



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:08 PM UTC

PDB ID : 8XER / pdb_00008xer
EMDB ID : EMD-38296
Title : Cryo-EM structure of integrin ITGAV, ITGB3 and Cilengitide TFA complex, conformation 1
Authors : Xi, Z.
Deposited on : 2023-12-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

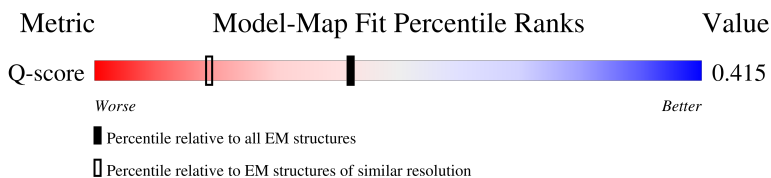
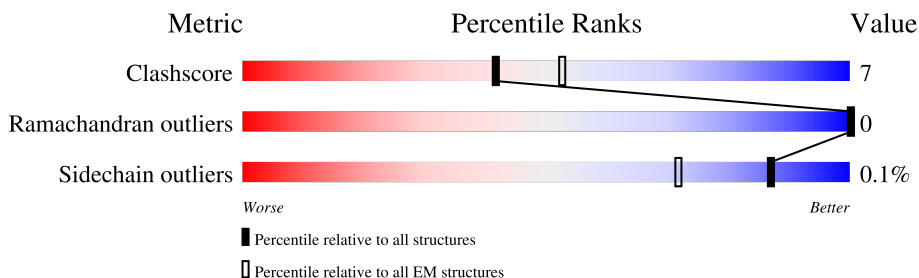
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1048	
2	B	788	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10933 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.

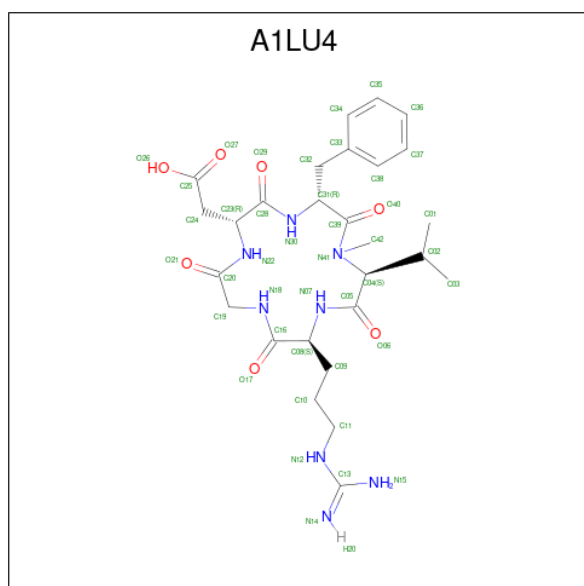
- Molecule 1 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	924	7185	4549	1220	1381	35	0	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	481	3706	2303	632	736	35	0	0

- Molecule 3 is 2-[(2 {R},5 {R},8 {S},11 {S})-11-(3-carbamimidamidopropyl)-7-methyl-3,6,9,12,15-pentakis(oxidanylidene)-5-(phenylmethyl)-8-propan-2-yl-1,4,7,10,13-pentazacyclopentadec-2-yl]ethanoic acid (CCD ID: A1LU4) (formula: C₂₇H₄₀N₈O₇).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	42	27	8	7	0

D139	I140	M144	S147	M150	K151	I157	L164	M168	R169	T172	S173	F179	Y192	I193	S194	P195	P196	E197	T208	T209	V219	Q236	S237	V238	S239	R240	D243	M253	V257	E260	R265	H270	T275	H281	T322	V336	T337			
E338	N339	V340	V341	N342	I351	L359	N365	I370	S379	K380	V381	E382	L383	E390	S393	L394	A398	I406	L409	M413	T420	R430	E435	K438	I442	V445	V453	H472	R473	D503	Y504	S507	GLN	GLN	ASP	GLU	GLY	SER		
PRO	ARG	GLU	GLY	GLN	CYS	GLY	ARG	GLY	GLU	LEU	GLY	VAL	CYS	HIS	SER	SER	ASP	GLY	ILE	THR	GLY	CYS	ASP	PHE	SER	CYS	ARG	PRO	TYR	LYS	GLY	HIS	GLY	CYS	GLN	SER	CYS	GLY	ASP	CYS
LEU	CYS	ASP	SER	TRP	THR	TYR	CYS	THR	THR	ARG	THR	ASP	THR	MET	SER	ASN	LEU	CYS	SER	ARG	GLY	GLY	SER	VAL	CYS	ILE	GLN	PRO	TYR	CYS	GLU	LYS	PRO	THR	CYS	PRO	ASP	ALA		
CYS	THR	PHE	LYS	GLU	CYS	VAL	LYS	LYS	ASP	GLY	ALA	LEU	HIS	ASP	ASN	CYS	ARG	TYR	ARG	GLU	ILE	VAL	GLY	LEU	LYS	GLY	ASP	ALA	ASP	ALA	ASN	GLY	THR	LYS	ASP	VAL	VAL	ARG	PHE	
GLN	TYR	TYR	GLU	ASP	GLY	SER	ILE	LEU	VAL	GLU	PRO	PRO	GLU	LYS	GLY	PRO	ILE	VAL	LEU	LEU	VAL	GLY	ILE	LEU	ILE	LEU	ALA	ALA	LEU	LEU	ILE	THR	ILE	HIS	ASP	ARG	GLY	PHE		
ALA	LYS	PHE	GLU	GLU	ALA	ALA	LYS	THR	ASN	ASN	ASN	GLU	LEU	LYS	ALA	THR	PHE	ASN	ILE	ILE	THR	GLY	ALA	LEU	LEU	ALA	ALA	LEU	LEU	ILE	THR	ILE	LYS	ASP	ARG	LYS	GLU	PHE		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103938	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	0.379	Depositor
Minimum map value	-0.174	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1LU4

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	0.12	0/7340	0.28	0/9949
2	B	0.12	0/3775	0.28	0/5118
All	All	0.12	0/11115	0.28	0/15067

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	7185	0	7012	91	0
2	B	3706	0	3609	55	0
3	B	42	0	0	1	0
All	All	10933	0	10621	146	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 (146) 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:B:131:ARG:NH1	2:B:420:THR:OG1	2.11	0.83
1:A:624:LEU:O	1:A:669:TYR:OH	1.99	0.80
1:A:735:SER:OG	1:A:737:MET:SD	2.39	0.80
1:A:740:SER:OG	1:A:764:VAL:O	1.99	0.79
2:B:322:THR:HG22	2:B:351:ILE:HG23	1.67	0.77
2:B:147:SER:OG	3:B:801:A1LU4:O27	2.04	0.76
2:B:435:GLU:OE1	2:B:438:LYS:NZ	2.22	0.73
1:A:828:GLN:O	1:A:952:SER:OG	2.06	0.72
1:A:769:LEU:N	1:A:818:SER:OG	2.23	0.72
1:A:733:GLN:NE2	1:A:735:SER:O	2.23	0.71
1:A:673:LEU:HD21	1:A:675:VAL:HG23	1.72	0.71
2:B:260:GLU:OE1	2:B:260:GLU:N	2.25	0.70
1:A:105:THR:O	1:A:119:LYS:NZ	2.23	0.70
1:A:577:GLU:N	1:A:577:GLU:OE1	2.26	0.68
1:A:398:ASP:OD2	1:A:400:LYS:NZ	2.27	0.68
1:A:590:GLU:OE2	1:A:592:ARG:NH2	2.26	0.68
2:B:194:SER:HB2	2:B:195:PRO:HD3	1.76	0.67
1:A:169:TYR:OH	1:A:216:ASP:OD2	2.11	0.64
1:A:342:VAL:HG12	1:A:365:GLU:O	1.97	0.64
1:A:410:SER:O	1:A:411:THR:OG1	2.12	0.64
1:A:382:GLN:NE2	1:A:448:GLY:O	2.32	0.63
2:B:138:VAL:HG11	2:B:168:MET:CE	2.28	0.62
2:B:151:LYS:HG3	2:B:238:VAL:HG21	1.81	0.62
1:A:273:VAL:CG1	1:A:276:ALA:HB2	2.30	0.61
1:A:672:GLU:N	1:A:672:GLU:OE1	2.34	0.61
2:B:48:MET:N	2:B:48:MET:HE2	2.15	0.60
2:B:413:MET:HE3	2:B:413:MET:HA	1.82	0.60
1:A:54:ASP:OD1	1:A:55:PHE:N	2.34	0.60
1:A:829:TRP:N	1:A:910:LEU:O	2.32	0.60
2:B:253:MET:O	2:B:257:VAL:HG22	2.01	0.60
2:B:339:ASN:OD1	2:B:340:VAL:HG13	2.01	0.60
2:B:138:VAL:HG11	2:B:168:MET:HE2	1.84	0.60
1:A:148:MET:SD	1:A:148:MET:N	2.75	0.59
2:B:398:ALA:HB3	2:B:409:LEU:HD21	1.83	0.59
1:A:679:LEU:HD12	1:A:679:LEU:H	1.68	0.58
1:A:670:GLU:N	1:A:715:ASN:OD1	2.36	0.58
2:B:157:ILE:HG12	2:B:275:THR:HG21	1.85	0.57
2:B:169:ARG:O	2:B:169:ARG:NH1	2.38	0.56
1:A:38:PRO:CG	1:A:463:ILE:HD11	2.35	0.56
1:A:252:LEU:HA	1:A:273:VAL:HG22	1.88	0.56
1:A:300:GLU:N	1:A:300:GLU:OE1	2.39	0.56
2:B:136:TYR:HH	2:B:379:SER:HG	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:OD1	1:A:150:GLN:NE2	2.39	0.55
2:B:390:GLU:OE1	2:B:390:GLU:N	2.36	0.54
2:B:65:ASP:OD1	2:B:69:ASN:ND2	2.39	0.54
2:B:86:GLU:N	2:B:86:GLU:OE1	2.41	0.54
2:B:208:THR:HG22	2:B:209:THR:H	1.73	0.54
2:B:383:LEU:HD12	2:B:442:ILE:HG22	1.90	0.54
1:A:824:MET:SD	1:A:825:LEU:N	2.81	0.53
1:A:40:GLU:OE2	1:A:461:ARG:NE	2.40	0.53
1:A:314:ASP:OD2	1:A:319:ASP:N	2.41	0.53
2:B:164:LEU:HD22	2:B:370:ILE:CD1	2.39	0.53
1:A:244:GLN:OE1	1:A:244:GLN:N	2.41	0.52
2:B:365:ASN:OD1	2:B:365:ASN:C	2.52	0.52
1:A:273:VAL:HG11	1:A:276:ALA:HB2	1.92	0.52
2:B:65:ASP:OD1	2:B:66:LEU:N	2.40	0.51
2:B:197:GLU:N	2:B:197:GLU:OE1	2.43	0.51
2:B:92:ASP:OD1	2:B:110:SER:OG	2.25	0.51
1:A:680:GLN:O	1:A:732:HIS:N	2.43	0.51
1:A:273:VAL:HG12	1:A:276:ALA:HB2	1.92	0.51
1:A:647:ILE:O	1:A:767:ALA:N	2.39	0.51
2:B:380:LYS:HG3	2:B:413:MET:HE1	1.92	0.51
1:A:785:LEU:O	1:A:984:GLY:N	2.44	0.50
1:A:693:LEU:HD22	1:A:693:LEU:H	1.75	0.50
1:A:506:ARG:NH1	1:A:567:GLU:OE2	2.43	0.50
1:A:673:LEU:C	1:A:673:LEU:HD23	2.36	0.50
2:B:383:LEU:HD12	2:B:442:ILE:CG2	2.42	0.50
1:A:680:GLN:O	1:A:732:HIS:ND1	2.45	0.49
1:A:45:GLU:OE1	1:A:428:ARG:NH1	2.45	0.49
1:A:673:LEU:CD2	1:A:675:VAL:HG23	2.41	0.49
2:B:55:GLU:OE1	2:B:473:ARG:NH1	2.46	0.49
2:B:265:ARG:O	2:B:270:HIS:NE2	2.43	0.48
1:A:543:PHE:CE1	1:A:568:LEU:HD13	2.48	0.48
2:B:192:TYR:OH	2:B:240:ARG:NH2	2.46	0.48
1:A:673:LEU:HD21	1:A:675:VAL:CG2	2.42	0.48
1:A:508:CYS:CB	1:A:563:MET:HE2	2.44	0.48
1:A:535:LYS:HD2	1:A:535:LYS:N	2.28	0.48
1:A:846:ILE:HG23	1:A:850:MET:SD	2.54	0.47
2:B:151:LYS:CG	2:B:238:VAL:HG21	2.43	0.47
2:B:341:VAL:HG13	2:B:342:ASN:N	2.29	0.47
1:A:76:THR:O	1:A:76:THR:CG2	2.62	0.47
1:A:649:ILE:HG21	1:A:963:TYR:CE1	2.50	0.47
1:A:333:ARG:NH2	1:A:337:GLY:O	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:VAL:HG22	1:A:731:VAL:O	2.14	0.47
2:B:172:THR:OG1	2:B:173:SER:N	2.48	0.47
1:A:655:LEU:HD23	1:A:655:LEU:C	2.40	0.47
1:A:540:ARG:NH1	1:A:580:ASP:O	2.48	0.46
2:B:144:MET:HE1	2:B:236:GLN:HG3	1.98	0.46
1:A:655:LEU:O	1:A:729:PHE:N	2.49	0.46
1:A:673:LEU:HD23	1:A:673:LEU:O	2.16	0.46
1:A:53:VAL:HG12	1:A:68:VAL:HG22	1.97	0.46
1:A:76:THR:O	1:A:76:THR:HG22	2.15	0.46
1:A:508:CYS:HB2	1:A:563:MET:HE2	1.98	0.46
1:A:643:ASP:OD1	1:A:643:ASP:N	2.49	0.46
1:A:833:TYR:HB2	1:A:838:LEU:HD11	1.97	0.45
1:A:693:LEU:O	1:A:695:ARG:NH1	2.50	0.45
1:A:848:GLY:N	1:A:849:PRO:CD	2.80	0.45
2:B:430:ARG:O	2:B:430:ARG:CZ	2.65	0.44
1:A:545:TYR:C	1:A:545:TYR:CD1	2.96	0.44
2:B:92:ASP:OD1	2:B:93:ARG:N	2.46	0.44
2:B:150:MET:HE2	2:B:157:ILE:HD11	2.00	0.44
1:A:36:ASP:OD1	1:A:37:SER:N	2.51	0.43
1:A:480:TYR:HB2	1:A:481:PRO:HD3	2.01	0.43
1:A:836:ASN:CB	1:A:937:THR:HG23	2.49	0.43
2:B:243:ASP:OD2	2:B:281:HIS:NE2	2.44	0.43
1:A:402:ILE:HD11	1:A:420:ILE:CG2	2.49	0.43
2:B:338:GLU:O	2:B:341:VAL:HG12	2.18	0.43
1:A:430:MET:HG3	1:A:431:PRO:HD2	2.00	0.43
2:B:140:ILE:HD11	2:B:168:MET:HG3	2.01	0.43
2:B:194:SER:CB	2:B:195:PRO:HD3	2.45	0.43
1:A:190:SER:HB2	1:A:256:VAL:HG22	1.99	0.43
1:A:653:ASN:OD1	1:A:653:ASN:N	2.52	0.42
1:A:749:SER:OG	1:A:751:ASN:OD1	2.35	0.42
2:B:157:ILE:CG1	2:B:275:THR:HG21	2.49	0.42
2:B:336:VAL:O	2:B:359:LEU:N	2.44	0.42
2:B:109:VAL:HG21	2:B:128:ILE:HD11	2.01	0.42
1:A:625:ASP:OD1	1:A:626:CYS:N	2.46	0.42
1:A:663:ASN:OD1	1:A:664:GLN:N	2.52	0.42
1:A:902:LEU:O	1:A:951:LYS:N	2.52	0.42
2:B:114:ILE:HG12	2:B:453:VAL:HG22	2.01	0.42
1:A:349:LEU:HD21	1:A:412:GLY:HA2	2.00	0.42
1:A:939:MET:SD	1:A:939:MET:N	2.93	0.42
2:B:48:MET:HE2	2:B:48:MET:CA	2.50	0.42
2:B:382:GLU:O	2:B:445:VAL:N	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:LEU:CB	1:A:713:LEU:HD21	2.51	0.41
2:B:179:PHE:CZ	2:B:219:VAL:HG11	2.55	0.41
1:A:960:GLU:OE2	1:A:961:PHE:O	2.38	0.41
1:A:675:VAL:HG22	1:A:745:LEU:HB3	2.03	0.41
1:A:38:PRO:HG2	1:A:463:ILE:HD11	2.03	0.41
2:B:472:HIS:O	2:B:473:ARG:CB	2.68	0.41
1:A:177:ILE:O	1:A:178:ASP:HB2	2.20	0.41
2:B:393:SER:O	2:B:394:LEU:HD13	2.20	0.41
1:A:113:ASP:N	1:A:113:ASP:OD1	2.54	0.41
1:A:628:GLU:OE1	1:A:629:ASP:N	2.54	0.41
1:A:809:ILE:HD12	1:A:928:TYR:HD1	1.86	0.41
1:A:836:ASN:HB2	1:A:937:THR:HG23	2.02	0.41
2:B:136:TYR:HE1	2:B:379:SER:HG	1.69	0.41
2:B:406:ILE:HG12	2:B:409:LEU:HD22	2.02	0.41
1:A:712:ASP:C	1:A:713:LEU:HD23	2.46	0.41
1:A:856:MET:SD	1:A:910:LEU:HD12	2.61	0.41
1:A:673:LEU:HB3	1:A:713:LEU:HD21	2.03	0.40
1:A:136:LEU:HD22	1:A:199:VAL:HG21	2.03	0.40
1:A:194:THR:HG23	1:A:267:ASP:HB2	2.03	0.40
2:B:150:MET:HE3	2:B:150:MET:HB3	1.97	0.40
1:A:38:PRO:HG3	1:A:463:ILE:HD11	2.01	0.40
1:A:402:ILE:HD11	1:A:420:ILE:HG21	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	A	675/1048 (64%)	653 (97%)	22 (3%)	0	100	100
2	B	479/788 (61%)	457 (95%)	22 (5%)	0	100	100
All	All	1154/1836 (63%)	1110 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	766/890 (86%)	765 (100%)	1 (0%)	88	93
2	B	421/690 (61%)	421 (100%)	0	100	100
All	All	1187/1580 (75%)	1186 (100%)	1 (0%)	87	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	235	ASN
1	A	350	GLN
1	A	551	HIS
1	A	554	ASN
1	A	789	ASN
2	B	306	HIS
2	B	470	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1LU4	B	801	-	43,43,43	2.56	16 (37%)	57,58,58	1.86	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1LU4	B	801	-	-	18/60/60/60	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	A1LU4	C05-N07	6.24	1.47	1.34
3	B	801	A1LU4	C28-N30	5.78	1.46	1.34
3	B	801	A1LU4	C39-N41	5.67	1.48	1.35
3	B	801	A1LU4	C20-N22	5.63	1.46	1.34
3	B	801	A1LU4	C16-N18	5.60	1.46	1.33
3	B	801	A1LU4	C13-N14	3.91	1.46	1.32
3	B	801	A1LU4	C37-C38	3.56	1.45	1.38
3	B	801	A1LU4	C13-N15	3.17	1.46	1.34
3	B	801	A1LU4	C13-N12	-3.06	1.27	1.33
3	B	801	A1LU4	C37-C36	2.94	1.44	1.38
3	B	801	A1LU4	C36-C35	2.89	1.44	1.38
3	B	801	A1LU4	C38-C33	2.81	1.44	1.38
3	B	801	A1LU4	O06-C05	-2.49	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	A1LU4	O17-C16	-2.43	1.18	1.23
3	B	801	A1LU4	O29-C28	-2.42	1.18	1.23
3	B	801	A1LU4	O21-C20	-2.29	1.18	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	A1LU4	C35-C34-C33	7.64	131.35	120.61
3	B	801	A1LU4	C36-C35-C34	-5.76	113.13	120.24
3	B	801	A1LU4	C09-C08-C16	4.09	120.11	110.11
3	B	801	A1LU4	C38-C33-C34	-3.35	113.25	118.23
3	B	801	A1LU4	C16-C08-N07	-3.11	102.71	111.11
3	B	801	A1LU4	C36-C37-C38	-2.43	117.25	120.24
3	B	801	A1LU4	C09-C08-N07	2.13	115.12	110.91
3	B	801	A1LU4	O26-C25-C24	2.02	120.27	114.00

There are no chirality outliers.

All (18) torsion outliers are listed below:

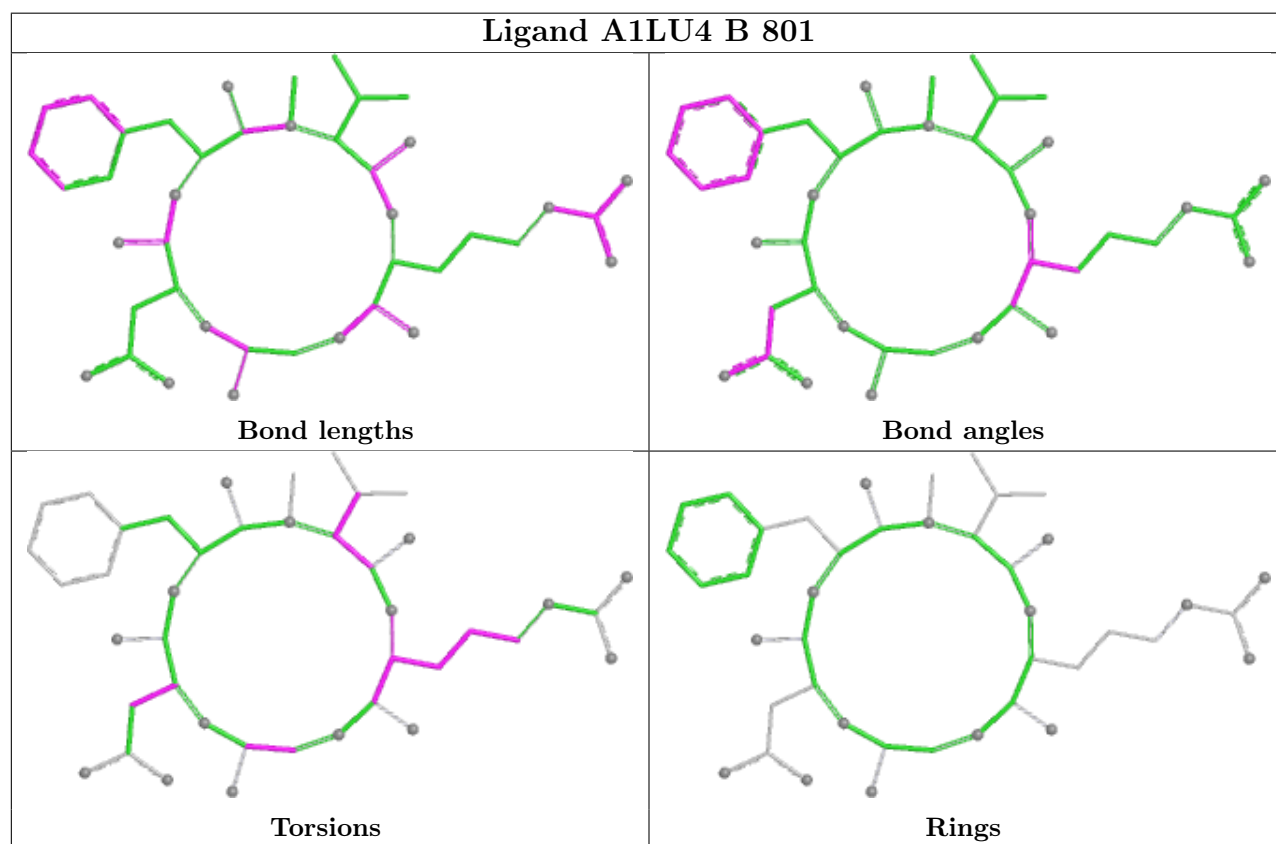
Mol	Chain	Res	Type	Atoms
3	B	801	A1LU4	C01-C02-C04-C05
3	B	801	A1LU4	N07-C08-C09-C10
3	B	801	A1LU4	C16-C08-C09-C10
3	B	801	A1LU4	C09-C08-N07-C05
3	B	801	A1LU4	C09-C10-C11-N12
3	B	801	A1LU4	C01-C02-C04-N41
3	B	801	A1LU4	C03-C02-C04-C05
3	B	801	A1LU4	C03-C02-C04-N41
3	B	801	A1LU4	N22-C23-C24-C25
3	B	801	A1LU4	N41-C04-C05-O06
3	B	801	A1LU4	N41-C04-C05-N07
3	B	801	A1LU4	N18-C19-C20-O21
3	B	801	A1LU4	C16-C08-N07-C05
3	B	801	A1LU4	C08-C09-C10-C11
3	B	801	A1LU4	N18-C19-C20-N22
3	B	801	A1LU4	C28-C23-C24-C25
3	B	801	A1LU4	N07-C08-C16-O17
3	B	801	A1LU4	N07-C08-C16-N18

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	A1LU4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

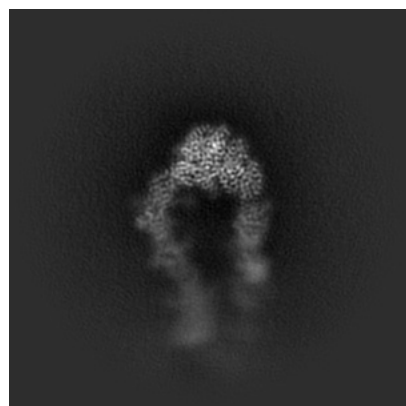
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38296. These allow visual inspection of the internal detail of the map and identification of artifacts.

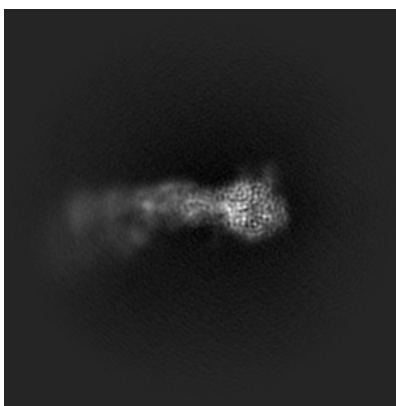
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

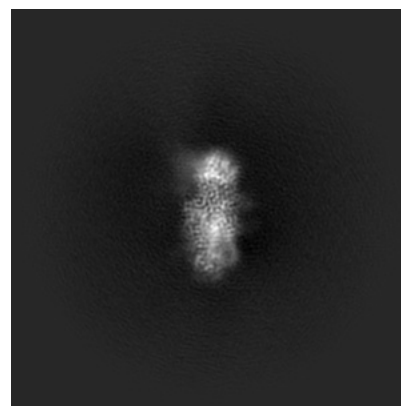
6.1.1 Primary map



X

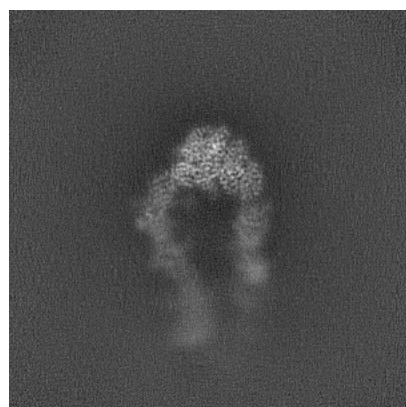


Y

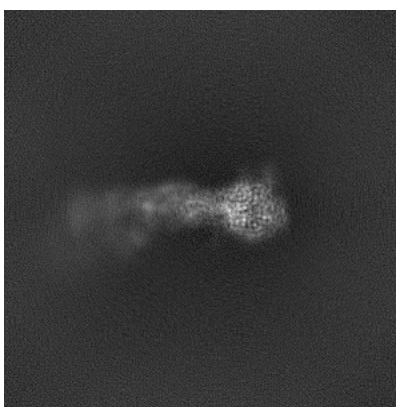


Z

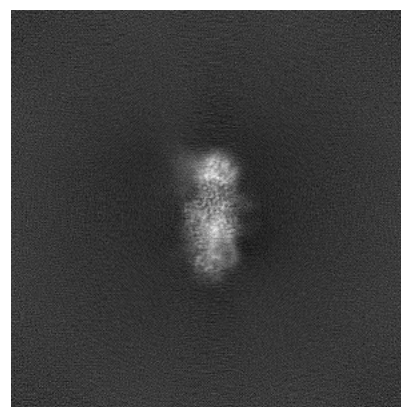
6.1.2 Raw map



X



Y

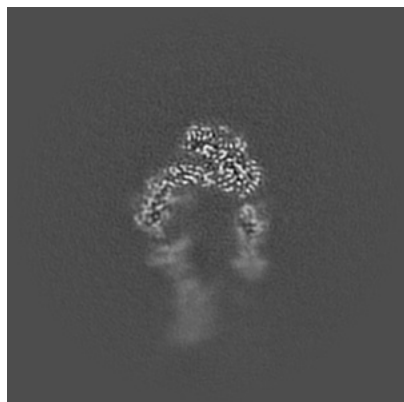


Z

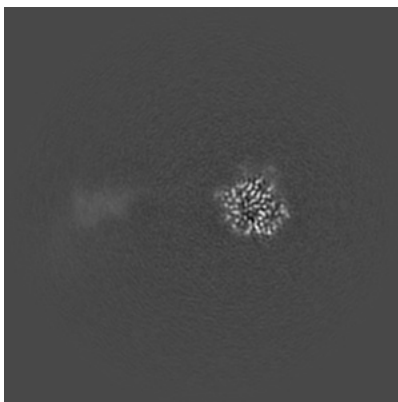
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

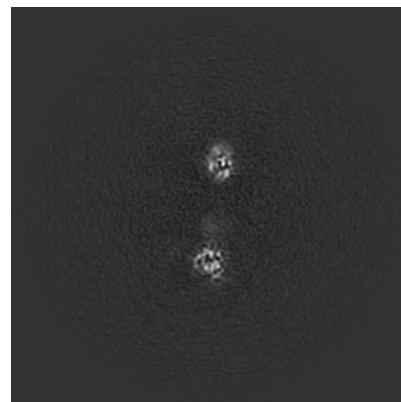
6.2.1 Primary map



X Index: 256



Y Index: 256

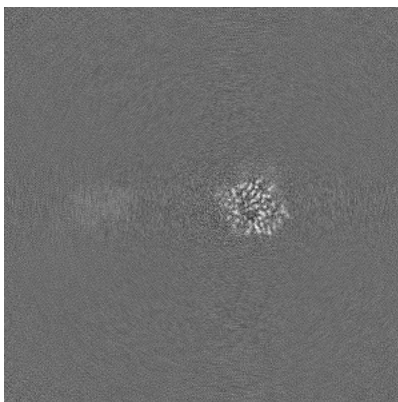


Z Index: 256

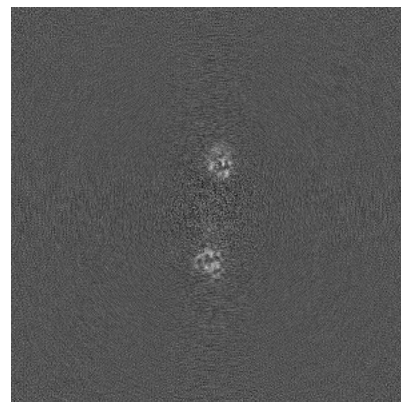
6.2.2 Raw map



X Index: 256



Y Index: 256

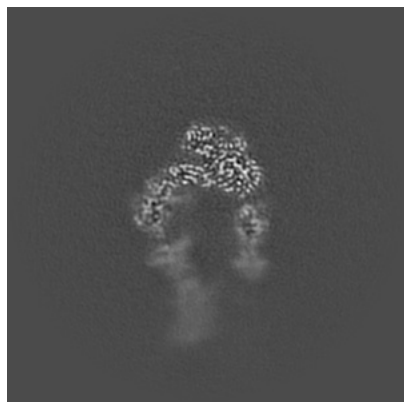


Z Index: 256

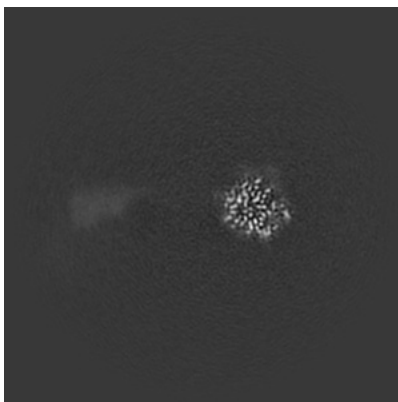
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

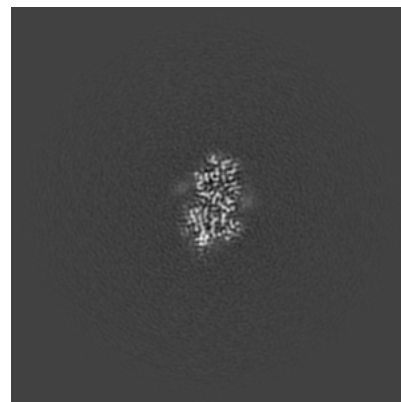
6.3.1 Primary map



X Index: 257

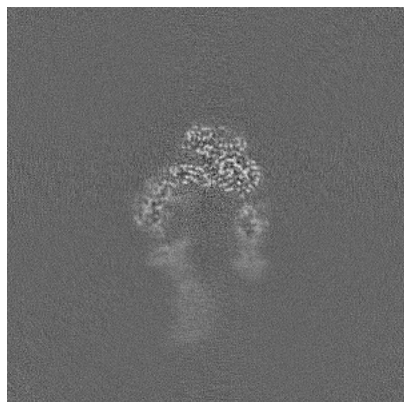


Y Index: 254

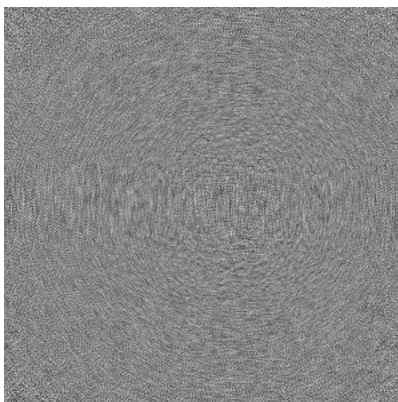


Z Index: 307

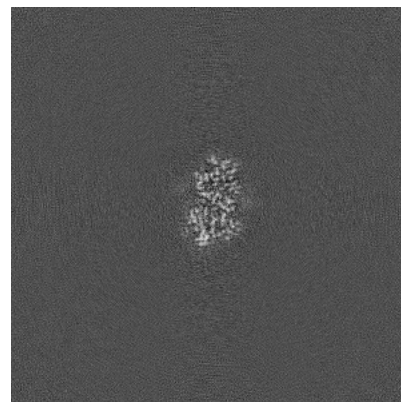
6.3.2 Raw map



X Index: 257



Y Index: 0

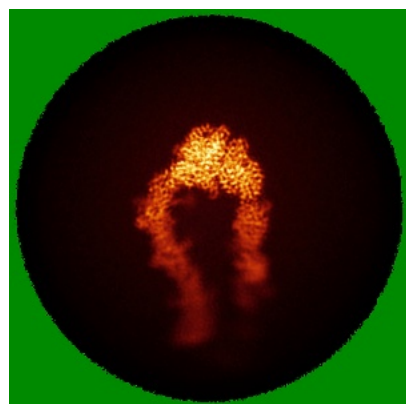


Z Index: 307

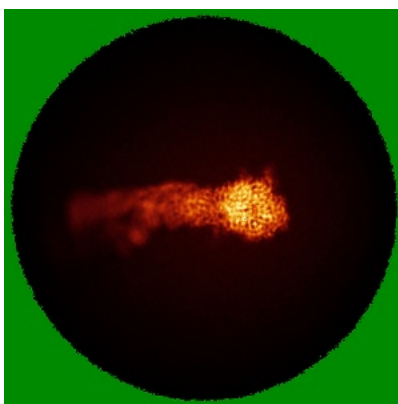
The images above show the largest variance slices of the map in three orthogonal directions.

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

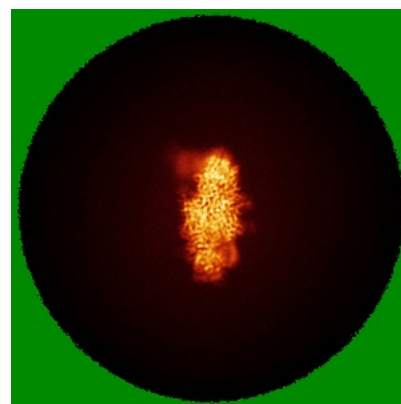
6.4.1 Primary map



X

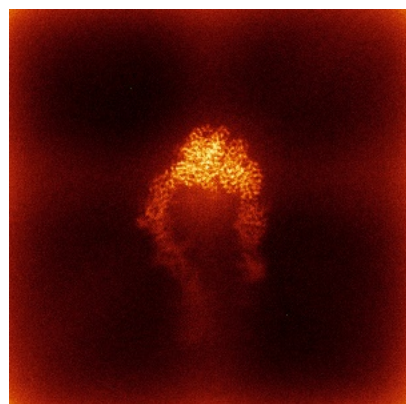


Y

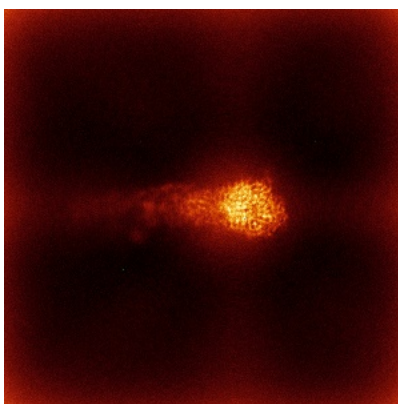


Z

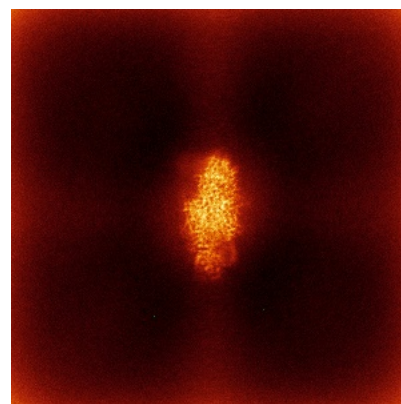
6.4.2 Raw map



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.

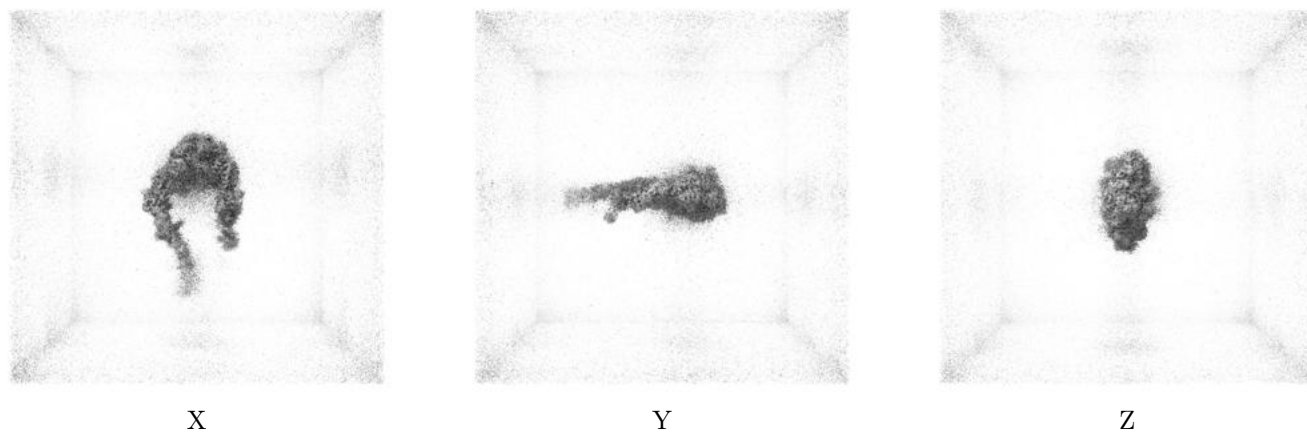
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

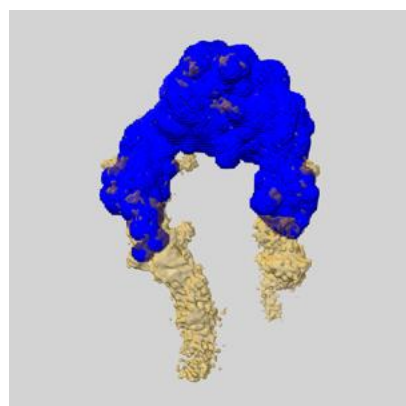
6.6 Mask visualisation [i](#)

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

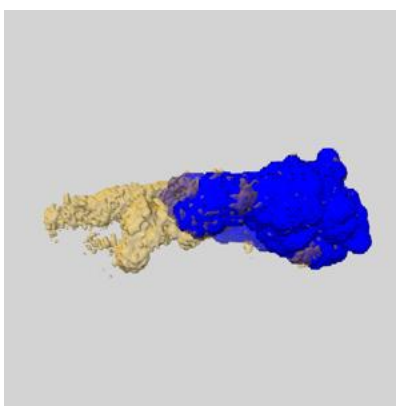
A mask typically either:

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

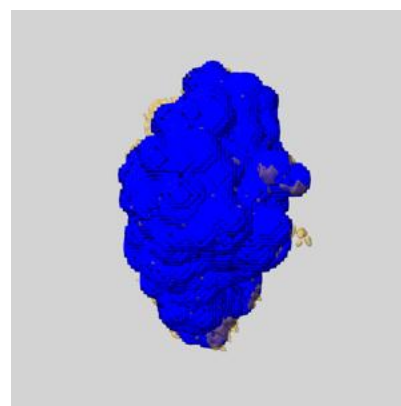
6.6.1 emd_38296_msk_1.map [i](#)



X



Y

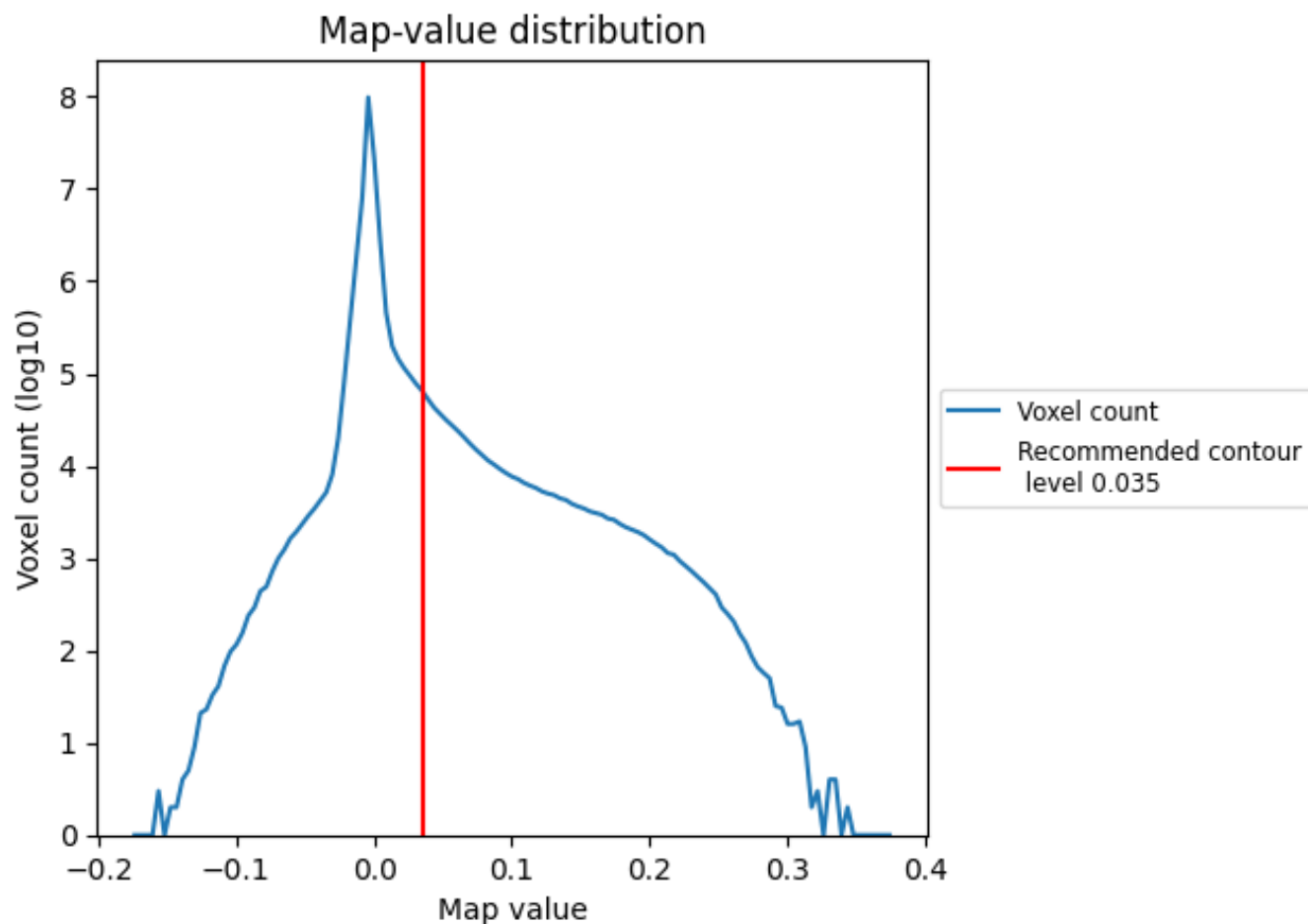


Z

7 Map analysis [i](#)

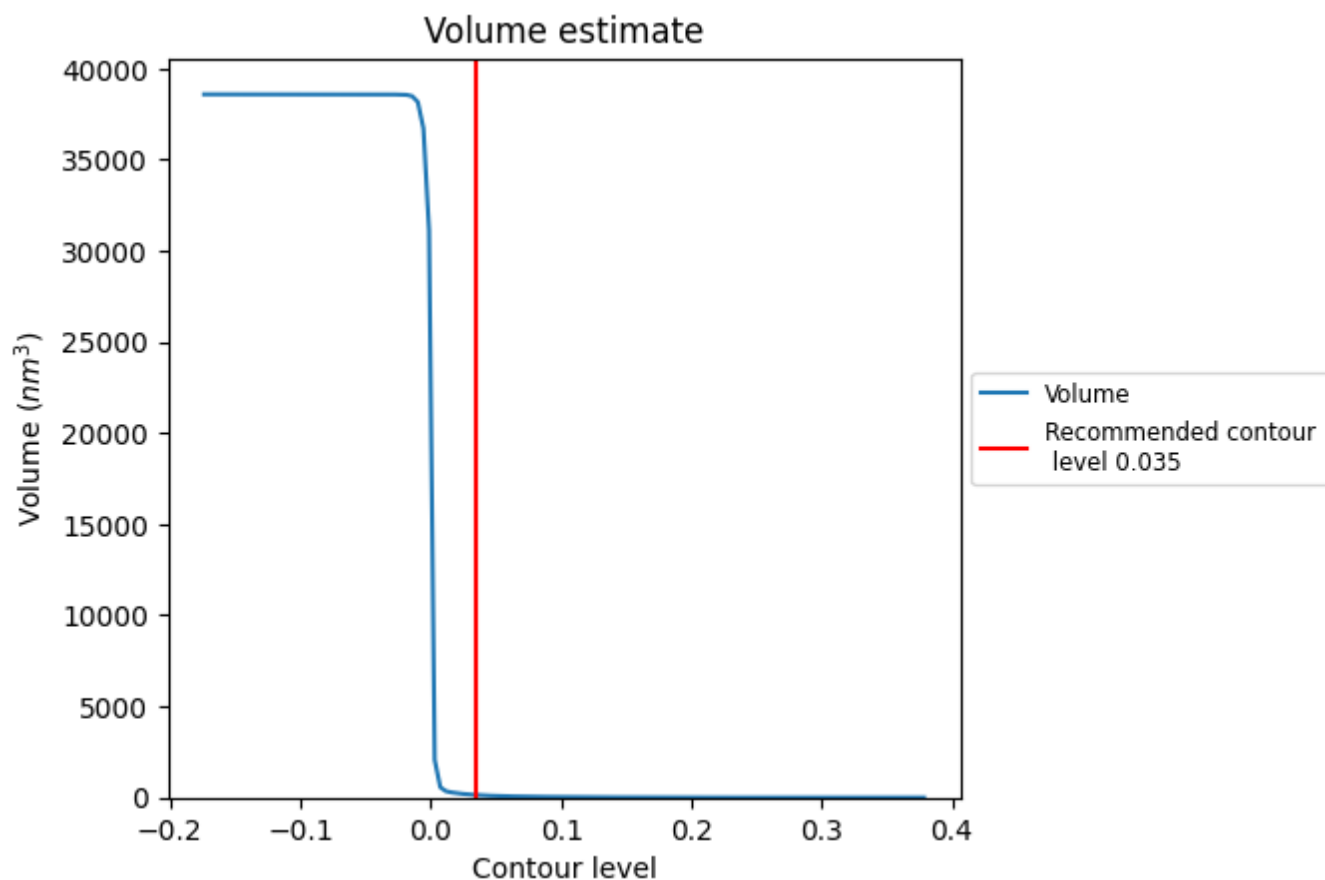
This section contains the results of statistical analysis of the map.

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.

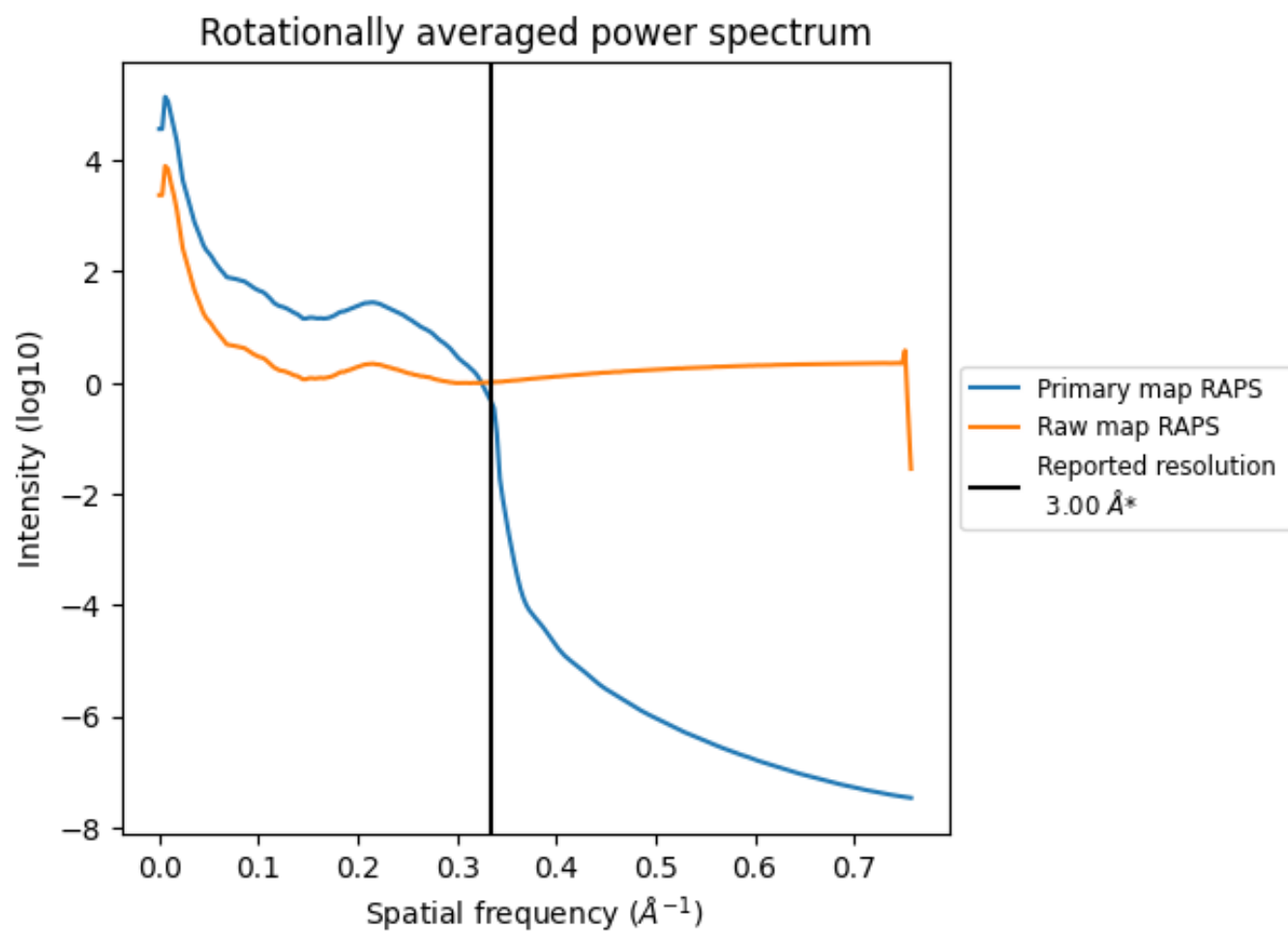
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 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 ⓘ

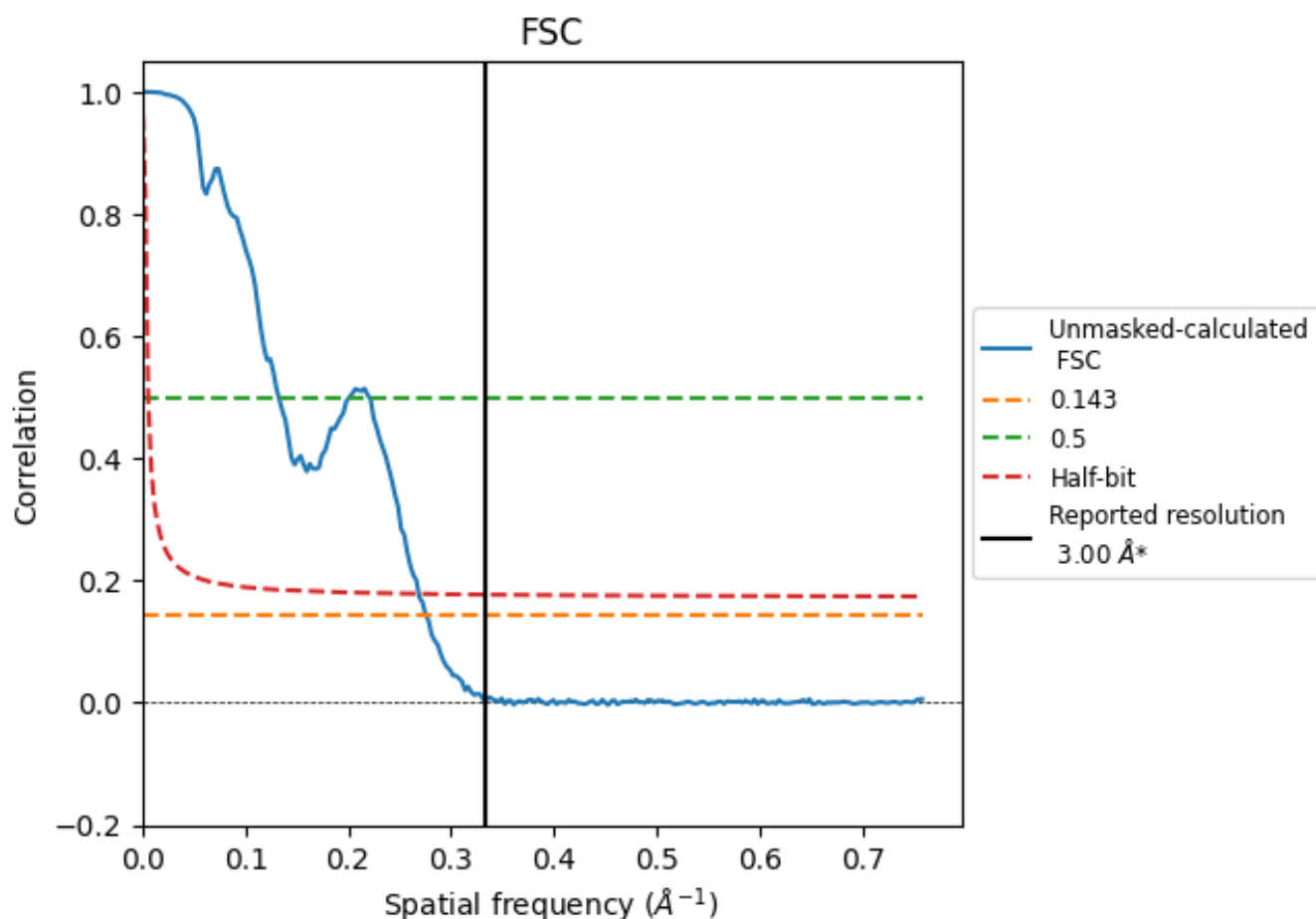


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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

8.2 Resolution estimates [i](#)

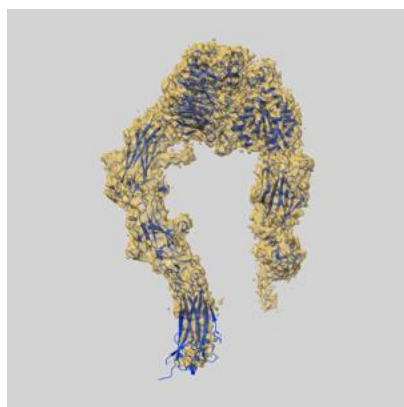
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	7.54	3.72

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

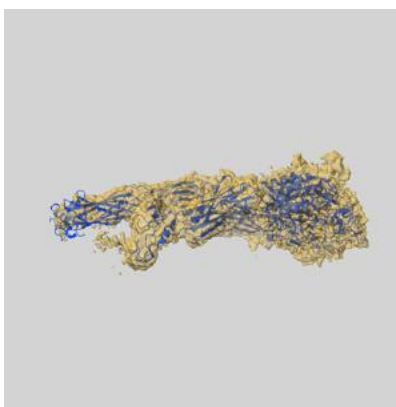
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38296 and PDB model 8XER. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

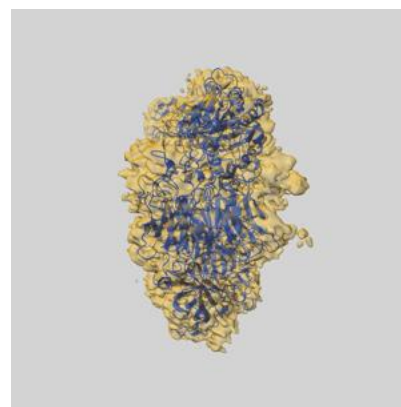
9.1 Map-model overlay [i](#)



X



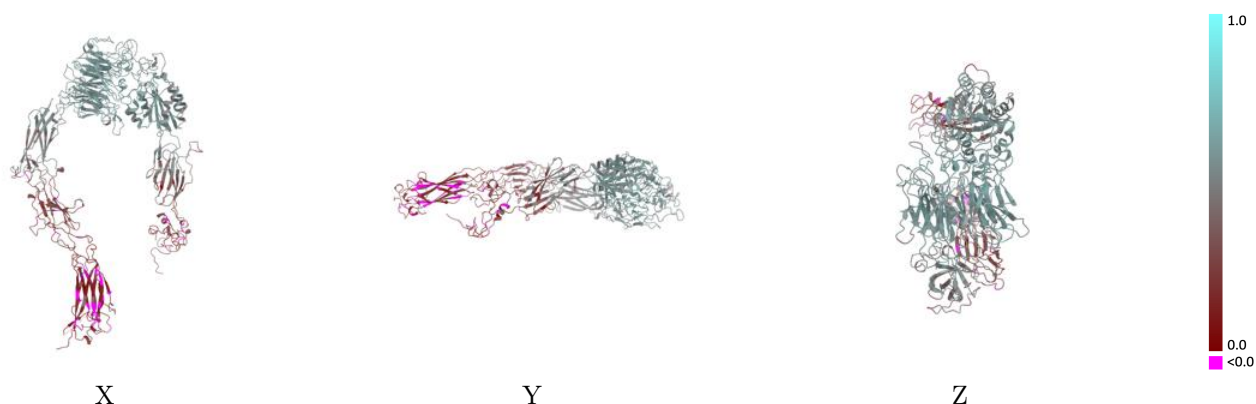
Y



Z

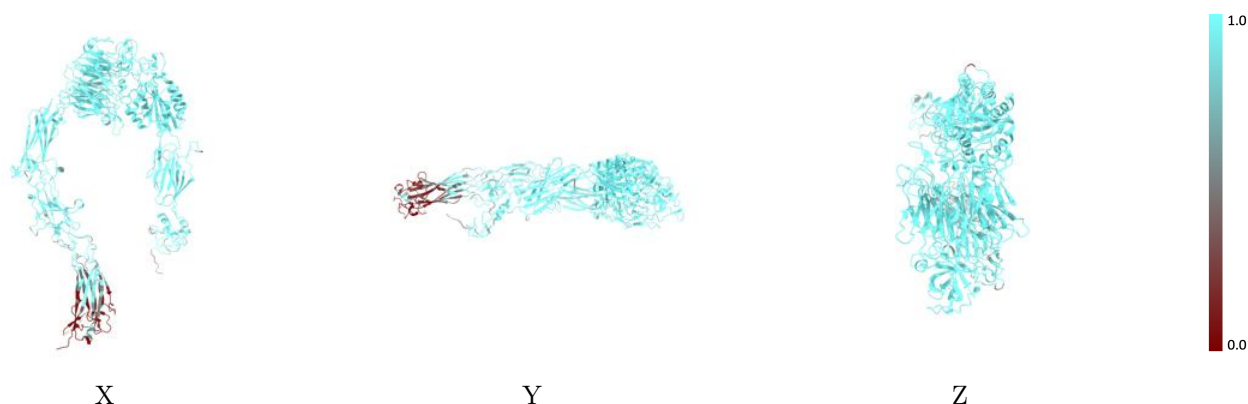
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



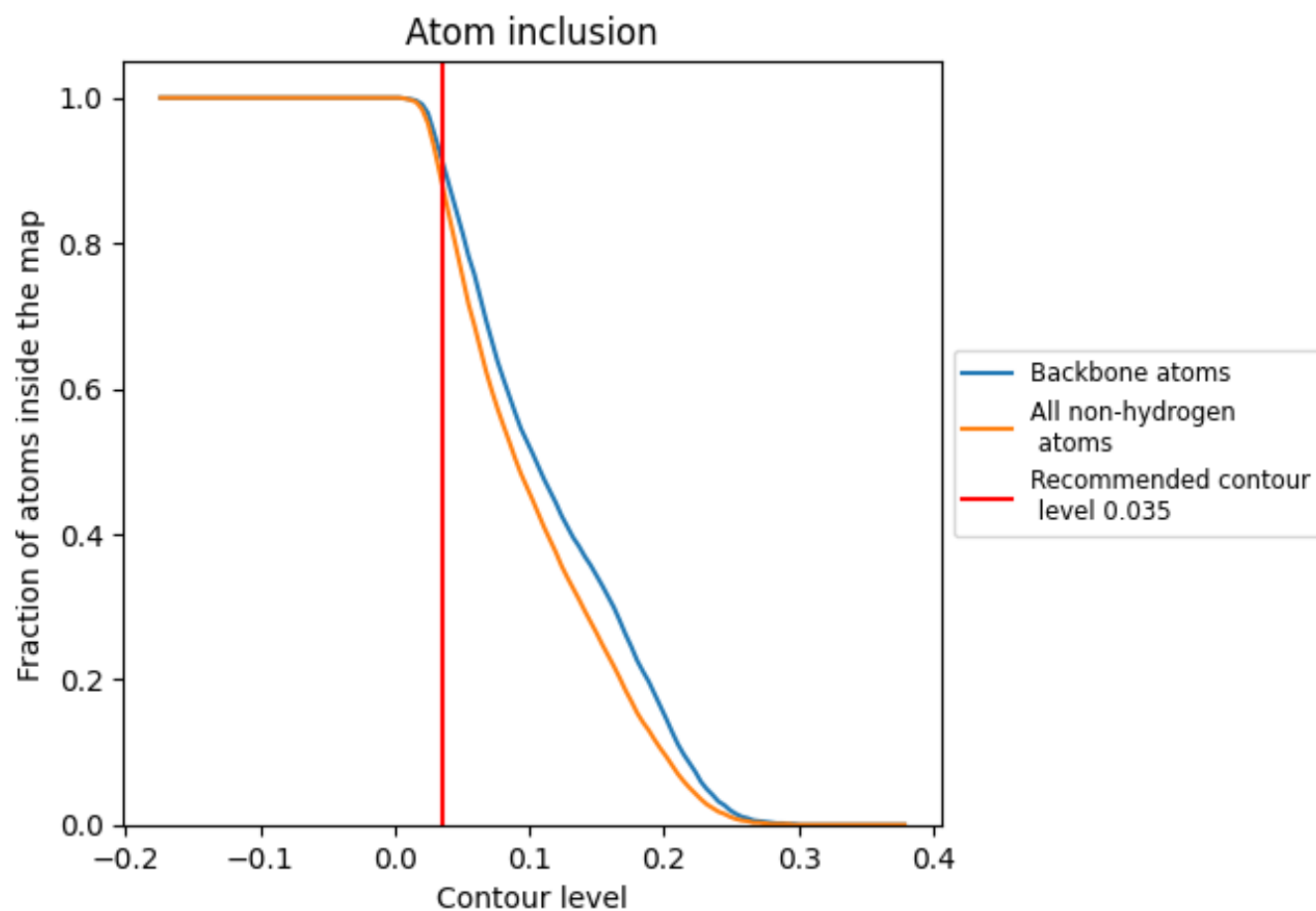
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.4150
A	0.8450	0.4050
B	0.9580	0.4360

