



Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 04:21 PM EDT

PDB ID : 9ZDX / pdb_00009zdx
EMDB ID : EMD-74076
Title : Dimer of ATPase BrxC containing a Walker B mutation and bound to ATP from the Acinetobacter BREX system
Authors : Doyle, L.A.; Stoddard, B.L.; Kaiser, B.; Kaiser, A.
Deposited on : 2025-11-26
Resolution : 2.95 Å(reported)
Based on initial model : .

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.dev133
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 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) : 2.50

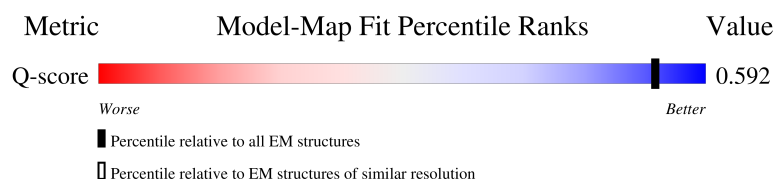
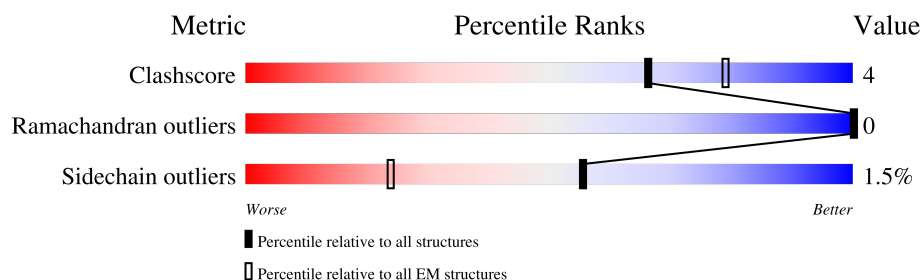
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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	13114 (2.45 - 3.45)

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	1228	
1	C	1228	

2 Entry composition [i](#)

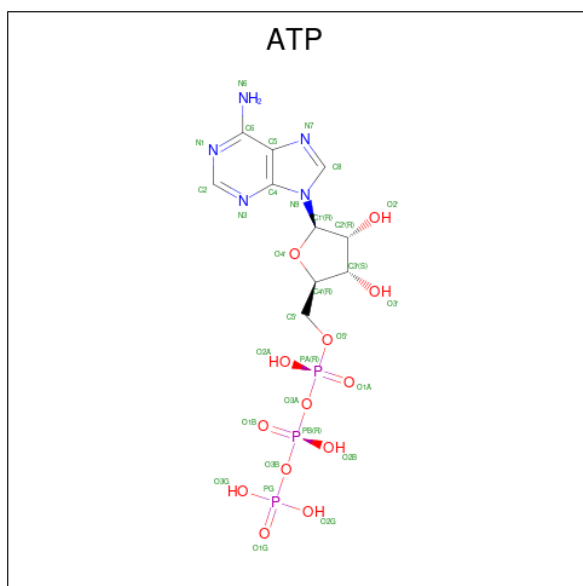
There are 4 unique types of molecules in this entry. The entry contains 17292 atoms, of which 8438 are hydrogens and 0 are deuteriums.

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 BREX system P-loop protein BrxC.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	C	550	8617	2793	4205	755	852	12	0	0
1	A	544	8607	2770	4233	747	846	11	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	C	1	31	10	5	13	3	0
2	A	1	31	10	5	13	3	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total 1	Mg 1	0
3	A	1	Total 1	Mg 1	0

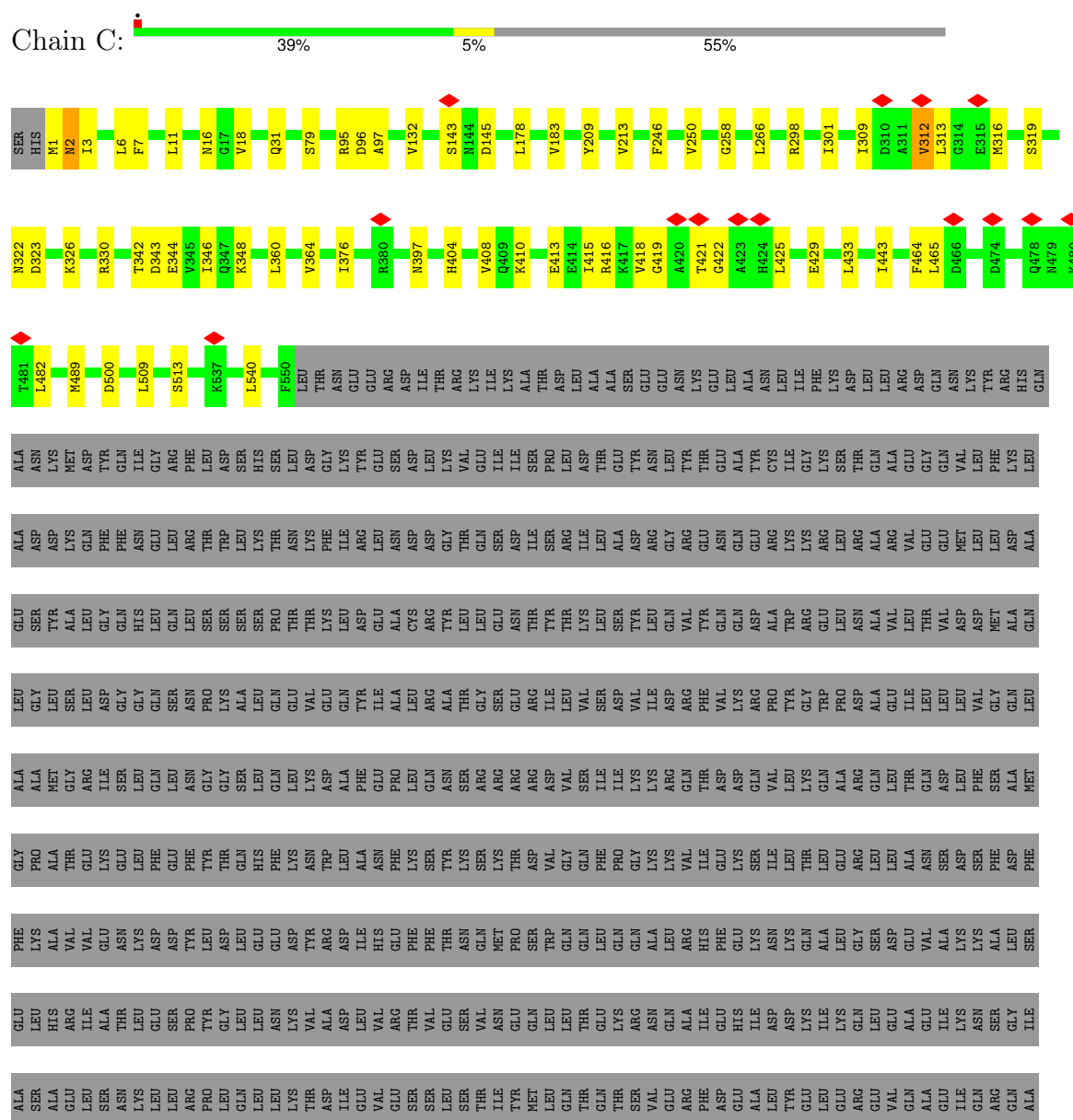
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	C	3	Total 3	O 3	0
4	A	1	Total 1	O 1	0

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: BREX system P-loop protein BrxC



TYR	LEU	GLU	THR	GLU	GLU	SER	VAL	ASP	GLN	PHE	VAL	ASP	ALA	LEU	LYS	ALA	GLU	LEU	LYS	LYS	ILE	VAL	GLY	ASP	LYS	LYS	ARG	VAL	ARG	ILE	ARG
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- Molecule 1: BREX system P-loop protein BrxC

Chain A:

Lys	Ser	Thr	Leu	Asp	Leu	Ala	Gln	Leu	Lys	Glu	Ser	His
Lys	Ser	Pro	Val	Leu	Ala	Asn	Thr	Asp	Leu	Glu	Met	Ser
Val	Ala	Ala	Glu	Arg	Phe	Pro	Thr	Ala	Asn	Leu	Ala	Met
Gly	Thr	Thr	Ser	Thr	Lys	Gln	Leu	Lys	Asp	Thr	Ala	N2
Lys	Ser	Ser	Val	Val	Thr	Gln	Ala	Arg	Leu	Arg	Thr	R13
Lys	Ala	Leu	Glu	Thr	Ser	Asn	Ala	Tyr	Lys	Val	Lys	R16
Lys	Pro	Ser	Ser	Ser	Lys	Ser	Thr	Leu	Thr	Gly	Lys	R17
Arg	Ala	Ala	Val	Val	Asn	Arg	Ser	Leu	Leu	Glu	Thr	R18
Val	Ala	Ala	Leu	Leu	Val	Ala	Ala	Tyr	Lys	Arg	Ala	R19
Val	Ala	Ala	Val	Val	Gln	Gln	Ala	Val	Thr	Val	Thr	R20
Arg	Pro	Thr	Thr	Gln	Leu	Phe	Thr	Leu	Thr	Glu	Val	R21
Val	Pro	Lys	Glu	His	Leu	Thr	Phe	Gln	Thr	Glu	Gly	R22
Val	Pro	Lys	Glu	Phe	Glu	Asp	Val	Asn	Thr	Leu	Val	R23
Val	Pro	Lys	Glu	His	Glu	Lys	Lys	Gln	Ala	Ala	Ala	R24
Val	Val	Val	Ala	Leu	Leu	Gln	Pro	Ala	Tyr	Asn	Thr	R25
Val	Val	Val	Ala	Asn	Leu	Val	Pro	Ala	Gly	Cys	Gly	R26
Glu	Glu	Glu	Lys	Asp	Lys	Leu	Tyr	Trp	Leu	Leu	Ala	R28
Val	Val	Glu	Lys	Lys	Thr	Leu	Gly	Arg	Lys	Phe	Ala	R29
Asp	Asp	Lys	Leu	Leu	Glu	Gln	Trp	Glu	Lys	Lys	Lys	Q189
Val	Val	Ala	Lys	Gln	Arg	Ala	Pro	Leu	Ser	Asp	Asp	F208
Ala	Ala	Ala	Gly	Gly	Arg	Arg	Asp	Asn	Arg	Leu	Leu	R230
Ser	Ser	Ser	Leu	Ser	Phe	Gln	Ala	Ala	Arg	Ala	Arg	R230
Leu	Leu	Val	Ala	Val	Ala	Thr	Leu	Val	Gly	Asp	Asp	F246
Lys	Lys	Ser	Glu	Leu	Leu	Gln	Leu	Val	Gln	Gln	Asn	V250
Ser	Ser	Ser	Asn	Asp	Asp	Phe	Pro	Asp	Val	Val	Lys	V250
Ser	Ser	Ser	Leu	Phe	Ser	Thr	Val	Asp	Arg	Leu	Tyr	D255
Ser	Ser	Ser	Gly	Arg	Arg	Ser	Gly	Met	Gly	Phe	Arg	D255
Val	Val	Val	Ala	Leu	Ala	Ala	Gln	Ala	Ala	Lys	His	L266
Thr	Thr	Val	Leu	Phe	Phe	Gly	Leu	Gln	Leu	Leu	Gln	V267
Leu	Leu	Val	Ser	Ser	Lys	Pro	Ala	Gly	Asp	Asn	Asn	V270
Glu	Glu	Thr	Ala	Ala	Ala	Ala	Ala	Leu	Lys	Asp	Lys	V270
Thr	Thr	Thr	Gln	Glu	Thr	Thr	Gly	Leu	Lys	Met	Met	R298
Glu	Glu	Glu	Leu	Val	Val	Glu	Arg	Leu	Gln	Asp	Asp	R298
Glu	Glu	Glu	Ala	Val	Val	Glu	Leu	Leu	Phe	Phe	Tyr	V303
Val	Val	Val	Asn	Asn	Asn	Glu	Ser	Gly	Gln	Gln	Gln	T304
Asp	Asp	Val	Lys	Lys	Lys	Phe	Leu	Gln	Asn	Leu	Leu	Q306
Gln	Gln	Phe	Leu	Asp	Asp	Phe	Leu	Gln	Leu	Arg	Phe	V303
Val	Val	Thr	Pro	Tyr	Thr	Phe	Asn	Leu	Arg	Thr	Leu	S319
Ala	Ala	Leu	Asp	Gly	Thr	Thr	Gly	Ser	Trp	Asp	Asp	S319
Lys	Lys	Asn	Leu	Leu	Glu	His	Leu	Ser	Leu	Lys	Lys	K320
Ala	Ala	Thr	Leu	Glu	Glu	Phe	Gln	Pro	Thr	Thr	Ser	K320
Glu	Glu	Thr	Val	Tyr	Asp	Lys	Leu	Val	Lys	Asn	Lys	A321
Leu	Leu	Thr	Thr	Arg	Arg	Lys	Thr	Val	Lys	Thr	Asp	S339
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Gly	Gly	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342
Val	Val	Thr	Thr	Thr	Val	Val	Thr	Thr	Lys	Lys	Phe	T342

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	477102	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	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	5.837	Depositor
Minimum map value	-3.324	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.38	Depositor
Map size ($\text{\AA}$)	403.91998, 403.91998, 403.91998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.122, 1.122, 1.122	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: MG, ATP

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	0.18	0/4460	0.26	0/6017
1	C	0.18	0/4499	0.38	4/6068 (0.1%)
All	All	0.18	0/8959	0.33	4/12085 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	VAL	CA-C-N	8.77	134.81	122.36
1	C	312	VAL	C-N-CA	8.77	134.81	122.36
1	C	323	ASP	CA-C-N	7.79	138.23	121.64
1	C	323	ASP	C-N-CA	7.79	138.23	121.64

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	4374	4233	4252	32	0
1	C	4412	4205	4302	38	0
2	A	31	0	12	0	0
2	C	31	0	12	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	C	3	0	0	0	0
All	All	8854	8438	8578	68	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 (68) 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:543:ARG:NH1	1:A:545:GLY:O	2.19	0.75
1:C:322:ASN:OD1	1:A:306:GLN:NE2	2.20	0.74
1:C:258:GLY:O	1:C:298:ARG:NH2	2.21	0.73
1:A:16:ASN:ND2	1:A:18:VAL:O	2.26	0.69
1:C:326:LYS:O	1:C:330:ARG:NH1	2.28	0.67
1:C:415:ILE:O	1:C:418:VAL:HG22	1.96	0.66
1:A:339:SER:O	1:A:342:THR:OG1	2.14	0.64
1:C:309:ILE:O	1:C:313:LEU:N	2.31	0.64
1:C:410:LYS:NZ	1:C:500:ASP:OD1	2.26	0.63
1:C:7:PHE:CE2	1:C:11:LEU:HD11	2.34	0.63
1:C:132:VAL:HG13	1:C:266:LEU:HD13	1.81	0.63
1:C:246:PHE:O	1:C:250:VAL:HG23	1.99	0.62
1:A:506:LEU:O	1:A:510:VAL:HG23	2.00	0.61
1:C:416:ARG:HG3	1:C:422:GLY:HA2	1.82	0.61
1:C:1:MET:HG2	1:C:2:ASN:N	2.16	0.61
1:C:415:ILE:O	1:C:421:THR:OG1	2.18	0.61
1:C:413:GLU:OE1	1:A:471:ARG:NH1	2.33	0.60
1:C:343:ASP:OD1	1:C:344:GLU:N	2.34	0.59
1:C:418:VAL:HG23	1:C:419:GLY:H	1.66	0.59
1:C:96:ASP:OD1	1:C:97:ALA:N	2.32	0.59
1:A:387:ASN:OD1	1:A:388:TYR:N	2.36	0.58
1:C:3:ILE:HG22	1:C:3:ILE:O	2.01	0.58
1:C:16:ASN:O	2:C:1301:ATP:O3'	2.22	0.58
1:C:2:ASN:O	1:C:6:LEU:HD13	2.06	0.56
1:C:143:SER:OG	1:C:145:ASP:OD1	2.24	0.56
1:C:418:VAL:HG23	1:C:419:GLY:N	2.21	0.56
1:A:186:ARG:NH1	1:A:189:GLN:OE1	2.40	0.54
1:A:404:HIS:O	1:A:408:VAL:HG23	2.07	0.54
1:A:398:TYR:CD1	1:A:399:PRO:HA	2.44	0.53
1:A:449:GLY:HA2	1:A:517:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HG13	1:A:303:VAL:HG22	1.90	0.53
1:C:404:HIS:O	1:C:408:VAL:HG23	2.08	0.53
1:C:421:THR:HG22	1:C:464:PHE:C	2.33	0.52
1:A:469:VAL:HG11	1:A:494:PHE:CE1	2.44	0.52
1:A:391:PRO:O	1:A:395:ILE:HD12	2.10	0.51
1:C:415:ILE:HG23	1:C:421:THR:HG21	1.93	0.51
1:C:313:LEU:HD23	1:C:316:MET:HE3	1.94	0.49
1:C:482:LEU:HD11	1:C:540:LEU:HD12	1.93	0.49
1:A:270:VAL:HG21	1:A:303:VAL:HG22	1.94	0.49
1:A:255:ASP:OD1	1:A:298:ARG:NH2	2.43	0.49
1:C:209:TYR:O	1:C:213:VAL:HG23	2.12	0.48
1:C:429:GLU:O	1:C:433:LEU:HB2	2.14	0.48
1:A:514:ILE:HD11	1:A:521:LYS:HD3	1.97	0.47
1:C:489:MET:HE1	1:C:513:SER:OG	2.15	0.46
1:A:132:VAL:HG13	1:A:266:LEU:HD13	1.98	0.46
1:C:301:ILE:HG23	1:C:301:ILE:O	2.15	0.46
1:C:342:THR:O	1:C:346:ILE:HG12	2.16	0.45
1:A:443:ILE:O	1:A:443:ILE:CG2	2.63	0.45
1:C:415:ILE:HG22	1:C:425:LEU:HD23	1.99	0.45
1:A:367:GLN:O	1:A:368:LYS:C	2.60	0.45
1:A:110:GLU:H	1:A:110:GLU:CD	2.25	0.44
1:A:246:PHE:O	1:A:250:VAL:HG23	2.18	0.44
1:C:178:LEU:HD22	1:C:183:VAL:HG23	2.00	0.43
1:C:376:ILE:O	1:C:376:ILE:CG2	2.66	0.43
1:A:13:ARG:NH2	1:A:349:ARG:O	2.43	0.43
1:A:507:ASP:N	1:A:507:ASP:OD1	2.52	0.43
1:C:16:ASN:ND2	1:C:18:VAL:O	2.51	0.43
1:A:24:ASP:C	1:A:24:ASP:OD2	2.62	0.43
1:A:399:PRO:HB2	1:A:452:VAL:HG23	2.01	0.43
1:A:489:MET:HA	1:A:489:MET:HE2	2.00	0.42
1:A:270:VAL:HB	1:A:303:VAL:HG13	2.00	0.42
1:C:360:LEU:O	1:C:364:VAL:HG23	2.20	0.42
1:A:23:GLN:O	1:A:83:LYS:NZ	2.36	0.42
1:A:267:VAL:HG22	1:A:270:VAL:CG2	2.49	0.42
1:A:267:VAL:CG1	1:A:303:VAL:HG22	2.50	0.41
1:A:142:SER:OG	1:A:143:SER:N	2.54	0.41
1:C:79:SER:OG	2:C:1301:ATP:O1B	2.38	0.41
1:C:1:MET:CG	1:C:2:ASN:N	2.83	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	540/1228 (44%)	527 (98%)	13 (2%)	0	100	100
1	C	548/1228 (45%)	523 (95%)	25 (5%)	0	100	100
All	All	1088/2456 (44%)	1050 (96%)	38 (4%)	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	473/1076 (44%)	469 (99%)	4 (1%)	73	85
1	C	476/1076 (44%)	466 (98%)	10 (2%)	47	69
All	All	949/2152 (44%)	935 (98%)	14 (2%)	55	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	ASN
1	C	31	GLN
1	C	95	ARG
1	C	312	VAL
1	C	319	SER
1	C	348	LYS
1	C	397	ASN
1	C	443	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	465	LEU
1	C	509	LEU
1	A	208	PHE
1	A	230	LYS
1	A	304	THR
1	A	507	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2	ASN
1	C	136	ASN
1	C	162	GLN
1	A	45	HIS
1	A	152	ASN
1	A	177	HIS
1	A	374	ASN
1	A	397	ASN
1	A	409	GLN
1	A	478	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
2	ATP	C	1301	3	32,33,33	0.57	1 (3%)	48,52,52	0.34	0
2	ATP	A	1301	3	32,33,33	0.57	1 (3%)	48,52,52	0.32	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
2	ATP	C	1301	3	-	2/22/38/38	0/3/3/3
2	ATP	A	1301	3	-	5/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ATP	PB-O3B	-2.23	1.57	1.59
2	C	1301	ATP	PB-O3B	-2.07	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

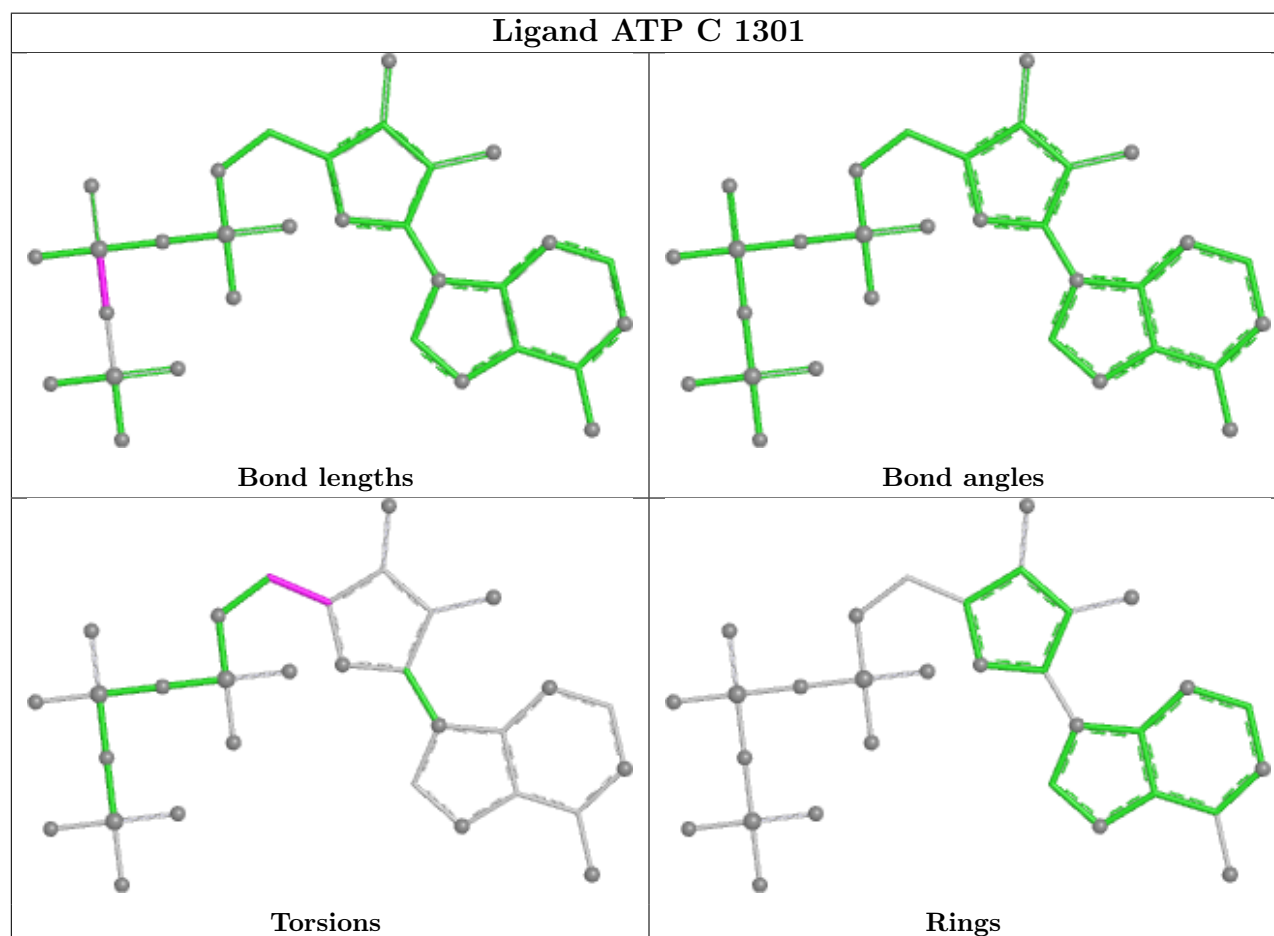
Mol	Chain	Res	Type	Atoms
2	A	1301	ATP	PB-O3B-PG-O2G
2	C	1301	ATP	O4'-C4'-C5'-O5'
2	A	1301	ATP	O4'-C4'-C5'-O5'
2	A	1301	ATP	C3'-C4'-C5'-O5'
2	C	1301	ATP	C3'-C4'-C5'-O5'
2	A	1301	ATP	PB-O3B-PG-O3G
2	A	1301	ATP	PG-O3B-PB-O2B

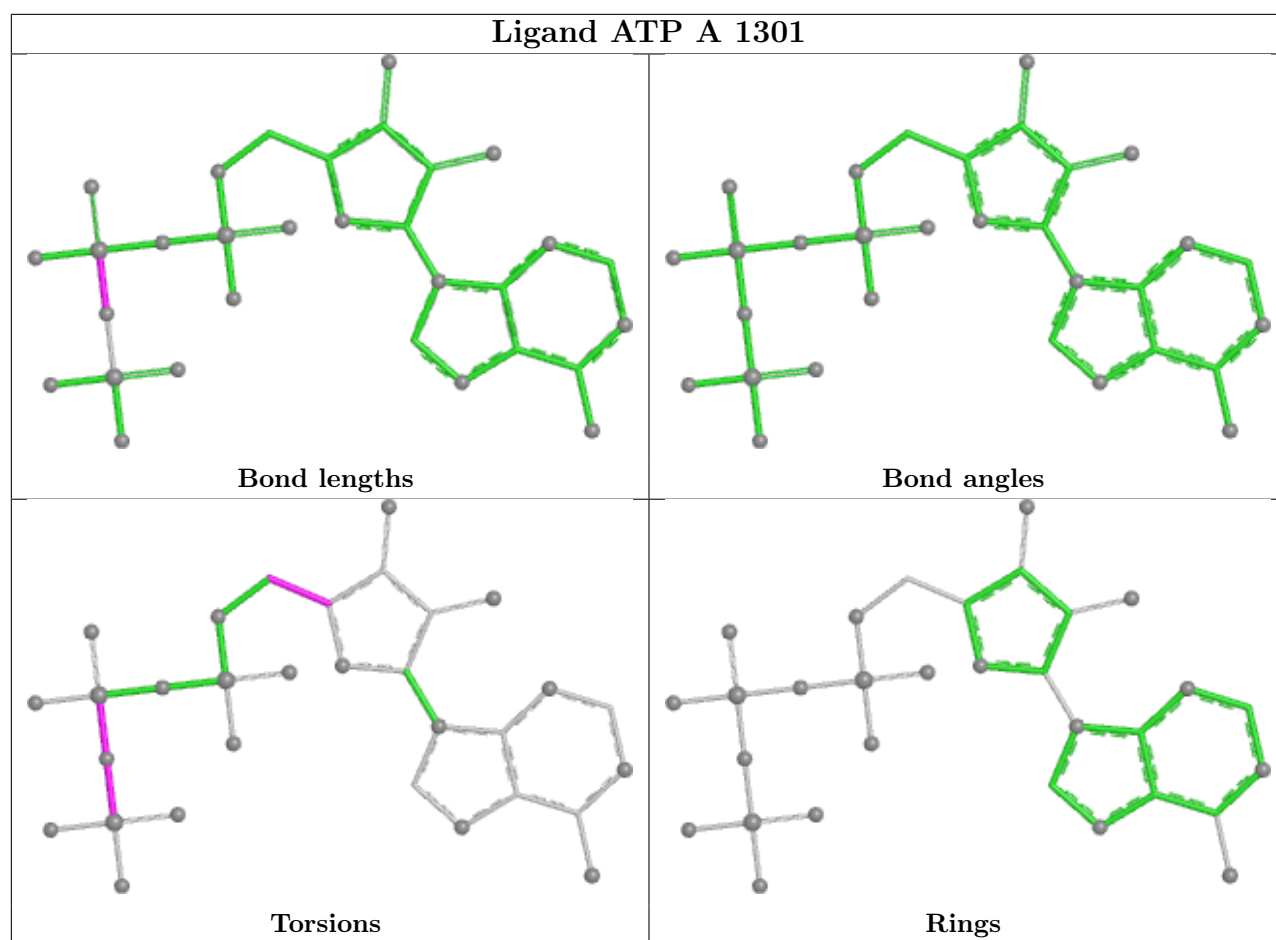
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1301	ATP	2	0

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.

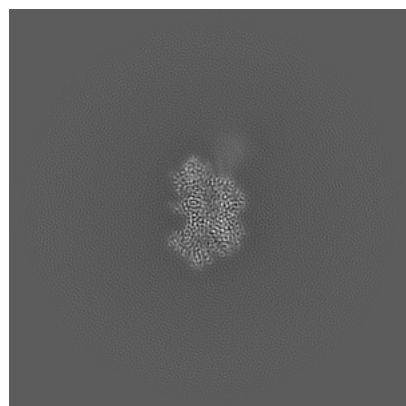
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74076. These allow visual inspection of the internal detail of the map and identification of artifacts.

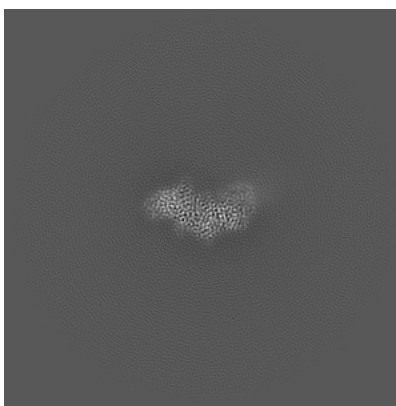
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

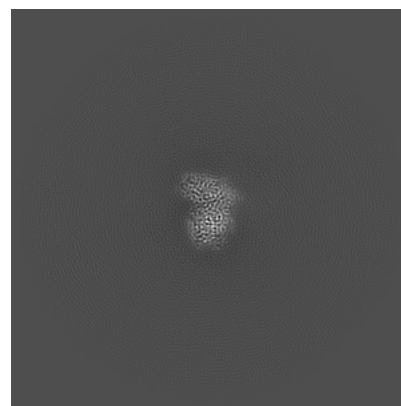
6.1.1 Primary map



X

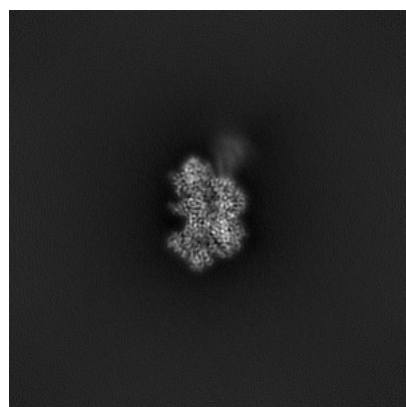


Y

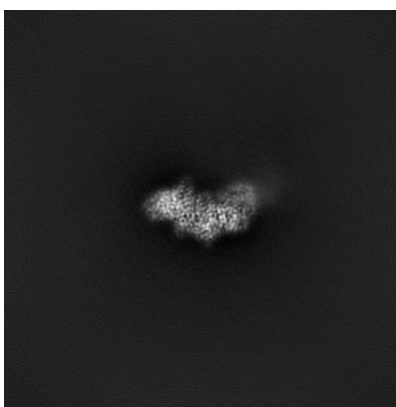


Z

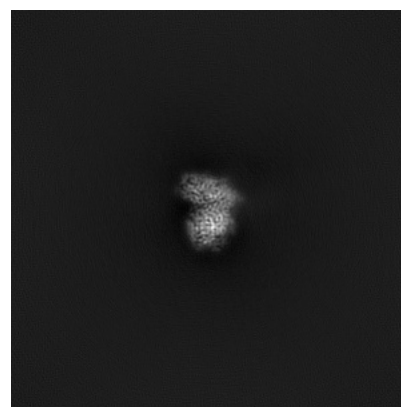
6.1.2 Raw map



X



Y

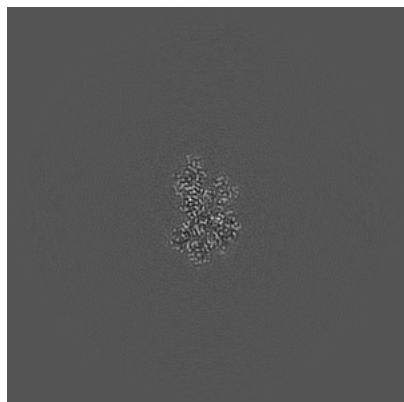


Z

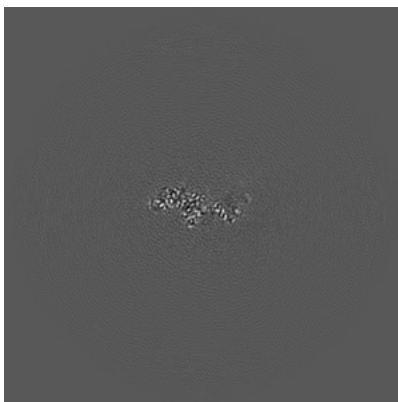
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

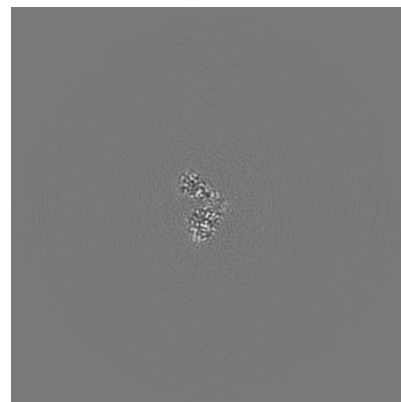
6.2.1 Primary map



X Index: 180

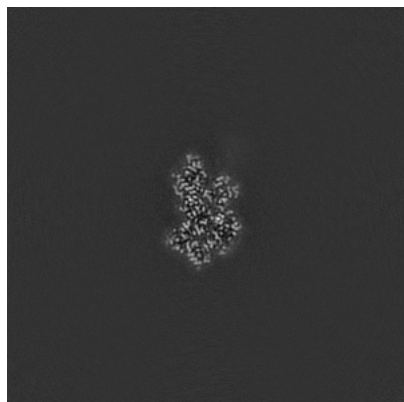


Y Index: 180

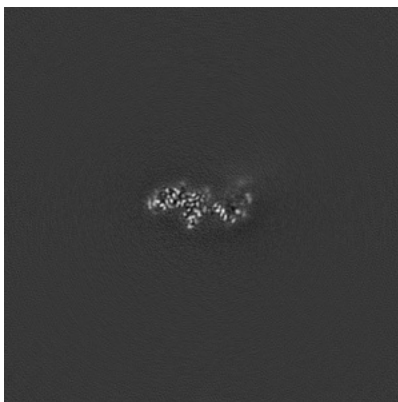


Z Index: 180

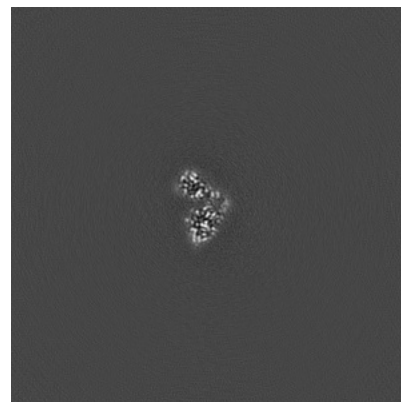
6.2.2 Raw map



X Index: 180



Y Index: 180

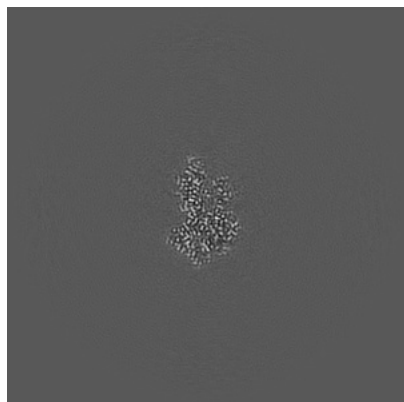


Z Index: 180

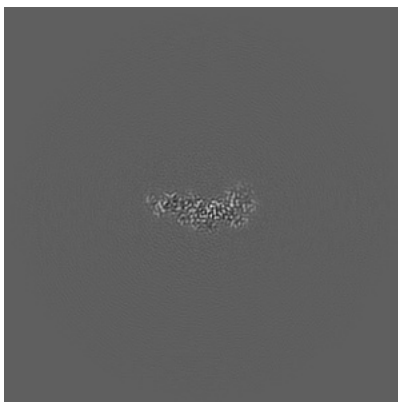
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

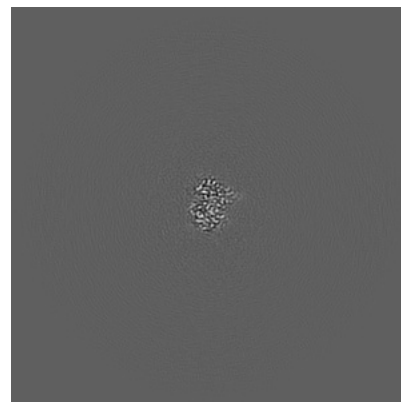
6.3.1 Primary map



X Index: 181

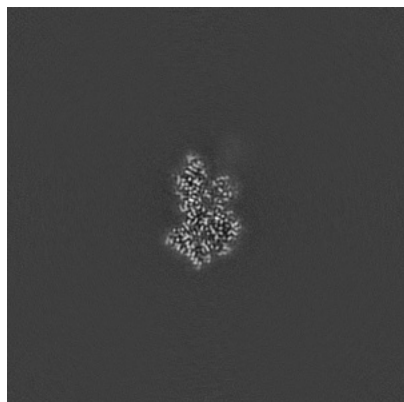


Y Index: 164

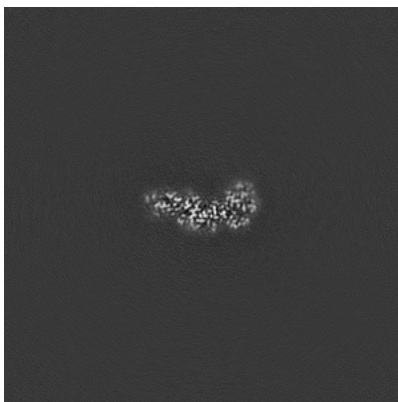


Z Index: 166

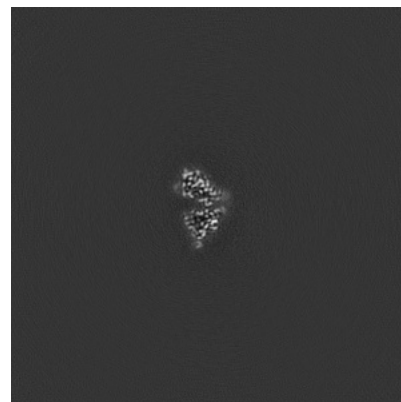
6.3.2 Raw map



X Index: 181



Y Index: 163

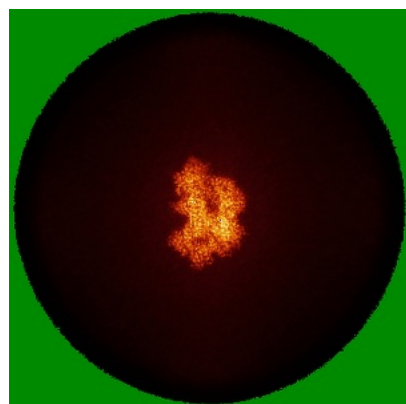


Z Index: 185

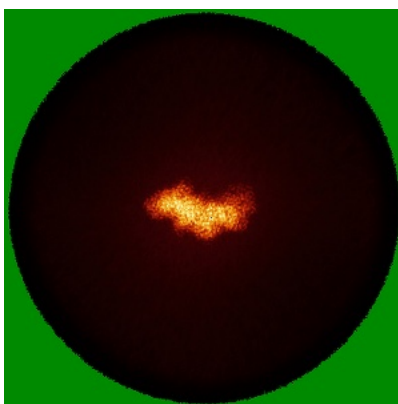
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

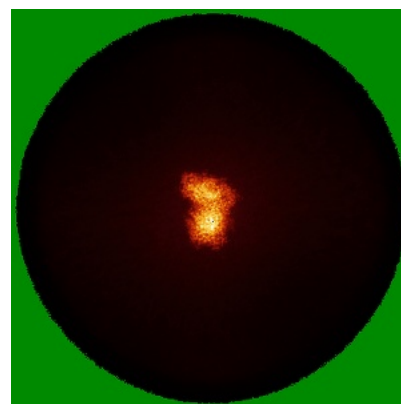
6.4.1 Primary map



X



Y

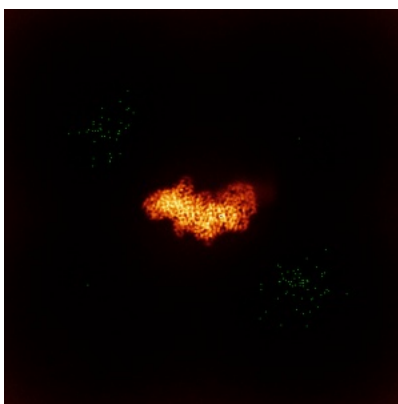


Z

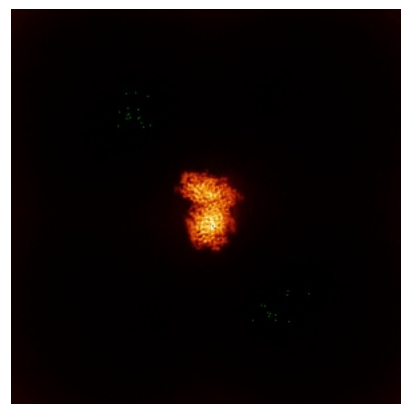
6.4.2 Raw map



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](#)

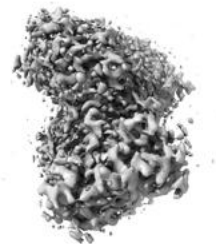
6.5.1 Primary map



X



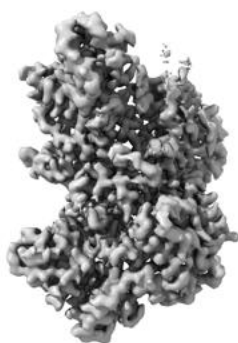
Y



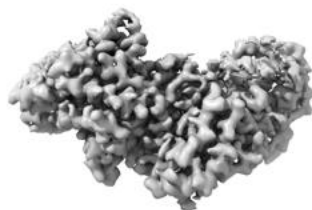
Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

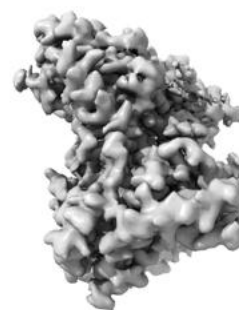
6.5.2 Raw map



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.

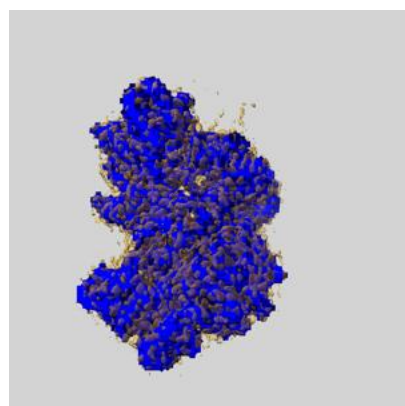
6.6 Mask visualisation [i](#)

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

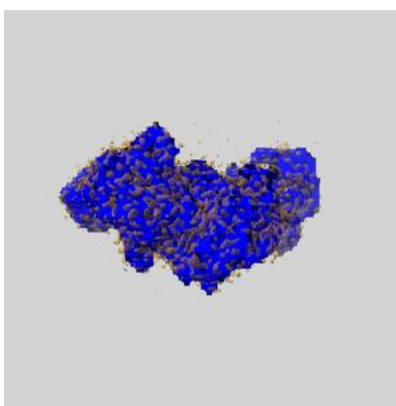
A mask typically either:

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

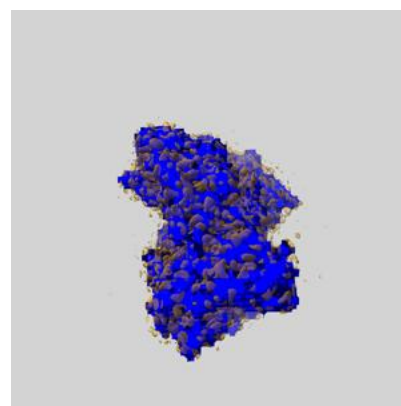
6.6.1 emd_74076_msk_1.map [i](#)



X



Y

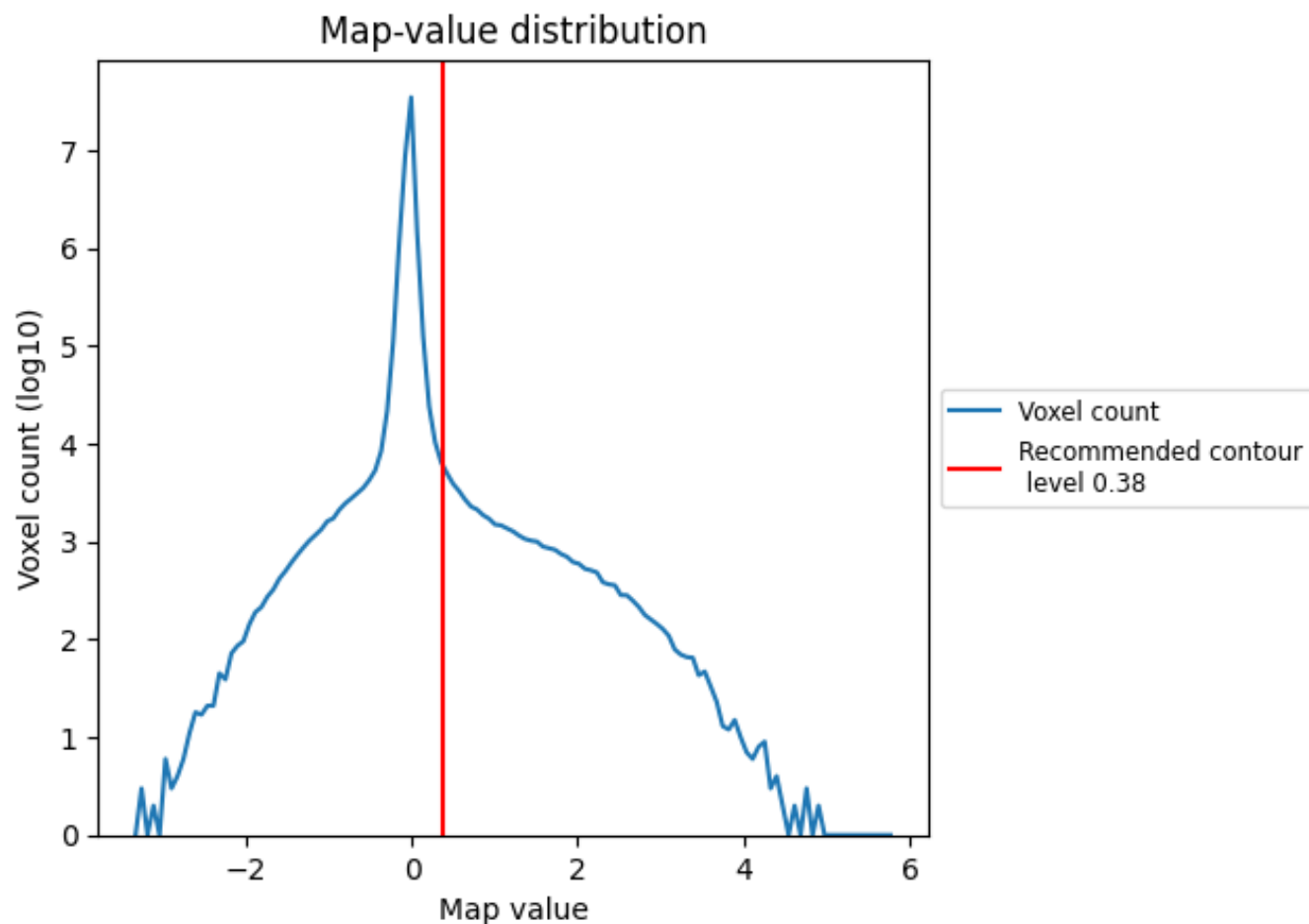


Z

7 Map analysis [i](#)

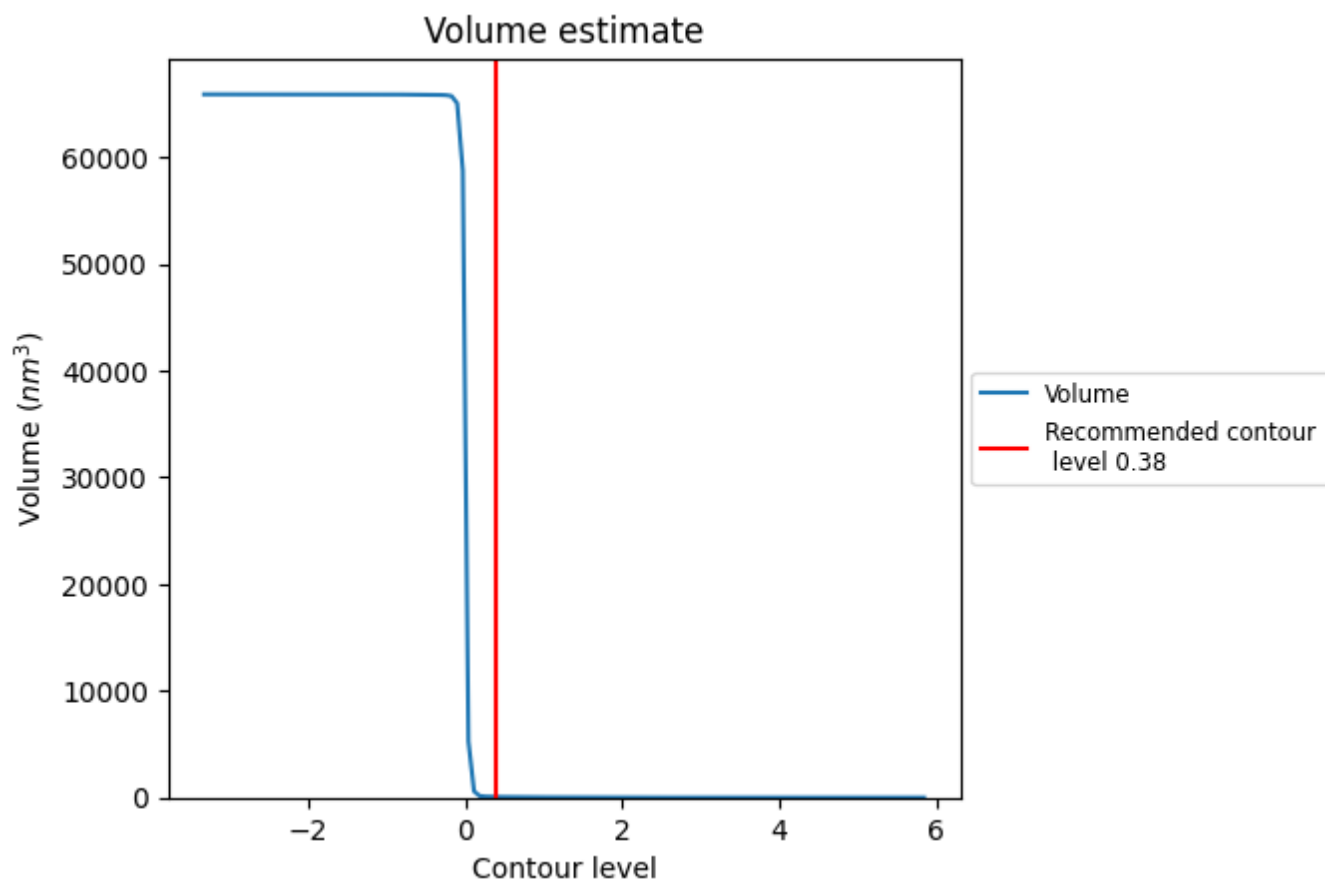
This section contains the results of statistical analysis of the map.

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.

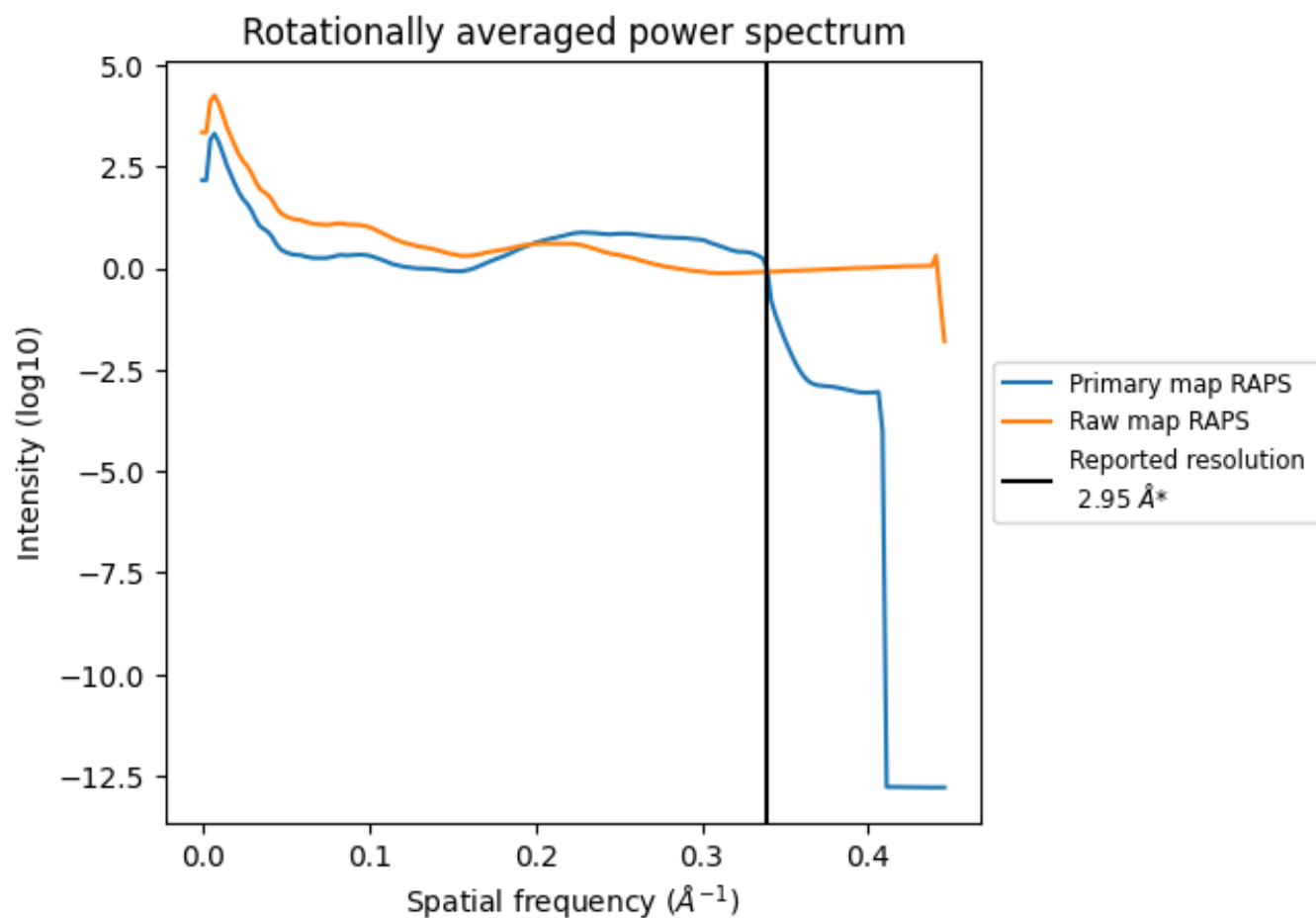
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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 ⓘ

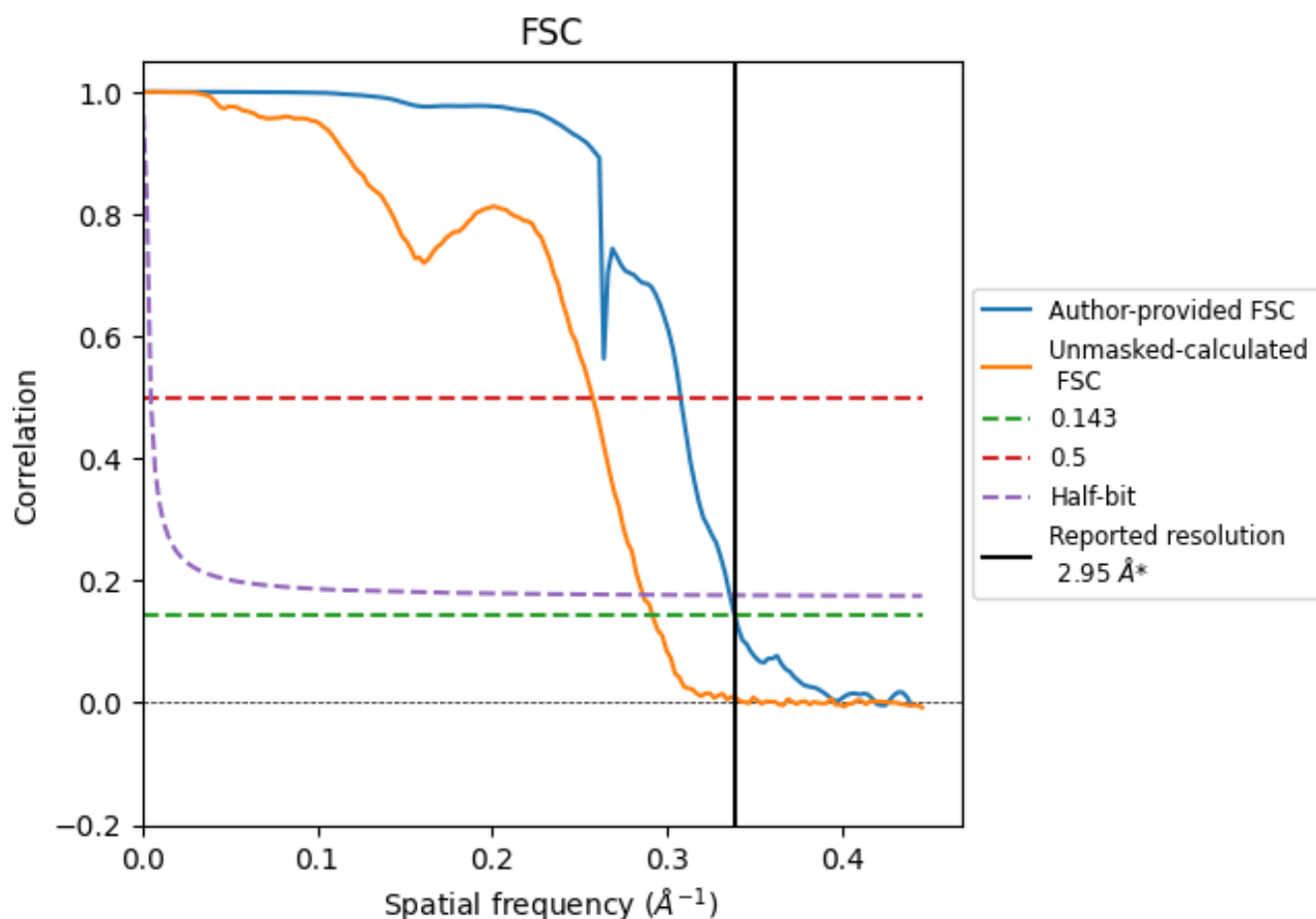


*Reported resolution corresponds to spatial frequency of 0.339 Å⁻¹

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 0.339 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

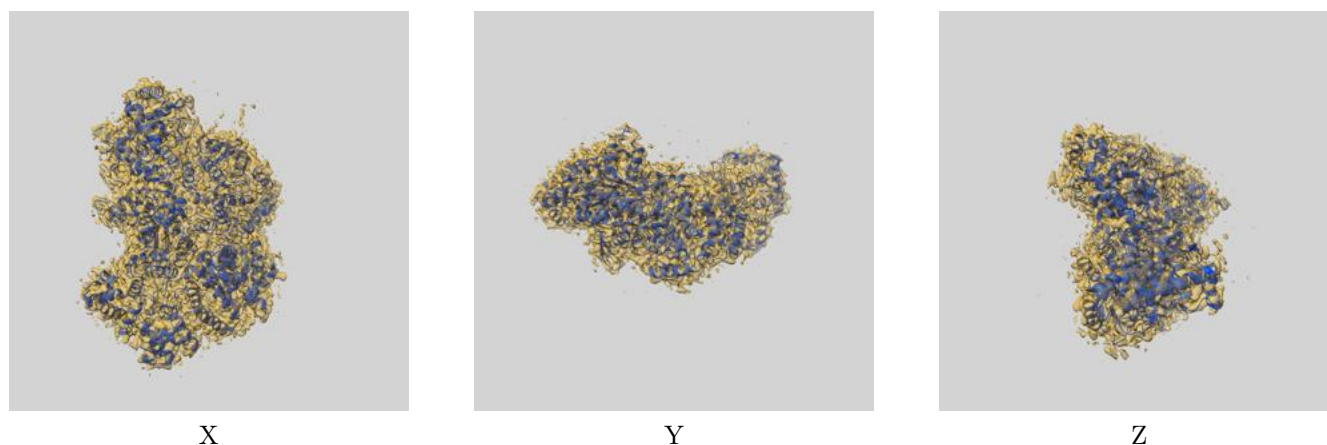
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.25	2.98
Unmasked-calculated*	3.43	3.89	3.49

*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 3.43 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

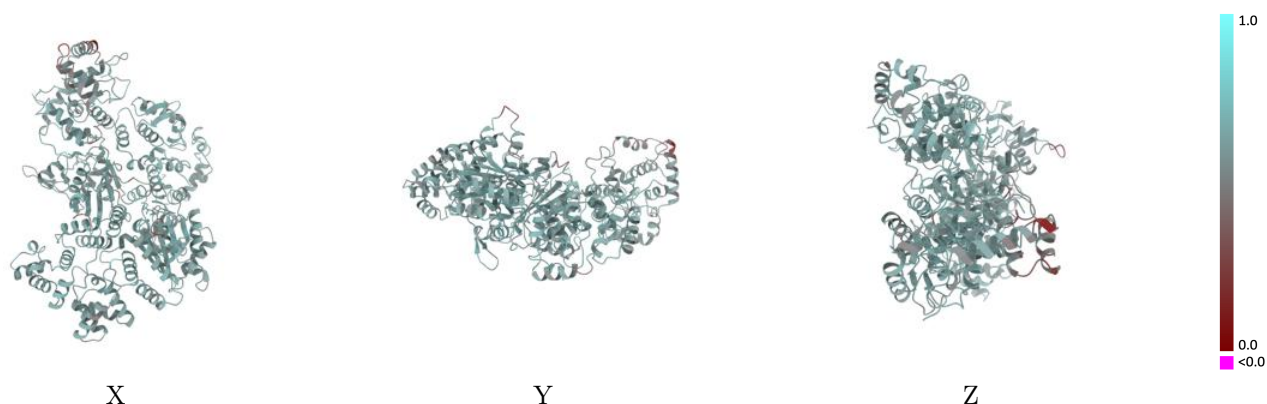
This section contains information regarding the fit between EMDB map EMD-74076 and PDB model 9ZDX. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



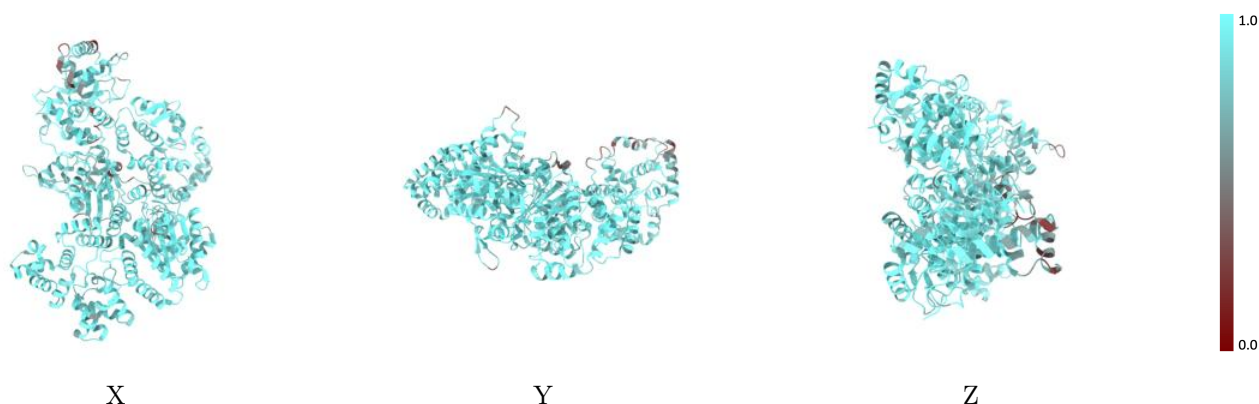
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



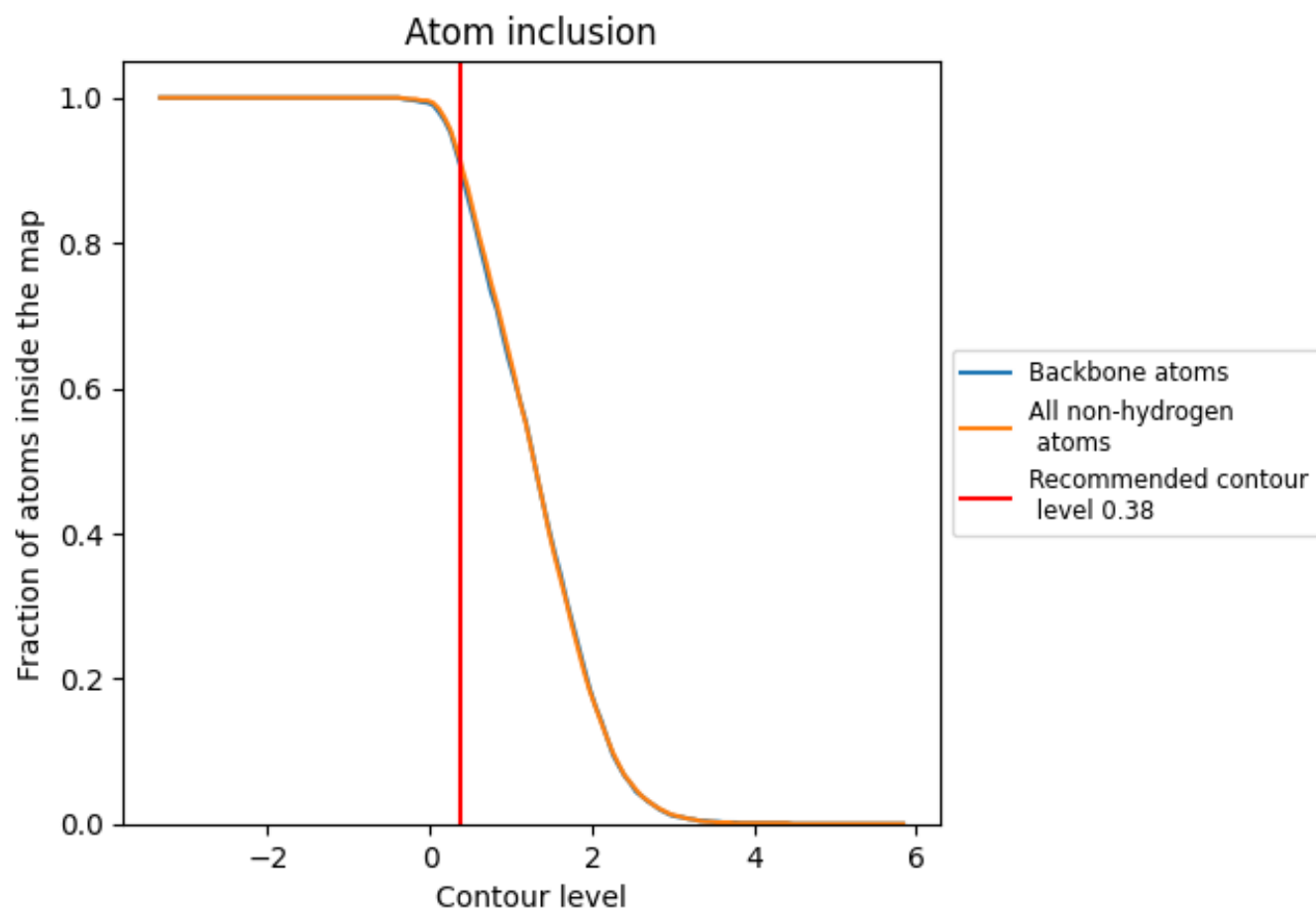
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.38).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9120	0.5920
A	0.9310	0.6010
C	0.8930	0.5830

