



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:20 AM UTC

PDB ID : 9C5T / pdb_00009c5t
EMDB ID : EMD-45224
Title : Cryo EM structure of DCAF2
Authors : McMahon, E.J.; Wang, W.
Deposited on : 2024-06-06
Resolution : 3.36 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.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

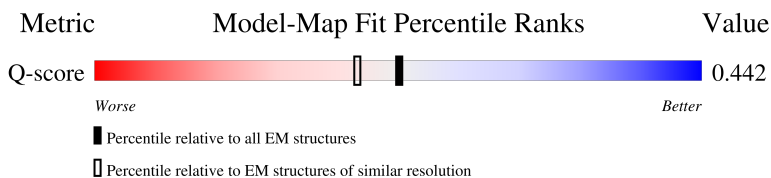
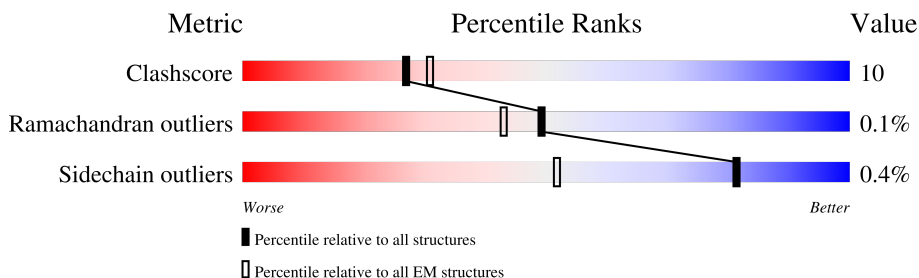
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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	471	 64% 18% 17%
2	B	1140	 74% 24% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11781 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 Denticleless protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	389	Total	C	N	O	S	0	0
			3036	1925	515	579	17		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	GLU	-	expression tag	UNP Q9NZJ0
A	460	ASN	-	expression tag	UNP Q9NZJ0
A	461	LEU	-	expression tag	UNP Q9NZJ0
A	462	TYR	-	expression tag	UNP Q9NZJ0
A	463	PHE	-	expression tag	UNP Q9NZJ0
A	464	GLN	-	expression tag	UNP Q9NZJ0
A	465	SER	-	expression tag	UNP Q9NZJ0
A	466	HIS	-	expression tag	UNP Q9NZJ0
A	467	HIS	-	expression tag	UNP Q9NZJ0
A	468	HIS	-	expression tag	UNP Q9NZJ0
A	469	HIS	-	expression tag	UNP Q9NZJ0
A	470	HIS	-	expression tag	UNP Q9NZJ0
A	471	HIS	-	expression tag	UNP Q9NZJ0

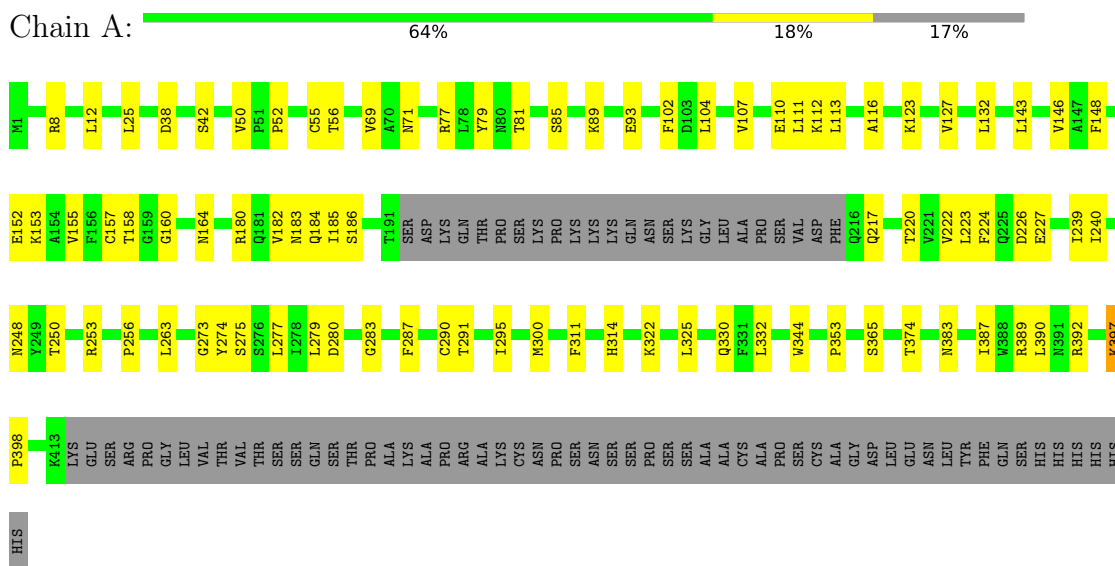
- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1117	Total	C	N	O	S	0	0
			8745	5538	1475	1685	47		

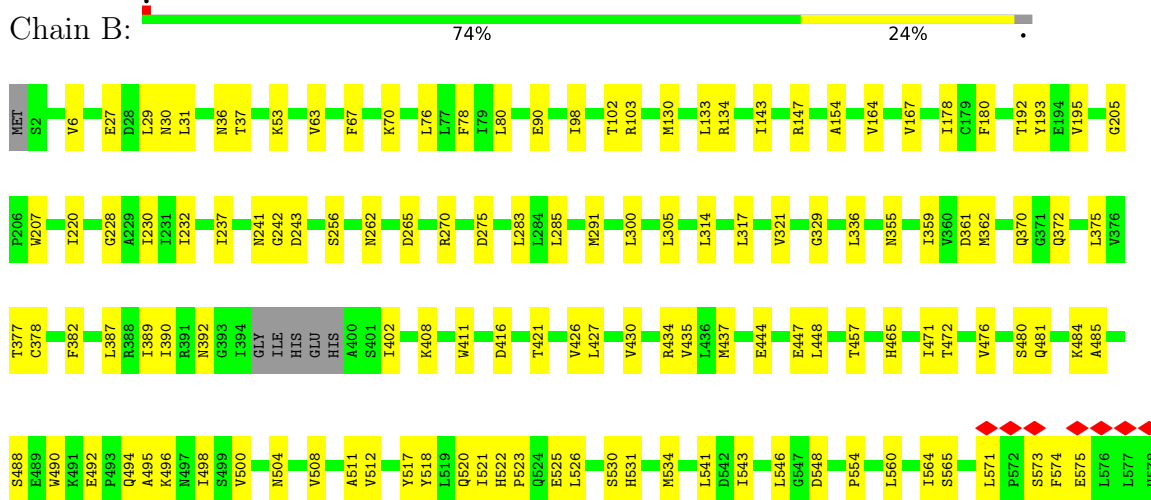
3 Residue-property plots

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: Denticless protein homolog



• Molecule 2: DNA damage-binding protein 1



S1075	F1076	H1077	I1089	L1093	V1109	A1110	N1111	L1112	GLN	TYR	ASP	ASP	GLY	SER	GLY	MET	R1121	D1128	L1129	V1132	V1133	E1134	T1137	R1138	I1139	H1140	D948	F949	N950	M954	V957	E969	N970	A971	F972	N973	D980	T984	T985	E988	R989	L992	Q993	E994	L997	F998	H999	E1002	S1011	L1012	V1013	M1014	Q1015	N1016	F1030	N1034	G1038	L1039	V1040	T1041	E1045	N1049	L1050	L1051	Q1055	N1056	R1057	V1065	L691	A692	L693	N696	S697	M698	I701	G702	THR	ILE	ASP	GLU	ILE	Q708	R713	Y718	E719	S720	I724	V735	L736	S737	I740	S765	L770	S773	SER	THR	ALA	PRO	H778	E785	V788	H789	N790	L791	L792	I793	I794	H803	E811	S815	L816	L821	D824	F825	N826	T827	Y828	F829	I830	V831	E842	F843	K844	R847	I848	V849	V850	D855	G856	K857	L858	E863	K864	E865	V866	M873	L880	L881	I884	N885	S886	L890	Y891	E892	W893	L899	N908	I909	M910	A911	L912	R928	S929	V930	L931	E944	I945	A946	R947	L582	P588	L592	M593	T594	Y601	L602	L603	L606	A610	G615	L616	N617	I618	G621	L622	L623	S624	L638	R639	T640	F641	E642	S643	N648	V649	G652	S653	D654	R655	P656	Y660	K665	N670	L673	K674	E675	M679	L682	Y687	S690
-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124770	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 ($e^-/\text{\AA}^2$)	51.87	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.333	Depositor
Minimum map value	-0.817	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.02092	Depositor
Map size (Å)	250.2, 250.2, 250.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	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	0.11	0/3113	0.31	0/4225
2	B	0.12	0/8902	0.28	0/12054
All	All	0.12	0/12015	0.29	0/16279

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

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	3036	0	2939	56	0
2	B	8745	0	8721	179	0
All	All	11781	0	11660	231	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 10.

All (231) 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:250:THR:O	1:A:253:ARG:NH2	2.15	0.78
2:B:457:THR:HA	2:B:472:THR:HA	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:VAL:HG22	2:B:1040:VAL:HG22	1.70	0.73
2:B:886:SER:HB2	2:B:910:MET:H	1.53	0.73
2:B:375:LEU:HG	2:B:1012:LEU:HD21	1.69	0.73
1:A:374:THR:HG23	1:A:390:LEU:H	1.53	0.72
2:B:494:GLN:HB3	2:B:496:LYS:HG3	1.73	0.71
2:B:1055:GLN:HG3	2:B:1093:LEU:HD23	1.73	0.70
2:B:690:SER:HB3	2:B:702:GLY:HA3	1.73	0.69
2:B:1128:ASP:O	2:B:1132:VAL:HG23	1.93	0.69
2:B:588:PRO:HA	2:B:606:LEU:HA	1.74	0.68
2:B:740:ILE:HD11	2:B:785:GLU:HB3	1.75	0.68
2:B:1057:ARG:NH2	2:B:1111:ASN:O	2.27	0.67
1:A:146:VAL:HG22	1:A:158:THR:HG22	1.76	0.67
2:B:656:PRO:O	2:B:670:ASN:ND2	2.30	0.65
2:B:361:ASP:OD1	2:B:362:MET:N	2.30	0.64
1:A:322:LYS:HB2	1:A:365:SER:HA	1.78	0.64
2:B:387:LEU:HD11	2:B:724:ILE:HD12	1.78	0.64
2:B:305:LEU:HD23	2:B:336:LEU:HD22	1.79	0.64
2:B:291:MET:SD	2:B:291:MET:N	2.64	0.63
1:A:290:CYS:SG	1:A:291:THR:N	2.72	0.63
2:B:665:LYS:HD2	2:B:1138:ARG:HH22	1.64	0.63
2:B:521:ILE:HD12	2:B:526:LEU:HG	1.81	0.63
2:B:411:TRP:HE1	2:B:426:VAL:HB	1.64	0.62
2:B:500:VAL:HG11	2:B:541:LEU:HB3	1.80	0.62
2:B:1109:VAL:HG22	2:B:1129:LEU:HD22	1.80	0.62
1:A:392:ARG:NH2	2:B:842:GLU:OE2	2.33	0.61
2:B:134:ARG:NH1	2:B:164:VAL:O	2.33	0.61
2:B:262:ASN:ND2	2:B:314:LEU:O	2.31	0.61
1:A:248:ASN:OD1	1:A:250:THR:OG1	2.20	0.60
2:B:382:PHE:H	2:B:720:SER:HB3	1.65	0.60
2:B:594:THR:HG21	2:B:603:LEU:HD12	1.82	0.60
2:B:985:THR:HA	2:B:989:ARG:HB2	1.83	0.60
1:A:52:PRO:HD3	1:A:383:ASN:HA	1.84	0.60
2:B:256:SER:OG	2:B:275:ASP:OD1	2.17	0.60
2:B:848:ILE:HD11	2:B:884:ILE:HD11	1.83	0.60
1:A:38:ASP:OD2	1:A:389:ARG:NH2	2.35	0.60
1:A:116:ALA:HB2	1:A:146:VAL:HG23	1.85	0.59
2:B:471:ILE:HG23	2:B:476:VAL:HG12	1.85	0.59
2:B:518:TYR:H	2:B:530:SER:HB2	1.68	0.58
2:B:816:LEU:HD12	2:B:831:VAL:HG22	1.85	0.58
2:B:389:ILE:HB	2:B:713:ARG:HB2	1.84	0.58
2:B:639:ARG:HH11	2:B:679:MET:HE3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:682:LEU:H	2:B:691:LEU:HD12	1.69	0.58
2:B:656:PRO:HG2	2:B:673:LEU:HB2	1.84	0.58
2:B:770:LEU:HD11	2:B:863:GLU:HB3	1.85	0.57
2:B:873:MET:HE3	2:B:880:LEU:HD11	1.86	0.57
2:B:167:VAL:HG12	2:B:180:PHE:HB3	1.86	0.56
2:B:103:ARG:HH21	2:B:147:ARG:HH22	1.53	0.56
2:B:594:THR:OG1	2:B:601:TYR:O	2.23	0.56
2:B:770:LEU:HD13	2:B:865:GLU:HB2	1.88	0.56
2:B:329:GLY:O	2:B:355:ASN:ND2	2.36	0.56
2:B:564:ILE:HG12	2:B:588:PRO:HD3	1.88	0.56
1:A:25:LEU:HD12	1:A:330:GLN:HE22	1.72	0.55
2:B:392:ASN:HB2	2:B:1012:LEU:HB3	1.88	0.55
2:B:573:SER:HB2	2:B:575:GLU:HG2	1.89	0.55
2:B:80:LEU:HD22	2:B:133:LEU:HD22	1.89	0.55
2:B:130:MET:HE1	2:B:195:VAL:HG11	1.88	0.54
2:B:143:ILE:HG12	2:B:154:ALA:HB2	1.89	0.54
1:A:223:LEU:HD21	1:A:279:LEU:HD11	1.90	0.54
2:B:931:LEU:HD21	2:B:944:GLU:HG2	1.89	0.54
2:B:886:SER:OG	2:B:908:ASN:O	2.22	0.53
2:B:317:LEU:HB2	2:B:321:VAL:HG23	1.90	0.53
2:B:560:LEU:HB2	2:B:565:SER:H	1.72	0.53
2:B:969:GLU:HG2	2:B:971:ALA:H	1.73	0.53
2:B:480:SER:OG	2:B:485:ALA:O	2.22	0.53
2:B:910:MET:HE3	2:B:912:LEU:HD21	1.90	0.53
1:A:77:ARG:HH11	1:A:93:GLU:HG2	1.74	0.53
2:B:648:ASN:HD21	2:B:660:TYR:HA	1.74	0.53
2:B:435:VAL:HB	2:B:447:GLU:HA	1.91	0.53
2:B:687:TYR:HB3	2:B:690:SER:HB2	1.90	0.53
2:B:793:ILE:HD11	2:B:858:LEU:HD21	1.90	0.53
1:A:77:ARG:HB2	1:A:79:TYR:HE1	1.73	0.52
2:B:1045:GLU:OE2	2:B:1049:ASN:ND2	2.42	0.52
1:A:110:GLU:OE1	1:A:112:LYS:NZ	2.38	0.52
2:B:554:PRO:HB3	2:B:571:LEU:HD22	1.92	0.51
2:B:648:ASN:OD1	2:B:649:VAL:N	2.43	0.51
1:A:104:LEU:HD22	1:A:113:LEU:HD11	1.92	0.51
2:B:402:ILE:H	2:B:698:THR:HB	1.74	0.51
2:B:653:SER:OG	2:B:654:ASP:N	2.44	0.51
2:B:693:LEU:HB3	2:B:702:GLY:H	1.75	0.51
2:B:594:THR:HG22	2:B:649:VAL:HG11	1.92	0.51
2:B:886:SER:OG	2:B:886:SER:O	2.28	0.51
2:B:980:ASP:OD2	2:B:993:GLN:NE2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:GLU:OE1	2:B:1034:ASN:ND2	2.39	0.51
1:A:295:ILE:HB	1:A:311:PHE:HB2	1.92	0.50
1:A:295:ILE:HG13	1:A:314:HIS:HE1	1.77	0.50
2:B:283:LEU:HD11	2:B:300:LEU:HD22	1.93	0.50
2:B:375:LEU:HB2	2:B:390:ILE:HB	1.92	0.50
2:B:736:LEU:HG	2:B:816:LEU:HD13	1.93	0.50
1:A:392:ARG:HG3	2:B:909:ILE:HG13	1.93	0.50
2:B:416:ASP:OD2	2:B:421:THR:OG1	2.27	0.50
2:B:931:LEU:HD12	2:B:947:ARG:HH21	1.77	0.50
2:B:504:ASN:ND2	2:B:543:ILE:O	2.44	0.49
2:B:192:THR:HG23	2:B:205:GLY:HA3	1.92	0.49
2:B:654:ASP:HA	2:B:675:GLU:HG2	1.93	0.49
2:B:370:GLN:HG2	2:B:372:GLN:H	1.77	0.49
1:A:180:ARG:NE	1:A:180:ARG:HA	2.27	0.49
1:A:185:ILE:HG23	1:A:256:PRO:HG2	1.95	0.48
2:B:498:ILE:HG13	2:B:512:VAL:HG13	1.95	0.48
2:B:735:VAL:HG21	2:B:794:ILE:HD12	1.96	0.48
1:A:182:VAL:HG12	1:A:183:ASN:OD1	2.13	0.48
2:B:891:TYR:HB3	2:B:899:LEU:HD22	1.95	0.48
2:B:950:ASN:ND2	2:B:994:GLU:OE2	2.42	0.48
2:B:265:ASP:OD2	2:B:270:ARG:NH1	2.47	0.48
2:B:984:THR:O	2:B:989:ARG:N	2.46	0.48
2:B:500:VAL:HB	2:B:511:ALA:HB3	1.96	0.48
2:B:950:ASN:OD1	2:B:950:ASN:N	2.45	0.48
2:B:243:ASP:OD1	2:B:243:ASP:N	2.47	0.48
2:B:692:ALA:HA	2:B:701:ILE:HG23	1.95	0.48
1:A:111:LEU:HG	1:A:127:VAL:HG23	1.96	0.47
1:A:239:ILE:HG23	1:A:263:LEU:HA	1.96	0.47
2:B:824:ASP:OD2	2:B:893:TRP:NE1	2.43	0.47
2:B:830:ILE:HG12	2:B:850:VAL:HG23	1.95	0.47
2:B:615:GLY:H	2:B:624:SER:HB2	1.78	0.47
2:B:665:LYS:HG2	2:B:1138:ARG:HH12	1.79	0.47
2:B:359:ILE:HG23	2:B:377:THR:HB	1.96	0.47
1:A:42:SER:HB3	1:A:52:PRO:HG3	1.97	0.47
2:B:548:ASP:OD1	2:B:548:ASP:N	2.47	0.47
1:A:164:ASN:HB3	1:A:186:SER:HA	1.96	0.47
2:B:232:ILE:HG22	2:B:237:ILE:HG12	1.97	0.47
2:B:1030:PHE:CE2	2:B:1038:GLY:HA3	2.49	0.47
2:B:490:TRP:HE3	2:B:526:LEU:HD23	1.80	0.47
2:B:508:VAL:HB	2:B:521:ILE:HG13	1.96	0.47
1:A:223:LEU:HD13	1:A:277:LEU:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:866:VAL:HG21	2:B:884:ILE:HD12	1.97	0.46
1:A:397:LYS:HB3	1:A:398:PRO:HD3	1.97	0.46
2:B:844:LYS:HD3	2:B:844:LYS:HA	1.66	0.46
2:B:29:LEU:C	2:B:30:ASN:HD22	2.24	0.46
2:B:63:VAL:HB	2:B:80:LEU:HB3	1.97	0.46
2:B:811:GLU:OE2	2:B:847:ARG:NH1	2.48	0.46
2:B:881:LEU:HB3	2:B:890:LEU:HD12	1.98	0.46
1:A:50:VAL:HG12	1:A:71:ASN:HB2	1.97	0.46
1:A:81:THR:HG22	1:A:387:ILE:HD13	1.98	0.46
2:B:928:ARG:HB3	2:B:947:ARG:HH22	1.81	0.46
2:B:1041:THR:HG21	2:B:1139:ILE:HD12	1.98	0.46
1:A:217:GLN:CD	1:A:217:GLN:H	2.24	0.46
2:B:492:GLU:OE1	2:B:495:ALA:N	2.48	0.46
2:B:592:LEU:HD22	2:B:638:LEU:HB3	1.97	0.46
2:B:512:VAL:HG23	2:B:517:TYR:HE2	1.81	0.45
2:B:803:HIS:ND1	2:B:858:LEU:HD12	2.31	0.45
2:B:815:SER:OG	2:B:873:MET:SD	2.74	0.45
2:B:31:LEU:HD13	2:B:317:LEU:HD21	1.99	0.45
2:B:791:LEU:HD22	2:B:831:VAL:HG21	1.98	0.45
2:B:855:ASP:O	2:B:857:LYS:NZ	2.40	0.45
2:B:130:MET:HE1	2:B:195:VAL:CG1	2.46	0.45
2:B:207:TRP:HB3	2:B:242:GLY:HA2	1.98	0.45
1:A:110:GLU:HG3	1:A:153:LYS:HE2	1.99	0.45
2:B:465:HIS:ND1	2:B:523:PRO:HG2	2.31	0.45
2:B:929:SER:HB3	2:B:948:ASP:HB3	1.97	0.45
2:B:27:GLU:OE2	2:B:27:GLU:N	2.49	0.45
2:B:370:GLN:N	2:B:370:GLN:OE1	2.49	0.45
2:B:520:GLN:HB3	2:B:522:HIS:CE1	2.51	0.45
2:B:571:LEU:HA	2:B:574:PHE:HE1	1.82	0.45
1:A:374:THR:HG21	2:B:928:ARG:HH21	1.81	0.45
1:A:344:TRP:CD1	1:A:353:PRO:HB3	2.52	0.45
2:B:582:LEU:HD11	2:B:623:LEU:HD13	1.99	0.45
2:B:826:ASN:HB2	2:B:828:TYR:CE1	2.52	0.45
1:A:8:ARG:HB3	1:A:12:LEU:HD12	1.99	0.44
2:B:582:LEU:HD21	2:B:623:LEU:HD13	1.99	0.44
1:A:184:GLN:H	1:A:250:THR:HG23	1.82	0.44
1:A:287:PHE:CE1	1:A:325:LEU:HD11	2.52	0.44
2:B:102:THR:OG1	2:B:1065:VAL:O	2.36	0.44
2:B:228:GLY:HA3	2:B:241:ASN:HB2	1.98	0.44
1:A:85:SER:O	1:A:89:LYS:HG2	2.17	0.44
2:B:517:TYR:HD1	2:B:531:HIS:HA	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ILE:HB	2:B:230:ILE:HB	1.99	0.44
1:A:273:GLY:O	1:A:291:THR:OG1	2.35	0.44
2:B:534:MET:SD	2:B:534:MET:N	2.91	0.44
2:B:639:ARG:NH1	2:B:652:CYS:SG	2.91	0.44
2:B:718:TYR:HB2	2:B:755:SER:HA	2.00	0.44
2:B:821:LEU:HB3	2:B:893:TRP:CG	2.53	0.44
2:B:946:ALA:HB1	2:B:992:LEU:HG	1.99	0.44
1:A:143:LEU:HA	1:A:160:GLY:HA2	1.99	0.43
2:B:90:GLU:OE1	2:B:103:ARG:NH1	2.51	0.43
2:B:675:GLU:HB3	2:B:696:ASN:ND2	2.32	0.43
1:A:102:PHE:N	1:A:116:ALA:O	2.38	0.43
1:A:55:CYS:HB3	1:A:69:VAL:HG23	1.99	0.43
2:B:1015:GLN:HG2	2:B:1016:ASN:H	1.82	0.43
2:B:571:LEU:HA	2:B:574:PHE:CE1	2.54	0.43
1:A:226:ASP:OD1	1:A:227:GLU:N	2.43	0.42
2:B:864:LYS:HD2	2:B:864:LYS:HA	1.64	0.42
2:B:997:LEU:HB3	2:B:1076:PHE:HB2	2.00	0.42
1:A:295:ILE:HG21	1:A:332:LEU:HD21	2.02	0.42
2:B:931:LEU:HD12	2:B:947:ARG:HE	1.84	0.42
2:B:378:CYS:SG	2:B:724:ILE:HB	2.59	0.42
2:B:53:LYS:HE2	2:B:98:ILE:HG22	2.02	0.42
2:B:76:LEU:HD22	2:B:90:GLU:HB2	2.02	0.42
2:B:606:LEU:HD12	2:B:610:ALA:HB3	2.01	0.42
2:B:70:LYS:HB3	2:B:70:LYS:HE3	1.85	0.42
1:A:392:ARG:HH21	2:B:910:MET:HG2	1.84	0.42
2:B:641:PHE:CE2	2:B:643:SER:HB3	2.55	0.42
2:B:857:LYS:HE2	2:B:857:LYS:HB2	1.89	0.42
1:A:240:ILE:HD11	1:A:274:TYR:CZ	2.55	0.42
1:A:107:VAL:HG22	1:A:148:PHE:CE2	2.55	0.42
2:B:427:LEU:N	2:B:434:ARG:O	2.50	0.42
2:B:973:ASN:OD1	2:B:999:HIS:ND1	2.42	0.42
2:B:788:VAL:HG12	2:B:790:ASN:HD21	1.84	0.41
2:B:522:HIS:HB2	2:B:525:GLU:HB3	2.01	0.41
2:B:945:ILE:HD13	2:B:945:ILE:HA	1.89	0.41
1:A:374:THR:HG22	1:A:389:ARG:HG2	2.03	0.41
2:B:36:ASN:ND2	2:B:37:THR:HG23	2.35	0.41
2:B:546:LEU:HD22	2:B:618:ILE:HD12	2.02	0.41
1:A:123:LYS:HB3	1:A:132:LEU:HD11	2.02	0.41
2:B:617:ASN:H	2:B:621:GLY:HA2	1.85	0.41
2:B:679:MET:HE3	2:B:679:MET:HB3	1.97	0.41
1:A:390:LEU:HD12	1:A:390:LEU:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:LEU:HD23	2:B:481:GLN:NE2	2.35	0.41
2:B:484:LYS:HD3	2:B:484:LYS:HA	1.87	0.41
1:A:152:GLU:HG3	1:A:155:VAL:HB	2.02	0.41
2:B:655:ARG:HE	2:B:1014:MET:HE1	1.85	0.41
2:B:67:PHE:HE1	2:B:78:PHE:HB2	1.86	0.41
2:B:1089:ILE:HD13	2:B:1089:ILE:HA	1.94	0.41
1:A:77:ARG:HB2	1:A:79:TYR:CE1	2.54	0.41
2:B:408:LYS:HE3	2:B:430:VAL:HG22	2.03	0.41
2:B:954:MET:HE2	2:B:957:VAL:HG12	2.03	0.41
2:B:973:ASN:ND2	2:B:1077:HIS:O	2.50	0.41
2:B:984:THR:HB	2:B:988:GLU:OE1	2.20	0.41
2:B:488:SER:HB3	2:B:526:LEU:HD22	2.03	0.41
2:B:1134:GLU:O	2:B:1137:THR:HG22	2.21	0.41
1:A:220:THR:HG21	1:A:275:SER:HA	2.02	0.40
2:B:437:MET:N	2:B:444:GLU:O	2.54	0.40
2:B:999:HIS:HB2	2:B:1075:SER:O	2.21	0.40
1:A:157:CYS:HB3	1:A:224:PHE:HE2	1.86	0.40
2:B:178:ILE:HG22	2:B:193:TYR:HB2	2.04	0.40
2:B:985:THR:HG23	2:B:989:ARG:HH11	1.87	0.40
2:B:1051:LEU:HD13	2:B:1089:ILE:HG21	2.02	0.40
1:A:157:CYS:SG	1:A:222:VAL:HG11	2.61	0.40
1:A:280:ASP:OD1	1:A:283:GLY:N	2.54	0.40
2:B:719:GLU:OE2	2:B:737:SER:OG	2.23	0.40
2:B:972:PHE:HB3	2:B:1002:GLU:N	2.37	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	385/471 (82%)	364 (94%)	20 (5%)	1 (0%)	36 63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1107/1140 (97%)	1045 (94%)	62 (6%)	0	100	100
All	All	1492/1611 (93%)	1409 (94%)	82 (6%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	LYS

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	335/406 (82%)	333 (99%)	2 (1%)	78	79
2	B	980/999 (98%)	977 (100%)	3 (0%)	86	84
All	All	1315/1405 (94%)	1310 (100%)	5 (0%)	81	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	300	MET
2	B	285	LEU
2	B	821	LEU
2	B	1011	SER

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	228	ASN
2	B	183	GLN
2	B	186	GLN
2	B	456	GLN
2	B	497	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	677	ASN
2	B	743	GLN
2	B	759	GLN
2	B	803	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

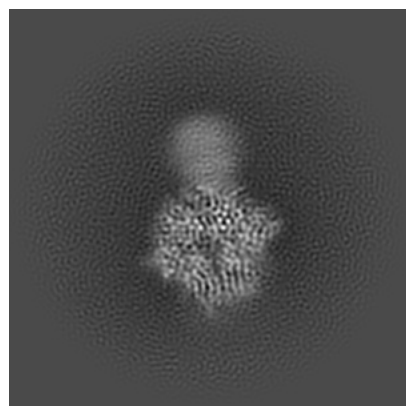
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45224. These allow visual inspection of the internal detail of the map and identification of artifacts.

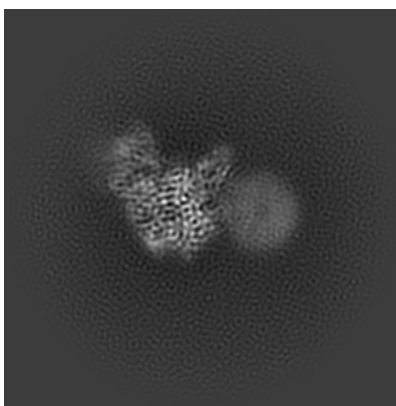
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

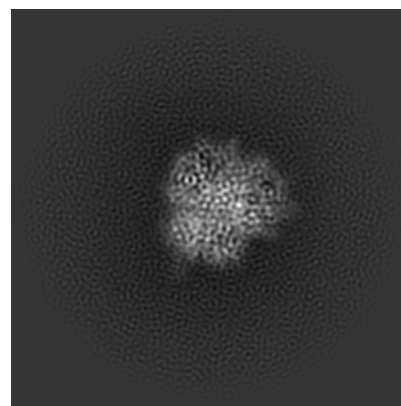
6.1.1 Primary map



X

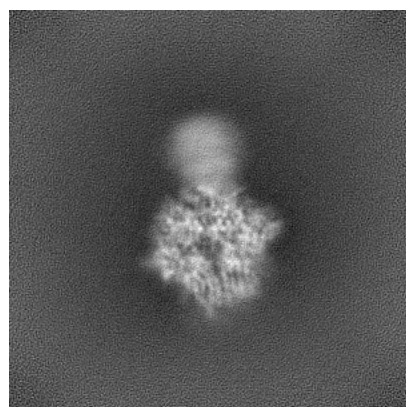


Y

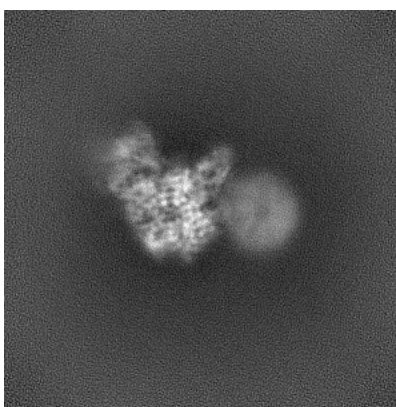


Z

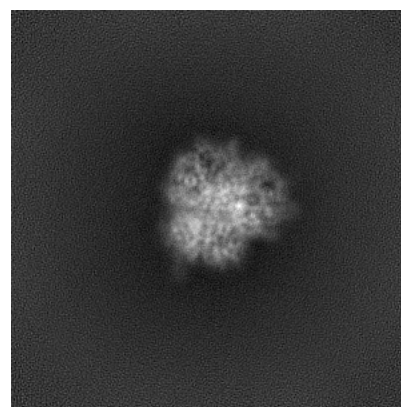
6.1.2 Raw map



X



Y

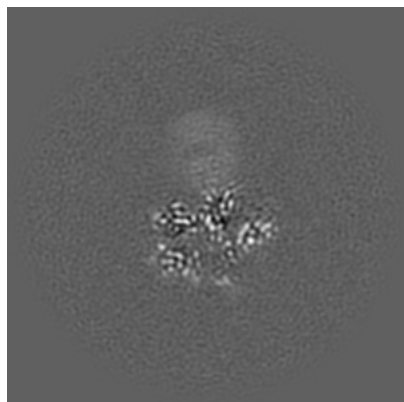


Z

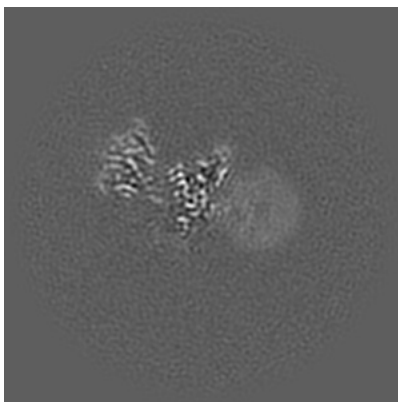
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

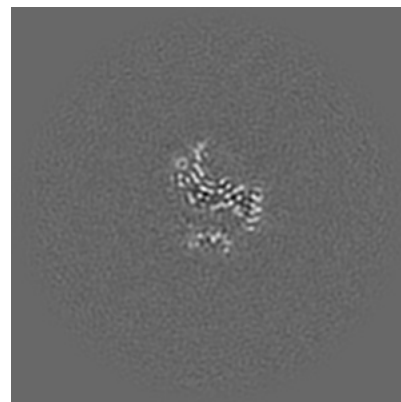
6.2.1 Primary map



X Index: 150



Y Index: 150

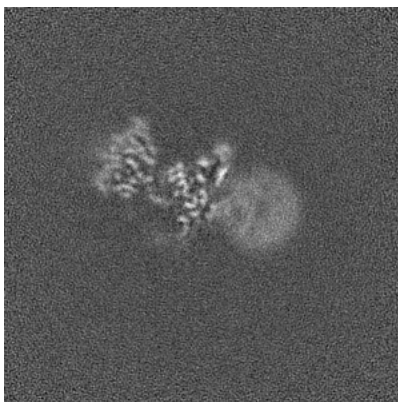


Z Index: 150

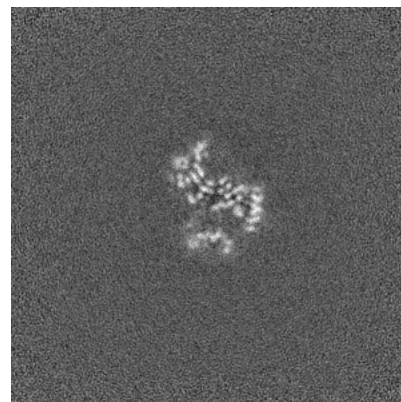
6.2.2 Raw map



X Index: 150



Y Index: 150

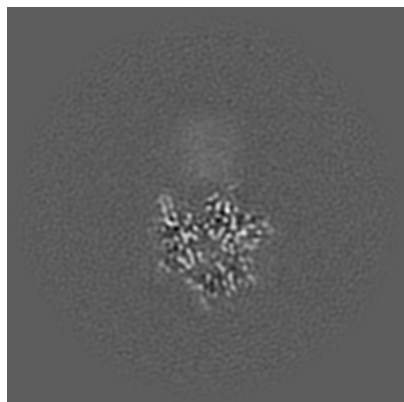


Z Index: 150

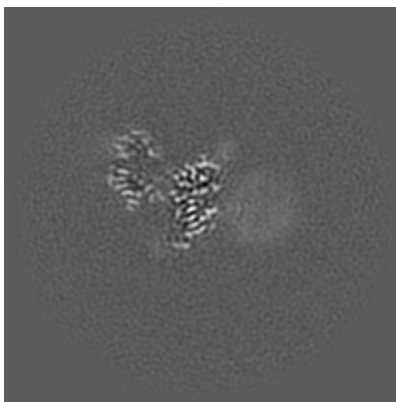
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

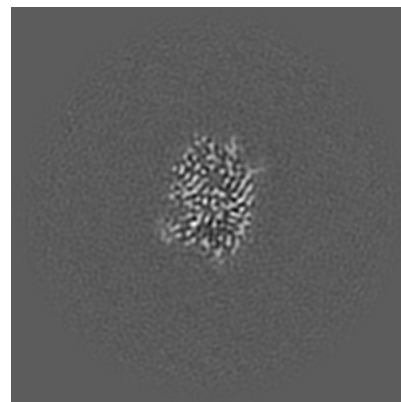
6.3.1 Primary map



X Index: 162

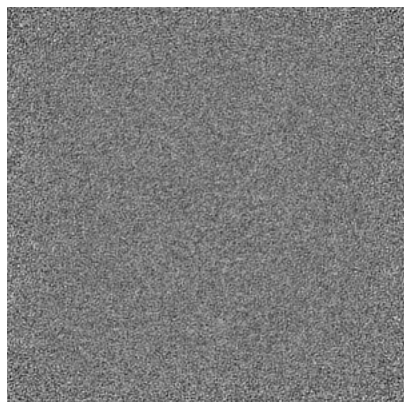


Y Index: 157

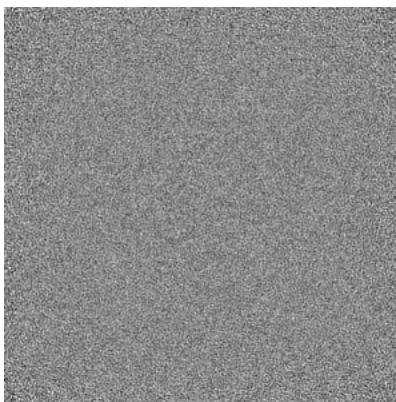


Z Index: 136

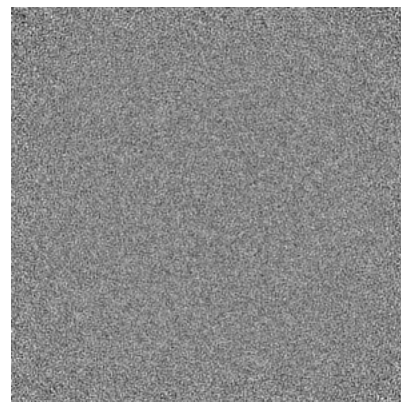
6.3.2 Raw map



X Index: 0



Y Index: 0

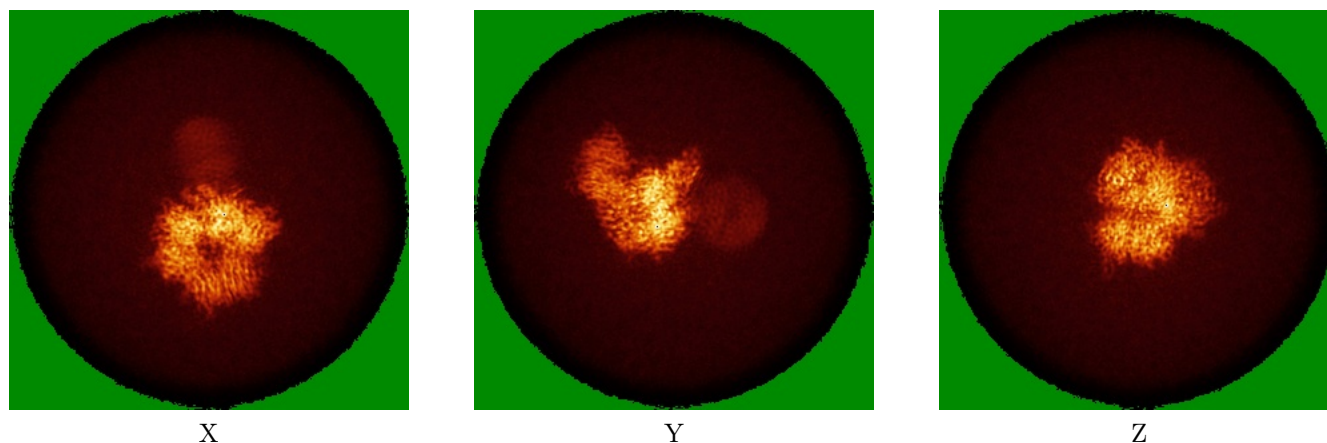


Z Index: 0

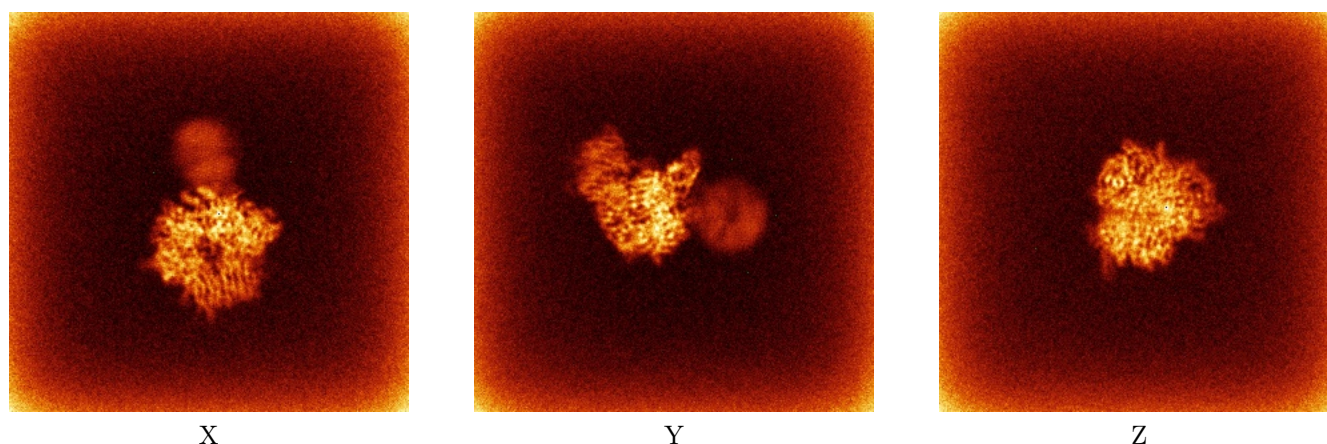
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

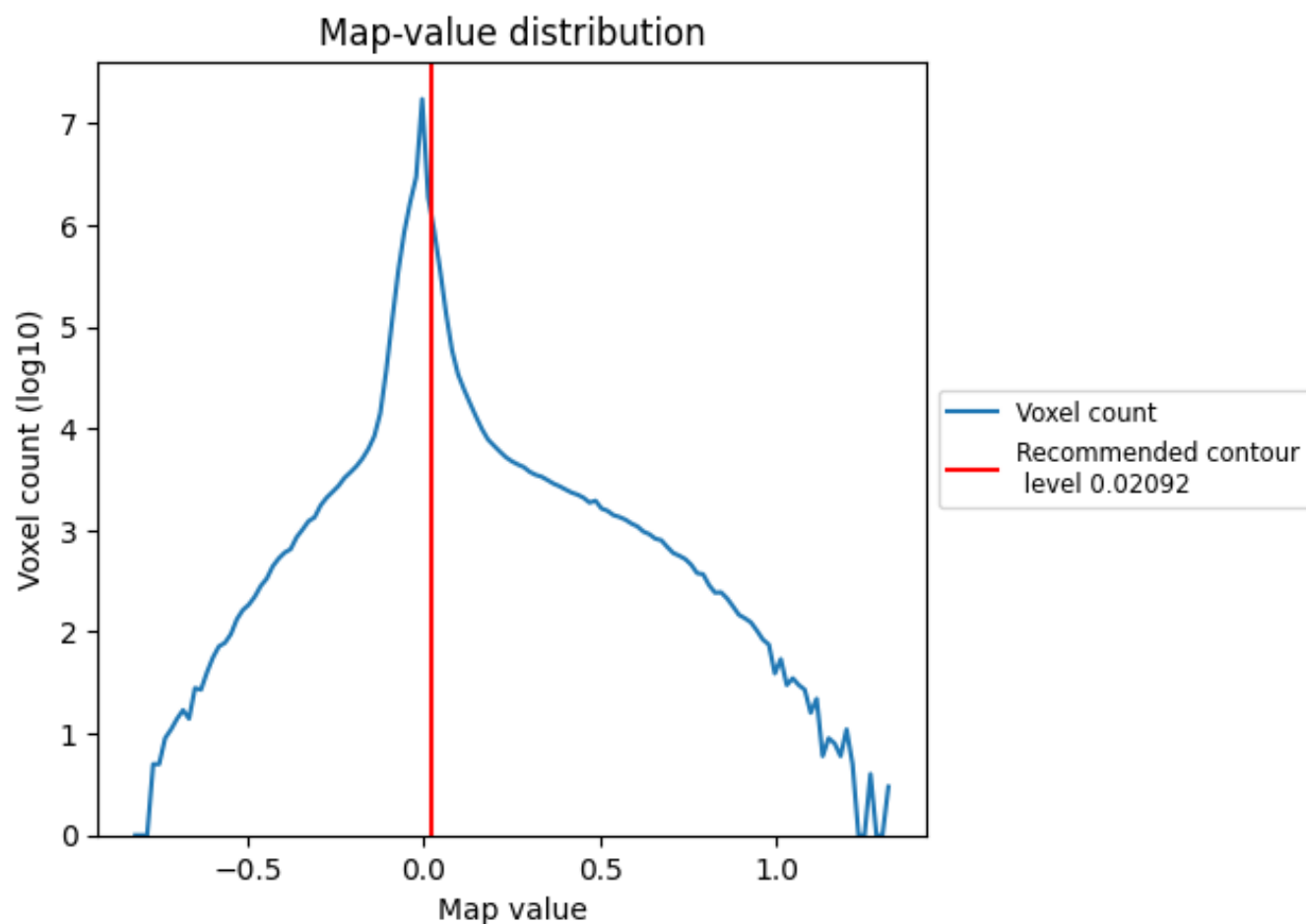
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

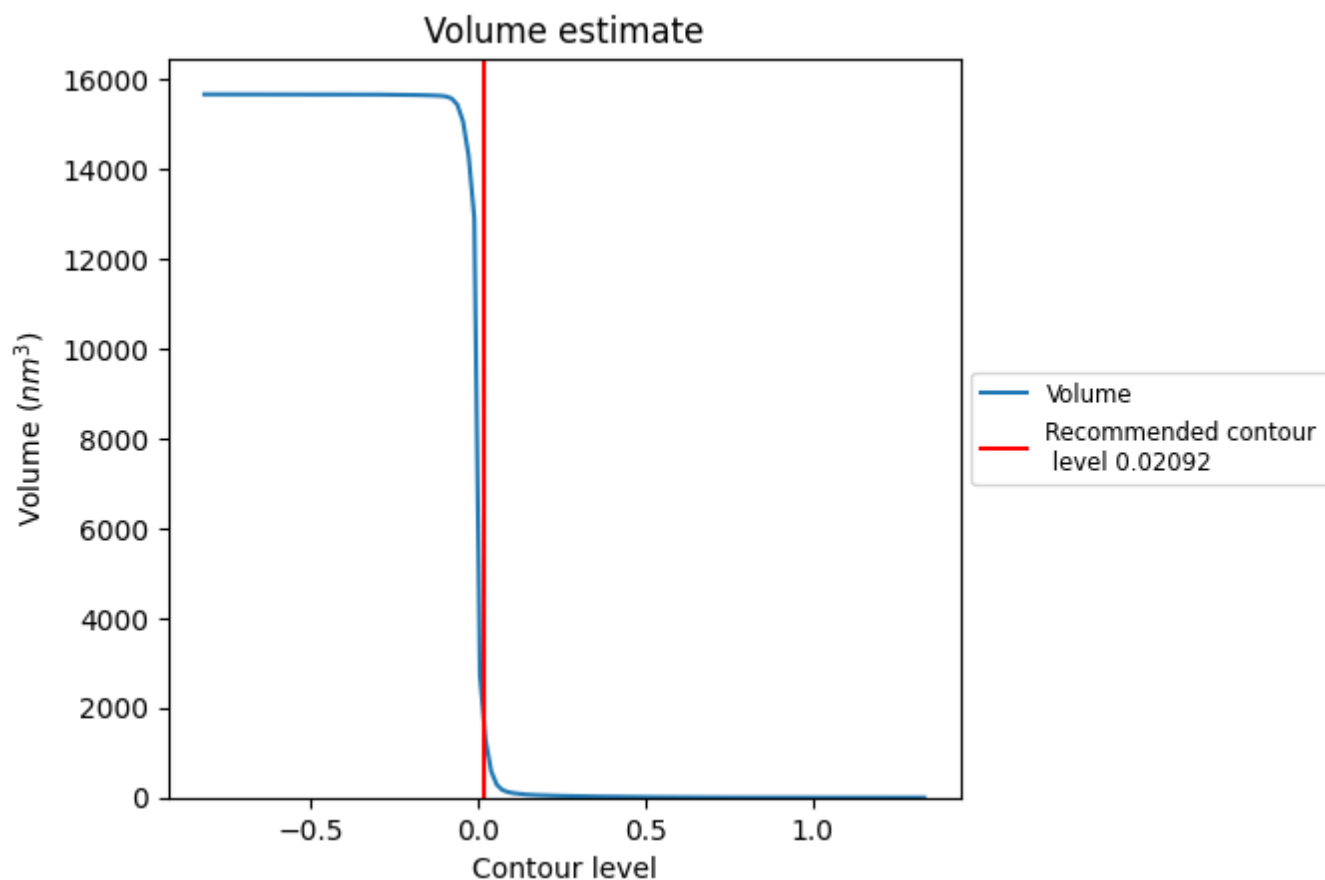
This section contains the results of statistical analysis of the map.

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.

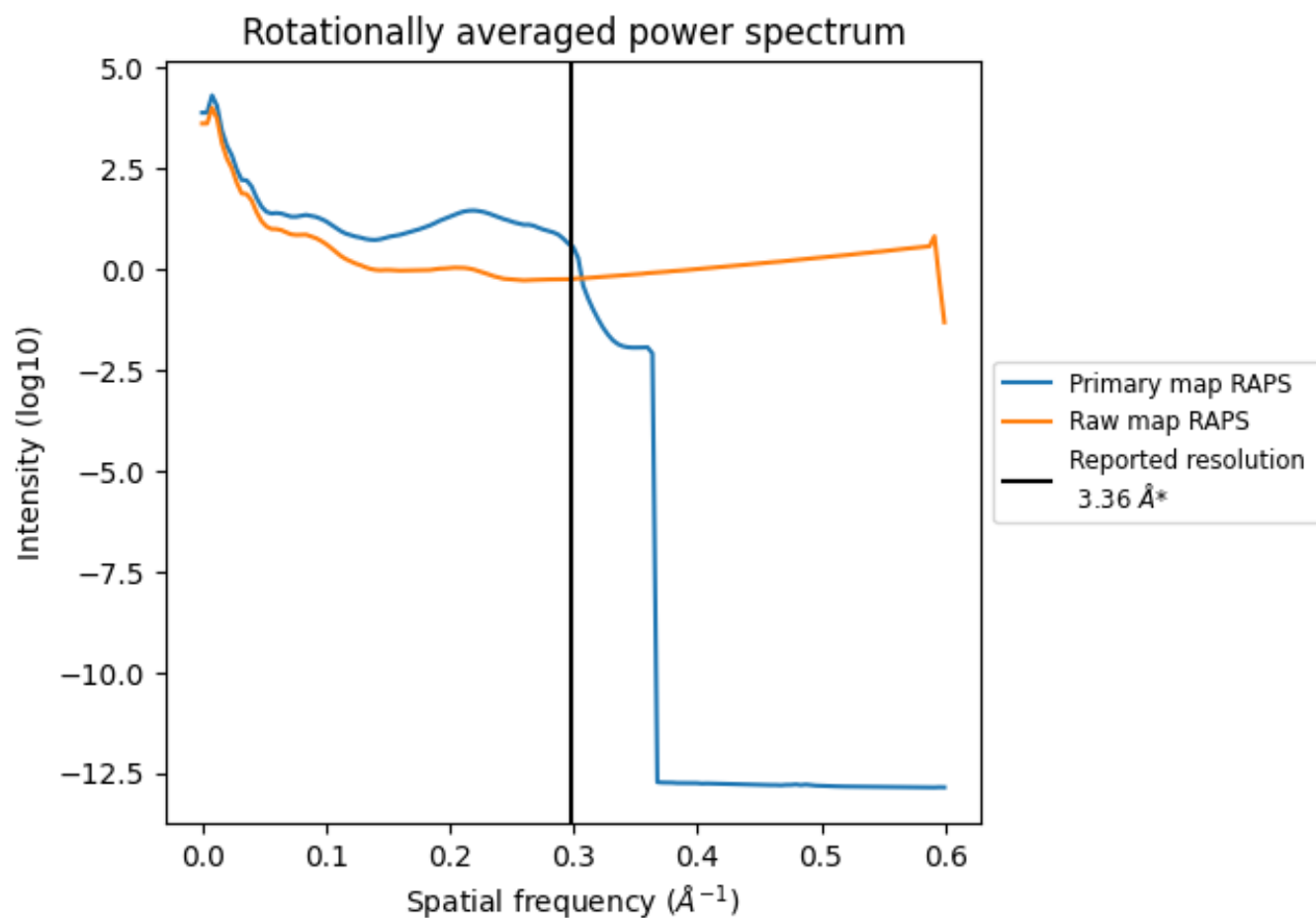
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1450 nm³; this corresponds to an approximate mass of 1309 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 ⓘ

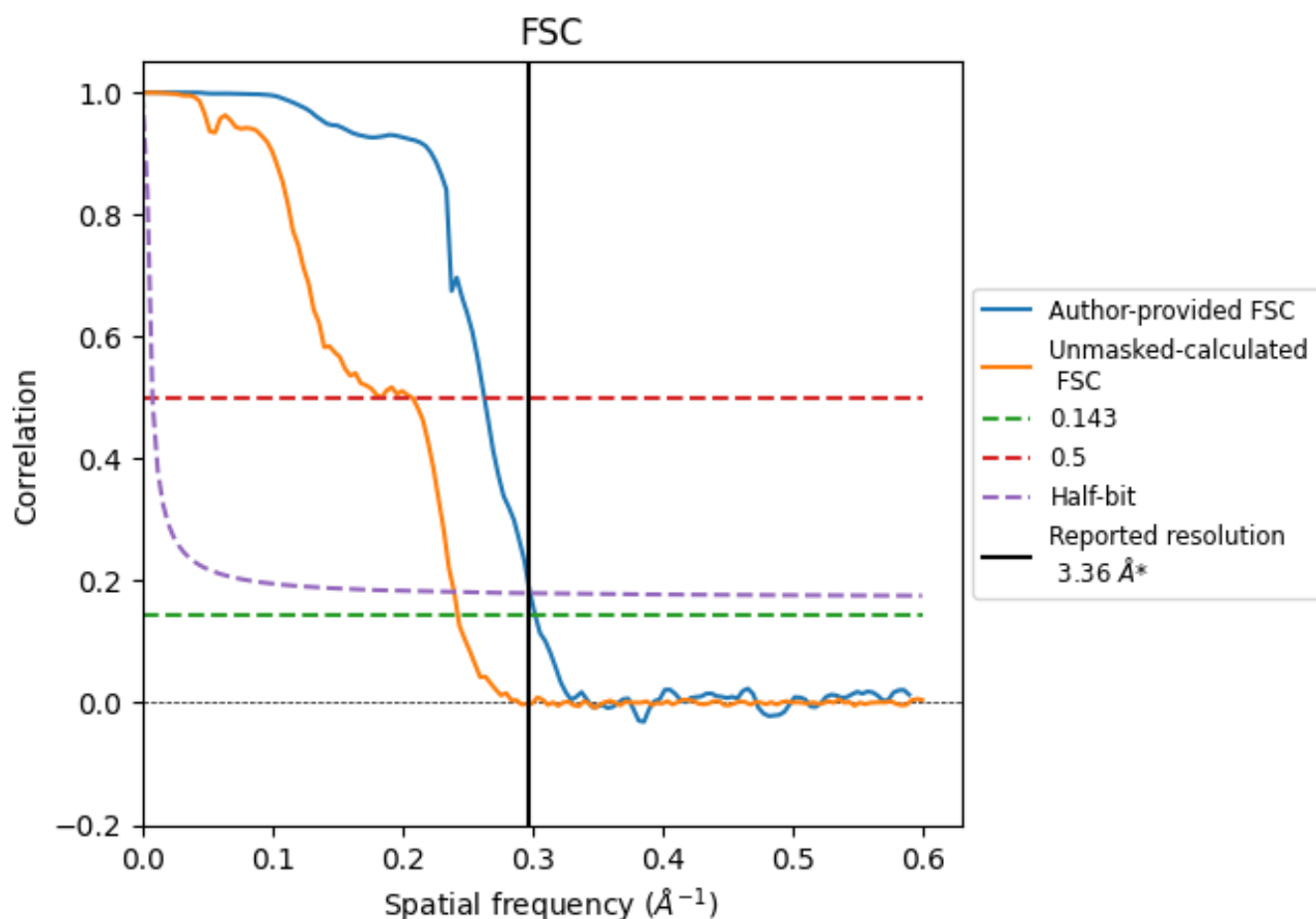


*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

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 $0.298 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.31	3.80	3.35
Unmasked-calculated*	4.12	5.45	4.17

*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 4.12 differs from the reported value 3.36 by more than 10 %

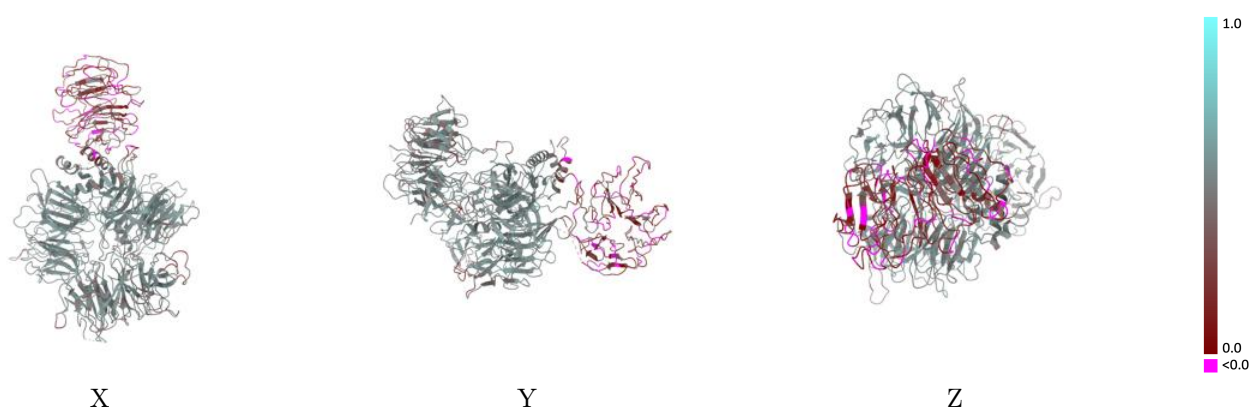
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-45224 and PDB model 9C5T. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

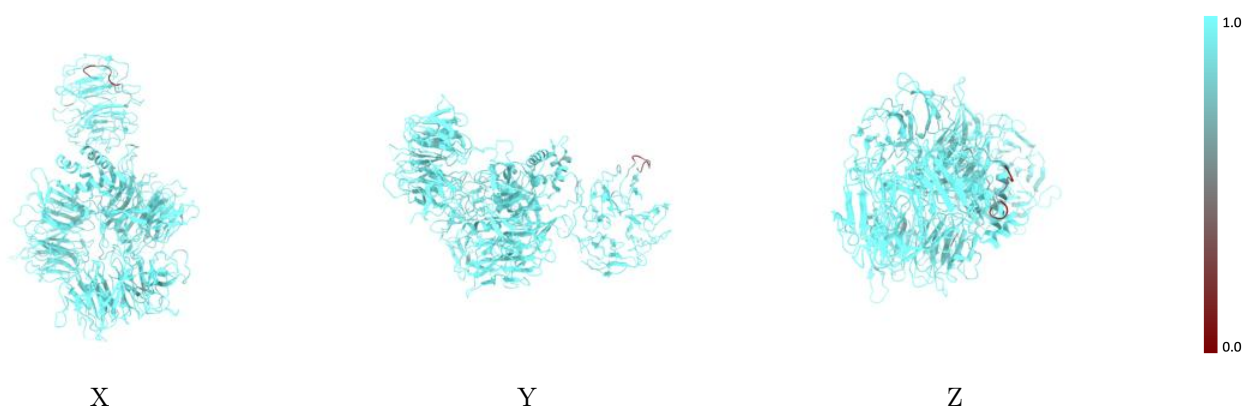
This section was not generated.

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



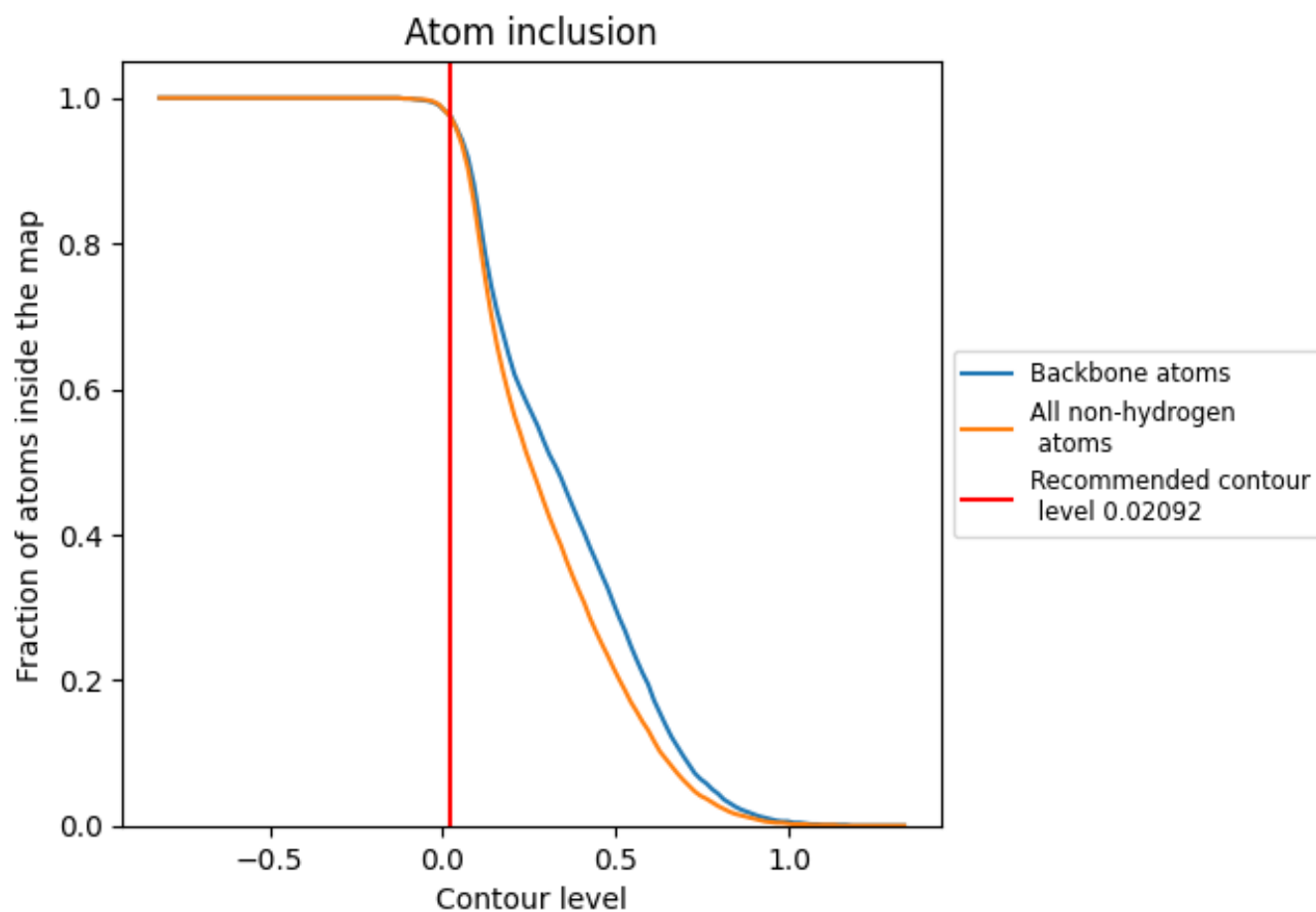
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02092).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.02092) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.4420
A	0.9780	0.4990
B	0.9740	0.4220

