



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:16 AM UTC

PDB ID : 9NWT / pdb_00009nwt
EMDB ID : EMD-49893
Title : Cryo-EM structure of DDB1dB:CRBN:mezigdomide:SALL4(392-449;G416A)
Authors : Park, J.; Hunkeler, M.; Roy Burman, S.S.; Fischer, E.S.
Deposited on : 2025-03-24
Resolution : 2.70 Å(reported)
Based on initial models : 8TNQ, 8D7Z, 8U17

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

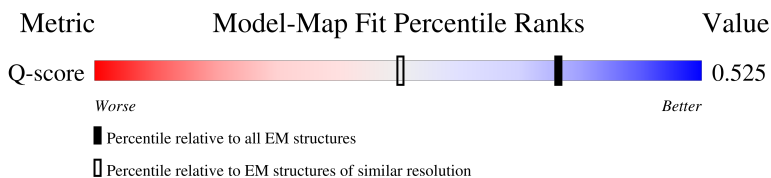
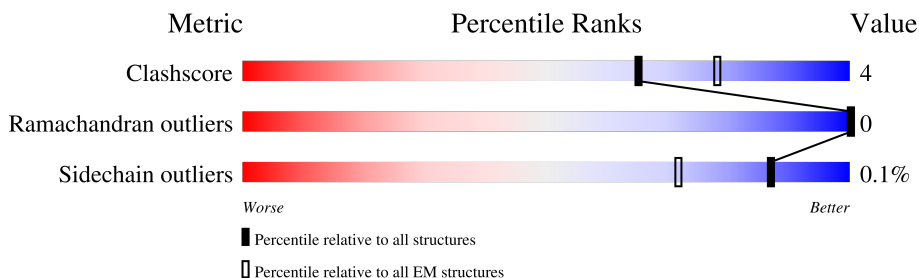
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	102	21% 25% 5% 71%
2	A	860	5% 84% 9% 7%
3	B	485	18% 68% 10% 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19275 atoms, of which 9620 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 Sal-like protein 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	30	Total	C	H	N	O	S	0	0
			484	155	241	50	36	2		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	348	MET	-	expression tag	UNP Q9UJQ4
C	349	ASP	-	expression tag	UNP Q9UJQ4
C	350	TRP	-	expression tag	UNP Q9UJQ4
C	351	SER	-	expression tag	UNP Q9UJQ4
C	352	HIS	-	expression tag	UNP Q9UJQ4
C	353	PRO	-	expression tag	UNP Q9UJQ4
C	354	GLN	-	expression tag	UNP Q9UJQ4
C	355	PHE	-	expression tag	UNP Q9UJQ4
C	356	GLU	-	expression tag	UNP Q9UJQ4
C	357	LYS	-	expression tag	UNP Q9UJQ4
C	358	SER	-	expression tag	UNP Q9UJQ4
C	359	ALA	-	expression tag	UNP Q9UJQ4
C	360	VAL	-	expression tag	UNP Q9UJQ4
C	361	GLY	-	expression tag	UNP Q9UJQ4
C	362	LEU	-	expression tag	UNP Q9UJQ4
C	363	ASN	-	expression tag	UNP Q9UJQ4
C	364	ASP	-	expression tag	UNP Q9UJQ4
C	365	ILE	-	expression tag	UNP Q9UJQ4
C	366	PHE	-	expression tag	UNP Q9UJQ4
C	367	GLU	-	expression tag	UNP Q9UJQ4
C	368	ALA	-	expression tag	UNP Q9UJQ4
C	369	GLN	-	expression tag	UNP Q9UJQ4
C	370	LYS	-	expression tag	UNP Q9UJQ4
C	371	ILE	-	expression tag	UNP Q9UJQ4
C	372	GLU	-	expression tag	UNP Q9UJQ4
C	373	TRP	-	expression tag	UNP Q9UJQ4
C	374	HIS	-	expression tag	UNP Q9UJQ4
C	375	GLU	-	expression tag	UNP Q9UJQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	376	GLY	-	expression tag	UNP Q9UJQ4
C	377	GLY	-	expression tag	UNP Q9UJQ4
C	378	GLY	-	expression tag	UNP Q9UJQ4
C	379	GLY	-	expression tag	UNP Q9UJQ4
C	380	SER	-	expression tag	UNP Q9UJQ4
C	381	GLY	-	expression tag	UNP Q9UJQ4
C	382	GLU	-	expression tag	UNP Q9UJQ4
C	383	ASN	-	expression tag	UNP Q9UJQ4
C	384	LEU	-	expression tag	UNP Q9UJQ4
C	385	TYR	-	expression tag	UNP Q9UJQ4
C	386	PHE	-	expression tag	UNP Q9UJQ4
C	387	GLN	-	expression tag	UNP Q9UJQ4
C	388	GLY	-	expression tag	UNP Q9UJQ4
C	389	GLY	-	expression tag	UNP Q9UJQ4
C	390	GLY	-	expression tag	UNP Q9UJQ4
C	391	ARG	-	expression tag	UNP Q9UJQ4
C	416	ALA	GLY	engineered mutation	UNP Q9UJQ4

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	801	Total	C	H	N	O	S	0	0
			12625	4011	6307	1065	1208	34		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q16531
A	-22	GLY	-	expression tag	UNP Q16531
A	-21	SER	-	expression tag	UNP Q16531
A	-20	SER	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	SER	-	expression tag	UNP Q16531
A	-12	ALA	-	expression tag	UNP Q16531
A	-11	VAL	-	expression tag	UNP Q16531
A	-10	ASP	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

- Molecule 3 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	378	Total	C	H	N	O	S	0	0
			6102	1949	3052	522	556	23		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-42	MET	-	expression tag	UNP Q96SW2
B	-41	ASP	-	expression tag	UNP Q96SW2
B	-40	TYR	-	expression tag	UNP Q96SW2
B	-39	LYS	-	expression tag	UNP Q96SW2
B	-38	ASP	-	expression tag	UNP Q96SW2
B	-37	ASP	-	expression tag	UNP Q96SW2
B	-36	ASP	-	expression tag	UNP Q96SW2
B	-35	ASP	-	expression tag	UNP Q96SW2
B	-34	LYS	-	expression tag	UNP Q96SW2
B	-33	SER	-	expression tag	UNP Q96SW2
B	-32	ALA	-	expression tag	UNP Q96SW2
B	-31	VAL	-	expression tag	UNP Q96SW2
B	-30	ASP	-	expression tag	UNP Q96SW2
B	-29	GLU	-	expression tag	UNP Q96SW2
B	-28	ASN	-	expression tag	UNP Q96SW2
B	-27	LEU	-	expression tag	UNP Q96SW2
B	-26	TYR	-	expression tag	UNP Q96SW2

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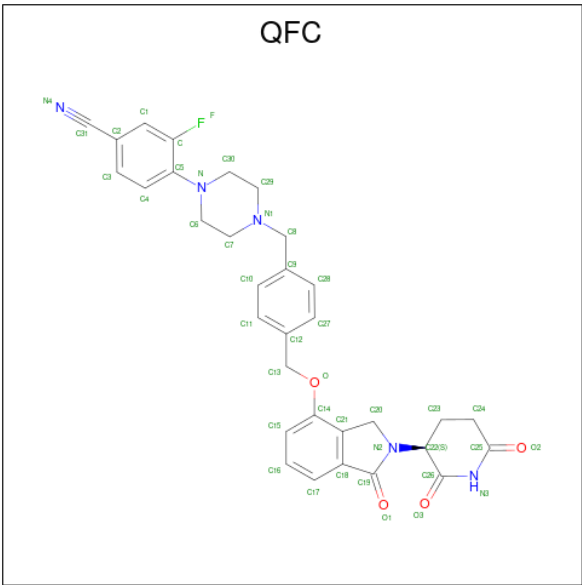
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-25	PHE	-	expression tag	UNP Q96SW2
B	-24	GLN	-	expression tag	UNP Q96SW2
B	-23	GLY	-	expression tag	UNP Q96SW2
B	-22	GLY	-	expression tag	UNP Q96SW2
B	-21	GLY	-	expression tag	UNP Q96SW2
B	-20	ARG	-	expression tag	UNP Q96SW2
B	-19	GLY	-	expression tag	UNP Q96SW2
B	-18	GLY	-	expression tag	UNP Q96SW2
B	-17	SER	-	expression tag	UNP Q96SW2
B	-16	ALA	-	expression tag	UNP Q96SW2
B	-15	HIS	-	expression tag	UNP Q96SW2
B	-14	ILE	-	expression tag	UNP Q96SW2
B	-13	VAL	-	expression tag	UNP Q96SW2
B	-12	MET	-	expression tag	UNP Q96SW2
B	-11	VAL	-	expression tag	UNP Q96SW2
B	-10	ASP	-	expression tag	UNP Q96SW2
B	-9	ALA	-	expression tag	UNP Q96SW2
B	-8	TYR	-	expression tag	UNP Q96SW2
B	-7	LYS	-	expression tag	UNP Q96SW2
B	-6	PRO	-	expression tag	UNP Q96SW2
B	-5	THR	-	expression tag	UNP Q96SW2
B	-4	LYS	-	expression tag	UNP Q96SW2
B	-3	GLY	-	expression tag	UNP Q96SW2
B	-2	GLY	-	expression tag	UNP Q96SW2
B	-1	SER	-	expression tag	UNP Q96SW2
B	0	GLY	-	expression tag	UNP Q96SW2

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	

- Molecule 5 is Mezigidomide (CCD ID: QFC) (formula: C₃₂H₃₀FN₅O₄) (labeled as "Ligand of Interest" by depositor).

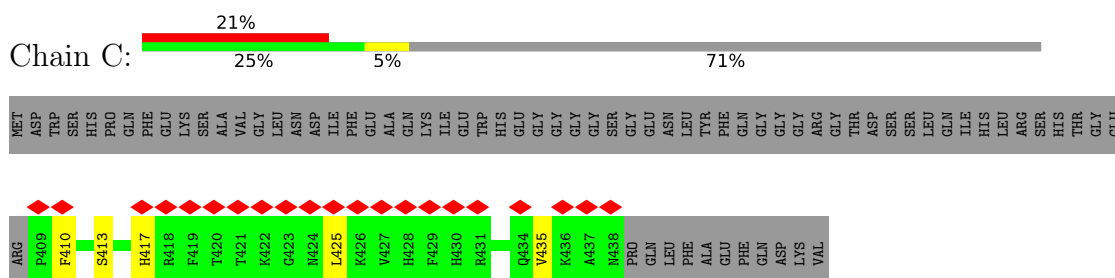


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
5	B	1	62	32	1	20	5	4	0

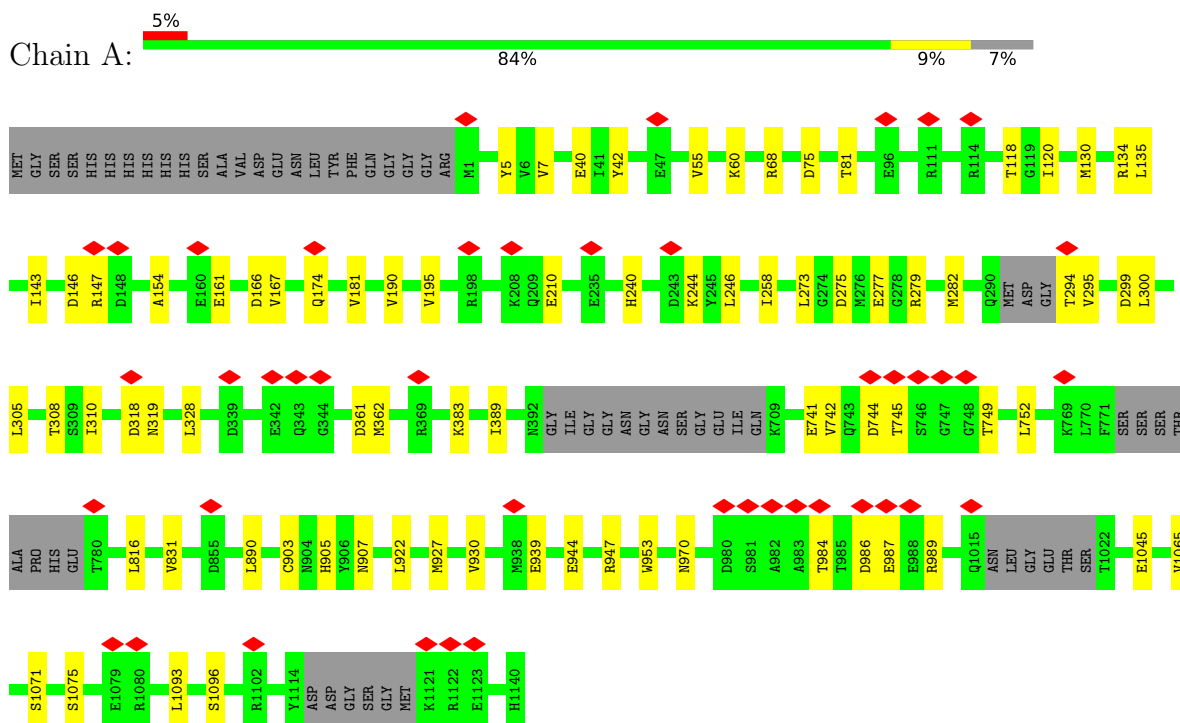
3 Residue-property plots [i](#)

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: Sal-like protein 4

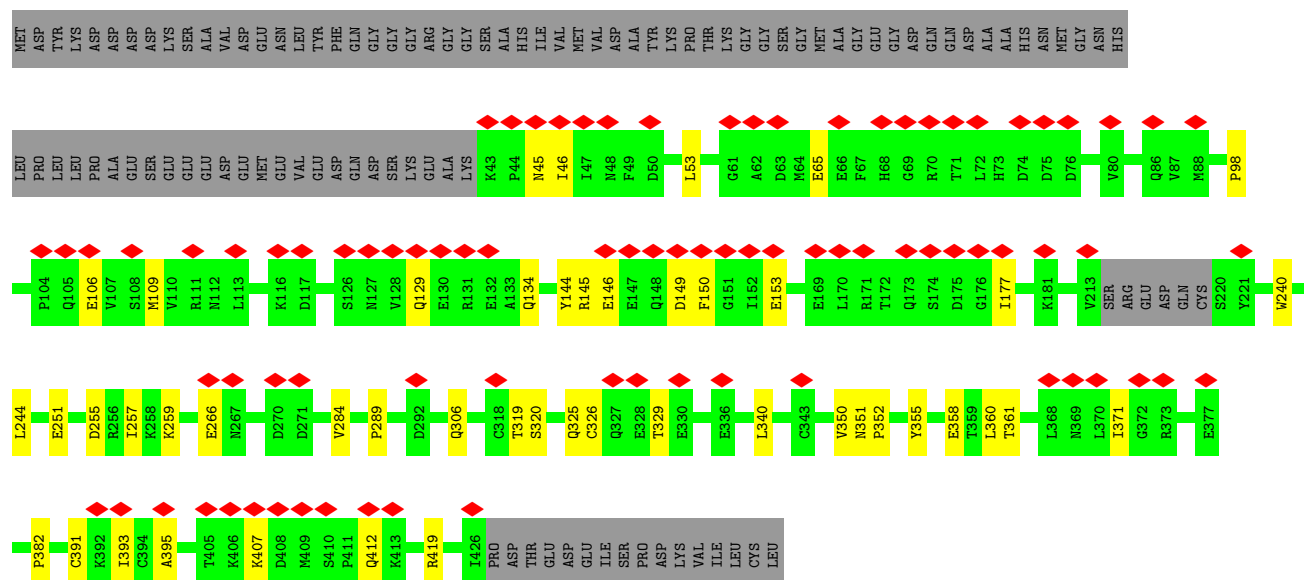


- Molecule 2: DNA damage-binding protein 1



- Molecule 3: Protein cereblon





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	479953	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.797	Depositor
Minimum map value	-0.520	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	278.88, 278.88, 278.88	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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, QFC

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	C	0.11	0/251	0.30	0/337
2	A	0.10	0/6429	0.25	0/8689
3	B	0.09	0/3123	0.25	0/4236
All	All	0.10	0/9803	0.25	0/13262

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	C	243	241	241	3	0
2	A	6318	6307	6309	46	0
3	B	3050	3052	3052	30	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	42	20	0	0	0
All	All	9655	9620	9602	76	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 4.

All (76) 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:A:986:ASP:OD1	2:A:989:ARG:NH2	2.19	0.76
2:A:275:ASP:OD1	2:A:279:ARG:N	2.19	0.75
2:A:1045:GLU:OE1	2:A:1045:GLU:N	2.23	0.72
3:B:407:LYS:O	3:B:412:GLN:NE2	2.24	0.71
3:B:153:GLU:N	3:B:153:GLU:OE1	2.24	0.70
3:B:145:ARG:NH1	3:B:146:GLU:O	2.25	0.69
2:A:181:VAL:HG22	2:A:190:VAL:HG22	1.75	0.69
3:B:65:GLU:N	3:B:144:TYR:O	2.26	0.68
2:A:161:GLU:OE1	2:A:161:GLU:N	2.25	0.68
2:A:299:ASP:OD1	2:A:300:LEU:N	2.26	0.68
3:B:266:GLU:OE1	3:B:266:GLU:N	2.26	0.68
2:A:210:GLU:OE1	2:A:240:HIS:ND1	2.27	0.67
2:A:174:GLN:N	2:A:174:GLN:OE1	2.26	0.66
3:B:129:GLN:N	3:B:129:GLN:OE1	2.28	0.65
1:C:413:SER:O	3:B:351:ASN:ND2	2.30	0.65
3:B:45:ASN:OD1	3:B:46:ILE:N	2.30	0.64
2:A:318:ASP:OD1	2:A:319:ASN:N	2.31	0.63
2:A:741:GLU:OE1	2:A:749:THR:OG1	2.07	0.62
3:B:351:ASN:OD1	3:B:355:TYR:N	2.33	0.62
2:A:244:LYS:HE3	2:A:246:LEU:HD11	1.84	0.60
3:B:358:GLU:OE1	3:B:419:ARG:NE	2.25	0.60
2:A:361:ASP:OD1	2:A:362:MET:N	2.35	0.59
1:C:410:PHE:HB3	1:C:425:LEU:HD22	1.85	0.58
2:A:118:THR:OG1	2:A:134:ARG:NH2	2.35	0.58
3:B:329:THR:HG21	3:B:393:ILE:HG21	1.87	0.57
2:A:166:ASP:OD1	2:A:167:VAL:N	2.39	0.56
3:B:391:CYS:O	3:B:395:ALA:N	2.34	0.56
3:B:240:TRP:HB3	3:B:244:LEU:HD23	1.87	0.56
3:B:149:ASP:OD1	3:B:150:PHE:N	2.38	0.55
2:A:939:GLU:N	2:A:939:GLU:OE1	2.40	0.54
3:B:325:GLN:N	3:B:325:GLN:OE1	2.41	0.53
3:B:134:GLN:N	3:B:134:GLN:OE1	2.41	0.53
2:A:987:GLU:OE1	2:A:987:GLU:N	2.40	0.52
2:A:1071:SER:O	2:A:1075:SER:OG	2.25	0.51
3:B:53:LEU:HD21	3:B:382:PRO:HB2	1.93	0.51
3:B:251:GLU:OE1	3:B:251:GLU:N	2.40	0.51
3:B:319:THR:OG1	3:B:320:SER:N	2.42	0.51
2:A:146:ASP:OD1	2:A:147:ARG:N	2.44	0.50
2:A:277:GLU:OE1	2:A:279:ARG:NH1	2.46	0.49
2:A:294:THR:OG1	2:A:295:VAL:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1093:LEU:O	2:A:1096:SER:OG	2.28	0.49
2:A:744:ASP:OD1	2:A:745:THR:N	2.43	0.47
2:A:120:ILE:HG23	2:A:135:LEU:CD2	2.44	0.47
2:A:922:LEU:HD11	2:A:930:VAL:HG13	1.97	0.47
2:A:816:LEU:HD13	2:A:831:VAL:HG22	1.97	0.46
2:A:984:THR:HG22	2:A:984:THR:O	2.17	0.45
2:A:120:ILE:HG23	2:A:135:LEU:HD23	1.98	0.45
2:A:282:MET:HE2	2:A:305:LEU:HD11	1.99	0.45
2:A:143:ILE:HG12	2:A:154:ALA:HB2	1.99	0.44
2:A:953:TRP:O	2:A:970:ASN:N	2.51	0.44
2:A:60:LYS:O	2:A:81:THR:HA	2.18	0.44
1:C:417:HIS:CE1	3:B:371:ILE:HG21	2.52	0.44
2:A:742:VAL:CG2	2:A:752:LEU:HD21	2.48	0.44
3:B:289:PRO:HB3	3:B:360:LEU:HD22	1.99	0.43
3:B:257:ILE:HG21	3:B:284:VAL:HG21	2.01	0.43
2:A:40:GLU:OE1	2:A:42:TYR:OH	2.19	0.43
2:A:258:ILE:HD13	2:A:273:LEU:HD13	2.01	0.43
3:B:326:CYS:SG	3:B:393:ILE:HG23	2.58	0.43
2:A:310:ILE:HG21	2:A:328:LEU:HD12	2.01	0.43
2:A:130:MET:SD	2:A:195:VAL:HG11	2.58	0.42
2:A:55:VAL:HG11	2:A:1065:VAL:HG21	2.01	0.42
2:A:5:TYR:CE2	2:A:7:VAL:HG13	2.54	0.42
2:A:308:THR:O	2:A:383:LYS:NZ	2.45	0.42
2:A:944:GLU:OE2	2:A:947:ARG:NE	2.52	0.42
2:A:905:HIS:ND1	2:A:907:ASN:OD1	2.52	0.42
3:B:340:LEU:HD12	3:B:361:THR:HG21	2.00	0.42
2:A:55:VAL:CG1	2:A:1065:VAL:HG21	2.50	0.41
2:A:890:LEU:HB3	2:A:903:CYS:SG	2.60	0.41
2:A:927:MET:HE2	3:B:306:GLN:HG3	2.02	0.41
2:A:389:ILE:HD12	2:A:389:ILE:N	2.35	0.41
3:B:351:ASN:HB2	3:B:352:PRO:HD2	2.03	0.41
3:B:106:GLU:O	3:B:109:MET:HG2	2.21	0.41
2:A:68:ARG:NE	2:A:75:ASP:OD1	2.41	0.40
3:B:255:ASP:OD2	3:B:259:LYS:NZ	2.53	0.40
3:B:98:PRO:HG2	3:B:350:VAL:HG23	2.03	0.40
3:B:109:MET:SD	3:B:177:ILE:HD12	2.62	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	C	28/102 (28%)	28 (100%)	0	0	100	100
2	A	789/860 (92%)	767 (97%)	22 (3%)	0	100	100
3	B	374/485 (77%)	369 (99%)	5 (1%)	0	100	100
All	All	1191/1447 (82%)	1164 (98%)	27 (2%)	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	C	27/85 (32%)	26 (96%)	1 (4%)	30	59
2	A	702/746 (94%)	702 (100%)	0	100	100
3	B	342/430 (80%)	342 (100%)	0	100	100
All	All	1071/1261 (85%)	1070 (100%)	1 (0%)	87	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	435	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	964	ASN
2	A	978	GLN
3	B	95	GLN
3	B	390	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	QFC	B	502	-	47,47,47	0.14	0	65,67,67	0.35	0

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
5	QFC	B	502	-	-	8/19/54/54	0/6/6/6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

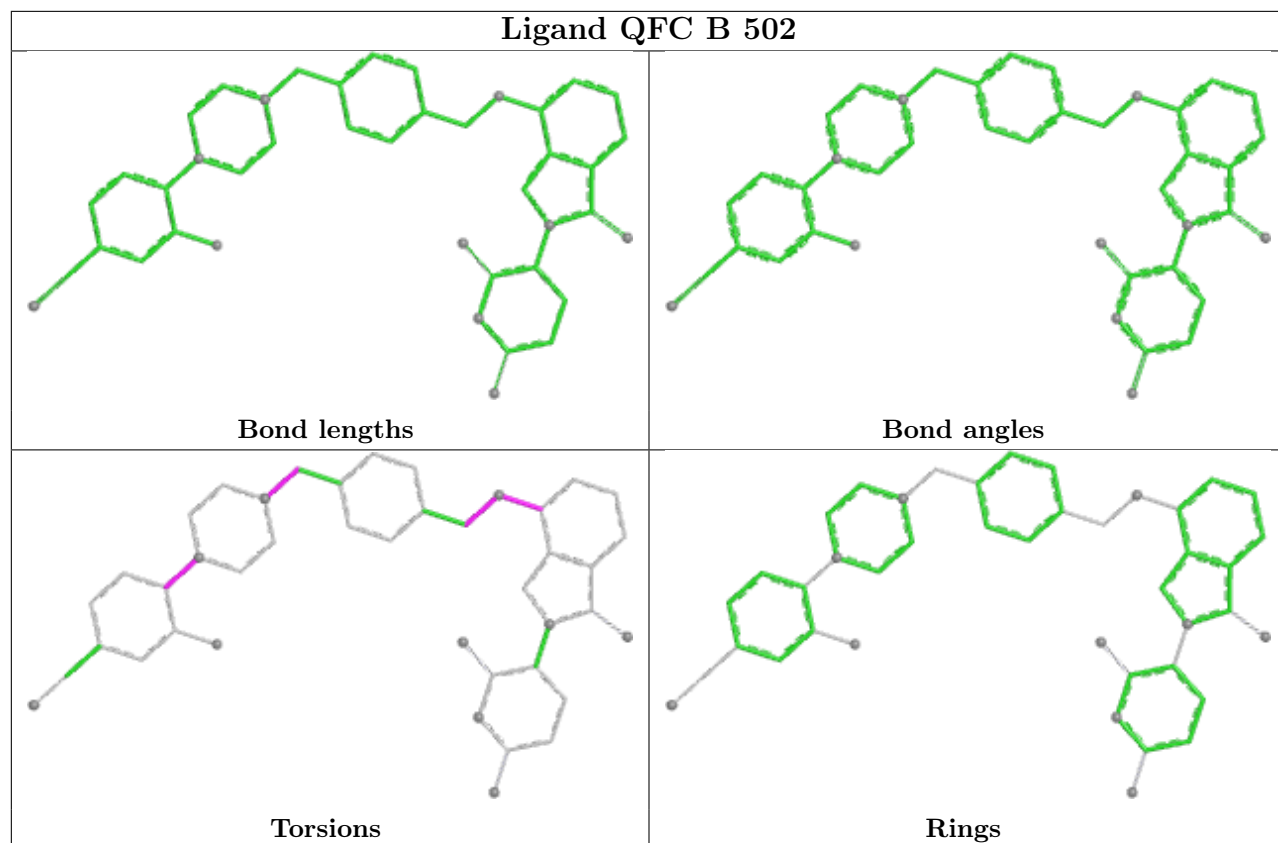
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	502	QFC	C-C5-N-C30
5	B	502	QFC	C-C5-N-C6
5	B	502	QFC	C9-C8-N1-C29
5	B	502	QFC	C9-C8-N1-C7
5	B	502	QFC	C21-C14-O-C13
5	B	502	QFC	C15-C14-O-C13
5	B	502	QFC	C12-C13-O-C14
5	B	502	QFC	C4-C5-N-C6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

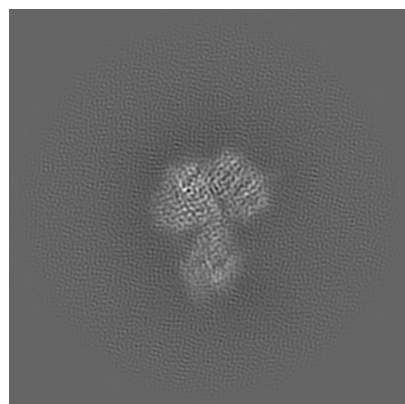
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49893. These allow visual inspection of the internal detail of the map and identification of artifacts.

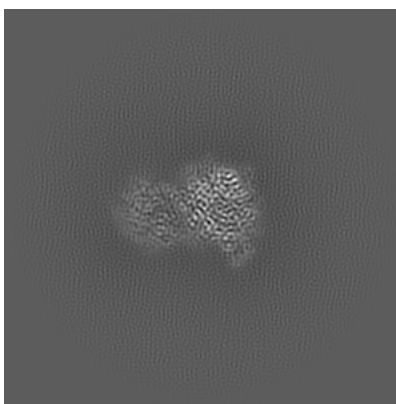
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

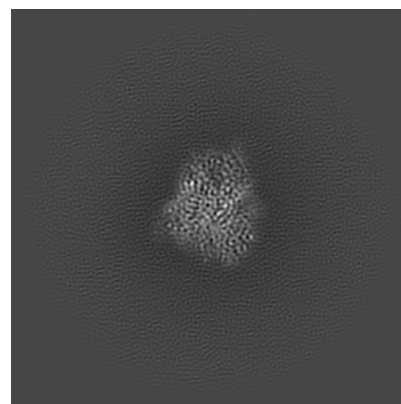
6.1.1 Primary map



X

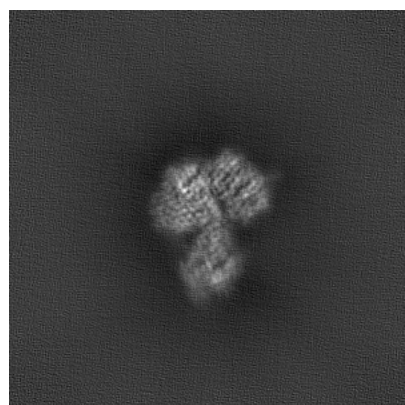


Y

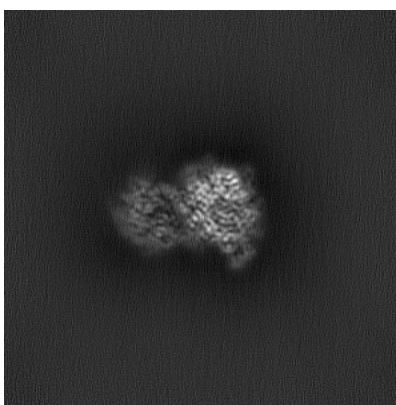


Z

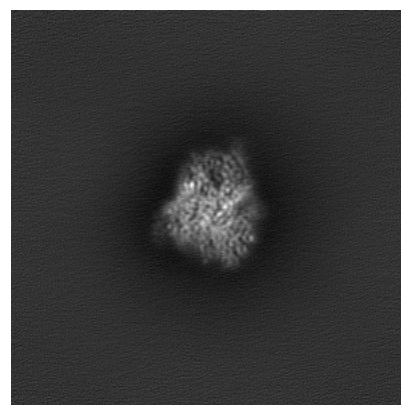
6.1.2 Raw map



X



Y

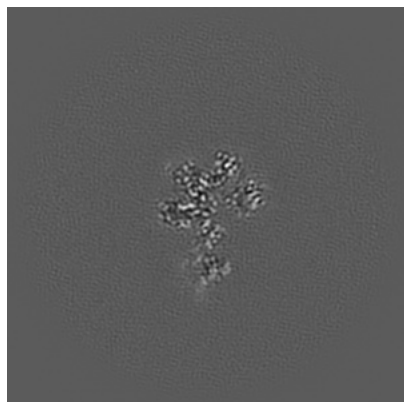


Z

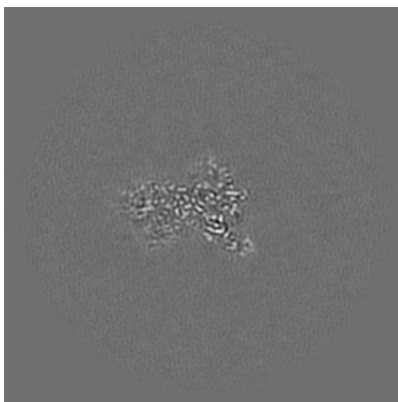
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

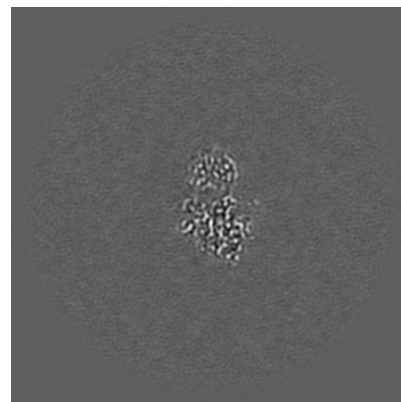
6.2.1 Primary map



X Index: 168

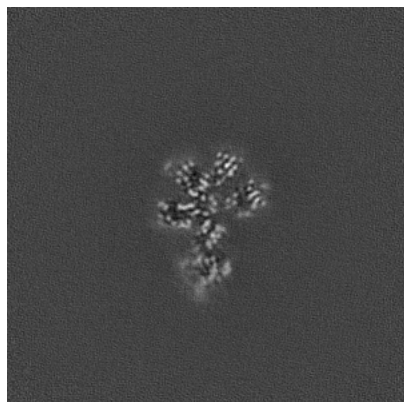


Y Index: 168

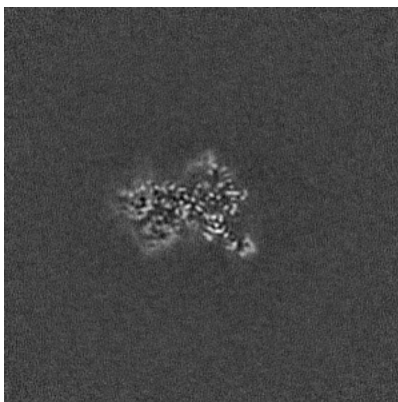


Z Index: 168

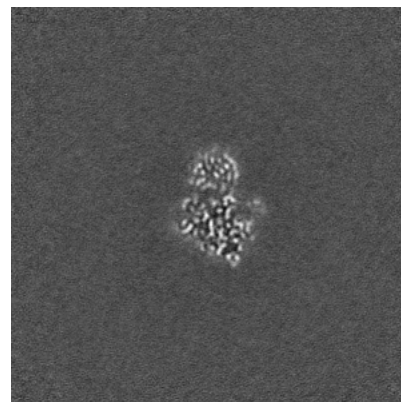
6.2.2 Raw map



X Index: 168



Y Index: 168

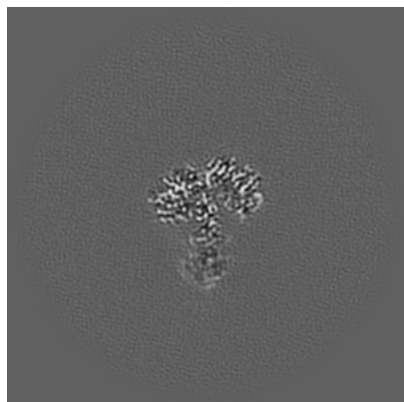


Z Index: 168

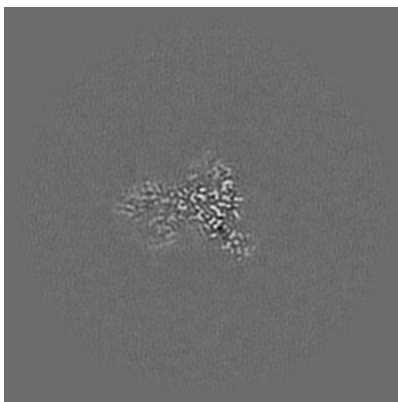
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

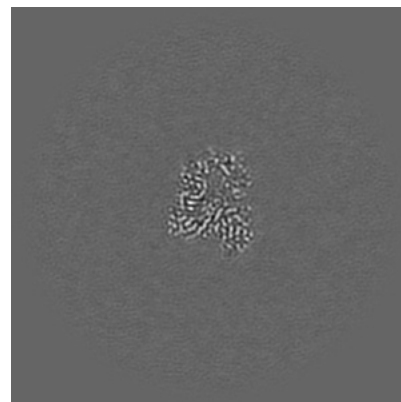
6.3.1 Primary map



X Index: 179

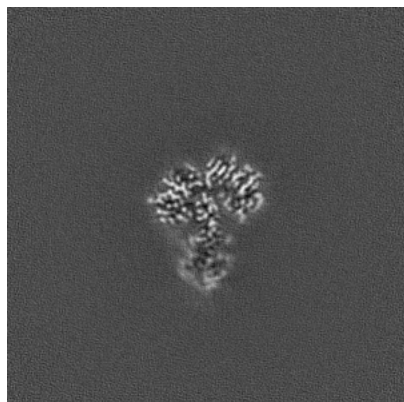


Y Index: 165

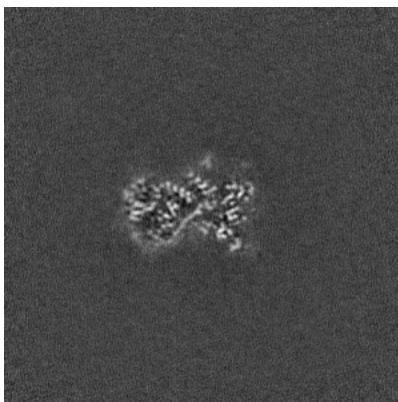


Z Index: 185

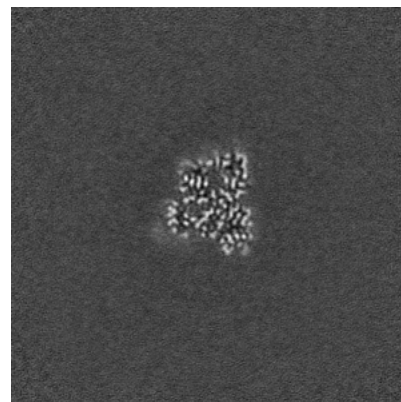
6.3.2 Raw map



X Index: 179



Y Index: 173

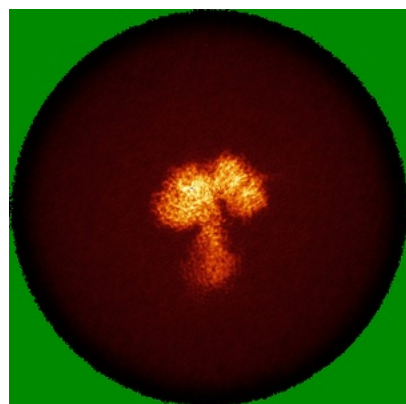


Z Index: 189

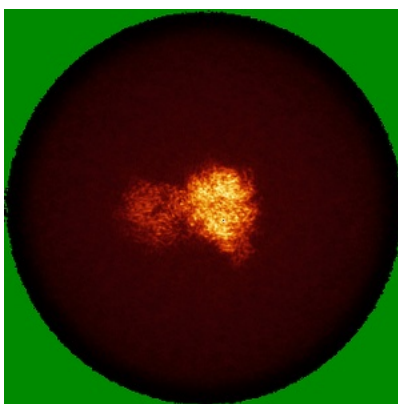
The images above show the largest variance slices of the map in three orthogonal directions.

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

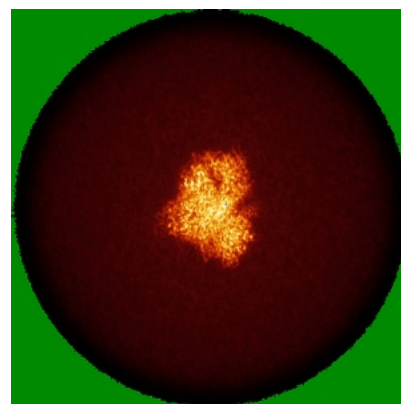
6.4.1 Primary map



X

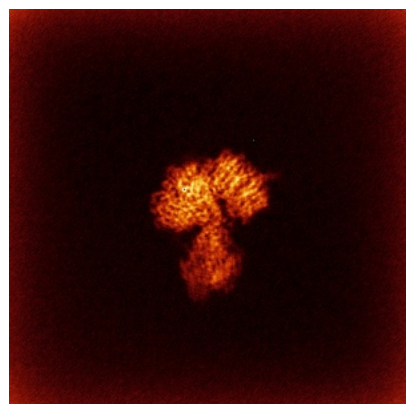


Y

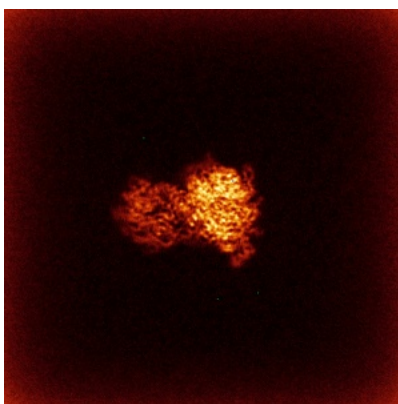


Z

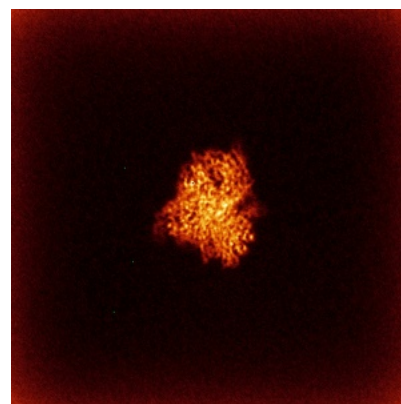
6.4.2 Raw map



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



X



Y



Z

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



X



Y



Z

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.

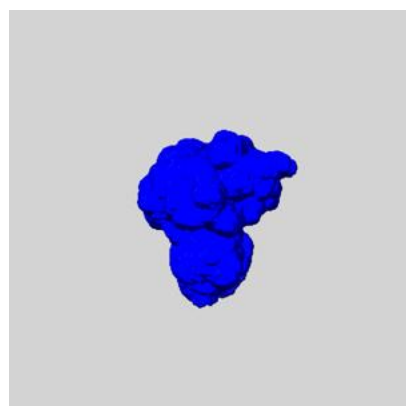
6.6 Mask visualisation [i](#)

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

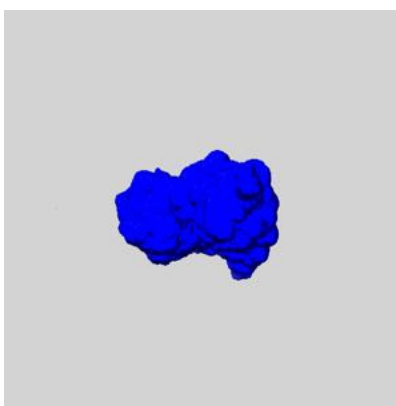
A mask typically either:

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

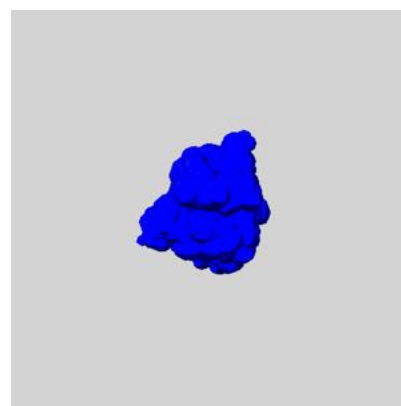
6.6.1 emd_49893_msk_1.map [i](#)



X



Y

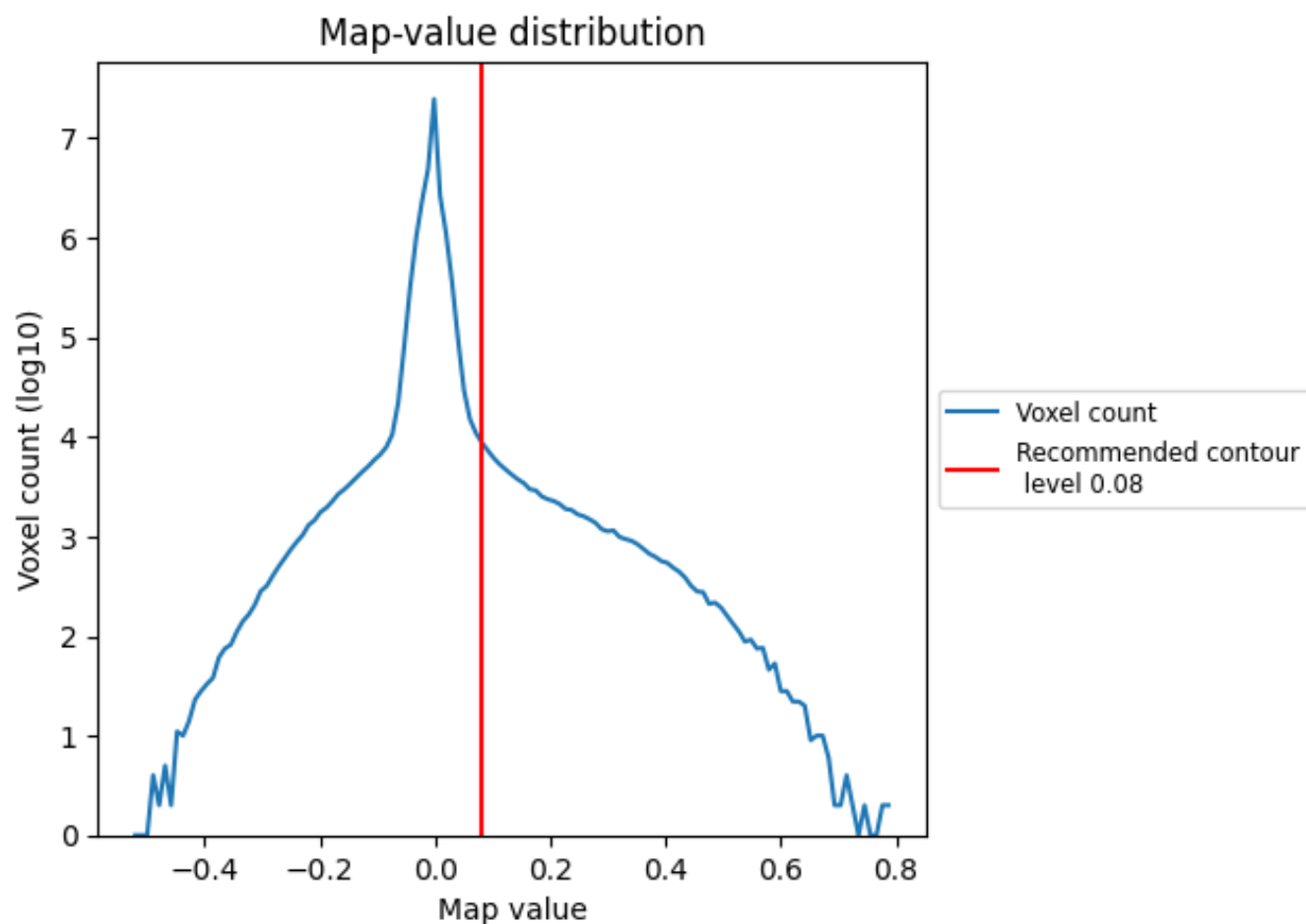


Z

7 Map analysis [i](#)

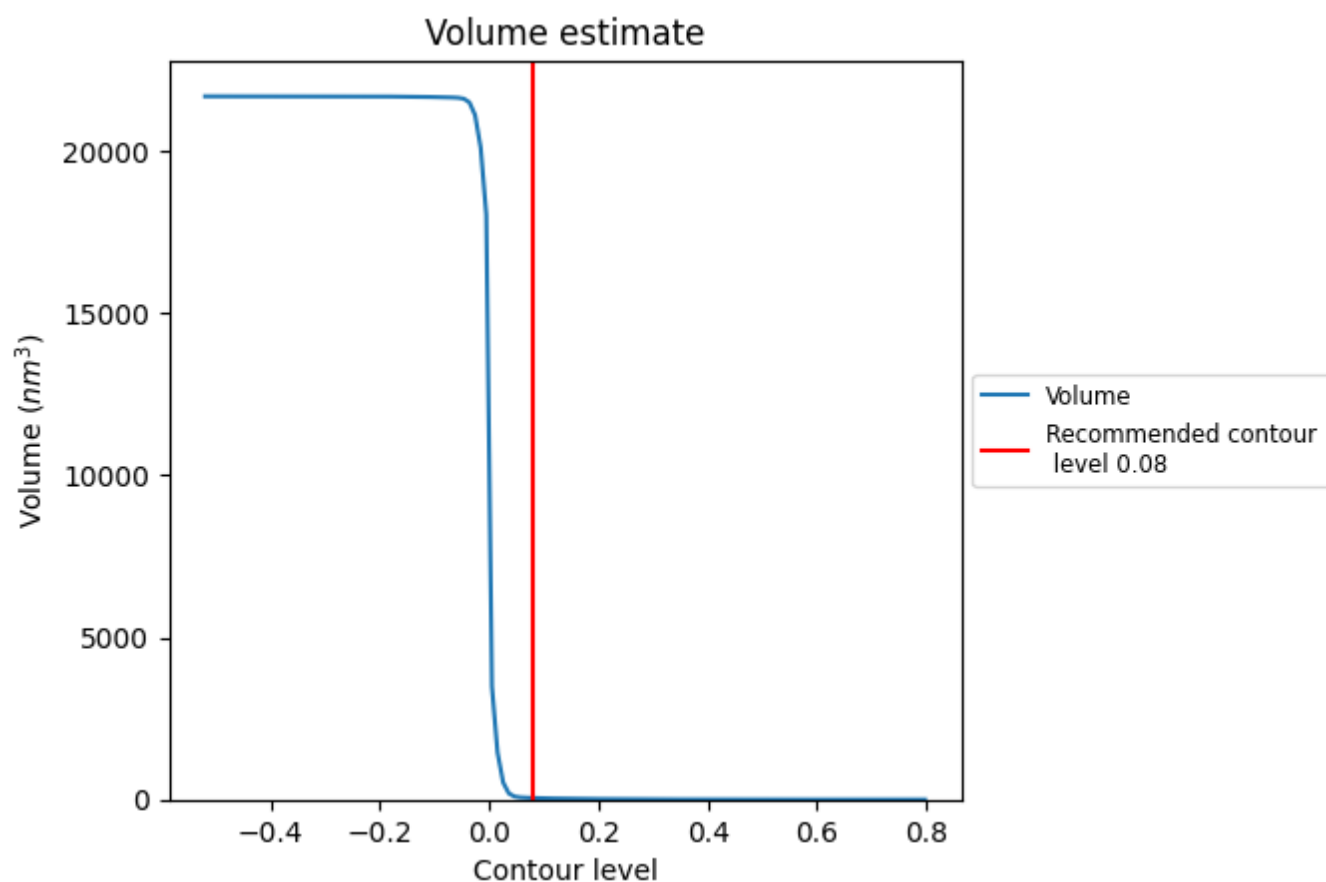
This section contains the results of statistical analysis of the map.

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.

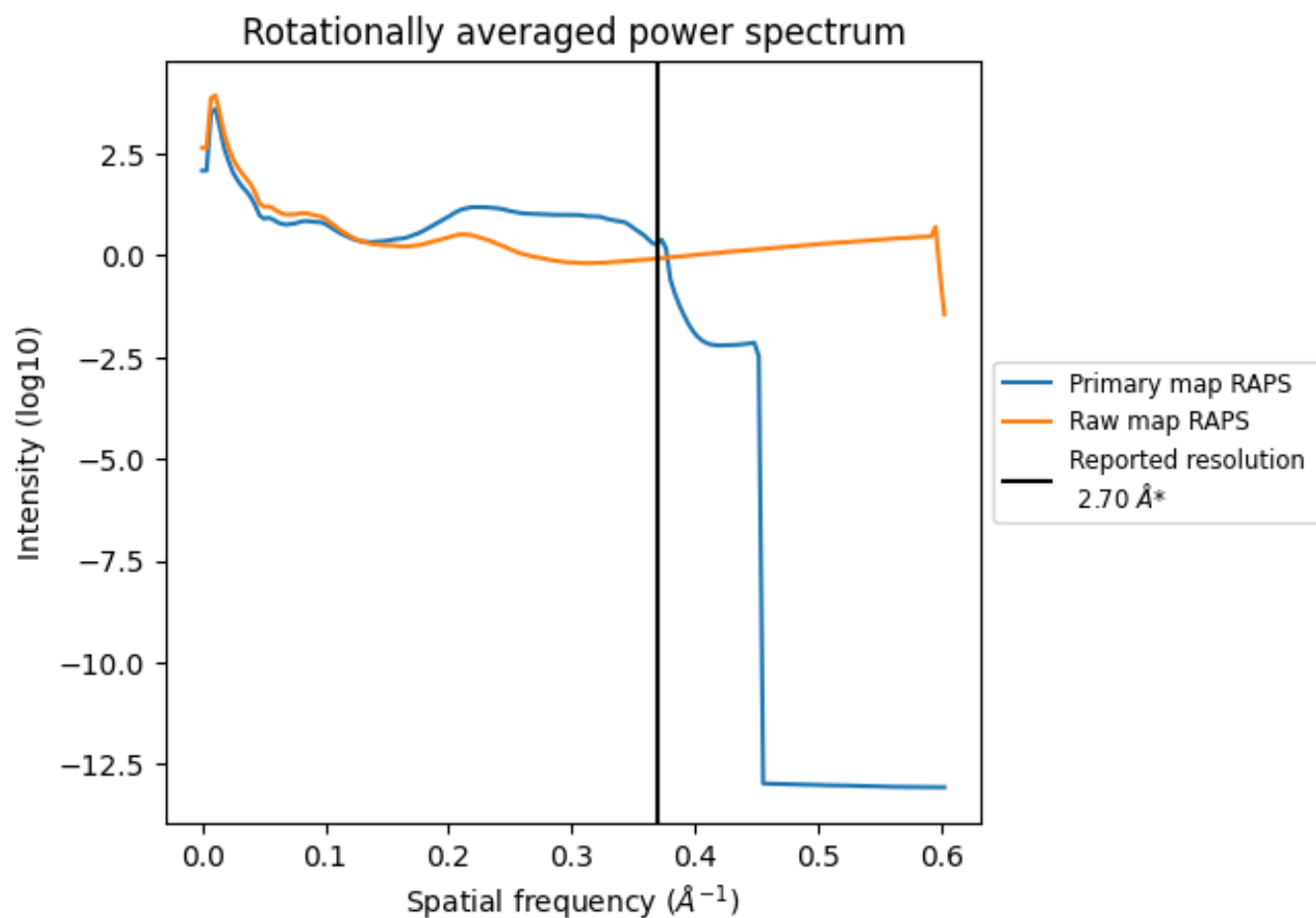
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm^3 ; this corresponds to an approximate mass of 44 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

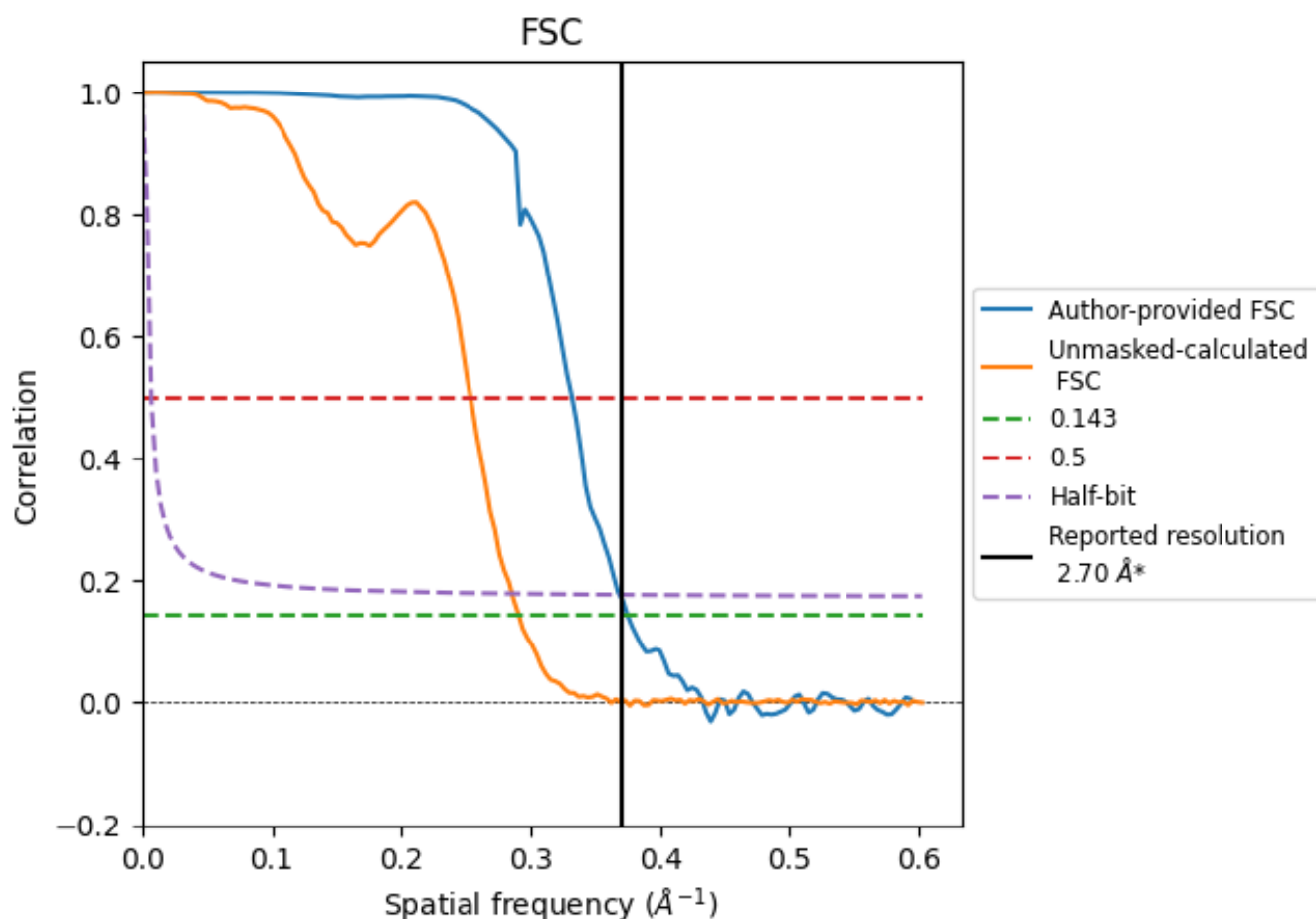


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

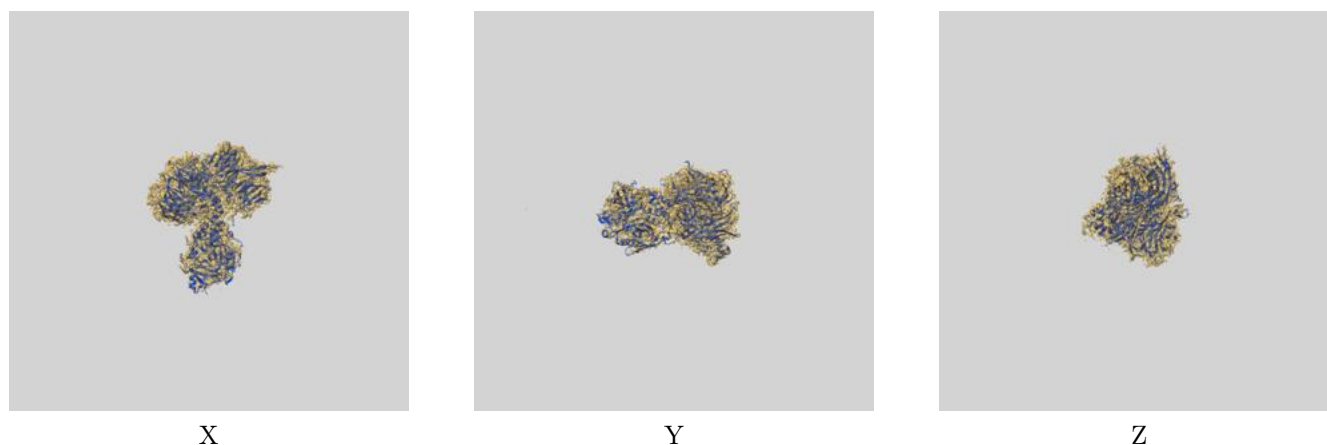
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.01	2.71
Unmasked-calculated*	3.44	3.94	3.50

*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 3.44 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

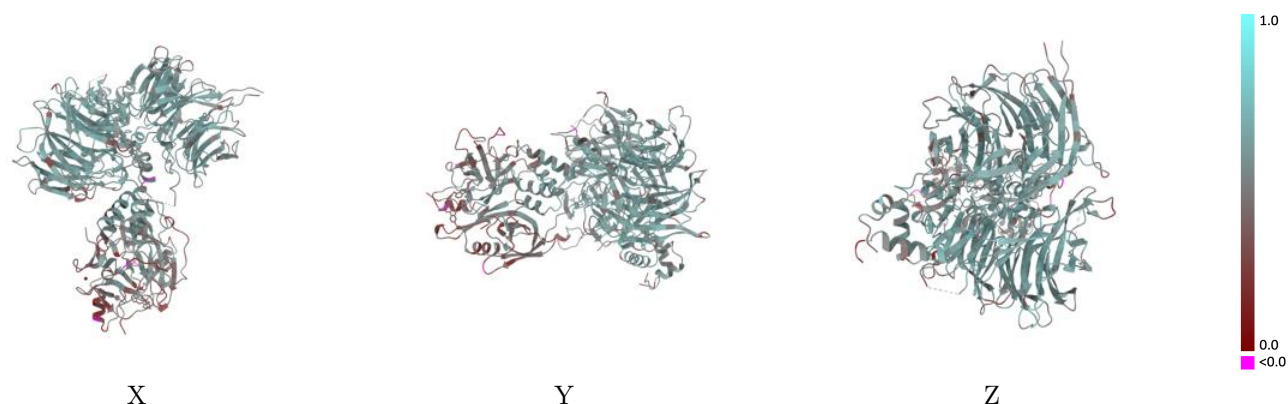
This section contains information regarding the fit between EMDB map EMD-49893 and PDB model 9NWT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



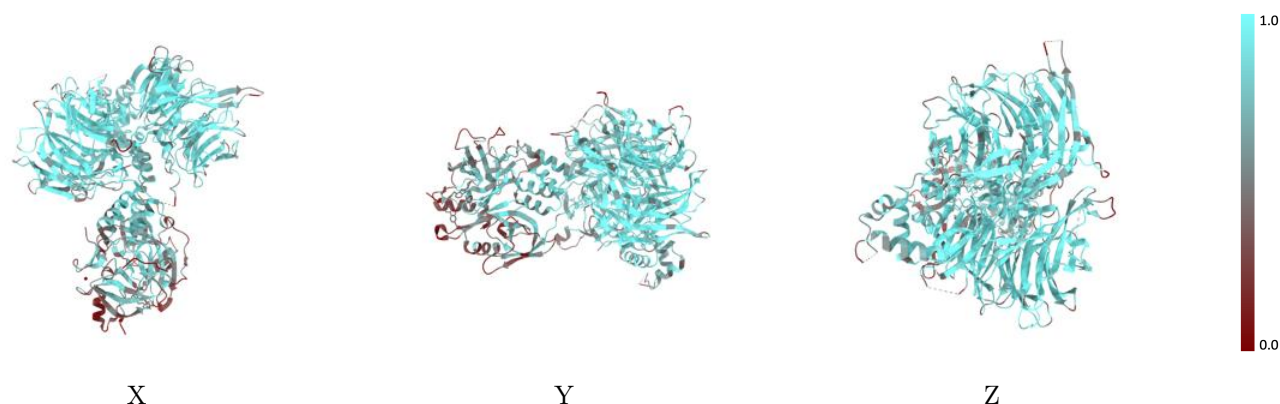
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



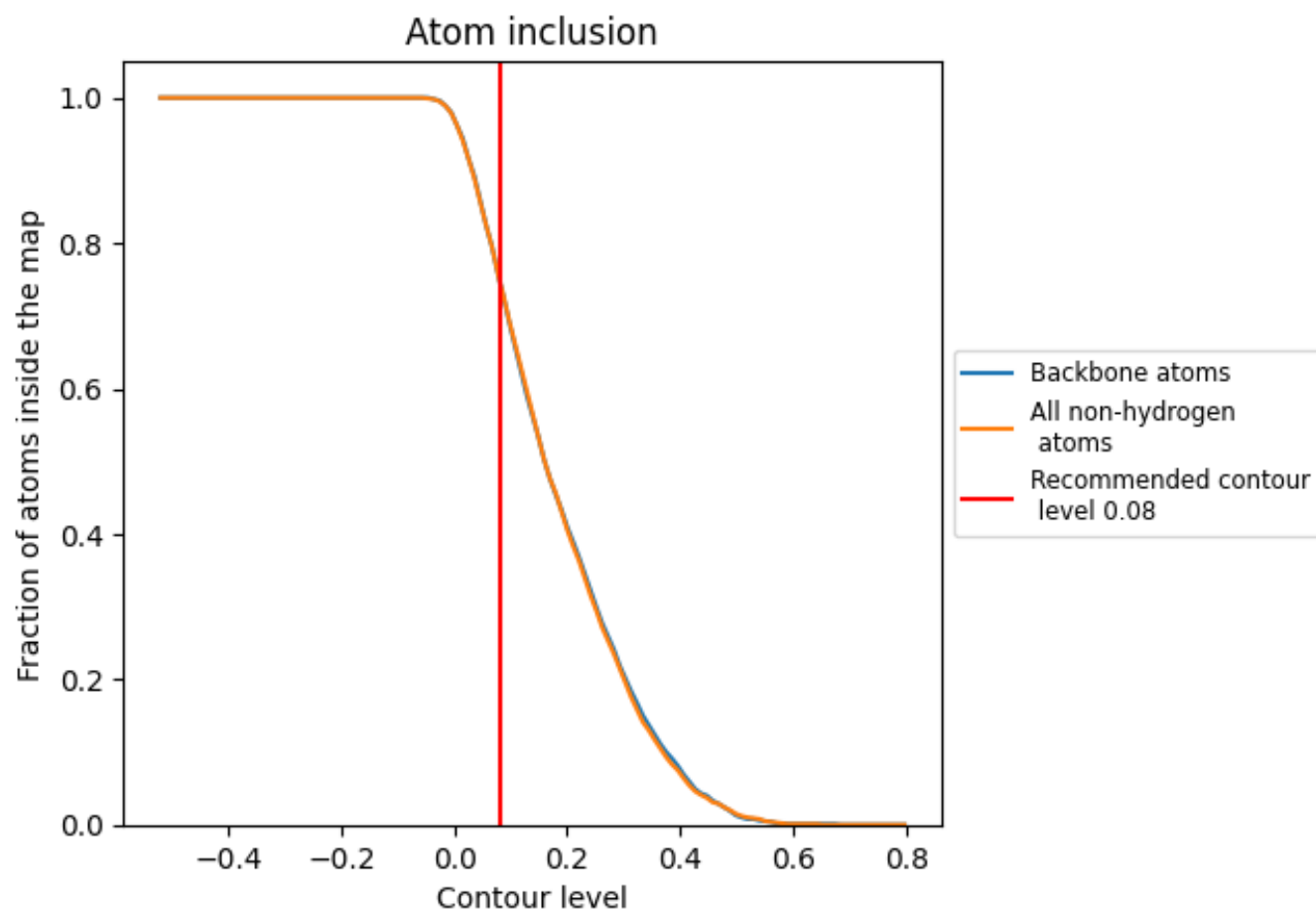
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 75% of all backbone atoms, 75% 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	0.7490	0.5250
A	0.8350	0.5650
B	0.6320	0.4610
C	0.3080	0.3020

