



Full wwPDB EM Validation Report ⓘ

Mar 16, 2025 – 12:18 PM EDT

PDB ID : 9DIL
EMDB ID : EMD-46912
Title : Cryo-EM structure of VCP/p97 in complex with VCPIP1 (VCIP135)
Authors : Vostal, L.E.; Reynolds, M.J.; Kapoor, T.M.
Deposited on : 2024-09-05
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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

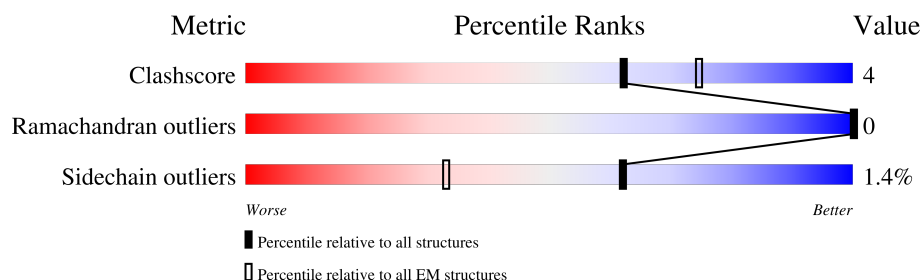
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	806	<div> <div>5%</div> <div>63%</div> <div>7%</div> <div>30%</div> </div>
1	B	806	<div> <div>5%</div> <div>62%</div> <div>7%</div> <div>31%</div> </div>
2	C	1222	<div> <div>8%</div> <div>91%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9783 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.

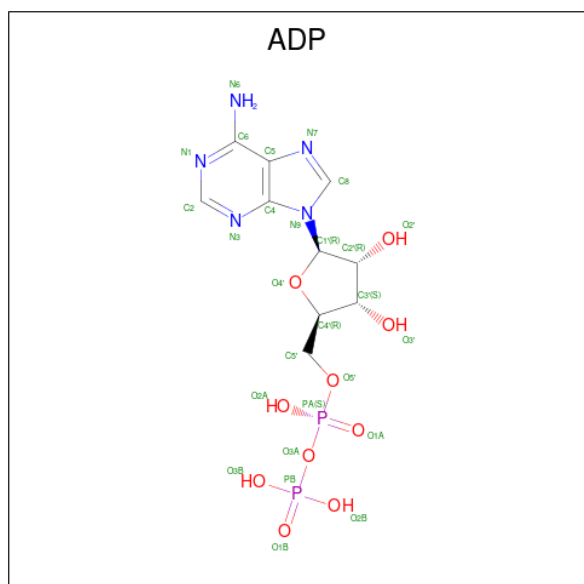
- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	566	Total	C	N	O	S	0	0
			4418	2778	784	834	22		
1	B	559	Total	C	N	O	S	0	0
			4362	2741	774	825	22		

- Molecule 2 is a protein called Deubiquitinating protein VCIPI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	111	Total	C	N	O	S	0	0
			895	572	150	170	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	380000	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 ($e^-/\text{\AA}^2$)	44.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	304.92, 304.92, 304.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84700006, 0.84700006, 0.84700006	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: ADP

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	0.27	0/4492	0.48	0/6059
1	B	0.27	0/4433	0.47	0/5980
2	C	0.27	0/921	0.42	0/1250
All	All	0.27	0/9846	0.47	0/13289

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	4418	0	4456	36	0
1	B	4362	0	4405	39	0
2	C	895	0	848	6	0
3	A	54	0	24	3	0
3	B	54	0	24	4	0
All	All	9783	0	9757	80	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 (80) 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:B:489:LEU:HB3	1:B:531:ILE:HG12	1.80	0.63
1:A:476:TRP:HE1	1:A:534:GLU:HG3	1.63	0.62
1:B:479:ILE:HD13	3:B:902:ADP:HN62	1.67	0.60
1:A:761:THR:HG21	2:C:623:TYR:HB2	1.83	0.60
1:A:656:ILE:HG12	3:A:902:ADP:C2	2.39	0.57
1:A:484:ASP:N	1:A:484:ASP:OD1	2.38	0.56
1:B:427:MET:HA	1:B:430:ILE:HG22	1.87	0.56
1:A:253:LEU:HD22	3:A:901:ADP:H2'	1.89	0.55
1:B:317:HIS:O	1:B:322:ARG:NH1	2.38	0.55
2:C:605:GLU:HG2	2:C:629:LEU:HD11	1.90	0.53
1:B:640:ASP:N	1:B:640:ASP:OD1	2.41	0.53
1:A:319:GLU:OE2	1:A:323:ARG:NH2	2.40	0.53
1:A:438:ASP:OD1	1:A:438:ASP:N	2.43	0.52
2:C:587:ASN:ND2	2:C:612:TYR:O	2.43	0.52
1:A:556:GLU:OE2	1:A:599:ARG:NH1	2.44	0.51
1:A:652:SER:O	1:A:656:ILE:HG13	2.11	0.51
1:A:405:GLY:O	1:A:461:PRO:HB3	2.11	0.50
1:B:501:ASP:OD1	1:B:501:ASP:N	2.44	0.50
1:B:653:ARG:NH1	1:B:676:ALA:O	2.44	0.50
1:A:294:GLU:HG3	1:A:338:ARG:HD3	1.94	0.49
1:B:244:TYR:CE2	1:B:350:PRO:HG3	2.48	0.49
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.95	0.48
1:B:312:LYS:NZ	1:B:351:ASN:O	2.42	0.48
1:B:605:LEU:HD22	1:B:638:ARG:HD3	1.96	0.48
1:A:204:ASP:N	1:A:204:ASP:OD1	2.44	0.47
1:B:333:ASP:OD2	1:B:362:ARG:NH2	2.37	0.47
1:B:548:LEU:HD23	1:B:582:ILE:HD13	1.95	0.47
1:A:428:ASP:N	1:A:428:ASP:OD1	2.47	0.47
1:B:476:TRP:HE3	1:B:486:LYS:HZ2	1.62	0.47
1:B:493:VAL:HG11	1:B:531:ILE:HG13	1.97	0.47
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.51	0.46
1:B:203:TYR:HB2	1:B:261:GLU:HG3	1.97	0.46
1:A:480:GLY:HA3	1:A:652:SER:HA	1.96	0.46
1:B:656:ILE:HG12	3:B:902:ADP:N1	2.30	0.46
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.55	0.46
1:B:653:ARG:NH2	1:B:680:ASN:O	2.49	0.46
1:A:624:ASN:OD1	1:A:624:ASN:N	2.49	0.45
1:B:751:ASP:N	1:B:751:ASP:OD1	2.48	0.45
1:B:543:LYS:HB3	1:B:545:PRO:HD2	1.98	0.45
1:A:336:LYS:O	1:A:338:ARG:N	2.49	0.45
1:B:476:TRP:HE1	1:B:534:GLU:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:HH11	1:B:210:ARG:HA	1.81	0.45
2:C:596:LEU:O	2:C:602:VAL:HA	2.17	0.44
1:A:516:PHE:HE1	1:A:643:ILE:HD12	1.82	0.44
1:B:408:GLY:HA3	3:B:901:ADP:C8	2.53	0.44
1:B:485:VAL:HG11	1:B:527:LEU:HD13	1.99	0.44
1:A:745:ARG:NH2	1:A:749:ASP:OD1	2.51	0.44
1:A:362:ARG:O	1:A:364:ASP:N	2.51	0.44
1:B:206:ILE:HG21	1:B:213:LEU:HD23	2.00	0.44
1:B:726:ASP:N	1:B:726:ASP:OD1	2.50	0.44
1:B:364:ASP:N	1:B:364:ASP:OD1	2.49	0.44
1:A:682:PHE:HB3	1:A:686:ASP:HB2	2.00	0.44
1:A:501:ASP:N	1:A:501:ASP:OD1	2.51	0.43
1:B:750:ASN:O	1:B:754:LYS:HG3	2.18	0.43
1:B:650:GLU:OE1	1:B:653:ARG:NH1	2.52	0.43
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.59	0.43
1:A:307:ASP:N	1:A:307:ASP:OD1	2.50	0.43
1:A:513:GLY:HA2	1:A:619:ILE:O	2.19	0.43
1:B:469:VAL:HG22	1:B:540:ILE:HG12	2.00	0.43
1:A:638:ARG:O	1:A:639:LEU:HD12	2.19	0.43
1:A:653:ARG:NH1	1:A:680:ASN:O	2.52	0.43
1:A:408:GLY:HA3	3:A:901:ADP:C8	2.54	0.42
2:C:564:ASN:OD1	2:C:564:ASN:N	2.45	0.42
1:A:479:ILE:HD11	1:A:526:LEU:HG	2.00	0.42
1:A:489:LEU:HB3	1:A:531:ILE:HG12	2.00	0.42
1:A:679:THR:HG21	1:A:687:LEU:HD21	2.01	0.42
1:B:365:ARG:HH11	1:B:365:ARG:HA	1.84	0.42
1:B:286:LEU:HD12	1:B:286:LEU:HA	1.94	0.42
2:C:598:TRP:HB2	2:C:643:LEU:HD22	2.00	0.42
1:B:497:VAL:HG13	1:B:498:GLU:HG3	2.02	0.41
1:B:603:GLN:HA	1:B:606:THR:HG22	2.02	0.41
1:B:652:SER:O	1:B:656:ILE:HG13	2.20	0.41
1:B:253:LEU:HD22	3:B:901:ADP:H2'	2.01	0.41
1:B:236:LYS:HG2	1:B:338:ARG:NH2	2.35	0.41
1:A:292:GLU:OE2	1:A:296:ASN:ND2	2.53	0.41
1:A:540:ILE:HG22	1:A:572:CYS:SG	2.61	0.41
1:A:210:ARG:HH11	1:A:210:ARG:HA	1.86	0.41
1:B:482:LEU:O	1:B:486:LYS:HG3	2.21	0.40
1:A:592:ASP:OD1	1:A:592:ASP:N	2.53	0.40
1:A:615:LYS:HE2	1:A:615:LYS:HB2	1.92	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	562/806 (70%)	543 (97%)	19 (3%)	0	100	100
1	B	555/806 (69%)	533 (96%)	22 (4%)	0	100	100
2	C	109/1222 (9%)	103 (94%)	6 (6%)	0	100	100
All	All	1226/2834 (43%)	1179 (96%)	47 (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	471/678 (70%)	464 (98%)	7 (2%)	60	77
1	B	465/678 (69%)	459 (99%)	6 (1%)	65	79
2	C	98/1045 (9%)	97 (99%)	1 (1%)	73	84
All	All	1034/2401 (43%)	1020 (99%)	14 (1%)	62	78

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

Mol	Chain	Res	Type
1	A	230	PHE
1	A	236	LYS
1	A	484	ASP
1	A	589	ASN
1	A	602	ASN

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Mol	Chain	Res	Type
1	A	639	LEU
1	A	710	GLU
1	B	213	LEU
1	B	274	ILE
1	B	337	GLN
1	B	351	ASN
1	B	493	VAL
1	B	766	ARG
2	C	559	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	A	398	GLN
1	A	533	ASN
1	A	568	GLN
1	A	589	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	B	902	-	24,29,29	0.90	0	29,45,45	1.22	2 (6%)
3	ADP	A	901	-	24,29,29	0.86	0	29,45,45	1.17	2 (6%)
3	ADP	A	902	-	24,29,29	0.89	0	29,45,45	1.20	2 (6%)
3	ADP	B	901	-	24,29,29	0.86	0	29,45,45	1.21	2 (6%)

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
3	ADP	B	902	-	-	5/12/32/32	0/3/3/3
3	ADP	A	901	-	-	2/12/32/32	0/3/3/3
3	ADP	A	902	-	-	3/12/32/32	0/3/3/3
3	ADP	B	901	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	ADP	N3-C2-N1	-3.73	123.61	128.67
3	B	902	ADP	N3-C2-N1	-3.70	123.66	128.67
3	A	902	ADP	N3-C2-N1	-3.56	123.84	128.67
3	A	901	ADP	N3-C2-N1	-3.54	123.87	128.67
3	B	901	ADP	C4-C5-N7	-2.60	106.59	109.34
3	A	901	ADP	C4-C5-N7	-2.57	106.62	109.34
3	A	902	ADP	C4-C5-N7	-2.45	106.75	109.34
3	B	902	ADP	C4-C5-N7	-2.31	106.89	109.34

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ADP	C5'-O5'-PA-O3A
3	A	902	ADP	C5'-O5'-PA-O1A

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Continued from previous page...

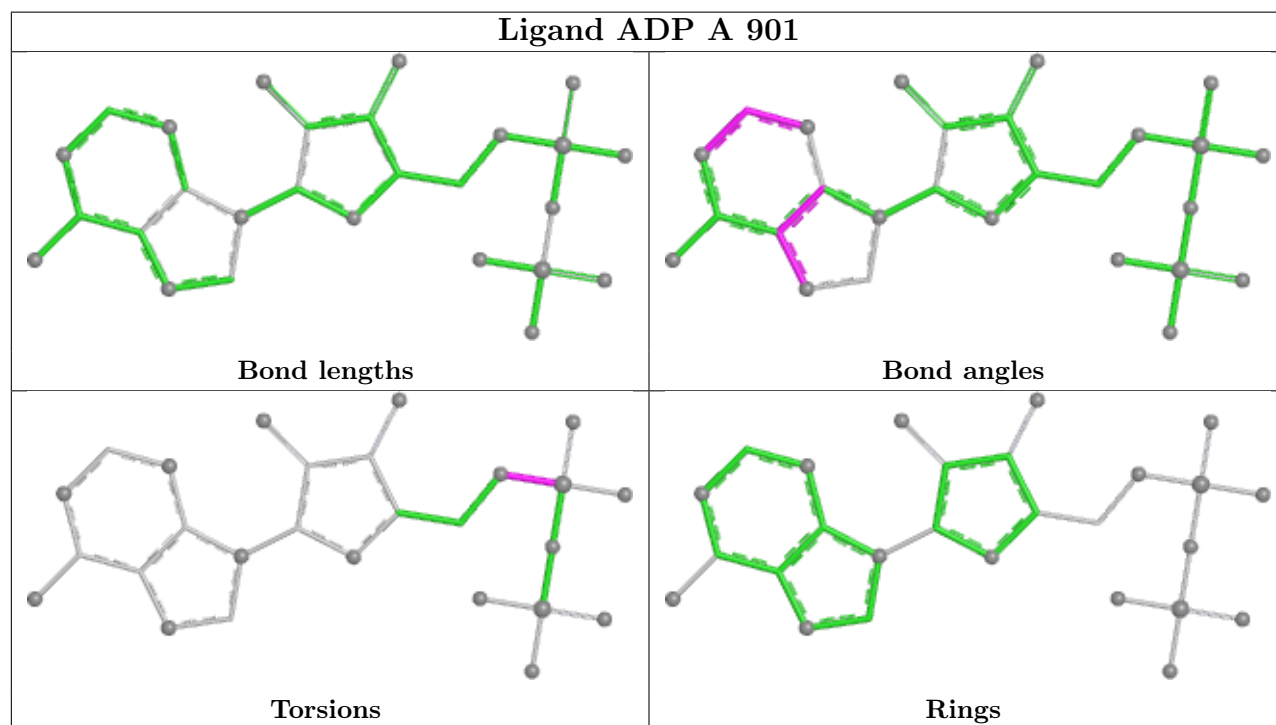
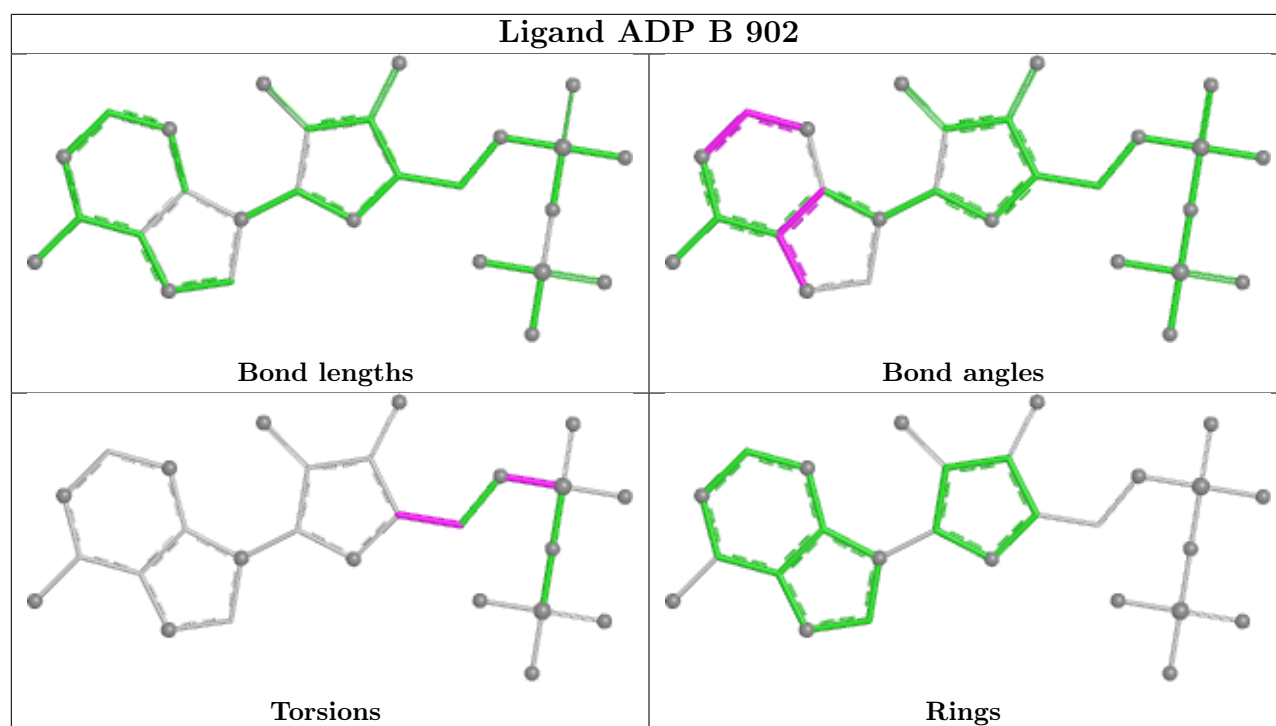
Mol	Chain	Res	Type	Atoms
3	A	902	ADP	O4'-C4'-C5'-O5'
3	B	901	ADP	C5'-O5'-PA-O3A
3	B	902	ADP	C5'-O5'-PA-O1A
3	B	902	ADP	C5'-O5'-PA-O3A
3	B	902	ADP	O4'-C4'-C5'-O5'
3	A	902	ADP	C3'-C4'-C5'-O5'
3	B	902	ADP	C3'-C4'-C5'-O5'
3	A	901	ADP	C5'-O5'-PA-O1A
3	B	901	ADP	C5'-O5'-PA-O1A
3	B	902	ADP	C5'-O5'-PA-O2A

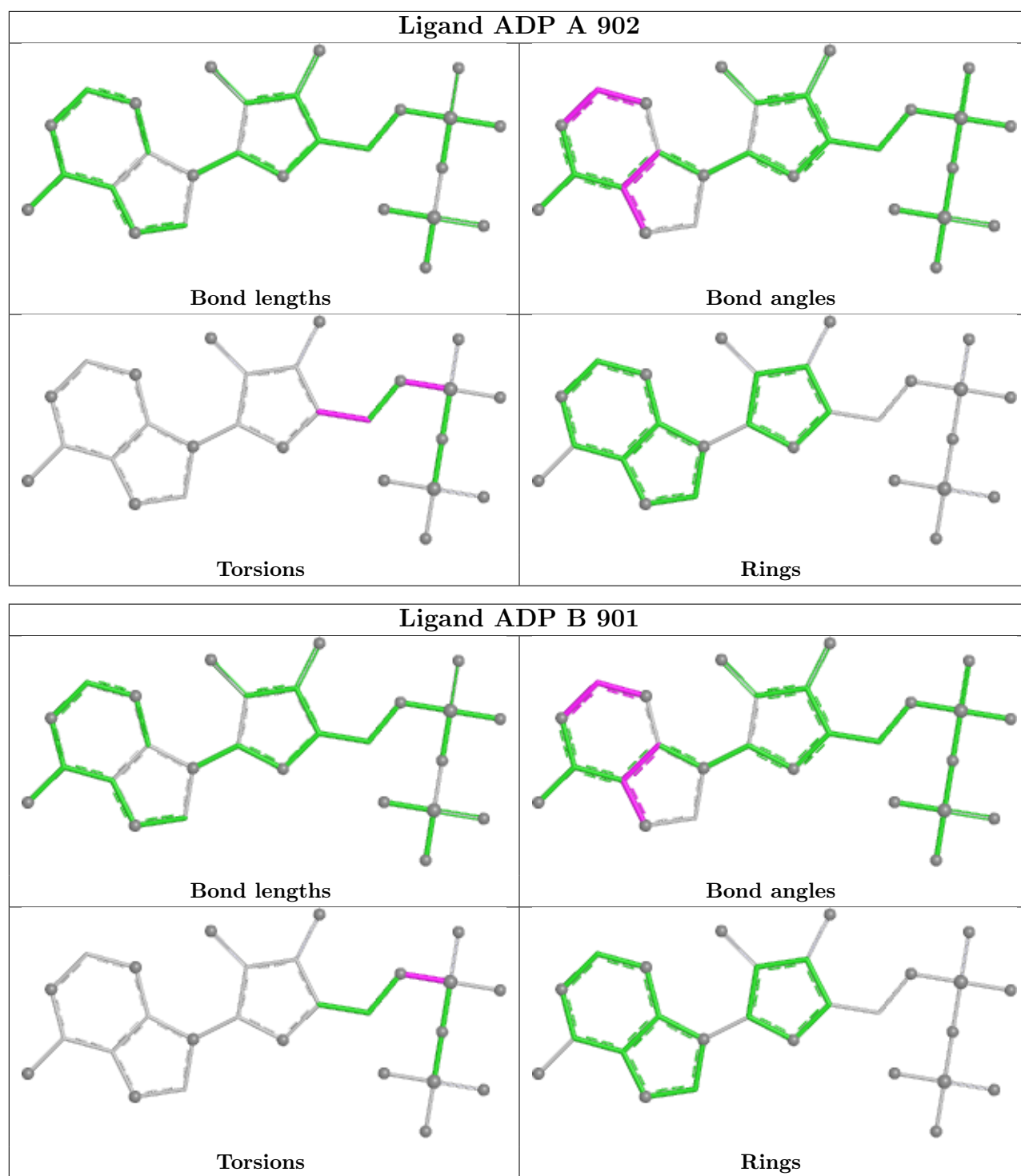
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	ADP	2	0
3	A	901	ADP	2	0
3	A	902	ADP	1	0
3	B	901	ADP	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 ⓘ

There are no chain breaks in this entry.

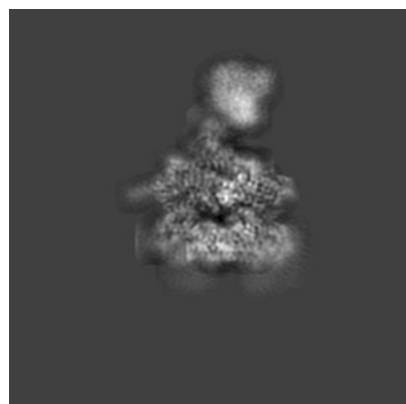
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46912. These allow visual inspection of the internal detail of the map and identification of artifacts.

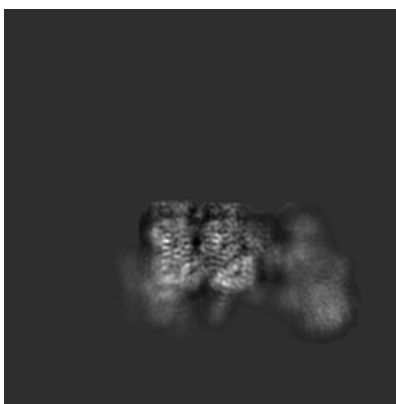
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

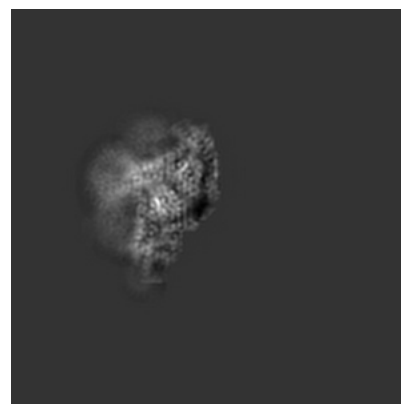
6.1.1 Primary map



X

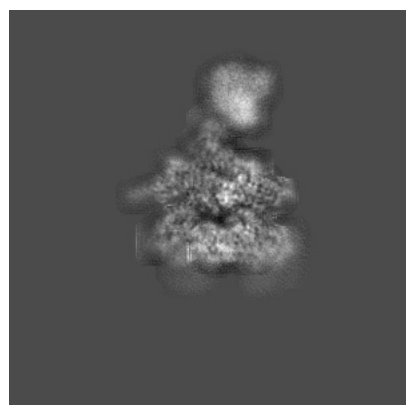


Y

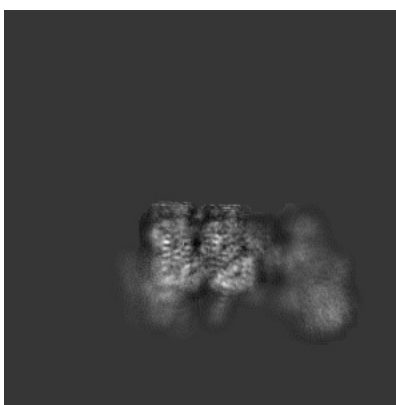


Z

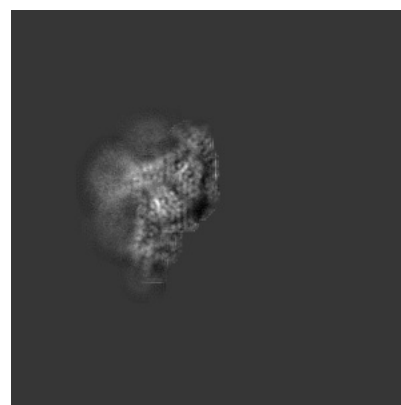
6.1.2 Raw map



X



Y

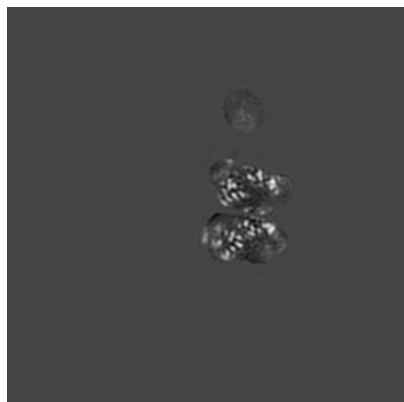


Z

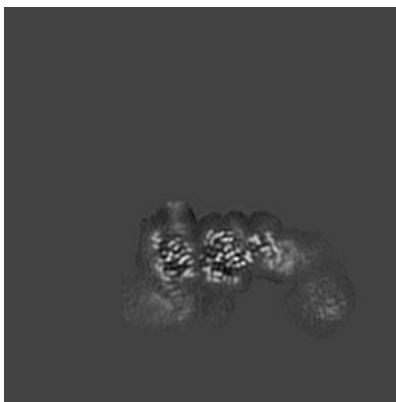
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

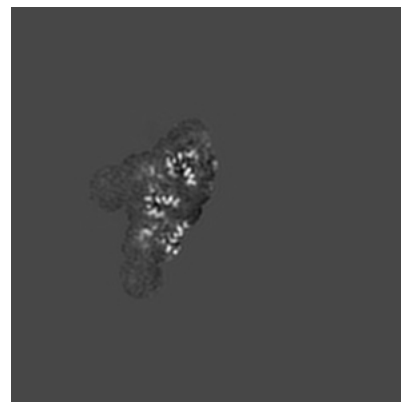
6.2.1 Primary map



X Index: 180

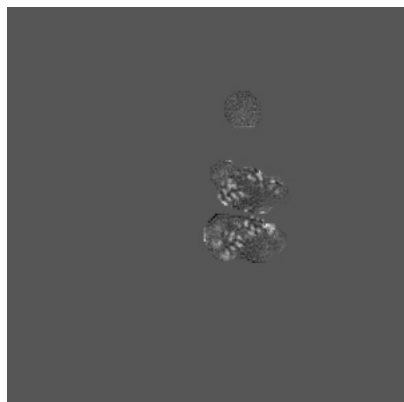


Y Index: 180

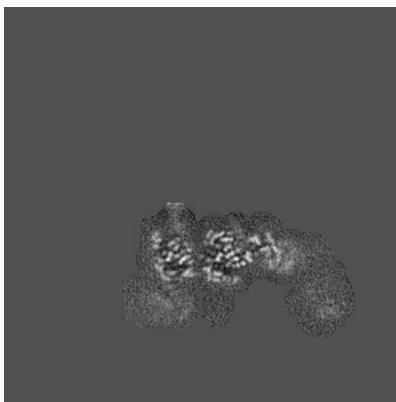


Z Index: 180

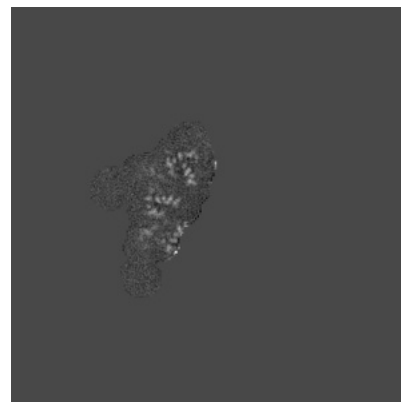
6.2.2 Raw map



X Index: 180



Y Index: 180

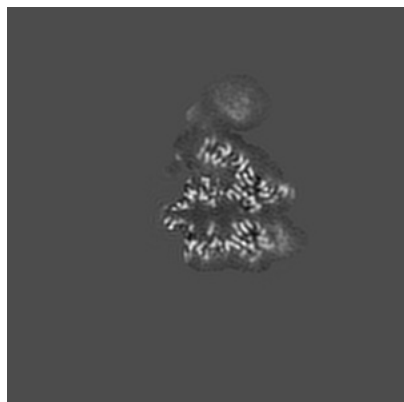


Z Index: 180

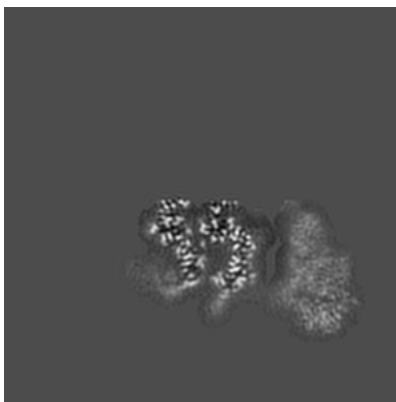
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

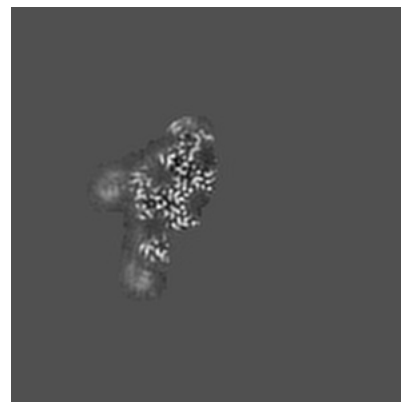
6.3.1 Primary map



X Index: 151

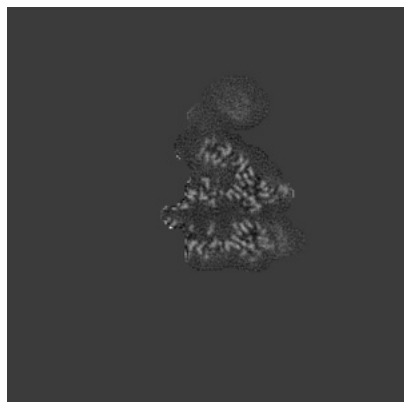


Y Index: 208

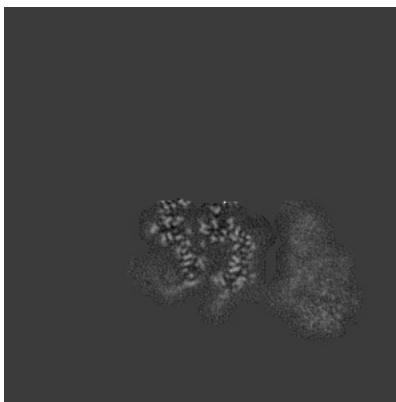


Z Index: 192

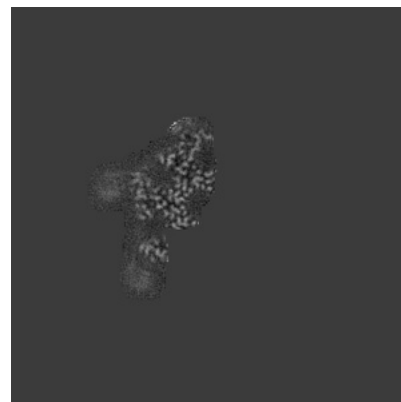
6.3.2 Raw map



X Index: 151



Y Index: 208

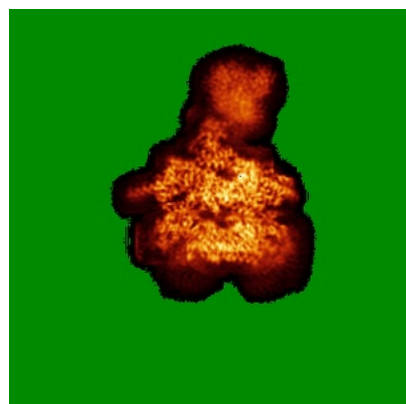


Z Index: 192

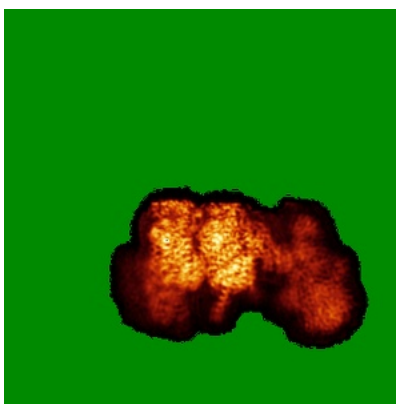
The images above show the largest variance slices of the map in three orthogonal directions.

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

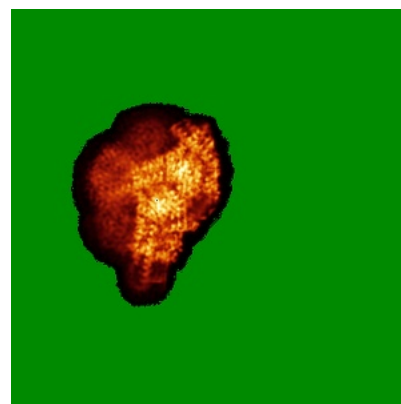
6.4.1 Primary map



X

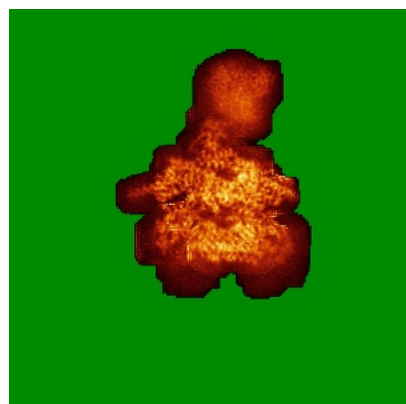


Y

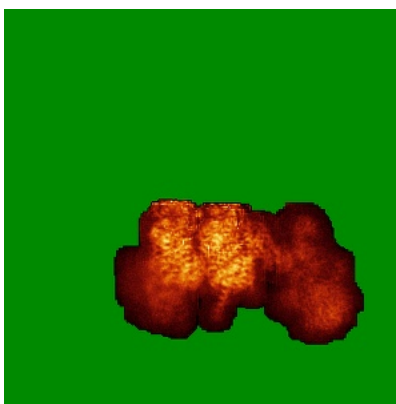


Z

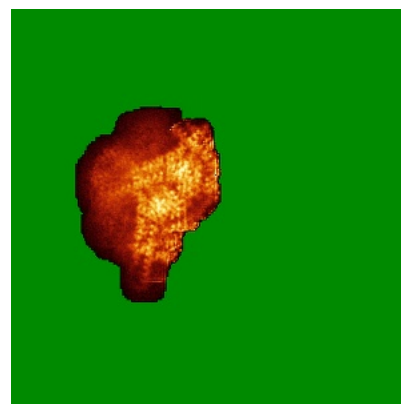
6.4.2 Raw map



X



Y

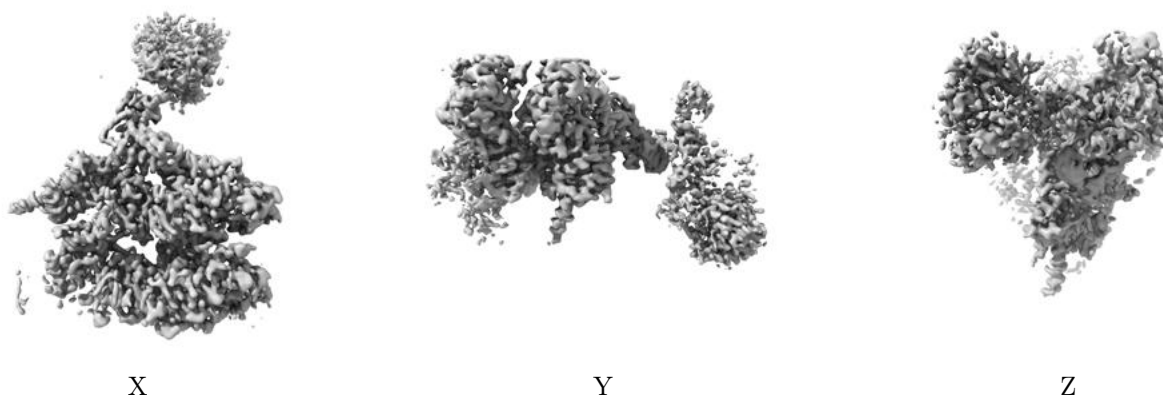


Z

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.

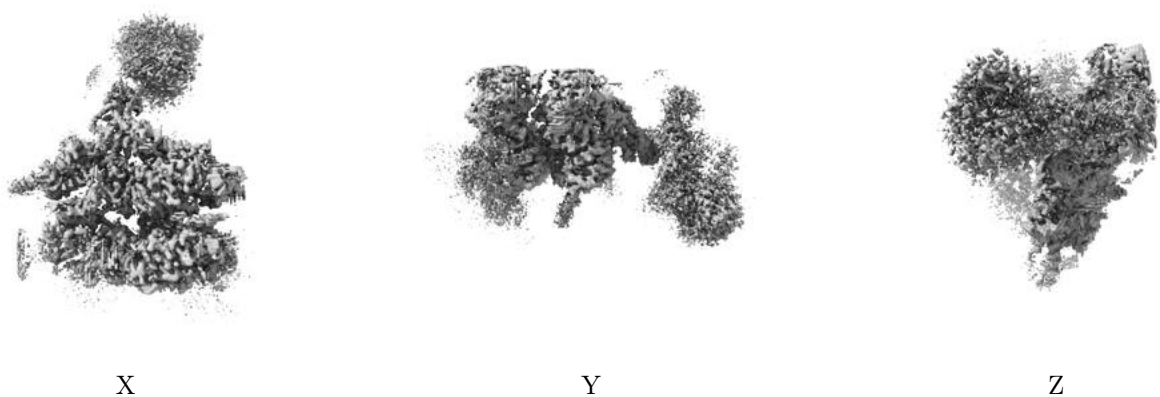
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

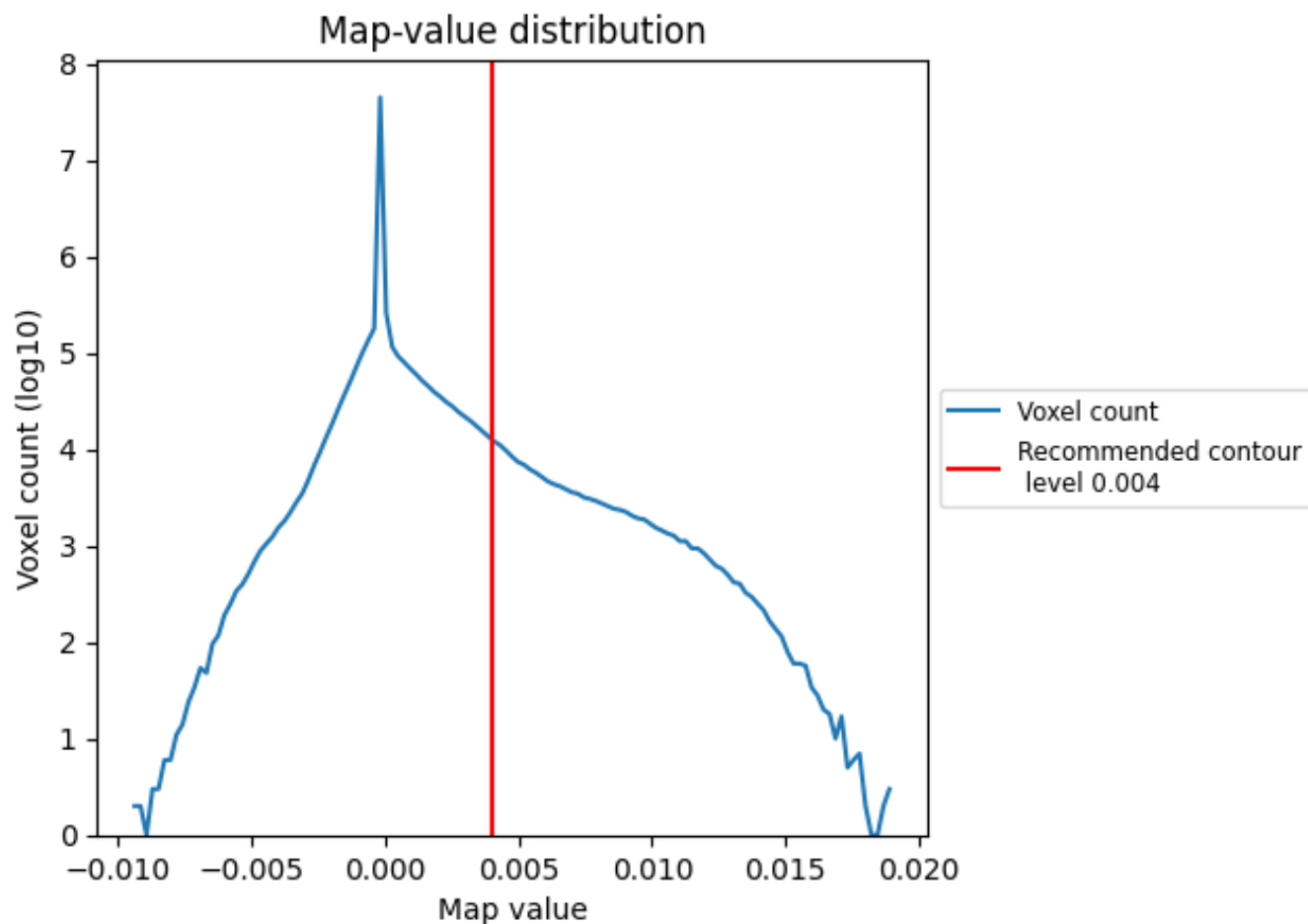
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

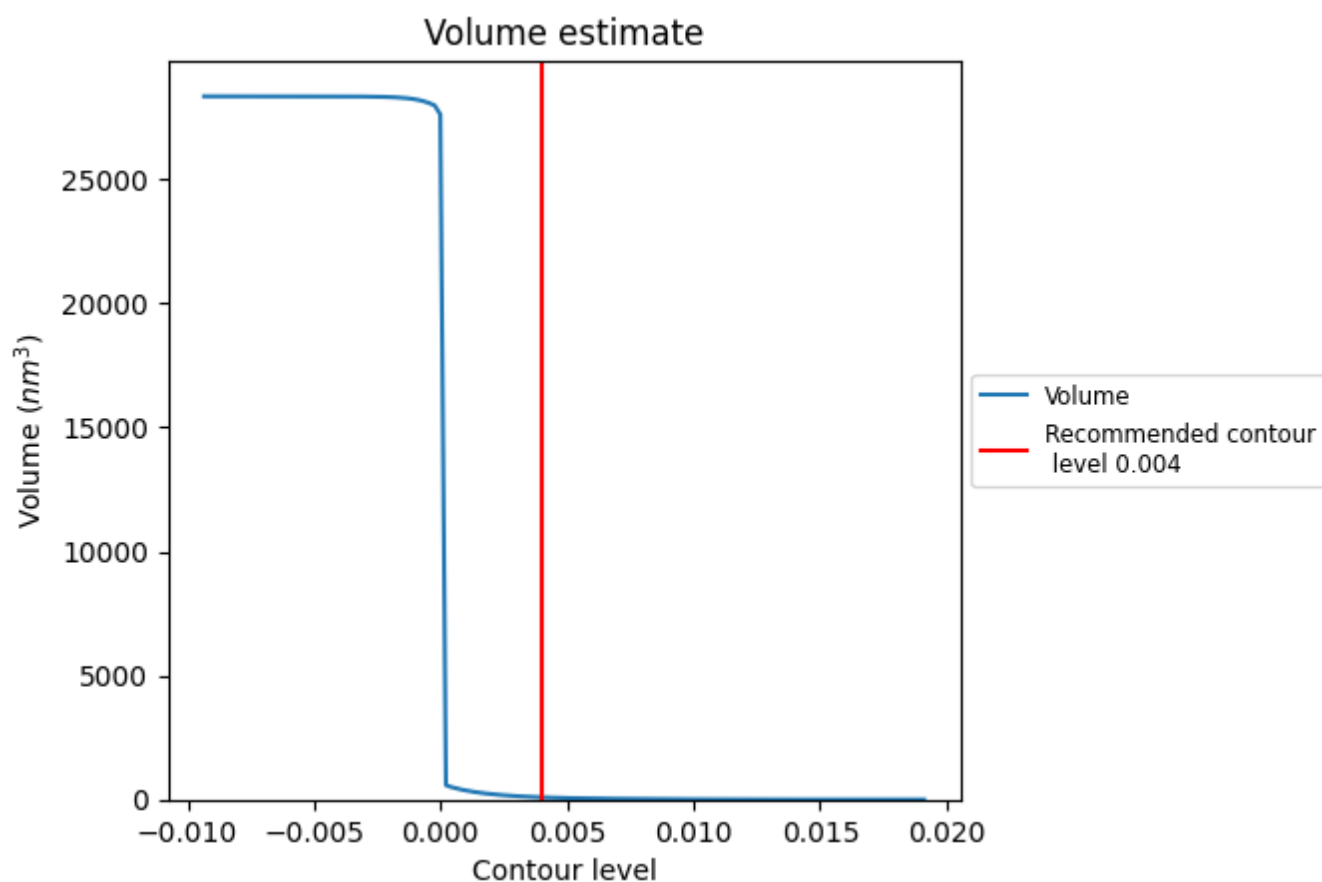
This section contains the results of statistical analysis of the map.

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.

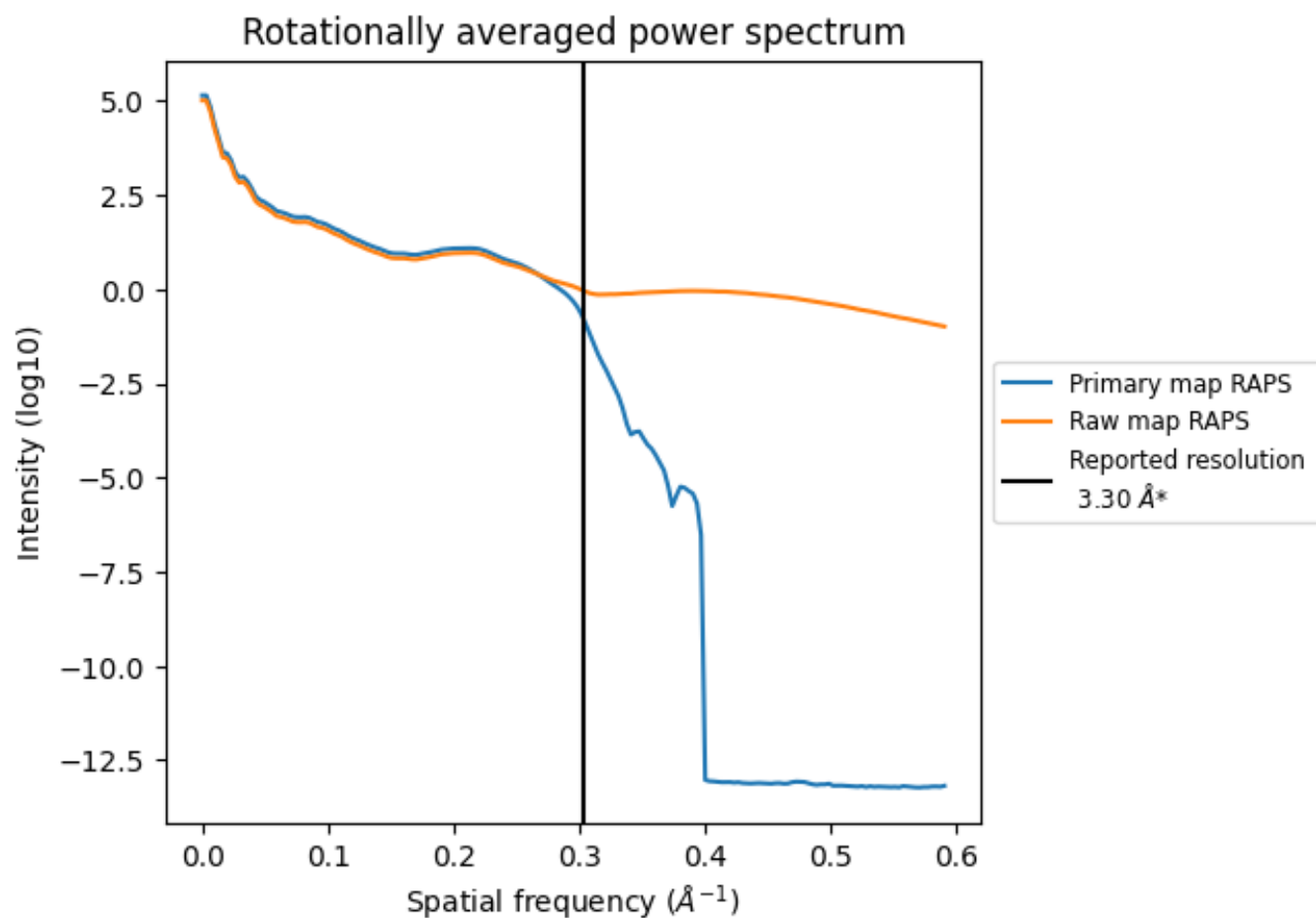
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm^3 ; this corresponds to an approximate mass of 81 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 ⓘ

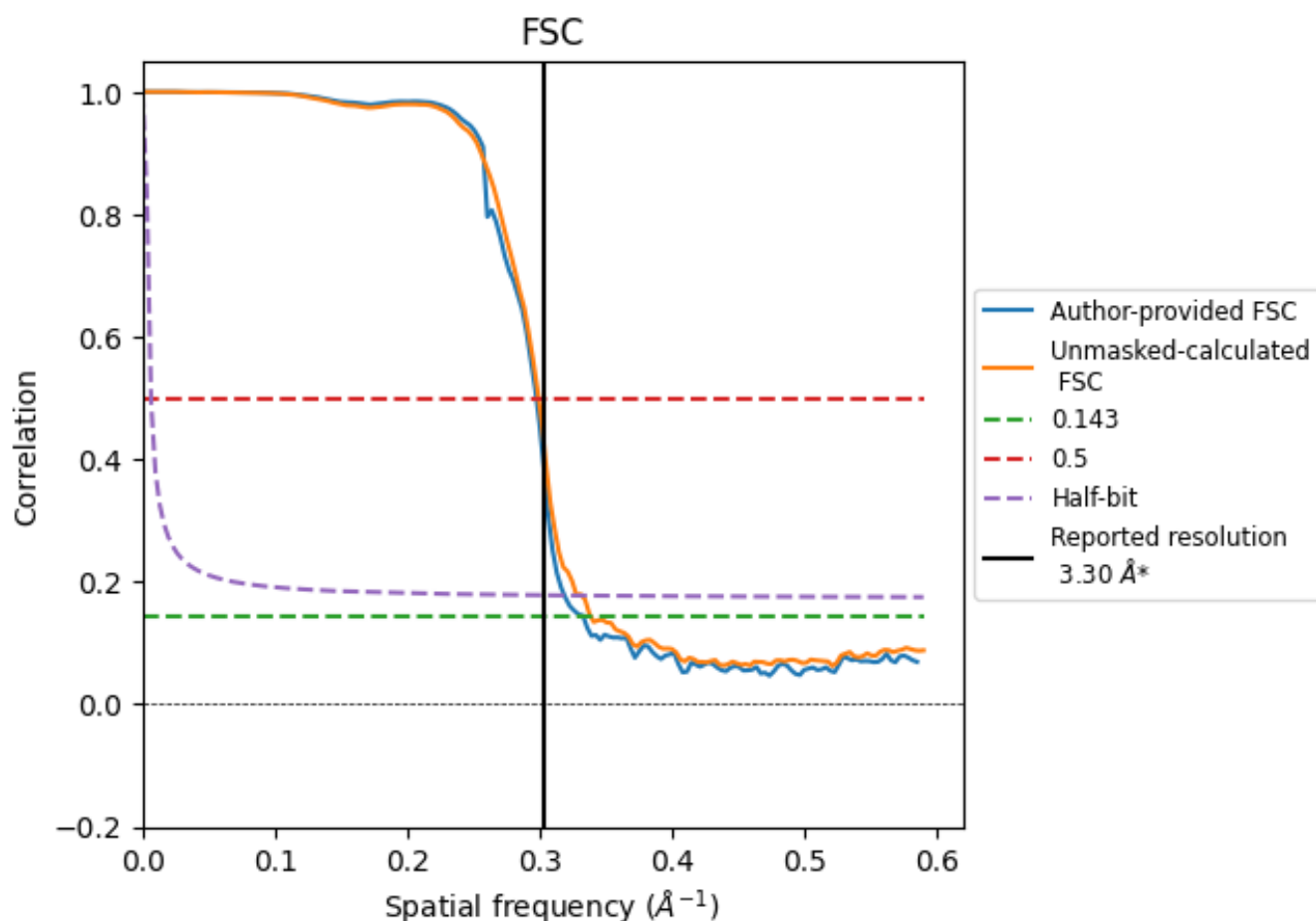


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

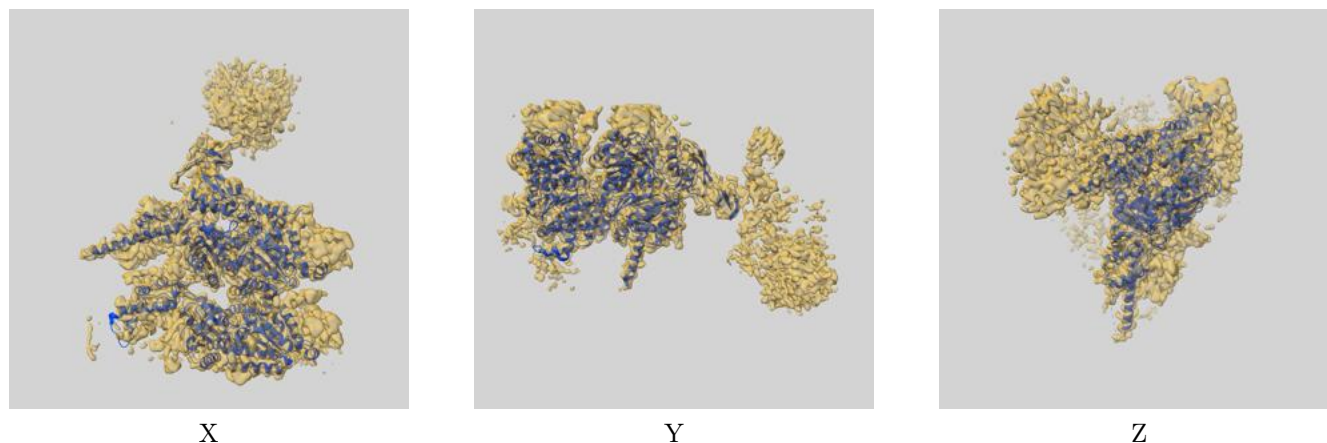
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.00	3.36	3.14
Unmasked-calculated*	2.95	3.34	3.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.95 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

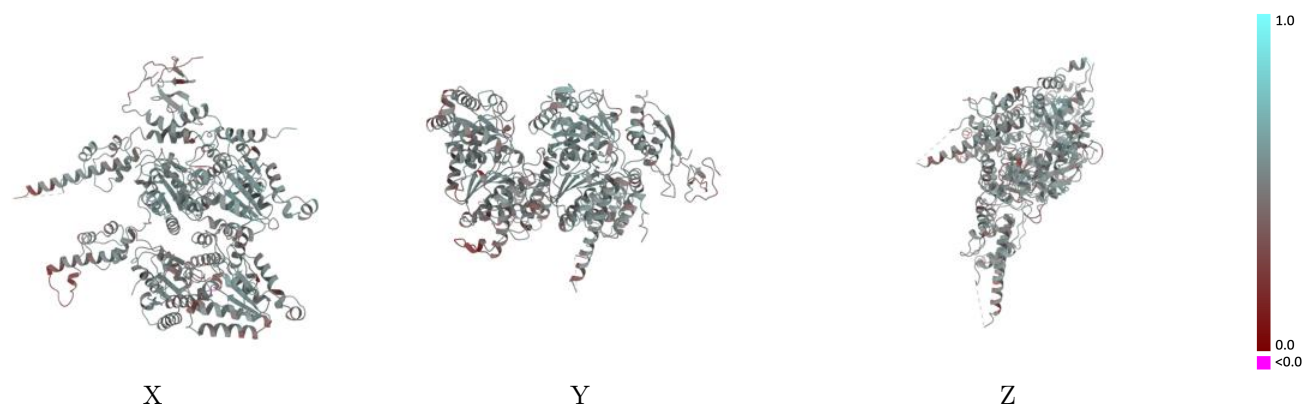
This section contains information regarding the fit between EMDB map EMD-46912 and PDB model 9DIL. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



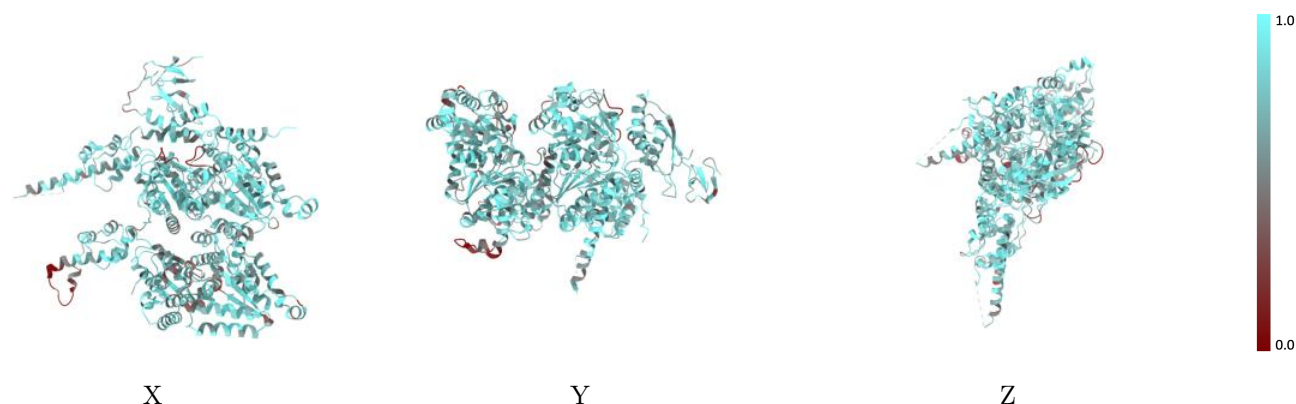
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



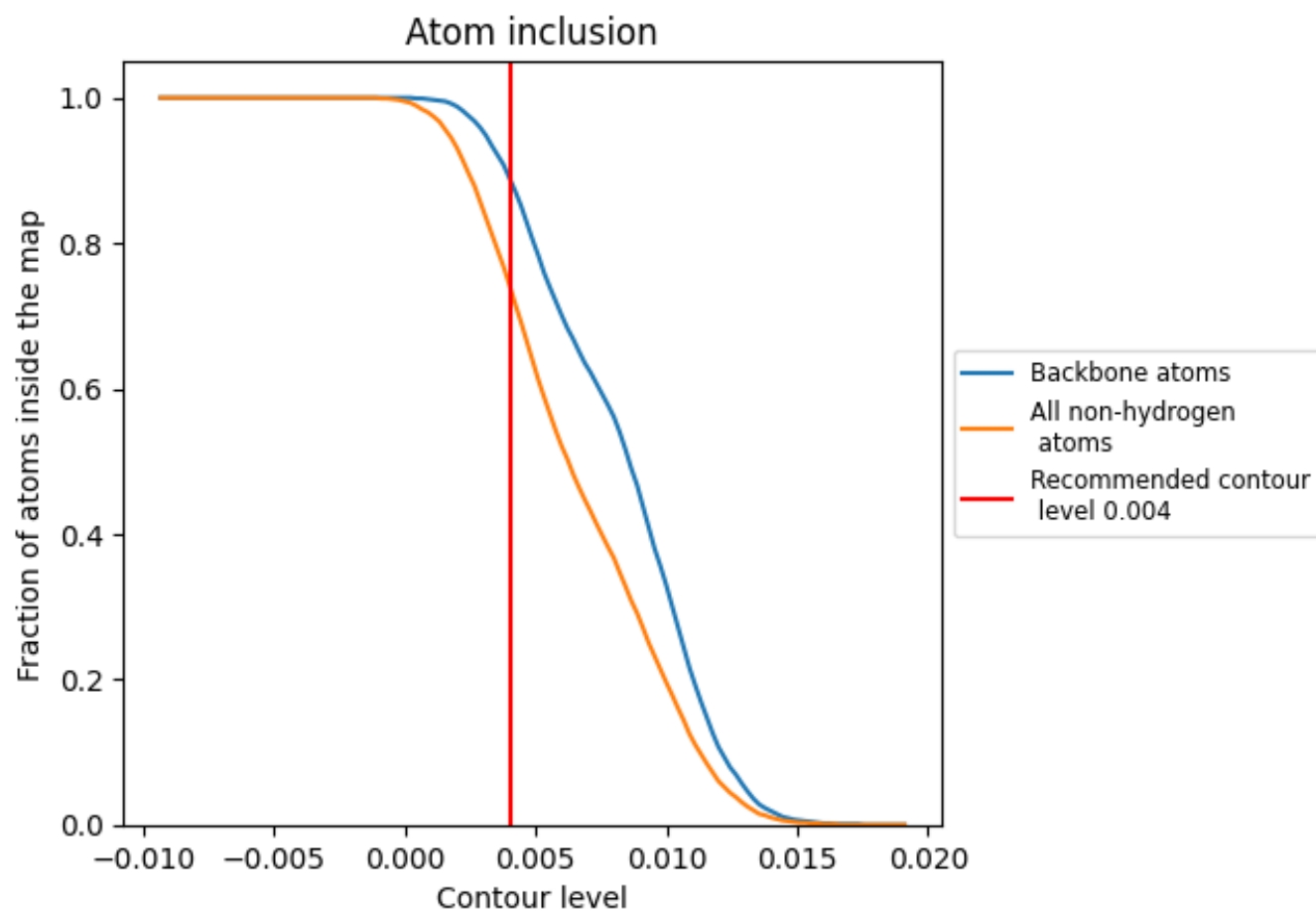
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7420	<div></div> 0.4940
A	<div></div> 0.7440	<div></div> 0.4970
B	<div></div> 0.7400	<div></div> 0.4960
C	<div></div> 0.7440	<div></div> 0.4700

