



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:41 AM UTC

PDB ID : 6TNI / pdb_00006tni
EMDB ID : EMD-10534
Title : Structure of FANCD2 homodimer
Authors : Alcon, P.; Shakeel, S.; Passmore, L.A.
Deposited on : 2019-12-08
Resolution : 3.40 Å(reported)
Based on initial model : 3S4W

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

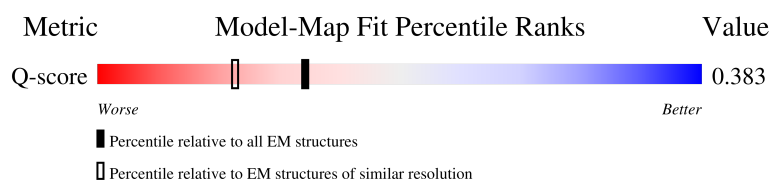
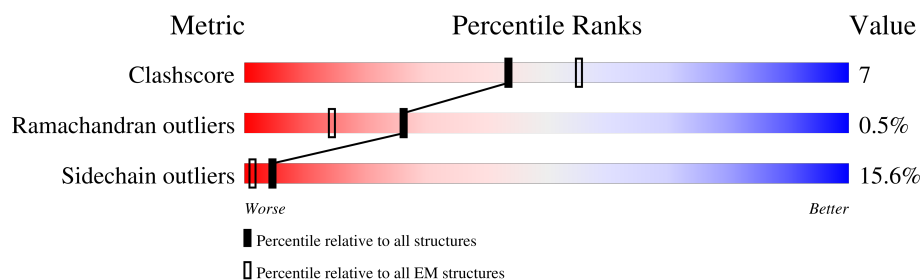
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1475	10% 64% 7% 28%
1	a	1475	11% 64% 7% 28%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11625 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1067	Total	C	N	O	S	0	0
			5815	3543	1118	1143	11		
1	a	1067	Total	C	N	O	S	0	0
			5810	3540	1116	1143	11		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1437	ALA	GLY	conflict	UNP F1NP22
A	1439	ARG	-	expression tag	UNP F1NP22
A	1440	LEU	-	expression tag	UNP F1NP22
A	1441	GLU	-	expression tag	UNP F1NP22
A	1442	VAL	-	expression tag	UNP F1NP22
A	1443	LEU	-	expression tag	UNP F1NP22
A	1444	PHE	-	expression tag	UNP F1NP22
A	1445	GLN	-	expression tag	UNP F1NP22
A	1446	GLY	-	expression tag	UNP F1NP22
A	1447	PRO	-	expression tag	UNP F1NP22
A	1448	TRP	-	expression tag	UNP F1NP22
A	1449	SER	-	expression tag	UNP F1NP22
A	1450	HIS	-	expression tag	UNP F1NP22
A	1451	PRO	-	expression tag	UNP F1NP22
A	1452	GLN	-	expression tag	UNP F1NP22
A	1453	PHE	-	expression tag	UNP F1NP22
A	1454	GLU	-	expression tag	UNP F1NP22
A	1455	LYS	-	expression tag	UNP F1NP22
A	1456	GLY	-	expression tag	UNP F1NP22
A	1457	SER	-	expression tag	UNP F1NP22
A	1458	ALA	-	expression tag	UNP F1NP22
A	1459	GLY	-	expression tag	UNP F1NP22
A	1460	SER	-	expression tag	UNP F1NP22
A	1461	ALA	-	expression tag	UNP F1NP22
A	1462	ALA	-	expression tag	UNP F1NP22
A	1463	GLY	-	expression tag	UNP F1NP22

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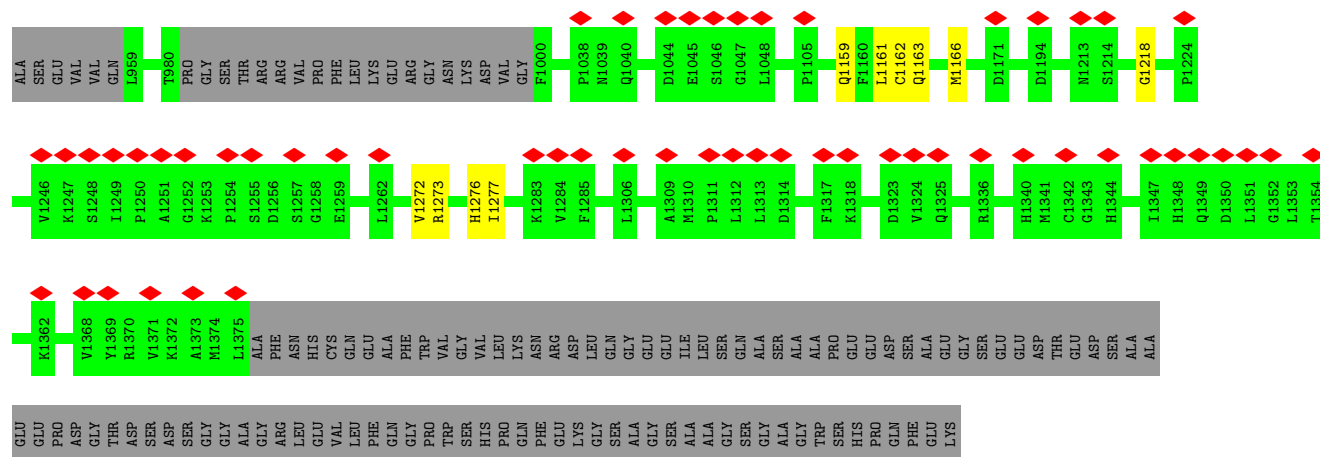
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1464	SER	-	expression tag	UNP F1NP22
A	1465	GLY	-	expression tag	UNP F1NP22
A	1466	ALA	-	expression tag	UNP F1NP22
A	1467	GLY	-	expression tag	UNP F1NP22
A	1468	TRP	-	expression tag	UNP F1NP22
A	1469	SER	-	expression tag	UNP F1NP22
A	1470	HIS	-	expression tag	UNP F1NP22
A	1471	PRO	-	expression tag	UNP F1NP22
A	1472	GLN	-	expression tag	UNP F1NP22
A	1473	PHE	-	expression tag	UNP F1NP22
A	1474	GLU	-	expression tag	UNP F1NP22
A	1475	LYS	-	expression tag	UNP F1NP22
a	1437	ALA	GLY	conflict	UNP F1NP22
a	1439	ARG	-	expression tag	UNP F1NP22
a	1440	LEU	-	expression tag	UNP F1NP22
a	1441	GLU	-	expression tag	UNP F1NP22
a	1442	VAL	-	expression tag	UNP F1NP22
a	1443	LEU	-	expression tag	UNP F1NP22
a	1444	PHE	-	expression tag	UNP F1NP22
a	1445	GLN	-	expression tag	UNP F1NP22
a	1446	GLY	-	expression tag	UNP F1NP22
a	1447	PRO	-	expression tag	UNP F1NP22
a	1448	TRP	-	expression tag	UNP F1NP22
a	1449	SER	-	expression tag	UNP F1NP22
a	1450	HIS	-	expression tag	UNP F1NP22
a	1451	PRO	-	expression tag	UNP F1NP22
a	1452	GLN	-	expression tag	UNP F1NP22
a	1453	PHE	-	expression tag	UNP F1NP22
a	1454	GLU	-	expression tag	UNP F1NP22
a	1455	LYS	-	expression tag	UNP F1NP22
a	1456	GLY	-	expression tag	UNP F1NP22
a	1457	SER	-	expression tag	UNP F1NP22
a	1458	ALA	-	expression tag	UNP F1NP22
a	1459	GLY	-	expression tag	UNP F1NP22
a	1460	SER	-	expression tag	UNP F1NP22
a	1461	ALA	-	expression tag	UNP F1NP22
a	1462	ALA	-	expression tag	UNP F1NP22
a	1463	GLY	-	expression tag	UNP F1NP22
a	1464	SER	-	expression tag	UNP F1NP22
a	1465	GLY	-	expression tag	UNP F1NP22
a	1466	ALA	-	expression tag	UNP F1NP22
a	1467	GLY	-	expression tag	UNP F1NP22

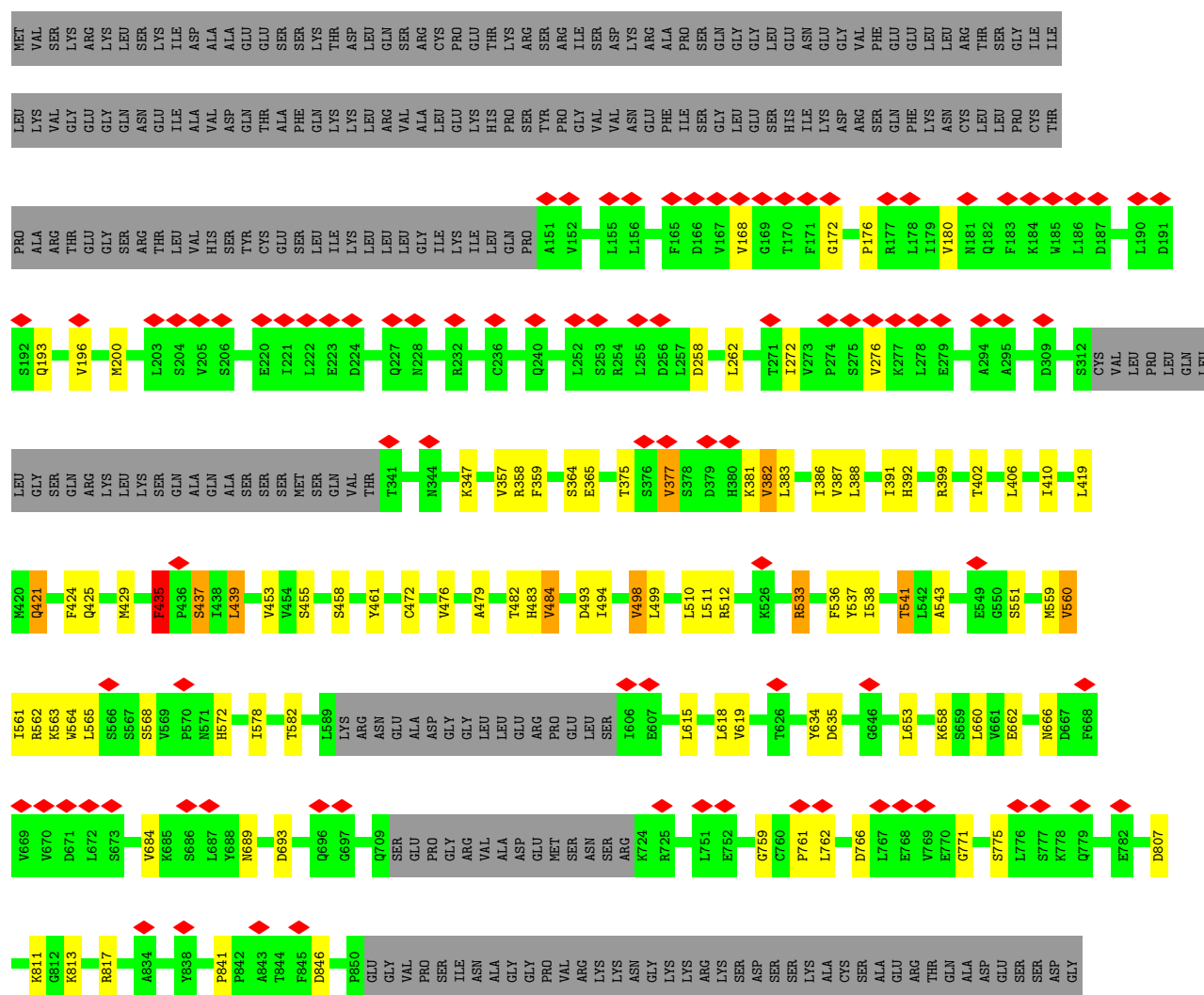
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Chain	Residue	Modelled	Actual	Comment	Reference
a	1468	TRP	-	expression tag	UNP F1NP22
a	1469	SER	-	expression tag	UNP F1NP22
a	1470	HIS	-	expression tag	UNP F1NP22
a	1471	PRO	-	expression tag	UNP F1NP22
a	1472	GLN	-	expression tag	UNP F1NP22
a	1473	PHE	-	expression tag	UNP F1NP22
a	1474	GLU	-	expression tag	UNP F1NP22
a	1475	LYS	-	expression tag	UNP F1NP22



• Molecule 1: Uncharacterized protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	901085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.0	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0134	Depositor
Map size (Å)	476.99997, 476.99997, 476.99997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	0.46	1/5835 (0.0%)	0.82	10/8080 (0.1%)
1	a	0.44	1/5829 (0.0%)	0.78	5/8072 (0.1%)
All	All	0.45	2/11664 (0.0%)	0.80	15/16152 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	921	ARG	C-N	-10.93	1.23	1.33
1	a	921	ARG	C-N	-9.78	1.23	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	MET	N-CA-C	-8.11	102.52	111.36
1	a	560	VAL	N-CA-C	-7.69	101.44	111.05
1	a	658	LYS	N-CA-C	-7.32	105.53	114.75
1	A	658	LYS	N-CA-C	-7.01	105.91	114.75
1	A	920	TYR	N-CA-C	-6.39	100.80	110.70
1	A	562	ARG	N-CA-C	-6.36	104.35	111.28
1	A	462	LYS	N-CA-C	-6.19	106.05	113.97
1	A	193	GLN	N-CA-C	-5.61	108.22	114.62
1	a	193	GLN	N-CA-C	-5.51	108.33	114.62
1	A	460	MET	CA-C-N	-5.50	114.35	122.83
1	A	460	MET	C-N-CA	-5.50	114.35	122.83
1	A	560	VAL	N-CA-C	-5.49	105.02	110.62
1	a	435	PHE	CA-C-O	-5.26	112.95	120.16
1	a	915	ALA	CB-CA-C	-5.21	102.69	110.50
1	A	566	SER	CA-C-O	-5.04	115.21	120.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5815	0	3387	62	0
1	a	5810	0	3382	60	0
All	All	11625	0	6769	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (120) 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:461:TYR:HD1	1:a:476:VAL:HG23	1.46	0.80
1:A:359:PHE:HA	1:a:482:THR:HG22	1.70	0.73
1:A:482:THR:HG22	1:a:359:PHE:HA	1.76	0.68
1:a:561:ILE:O	1:a:565:LEU:N	2.26	0.68
1:A:429:MET:N	1:A:429:MET:SD	2.66	0.67
1:a:916:GLN:O	1:a:918:GLN:N	2.30	0.65
1:a:429:MET:SD	1:a:429:MET:N	2.72	0.63
1:A:558:HIS:HA	1:A:561:ILE:CB	2.28	0.62
1:a:578:ILE:O	1:a:582:THR:OG1	2.15	0.62
1:A:578:ILE:O	1:A:582:THR:OG1	2.14	0.62
1:a:479:ALA:O	1:a:483:HIS:HB2	2.00	0.61
1:a:421:GLN:O	1:a:424:PHE:O	2.18	0.61
1:A:916:GLN:O	1:A:918:GLN:N	2.29	0.60
1:a:392:HIS:CD2	1:a:399:ARG:HB2	2.38	0.59
1:a:759:GLY:H	1:a:762:LEU:HA	1.68	0.59
1:A:759:GLY:H	1:A:762:LEU:HA	1.68	0.59
1:a:424:PHE:CZ	1:a:439:LEU:HD11	2.38	0.58
1:a:461:TYR:CD1	1:a:476:VAL:HG23	2.35	0.58
1:a:562:ARG:CB	1:a:618:LEU:HD23	2.34	0.58
1:A:479:ALA:O	1:A:483:HIS:HB2	2.04	0.57
1:A:693:ASP:N	1:A:766:ASP:O	2.36	0.57
1:a:537:TYR:O	1:a:541:THR:OG1	2.22	0.57
1:A:392:HIS:CD2	1:A:399:ARG:HB2	2.39	0.56
1:A:1161:LEU:HA	1:A:1218:GLY:HA2	1.87	0.56
1:a:347:LYS:HA	1:a:383:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:TYR:O	1:A:541:THR:OG1	2.22	0.56
1:A:258:ASP:O	1:A:262:LEU:N	2.39	0.56
1:a:813:LYS:O	1:a:817:ARG:N	2.39	0.55
1:A:1273:ARG:O	1:A:1277:ILE:N	2.39	0.55
1:A:386:ILE:HG13	1:A:427:HIS:HE1	1.71	0.55
1:a:392:HIS:HD2	1:a:399:ARG:HB2	1.72	0.55
1:A:662:GLU:O	1:A:666:ASN:ND2	2.40	0.55
1:A:813:LYS:O	1:A:817:ARG:N	2.40	0.55
1:a:693:ASP:N	1:a:766:ASP:O	2.37	0.54
1:a:484:VAL:HB	1:a:494:ILE:HG21	1.87	0.54
1:a:1161:LEU:HA	1:a:1218:GLY:HA2	1.89	0.54
1:a:662:GLU:O	1:a:666:ASN:ND2	2.39	0.54
1:A:561:ILE:O	1:A:565:LEU:N	2.26	0.54
1:a:258:ASP:O	1:a:262:LEU:N	2.41	0.54
1:A:168:VAL:O	1:A:172:GLY:N	2.41	0.54
1:a:559:MET:C	1:a:562:ARG:H	2.16	0.53
1:A:398:ASN:O	1:A:402:THR:OG1	2.25	0.53
1:a:689:ASN:HA	1:a:771:GLY:HA2	1.91	0.52
1:a:1355:ASN:O	1:a:1359:LEU:N	2.41	0.52
1:a:1325:GLN:O	1:a:1329:LYS:CB	2.57	0.52
1:A:386:ILE:HG13	1:A:427:HIS:CE1	2.44	0.52
1:A:1162:CYS:O	1:A:1166:MET:N	2.36	0.52
1:a:559:MET:O	1:a:562:ARG:N	2.38	0.52
1:A:689:ASN:HA	1:A:771:GLY:HA2	1.93	0.51
1:a:499:LEU:HA	1:a:538:ILE:HD11	1.91	0.51
1:A:560:VAL:O	1:A:563:LYS:HB3	2.10	0.51
1:a:272:ILE:O	1:a:276:VAL:N	2.41	0.51
1:A:499:LEU:HA	1:A:538:ILE:HD11	1.92	0.50
1:a:382:VAL:HG13	1:a:383:LEU:HD12	1.92	0.50
1:a:807:ASP:O	1:a:811:LYS:N	2.43	0.50
1:a:406:LEU:O	1:a:410:ILE:HG13	2.12	0.49
1:A:484:VAL:HB	1:A:494:ILE:HG21	1.93	0.49
1:a:435:PHE:O	1:a:437:SER:N	2.46	0.49
1:A:406:LEU:O	1:A:410:ILE:HG13	2.12	0.49
1:a:364:SER:OG	1:a:365:GLU:N	2.45	0.49
1:a:543:ALA:HB1	1:a:551:SER:HA	1.95	0.49
1:A:533:ARG:HH11	1:A:533:ARG:HB2	1.78	0.48
1:A:556:ASP:O	1:A:560:VAL:N	2.41	0.48
1:A:558:HIS:O	1:A:562:ARG:N	2.46	0.48
1:A:442:ALA:O	1:A:446:LEU:N	2.47	0.48
1:A:364:SER:OG	1:A:365:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:SER:O	1:A:462:LYS:HB2	2.14	0.47
1:A:272:ILE:O	1:A:276:VAL:N	2.41	0.47
1:A:381:LYS:O	1:A:385:LEU:N	2.48	0.46
1:A:841:PRO:O	1:A:846:ASP:N	2.49	0.46
1:A:382:VAL:O	1:A:386:ILE:HG12	2.14	0.46
1:a:377:VAL:O	1:a:381:LYS:N	2.45	0.46
1:a:533:ARG:HH11	1:a:533:ARG:HB2	1.81	0.46
1:A:494:ILE:O	1:A:498:VAL:HG23	2.16	0.46
1:A:435:PHE:O	1:A:437:SER:N	2.49	0.46
1:A:1159:GLN:O	1:A:1163:GLN:N	2.35	0.45
1:a:494:ILE:O	1:a:498:VAL:HG23	2.16	0.45
1:A:424:PHE:CZ	1:A:439:LEU:HD11	2.51	0.45
1:a:424:PHE:HZ	1:a:439:LEU:HD11	1.82	0.45
1:a:168:VAL:O	1:a:172:GLY:N	2.50	0.45
1:a:387:VAL:O	1:a:391:ILE:HG12	2.16	0.45
1:a:559:MET:C	1:a:561:ILE:N	2.72	0.44
1:A:919:SER:C	1:A:921:ARG:N	2.76	0.44
1:A:176:PRO:O	1:A:180:VAL:N	2.45	0.44
1:a:564:TRP:HA	1:a:568:SER:OG	2.18	0.44
1:a:560:VAL:O	1:a:563:LYS:HG3	2.18	0.44
1:a:196:VAL:O	1:a:200:MET:CB	2.66	0.44
1:A:533:ARG:HB2	1:A:533:ARG:NH1	2.33	0.43
1:a:1162:CYS:O	1:a:1166:MET:N	2.36	0.43
1:A:477:VAL:HG11	1:A:512:ARG:O	2.18	0.43
1:a:1159:GLN:O	1:a:1163:GLN:N	2.36	0.43
1:A:612:LEU:O	1:A:616:LEU:HB2	2.19	0.43
1:A:478:CYS:O	1:A:482:THR:HG23	2.19	0.43
1:a:634:TYR:CE1	1:a:660:LEU:HB3	2.54	0.43
1:a:392:HIS:HB2	1:a:402:THR:HG21	2.01	0.42
1:a:1129:CYS:O	1:a:1133:LEU:N	2.52	0.42
1:a:841:PRO:O	1:a:846:ASP:N	2.52	0.42
1:A:555:ASP:O	1:A:559:MET:N	2.52	0.42
1:A:634:TYR:CE1	1:A:660:LEU:HB3	2.54	0.42
1:A:364:SER:HB2	1:A:391:ILE:HD12	2.00	0.42
1:A:360:GLN:H	1:A:360:GLN:HG3	1.67	0.42
1:A:760:CYS:N	1:A:763:TYR:O	2.42	0.42
1:a:176:PRO:O	1:a:180:VAL:CB	2.67	0.42
1:A:468:PHE:HB3	1:A:472:CYS:SG	2.60	0.42
1:A:1272:VAL:O	1:A:1276:HIS:CB	2.68	0.42
1:a:455:SER:O	1:a:455:SER:OG	2.35	0.42
1:a:533:ARG:HB2	1:a:533:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:916:GLN:C	1:a:918:GLN:H	2.26	0.42
1:A:388:LEU:HD12	1:A:402:THR:HG23	2.02	0.42
1:A:367:TRP:O	1:A:371:ILE:HB	2.21	0.41
1:a:684:VAL:HB	1:a:775:SER:C	2.46	0.41
1:A:392:HIS:CD2	1:A:399:ARG:HE	2.39	0.41
1:A:493:ASP:O	1:A:497:ASP:HB2	2.20	0.41
1:A:684:VAL:HB	1:A:775:SER:C	2.46	0.41
1:a:419:LEU:HD12	1:a:419:LEU:HA	1.90	0.41
1:A:387:VAL:O	1:A:391:ILE:HG12	2.21	0.41
1:a:561:ILE:HA	1:a:564:TRP:CB	2.51	0.40
1:A:392:HIS:HB2	1:A:402:THR:HG21	2.03	0.40
1:a:1167:LYS:O	1:a:1169:GLY:N	2.55	0.40
1:A:807:ASP:O	1:A:811:LYS:N	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1053/1475 (71%)	893 (85%)	155 (15%)	5 (0%)	24	54
1	a	1053/1475 (71%)	883 (84%)	165 (16%)	5 (0%)	24	54
All	All	2106/2950 (71%)	1776 (84%)	320 (15%)	10 (0%)	26	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	ILE
1	A	567	SER
1	A	569	VAL
1	a	435	PHE
1	a	917	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	917	LEU
1	a	425	GLN
1	a	437	SER
1	A	761	PRO
1	a	761	PRO

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	170/1311 (13%)	143 (84%)	27 (16%)	2	10
1	a	169/1311 (13%)	143 (85%)	26 (15%)	2	10
All	All	339/2622 (13%)	286 (84%)	53 (16%)	4	10

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	VAL
1	A	358	ARG
1	A	375	THR
1	A	378	SER
1	A	382	VAL
1	A	393	SER
1	A	427	HIS
1	A	439	LEU
1	A	453	VAL
1	A	458	SER
1	A	461	TYR
1	A	472	CYS
1	A	483	HIS
1	A	493	ASP
1	A	498	VAL
1	A	510	LEU
1	A	511	LEU
1	A	512	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	520	ILE
1	A	533	ARG
1	A	536	PHE
1	A	541	THR
1	A	572	HIS
1	A	582	THR
1	A	615	LEU
1	A	635	ASP
1	A	653	LEU
1	a	357	VAL
1	a	358	ARG
1	a	375	THR
1	a	377	VAL
1	a	382	VAL
1	a	386	ILE
1	a	388	LEU
1	a	421	GLN
1	a	439	LEU
1	a	453	VAL
1	a	458	SER
1	a	472	CYS
1	a	484	VAL
1	a	493	ASP
1	a	498	VAL
1	a	510	LEU
1	a	511	LEU
1	a	512	ARG
1	a	533	ARG
1	a	536	PHE
1	a	541	THR
1	a	572	HIS
1	a	615	LEU
1	a	619	VAL
1	a	635	ASP
1	a	653	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	HIS
1	A	427	HIS
1	A	447	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	483	HIS
1	A	651	GLN
1	a	392	HIS
1	a	425	GLN
1	a	483	HIS
1	a	651	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

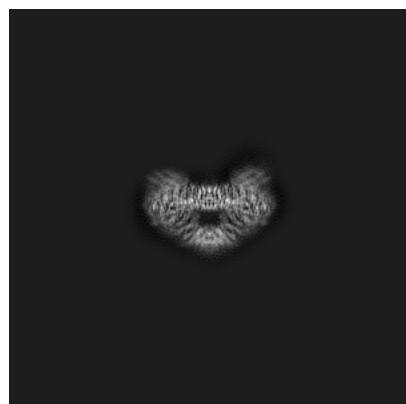
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10534. These allow visual inspection of the internal detail of the map and identification of artifacts.

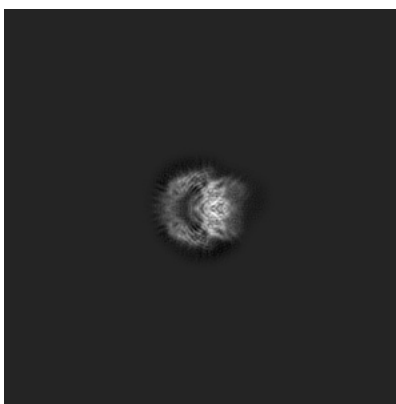
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

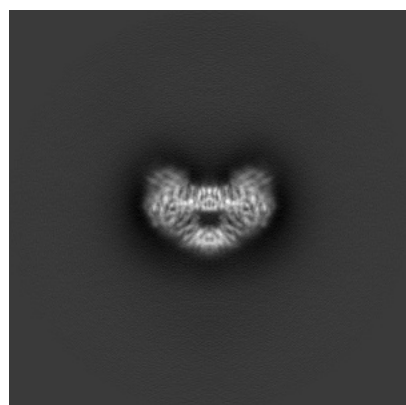


Y

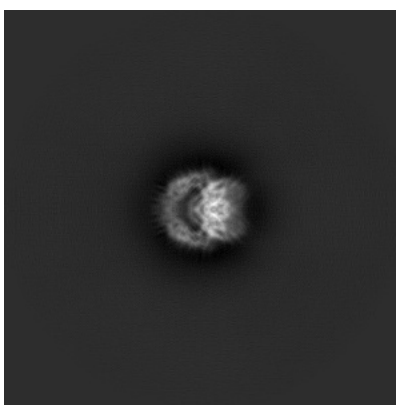


Z

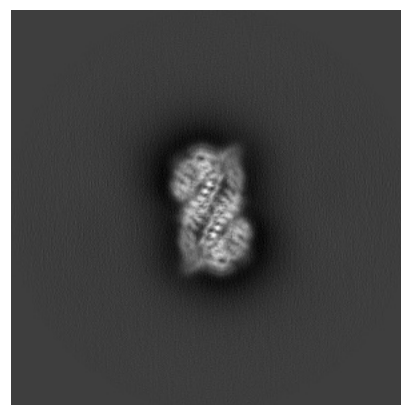
6.1.2 Raw map



X



Y

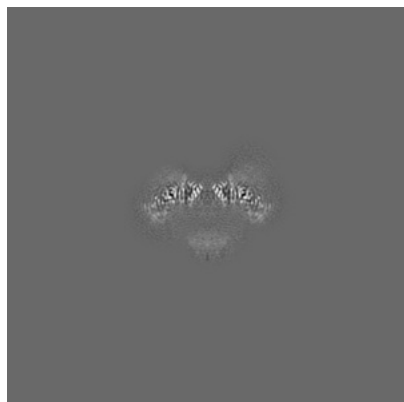


Z

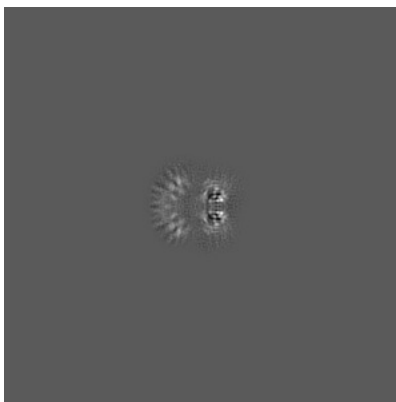
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

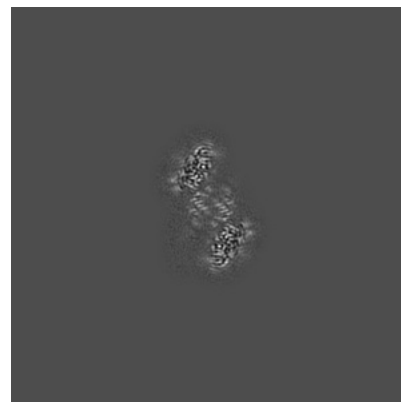
6.2.1 Primary map



X Index: 225

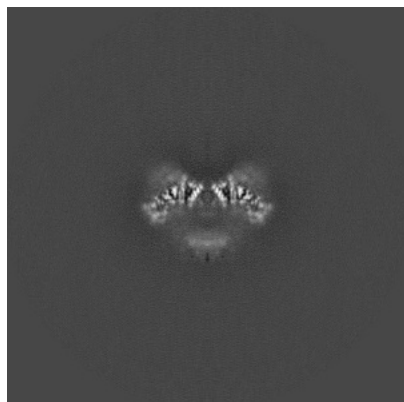


Y Index: 225

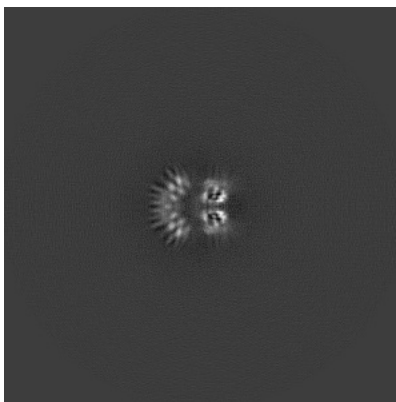


Z Index: 225

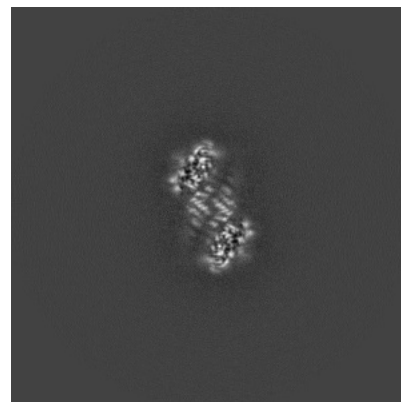
6.2.2 Raw map



X Index: 225



Y Index: 225

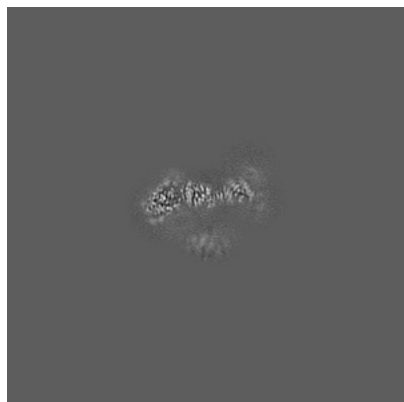


Z Index: 225

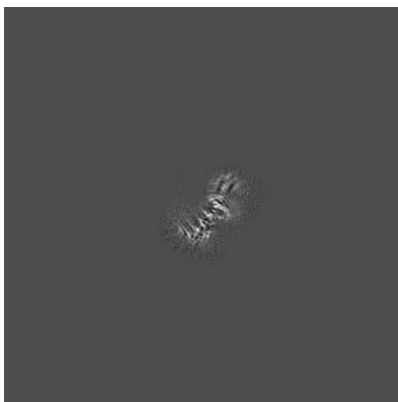
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

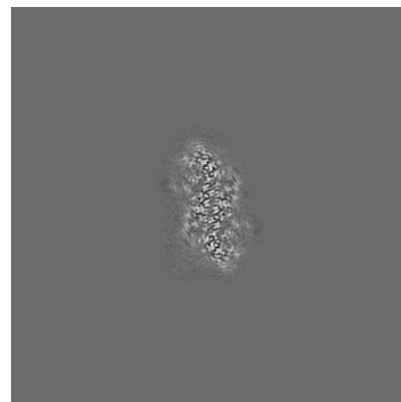
6.3.1 Primary map



X Index: 232

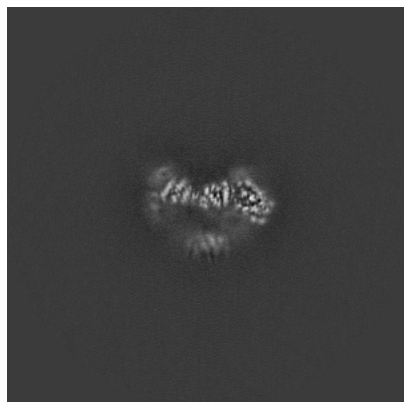


Y Index: 261

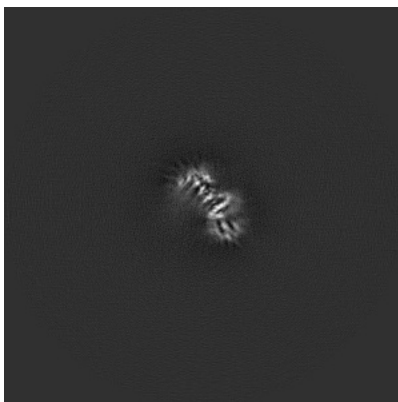


Z Index: 236

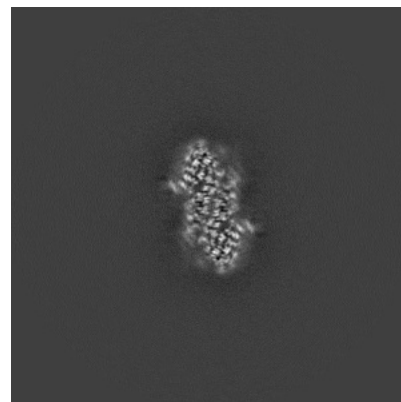
6.3.2 Raw map



X Index: 218



Y Index: 189

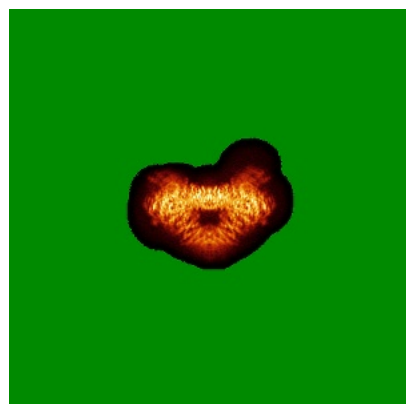


Z Index: 232

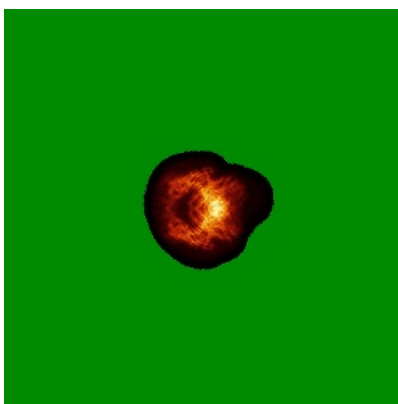
The images above show the largest variance slices of the map in three orthogonal directions.

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

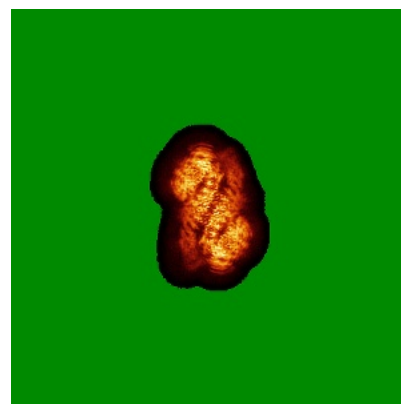
6.4.1 Primary map



X



Y

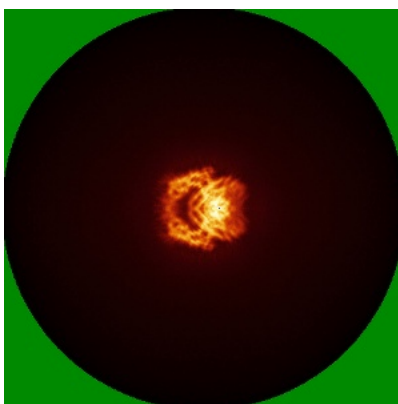


Z

6.4.2 Raw map



X



Y

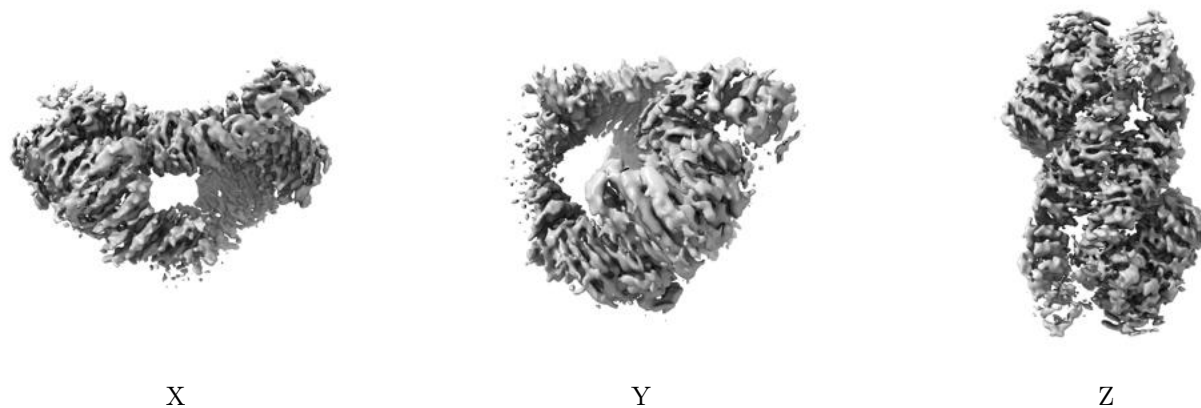


Z

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.

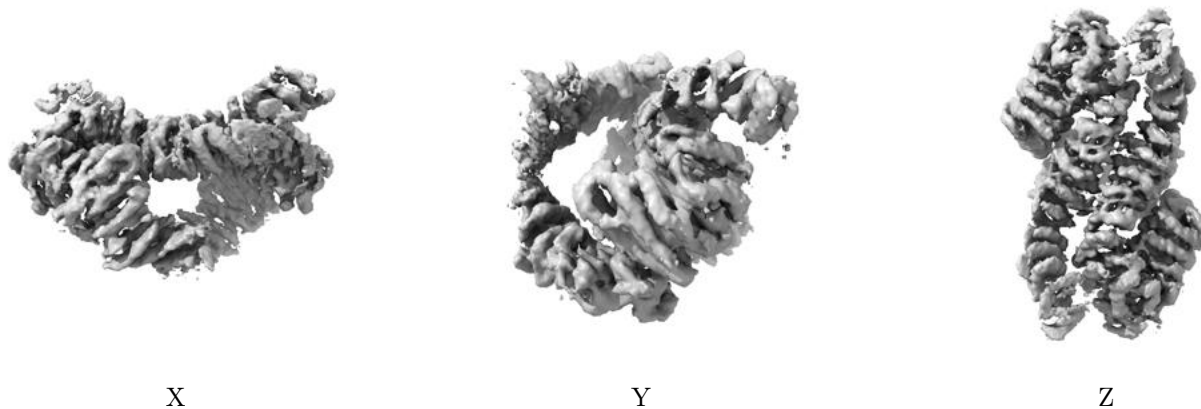
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0134. 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.

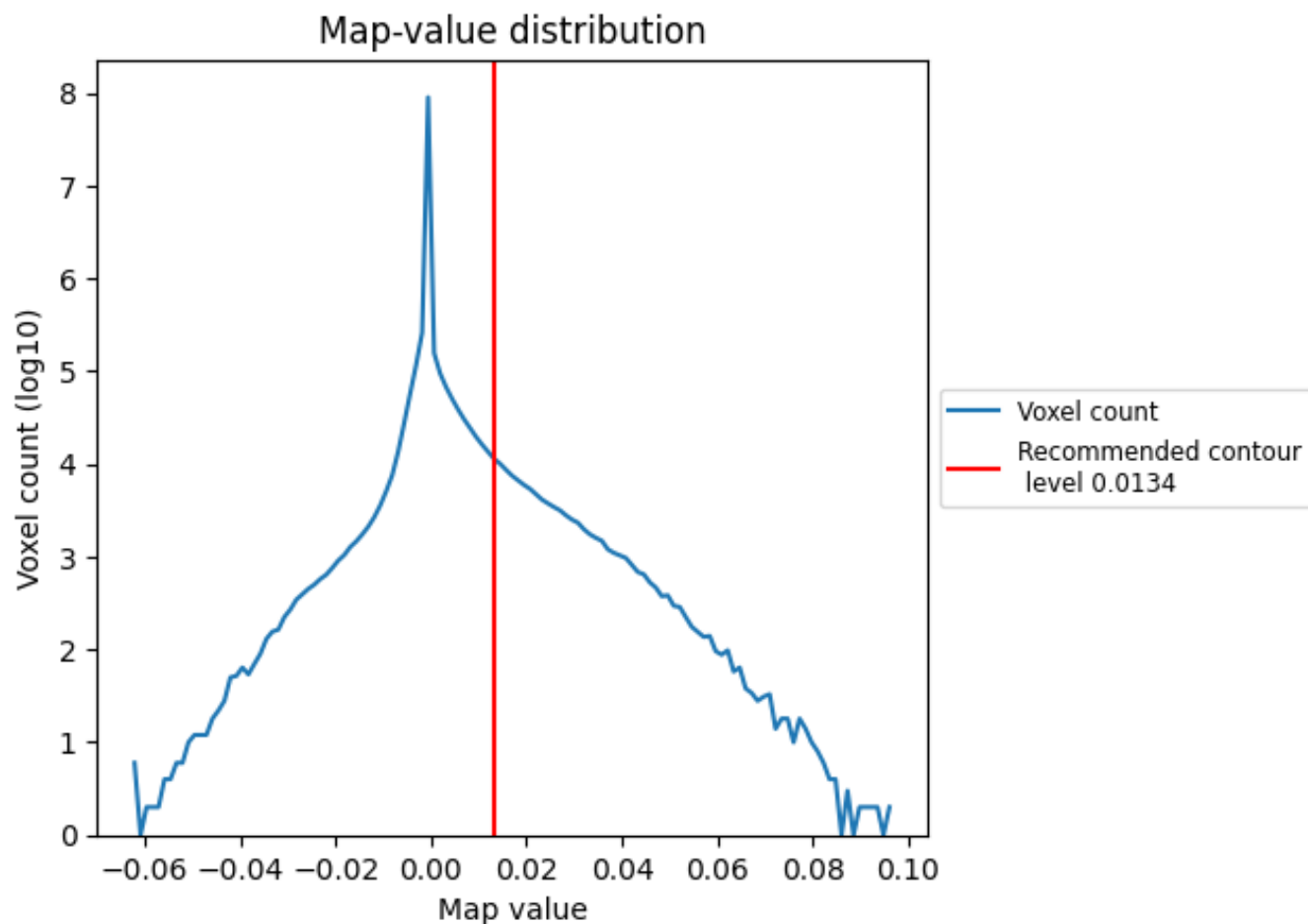
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

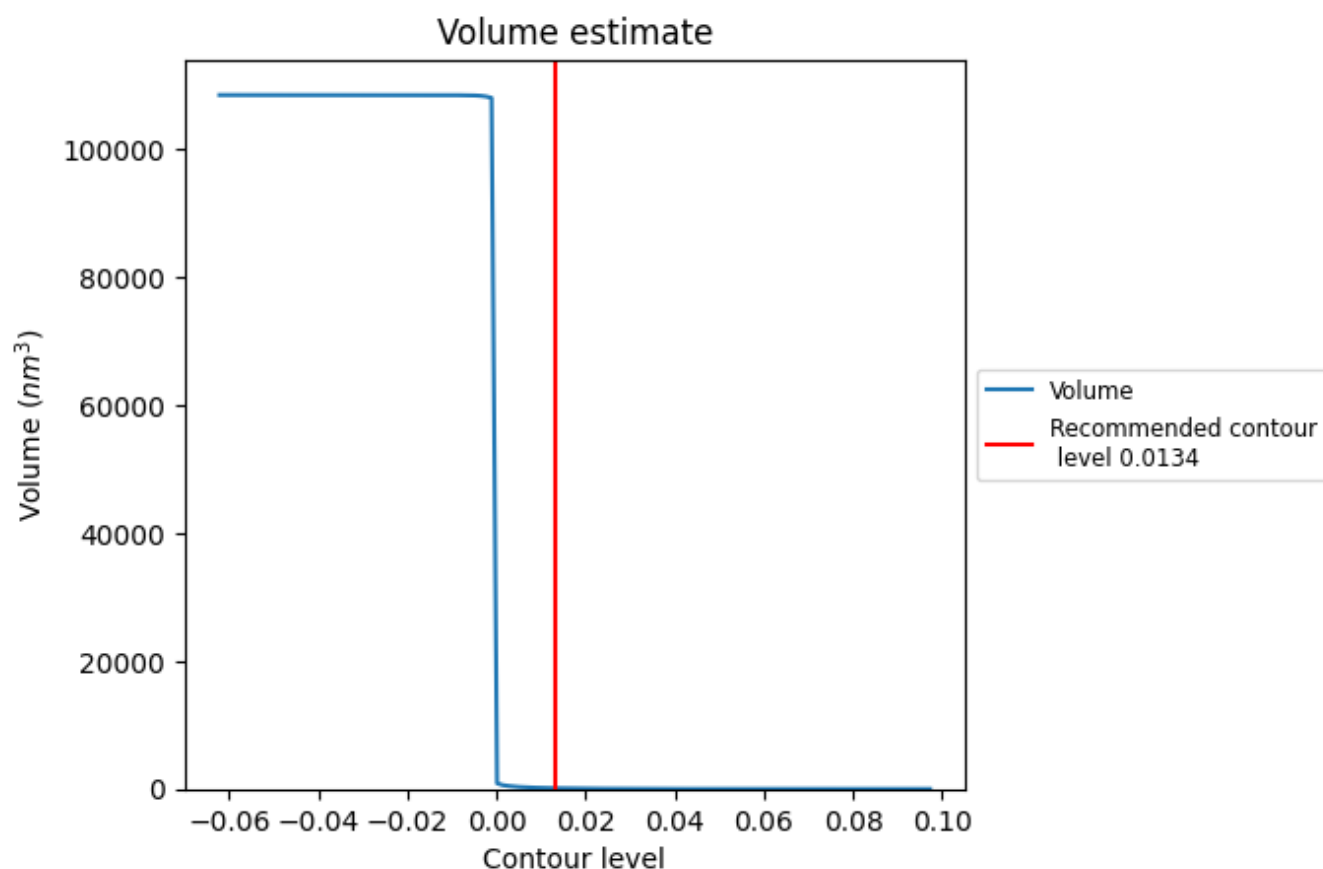
This section contains the results of statistical analysis of the map.

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.

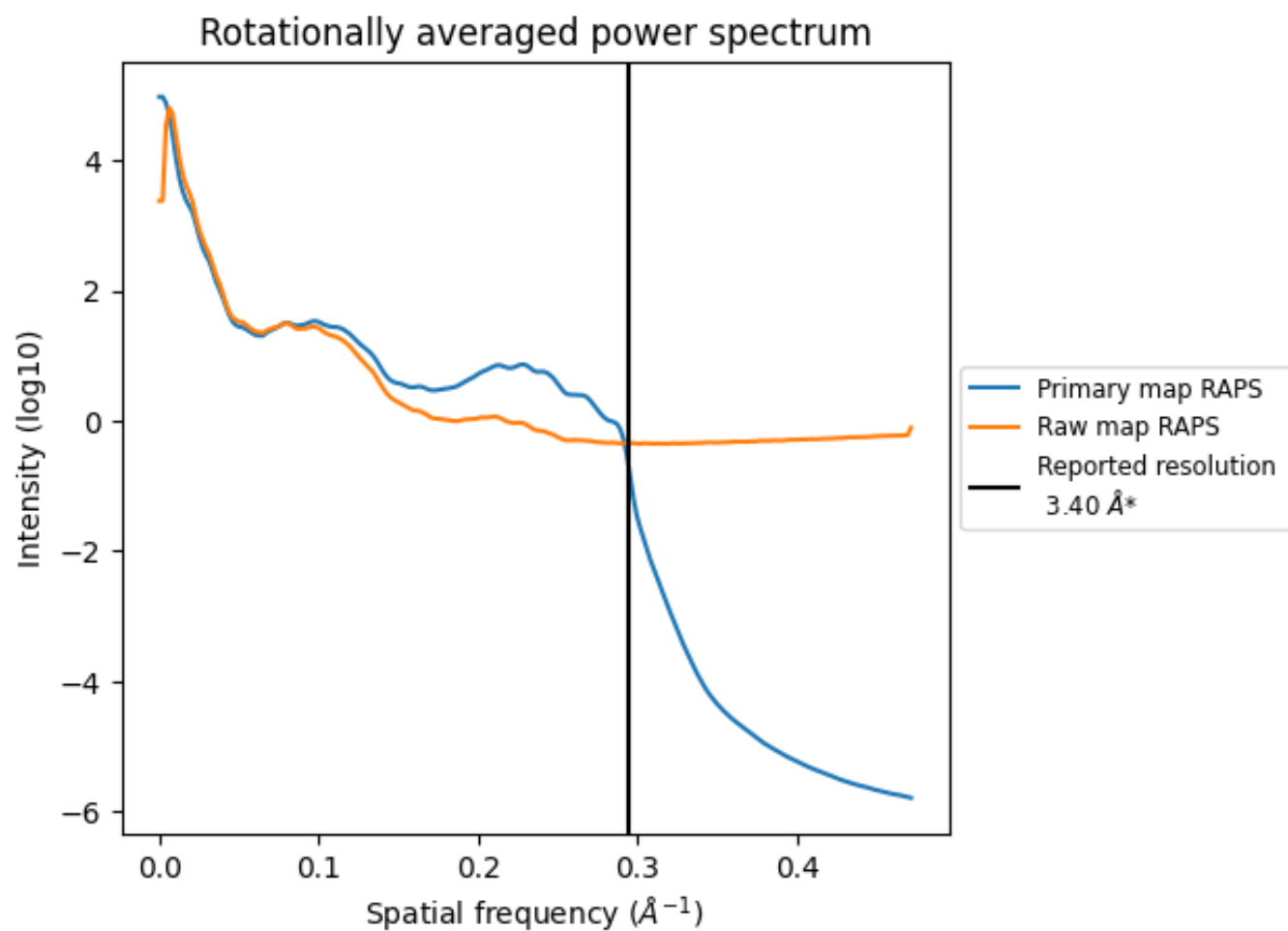
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm^3 ; this corresponds to an approximate mass of 106 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 ⓘ

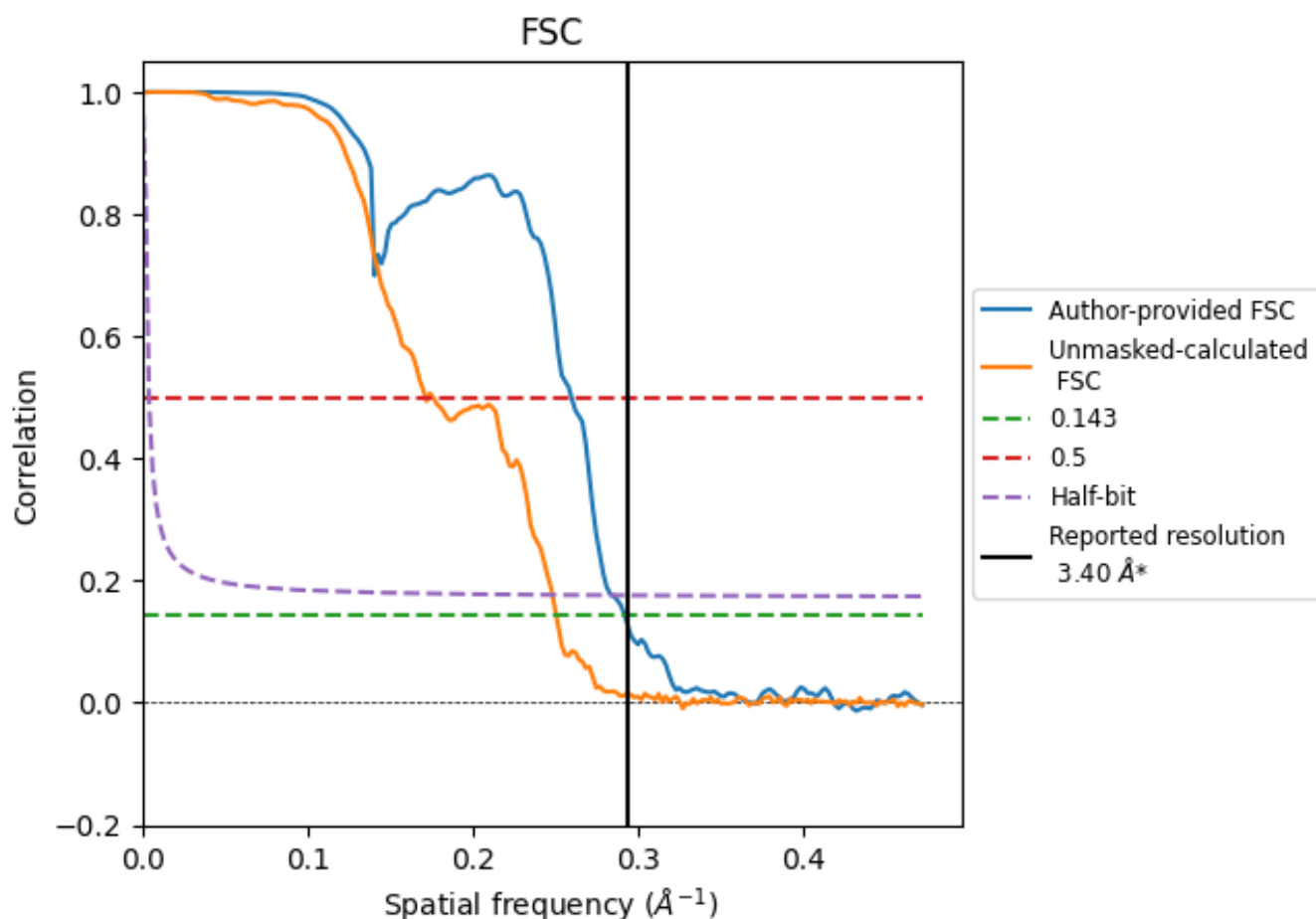


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

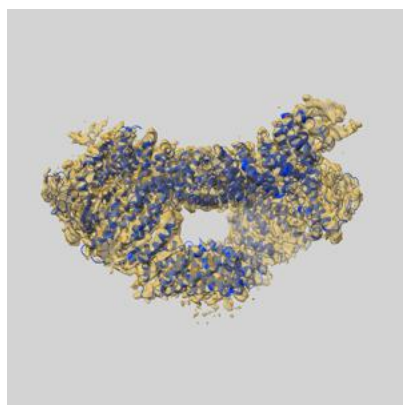
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.85	3.51
Unmasked-calculated*	3.99	5.84	4.03

*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 3.99 differs from the reported value 3.4 by more than 10 %

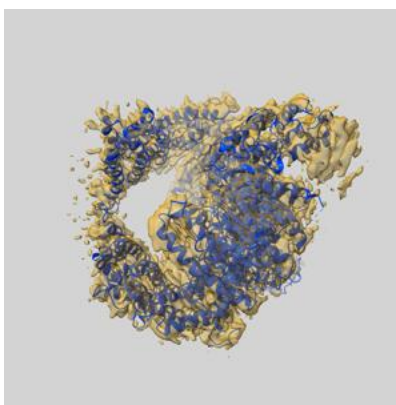
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10534 and PDB model 6TNI. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

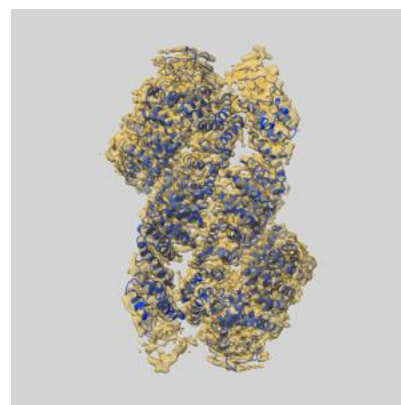
9.1 Map-model overlay [i](#)



X



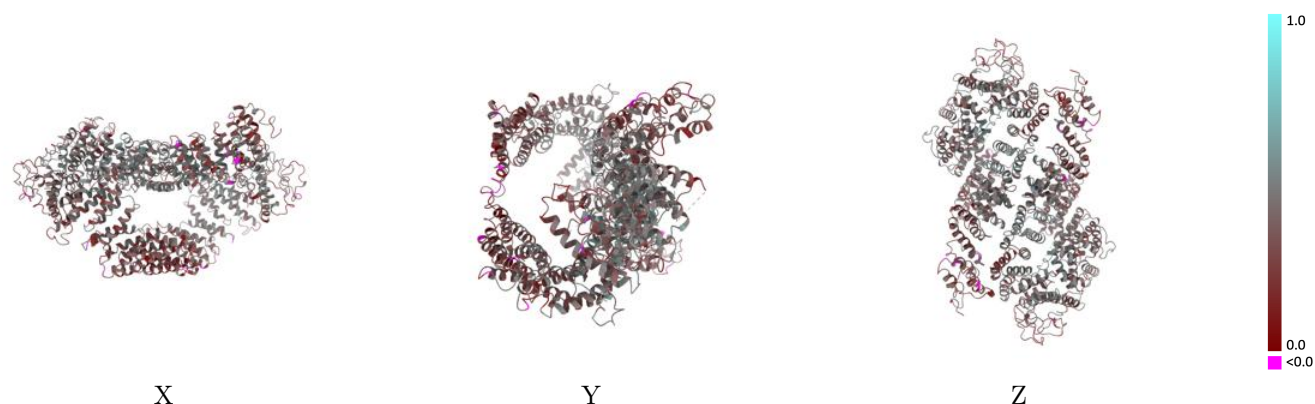
Y



Z

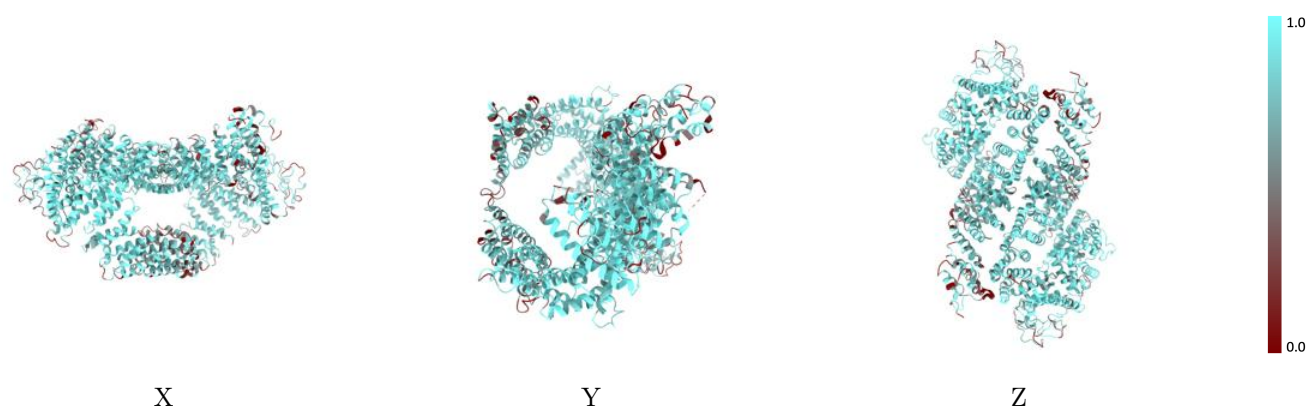
The images above show the 3D surface view of the map at the recommended contour level 0.0134 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



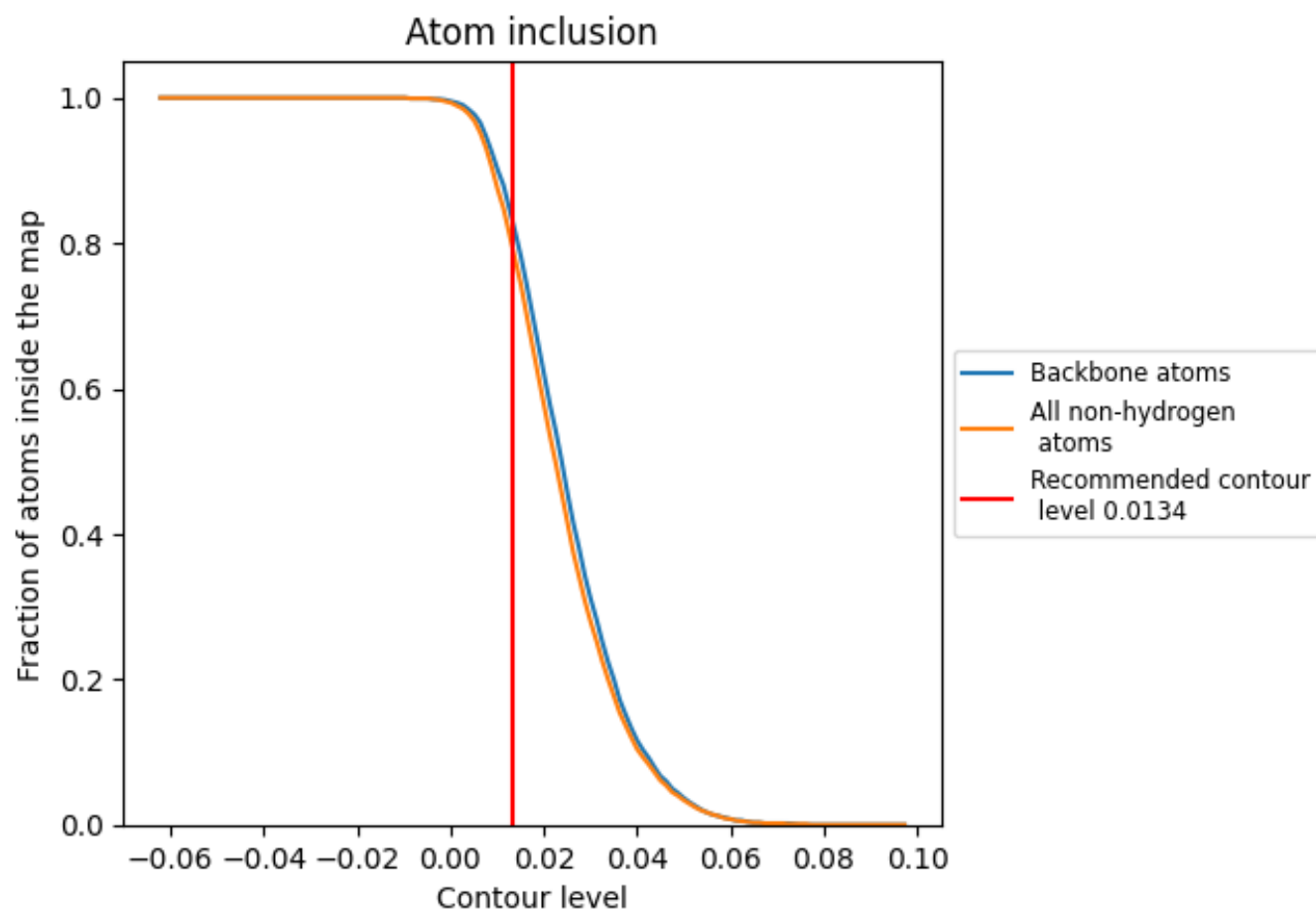
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0134).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.0134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7920	0.3830
A	0.7940	0.3830
a	0.7890	0.3840

