Full wwPDB EM Validation Report ⓘ

Oct 27, 2026 – 04:22 PM EDT

PDB ID	:	38YK / pdb_000038yk
EMDB ID	:	EMD-79237
Title	:	Cryo-EM structure of pSTAT1 bound to importin alpha 5 (2:1 assembly)
Authors	:	Kumar, P.; Vinkemeier, U.; Cingolani, G.
Deposited on	:	2026-09-23
Resolution	:	3.60 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:

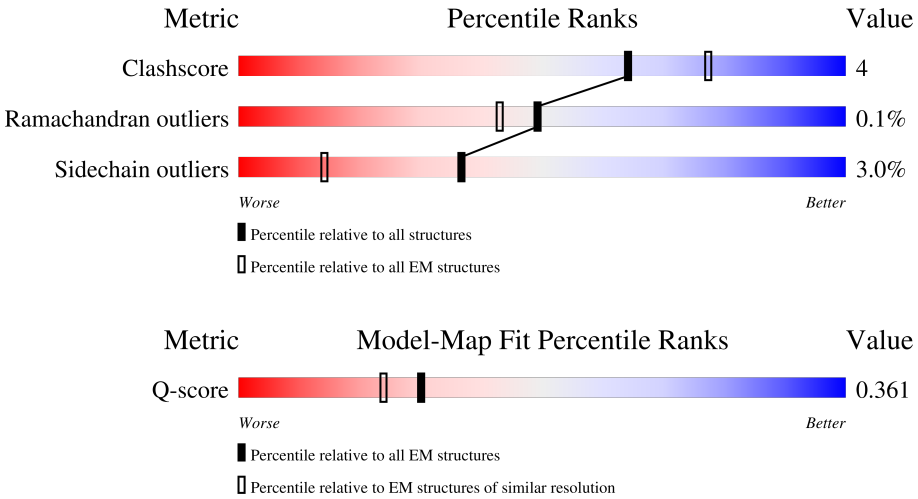
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.60 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	12797 (3.10 - 4.10)

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 <=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	C	538	71% 7% 22%
2	A	750	80% 13% • 6%
2	B	750	81% 11% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14849 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 Importin subunit alpha-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	422	3283	2087	552	626	18	0	0

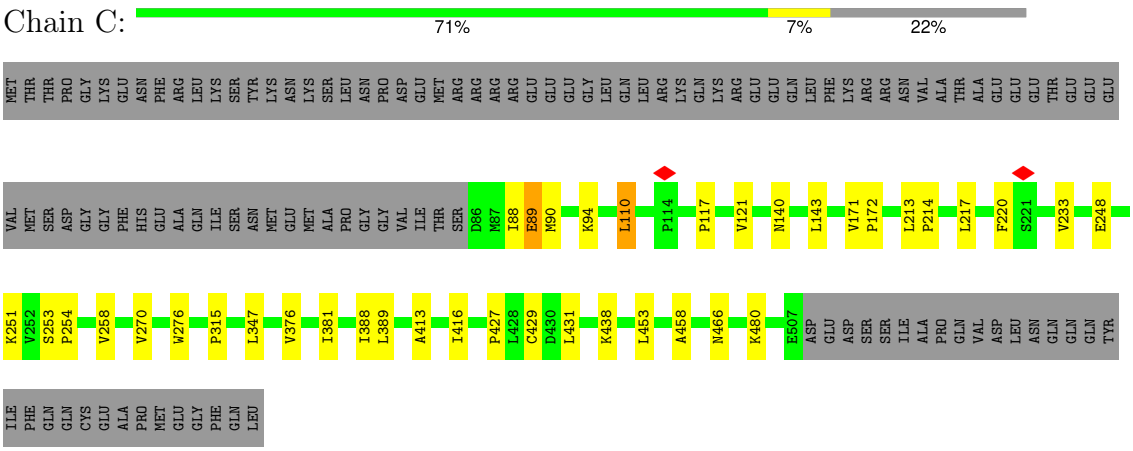
- Molecule 2 is a protein called Signal transducer and activator of transcription 1-alpha/beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
2	B	702	5779	3675	997	1082	1	24	0	0
			Total	C	N	O	P	S		
2	A	703	5787	3681	998	1083	1	24	0	0

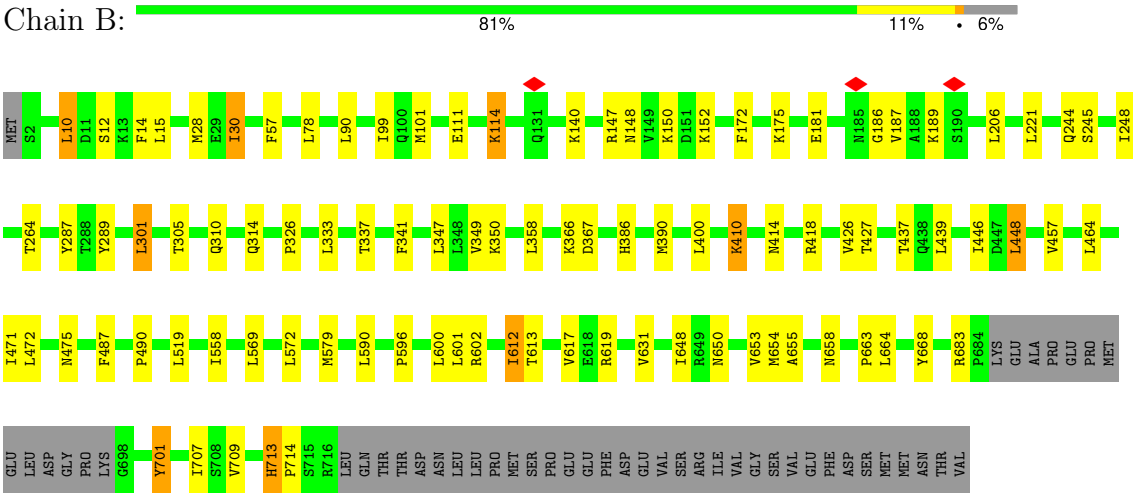
3 Residue-property plots (i)

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.

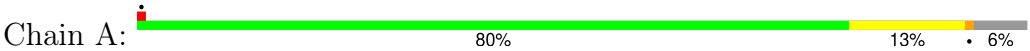
• Molecule 1: Importin subunit alpha-5

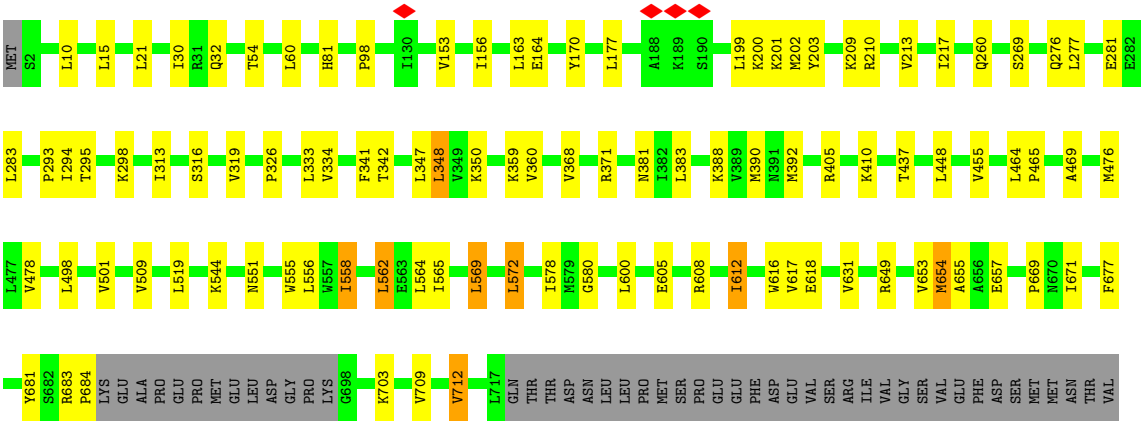


• Molecule 2: Signal transducer and activator of transcription 1-alpha/beta



• Molecule 2: Signal transducer and activator of transcription 1-alpha/beta




MET S2 L10 L15 L21 I30 R31 Q32 T54 L60 H81 P98 I130 V153 I156 L163 E164 Y170 L177 A188 K189 S190 L199 K200 K201 M202 Y203 K209 R210 V213 I217 Q260 S269 Q276 L277 E281 E282
L283 P293 I294 T295 K298 I313 S316 V319 P326 L333 V334 F341 T342 L347 L348 V349 K350 K359 V360 V368 R371 N381 I382 L383 K388 V389 M390 N391 M392 R405 K410 T437 L448 V455 L464 P465 A469 M476
L477 V478 L498 V501 V509 L519 K644 N551 W555 L556 W557 I568 L562 E563 L564 I565 L569 L572 I578 N579 G580 L600 E605 R608 I612 W616 V617 E618 V631 R649 V653 M654 A655 A656 E657 P669 N670 I671 F677
Y681 S682 R683 P684 LYS GLU ALA PRO GLU PRO MET GLU LEU ASP GLY PRO LYS G698 K703 V709 V712 L717 GLN THR THR ASP ASN LEU LEU PRO MET SER PRO GLU GLU PHE ASP GLU VAL SER ARG ILE VAL GLY SER VAL GLU PHE ASP SER MET MET ASN THR VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	246208	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	650	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	367.104, 367.104, 367.104	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.717, 0.717, 0.717	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.11	0/3341	0.34	0/4540
2	A	0.13	0/5893	0.34	0/7966
2	B	0.13	0/5885	0.34	0/7955
All	All	0.13	0/15119	0.34	0/20461

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	C	3283	0	3319	20	0
2	A	5787	0	5766	56	0
2	B	5779	0	5755	49	0
All	All	14849	0	14840	122	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 4.

All (122) 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:C:233:VAL:HG11	1:C:270:VAL:HA	1.73	0.71
2:A:156:ILE:HD11	2:A:213:VAL:HG13	1.76	0.68
2:B:683:ARG:HD3	2:B:683:ARG:H	1.57	0.67
2:A:54:THR:HG22	2:A:98:PRO:HG2	1.76	0.67
2:A:654:MET:HE1	2:A:657:GLU:H	1.60	0.66
1:C:110:LEU:HA	1:C:117:PRO:HD2	1.78	0.65
2:A:326:PRO:HD3	2:A:341:PHE:HA	1.79	0.65
2:B:326:PRO:HD3	2:B:341:PHE:HA	1.77	0.65
2:B:426:VAL:HG13	2:B:427:THR:HG23	1.80	0.63
2:B:314:GLN:HG3	2:B:446:ILE:HD11	1.82	0.62
2:B:111:GLU:HA	2:B:114:LYS:HE2	1.82	0.62
2:A:30:ILE:HD11	2:A:60:LEU:HD21	1.82	0.61
2:A:295:THR:HG23	2:A:298:LYS:HE2	1.84	0.59
1:C:413:ALA:HA	1:C:453:LEU:HD21	1.84	0.59
2:A:383:LEU:HD11	2:A:410:LYS:HB2	1.85	0.58
2:B:439:LEU:HB3	2:B:446:ILE:HG23	1.86	0.58
2:A:164:GLU:HG3	2:A:283:LEU:HD21	1.85	0.58
2:B:654:MET:HE3	2:B:709:VAL:HG21	1.84	0.58
2:B:181:GLU:HA	2:B:187:VAL:HG11	1.86	0.57
2:B:78:LEU:HD11	2:A:32:GLN:HG3	1.86	0.57
2:B:310:GLN:HG3	2:B:446:ILE:HD13	1.88	0.56
2:A:551:ASN:HB2	2:A:608:ARG:HH22	1.71	0.56
1:C:376:VAL:HG13	1:C:381:ILE:HD12	1.86	0.56
1:C:110:LEU:HD23	1:C:121:VAL:HG21	1.88	0.56
2:A:578:ILE:HG22	2:A:580:GLY:H	1.72	0.55
2:A:655:ALA:HB2	2:A:712:VAL:HG22	1.89	0.54
2:A:342:THR:HG22	2:A:405:ARG:HA	1.90	0.54
2:A:313:ILE:HG22	2:A:448:LEU:HD11	1.89	0.53
2:A:683:ARG:HD2	2:A:684:PRO:HD2	1.90	0.53
1:C:416:ILE:HD12	1:C:453:LEU:HD22	1.92	0.52
2:A:565:ILE:HD12	2:A:569:LEU:HB2	1.91	0.52
2:B:221:LEU:HD12	2:B:301:LEU:HD12	1.90	0.51
2:B:569:LEU:HD12	2:B:572:LEU:HD13	1.93	0.51
2:B:287:TYR:CE2	2:B:289:TYR:HB3	2.46	0.50
2:A:368:VAL:H	2:A:371:ARG:HH21	1.59	0.50
2:A:10:LEU:HB3	2:A:15:LEU:HD21	1.93	0.50
2:A:360:VAL:HG21	2:A:390:MET:HE2	1.93	0.50
2:B:487:PHE:O	2:B:490:PRO:HD3	2.12	0.50
2:A:170:TYR:HB3	2:A:202:MET:HE3	1.93	0.49
2:B:264:THR:HG22	2:B:350:LYS:H	1.77	0.49
1:C:140:ASN:HB3	1:C:143:LEU:HB3	1.94	0.49
2:B:314:GLN:HA	2:B:448:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:ASN:HA	2:B:418:ARG:HH22	1.78	0.49
2:A:153:VAL:HG21	2:A:269:SER:HB3	1.95	0.49
2:A:649:ARG:HB2	2:A:681:TYR:CE1	2.48	0.49
2:B:579:MET:HG2	2:B:600:LEU:HD12	1.94	0.48
2:B:713:HIS:H	2:B:713:HIS:CD2	2.31	0.48
2:A:260:GLN:NE2	2:A:350:LYS:HB2	2.28	0.48
1:C:389:LEU:HD23	1:C:427:PRO:HB2	1.96	0.47
2:A:316:SER:HB2	2:A:348:LEU:HB2	1.96	0.47
2:B:28:MET:HE2	2:A:81:HIS:HB3	1.96	0.47
1:C:276:TRP:CE2	1:C:315:PRO:HB3	2.50	0.47
2:A:572:LEU:HD21	2:A:677:PHE:HE1	1.78	0.47
2:B:172:PHE:HA	2:B:175:LYS:HE2	1.98	0.46
2:B:12:SER:HA	2:B:15:LEU:HD12	1.98	0.46
2:A:469:ALA:HB2	2:A:555:TRP:CD1	2.50	0.46
2:A:156:ILE:HG12	2:A:217:ILE:HD11	1.96	0.46
2:A:210:ARG:HD2	2:A:293:PRO:HG2	1.97	0.46
1:C:248:GLU:HB3	1:C:251:LYS:HE3	1.98	0.46
2:B:148:ASN:HD21	2:B:152:LYS:HE3	1.80	0.45
2:B:333:LEU:HB3	2:B:471:ILE:HD13	1.98	0.45
2:A:368:VAL:HB	2:A:371:ARG:HE	1.82	0.45
2:A:564:LEU:HD21	2:A:612:ILE:HG22	1.99	0.45
2:B:663:PRO:HG2	2:B:664:LEU:HD12	1.99	0.45
2:B:287:TYR:HE2	2:B:289:TYR:HB3	1.82	0.44
2:A:177:LEU:HD21	2:A:199:LEU:HD21	1.98	0.44
2:A:360:VAL:HA	2:A:437:THR:HB	1.99	0.44
1:C:217:LEU:HA	1:C:220:PHE:HD1	1.83	0.44
2:A:616:TRP:CD1	2:A:618:GLU:HG3	2.53	0.44
2:A:703:LYS:HB2	2:A:703:LYS:HE2	1.78	0.44
2:B:701:PTR:O2P	2:A:605:GLU:N	2.51	0.43
2:B:147:ARG:HA	2:B:150:LYS:HE2	1.99	0.43
2:A:350:LYS:HE3	2:A:392:MET:HE1	1.99	0.43
2:A:381:ASN:OD1	2:A:410:LYS:HB3	2.17	0.43
2:B:57:PHE:HB2	2:B:101:MET:HE3	2.01	0.43
2:A:210:ARG:HH11	2:A:294:ILE:HD11	1.83	0.43
2:B:186:GLY:HA2	2:B:189:LYS:HE3	2.01	0.43
2:A:277:LEU:O	2:A:281:GLU:HG3	2.19	0.43
1:C:217:LEU:HD22	1:C:258:VAL:HG21	2.01	0.43
2:A:359:LYS:HE3	2:A:359:LYS:HB3	1.84	0.43
2:A:163:LEU:HD21	2:A:209:LYS:HB3	2.01	0.43
1:C:171:VAL:HB	1:C:172:PRO:HD3	2.01	0.42
2:B:596:PRO:HB3	2:B:619:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:388:LYS:HE2	2:A:388:LYS:HB3	1.91	0.42
2:A:544:LYS:HD3	2:A:544:LYS:HA	1.66	0.42
1:C:89:GLU:H	1:C:89:GLU:HG3	1.56	0.42
2:A:156:ILE:HG23	2:A:276:GLN:HE22	1.84	0.42
2:B:366:LYS:HG2	2:B:367:ASP:OD1	2.19	0.42
2:B:650:ASN:HB2	2:B:707:ILE:HD12	2.01	0.42
2:A:201:LYS:HB3	2:A:201:LYS:HE3	1.71	0.42
2:A:476:MET:SD	2:A:501:VAL:HG21	2.60	0.42
2:A:551:ASN:HB2	2:A:608:ARG:HH12	1.84	0.42
1:C:347:LEU:HB3	1:C:388:ILE:HD11	2.01	0.42
2:B:655:ALA:HB3	2:B:658:ASN:HB2	2.02	0.42
2:A:200:LYS:HD3	2:A:203:TYR:HD2	1.84	0.42
2:B:10:LEU:HD13	2:B:14:PHE:HB2	2.02	0.41
2:B:358:LEU:HD12	2:B:390:MET:HG3	2.02	0.41
2:A:558:ILE:HD13	2:A:558:ILE:HA	1.95	0.41
2:A:519:LEU:HD12	2:A:519:LEU:HA	1.88	0.41
2:B:30:ILE:H	2:B:30:ILE:HG12	1.61	0.41
2:B:221:LEU:HD21	2:B:305:THR:HG22	2.02	0.41
2:B:590:LEU:HB3	2:B:668:TYR:CE1	2.56	0.41
2:A:347:LEU:HD23	2:A:390:MET:HE3	2.02	0.41
2:B:221:LEU:HD23	2:B:221:LEU:HA	1.83	0.41
2:B:437:THR:HG23	2:B:448:LEU:HB2	2.01	0.41
2:B:464:LEU:HD23	2:B:464:LEU:HA	1.85	0.41
2:B:601:LEU:HD11	2:B:648:ILE:HD11	2.02	0.41
2:A:509:VAL:HG21	2:A:562:LEU:HD11	2.03	0.41
2:B:244:GLN:HE21	2:B:475:ASN:HA	1.85	0.41
2:B:713:HIS:ND1	2:B:714:PRO:HD3	2.36	0.41
1:C:213:LEU:HB3	1:C:214:PRO:HD3	2.03	0.41
2:B:347:LEU:HD23	2:B:400:LEU:HD23	2.03	0.41
2:A:464:LEU:HB3	2:A:465:PRO:HD3	2.02	0.41
1:C:429:CYS:O	1:C:480:LYS:HD3	2.20	0.40
1:C:458:ALA:HB2	1:C:466:ASN:HA	2.03	0.40
2:B:140:LYS:HB3	2:B:140:LYS:HE3	1.83	0.40
2:B:410:LYS:HE2	2:B:410:LYS:HB3	1.70	0.40
1:C:253:SER:OG	1:C:254:PRO:HD3	2.21	0.40
2:B:602:ARG:O	2:B:612:ILE:HD12	2.21	0.40
2:A:333:LEU:HD23	2:A:333:LEU:HA	1.95	0.40
1:C:217:LEU:HA	1:C:220:PHE:CD1	2.56	0.40
2:A:669:PRO:HG2	2:A:671:ILE:HG13	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	C	420/538 (78%)	414 (99%)	5 (1%)	1 (0%)	43 72
2	A	698/750 (93%)	673 (96%)	25 (4%)	0	100 100
2	B	697/750 (93%)	663 (95%)	34 (5%)	0	100 100
All	All	1815/2038 (89%)	1750 (96%)	64 (4%)	1 (0%)	49 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	88	ILE

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	C	366/469 (78%)	360 (98%)	6 (2%)	55 69
2	A	651/695 (94%)	631 (97%)	20 (3%)	35 59
2	B	650/695 (94%)	626 (96%)	24 (4%)	30 56
All	All	1667/1859 (90%)	1617 (97%)	50 (3%)	37 59

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	89	GLU
1	C	90	MET

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Mol	Chain	Res	Type
1	C	94	LYS
1	C	110	LEU
1	C	431	LEU
1	C	438	LYS
2	B	10	LEU
2	B	30	ILE
2	B	90	LEU
2	B	99	ILE
2	B	114	LYS
2	B	206	LEU
2	B	245	SER
2	B	248	ILE
2	B	301	LEU
2	B	337	THR
2	B	349	VAL
2	B	386	HIS
2	B	410	LYS
2	B	448	LEU
2	B	457	VAL
2	B	472	LEU
2	B	519	LEU
2	B	558	ILE
2	B	612	ILE
2	B	613	THR
2	B	617	VAL
2	B	631	VAL
2	B	653	VAL
2	B	713	HIS
2	A	21	LEU
2	A	319	VAL
2	A	334	VAL
2	A	348	LEU
2	A	455	VAL
2	A	478	VAL
2	A	498	LEU
2	A	556	LEU
2	A	558	ILE
2	A	562	LEU
2	A	569	LEU
2	A	572	LEU
2	A	600	LEU
2	A	612	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	617	VAL
2	A	631	VAL
2	A	653	VAL
2	A	654	MET
2	A	709	VAL
2	A	712	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	494	GLN
2	B	228	GLN
2	B	291	HIS
2	B	322	GLN
2	B	463	GLN
2	B	551	ASN
2	B	658	ASN
2	A	82	ASN
2	A	89	ASN
2	A	310	GLN
2	A	314	GLN
2	A	372	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
2	PTR	A	701	2	15,16,17	0.52	0	17,22,24	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PTR	B	701	2	15,16,17	0.56	0	17,22,24	0.68	1 (5%)

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
2	PTR	A	701	2	-	5/10/11/13	0/1/1/1
2	PTR	B	701	2	-	4/10/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	PTR	O2P-P-OH	2.08	111.48	105.32

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	PTR	C-CA-CB-CG
2	A	701	PTR	C-CA-CB-CG
2	B	701	PTR	N-CA-CB-CG
2	A	701	PTR	N-CA-CB-CG
2	A	701	PTR	CA-CB-CG-CD2
2	A	701	PTR	CA-CB-CG-CD1
2	B	701	PTR	CA-CB-CG-CD1
2	B	701	PTR	CA-CB-CG-CD2
2	A	701	PTR	CZ-OH-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	PTR	1	0

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.

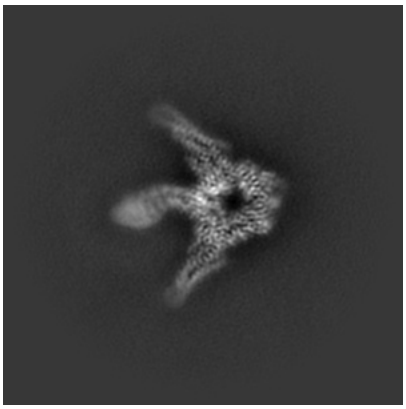
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-79237. These allow visual inspection of the internal detail of the map and identification of artifacts.

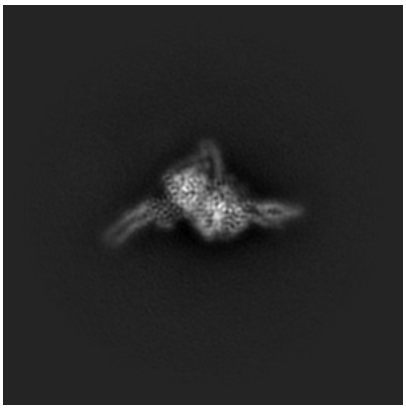
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

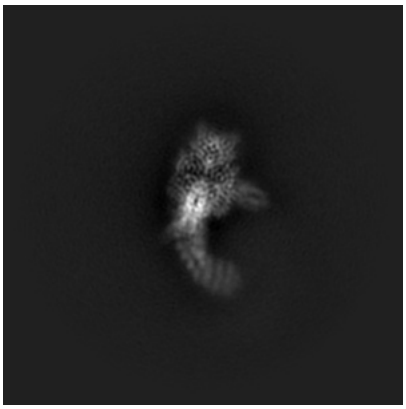
6.1.1 Primary map



X

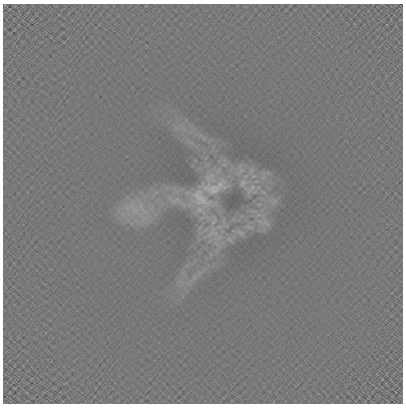


Y

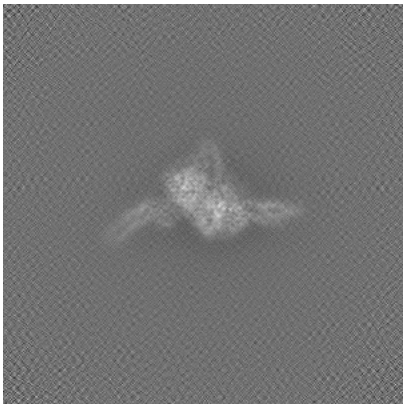


Z

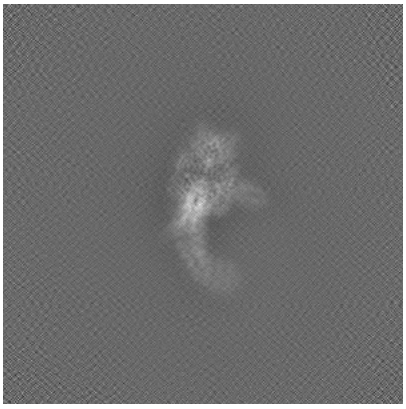
6.1.2 Raw map



X



Y

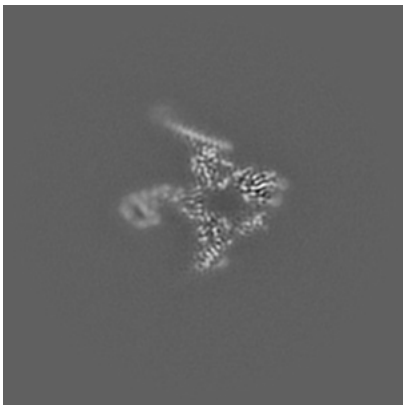


Z

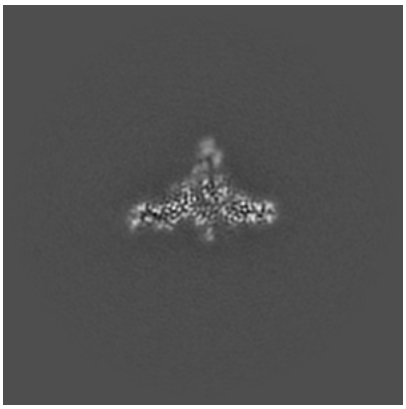
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

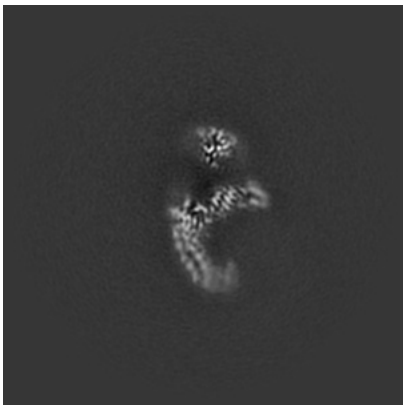
6.2.1 Primary map



X Index: 256

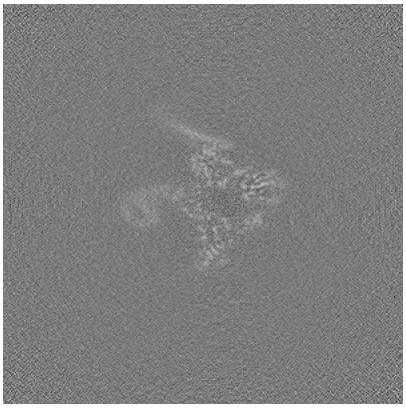


Y Index: 256

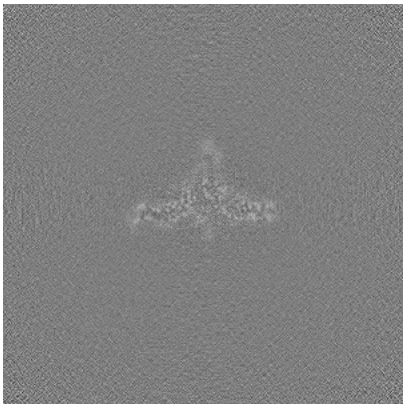


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

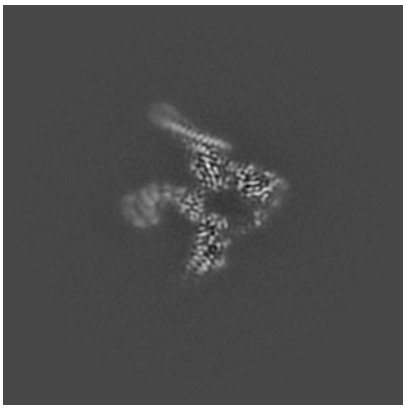


Z Index: 256

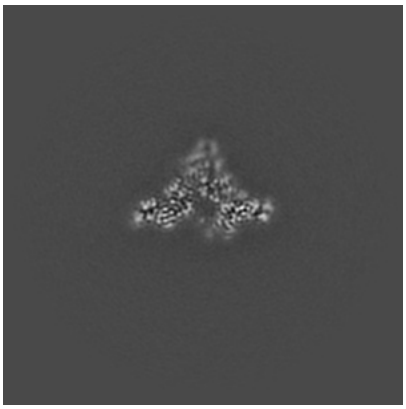
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 252

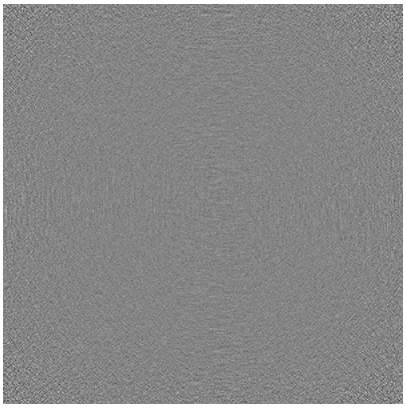


Y Index: 263

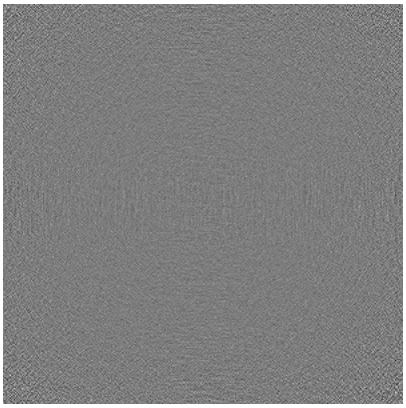


Z Index: 277

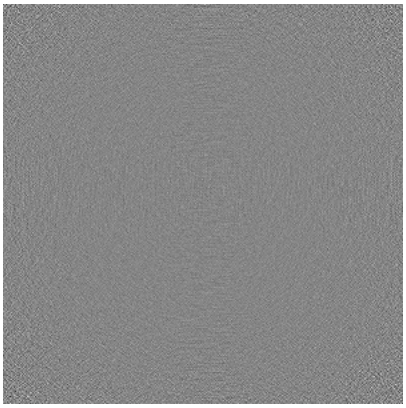
6.3.2 Raw map



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)

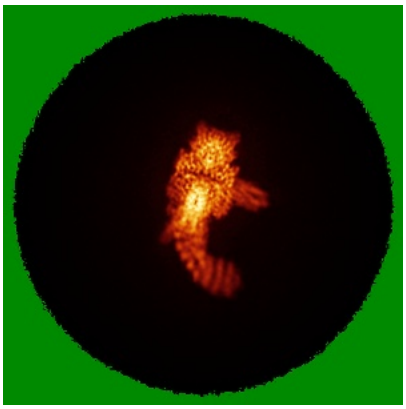
6.4.1 Primary map



X

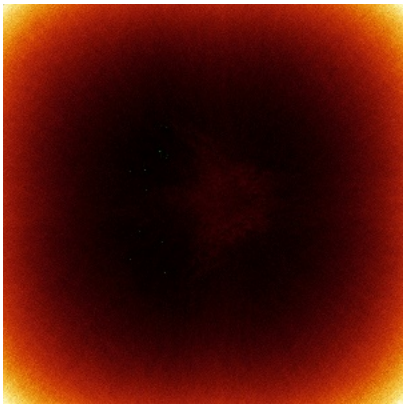


Y

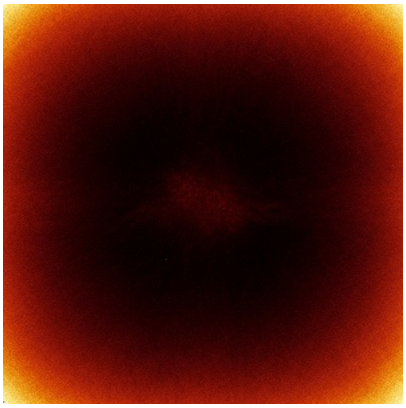


Z

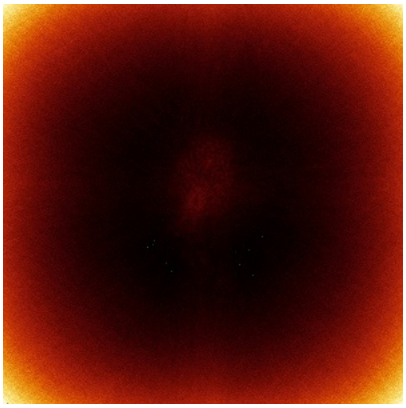
6.4.2 Raw map



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)

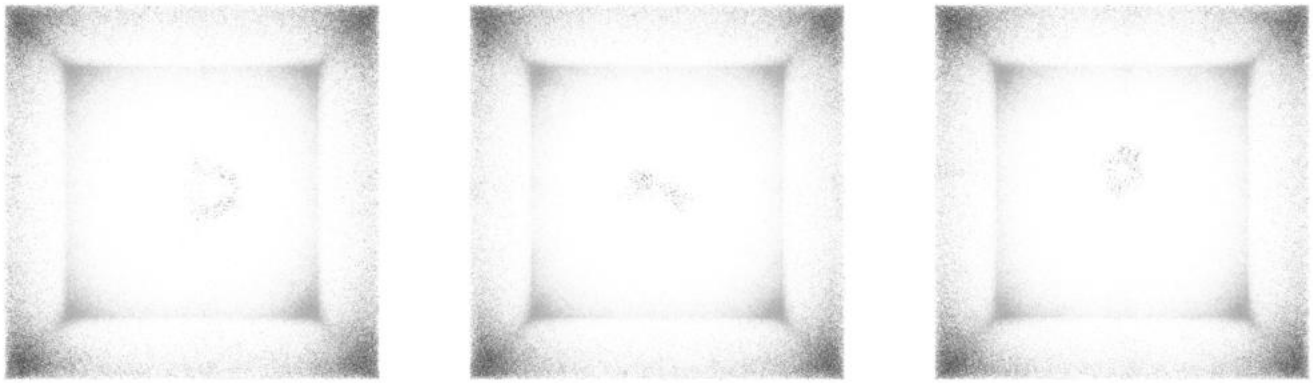
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



X Y Z

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.

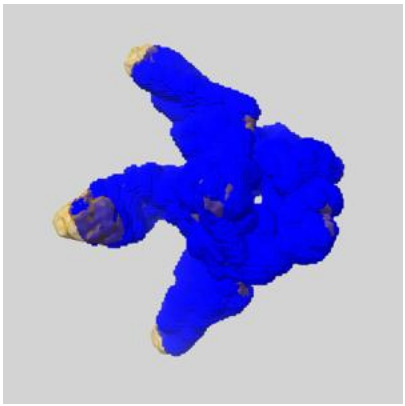
6.6 Mask visualisation (i)

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

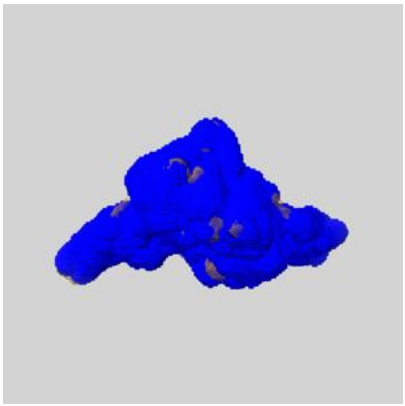
A mask typically either:

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

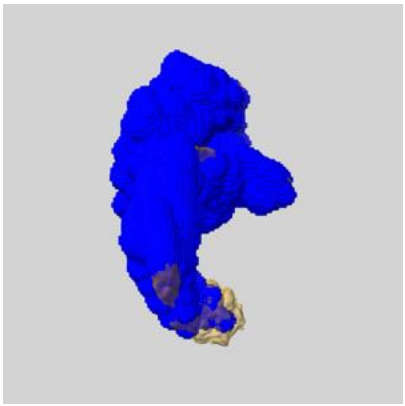
6.6.1 emd_79237_msk_1.map (i)



X



Y

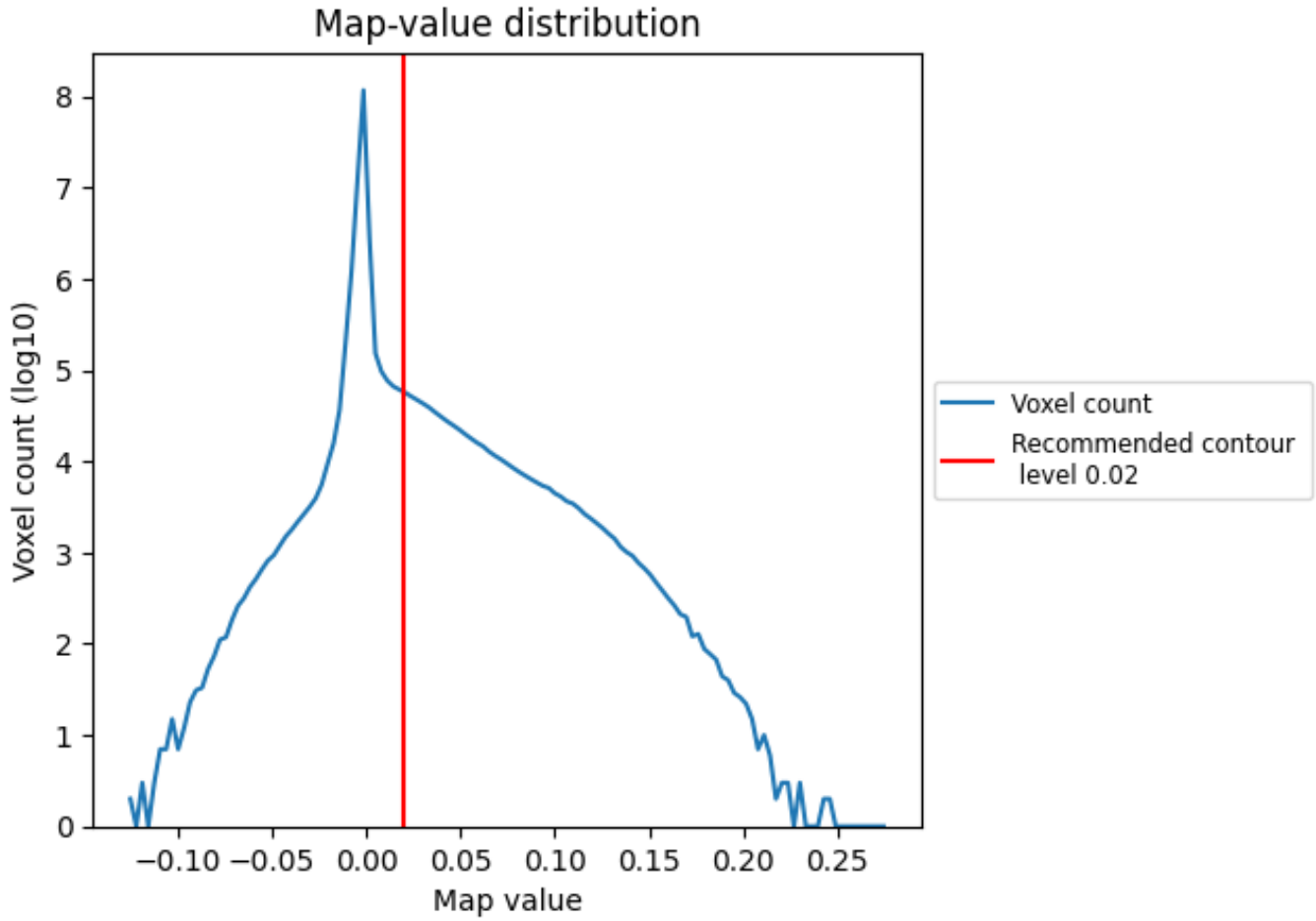


Z

7 Map analysis

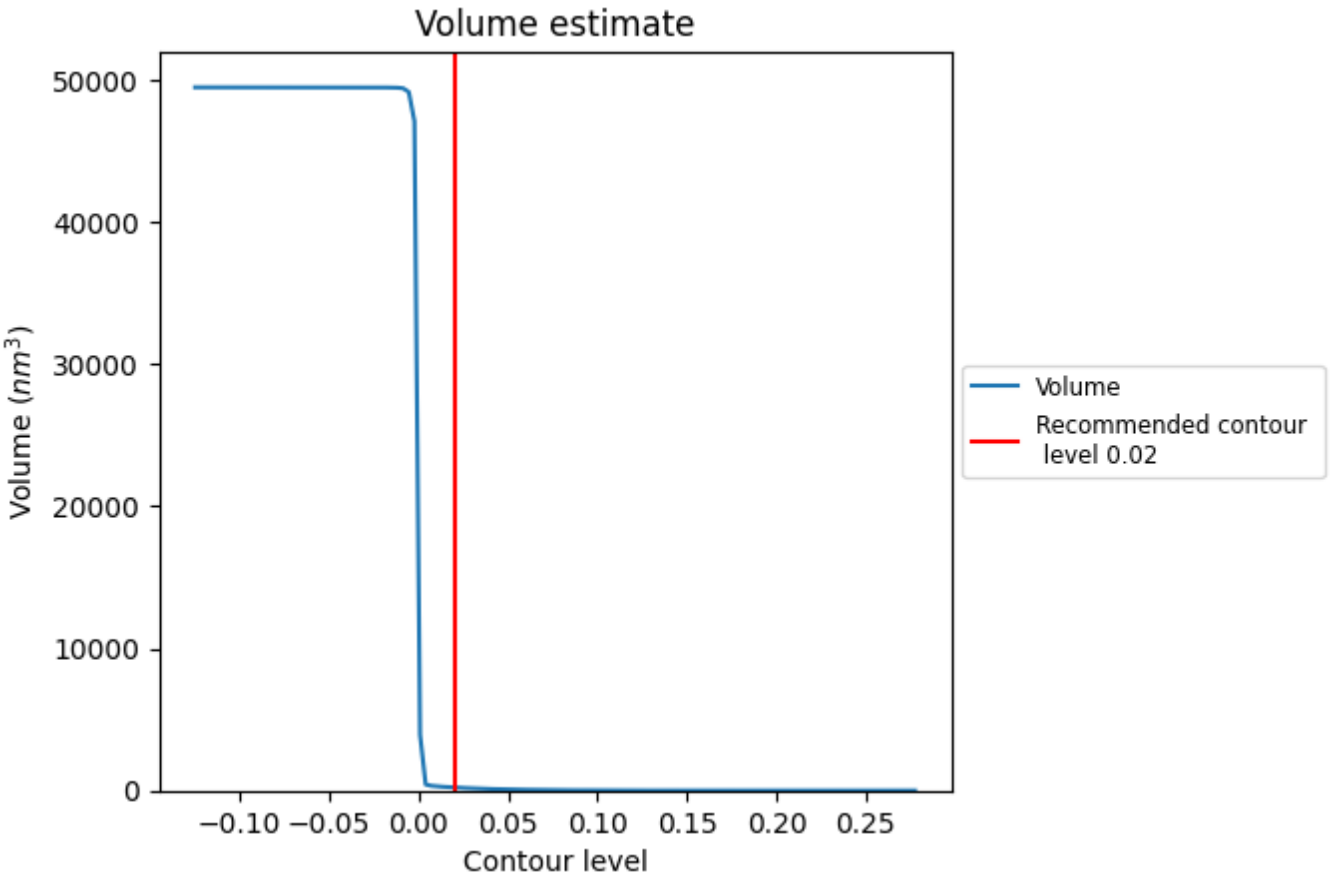
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

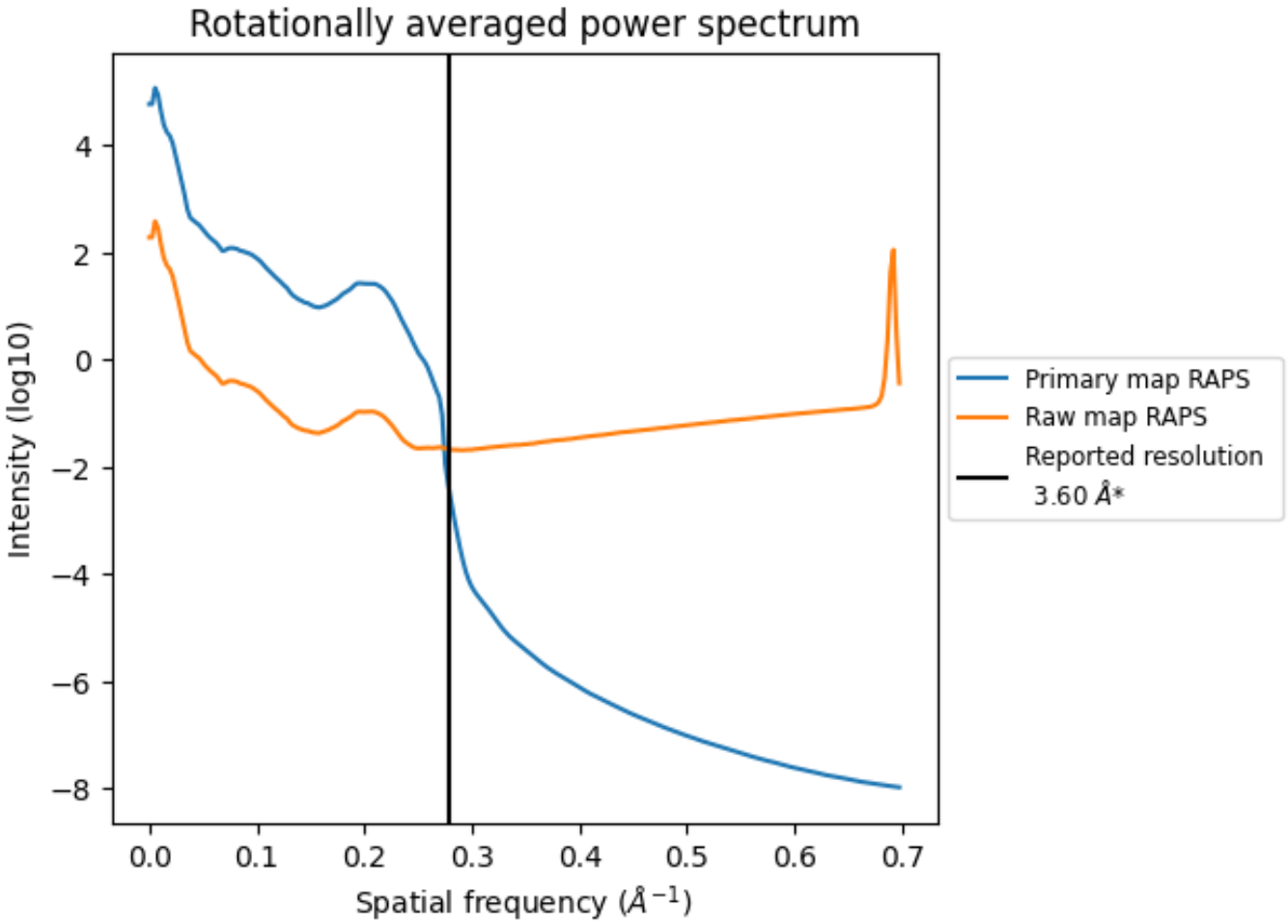
7.2 Volume estimate



The volume at the recommended contour level is 217 nm^3; this corresponds to an approximate mass of 196 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)

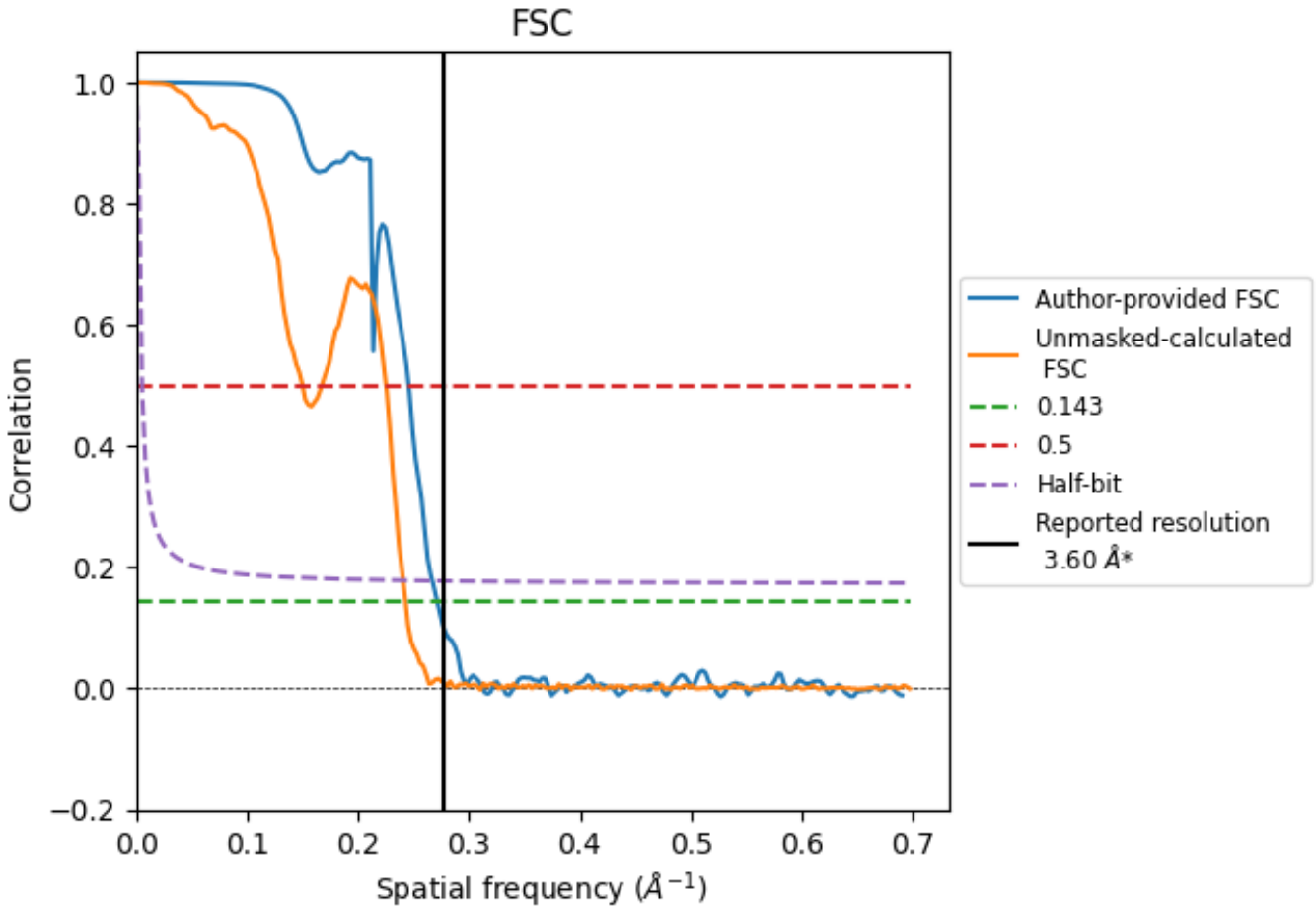


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

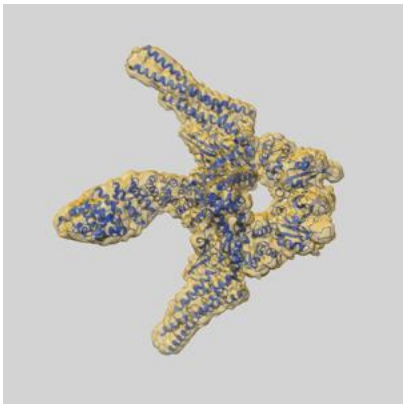
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.68	4.07	3.74
Unmasked-calculated*	4.12	6.67	4.15

*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 3.6 by more than 10 %

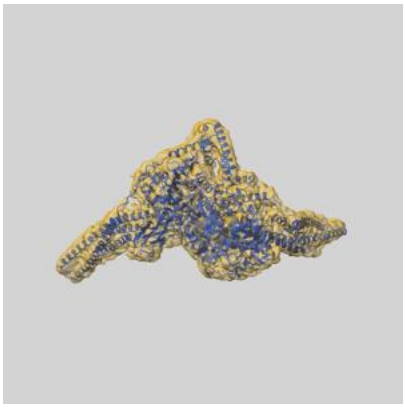
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-79237 and PDB model 38YK. Per-residue inclusion information can be found in section 3 on page 4.

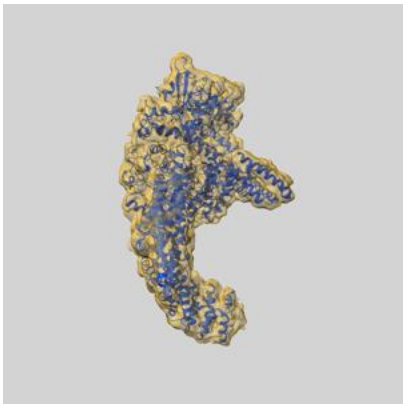
9.1 Map-model overlay



X



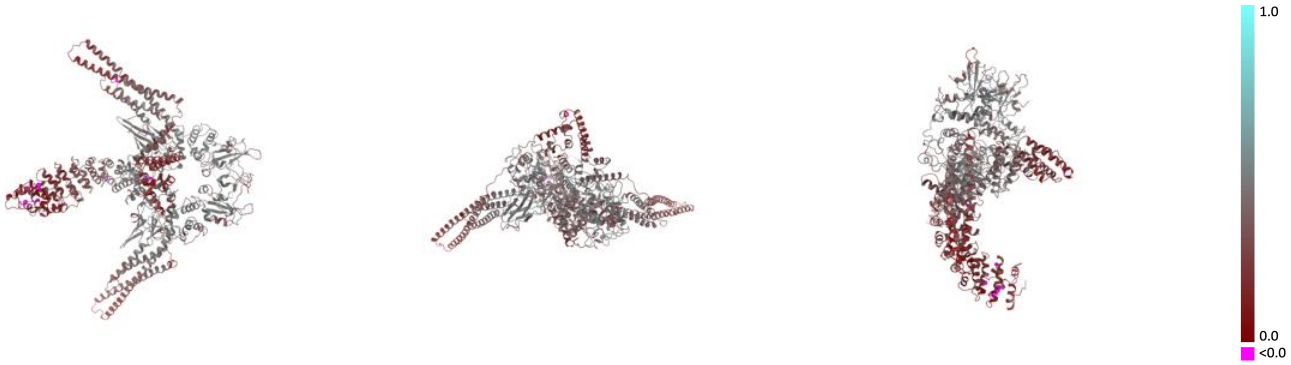
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

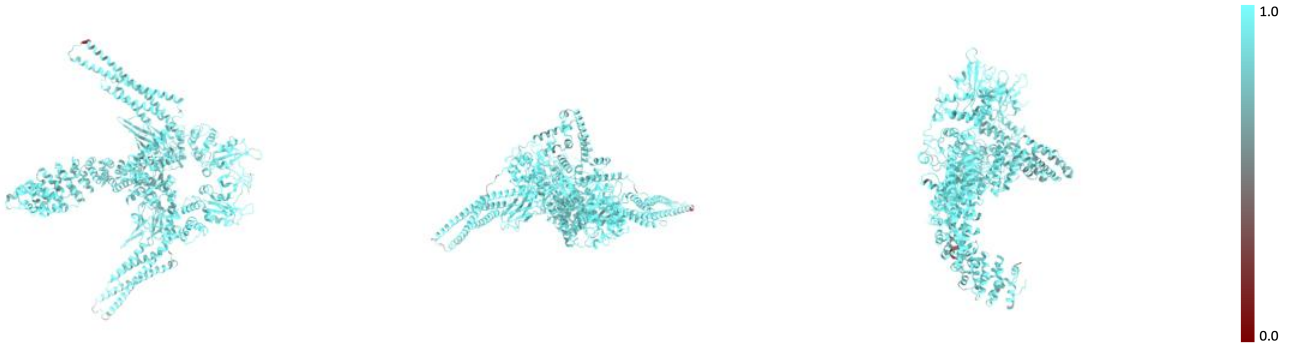
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

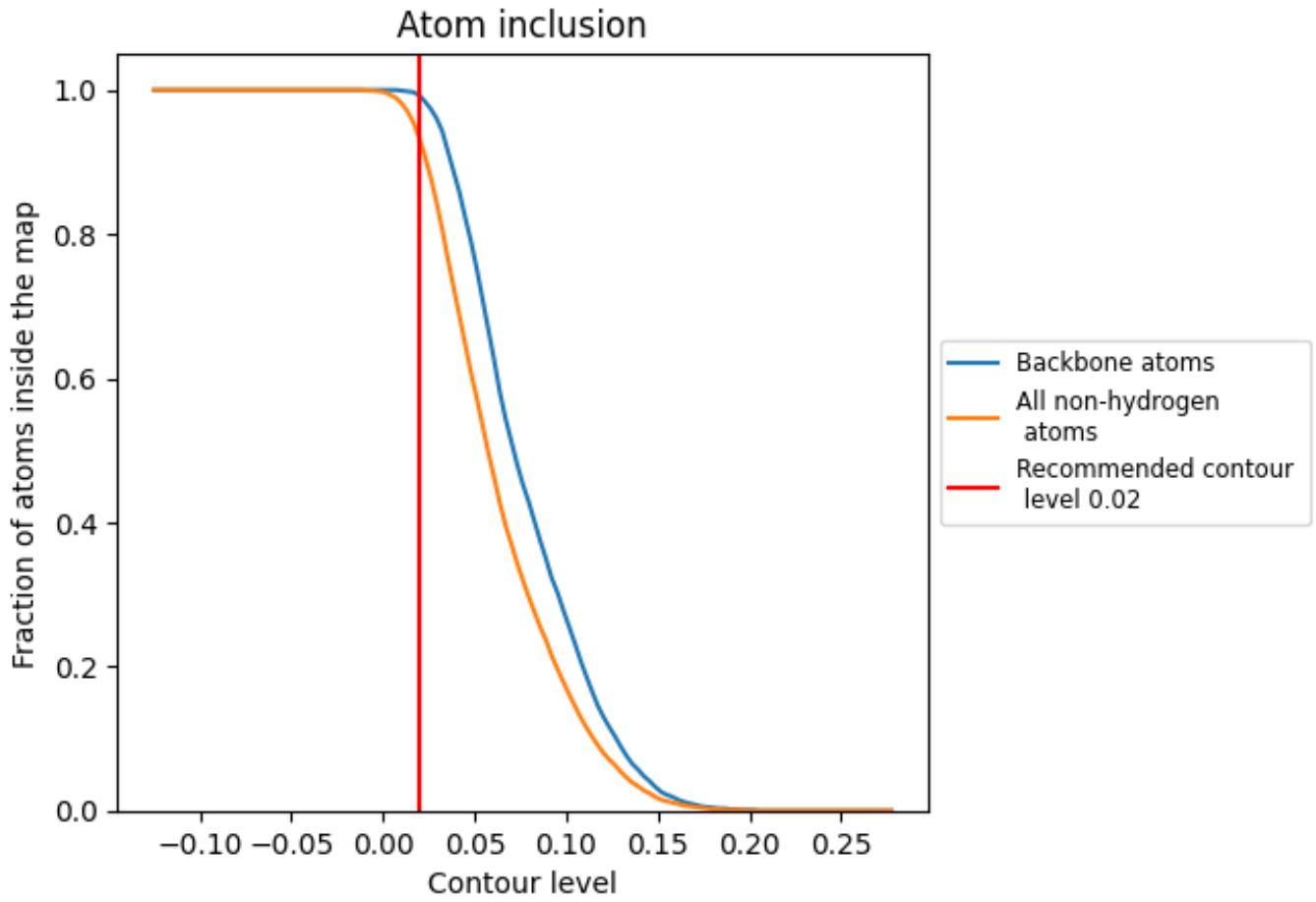
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.02) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9320	0.3610
A	0.9380	0.3960
B	0.9270	0.3760
C	0.9300	0.2730