



Full wwPDB EM Validation Report ⓘ

Feb 20, 2024 – 04:49 PM JST

PDB ID : 8IJ5
EMDB ID : EMD-35465
Title : Cryo-EM structure of Integrin AVB3
Authors : Xi, Z.; Cang, W.; Yuanzhu, G.
Deposited on : 2023-02-26
Resolution : 3.00 Å (reported)

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

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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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

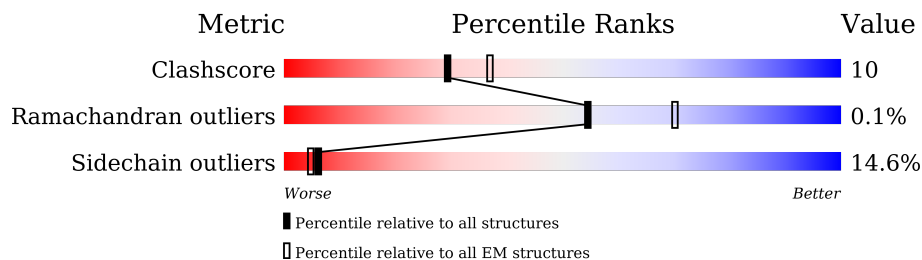
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	B	467	
2	E	593	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6815 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 Integrin beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	358	2804	1769	472	546	17	0	0

- Molecule 2 is a protein called Integrin alpha-V heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	520	4011	2545	672	775	19	0	0

ASN
GLN
ASP
ASN
ASN
LYS
THR
CYS
SER
LEU
PRO
GLY
THR
ALA
LEU
LYS
VAL
SER
C502
F503
R506
F507
C508
L509
K510
R511
D512
L517
P518
R519
Q524
V525
E526
L527
L528
LEU
ASP
LYS
LEU
LYS
GLN
LYS
GLY
ALA
ILE
ARG
ALA
LEU
PHE
LEU
TYR
SER
ARG
SER
PRO
SER
HIS

SER
LYS
ASN
MET
T556
I557
S558
L562
M563
Q564
C565
L568
I569
ALA
TYR
LEU
LEU
ARG
ASP
GLU
SER
GLU
PHE
ARG
ASP
LYS
LEU
THR
PRO
I585
E590
Y591
R592
T601
T602
N615
I616
SER
ARG
GLN
ALA
HIS
ILE
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69506	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.784	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	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	B	0.26	0/2852	0.53	0/3861
2	E	0.27	0/4100	0.52	0/5548
All	All	0.27	0/6952	0.52	0/9409

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	B	2804	0	2792	65	0
2	E	4011	0	3838	73	0
All	All	6815	0	6630	137	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 (137) 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)
2:E:508:CYS:HA	2:E:565:CYS:HB3	1.54	0.90
1:B:126:PHE:HB2	1:B:425:ILE:HB	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ILE:HG22	1:B:378:ARG:HD3	1.71	0.72
1:B:332:LEU:HB3	1:B:354:THR:HG22	1.74	0.70
1:B:142:TYR:HE1	1:B:144:MET:HG3	1.58	0.69
2:E:255:SER:HB2	2:E:310:VAL:HG22	1.74	0.68
1:B:191:MET:O	1:B:242:ARG:NH2	2.26	0.67
2:E:39:ALA:HB3	2:E:464:LEU:HB3	1.76	0.67
1:B:132:GLN:HB2	1:B:418:GLY:HA2	1.76	0.66
1:B:139:ASP:N	1:B:139:ASP:OD1	2.30	0.64
1:B:254:GLN:HE22	1:B:299:CYS:HA	1.62	0.63
2:E:334:GLY:N	2:E:338:LYS:O	2.23	0.61
1:B:361:MET:SD	1:B:361:MET:N	2.69	0.61
2:E:323:VAL:HG12	2:E:348:SER:HB2	1.84	0.60
2:E:168:GLU:OE2	2:E:173:ARG:NH2	2.34	0.60
1:B:241:ASN:ND2	1:B:243:ASP:O	2.35	0.60
2:E:502:CYS:HB3	2:E:569:ILE:HD11	1.84	0.59
1:B:194:SER:HB2	1:B:195:PRO:HD3	1.85	0.59
2:E:57:VAL:HG12	2:E:64:MET:HG2	1.84	0.59
1:B:404:GLU:HG2	1:B:406:ILE:HG12	1.84	0.58
2:E:171:PRO:HB2	2:E:214:ILE:HD13	1.86	0.57
1:B:253:MET:O	1:B:257:VAL:HG22	2.06	0.56
2:E:145:ARG:NH1	2:E:149:LYS:O	2.38	0.56
2:E:524:GLN:HB3	2:E:592:ARG:HG3	1.87	0.55
2:E:190:SER:HB2	2:E:256:VAL:HG22	1.89	0.55
2:E:106:GLY:O	2:E:119:LYS:NZ	2.40	0.55
2:E:117:GLU:HA	2:E:144:TRP:HA	1.88	0.54
2:E:279:THR:HG23	2:E:303:ALA:H	1.71	0.54
2:E:369:ARG:HG3	2:E:394:TYR:HD2	1.73	0.53
2:E:211:GLY:HA3	2:E:252:LEU:HB3	1.90	0.53
2:E:98:GLN:OE1	2:E:98:GLN:N	2.40	0.53
1:B:388:LEU:HD12	1:B:389:PRO:HD2	1.89	0.53
1:B:144:MET:HA	1:B:275:THR:HG23	1.91	0.53
2:E:116:LEU:O	2:E:145:ARG:N	2.32	0.53
2:E:270:VAL:HG13	2:E:285:ILE:HG12	1.89	0.53
2:E:400:LYS:HA	2:E:432:PRO:HG2	1.92	0.52
1:B:113:ARG:HH11	1:B:454:GLN:HE21	1.58	0.52
2:E:34:ASP:OD2	2:E:35:VAL:N	2.43	0.52
2:E:313:THR:OG1	2:E:314:ASP:N	2.42	0.52
2:E:454:VAL:HB	2:E:463:ILE:HG22	1.91	0.52
1:B:108:GLN:HG3	1:B:449:ASP:OD2	2.10	0.52
1:B:109:VAL:O	1:B:112:GLN:NE2	2.35	0.51
2:E:377:LEU:HD11	2:E:389:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:VAL:HG23	1:B:299:CYS:HB2	1.93	0.51
1:B:145:ASP:HB2	1:B:182:PHE:CZ	2.46	0.50
1:B:164:LEU:HD23	1:B:177:ILE:HD12	1.93	0.50
1:B:349:GLU:O	1:B:350:LEU:HD23	2.11	0.50
1:B:187:VAL:HG22	1:B:188:SER:H	1.75	0.50
1:B:267:ASP:N	1:B:267:ASP:OD1	2.44	0.50
2:E:207:PHE:HB3	2:E:242:THR:HG23	1.94	0.50
1:B:282:ILE:HD13	2:E:275:ARG:HH11	1.76	0.50
2:E:331:MET:HA	2:E:341:GLU:HA	1.94	0.50
2:E:314:ASP:O	2:E:386:ASN:HB2	2.12	0.50
1:B:119:ARG:HG3	1:B:120:PRO:HD2	1.93	0.50
2:E:154:PRO:HD2	2:E:184:PHE:CD1	2.46	0.50
1:B:88:ARG:HB2	1:B:115:ALA:HB3	1.95	0.49
1:B:128:ILE:HG22	1:B:423:PHE:H	1.76	0.49
2:E:33:LEU:HD12	2:E:405:ILE:HD11	1.95	0.49
1:B:271:LEU:HD21	1:B:374:TYR:HD1	1.77	0.49
1:B:114:ILE:HG22	1:B:453:VAL:HA	1.94	0.49
2:E:56:PHE:HB2	2:E:67:LEU:HG	1.94	0.49
2:E:210:GLN:HG2	2:E:247:PHE:O	2.13	0.49
2:E:407:ASN:OD1	2:E:407:ASN:N	2.41	0.49
2:E:345:VAL:HG21	2:E:390:ILE:HD13	1.95	0.48
2:E:377:LEU:HD13	2:E:380:LEU:HD22	1.95	0.48
2:E:87:LEU:HA	2:E:99:PRO:HA	1.94	0.48
2:E:278:ARG:O	2:E:279:THR:HG22	2.14	0.48
2:E:198:ARG:HH11	2:E:217:GLN:HG3	1.78	0.48
1:B:91:GLU:HG3	1:B:112:GLN:HB2	1.95	0.48
1:B:185:LYS:NZ	1:B:313:MET:O	2.47	0.48
2:E:348:SER:HB3	2:E:356:PHE:HD2	1.78	0.47
1:B:165:ALA:HB2	1:B:226:VAL:HG11	1.96	0.47
2:E:262:ASN:HB3	2:E:294:LEU:HD21	1.97	0.47
1:B:228:ARG:HA	1:B:231:GLU:HG2	1.97	0.47
2:E:381:ASP:OD1	2:E:381:ASP:N	2.44	0.47
1:B:90:LEU:HD22	1:B:113:ARG:HB3	1.96	0.47
2:E:466:ARG:NH2	2:E:602:THR:OG1	2.46	0.47
1:B:146:LEU:HB3	1:B:238:VAL:HG12	1.97	0.46
1:B:153:ASP:N	1:B:153:ASP:OD1	2.48	0.46
1:B:142:TYR:CE1	1:B:144:MET:HG3	2.45	0.46
1:B:125:ASN:OD1	1:B:125:ASN:N	2.48	0.46
1:B:443:LYS:HB3	1:B:450:SER:HB3	1.98	0.46
2:E:54:ASP:HA	2:E:439:LYS:HG2	1.98	0.46
1:B:131:ARG:HH11	1:B:131:ARG:HG2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:510:LYS:HD3	2:E:563:MET:SD	2.56	0.45
2:E:103:ASP:OD1	2:E:104:ALA:N	2.49	0.45
2:E:365:GLU:OE1	2:E:396:GLY:N	2.47	0.45
1:B:164:LEU:O	1:B:168:MET:HB2	2.16	0.45
2:E:136:LEU:HD13	2:E:160:LEU:HD12	1.98	0.45
1:B:110:SER:HB3	1:B:111:PRO:HD3	1.99	0.45
2:E:324:PHE:CE1	2:E:347:VAL:HG22	2.52	0.45
1:B:221:THR:O	1:B:223:THR:HG23	2.17	0.45
2:E:142:TYR:O	2:E:154:PRO:HA	2.17	0.44
1:B:224:ASP:OD2	1:B:224:ASP:N	2.36	0.44
1:B:244:ALA:HB3	1:B:245:PRO:HD3	2.00	0.44
1:B:384:GLU:CD	1:B:386:ARG:HH12	2.20	0.44
2:E:122:GLN:HA	2:E:141:LEU:O	2.16	0.44
2:E:143:HIS:NE2	2:E:154:PRO:HG3	2.32	0.44
2:E:459:VAL:O	2:E:461:ARG:HD3	2.17	0.44
1:B:121:ASP:OD1	1:B:431:GLY:N	2.51	0.44
2:E:519:ARG:H	2:E:519:ARG:HD2	1.83	0.44
2:E:41:TYR:HB2	2:E:462:ALA:HB3	1.99	0.44
1:B:401:LEU:HB3	1:B:402:ASN:H	1.59	0.44
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.33	0.43
1:B:160:LEU:HD23	1:B:229:PHE:HE2	1.83	0.43
1:B:159:ASN:N	1:B:159:ASN:OD1	2.52	0.43
1:B:113:ARG:HD3	1:B:454:GLN:HE21	1.83	0.43
2:E:44:PRO:HB2	2:E:47:SER:HB3	2.01	0.43
1:B:155:TRP:HA	1:B:158:GLN:HG2	2.01	0.42
1:B:396:PHE:CE2	1:B:425:ILE:HG12	2.54	0.42
1:B:254:GLN:O	1:B:258:CYS:HB2	2.19	0.42
1:B:116:LEU:HG	1:B:126:PHE:CE2	2.55	0.42
2:E:117:GLU:H	2:E:117:GLU:HG2	1.70	0.42
1:B:116:LEU:N	1:B:454:GLN:O	2.53	0.42
1:B:415:LEU:HD22	1:B:419:ASP:HB2	2.01	0.41
2:E:45:GLU:OE2	2:E:45:GLU:HA	2.20	0.41
2:E:194:THR:HG23	2:E:267:ASP:HB2	2.02	0.41
2:E:206:SER:HB2	2:E:212:GLN:HB2	2.02	0.41
1:B:142:TYR:CE1	1:B:275:THR:HG21	2.55	0.41
2:E:429:SER:OG	2:E:430:MET:N	2.53	0.41
2:E:286:TYR:HB3	2:E:291:MET:HG3	2.02	0.41
2:E:32:ASN:ND2	2:E:381:ASP:HB3	2.35	0.41
2:E:508:CYS:HB3	2:E:563:MET:HG3	2.02	0.41
2:E:270:VAL:HG22	2:E:285:ILE:HG23	2.02	0.41
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:GLY:HA2	2:E:209:TRP:HA	2.03	0.41
1:B:90:LEU:O	1:B:90:LEU:HD23	2.20	0.40
1:B:136:TYR:O	1:B:172:THR:OG1	2.36	0.40
2:E:178:ASP:OD2	2:E:178:ASP:N	2.53	0.40
2:E:76:THR:O	2:E:76:THR:OG1	2.36	0.40
2:E:139:ALA:HB3	2:E:157:THR:HG22	2.04	0.40
2:E:302:MET:HE2	2:E:302:MET:HB3	1.91	0.40
2:E:383:ASP:OD1	2:E:383:ASP:N	2.46	0.40
2:E:428:ARG:O	2:E:430:MET:N	2.52	0.40
1:B:153:ASP:O	1:B:157:ILE:HG23	2.21	0.40
2:E:427:ALA:HB2	2:E:432:PRO:HD3	2.03	0.40
1:B:146:LEU:HD22	1:B:154:LEU:HD11	2.03	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	B	350/467 (75%)	319 (91%)	31 (9%)	0	100	100
2	E	510/593 (86%)	462 (91%)	47 (9%)	1 (0%)	47	82
All	All	860/1060 (81%)	781 (91%)	78 (9%)	1 (0%)	54	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	148	MET

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	B	320/413 (78%)	269 (84%)	51 (16%)	2	12
2	E	420/486 (86%)	363 (86%)	57 (14%)	3	17
All	All	740/899 (82%)	632 (85%)	108 (15%)	6	15

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88	ARG
1	B	116	LEU
1	B	117	ARG
1	B	121	ASP
1	B	129	GLN
1	B	130	VAL
1	B	131	ARG
1	B	139	ASP
1	B	146	LEU
1	B	151	LYS
1	B	152	ASP
1	B	153	ASP
1	B	159	ASN
1	B	168	MET
1	B	170	LYS
1	B	185	LYS
1	B	227	THR
1	B	233	VAL
1	B	239	SER
1	B	259	ASP
1	B	261	LYS
1	B	273	VAL
1	B	275	THR
1	B	279	LYS
1	B	282	ILE
1	B	287	ARG
1	B	292	VAL

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Mol	Chain	Res	Type
1	B	299	CYS
1	B	303	SER
1	B	304	ASP
1	B	306	HIS
1	B	310	SER
1	B	317	SER
1	B	330	ILE
1	B	337	THR
1	B	338	GLU
1	B	340	VAL
1	B	348	SER
1	B	360	SER
1	B	361	MET
1	B	366	VAL
1	B	372	ASP
1	B	394	LEU
1	B	401	LEU
1	B	402	ASN
1	B	409	LEU
1	B	416	LYS
1	B	423	PHE
1	B	430	ARG
1	B	440	PHE
1	B	458	ASP
2	E	37	SER
2	E	53	VAL
2	E	63	ARG
2	E	90	ASP
2	E	91	TRP
2	E	98	GLN
2	E	118	PHE
2	E	120	SER
2	E	127	SER
2	E	144	TRP
2	E	145	ARG
2	E	147	GLU
2	E	148	MET
2	E	165	LYS
2	E	176	ASP
2	E	226	ASP
2	E	228	ASN
2	E	233	LYS

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Mol	Chain	Res	Type
2	E	248	ASP
2	E	255	SER
2	E	279	THR
2	E	309	SER
2	E	313	THR
2	E	314	ASP
2	E	319	ASP
2	E	323	VAL
2	E	333	ARG
2	E	338	LYS
2	E	348	SER
2	E	351	ARG
2	E	355	ASP
2	E	357	GLN
2	E	358	THR
2	E	366	VAL
2	E	369	ARG
2	E	379	ASP
2	E	397	GLU
2	E	418	SER
2	E	425	TRP
2	E	430	MET
2	E	473	VAL
2	E	502	CYS
2	E	503	PHE
2	E	506	ARG
2	E	510	LYS
2	E	512	ASP
2	E	517	LEU
2	E	519	ARG
2	E	526	GLU
2	E	558	SER
2	E	562	LEU
2	E	564	GLN
2	E	565	CYS
2	E	568	LEU
2	E	590	GLU
2	E	601	THR
2	E	615	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	454	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 [i](#)

There are no chain breaks in this entry.

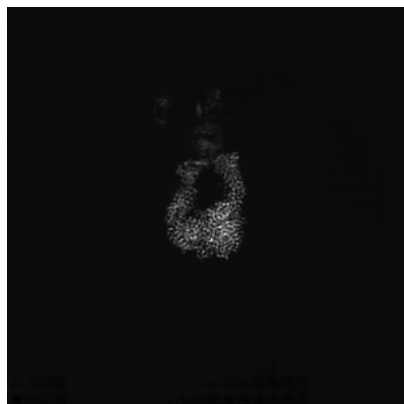
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35465. 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

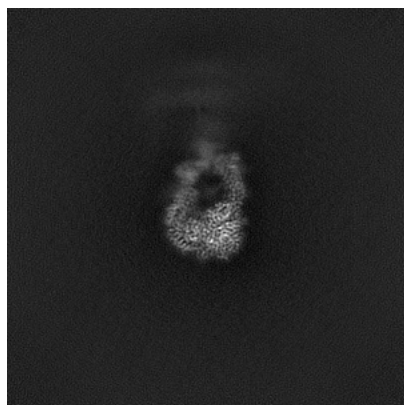


Y

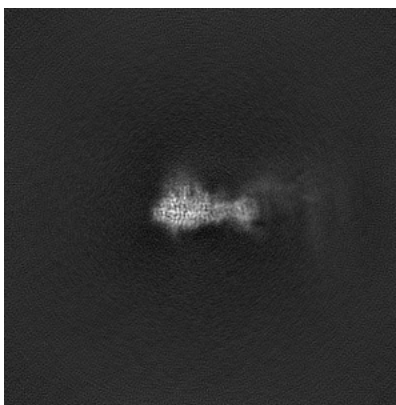


Z

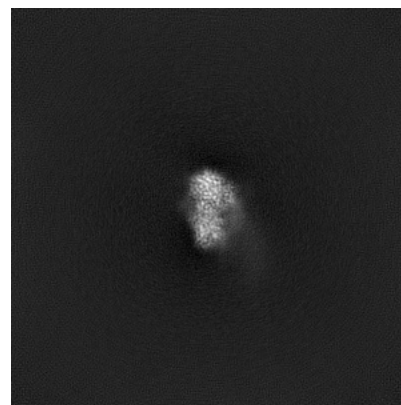
6.1.2 Raw map



X



Y

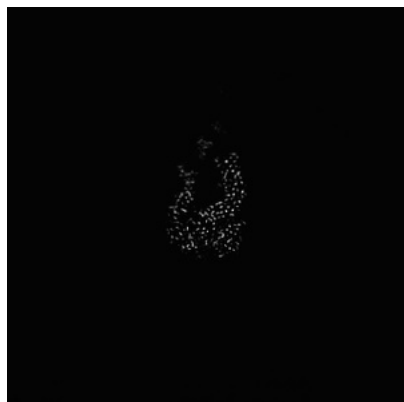


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

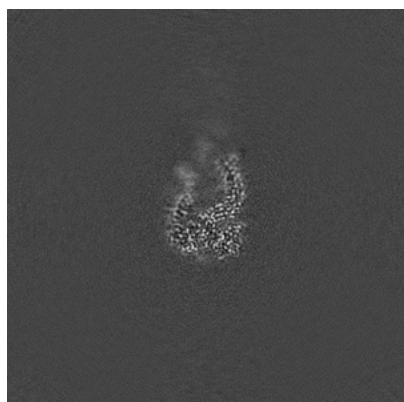


Y Index: 160

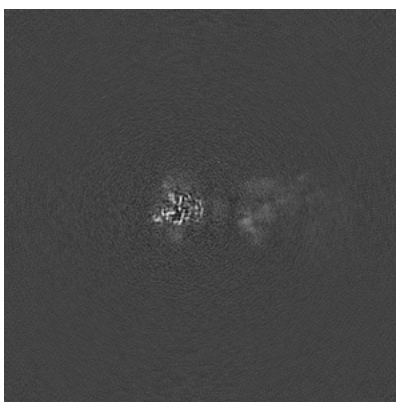


Z Index: 160

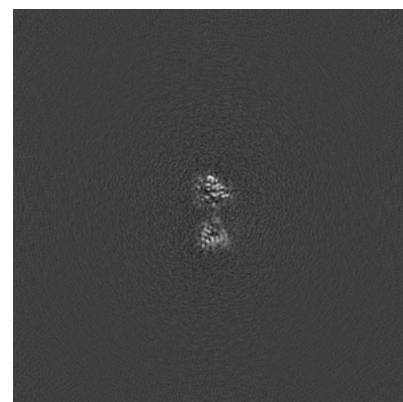
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 156

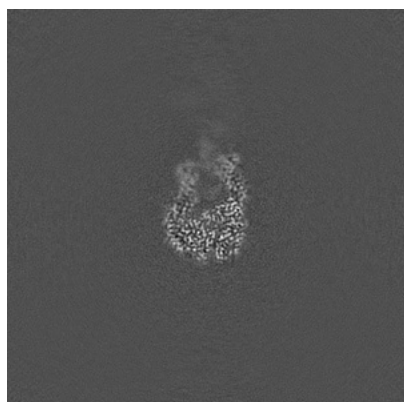


Y Index: 176

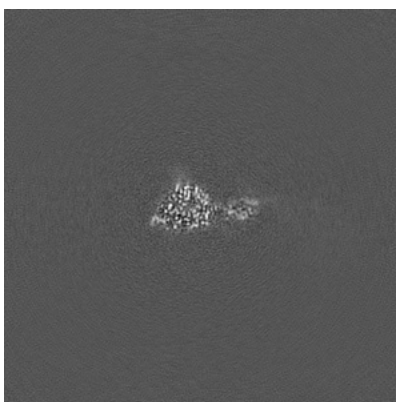


Z Index: 142

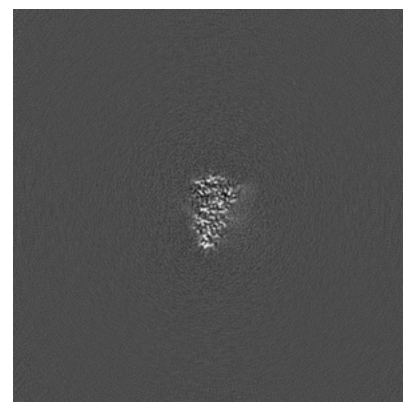
6.3.2 Raw map



X Index: 156



Y Index: 176



Z Index: 142

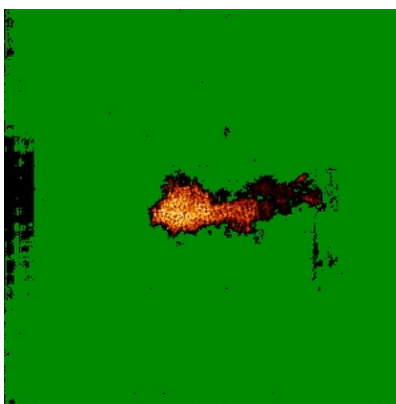
The images above show the largest variance slices of the map in three orthogonal directions.

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

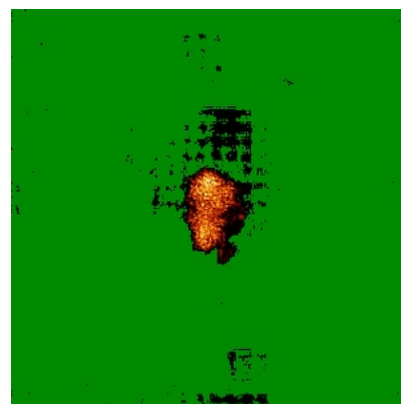
6.4.1 Primary map



X

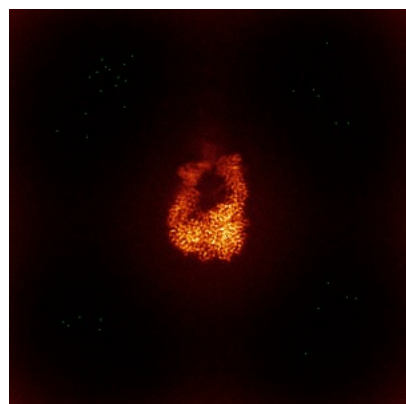


Y

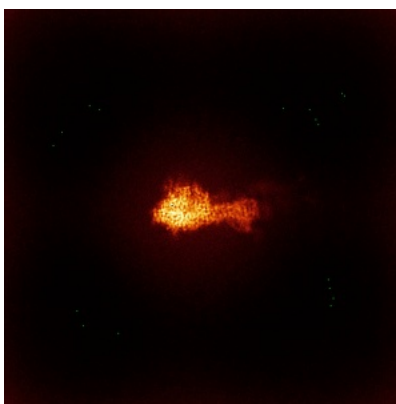


Z

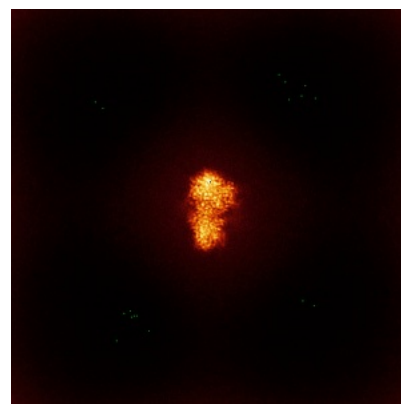
6.4.2 Raw map



X



Y

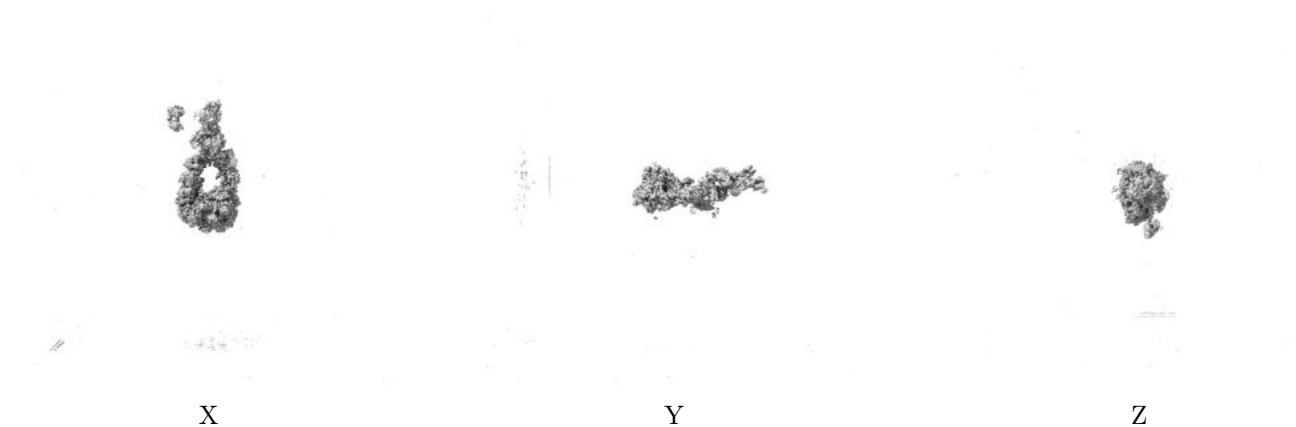


Z

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.

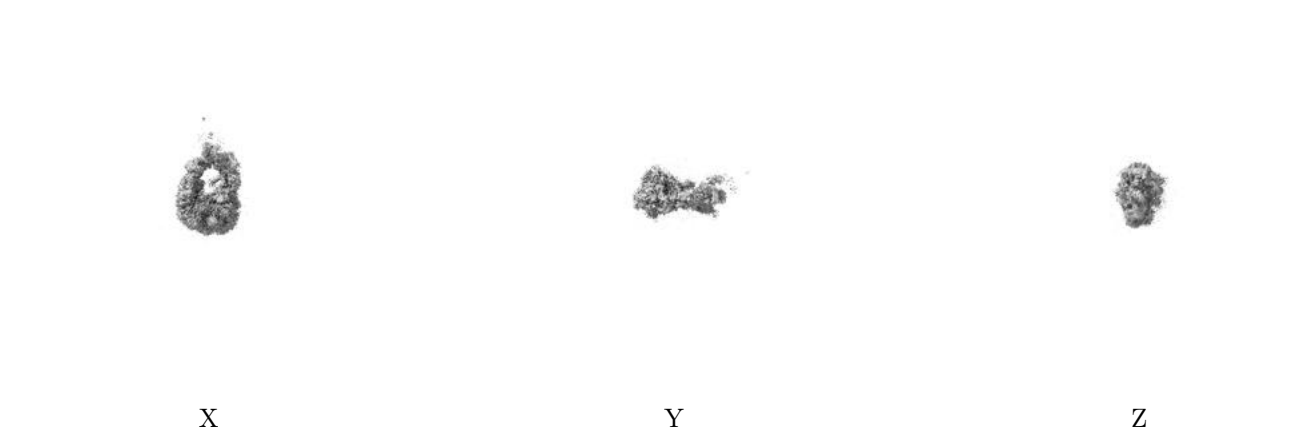
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

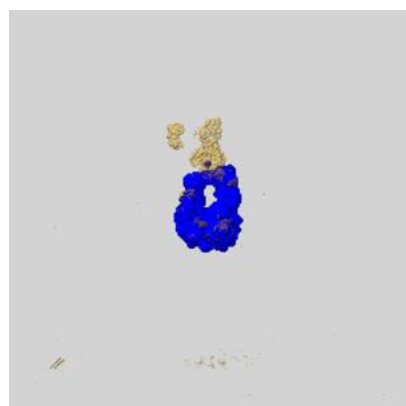
6.6 Mask visualisation [i](#)

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

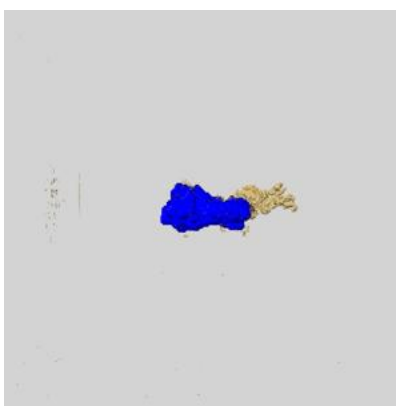
A mask typically either:

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

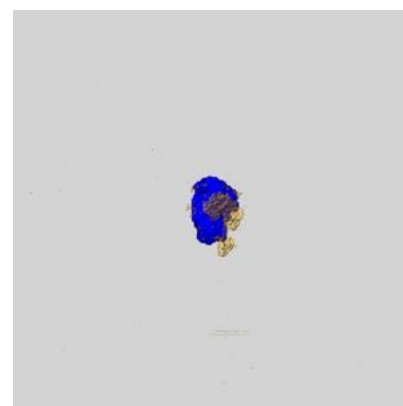
6.6.1 emd_35465_msk_1.map [i](#)



X



Y

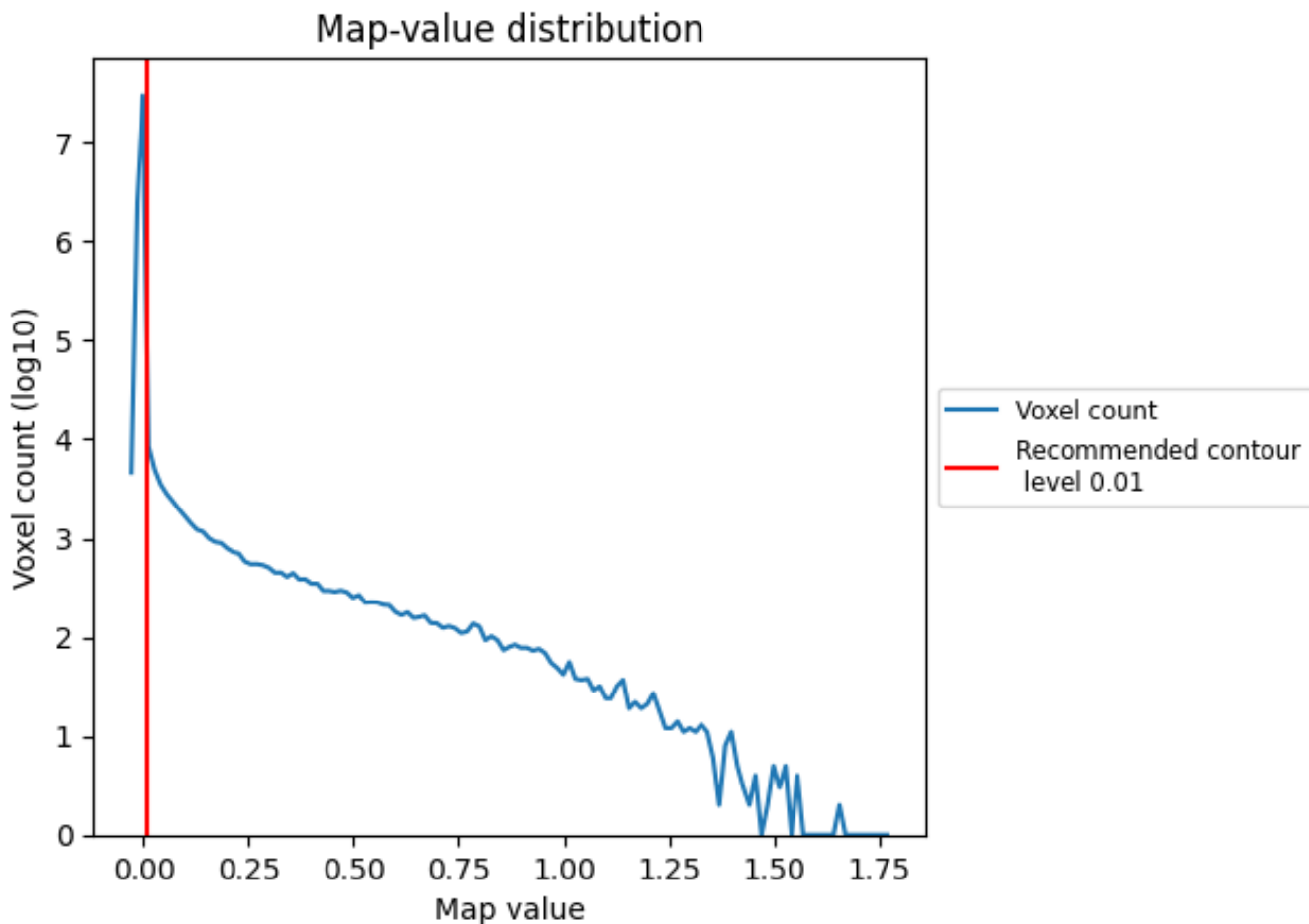


Z

7 Map analysis [i](#)

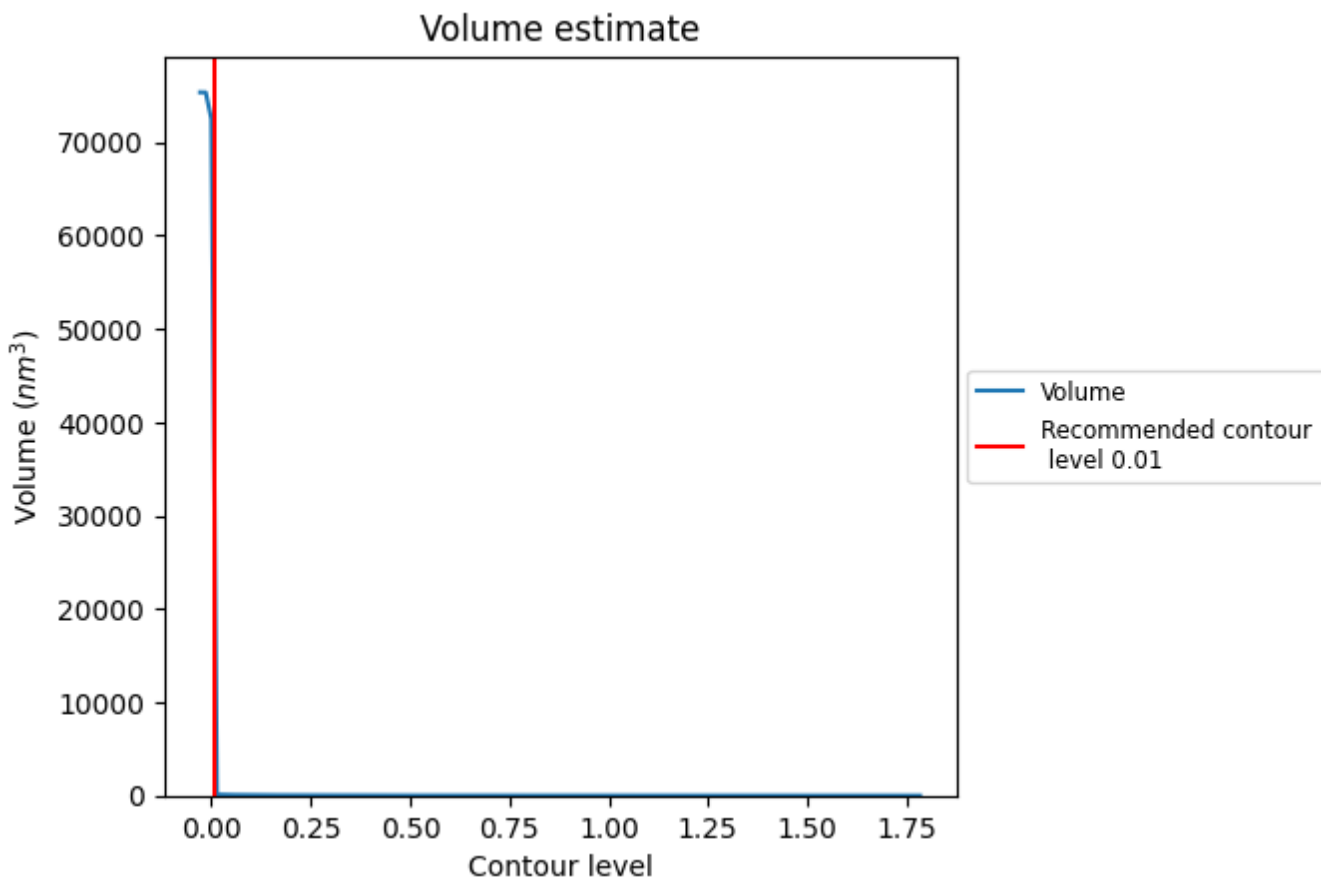
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

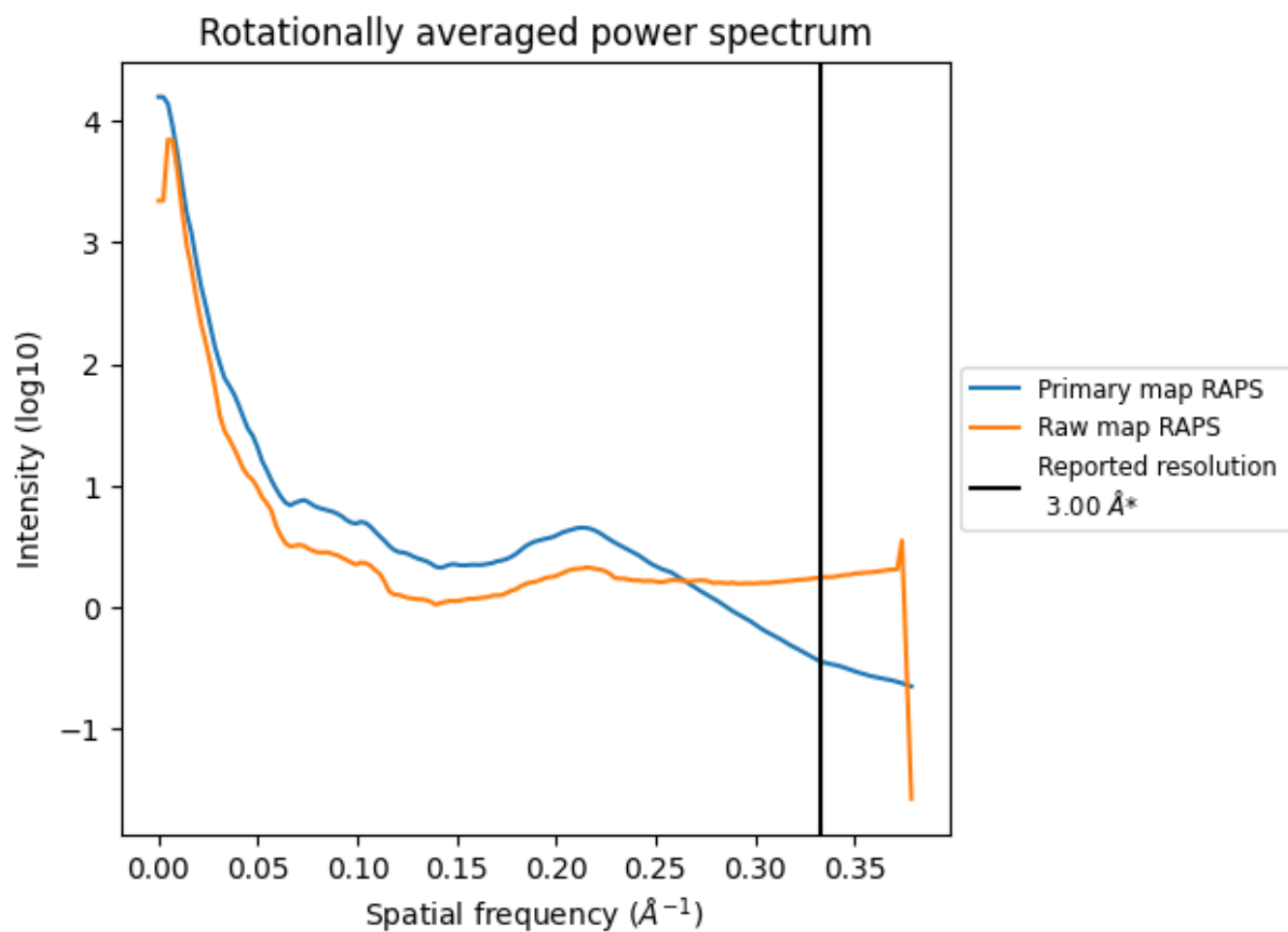
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 19562 nm^3 ; this corresponds to an approximate mass of 17671 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 i

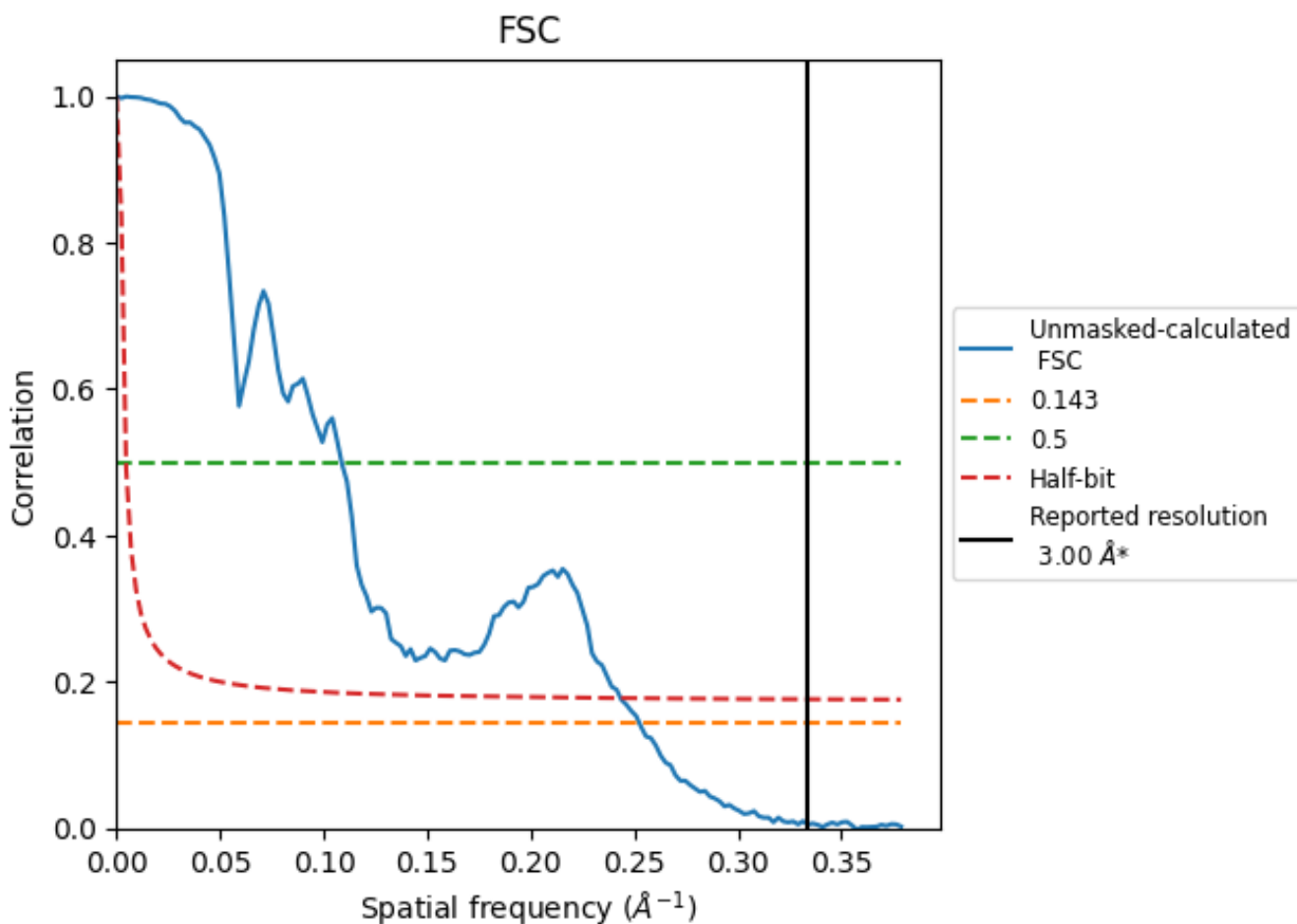


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

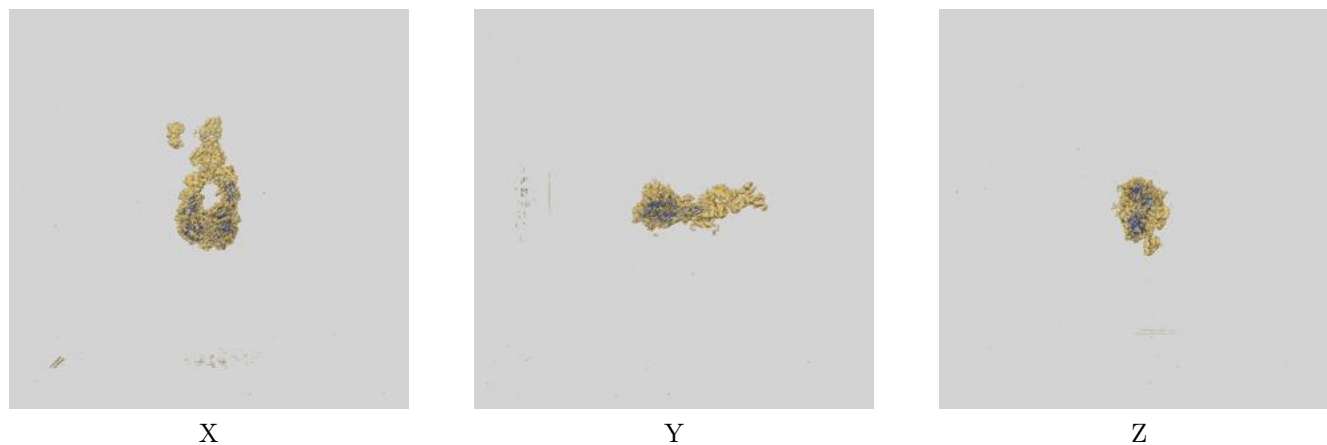
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	9.20	4.11

*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 3.96 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

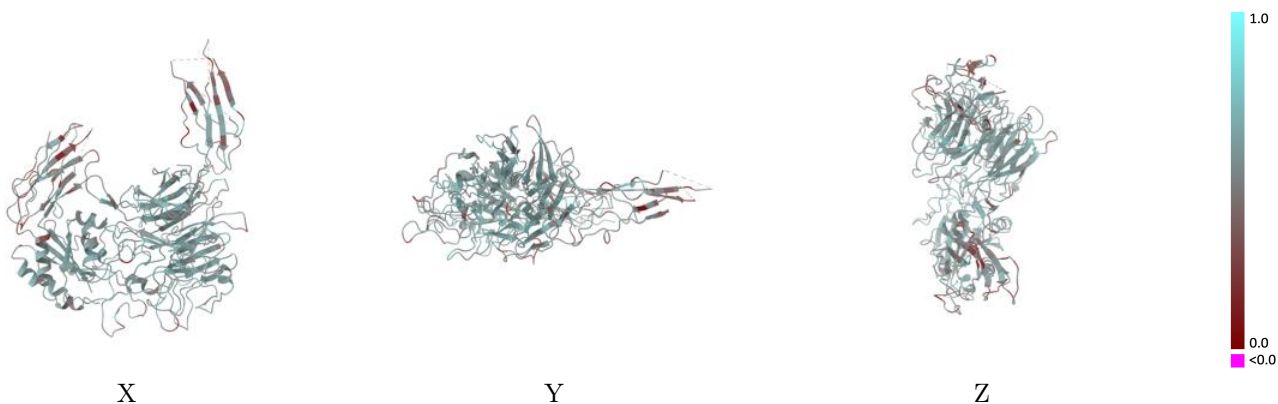
This section contains information regarding the fit between EMDB map EMD-35465 and PDB model 8IJ5. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



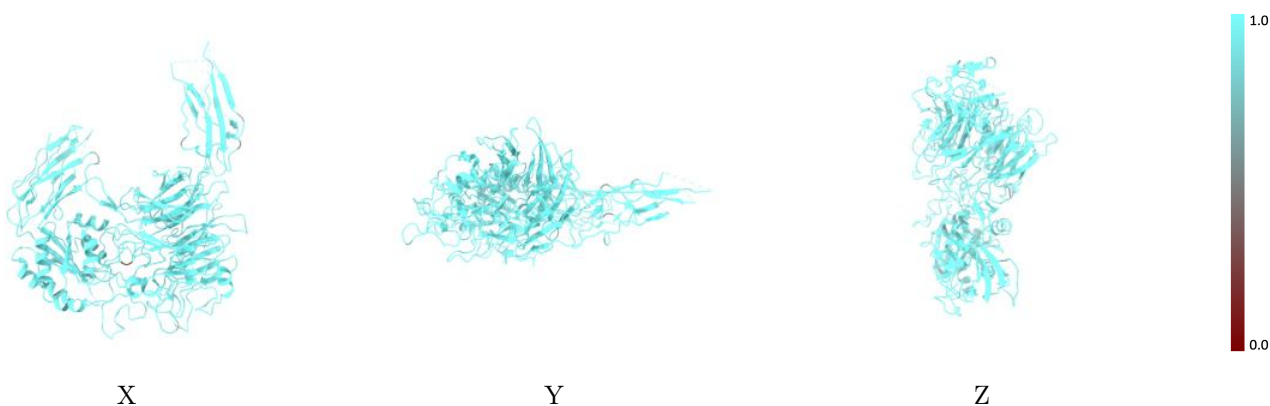
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



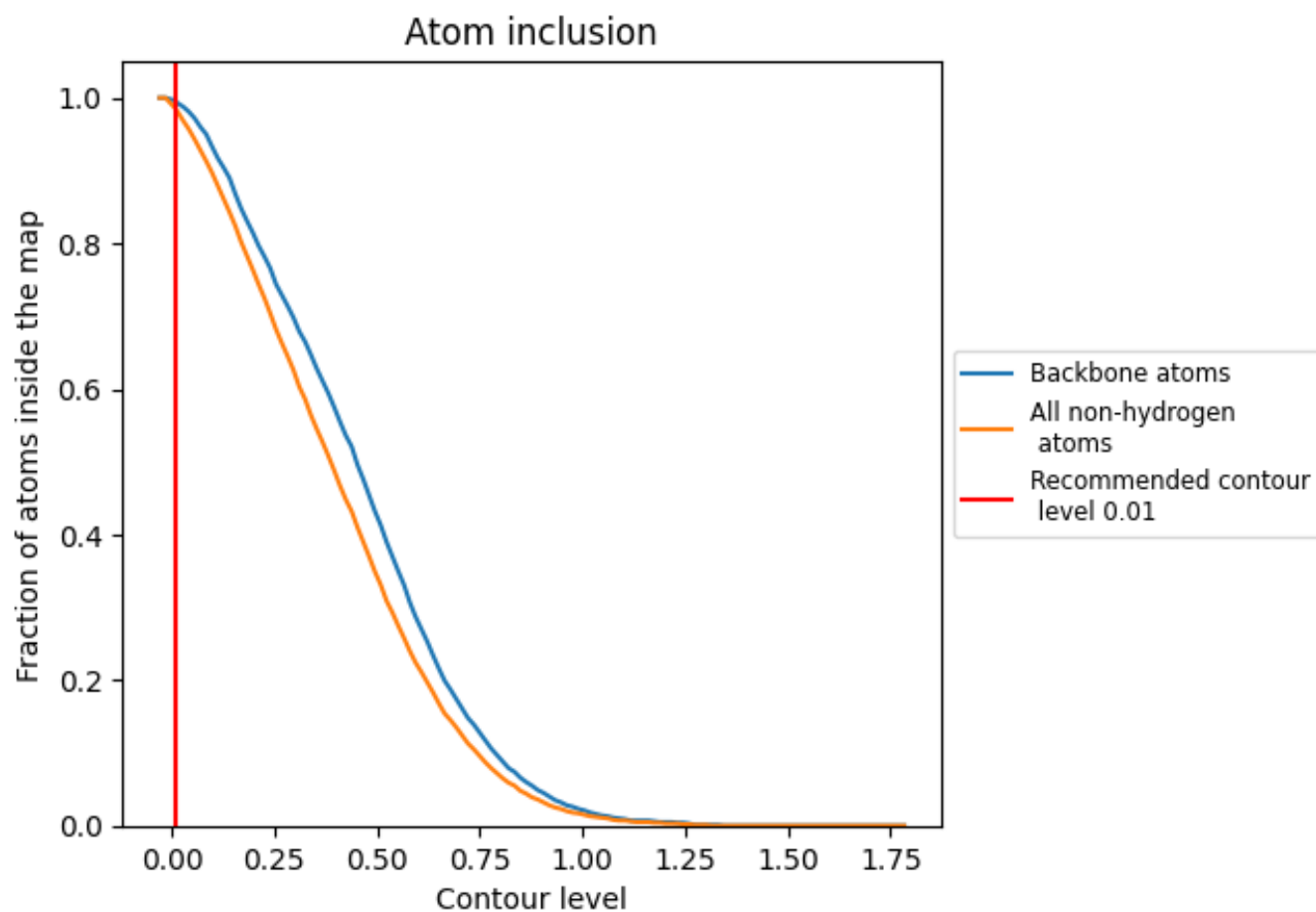
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).






9.4 Atom inclusion [i](#)



At the recommended contour level, 100% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9850	 0.5380
B	 0.9830	 0.5290
E	 0.9870	 0.5450

