



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:55 PM UTC

PDB ID : 8JAL / pdb_00008jal
EMDB ID : EMD-36129
Title : Structure of CRL2APPBP2 bound with RxxGP degron (dimer)
Authors : Zhao, S.; Zhang, K.; Xu, C.
Deposited on : 2023-05-06
Resolution : 3.30 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:

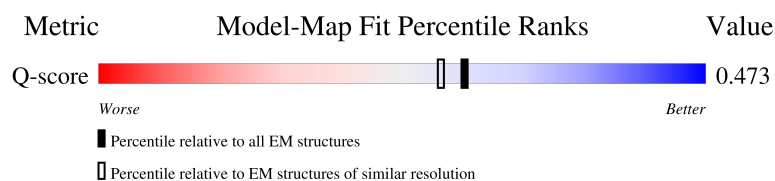
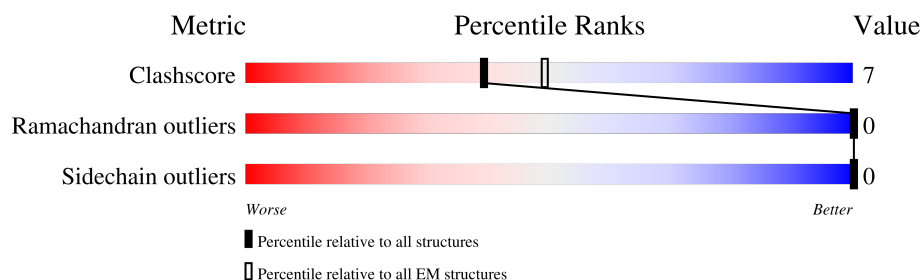
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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.



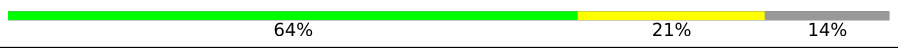
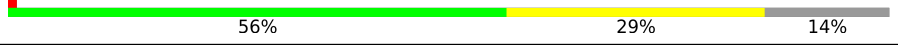
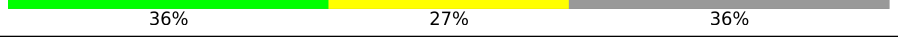
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	585	 83% 15% .
1	B	585	 81% 17% .
2	E	745	 27% 10% 62%
2	I	745	 31% 7% 62%

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Mol	Chain	Length	Quality of chain
3	C	118	
3	G	118	
4	D	112	
4	H	112	
5	F	11	
5	S	11	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17226 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 Amyloid protein-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	571	Total	C	N	O	S	0	0
			4613	2946	796	850	21		
1	B	573	Total	C	N	O	S	0	0
			4630	2955	799	855	21		

- Molecule 2 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	282	Total	C	N	O	S	0	0
			2382	1526	407	432	17		
2	I	282	Total	C	N	O	S	0	0
			2382	1526	407	432	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	THR	-	expression tag	UNP Q13617
I	1	THR	-	expression tag	UNP Q13617

- Molecule 3 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	105	Total	C	N	O	S	0	0
			830	525	140	161	4		
3	G	96	Total	C	N	O	S	0	0
			758	479	129	147	3		

- Molecule 4 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			760	487	122	145	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	96	Total	C	N	O	S	0	0
			760	487	122	145	6		

- Molecule 5 is a protein called LEU-THR-ARG-ASN-LYS-GLY-PRO.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	7	Total	C	N	O	0	0
			55	33	12	10		
5	F	7	Total	C	N	O	0	0
			55	33	12	10		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

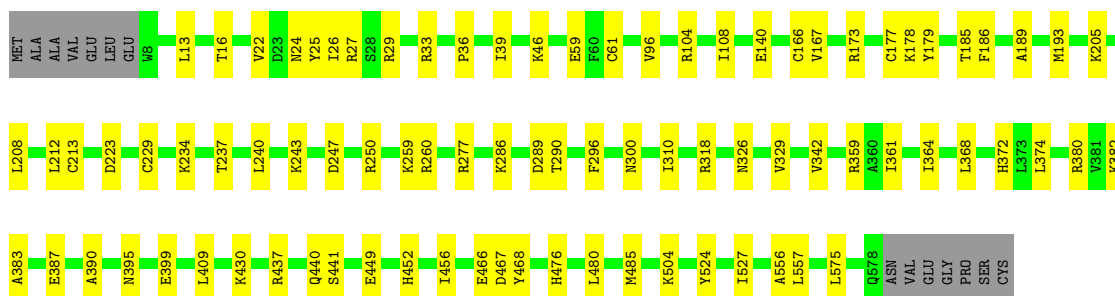
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Zn	0
			1	1	

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: Amyloid protein-binding protein 2

Chain A: 



• Molecule 1: Amyloid protein-binding protein 2

Chain B: 



• Molecule 2: Cullin-2

Chain E: 



ALA	VAL	ASN	PHE	SER	LEU	GLN	ALA	ARG	PHE	ASN	ASN	LYS	PHE	SER	THR	THR	VAL	SER	TYR	LYS	GLU	LEU	LYS	GLN	ASP	SER	THR	GLN	LYS	THR	ARG	GLU	THR	ILE	LYS	SER	ARG	LYS	LEU	MET	ASN	GLU	GLY	LYS	THR	GLN	VAL	THR	ALA	ILE	TYR	VAL	GLN	LEU	ASP	TYR	MET	ALA	ILE	ASN	HIS	ASP	SER	GLU	LYS	LYS	ALA	GLU	ASP	ILE	ASP	VAL	ASP	ALA	ARG	VAL	ARG	ILE	MET	LYS	VAL	ASP	LEU	ARG	HIS	GLU	SER	ASN	ALA	PHE	SER	LEU	ILE	GLN	ASN	GLU	MET
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• Molecule 3: Elongin-B



MET	D2	V3	F4	R8	K11	T23	K28	I34	L35	Q42	R43	I44	Y45	D52	D53	T56	F62	Q65	R68	P69	G76	R80	A81	D82	F85	I90	E91	S94	L99	V102	M103	K104	P105	Q106	ASP	SER	GLY	SER	SER	ALA	ALA	ASN
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• Molecule 3: Elongin-B



MET	D2	V3	F4	L5	M6	I7	R8	K11	T12	T13	I14	T23	E26	L27	K28	V31	G32	G33	I34	L35	K46	D47	D52	K55	T56	T63	S64	Q65	R68	P72	A81	D82	P97	GLU	LEU	PRO	ASP	VAL	MET	LYS	PRO	GLN	ASP	SER	GLY	SER	SER
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• Molecule 4: Elongin-C



MET	ASP	GLY	GLU	LYS	THR	TYR	GLY	GLY	CYS	GLU	GLY	PRO	ASP	ALA	M17	K20	D25	G26	H27	I30	R33	E34	H35	A36	S39	G40	T41	I42	G50	A53	N58	F62	R63	E64	H68	V81	R82	F93	E102	L103	L110	D111	C112
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• Molecule 4: Elongin-C



MET	ASP	GLY	GLU	LYS	THR	TYR	GLY	GLY	CYS	GLU	GLY	PRO	ASP	ALA	M17	K20	L21	I22	S23	S24	D25	G26	H27	E28	F29	I30	R33	E34	H35	T41	M45	G48	E56	E59	R63	S67	L70	S71	K72	M75	V81	R82	Y83	I90
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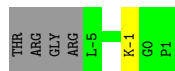
• Molecule 5: LEU-THR-ARG-ASN-LYS-GLY-PRO



THR	ARG	GLY	ARG	L-5	T-4	R-3	N-2	K-1	G0	P1
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- Molecule 5: LEU-THR-ARG-ASN-LYS-GLY-PRO

Chain F:  55% 9% 36%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	273296	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.347	Depositor
Minimum map value	-0.772	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.15	0/4712	0.33	0/6358
1	B	0.15	0/4729	0.33	0/6381
2	E	0.14	0/2436	0.35	0/3282
2	I	0.16	0/2436	0.36	0/3282
3	C	0.17	0/847	0.45	0/1146
3	G	0.17	0/773	0.46	0/1045
4	D	0.17	0/777	0.37	0/1050
4	H	0.17	0/777	0.41	0/1050
5	F	0.14	0/55	0.33	0/71
5	S	0.13	0/55	0.40	0/71
All	All	0.15	0/17597	0.35	0/23736

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	4613	0	4556	53	0
1	B	4630	0	4568	59	0
2	E	2382	0	2368	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	2382	0	2368	30	0
3	C	830	0	827	19	0
3	G	758	0	753	17	0
4	D	760	0	749	17	0
4	H	760	0	749	29	0
5	F	55	0	62	1	0
5	S	55	0	62	5	0
6	B	1	0	0	0	0
All	All	17226	0	17062	246	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 (246) 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:22:VAL:O	1:A:25:TYR:HB2	1.82	0.80
2:E:285:ILE:HG13	2:E:290:LYS:HB2	1.70	0.74
3:C:80:ARG:HA	3:C:85:PHE:HA	1.75	0.67
1:B:247:ASP:OD1	1:B:286:LYS:NZ	2.25	0.67
2:I:18:LEU:HA	2:I:21:ILE:HG22	1.78	0.66
4:D:63:ARG:NH1	4:D:64:GLU:OE2	2.30	0.65
2:E:86:MET:SD	2:E:89:ARG:NH2	2.71	0.63
2:I:111:GLN:HA	2:I:115:LYS:HD3	1.80	0.63
4:H:59:GLU:OE1	2:I:32:ARG:NH1	2.31	0.63
3:G:68:ARG:NH2	4:H:83:TYR:OH	2.32	0.63
2:I:27:LEU:HD21	2:I:96:LYS:HB2	1.80	0.62
1:B:510:TYR:HB3	1:B:513:LEU:HG	1.81	0.62
1:A:24:ASN:OD1	1:A:27:ARG:NH1	2.33	0.62
2:E:17:LEU:HD23	2:E:38:ARG:HD3	1.80	0.62
3:G:6:MET:HE1	4:H:75:MET:HE2	1.82	0.62
1:B:38:ASN:OD1	4:H:108:ASN:ND2	2.33	0.61
3:G:14:ILE:HD11	3:G:34:ILE:HD13	1.83	0.60
3:G:6:MET:HE3	3:G:72:PRO:HG2	1.83	0.60
1:B:264:LYS:NZ	1:B:577:SER:OG	2.35	0.60
1:B:482:ASN:ND2	1:B:519:GLY:O	2.33	0.60
1:A:372:HIS:HE1	1:A:374:LEU:HD23	1.67	0.59
1:B:383:ALA:HB2	1:B:409:LEU:HB2	1.85	0.59
4:H:63:ARG:NH2	2:I:41:ASP:OD1	2.36	0.59
1:B:403:LEU:HD23	1:B:442:MET:HG2	1.85	0.59
2:I:17:LEU:HD12	2:I:38:ARG:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ARG:NE	1:B:293:ASP:OD2	2.36	0.58
1:A:364:ILE:HG23	1:A:368:LEU:HD12	1.86	0.58
4:H:20:LYS:HB3	4:H:59:GLU:HA	1.86	0.57
3:G:12:THR:HA	4:H:28:GLU:HB2	1.86	0.57
3:C:23:THR:HA	3:C:56:THR:HA	1.86	0.57
3:C:43:ARG:NH2	3:C:45:TYR:OH	2.38	0.57
4:H:96:ALA:HB3	4:H:99:ILE:HG12	1.86	0.57
1:A:260:ARG:NH1	1:A:467:ASP:OD1	2.36	0.57
2:E:204:GLN:HA	2:E:208:GLU:HB3	1.86	0.57
1:B:488:TYR:HD2	1:B:523:LEU:HD12	1.69	0.57
4:H:111:ASP:OD2	2:I:106:ARG:NH1	2.38	0.57
1:B:386:LEU:HD22	1:B:402:LEU:HD22	1.86	0.56
1:A:173:ARG:NH1	1:A:185:THR:OG1	2.36	0.56
1:A:36:PRO:HD2	1:A:39:ILE:HD12	1.88	0.56
2:E:20:THR:HG21	2:E:38:ARG:HG3	1.87	0.56
1:B:103:ARG:NH1	1:B:107:TYR:OH	2.38	0.56
1:B:35:LEU:HD11	4:H:101:LEU:HD11	1.87	0.56
4:H:20:LYS:HD2	4:H:30:ILE:HG12	1.88	0.56
1:A:387:GLU:OE2	5:S:-3:ARG:NH2	2.39	0.56
2:I:109:ASN:HA	2:I:113:ILE:HB	1.88	0.55
1:B:296:PHE:O	1:B:300:ASN:ND2	2.39	0.55
1:A:524:TYR:HA	1:A:527:ILE:HG22	1.88	0.55
1:A:140:GLU:OE1	1:A:178:LYS:NZ	2.38	0.55
1:A:289:ASP:OD1	1:A:318:ARG:NH2	2.36	0.55
1:B:478:ALA:HB2	1:B:494:LEU:HB2	1.89	0.54
3:C:8:ARG:NH2	3:C:91:GLU:O	2.40	0.54
3:G:52:ASP:HB3	3:G:55:LYS:HD2	1.90	0.54
2:I:105:TYR:O	2:I:109:ASN:ND2	2.41	0.54
1:A:380:ARG:NH1	5:S:1:PRO:O	2.41	0.53
4:H:41:THR:O	4:H:45:MET:HG3	2.07	0.53
4:D:53:ALA:HB3	4:D:58:ASN:HD22	1.72	0.53
1:B:375:LEU:HB3	1:B:379:LYS:HD2	1.90	0.53
2:I:245:ASP:HA	2:I:248:ILE:HD12	1.91	0.53
2:E:148:ARG:HB2	2:E:191:VAL:HG11	1.91	0.53
1:A:383:ALA:HB2	1:A:409:LEU:HB2	1.90	0.53
2:E:299:VAL:HG23	2:E:300:LEU:HD12	1.91	0.53
4:D:33:ARG:NH2	4:D:58:ASN:OD1	2.41	0.52
1:A:296:PHE:O	1:A:300:ASN:ND2	2.42	0.52
1:B:173:ARG:NH1	1:B:185:THR:OG1	2.42	0.52
4:H:83:TYR:HD2	4:H:90:ILE:HG12	1.73	0.52
2:E:76:VAL:HG23	2:E:86:MET:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:GLY:HA2	1:B:515:TYR:HD2	1.73	0.52
4:H:35:HIS:CD2	4:H:81:VAL:HG11	2.45	0.52
1:A:243:LYS:HG3	1:A:286:LYS:HE3	1.91	0.52
1:A:390:ALA:HB1	1:A:399:GLU:HA	1.92	0.52
1:A:440:GLN:HB2	1:A:480:LEU:HD13	1.92	0.52
2:E:102:ASP:OD1	2:E:109:ASN:ND2	2.43	0.52
1:B:9:ILE:HD12	1:B:10:PRO:HD2	1.92	0.52
4:H:21:LEU:HD23	4:H:70:LEU:HD11	1.92	0.52
4:H:72:LYS:NZ	4:H:94:PRO:O	2.33	0.52
3:G:46:LYS:NZ	3:G:47:ASP:OD2	2.44	0.51
1:A:372:HIS:CE1	1:A:374:LEU:HD23	2.45	0.51
2:E:182:HIS:ND1	2:E:252:LYS:O	2.43	0.51
3:C:3:VAL:HG21	3:C:62:PHE:HB3	1.91	0.51
2:E:225:ASN:HA	2:E:228:GLN:HG2	1.93	0.51
1:B:84:GLN:HG2	1:B:323:GLY:H	1.74	0.51
2:E:291:LYS:HE2	2:E:294:MET:HE2	1.92	0.51
1:B:452:HIS:O	1:B:456:ILE:HG12	2.11	0.51
3:G:63:THR:HG23	3:G:65:GLN:H	1.74	0.51
2:I:239:VAL:HG22	2:I:270:MET:HE3	1.93	0.50
1:B:13:LEU:HD21	4:H:103:LEU:HD11	1.94	0.50
1:B:382:LYS:HE2	1:B:386:LEU:HD11	1.93	0.50
4:H:25:ASP:OD1	4:H:67:SER:OG	2.29	0.50
2:E:226:LEU:HD12	2:E:238:LYS:HD3	1.94	0.50
1:A:441:SER:OG	5:S:-3:ARG:NH2	2.45	0.50
2:E:164:LEU:HD21	2:E:211:PHE:HA	1.93	0.50
4:H:20:LYS:HE2	4:H:28:GLU:HB3	1.94	0.50
1:A:13:LEU:HD21	4:D:103:LEU:HD11	1.93	0.49
2:E:147:TRP:O	2:E:151:MET:HB3	2.12	0.49
1:B:32:ILE:HD13	1:B:43:VAL:HG11	1.93	0.49
1:A:342:VAL:HG22	5:S:-1:LYS:HD2	1.95	0.49
3:C:34:ILE:HG22	3:C:35:LEU:HD12	1.93	0.49
4:D:39:SER:HB3	4:D:112:CYS:HB3	1.93	0.49
1:B:410:HIS:CE1	1:B:434:ASN:HB3	2.47	0.49
1:B:36:PRO:HD2	1:B:39:ILE:HD12	1.93	0.49
1:A:189:ALA:O	1:A:193:MET:HG3	2.13	0.49
2:E:76:VAL:HG22	2:E:83:VAL:HG23	1.94	0.49
1:B:13:LEU:HD11	4:H:103:LEU:HD21	1.94	0.49
3:C:11:LYS:HB3	4:D:27:HIS:HA	1.95	0.49
1:B:306:GLN:NE2	1:B:554:THR:O	2.46	0.49
2:E:148:ARG:HA	2:E:152:VAL:HG12	1.95	0.48
1:A:430:LYS:HB2	5:S:1:PRO:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:PHE:HZ	4:H:82:ARG:HG3	1.79	0.48
3:C:94:SER:OG	4:D:25:ASP:OD2	2.26	0.48
1:A:361:ILE:HD12	1:A:382:LYS:HD2	1.95	0.48
2:I:26:MET:HA	2:I:93:GLU:HB3	1.96	0.48
2:I:148:ARG:HB2	2:I:191:VAL:HG11	1.96	0.48
1:A:16:THR:HG21	4:D:93:PHE:HB3	1.96	0.48
1:A:234:LYS:HA	1:A:575:LEU:HD11	1.94	0.48
3:G:23:THR:HA	3:G:56:THR:HA	1.96	0.48
1:A:22:VAL:HG21	1:A:46:LYS:HB3	1.96	0.47
1:B:74:ASP:OD1	1:B:75:LYS:N	2.47	0.47
1:B:449:GLU:HB3	1:B:485:MET:HE1	1.95	0.47
2:E:138:GLU:O	2:E:142:LEU:N	2.39	0.47
1:B:439:TYR:HA	1:B:442:MET:HB2	1.95	0.47
1:A:26:ILE:HA	1:A:29:ARG:HB3	1.95	0.47
4:D:20:LYS:HG3	4:D:30:ILE:HG13	1.97	0.47
3:G:11:LYS:HB3	4:H:27:HIS:HA	1.96	0.47
2:I:27:LEU:HD23	2:I:93:GLU:HA	1.97	0.47
3:C:65:GLN:O	3:C:68:ARG:NH1	2.44	0.47
4:H:17:MET:HE3	4:H:33:ARG:HD3	1.96	0.47
2:I:138:GLU:O	2:I:142:LEU:N	2.46	0.47
2:I:268:GLN:HA	2:I:272:ALA:HB3	1.96	0.47
2:E:37:ASP:OD1	4:D:63:ARG:NH2	2.46	0.47
3:G:28:LYS:O	3:G:32:GLU:HG3	2.15	0.47
1:B:331:THR:HA	1:B:334:GLU:HG2	1.97	0.46
1:A:61:CYS:HB3	1:A:96:VAL:HG11	1.97	0.46
3:C:52:ASP:OD1	3:C:53:ASP:N	2.47	0.46
1:B:355:PHE:HE1	1:B:359:ARG:HH21	1.63	0.46
2:E:184:VAL:O	2:E:187:SER:OG	2.30	0.46
2:E:247:GLU:OE2	2:E:251:ARG:NH1	2.48	0.46
2:E:32:ARG:HG2	4:D:50:GLY:HA2	1.98	0.46
2:E:65:LEU:O	2:E:69:VAL:HG22	2.15	0.46
2:E:148:ARG:HH12	2:E:195:LYS:HE3	1.80	0.46
2:E:292:ASN:OD1	2:E:293:ASP:N	2.48	0.46
1:A:449:GLU:HB2	1:A:485:MET:HE1	1.98	0.46
1:B:364:ILE:HG23	1:B:368:LEU:HD12	1.98	0.46
1:A:247:ASP:OD1	1:A:250:ARG:NH1	2.49	0.46
1:A:359:ARG:HD2	1:A:359:ARG:HA	1.83	0.46
2:E:96:LYS:HB3	2:E:96:LYS:HE2	1.82	0.46
2:I:166:GLU:OE2	2:I:169:ASN:ND2	2.48	0.46
2:E:198:PHE:HB3	2:E:201:LYS:HB2	1.98	0.45
2:I:84:LEU:HD21	2:I:181:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:HIS:CE1	2:E:183:GLY:HA3	2.51	0.45
1:B:213:CYS:SG	1:B:229:CYS:HB3	2.57	0.45
3:C:104:LYS:HE2	3:C:104:LYS:HB2	1.81	0.45
4:H:101:LEU:HD12	4:H:104:LEU:HD23	1.99	0.45
2:E:61:THR:HG21	2:E:139:ILE:HD12	1.99	0.45
2:E:177:ASN:HB3	2:E:180:VAL:HB	1.99	0.45
2:E:246:GLU:HA	2:E:249:ARG:HG2	1.99	0.45
1:B:474:VAL:HG23	1:B:498:SER:HB2	1.98	0.45
1:A:33:ARG:NH2	1:A:59:GLU:OE1	2.49	0.45
1:B:342:VAL:HG22	5:F:-1:LYS:HD2	1.99	0.45
1:B:440:GLN:NE2	1:B:484:ASP:OD2	2.50	0.45
1:B:472:LEU:HG	1:B:476:HIS:CE1	2.52	0.45
3:G:23:THR:OG1	3:G:26:GLU:OE1	2.28	0.45
3:C:76:GLY:HA2	3:C:90:ILE:HD11	1.97	0.45
1:B:193:MET:SD	1:B:205:LYS:HG2	2.57	0.45
1:B:266:GLU:HB3	1:B:297:TYR:CZ	2.52	0.45
2:I:177:ASN:O	2:I:253:TYR:OH	2.28	0.45
1:A:466:GLU:HG2	1:A:504:LYS:HE3	1.99	0.45
2:I:221:GLN:OE1	2:I:225:ASN:ND2	2.50	0.45
4:D:68:HIS:NE2	4:D:102:GLU:OE1	2.45	0.45
1:B:521:ILE:HG23	1:B:533:VAL:HG13	1.99	0.45
2:I:273:ASP:N	2:I:273:ASP:OD1	2.50	0.45
1:B:325:LYS:HD3	1:B:363:ILE:HG12	1.98	0.44
4:H:48:GLY:HA2	2:I:100:TYR:CD1	2.53	0.44
3:G:8:ARG:HD3	3:G:13:THR:HG23	1.99	0.44
1:B:266:GLU:HB3	1:B:297:TYR:OH	2.18	0.44
1:A:213:CYS:SG	1:A:229:CYS:HB3	2.57	0.44
1:A:250:ARG:HD2	1:A:290:THR:HG22	2.00	0.44
2:E:156:GLN:HE21	2:E:206:ILE:HG23	1.82	0.44
3:C:4:PHE:CE1	3:C:69:PRO:HG3	2.53	0.44
4:H:27:HIS:ND1	4:H:67:SER:OG	2.51	0.44
2:I:219:TYR:HE1	2:I:242:ARG:HE	1.64	0.44
1:A:186:PHE:CG	1:A:212:LEU:HD13	2.52	0.44
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.88	0.44
2:E:38:ARG:NH2	2:E:41:ASP:OD2	2.48	0.44
2:E:163:LEU:HD21	2:E:185:ILE:HG12	2.00	0.44
4:D:35:HIS:HA	4:D:81:VAL:HG21	1.99	0.44
1:B:153:HIS:HB2	1:B:158:HIS:CE1	2.53	0.44
1:B:159:TRP:HE1	1:B:195:LYS:HD2	1.82	0.44
1:A:467:ASP:OD1	1:A:468:TYR:N	2.48	0.43
2:E:10:PHE:CE2	2:E:60:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:THR:HB	4:D:110:LEU:HA	2.00	0.43
2:I:77:LEU:HD13	2:I:155:LEU:HD21	2.00	0.43
1:B:524:TYR:O	1:B:528:GLY:N	2.50	0.43
3:G:31:VAL:HG13	3:G:35:LEU:HD13	2.00	0.43
1:A:104:ARG:O	1:A:108:ILE:HG12	2.18	0.43
2:E:169:ASN:HB3	2:E:174:GLU:HG3	2.00	0.43
3:C:103:MET:HG2	1:B:33:ARG:HD2	2.01	0.43
1:A:237:THR:H	1:A:240:LEU:HD23	1.83	0.43
1:A:326:ASN:HB3	1:A:329:VAL:HG12	1.99	0.43
2:E:148:ARG:NH1	2:E:195:LYS:HE3	2.34	0.43
1:B:299:LEU:HD12	1:B:304:ILE:HD12	2.01	0.43
2:E:102:ASP:HB2	2:E:140:GLY:HA3	2.01	0.42
1:B:438:LEU:O	1:B:442:MET:N	2.44	0.42
1:A:177:CYS:SG	1:A:179:TYR:OH	2.65	0.42
2:I:226:LEU:HD11	2:I:238:LYS:HB3	2.01	0.42
2:E:107:TYR:CZ	2:E:111:GLN:HG3	2.54	0.42
1:B:167:VAL:HG12	1:B:208:LEU:HB2	2.00	0.42
3:G:27:LEU:O	3:G:31:VAL:HG23	2.19	0.42
1:A:395:ASN:OD1	1:B:395:ASN:ND2	2.52	0.42
1:B:322:PHE:HB3	1:B:326:ASN:HD22	1.85	0.42
2:E:25:VAL:HA	2:E:97:GLY:HA3	2.01	0.42
1:B:12:THR:HG22	1:B:14:TYR:H	1.85	0.42
2:I:236:MET:HA	2:I:239:VAL:HB	2.01	0.42
2:E:167:ILE:HD11	2:E:249:ARG:HD3	2.01	0.42
4:D:36:ALA:HB1	4:D:42:ILE:HG21	2.01	0.42
4:D:42:ILE:HG12	4:D:62:PHE:HZ	1.84	0.42
1:B:41:PHE:HE2	1:B:79:LEU:HB2	1.84	0.42
1:A:277:ARG:HH22	1:A:557:LEU:HB3	1.84	0.42
3:C:28:LYS:NZ	3:C:42:GLN:O	2.44	0.42
1:B:270:LYS:HG2	1:B:560:VAL:HG12	2.02	0.42
1:A:310:ILE:HD11	1:A:556:ALA:HB3	2.01	0.42
3:C:69:PRO:HG2	4:D:82:ARG:HD2	2.02	0.42
2:I:76:VAL:HG22	2:I:83:VAL:HG23	2.02	0.42
2:E:72:LEU:HD23	2:E:90:TYR:HB3	2.02	0.41
2:E:294:MET:HE3	2:E:294:MET:HB3	1.93	0.41
2:E:282:CYS:HA	2:E:285:ILE:HG22	2.02	0.41
1:B:22:VAL:O	1:B:25:TYR:HB2	2.20	0.41
2:I:107:TYR:CZ	2:I:111:GLN:HG3	2.56	0.41
3:C:99:LEU:HD12	3:C:99:LEU:HA	1.93	0.41
1:A:167:VAL:HG22	1:A:208:LEU:HB2	2.02	0.41
1:A:452:HIS:O	1:A:456:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:PHE:CZ	4:H:82:ARG:HG3	2.56	0.41
4:H:23:SER:OG	4:H:24:SER:N	2.54	0.41
1:A:166:CYS:HB3	1:A:189:ALA:HB2	2.03	0.41
3:C:102:VAL:O	1:B:30:ARG:NH1	2.54	0.41
1:B:22:VAL:HG21	1:B:46:LYS:HB3	2.03	0.41
1:A:193:MET:SD	1:A:205:LYS:HG2	2.61	0.41
1:A:223:ASP:OD1	1:A:259:LYS:NZ	2.36	0.41
2:I:10:PHE:HB2	2:I:53:LEU:HD13	2.03	0.41
2:E:21:ILE:HD11	2:E:104:LEU:HD22	2.03	0.41
2:E:149:LYS:HA	2:E:153:GLU:HG3	2.02	0.40
2:E:255:HIS:CD2	2:E:256:PRO:HD2	2.55	0.40
1:A:437:ARG:HD2	1:A:476:HIS:CD2	2.57	0.40
4:H:95:ILE:HG12	4:H:103:LEU:HD23	2.04	0.40
2:I:66:GLU:HG3	2:I:150:LEU:HD21	2.04	0.40
1:A:27:ARG:HG2	3:C:99:LEU:HG	2.03	0.40
1:B:445:PHE:CZ	1:B:484:ASP:HB3	2.56	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	
1	A	569/585 (97%)	556 (98%)	13 (2%)	0	100	100
1	B	571/585 (98%)	562 (98%)	9 (2%)	0	100	100
2	E	278/745 (37%)	270 (97%)	8 (3%)	0	100	100
2	I	278/745 (37%)	267 (96%)	11 (4%)	0	100	100
3	C	103/118 (87%)	96 (93%)	7 (7%)	0	100	100
3	G	94/118 (80%)	83 (88%)	11 (12%)	0	100	100
4	D	94/112 (84%)	91 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	94/112 (84%)	90 (96%)	4 (4%)	0	100	100
5	F	5/11 (46%)	5 (100%)	0	0	100	100
5	S	5/11 (46%)	5 (100%)	0	0	100	100
All	All	2091/3142 (66%)	2025 (97%)	66 (3%)	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	491/502 (98%)	491 (100%)	0	100	100
1	B	493/502 (98%)	493 (100%)	0	100	100
2	E	263/681 (39%)	263 (100%)	0	100	100
2	I	263/681 (39%)	263 (100%)	0	100	100
3	C	93/103 (90%)	93 (100%)	0	100	100
3	G	84/103 (82%)	84 (100%)	0	100	100
4	D	85/96 (88%)	85 (100%)	0	100	100
4	H	85/96 (88%)	85 (100%)	0	100	100
5	F	6/9 (67%)	6 (100%)	0	100	100
5	S	6/9 (67%)	6 (100%)	0	100	100
All	All	1869/2782 (67%)	1869 (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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	400	GLN
1	A	404	GLN

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Mol	Chain	Res	Type
1	A	427	GLN
1	A	452	HIS
1	A	465	GLN
1	A	482	ASN
1	A	486	ASN
2	E	109	ASN
2	E	221	GLN
2	E	225	ASN
2	E	228	GLN
2	E	264	HIS
2	E	279	HIS
2	E	296	ASN
4	D	27	HIS
1	B	38	ASN
1	B	153	HIS
1	B	158	HIS
1	B	202	GLN
1	B	537	HIS
4	H	108	ASN
2	I	71	HIS
2	I	109	ASN
2	I	111	GLN
2	I	156	GLN
2	I	274	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

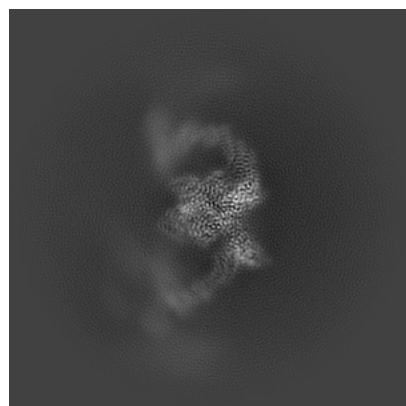
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36129. These allow visual inspection of the internal detail of the map and identification of artifacts.

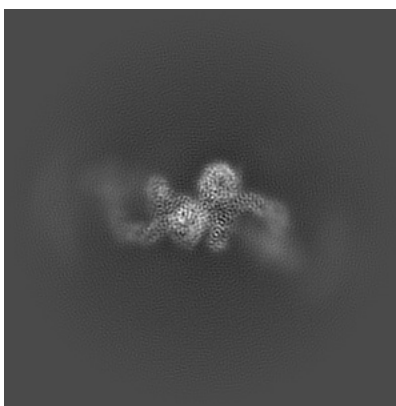
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

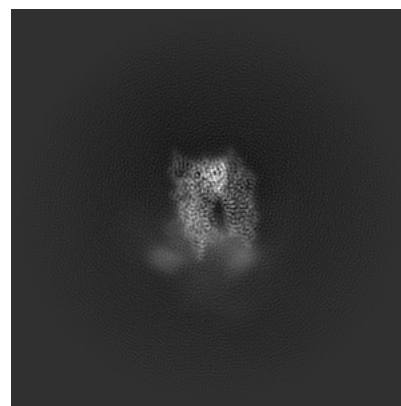
6.1.1 Primary map



X

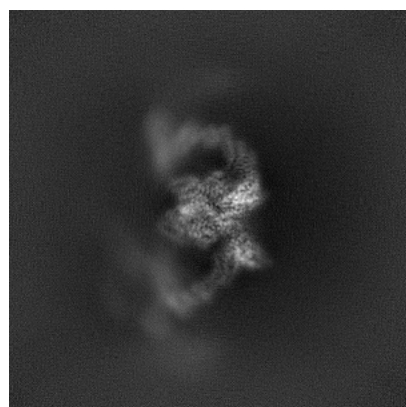


Y

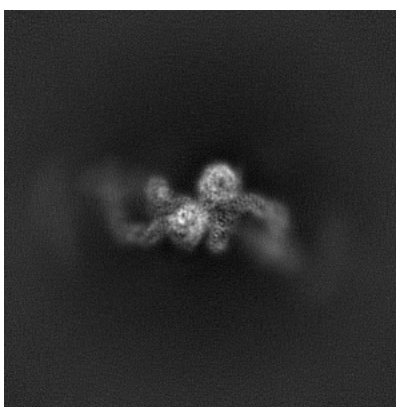


Z

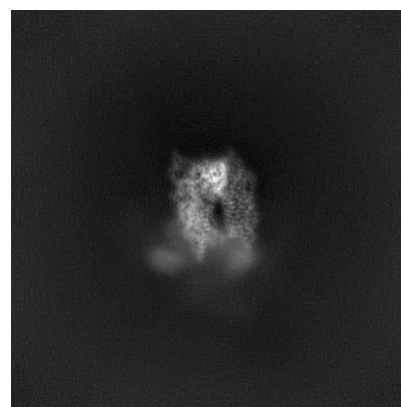
6.1.2 Raw map



X



Y

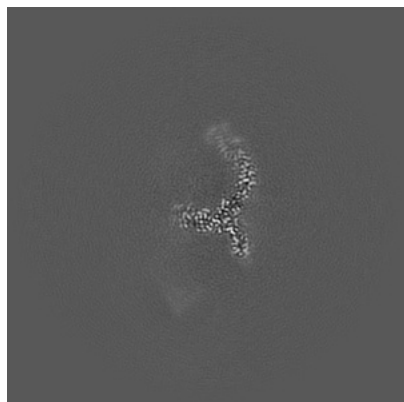


Z

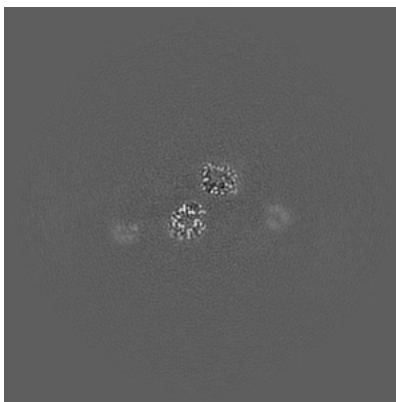
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

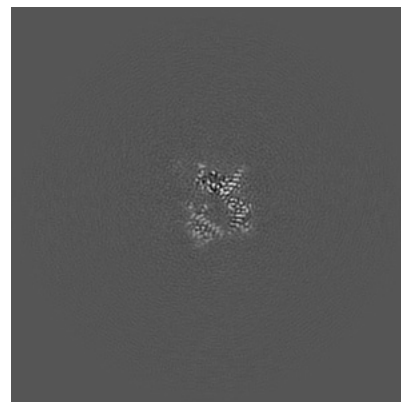
6.2.1 Primary map



X Index: 256

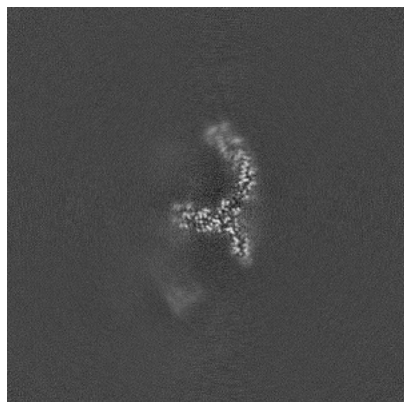


Y Index: 256

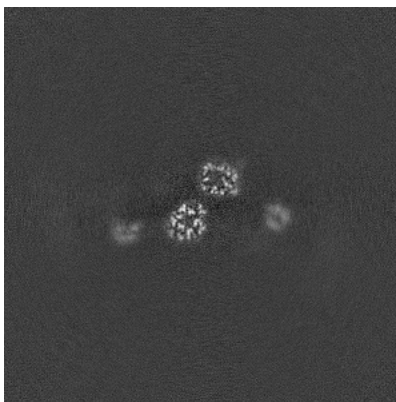


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

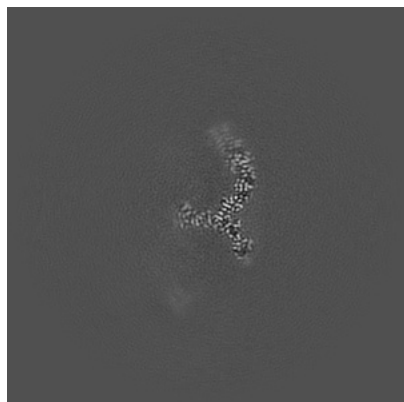


Z Index: 256

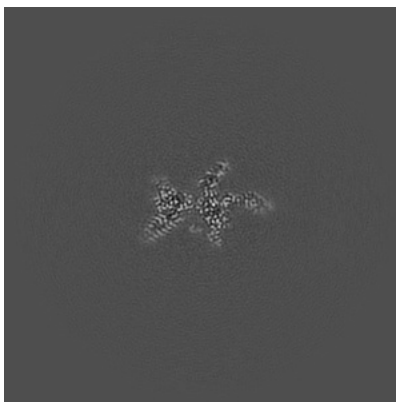
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

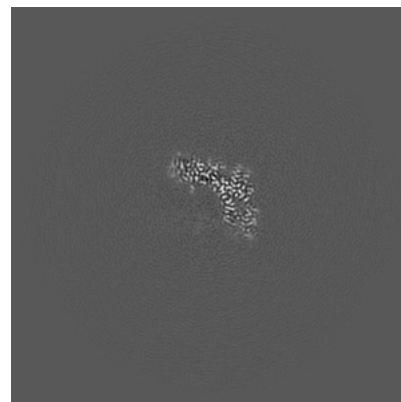
6.3.1 Primary map



X Index: 259

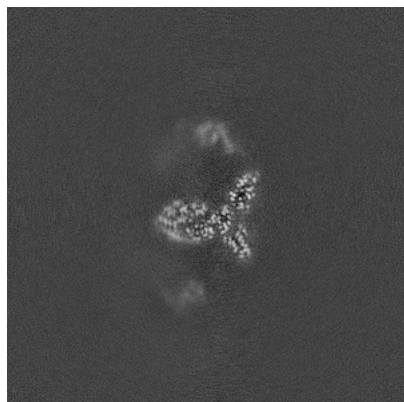


Y Index: 293

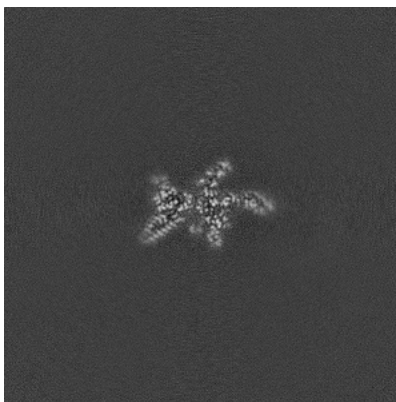


Z Index: 267

6.3.2 Raw map



X Index: 245



Y Index: 293

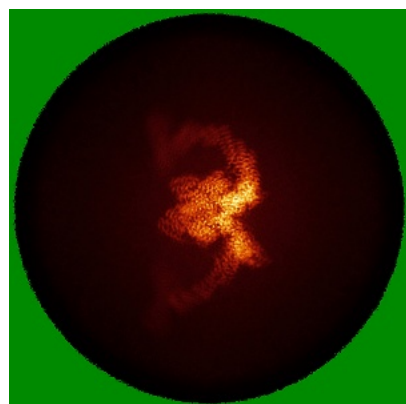


Z Index: 267

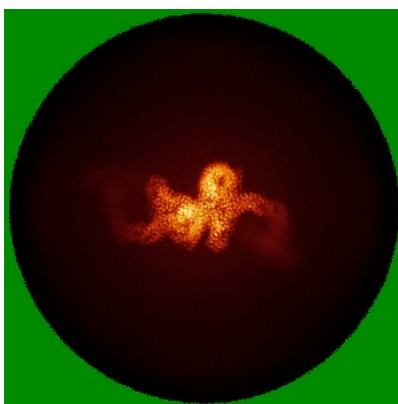
The images above show the largest variance slices of the map in three orthogonal directions.

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

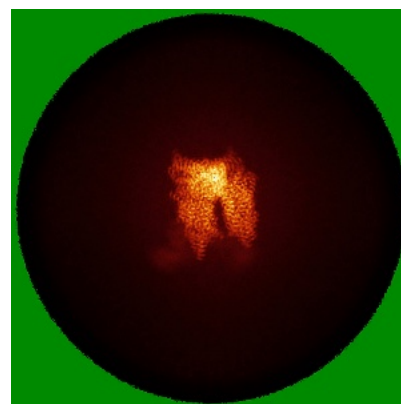
6.4.1 Primary map



X

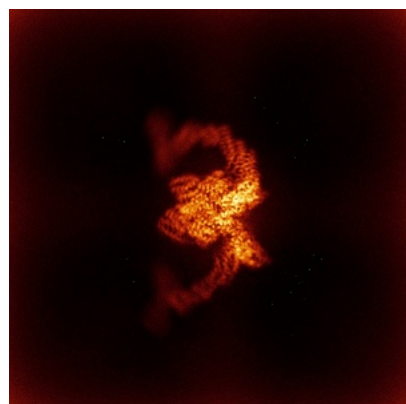


Y

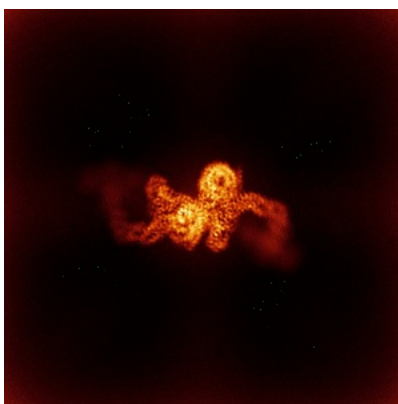


Z

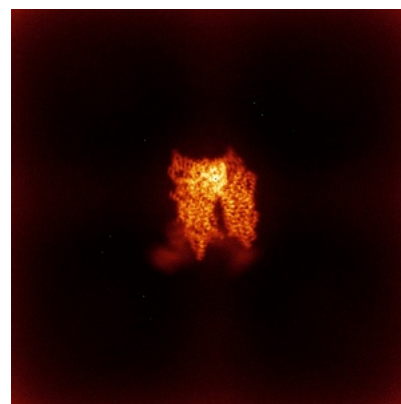
6.4.2 Raw map



X



Y

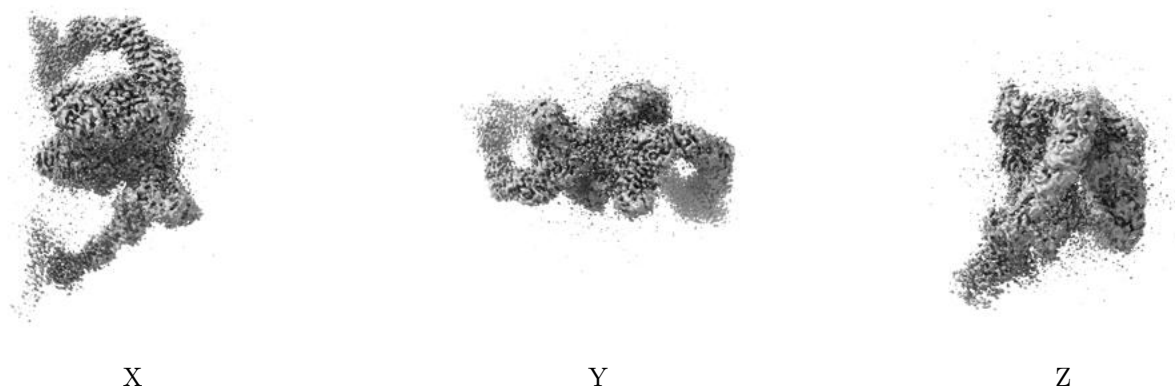


Z

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.

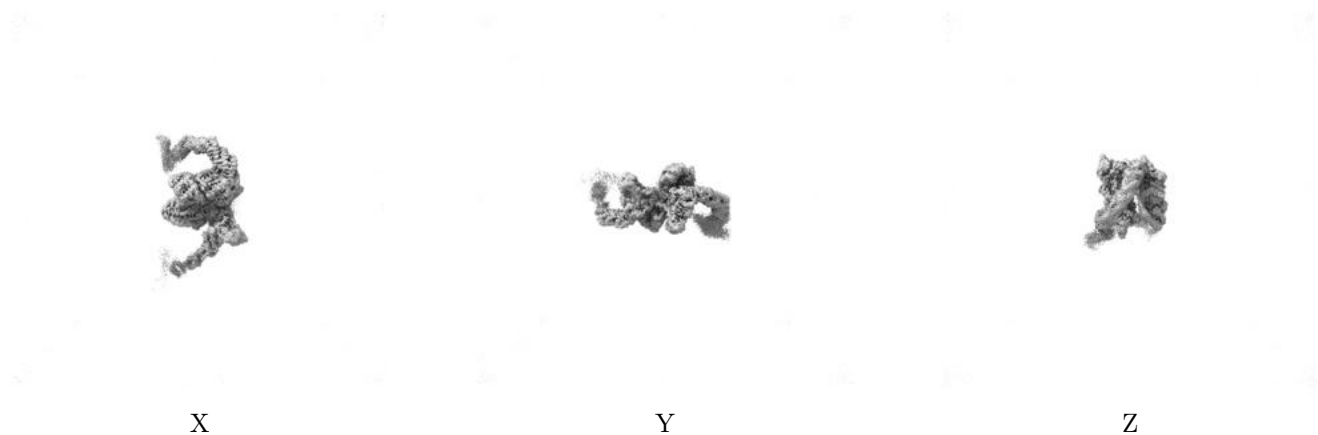
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

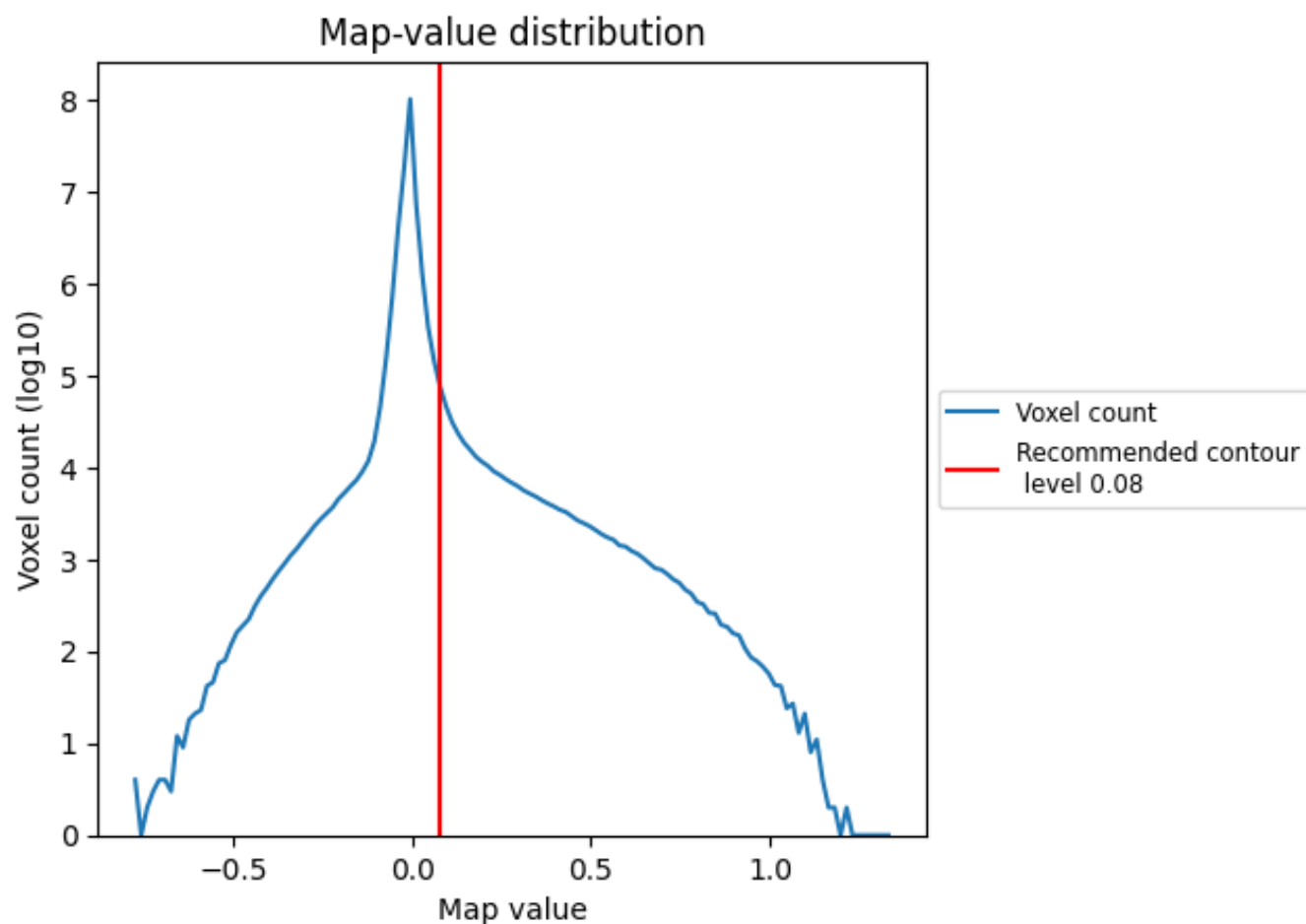
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

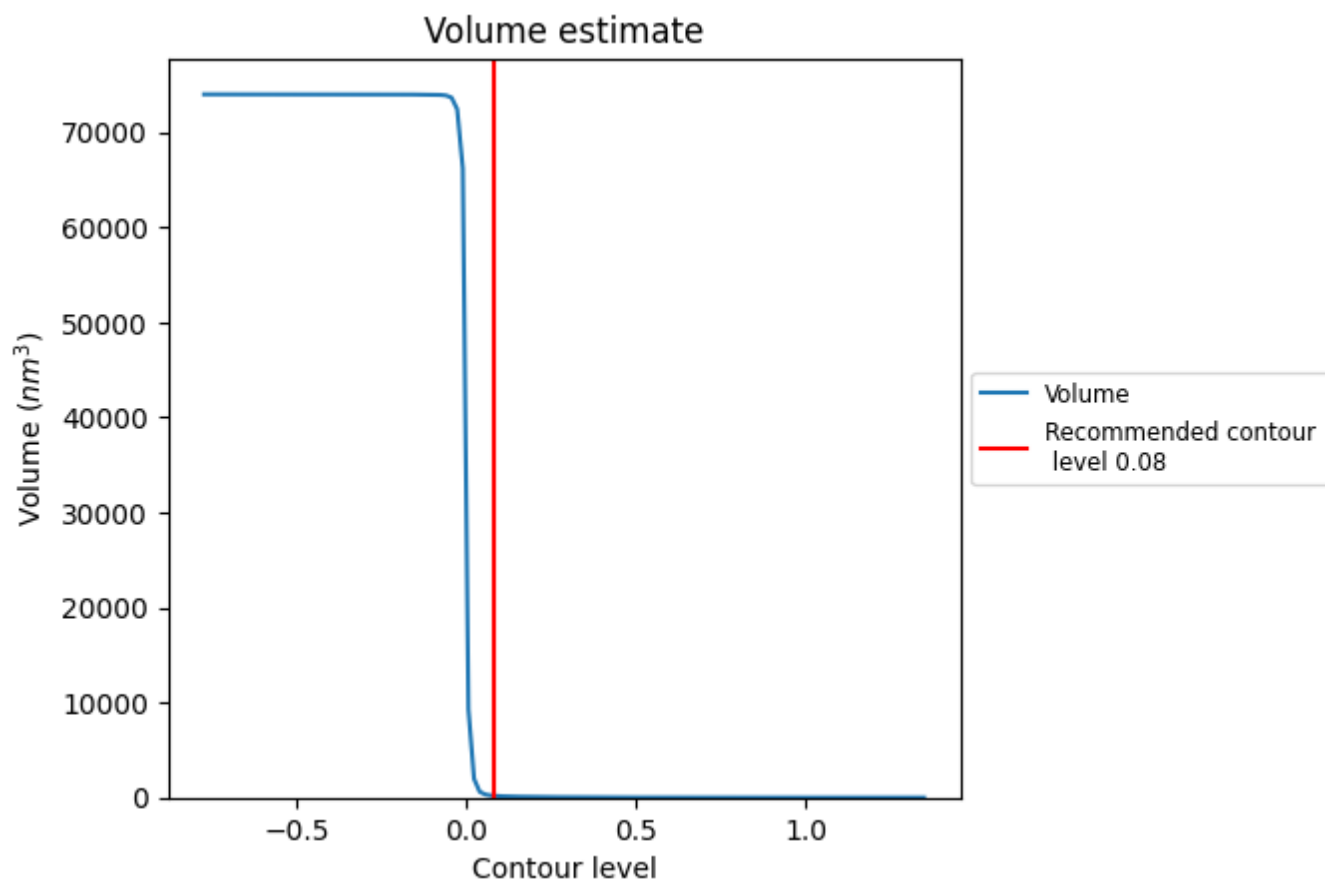
This section contains the results of statistical analysis of the map.

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.

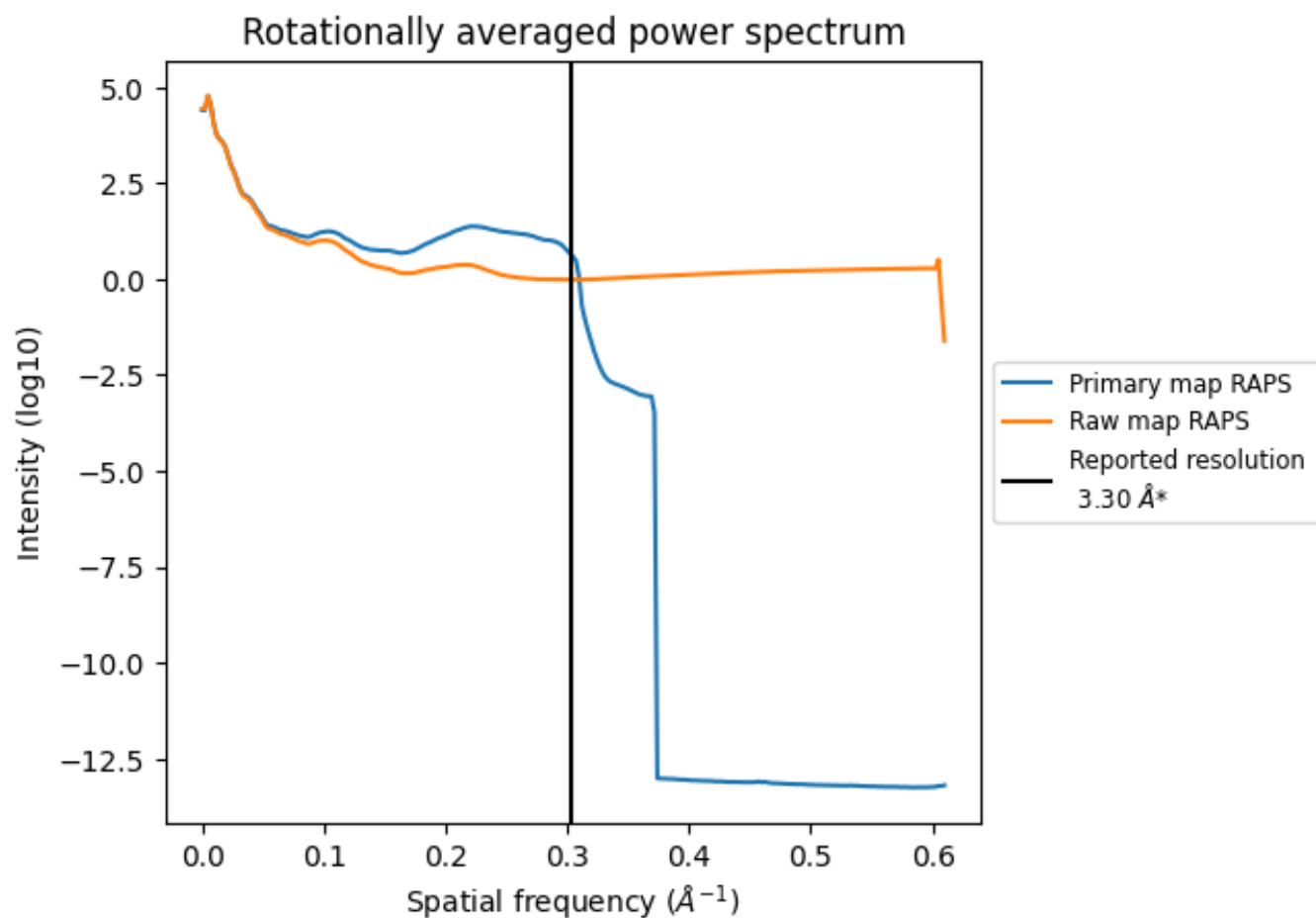
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm³; this corresponds to an approximate mass of 174 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 ⓘ

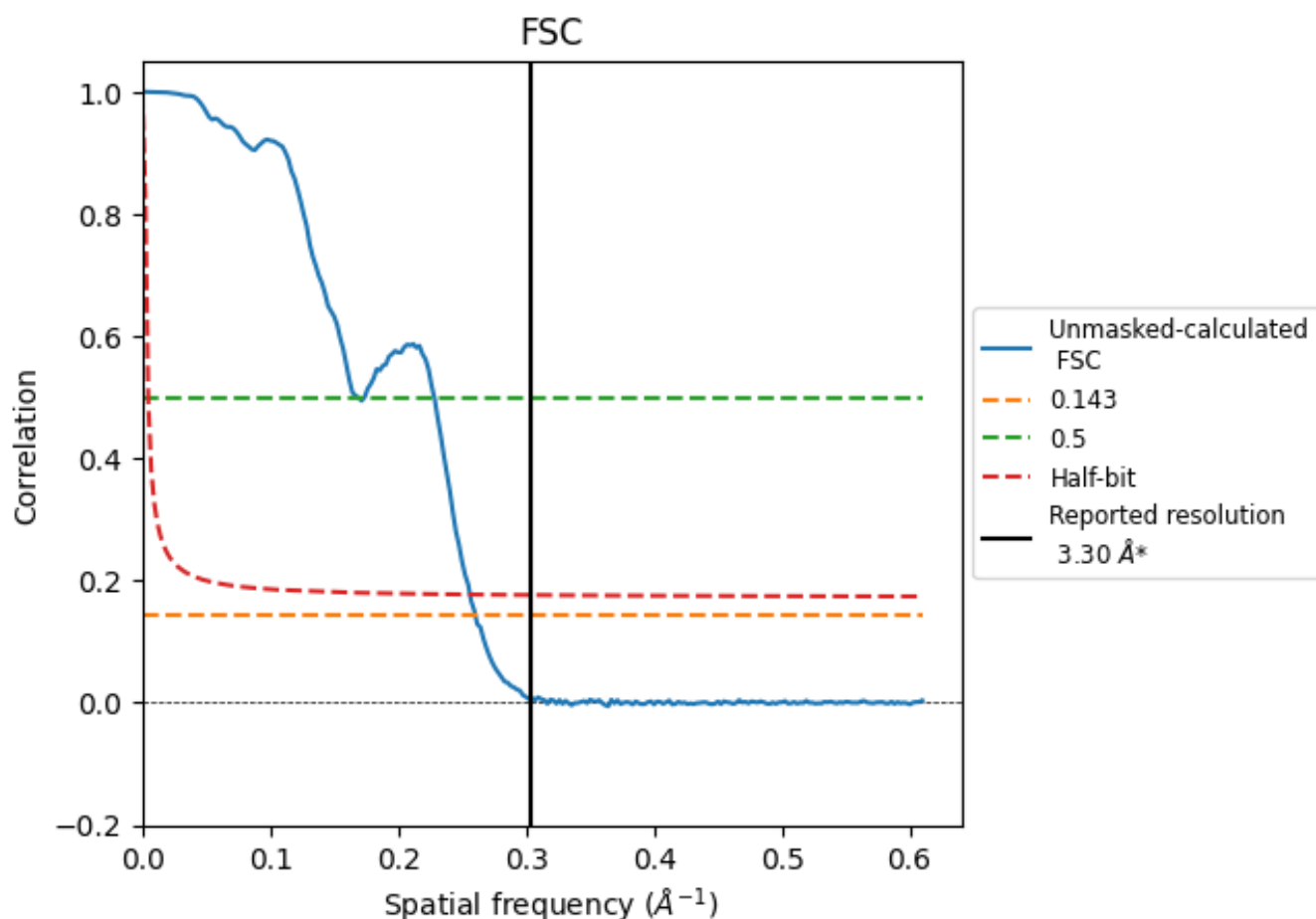


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

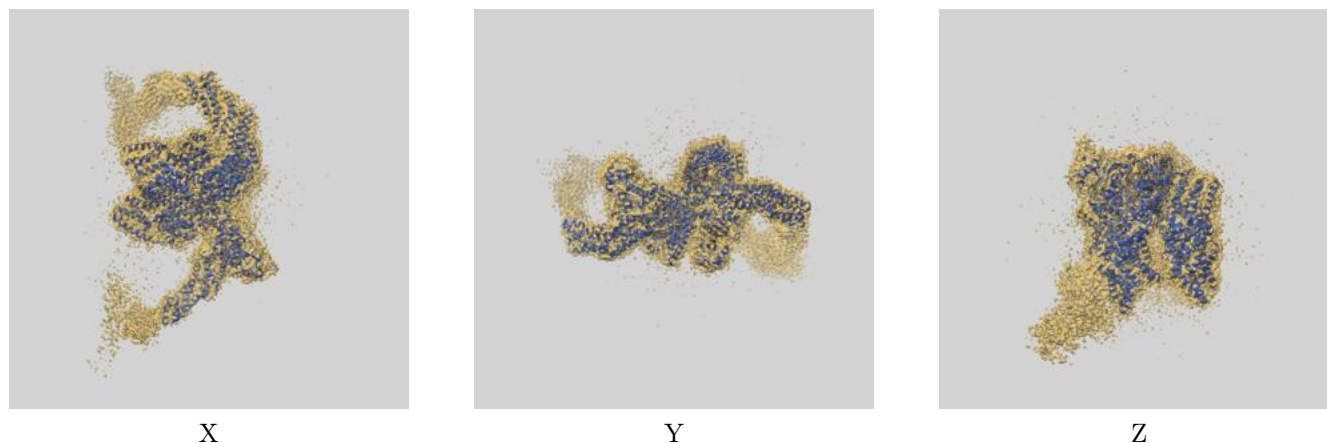
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.84	5.93	3.90

*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 3.84 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

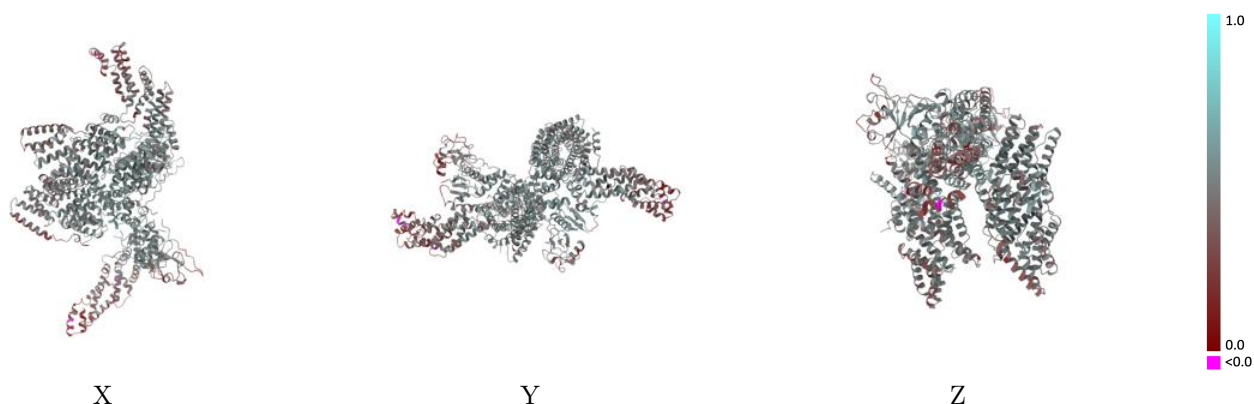
This section contains information regarding the fit between EMDB map EMD-36129 and PDB model 8JAL. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



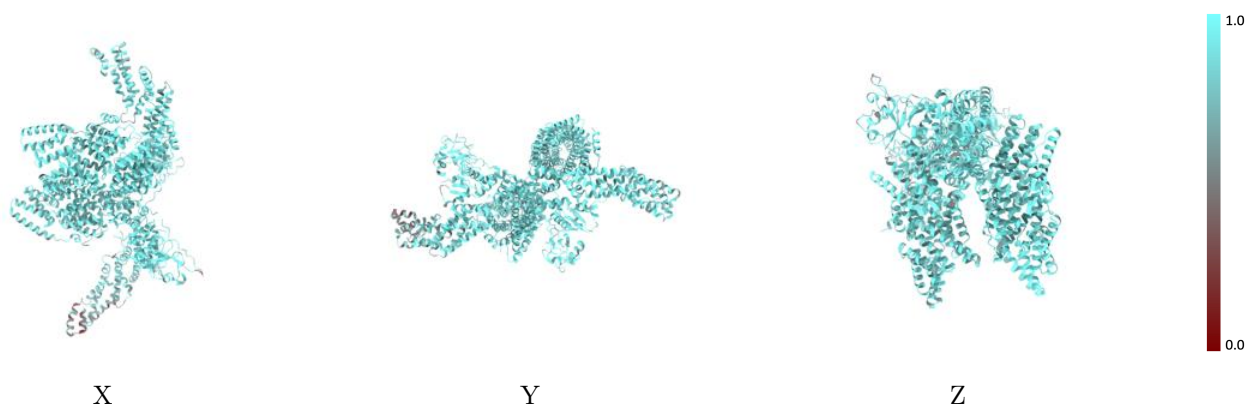
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



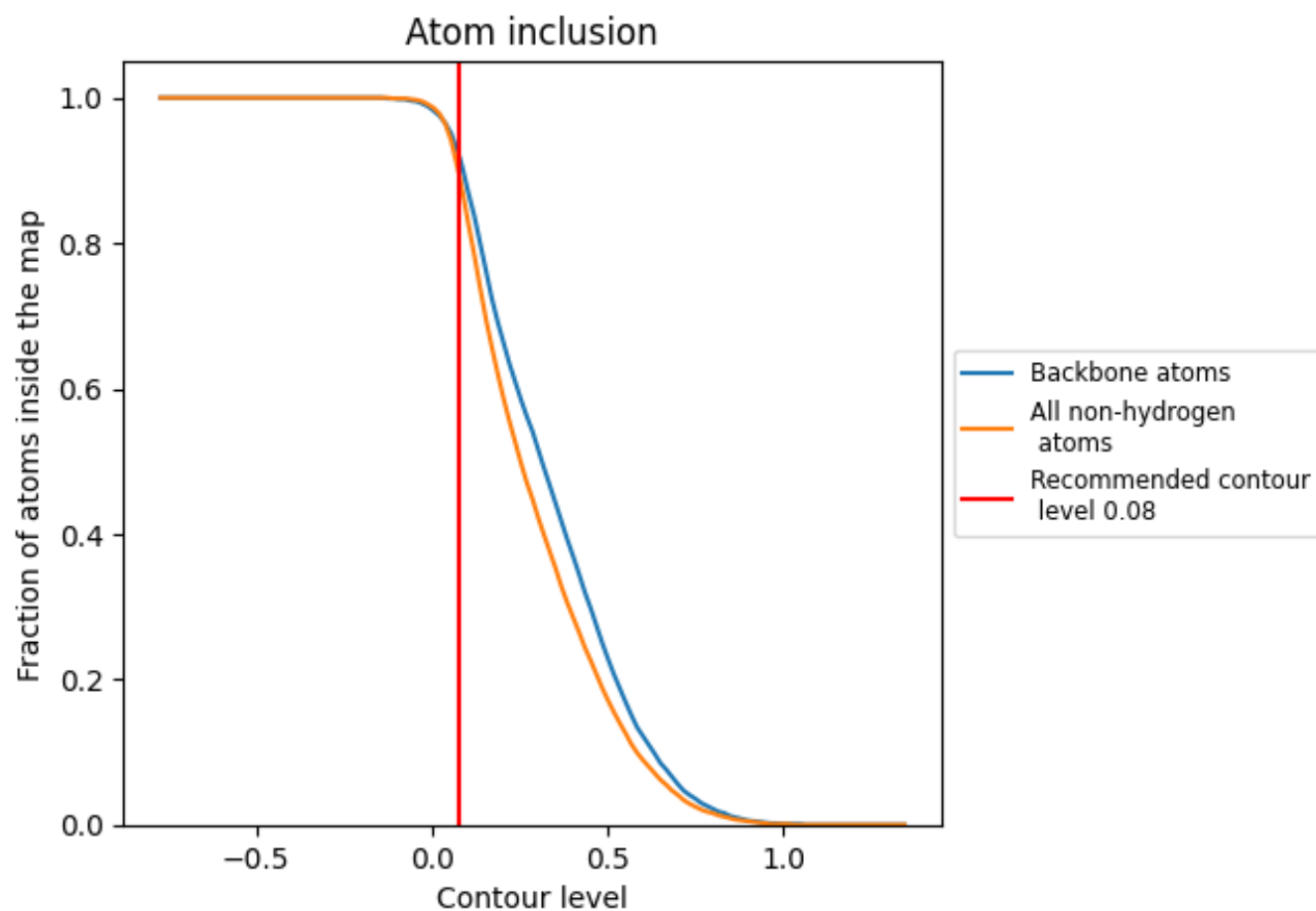
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.4730
A	0.9220	0.5070
B	0.9110	0.4960
C	0.8930	0.4490
D	0.9130	0.5270
E	0.8810	0.4380
F	0.9430	0.5100
G	0.8630	0.3810
H	0.9030	0.4870
I	0.7950	0.4100
S	0.9060	0.5130

1.0

0.0

<0.0