



Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 11:31 PM EST

PDB ID : 7U5T
EMDB ID : EMD-26358
Title : Structure of DHQS/EPSPS dimer from *Candida albicans* Aro1
Authors : Quade, B.; Borek, D.; Otwinowski, Z.
Deposited on : 2022-03-02
Resolution : 3.43 Å (reported)
Based on initial models : 7TBV, 6C5C, 7TBU

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

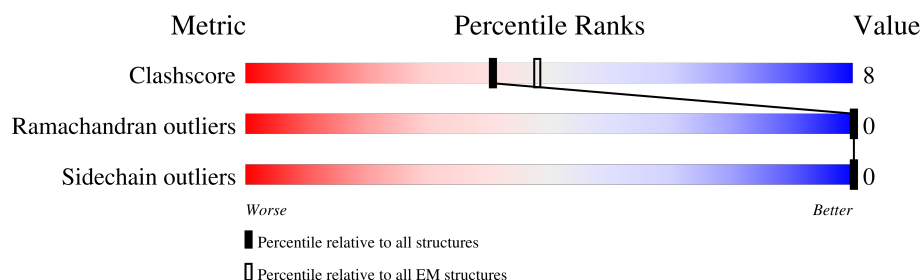
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1551	
1	B	1551	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9093 atoms, of which 0 are hydrogens and 0 are deuteriums.

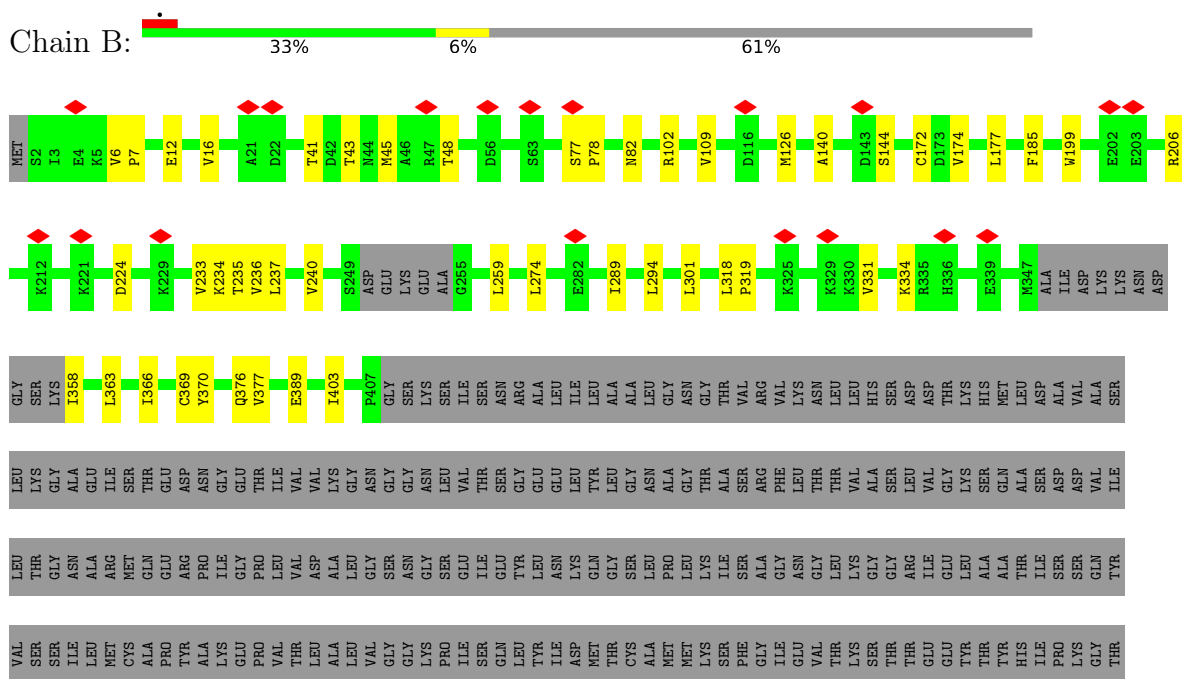
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pentafunctional AROM polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	592	Total	C	N	O	S	0	0
			4529	2891	764	850	24		
1	B	598	Total	C	N	O	S	0	0
			4564	2912	770	858	24		

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

- Molecule 1: Pentafunctional AROM polypeptide





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87484	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 ($e^-/\text{\AA}^2$)	83.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.608	Depositor
Minimum map value	-0.897	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.211	Depositor
Map size (Å)	499.80002, 499.80002, 499.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2495, 1.2495, 1.2495	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/4613	0.56	0/6255
1	B	0.42	0/4650	0.57	0/6307
All	All	0.43	0/9263	0.57	0/12562

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	4529	0	4648	90	0
1	B	4564	0	4683	49	0
All	All	9093	0	9331	139	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 8.

All (139) 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:800:LYS:CD	1:A:830:GLU:HB3	1.74	1.18
1:A:757:ILE:CG2	1:A:768:ILE:HD11	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:TYR:CE1	1:A:738:THR:HG22	1.88	1.08
1:A:733:THR:HA	1:A:736:PHE:HE2	1.23	1.04
1:A:730:GLU:O	1:A:733:THR:HG23	1.62	0.99
1:A:757:ILE:HG21	1:A:768:ILE:HD11	1.46	0.96
1:A:733:THR:HA	1:A:736:PHE:CE2	2.01	0.93
1:A:800:LYS:HD2	1:A:830:GLU:HB3	1.50	0.92
1:A:800:LYS:HD3	1:A:830:GLU:HB3	1.53	0.87
1:A:737:LEU:HD21	1:A:767:ARG:HB3	1.62	0.82
1:A:664:TYR:CE1	1:A:738:THR:CG2	2.68	0.77
1:A:757:ILE:HG22	1:A:768:ILE:HD11	1.68	0.74
1:A:664:TYR:CZ	1:A:738:THR:CG2	2.71	0.73
1:B:715:THR:HG22	1:B:742:GLN:HE21	1.56	0.70
1:A:737:LEU:HD11	1:A:767:ARG:HD2	1.73	0.69
1:A:664:TYR:CZ	1:A:738:THR:HG22	2.28	0.68
1:A:93:ASP:O	1:A:97:GLN:HG3	1.95	0.67
1:A:730:GLU:O	1:A:733:THR:CG2	2.41	0.65
1:A:736:PHE:CD1	1:A:757:ILE:HG12	2.32	0.64
1:B:140:ALA:HA	1:B:144:SER:HB2	1.80	0.64
1:A:391:LEU:HD12	1:A:832:VAL:O	1.99	0.63
1:B:358:ILE:N	1:B:376:GLN:OE1	2.33	0.62
1:B:798:ARG:HH12	1:B:825:THR:HG21	1.64	0.61
1:A:192:VAL:HG13	1:A:239:SER:HB2	1.82	0.61
1:A:389:GLU:HG2	1:A:835:LEU:HA	1.81	0.61
1:B:765:ASN:ND2	1:B:772:GLU:OE1	2.34	0.61
1:A:692:PHE:HD1	1:A:732:MET:CE	2.14	0.61
1:B:7:PRO:HA	1:B:12:GLU:HA	1.83	0.61
1:A:800:LYS:CE	1:A:830:GLU:HB3	2.31	0.60
1:B:389:GLU:HG2	1:B:817:LEU:HA	1.83	0.60
1:A:729:MET:HB3	1:A:732:MET:HB2	1.84	0.58
1:A:757:ILE:HG22	1:A:757:ILE:O	2.02	0.57
1:B:12:GLU:O	1:B:12:GLU:HG3	2.05	0.56
1:A:736:PHE:HD1	1:A:754:ILE:CG2	2.18	0.56
1:B:685:LYS:HB2	1:B:696:THR:HB	1.88	0.56
1:A:736:PHE:CD1	1:A:757:ILE:CG1	2.90	0.55
1:A:736:PHE:CG	1:A:757:ILE:HG12	2.42	0.54
1:A:182:ALA:HA	1:A:185:PHE:HD2	1.73	0.54
1:A:783:ASN:ND2	1:A:790:GLU:OE1	2.38	0.54
1:B:665:SER:HB3	1:B:688:GLN:HG2	1.90	0.54
1:A:757:ILE:HG21	1:A:768:ILE:CD1	2.28	0.54
1:B:663:ILE:HG21	1:B:669:GLN:HE21	1.73	0.54
1:A:140:ALA:HA	1:A:144:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:CYS:SG	1:B:370:TYR:N	2.80	0.54
1:B:102:ARG:HG2	1:B:126:MET:HB3	1.90	0.54
1:B:77:SER:OG	1:B:82:ASN:ND2	2.42	0.53
1:B:719:LEU:HD21	1:B:749:ARG:HB3	1.91	0.52
1:A:274:LEU:HD22	1:A:331:VAL:HG21	1.91	0.52
1:B:767:LEU:HD23	1:B:769:ASP:H	1.75	0.52
1:A:760:GLN:HA	1:A:763:LYS:HB2	1.91	0.52
1:B:749:ARG:NH1	1:B:796:ASP:OD1	2.43	0.52
1:A:667:ALA:HB1	1:A:742:VAL:CG2	2.39	0.52
1:A:32:LEU:HD22	1:A:130:ARG:HH11	1.76	0.51
1:A:378:SER:OG	1:A:379:LYS:N	2.44	0.51
1:A:790:GLU:OE2	1:A:792:HIS:NE2	2.44	0.50
1:A:737:LEU:HD21	1:A:767:ARG:CB	2.38	0.50
1:B:710:ASP:OD1	1:B:737:THR:OG1	2.32	0.48
1:A:815:HIS:HB3	1:A:840:THR:HA	1.95	0.48
1:A:692:PHE:HD1	1:A:732:MET:HE2	1.79	0.48
1:B:294:LEU:HD21	1:B:377:VAL:HG21	1.95	0.48
1:A:45:MET:O	1:A:48:THR:OG1	2.28	0.48
1:A:764:GLU:HB2	1:A:767:ARG:HH21	1.77	0.48
1:A:703:LYS:HB2	1:A:714:THR:HB	1.95	0.48
1:A:380:GLN:HG3	1:A:860:ASP:HB3	1.95	0.48
1:A:667:ALA:HB1	1:A:742:VAL:HG21	1.95	0.48
1:B:206:ARG:HH22	1:B:235:THR:HG22	1.78	0.48
1:A:199:TRP:HZ3	1:A:259:LEU:HD12	1.78	0.47
1:B:16:VAL:HG22	1:B:172:CYS:HB2	1.97	0.47
1:B:690:THR:HG23	1:B:691:THR:HG23	1.95	0.47
1:A:736:PHE:CD1	1:A:754:ILE:CG2	2.98	0.46
1:A:785:LEU:HD12	1:A:787:ASP:H	1.80	0.46
1:A:841:GLY:HA2	1:A:845:PRO:HB3	1.96	0.46
1:B:706:LEU:HD13	1:B:709:VAL:HG13	1.97	0.46
1:A:29:ILE:HD11	1:A:65:LYS:HD3	1.98	0.46
1:A:692:PHE:HD1	1:A:732:MET:HE1	1.81	0.46
1:B:41:THR:HG22	1:B:109:VAL:HB	1.98	0.46
1:A:32:LEU:HD22	1:A:130:ARG:HD3	1.98	0.46
1:B:199:TRP:HZ3	1:B:259:LEU:HD12	1.81	0.46
1:A:733:THR:CA	1:A:736:PHE:HE2	2.10	0.46
1:B:174:VAL:HG11	1:B:236:VAL:HG21	1.97	0.46
1:A:32:LEU:CD2	1:A:130:ARG:HH11	2.29	0.45
1:B:823:GLY:HA2	1:B:827:PRO:HB3	1.97	0.45
1:A:154:THR:HG22	1:A:156:LEU:H	1.82	0.45
1:A:838:SER:O	1:A:838:SER:OG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:HG21	1:B:233:VAL:HG12	1.99	0.45
1:B:224:ASP:OD2	1:B:224:ASP:N	2.47	0.45
1:B:45:MET:O	1:B:48:THR:OG1	2.31	0.45
1:A:860:ASP:N	1:A:860:ASP:OD1	2.46	0.44
1:A:234:LYS:HA	1:A:237:LEU:HB3	1.99	0.44
1:A:747:LYS:HG2	1:A:748:GLY:N	2.32	0.44
1:A:736:PHE:CE1	1:A:757:ILE:HG12	2.52	0.44
1:B:797:HIS:HB3	1:B:822:THR:HA	1.99	0.44
1:A:369:CYS:SG	1:A:370:TYR:N	2.90	0.44
1:A:394:PRO:HA	1:A:826:GLY:HA2	2.00	0.44
1:B:687:GLU:HG2	1:B:694:THR:HB	1.98	0.44
1:A:729:MET:O	1:A:736:PHE:CZ	2.71	0.43
1:B:6:VAL:HG11	1:B:240:VAL:HG12	2.00	0.43
1:A:736:PHE:HD1	1:A:754:ILE:HG21	1.81	0.43
1:A:737:LEU:CD1	1:A:816:ARG:CB	2.95	0.43
1:B:177:LEU:HB3	1:B:185:PHE:HE1	1.84	0.43
1:A:672:THR:HG23	1:A:718:ARG:HH21	1.84	0.43
1:A:737:LEU:HD12	1:A:816:ARG:CB	2.49	0.43
1:A:224:ASP:OD2	1:A:224:ASP:N	2.51	0.43
1:A:288:MET:HE3	1:A:313:LEU:HD11	2.01	0.43
1:B:786:ILE:HG21	1:B:815:LEU:H	1.84	0.42
1:A:736:PHE:CE1	1:A:757:ILE:CG1	3.01	0.42
1:B:784:PRO:HG3	1:B:814:VAL:HG22	2.02	0.42
1:A:737:LEU:CD1	1:A:816:ARG:HB2	2.49	0.42
1:A:272:ALA:HB3	1:A:346:LYS:HD3	2.02	0.42
1:B:234:LYS:HA	1:B:237:LEU:HB3	2.02	0.42
1:A:62:LEU:HD12	1:A:62:LEU:HA	1.80	0.42
1:A:810:SER:HB3	1:A:835:LEU:HD12	2.00	0.42
1:A:379:LYS:HB2	1:A:379:LYS:HE3	1.95	0.42
1:A:194:LYS:HE2	1:A:194:LYS:HB3	1.88	0.41
1:A:724:LEU:HA	1:A:725:PRO:HD3	1.90	0.41
1:A:84:ASN:OD1	1:A:84:ASN:N	2.53	0.41
1:A:851:LEU:HA	1:A:855:PHE:HB2	2.02	0.41
1:B:43:THR:HB	1:B:78:PRO:HG3	2.01	0.41
1:B:301:LEU:HD13	1:B:363:LEU:HB3	2.01	0.41
1:A:800:LYS:HE2	1:A:830:GLU:HB3	2.03	0.41
1:B:366:ILE:HD13	1:B:366:ILE:HA	1.94	0.41
1:B:289:ILE:HD12	1:B:289:ILE:HA	1.86	0.41
1:B:714:MET:HB3	1:B:717:ALA:HB3	2.03	0.41
1:B:739:ILE:HG22	1:B:742:GLN:HB2	2.03	0.41
1:A:294:LEU:HD21	1:A:377:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:THR:CA	1:A:736:PHE:CE2	2.90	0.41
1:B:274:LEU:HD13	1:B:331:VAL:HG21	2.02	0.41
1:B:776:ILE:HD12	1:B:776:ILE:HA	1.94	0.40
1:A:747:LYS:HG2	1:A:748:GLY:H	1.87	0.40
1:B:648:LEU:HD22	1:B:695:VAL:HG13	2.04	0.40
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.89	0.40
1:A:391:LEU:HG	1:A:831:PRO:HB2	2.02	0.40
1:A:763:LYS:HE3	1:A:763:LYS:HB3	1.92	0.40
1:B:318:LEU:HA	1:B:319:PRO:HD3	1.93	0.40
1:A:173:ASP:OD1	1:A:175:SER:OG	2.38	0.40
1:A:737:LEU:HD13	1:A:816:ARG:HB2	2.04	0.40
1:A:767:ARG:O	1:A:771:MET:HG2	2.22	0.40
1:B:334:LYS:HE3	1:B:334:LYS:HB3	1.93	0.40
1:B:403:ILE:HD11	1:B:661:PRO:HG3	2.02	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	582/1551 (38%)	550 (94%)	32 (6%)	0	100	100
1	B	590/1551 (38%)	547 (93%)	43 (7%)	0	100	100
All	All	1172/3102 (38%)	1097 (94%)	75 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	506/1311 (39%)	506 (100%)	0	100	100
1	B	510/1311 (39%)	510 (100%)	0	100	100
All	All	1016/2622 (39%)	1016 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	706	GLN
1	B	82	ASN
1	B	376	GLN
1	B	669	GLN
1	B	742	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 monosaccharides 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 ⓘ

There are no chain breaks in this entry.

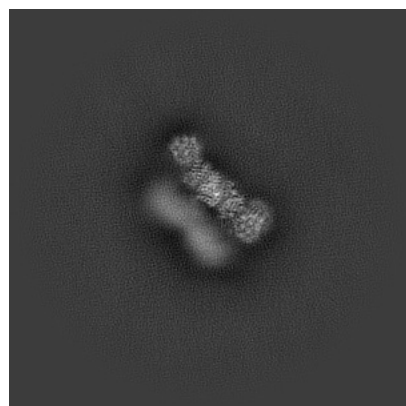
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26358. These allow visual inspection of the internal detail of the map and identification of artifacts.

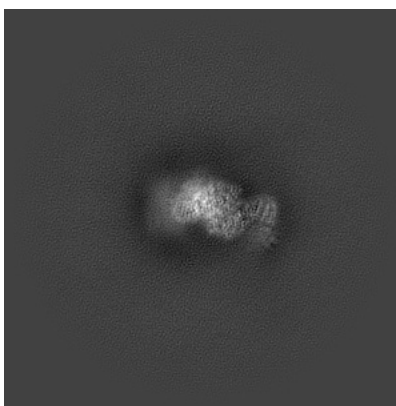
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

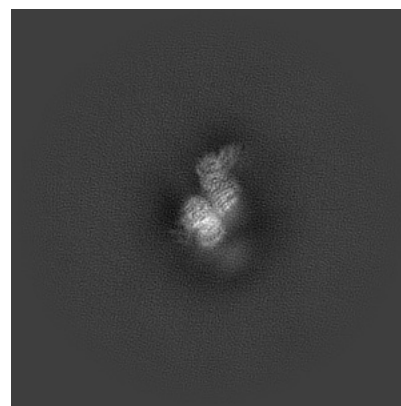
6.1.1 Primary map



X

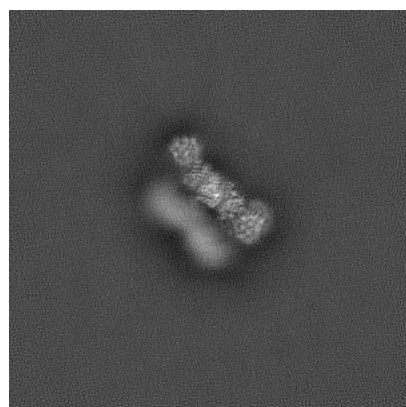


Y

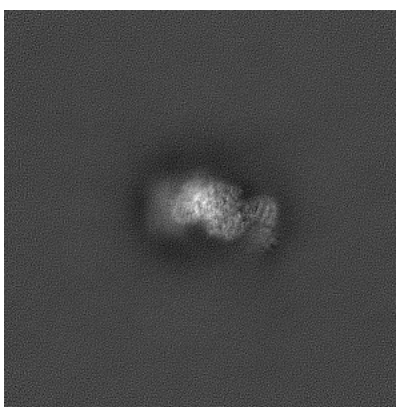


Z

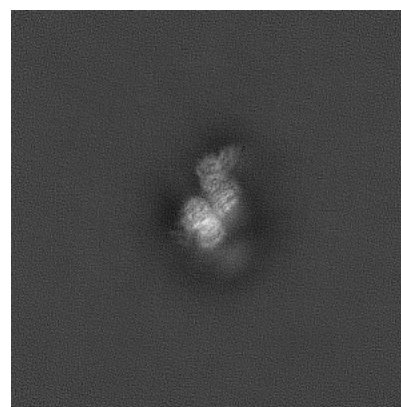
6.1.2 Raw map



X



Y

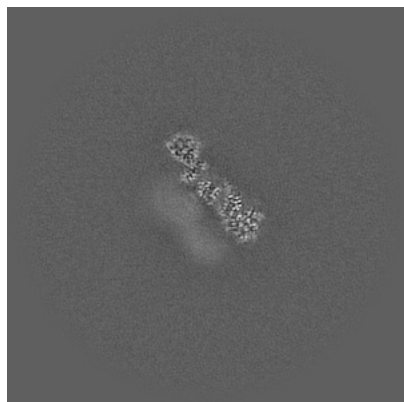


Z

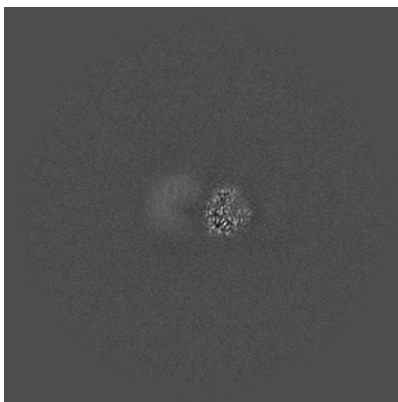
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

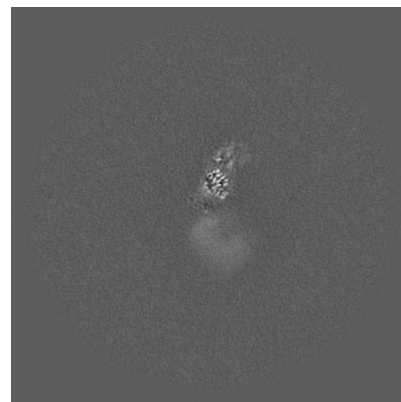
6.2.1 Primary map



X Index: 200

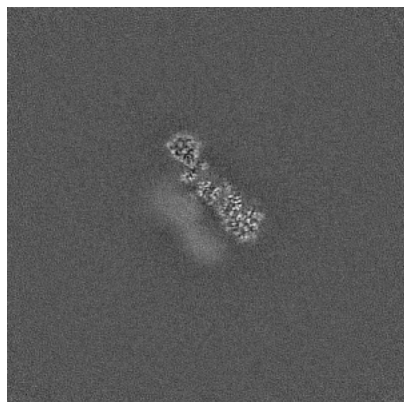


Y Index: 200

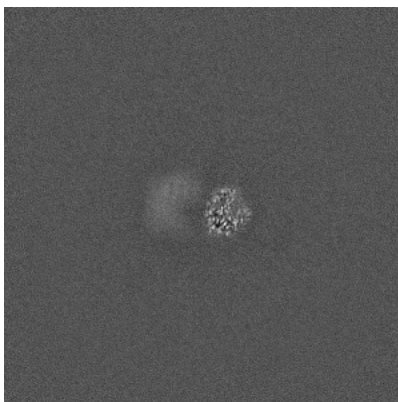


Z Index: 200

6.2.2 Raw map



X Index: 200



Y Index: 200

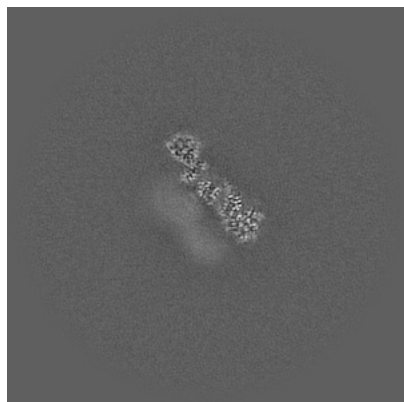


Z Index: 200

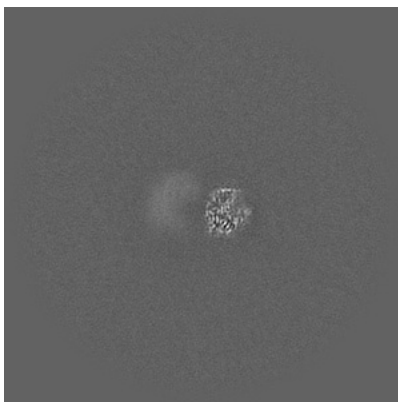
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

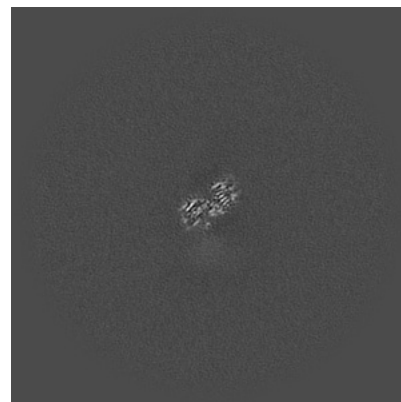
6.3.1 Primary map



X Index: 200

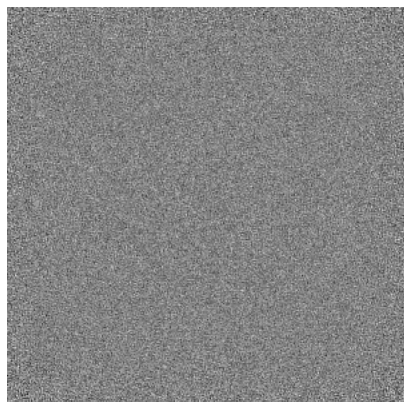


Y Index: 201

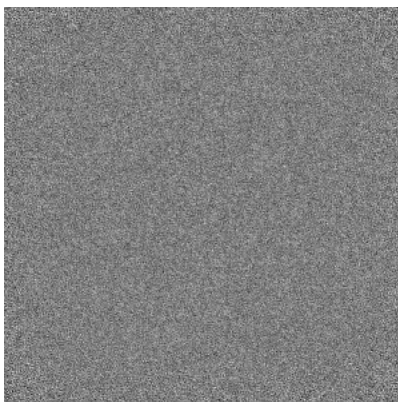


Z Index: 223

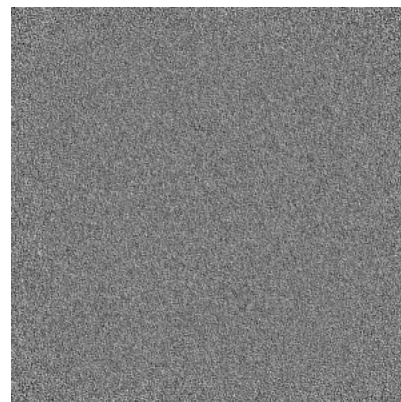
6.3.2 Raw map



X Index: 0



Y Index: 0

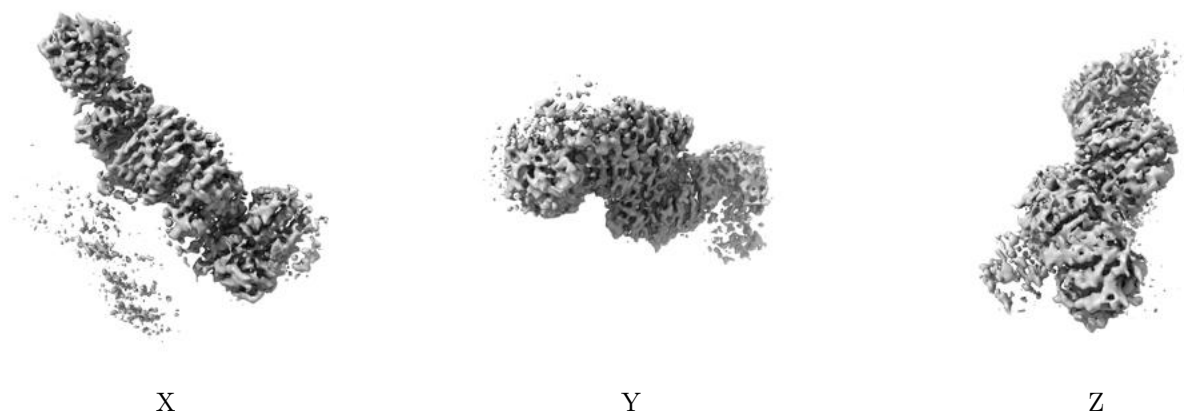


Z Index: 0

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

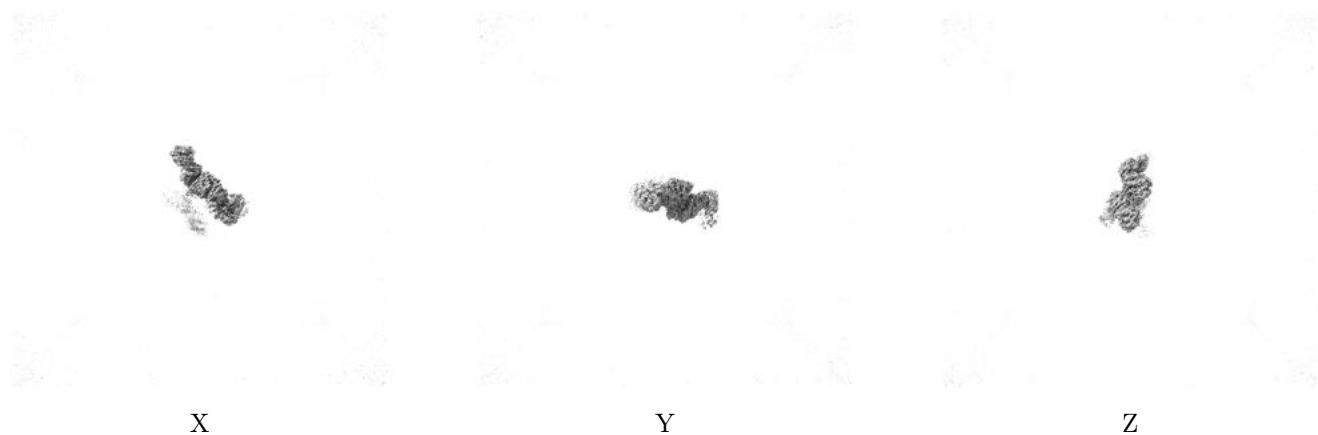
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.211. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

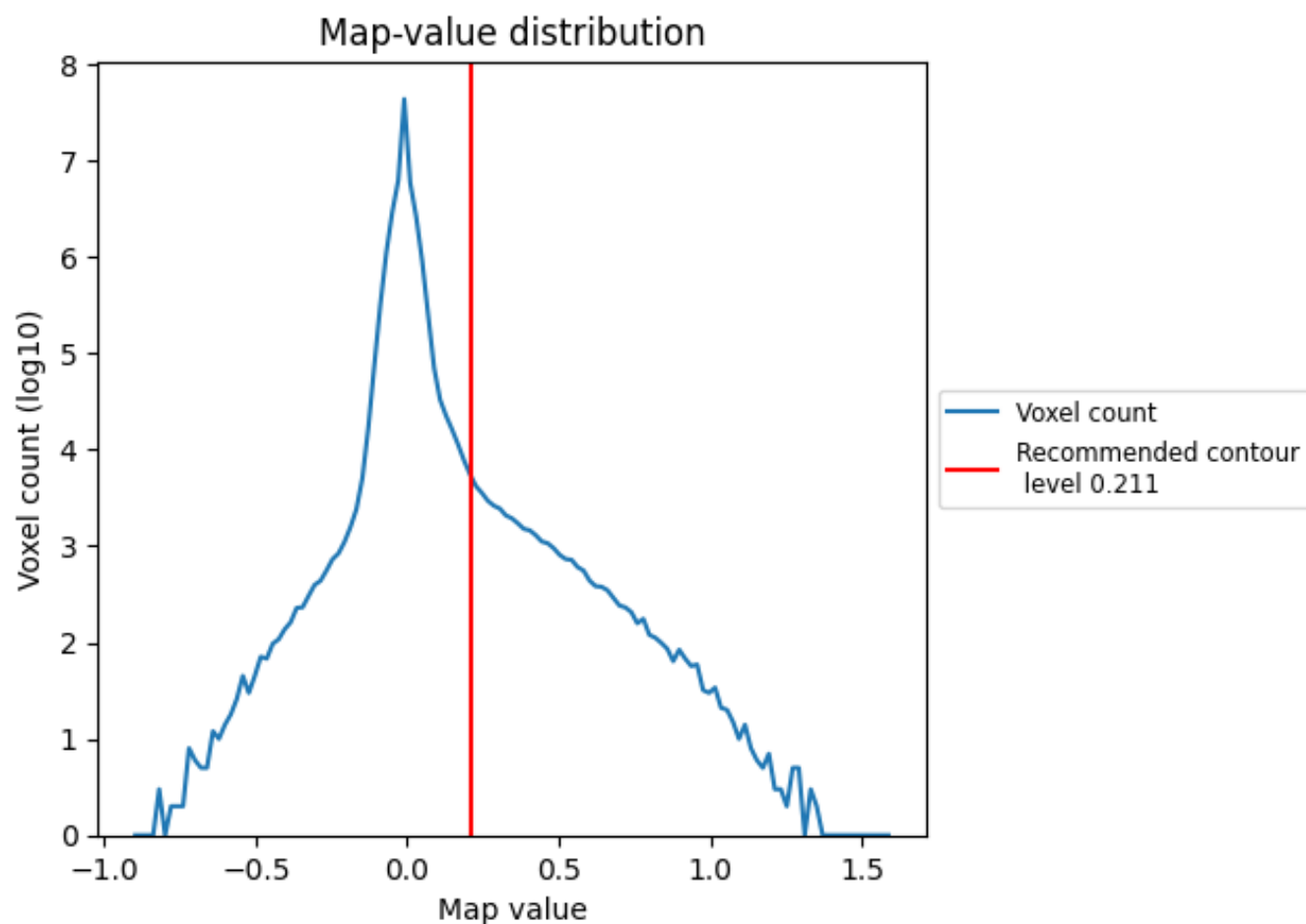
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

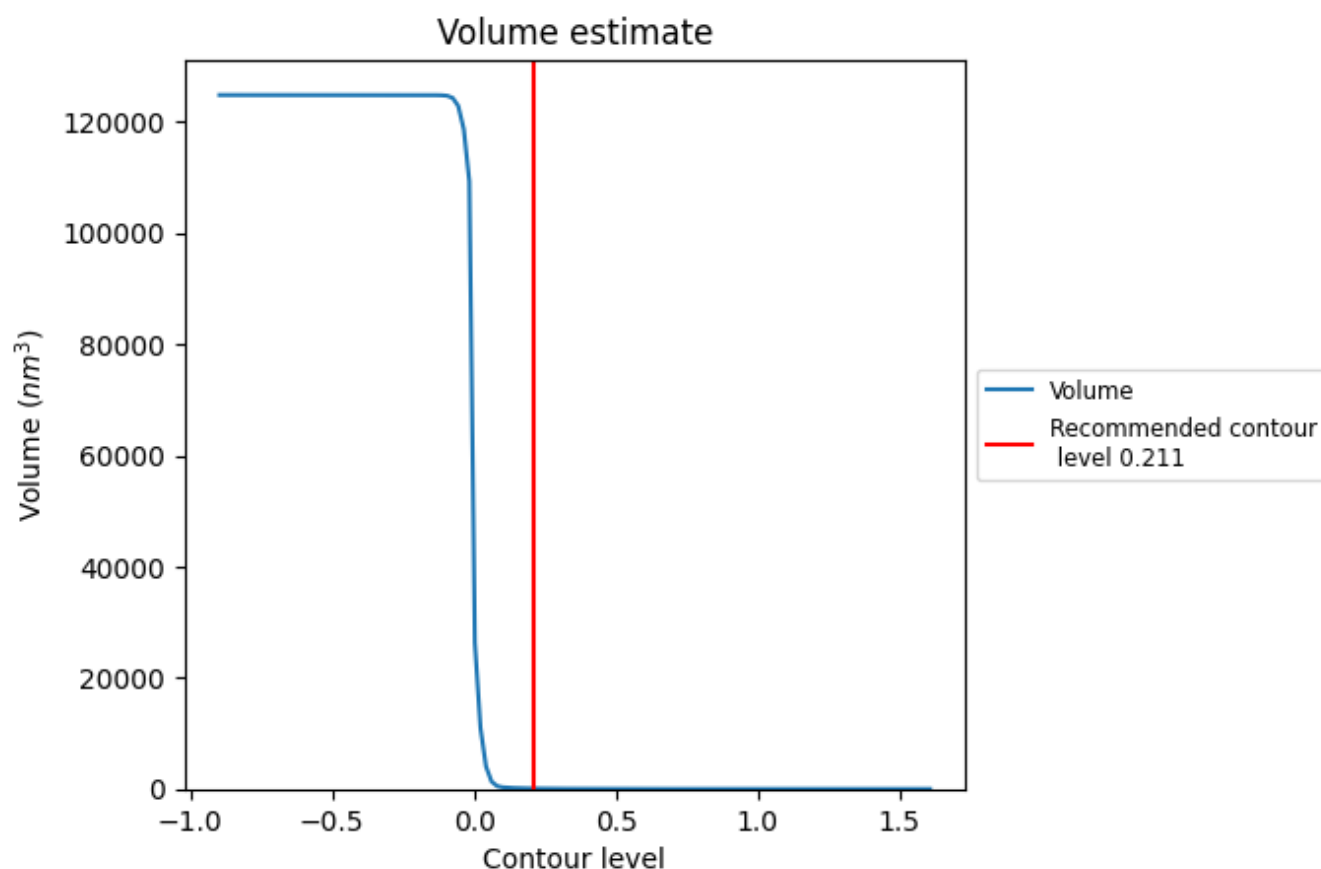
This section contains the results of statistical analysis of the map.

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.

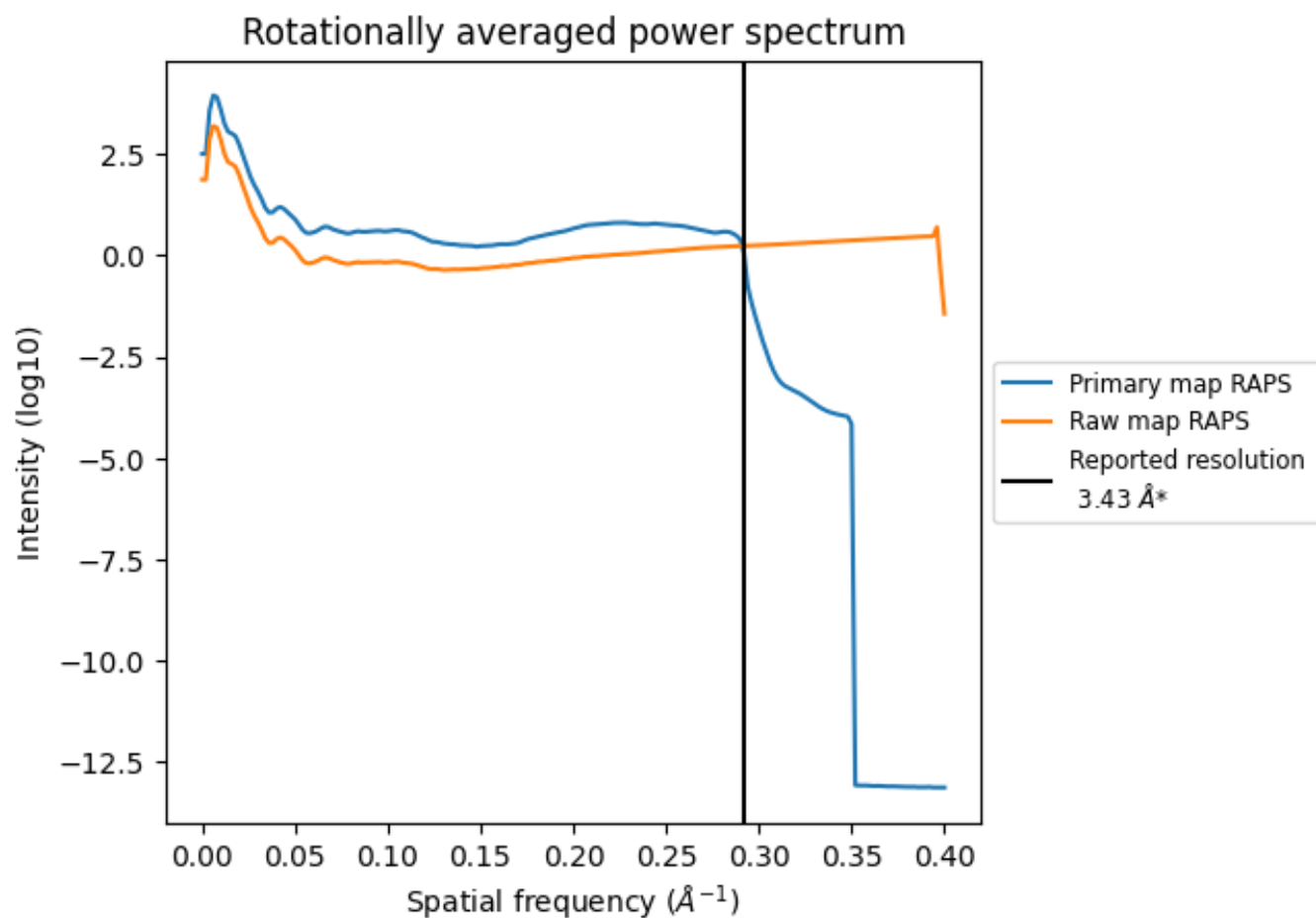
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm^3 ; this corresponds to an approximate mass of 72 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 ⓘ

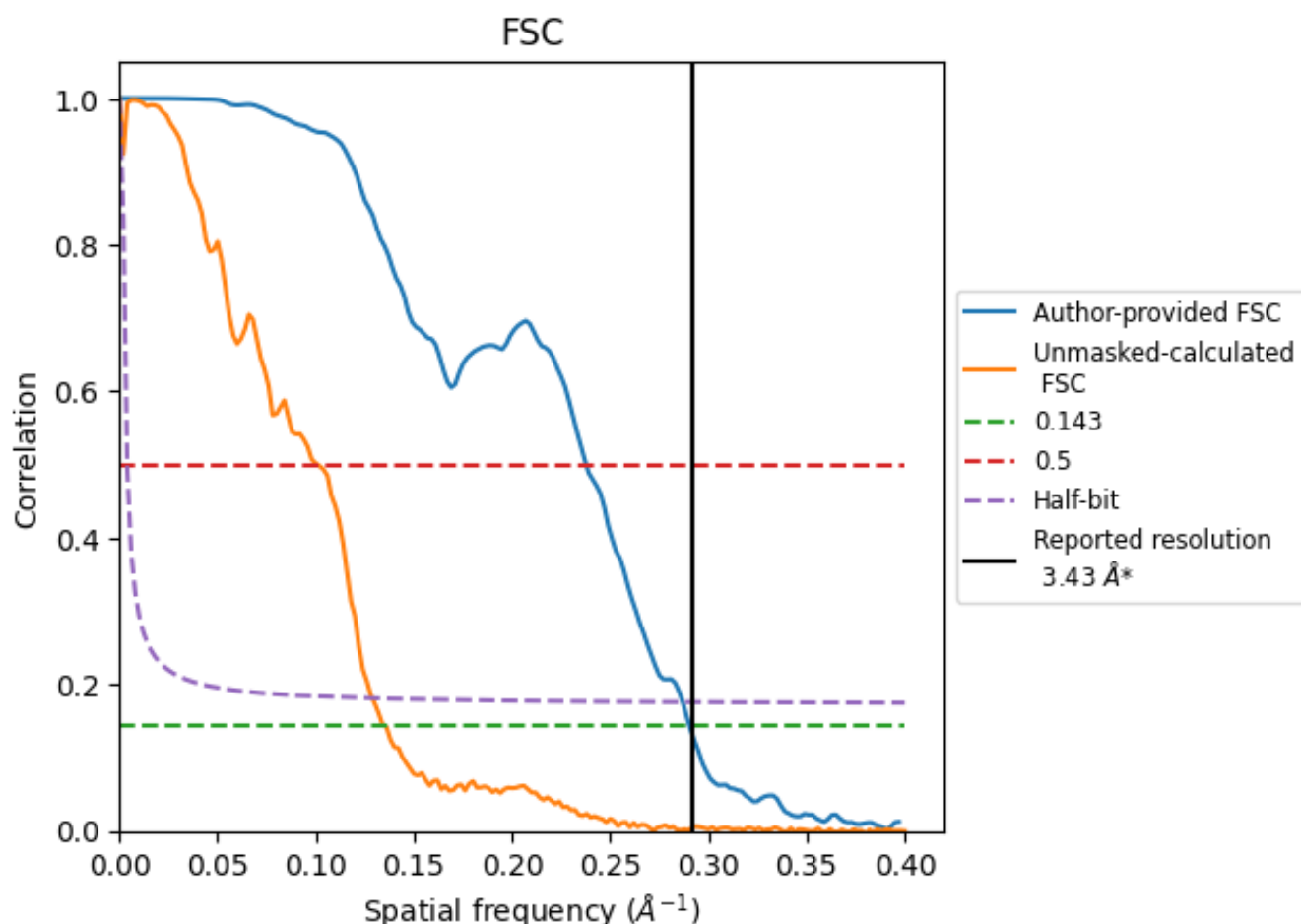


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

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 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

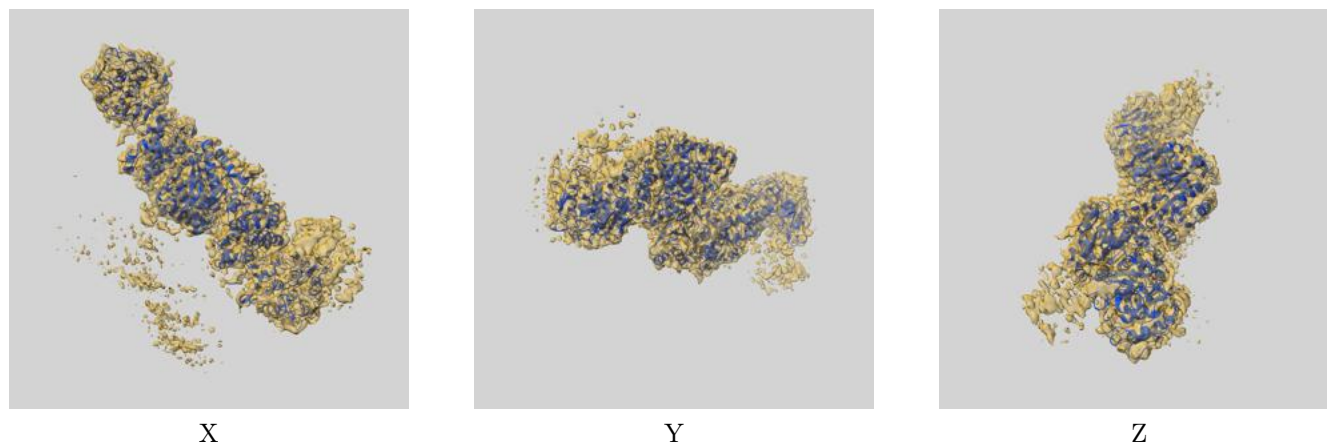
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	3.44	4.21	3.48
Unmasked-calculated*	7.40	9.91	7.76

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

9 Map-model fit [i](#)

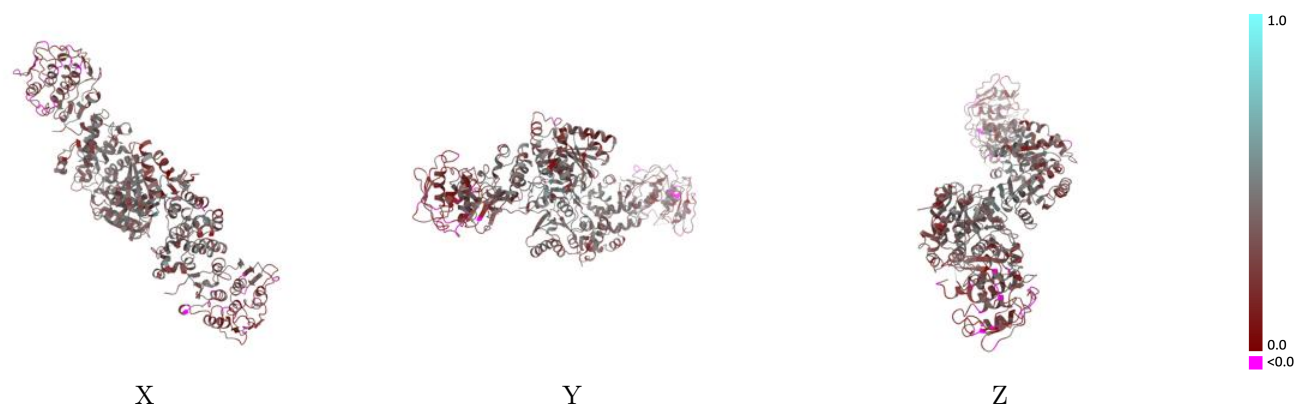
This section contains information regarding the fit between EMDB map EMD-26358 and PDB model 7U5T. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



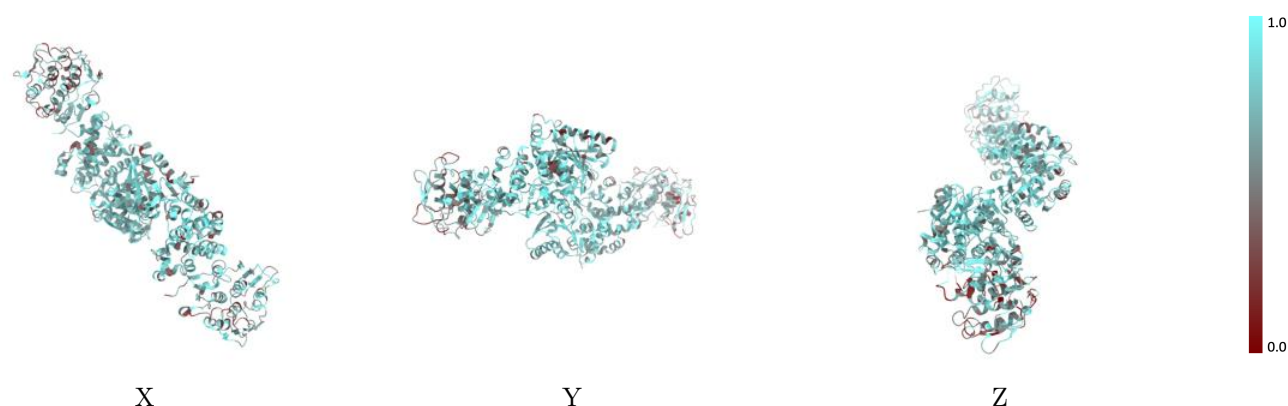
The images above show the 3D surface view of the map at the recommended contour level 0.211 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



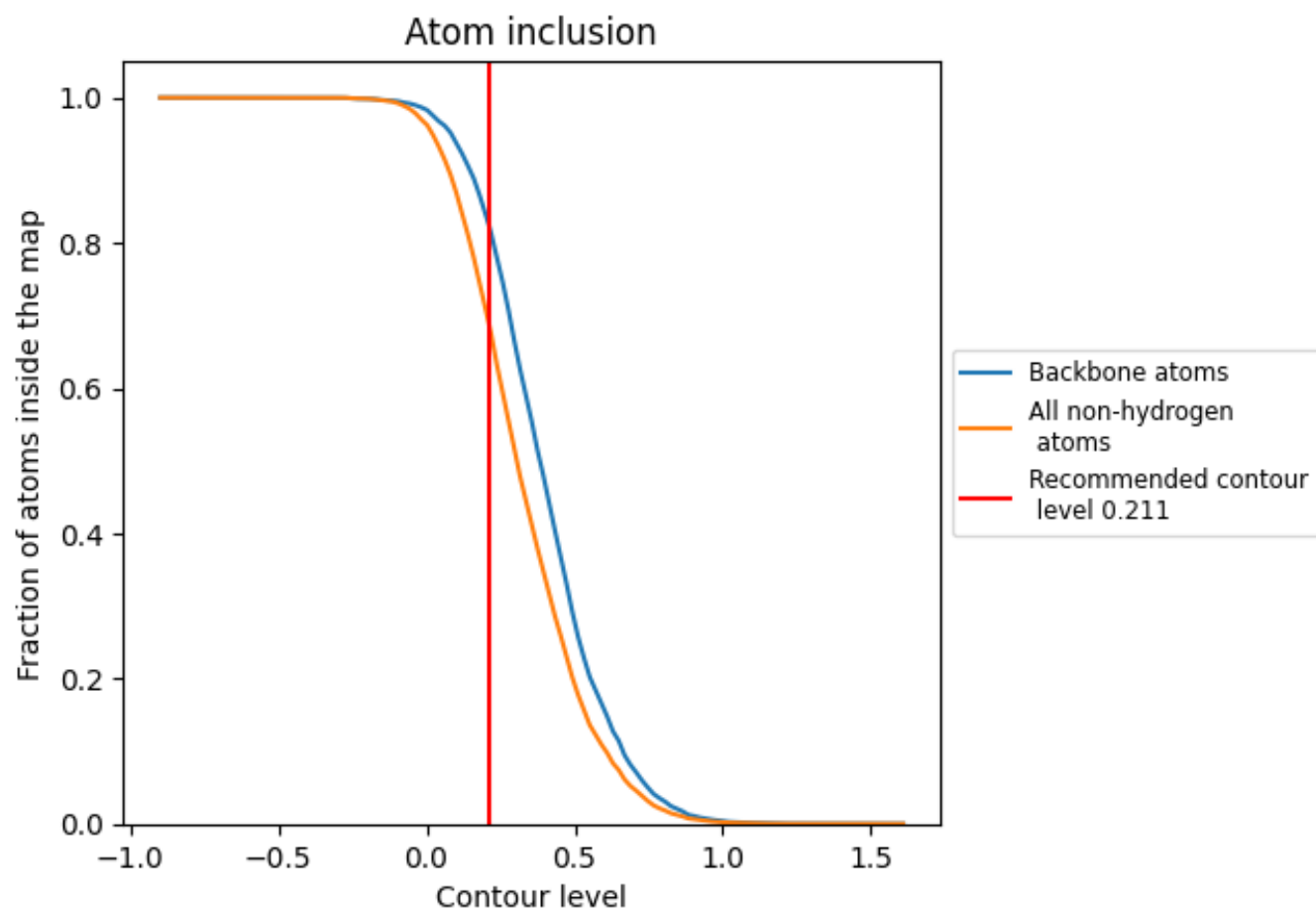
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.211).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.211) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6902	<div></div> 0.3330
A	<div></div> 0.6802	<div></div> 0.3360
B	<div></div> 0.7000	<div></div> 0.3310

