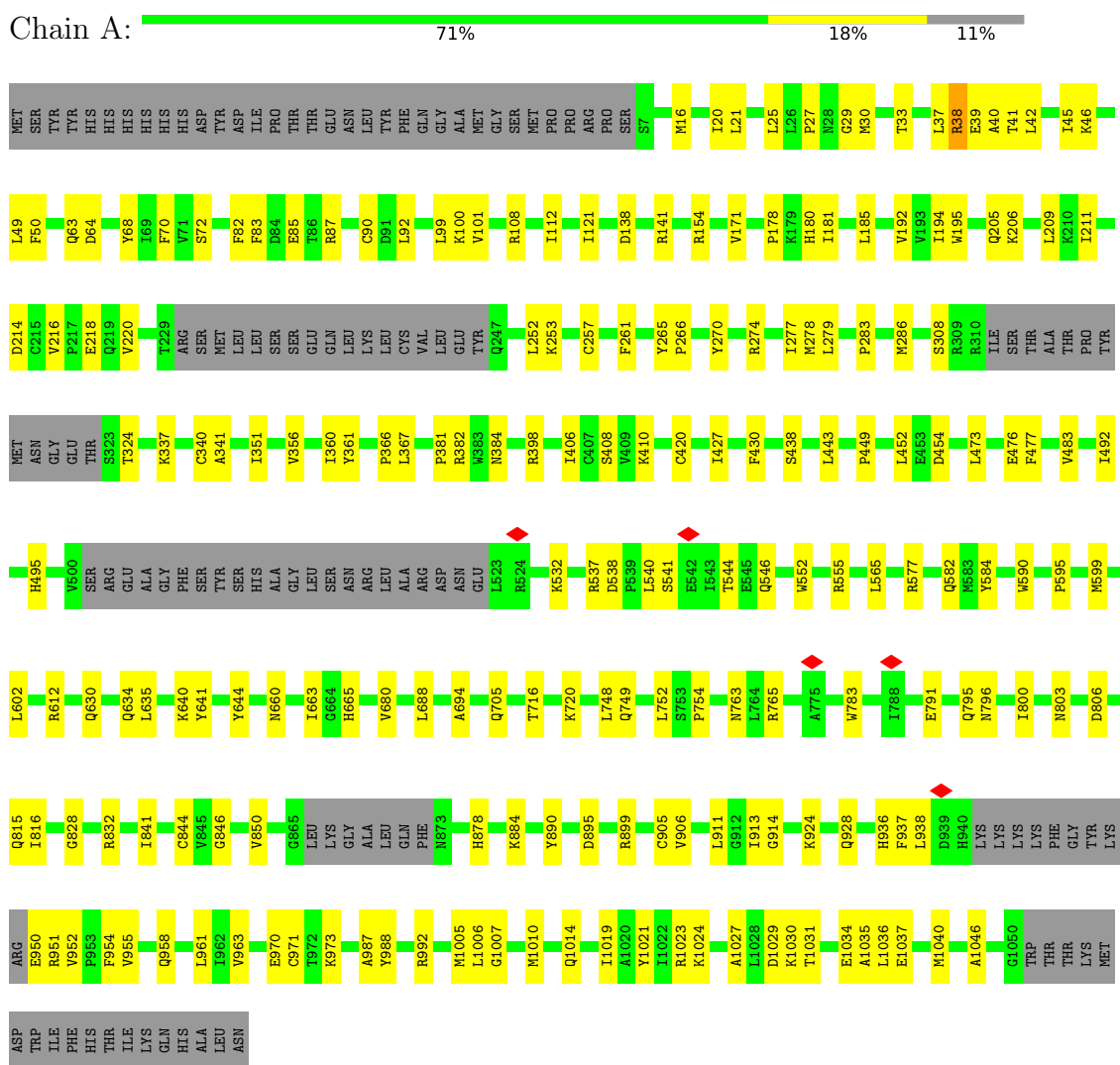
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	8	Total	O	0
			8	8	

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



THR	THR	PHE	LEU	TYR	GLN	GLN	R461	LEU	HIS
ALA	ALA	ALA	ALA	LEU	PRO	PRO	E462	VAL	CYS
PRO	PRO	PRO	ASP	LEU	ALA	ALA	R465	GLU	ILE
GLY	GLY	ASP	PHE	LYS	ALA	ALA	T473	ASP	ASN
TYR	ARG	ILE	ARG	PHE	LEU	PRO	T477	GLU	THR
GLY	ASP	ALA	TYR	LEU	PRO	PRO	K480	ASP	ALA
ARG	PHE	PRO	TYR	LYS	LEU	LEU	I484	PRO	ALA
THR	PRO	LEU	ASP	THR	LEU	LEU	F487	LEU	THR
GLY	ASP	LEU	LEU	LEU	LEU	LEU	I491	LEU	THR
THR	THR	LEU	LEU	THR	ASN	ASN	K492	LEU	HIS
VAL	VAL	LEU	LEU	LEU	ALA	ALA	I493	GLY	TYR
GLU	GLU	LEU	LEU	LEU	ASN	ASN	Q497	ASP	GLY
LEU	LEU	LEU	LEU	LEU	ASN	ASN	K501	GLY	PHE
LEU	LEU	LEU	LEU	LEU	ALA	ALA	K506	LEU	ALA
LEU	LEU	LEU	LEU	LEU	GLY	GLY	E507	LEU	ALA
LEU	LEU	LEU	LEU	LEU	MET	MET	E520	LEU	VAL
LEU	LEU	LEU	LEU	LEU	N323	N324	R523	LEU	ASN
LEU	LEU	LEU	LEU	LEU	N344	N344	R527	LEU	THR
LEU	LEU	LEU	LEU	LEU	L347	L347	K532	LEU	GLY
LEU	LEU	LEU	LEU	LEU	R348	R348	I535	LEU	THR
LEU	LEU	LEU	LEU	LEU	F855	F855	L549	LEU	PHE
LEU	LEU	LEU	LEU	LEU	T371	T371	Y580	LEU	ASP
LEU	LEU	LEU	LEU	LEU	L372	L372	L581	LEU	VAL
LEU	LEU	LEU	LEU	LEU	R373	R373	M582	LEU	ARG
LEU	LEU	LEU	LEU	LEU	N878	N878	R590	LEU	GLU
LEU	LEU	LEU	LEU	LEU	K382	K382	E591	LEU	GLY
LEU	LEU	LEU	LEU	LEU	I405	I405	K593	LEU	GLN
LEU	LEU	LEU	LEU	LEU	Y408	Y408	E596	LEU	ALA
LEU	LEU	LEU	LEU	LEU	R409	R409	M597	LEU	TYR
LEU	LEU	LEU	LEU	LEU	L413	L413	L598	LEU	ALA
LEU	LEU	LEU	LEU	LEU	L424	L424	GLY	LEU	SER
LEU	LEU	LEU	LEU	LEU	K430	K430	ASN	LEU	VAL
LEU	LEU	LEU	LEU	LEU	Q433	Q433	GLU	LEU	VAL
LEU	LEU	LEU	LEU	LEU	E439	E439	ASN	LEU	VAL
LEU	LEU	LEU	LEU	LEU	D440	D440	GLU	LEU	VAL
LEU	LEU	LEU	LEU	LEU	L449	L449	ASN	LEU	VAL
LEU	LEU	LEU	LEU	LEU	H450	H450	THR	LEU	VAL
LEU	LEU	LEU	LEU	LEU	E458	E458	ASP	LEU	VAL
LEU	LEU	LEU	LEU	LEU	GLN	GLN	TYR	LEU	LYS
LEU	LEU	LEU	LEU	LEU	TYR	TYR	SER	LEU	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	332105	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	46685	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.047	Depositor
Minimum map value	-3.780	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.394	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	105.545, 141.075, 115.994995	wwPDB
Map dimensions	111, 135, 101	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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	0.26	0/8252	0.52	0/11152
2	B	0.25	0/2386	0.55	1/3197 (0.0%)
All	All	0.26	0/10638	0.53	1/14349 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	413	LEU	CA-CB-CG	5.15	127.14	115.30

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	8072	0	8074	121	0
2	B	2346	0	2321	29	0
3	A	8	0	0	0	0
All	All	10426	0	10395	143	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 7.

All (143) 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:A:37:LEU:HB3	1:A:40:ALA:HB2	1.75	0.67
1:A:544:THR:HG21	2:B:382:LYS:HB2	1.77	0.66
1:A:716:THR:HG21	1:A:803:ASN:HB3	1.78	0.64
1:A:454:ASP:OD1	2:B:348:ARG:NH1	2.30	0.64
1:A:356:VAL:HG22	1:A:406:ILE:HG12	1.78	0.64
1:A:100:LYS:HE3	2:B:493:ILE:HG23	1.80	0.63
1:A:878:HIS:HE2	1:A:890:TYR:HH	1.45	0.63
1:A:1010:MET:O	1:A:1014:GLN:NE2	2.32	0.63
1:A:38:ARG:NH1	1:A:90:CYS:SG	2.72	0.62
1:A:640:LYS:HE2	1:A:680:VAL:HG21	1.82	0.62
1:A:1023:ARG:NH2	1:A:1029:ASP:OD1	2.34	0.60
1:A:895:ASP:OD2	1:A:899:ARG:NH1	2.35	0.59
1:A:252:LEU:HB2	1:A:261:PHE:HB2	1.84	0.58
1:A:546:GLN:NE2	2:B:382:LYS:O	2.36	0.58
1:A:138:ASP:OD1	1:A:141:ARG:NH2	2.36	0.58
1:A:992:ARG:NH2	1:A:1030:LYS:O	2.38	0.57
1:A:537:ARG:NE	1:A:541:SER:OG	2.38	0.56
1:A:340:CYS:HB3	1:A:382:ARG:HD2	1.86	0.56
1:A:427:ILE:HD11	1:A:443:LEU:HD22	1.87	0.55
1:A:337:LYS:HB3	1:A:476:GLU:HB3	1.87	0.55
1:A:185:LEU:HD21	1:A:277:ILE:HD12	1.88	0.55
1:A:988:TYR:HE1	1:A:1035:ALA:HB1	1.72	0.55
1:A:716:THR:HG22	1:A:720:LYS:HD2	1.89	0.54
2:B:458:GLU:HA	2:B:461:ARG:HG2	1.90	0.54
1:A:954[B]:PHE:HB3	1:A:1046:ALA:HB2	1.90	0.54
2:B:347:LEU:HD12	2:B:373:ARG:HB2	1.89	0.53
1:A:25:LEU:HB2	1:A:100:LYS:HA	1.90	0.53
1:A:351:ILE:HG21	1:A:408:SER:HB2	1.89	0.53
2:B:430:LYS:O	2:B:433:GLN:NE2	2.42	0.53
1:A:16:MET:HB2	1:A:20:ILE:HD11	1.90	0.53
1:A:214:ASP:HA	1:A:266:PRO:HB3	1.91	0.52
1:A:540:LEU:HB2	1:A:1023:ARG:HD2	1.91	0.52
1:A:121:ILE:HG12	1:A:688:LEU:HB3	1.91	0.52
1:A:42:LEU:HD21	1:A:92:LEU:HD11	1.92	0.52
1:A:216:VAL:HG12	1:A:218:GLU:H	1.75	0.52
2:B:590:ARG:HG2	2:B:593:LYS:H	1.75	0.51
1:A:253:LYS:NZ	1:A:257:CYS:O	2.41	0.51
1:A:806:ASP:HA	1:A:844:CYS:HA	1.93	0.51
2:B:532:LYS:HD3	2:B:535:ILE:HD11	1.92	0.51
1:A:913:ILE:HA	1:A:937:PHE:HA	1.92	0.51
1:A:29:GLY:O	2:B:501:GLN:NE2	2.44	0.51
1:A:141:ARG:HG2	1:A:308:SER:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:LYS:HB3	2:B:549:LEU:HD12	1.93	0.51
2:B:449:LEU:HD12	2:B:580:TYR:HB3	1.93	0.50
1:A:602:LEU:O	1:A:612:ARG:NH2	2.40	0.50
1:A:660:ASN:HB3	1:A:663:ILE:HB	1.94	0.50
1:A:961:LEU:HD12	1:A:971:CYS:HB3	1.94	0.50
1:A:552:TRP:O	1:A:555:ARG:NH1	2.39	0.50
1:A:194:ILE:HD12	1:A:209:LEU:HD13	1.94	0.49
1:A:41:THR:OG1	1:A:85:GLU:O	2.29	0.49
1:A:398:ARG:NH1	1:A:644:TYR:OH	2.32	0.49
1:A:72:SER:HB2	1:A:99:LEU:HD23	1.94	0.49
2:B:520:GLU:HA	2:B:523:ARG:HG2	1.94	0.49
1:A:253:LYS:HB3	1:A:286:MET:HB2	1.95	0.49
1:A:924:LYS:HD3	1:A:928:GLN:HB3	1.94	0.49
1:A:68:TYR:HB3	1:A:101:VAL:HG13	1.95	0.49
1:A:154:ARG:NH2	1:A:694:ALA:O	2.42	0.48
1:A:25:LEU:HD12	2:B:497:GLN:HG2	1.96	0.48
1:A:878:HIS:HB2	1:A:963:VAL:HG22	1.95	0.48
1:A:951[B]:ARG:HB2	1:A:1021:TYR:HE1	1.77	0.48
1:A:1037:GLU:N	1:A:1037:GLU:OE1	2.47	0.48
1:A:538:ASP:OD2	1:A:1023:ARG:NE	2.35	0.48
1:A:800:ILE:HG12	1:A:850:VAL:HG22	1.95	0.48
1:A:958:GLN:HA	1:A:961:LEU:HB2	1.95	0.48
1:A:37:LEU:HD23	1:A:39:GLU:H	1.79	0.47
1:A:360:ILE:HG22	1:A:367:LEU:HD12	1.96	0.47
1:A:937:PHE:HD1	1:A:938:LEU:HD13	1.78	0.47
1:A:495:HIS:CE1	1:A:577:ARG:HE	2.33	0.47
1:A:791:GLU:HA	1:A:795:GLN:HG2	1.96	0.47
1:A:30:MET:SD	2:B:527:ASN:ND2	2.88	0.47
2:B:405:ILE:O	2:B:409:ARG:HB2	2.15	0.47
1:A:21:LEU:HD12	1:A:33:THR:HG22	1.98	0.46
1:A:45:ILE:O	1:A:49:LEU:HB2	2.14	0.46
1:A:408:SER:OG	1:A:420:CYS:SG	2.68	0.46
1:A:279:LEU:HA	1:A:832:ARG:HH12	1.82	0.45
1:A:438:SER:HA	1:A:477:PHE:HB2	1.98	0.45
1:A:449:PRO:HD2	1:A:452:LEU:HD22	1.98	0.45
1:A:178:PRO:HD2	1:A:181:ILE:HD11	1.96	0.45
1:A:361:TYR:CZ	1:A:366:PRO:HG3	2.50	0.45
1:A:634:GLN:HG3	1:A:1005:MET:HG2	1.98	0.45
2:B:473:THR:O	2:B:477:ILE:HG12	2.16	0.45
2:B:408:TYR:HB3	2:B:424:LEU:HD13	1.99	0.45
1:A:63:GLN:HG3	1:A:64:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:GLN:O	1:A:815:GLN:NE2	2.50	0.45
1:A:992:ARG:NH2	1:A:1027:ALA:O	2.50	0.45
2:B:487:PHE:O	2:B:491:ILE:HG12	2.17	0.45
1:A:748:LEU:HD12	1:A:783:TRP:HZ2	1.82	0.45
1:A:906:VAL:HG21	1:A:987:ALA:HB3	1.98	0.45
1:A:816:ILE:HG21	1:A:911:LEU:HD21	1.98	0.45
1:A:42:LEU:HB2	1:A:85:GLU:HA	2.00	0.44
1:A:905:CYS:HB3	1:A:954[B]:PHE:CZ	2.53	0.44
1:A:430:PHE:O	1:A:644:TYR:OH	2.28	0.44
1:A:555:ARG:NH2	1:A:582:GLN:OE1	2.47	0.44
2:B:462:GLU:OE1	2:B:465:ARG:NH2	2.51	0.44
1:A:1006:LEU:HD21	1:A:1019:ILE:HD11	1.98	0.44
1:A:950[B]:GLU:HG3	1:A:1024:LYS:HD2	2.00	0.44
1:A:410:LYS:HA	1:A:410:LYS:HD2	1.87	0.44
1:A:46:LYS:HB2	1:A:46:LYS:HE3	1.66	0.43
1:A:50:PHE:HZ	1:A:68:TYR:HD2	1.65	0.43
1:A:841:ILE:HG12	1:A:846:GLY:HA2	2.00	0.43
1:A:83:PHE:CD2	1:A:108:ARG:HA	2.54	0.43
2:B:506:LYS:HD2	2:B:506:LYS:HA	1.81	0.43
1:A:42:LEU:HD23	1:A:45:ILE:HD12	2.00	0.43
1:A:914:GLY:N	1:A:936:HIS:O	2.52	0.43
1:A:324:THR:HG22	1:A:483:VAL:HB	2.01	0.43
1:A:382:ARG:NH1	1:A:384:ASN:HB2	2.34	0.43
1:A:1031:THR:HG23	1:A:1034:GLU:H	1.84	0.43
1:A:195:TRP:CZ3	1:A:206:LYS:HB3	2.54	0.43
2:B:480:LYS:O	2:B:484:ILE:HG12	2.18	0.43
1:A:340:CYS:O	1:A:473:LEU:HD12	2.18	0.42
1:A:641:TYR:OH	1:A:1007:GLY:N	2.52	0.42
1:A:705:GLN:HE21	1:A:752:LEU:HB2	1.84	0.42
1:A:83:PHE:HB2	1:A:112:ILE:HD11	2.01	0.42
1:A:171:VAL:HG11	1:A:265:TYR:HD2	1.83	0.42
2:B:440:ASP:N	2:B:440:ASP:OD1	2.53	0.42
1:A:749:GLN:HE22	1:A:763:ASN:HA	1.84	0.42
2:B:450:HIS:HD2	2:B:597:TRP:HB3	1.85	0.42
1:A:341:ALA:HB3	1:A:381:PRO:HB2	2.01	0.42
1:A:884:LYS:HD2	1:A:884:LYS:HA	1.80	0.42
1:A:970:GLU:OE1	1:A:973:LYS:NZ	2.49	0.42
1:A:532:LYS:HB3	1:A:532:LYS:HE3	1.86	0.42
2:B:532:LYS:HA	2:B:535:ILE:HG12	2.02	0.42
1:A:595:PRO:O	1:A:599:MET:HG3	2.19	0.42
1:A:87:ARG:HE	1:A:92:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ILE:HG21	1:A:584:TYR:HD2	1.84	0.41
2:B:344:ASN:OD1	2:B:378:ASN:ND2	2.39	0.41
1:A:192:VAL:HG23	1:A:283:PRO:HB2	2.02	0.41
1:A:765:ARG:NH1	1:A:796:ASN:OD1	2.53	0.41
1:A:82:PHE:CE1	1:A:92:LEU:HD22	2.55	0.41
1:A:171:VAL:HG12	1:A:270:TYR:HA	2.02	0.41
2:B:598:LEU:HD23	2:B:598:LEU:HA	1.93	0.41
1:A:665:HIS:CE1	1:A:754:PRO:HA	2.56	0.41
1:A:27:PRO:HD3	1:A:101:VAL:HB	2.02	0.41
1:A:42:LEU:HD22	1:A:70:PHE:HD2	1.86	0.41
1:A:180:HIS:HD2	1:A:828:GLY:HA2	1.86	0.41
1:A:1036:LEU:O	1:A:1040:MET:HG2	2.21	0.41
1:A:635:LEU:HD23	1:A:635:LEU:HA	1.96	0.41
1:A:274:ARG:O	1:A:278:MET:HG2	2.20	0.40
1:A:565:LEU:HD13	1:A:590:TRP:CE2	2.56	0.40
2:B:355:PHE:HA	2:B:371:THR:O	2.21	0.40
2:B:592:LYS:HA	2:B:592:LYS:HD2	1.91	0.40
1:A:688:LEU:HD23	1:A:688:LEU:HA	1.86	0.40
1:A:211:ILE:HD12	1:A:220:VAL:HG22	2.03	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	975/1096 (89%)	950 (97%)	25 (3%)	0	100	100
2	B	274/723 (38%)	270 (98%)	4 (2%)	0	100	100
All	All	1249/1819 (69%)	1220 (98%)	29 (2%)	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	904/999 (90%)	898 (99%)	6 (1%)	84	95
2	B	257/653 (39%)	257 (100%)	0	100	100
All	All	1161/1652 (70%)	1155 (100%)	6 (0%)	92	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	205	GLN
1	A	952[A]	VAL
1	A	952[B]	VAL
1	A	955[A]	VAL
1	A	955[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1014	GLN
2	B	385	HIS

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 monosaccharides 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.

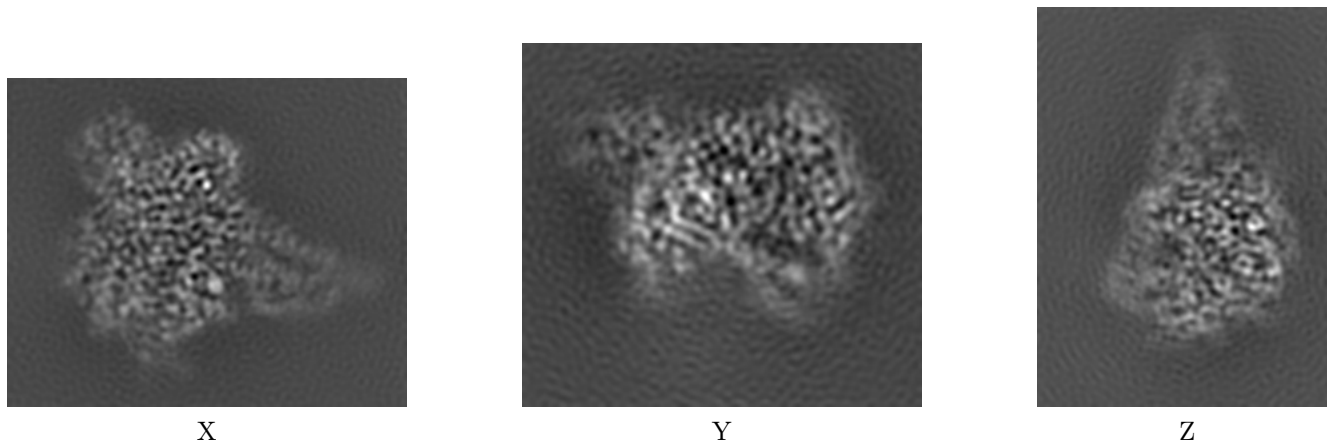
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24081. These allow visual inspection of the internal detail of the map and identification of artifacts.

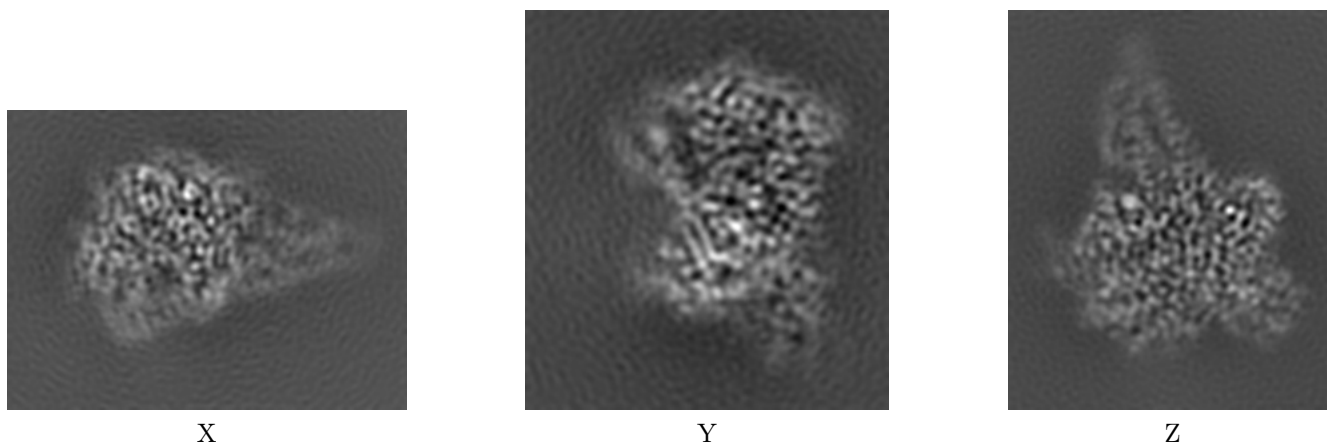
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



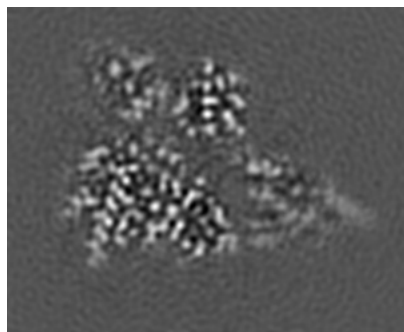
6.1.2 Raw map



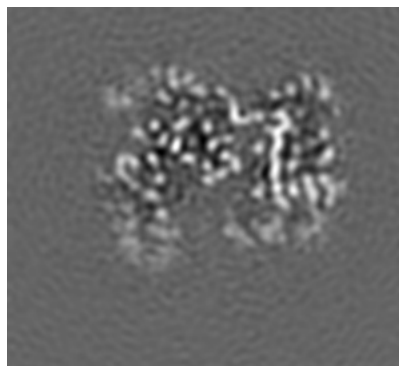
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

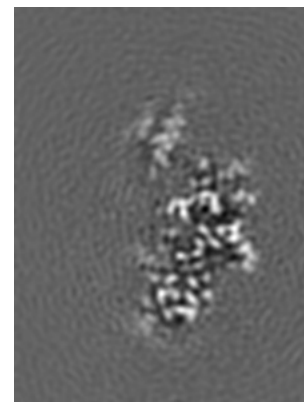
6.2.1 Primary map



X Index: 50

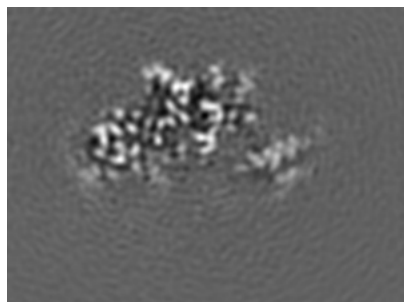


Y Index: 67

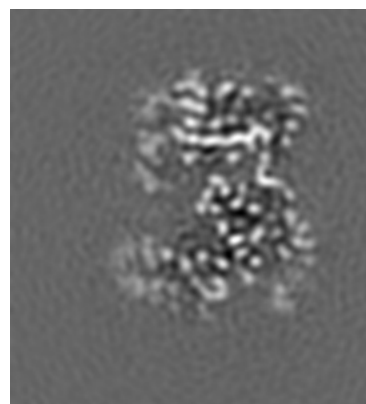


Z Index: 55

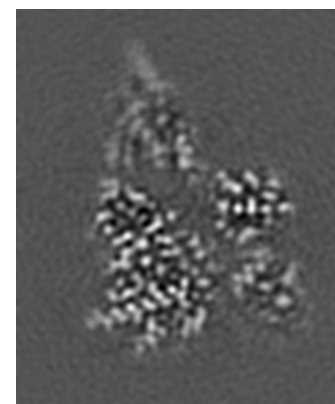
6.2.2 Raw map



X Index: 55



Y Index: 67

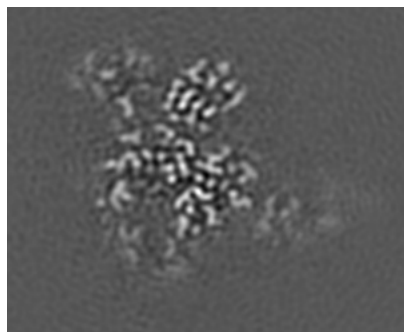


Z Index: 50

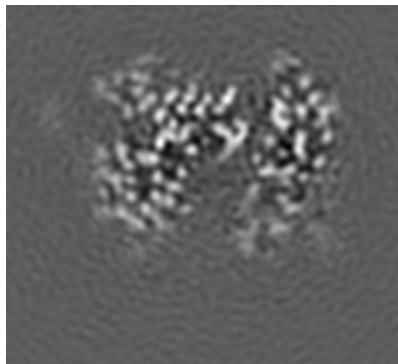
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

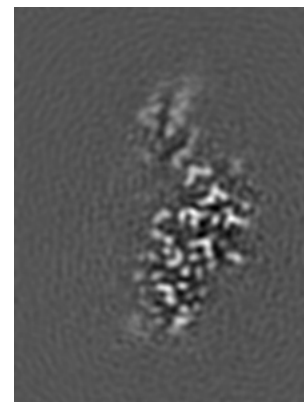
6.3.1 Primary map



X Index: 63

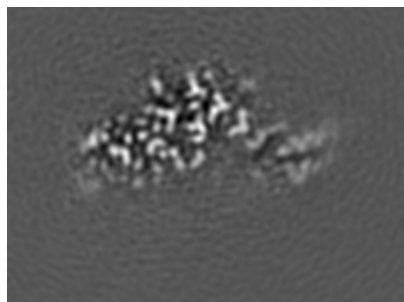


Y Index: 61

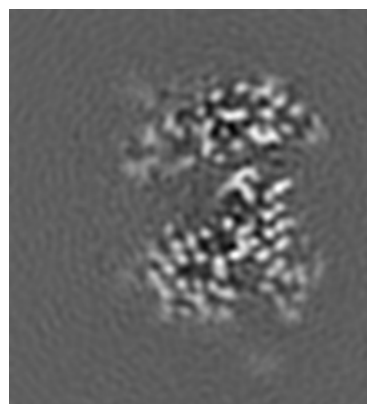


Z Index: 52

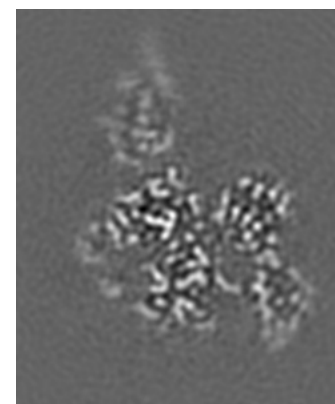
6.3.2 Raw map



X Index: 52



Y Index: 61

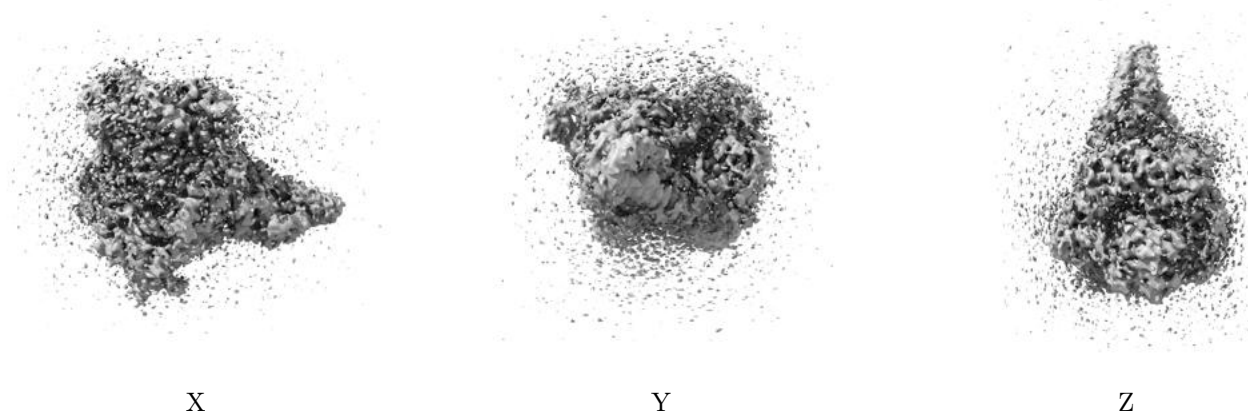


Z Index: 60

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

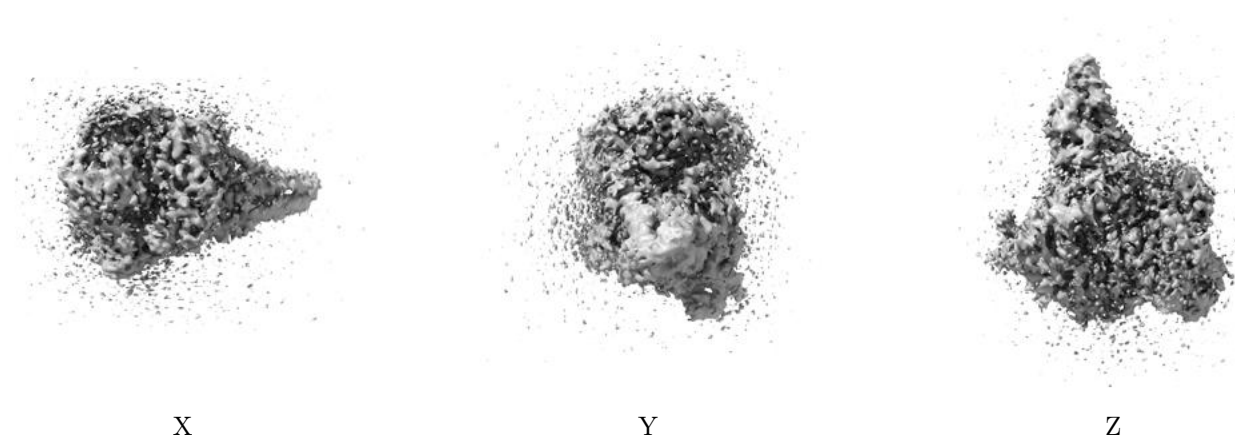
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

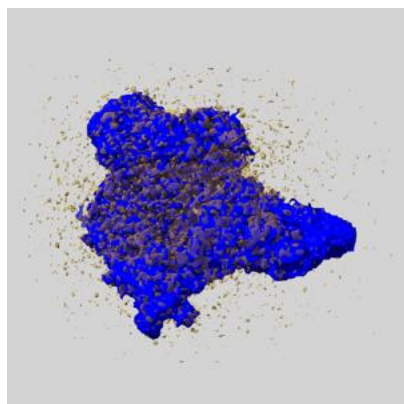
6.5 Mask visualisation [i](#)

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

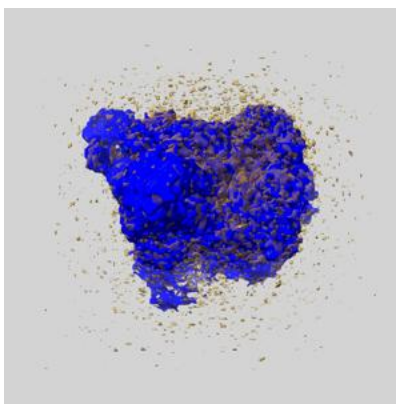
A mask typically either:

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

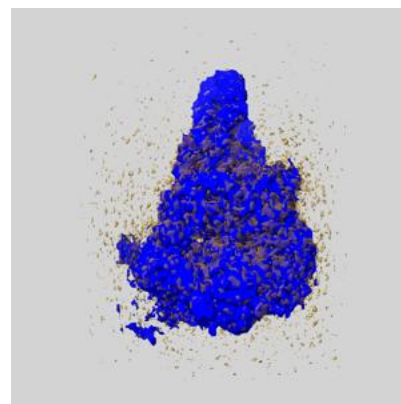
6.5.1 emd_24081_msk_1.map [i](#)



X



Y

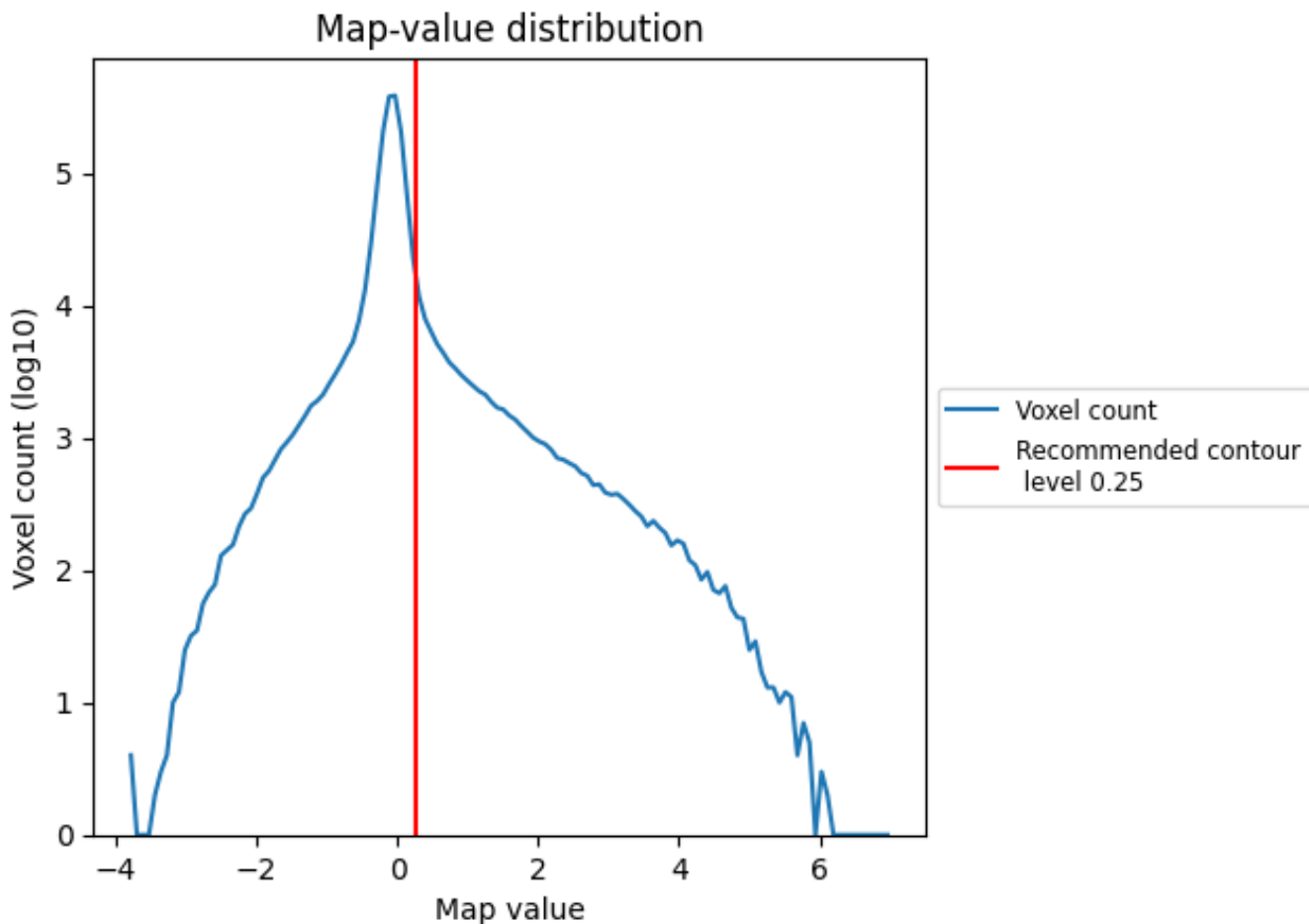


Z

7 Map analysis [i](#)

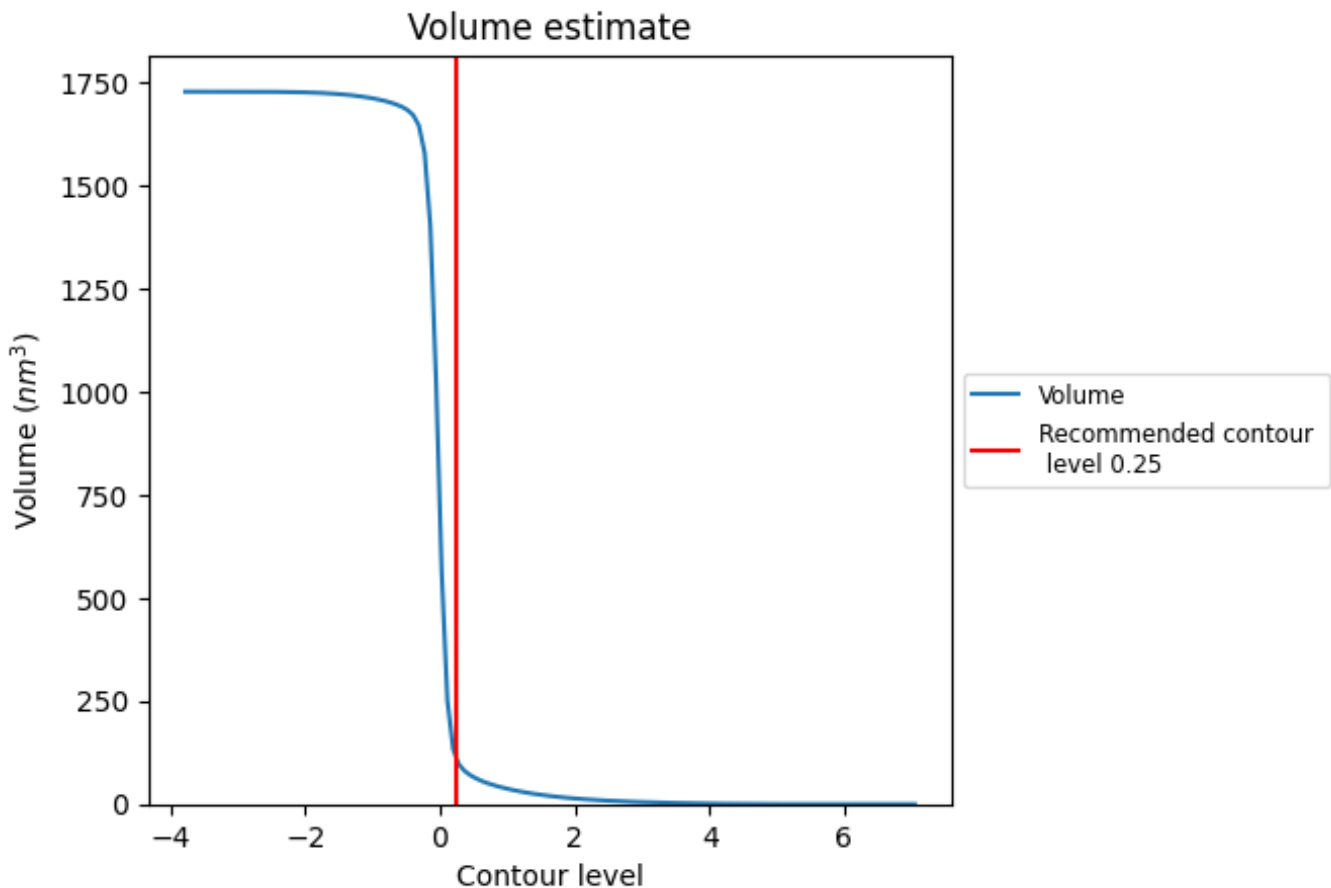
This section contains the results of statistical analysis of the map.

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 110 nm³; this corresponds to an approximate mass of 99 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.

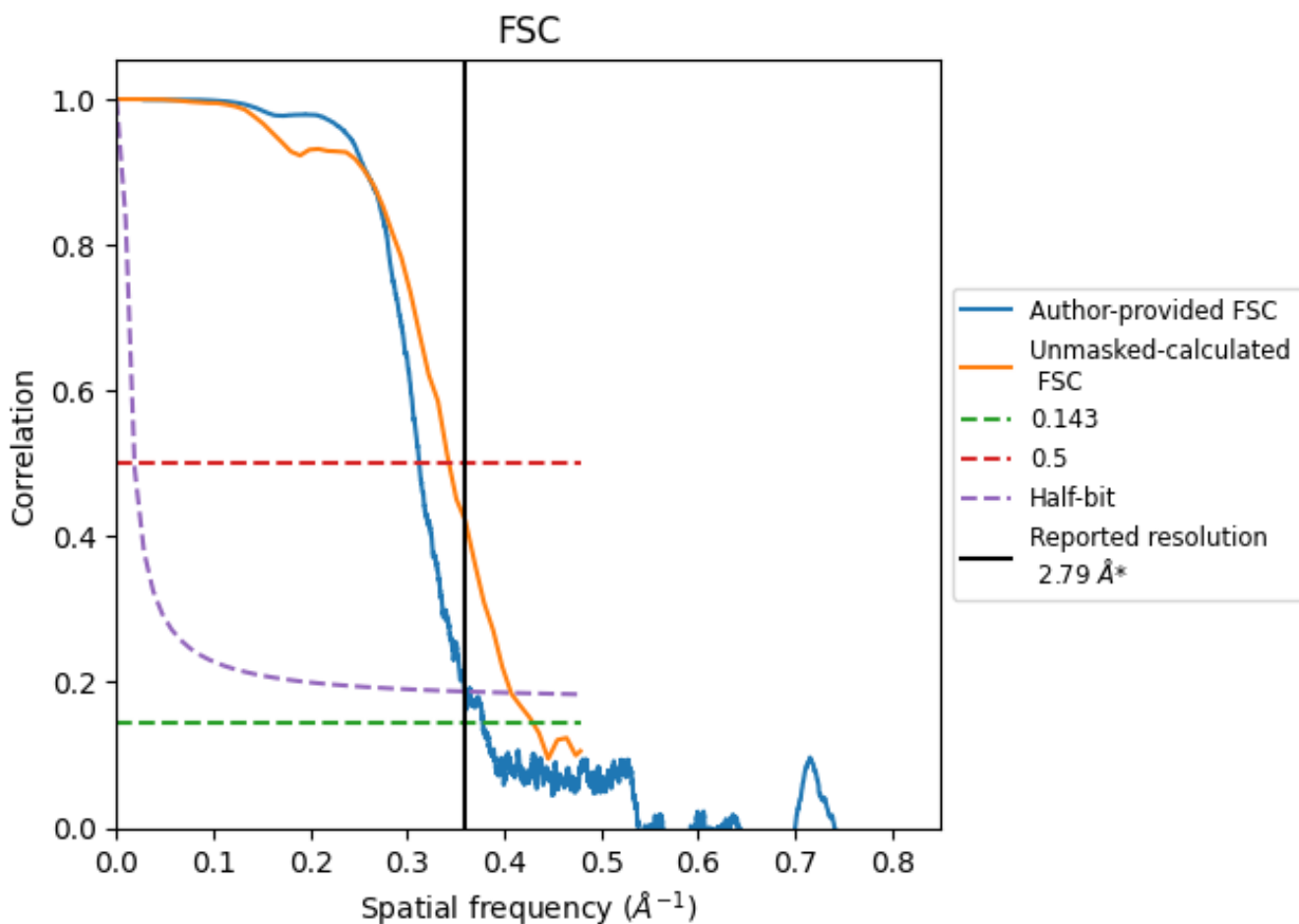
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.358 Å⁻¹

8.2 Resolution estimates [i](#)

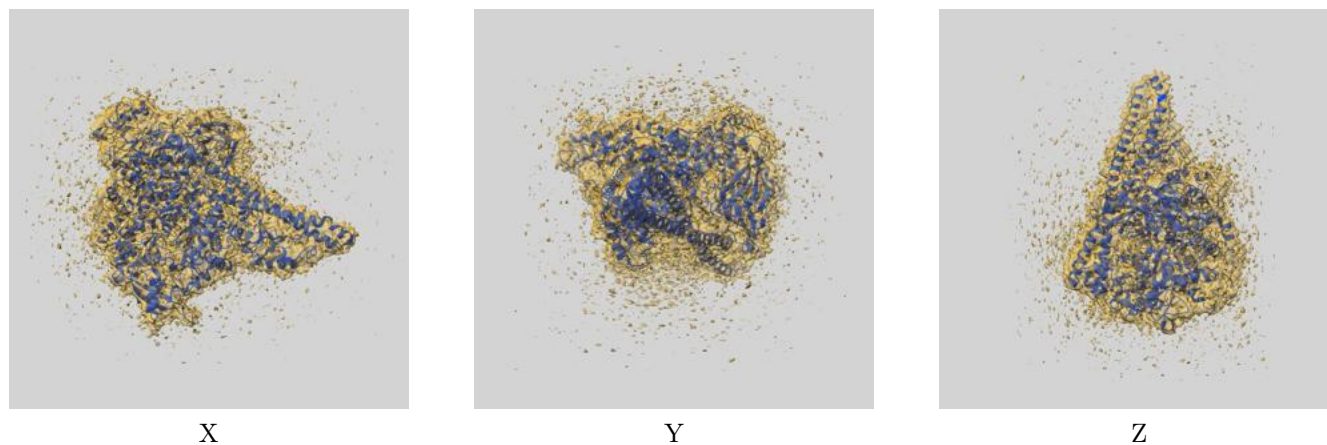
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.65	3.20	2.78
Unmasked-calculated*	2.33	2.92	2.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.33 differs from the reported value 2.79 by more than 10 %

9 Map-model fit [i](#)

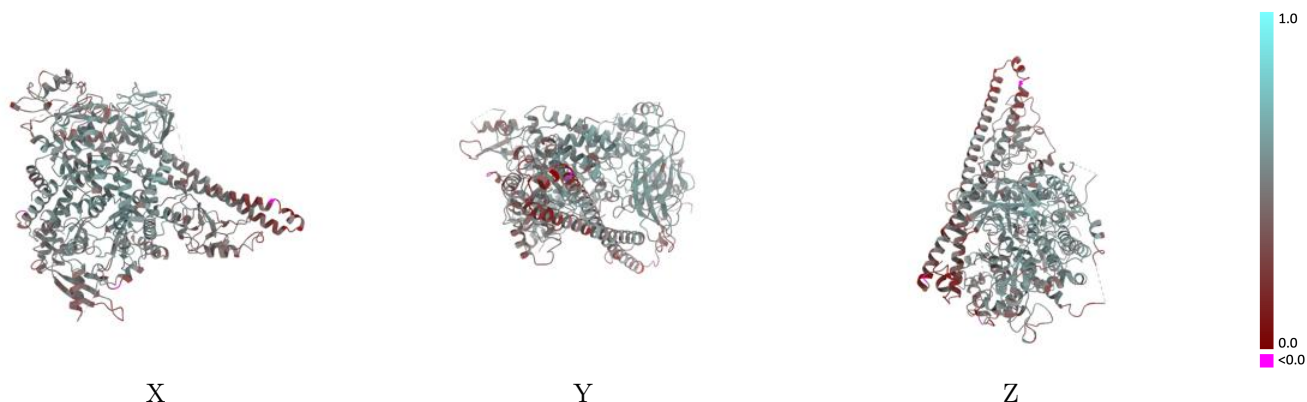
This section contains information regarding the fit between EMDB map EMD-24081 and PDB model 7MYN. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.25 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](#)



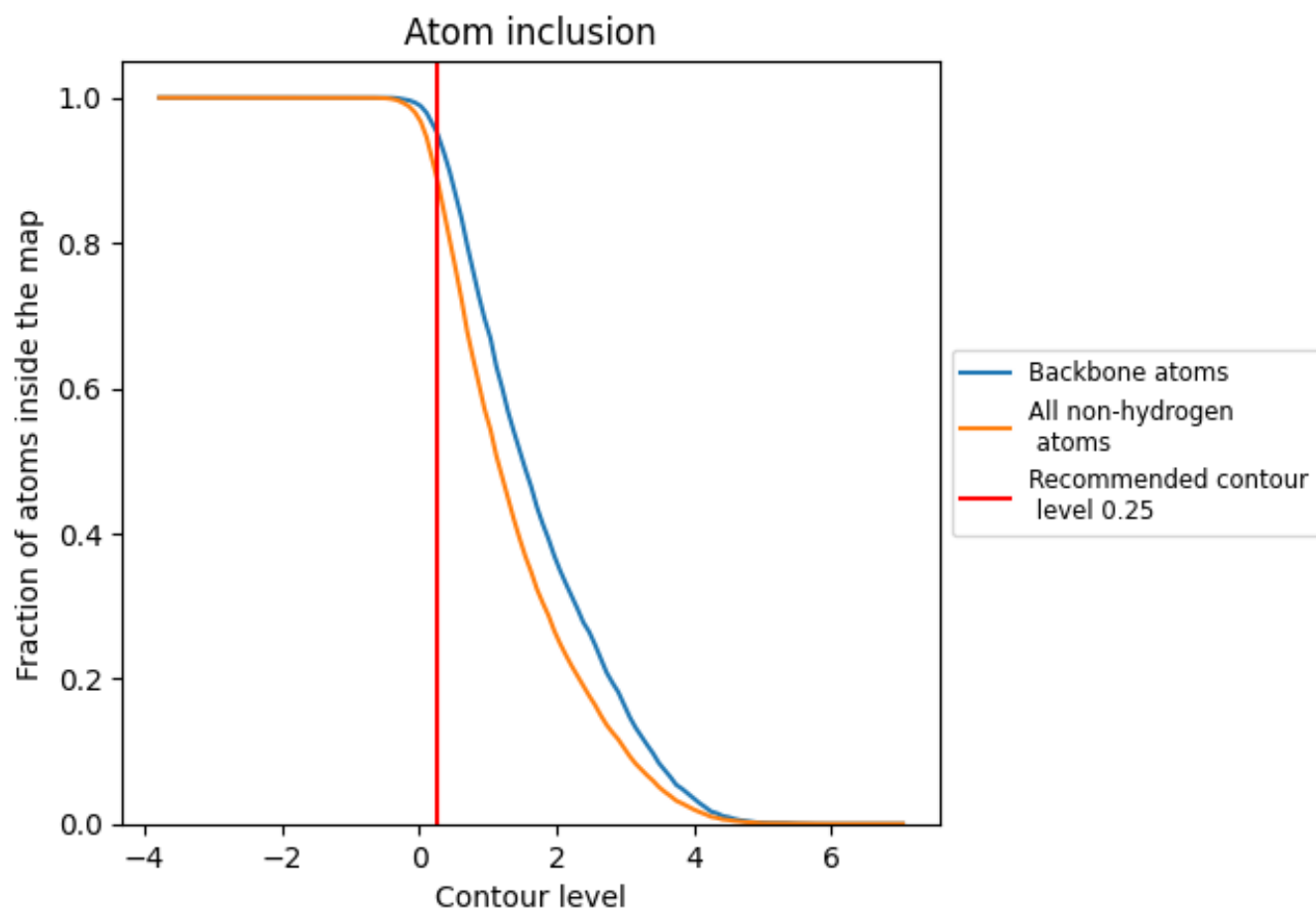
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).







9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8932	 0.4720
A	 0.9068	 0.4950
B	 0.8462	 0.3930

