



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:29 PM UTC

PDB ID : 7PPO / pdb\_00007ppo  
EMDB ID : EMD-13583  
Title : Structure of SidJ/CaM bound to SdeA in pre-glutamylation state  
Authors : Adams, M.; Bhogaraju, S.  
Deposited on : 2021-09-14  
Resolution : 2.91 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](mailto: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>.

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

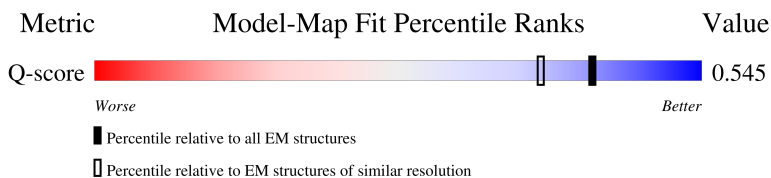
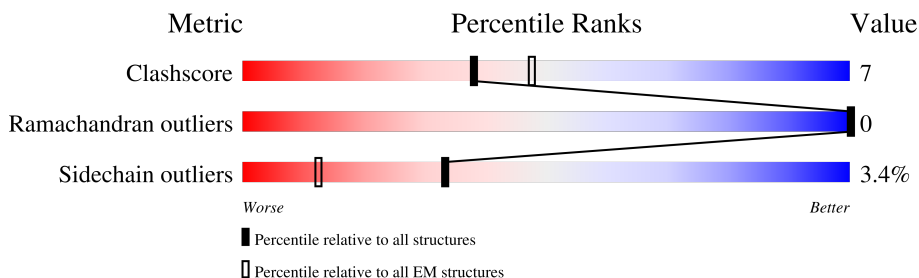
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 2.91 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	12972 ( 2.41 - 3.41 )

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  $\geq 3$ , 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	979	 5% 38% 12% • 49%
2	C	794	 77% 17% • 6%
3	B	168	 10% 64% 15% • 20%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10990 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 Ubiquitinating/deubiquitinating enzyme SdeA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
1	A	500	4003	2524	695	769	1	14	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	HIS	-	expression tag	UNP Q5ZTK4
A	213	HIS	-	expression tag	UNP Q5ZTK4
A	214	HIS	-	expression tag	UNP Q5ZTK4
A	215	HIS	-	expression tag	UNP Q5ZTK4
A	216	HIS	-	expression tag	UNP Q5ZTK4
A	217	HIS	-	expression tag	UNP Q5ZTK4
A	218	SER	-	expression tag	UNP Q5ZTK4
A	219	ALA	-	expression tag	UNP Q5ZTK4
A	220	GLY	-	expression tag	UNP Q5ZTK4
A	221	LEU	-	expression tag	UNP Q5ZTK4
A	222	GLU	-	expression tag	UNP Q5ZTK4
A	223	VAL	-	expression tag	UNP Q5ZTK4
A	224	LEU	-	expression tag	UNP Q5ZTK4
A	225	PHE	-	expression tag	UNP Q5ZTK4
A	226	GLN	-	expression tag	UNP Q5ZTK4
A	227	GLY	-	expression tag	UNP Q5ZTK4
A	228	PRO	-	expression tag	UNP Q5ZTK4
A	229	MET	-	expression tag	UNP Q5ZTK4
A	230	VAL	-	expression tag	UNP Q5ZTK4

- Molecule 2 is a protein called Calmodulin-dependent glutamylase SidJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	749	6099	3901	1033	1150	15	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	81	HIS	-	expression tag	UNP Q5ZTK6
C	82	HIS	-	expression tag	UNP Q5ZTK6
C	83	HIS	-	expression tag	UNP Q5ZTK6
C	84	HIS	-	expression tag	UNP Q5ZTK6
C	85	HIS	-	expression tag	UNP Q5ZTK6
C	86	HIS	-	expression tag	UNP Q5ZTK6
C	87	SER	-	expression tag	UNP Q5ZTK6
C	88	ALA	-	expression tag	UNP Q5ZTK6
C	89	GLY	-	expression tag	UNP Q5ZTK6
C	90	LEU	-	expression tag	UNP Q5ZTK6
C	91	GLU	-	expression tag	UNP Q5ZTK6
C	92	VAL	-	expression tag	UNP Q5ZTK6
C	93	LEU	-	expression tag	UNP Q5ZTK6
C	94	PHE	-	expression tag	UNP Q5ZTK6
C	95	GLN	-	expression tag	UNP Q5ZTK6
C	96	GLY	-	expression tag	UNP Q5ZTK6
C	97	PRO	-	expression tag	UNP Q5ZTK6
C	98	MET	-	expression tag	UNP Q5ZTK6
C	138	THR	ALA	variant	UNP Q5ZTK6
C	151	VAL	ILE	variant	UNP Q5ZTK6
C	153	GLN	LYS	variant	UNP Q5ZTK6
C	200	ILE	THR	variant	UNP Q5ZTK6
C	212	THR	MET	variant	UNP Q5ZTK6
C	371	ARG	LYS	variant	UNP Q5ZTK6
C	383	GLN	GLU	variant	UNP Q5ZTK6
C	393	SER	ARG	variant	UNP Q5ZTK6
C	398	TYR	HIS	variant	UNP Q5ZTK6
C	433	GLY	ASP	variant	UNP Q5ZTK6
C	447	LEU	GLN	variant	UNP Q5ZTK6
C	448	THR	SER	variant	UNP Q5ZTK6
C	483	MET	VAL	variant	UNP Q5ZTK6
C	565	ALA	GLU	engineered mutation	UNP Q5ZTK6
C	725	THR	VAL	variant	UNP Q5ZTK6
C	767	GLN	GLU	variant	UNP Q5ZTK6
C	798	ARG	GLY	variant	UNP Q5ZTK6
C	834	LYS	ARG	variant	UNP Q5ZTK6
C	848	THR	ALA	variant	UNP Q5ZTK6
C	855	ASN	LYS	variant	UNP Q5ZTK6
C	859	GLU	ASP	variant	UNP Q5ZTK6
C	874	LYS	-	variant	UNP Q5ZTK6

- Molecule 3 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	134	886	549	147	184	6	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP P0DP24
B	-17	HIS	-	expression tag	UNP P0DP24
B	-16	HIS	-	expression tag	UNP P0DP24
B	-15	HIS	-	expression tag	UNP P0DP24
B	-14	HIS	-	expression tag	UNP P0DP24
B	-13	HIS	-	expression tag	UNP P0DP24
B	-12	SER	-	expression tag	UNP P0DP24
B	-11	SER	-	expression tag	UNP P0DP24
B	-10	GLY	-	expression tag	UNP P0DP24
B	-9	LEU	-	expression tag	UNP P0DP24
B	-8	GLU	-	expression tag	UNP P0DP24
B	-7	VAL	-	expression tag	UNP P0DP24
B	-6	LEU	-	expression tag	UNP P0DP24
B	-5	PHE	-	expression tag	UNP P0DP24
B	-4	GLN	-	expression tag	UNP P0DP24
B	-3	GLY	-	expression tag	UNP P0DP24
B	-2	PRO	-	expression tag	UNP P0DP24
B	-1	HIS	-	expression tag	UNP P0DP24
B	0	MET	-	expression tag	UNP P0DP24

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Mg	0
			1	1	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Ca	0
			1	1	





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140022	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 ( $e^-/\text{\AA}^2$ )	47.45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.165	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	282.24, 282.24, 282.24	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.008, 1.008, 1.008	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, 86N

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	0.17	0/4055	0.33	0/5469
2	C	0.28	0/6239	0.35	0/8439
3	B	0.19	0/892	0.37	0/1211
All	All	0.24	0/11186	0.35	0/15119

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4003	0	3878	74	0
2	C	6099	0	6064	80	0
3	B	886	0	723	14	0
4	C	1	0	0	0	0
5	B	1	0	0	0	0
All	All	10990	0	10665	160	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 (160) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:GLU:HG3	1:A:803:LYS:HE3	1.62	0.81
1:A:306:LEU:HB3	1:A:314:THR:HG21	1.62	0.80
2:C:220:SER:OG	2:C:793:ASP:OD1	2.09	0.68
1:A:478:ILE:HA	1:A:484:PRO:HA	1.75	0.68
2:C:459:ASP:N	2:C:459:ASP:OD1	2.27	0.68
2:C:185:GLY:O	2:C:189:ASN:ND2	2.27	0.67
2:C:399:SER:OG	2:C:473:ASP:OD2	2.13	0.66
2:C:248:GLU:OE1	2:C:248:GLU:N	2.27	0.64
3:B:9:GLN:HE22	3:B:77:MET:HE1	1.63	0.64
1:A:330:GLN:HE21	1:A:403:ILE:HA	1.63	0.63
3:B:110:MET:HB3	3:B:117:LEU:HD12	1.80	0.63
2:C:176:ARG:O	2:C:180:ASN:ND2	2.27	0.63
1:A:397:THR:OG1	1:A:400:HIS:ND1	2.32	0.62
1:A:281:HIS:ND1	1:A:410:ASP:OD2	2.32	0.61
2:C:263:ASP:OD2	2:C:299:ASN:ND2	2.34	0.60
1:A:517:ASP:OD1	1:A:521:LYS:NZ	2.34	0.60
2:C:706:PRO:O	2:C:739:ARG:NH2	2.35	0.60
1:A:355:ARG:HG3	1:A:384:ALA:HB1	1.82	0.59
1:A:284:ARG:HD3	1:A:452:THR:HG21	1.84	0.59
1:A:236:THR:HB	2:C:293:ARG:HG2	1.84	0.59
1:A:434:GLY:O	1:A:438:THR:OG1	2.19	0.58
2:C:137:GLU:OE2	2:C:140:ARG:NE	2.36	0.58
2:C:626:MET:N	2:C:626:MET:SD	2.76	0.58
2:C:467:VAL:HG21	2:C:614:LEU:HD21	1.86	0.58
1:A:833:ASP:OD1	1:A:890:ARG:NH1	2.37	0.57
1:A:424:ARG:HG2	1:A:470:VAL:HB	1.87	0.57
1:A:759:LYS:NZ	2:C:711:THR:O	2.37	0.57
2:C:102:TYR:O	2:C:394:ARG:NH1	2.38	0.56
1:A:421:PHE:HA	1:A:470:VAL:HG21	1.87	0.56
2:C:552:LEU:HD22	2:C:598:LEU:HB3	1.88	0.56
2:C:340:GLN:H	2:C:340:GLN:CD	2.14	0.56
1:A:267:PHE:HB2	1:A:558:ALA:HB2	1.88	0.56
2:C:294:GLU:OE2	2:C:297:SER:OG	2.25	0.55
2:C:173:LEU:O	2:C:177:SER:OG	2.25	0.55
2:C:694:LEU:HD21	2:C:710:PHE:HZ	1.72	0.55
1:A:292:ILE:HG23	1:A:433:ILE:HD11	1.88	0.54
2:C:705:GLU:HB2	2:C:706:PRO:HD2	1.90	0.54
1:A:454:GLU:OE2	1:A:557:ARG:NH1	2.39	0.54
1:A:800:GLU:HA	1:A:803:LYS:HG2	1.88	0.54
1:A:874:VAL:HG23	1:A:896:VAL:HG13	1.90	0.54
2:C:180:ASN:O	2:C:790:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ASP:HA	1:A:550:ASN:HD21	1.72	0.53
3:B:37:MET:HG2	3:B:73:MET:HE1	1.88	0.53
2:C:557:ASP:OD1	2:C:557:ASP:N	2.39	0.53
1:A:547:ASP:OD2	1:A:547:ASP:N	2.42	0.53
2:C:453:LEU:O	2:C:458:GLN:NE2	2.42	0.53
1:A:248:TYR:HA	1:A:252:LEU:HB2	1.92	0.52
1:A:478:ILE:HD12	1:A:482:GLY:HA2	1.90	0.52
1:A:867:LEU:HD11	1:A:873:LEU:HG	1.90	0.52
2:C:502:ASP:OD1	2:C:502:ASP:N	2.42	0.52
1:A:771:SER:O	1:A:775:THR:OG1	2.22	0.52
3:B:27:THR:HB	3:B:63:THR:HB	1.92	0.52
2:C:368:VAL:HG12	2:C:440:VAL:HG12	1.92	0.51
2:C:492:HIS:CD2	2:C:493:THR:HG22	2.46	0.51
2:C:812:GLU:OE2	3:B:38:ARG:NH1	2.44	0.51
1:A:870:ASP:OD1	1:A:870:ASP:N	2.39	0.51
2:C:632:GLU:OE2	2:C:636:ARG:NH2	2.43	0.51
1:A:816:ARG:HH11	1:A:816:ARG:HA	1.77	0.50
1:A:844:ASP:N	1:A:844:ASP:OD1	2.44	0.50
2:C:205:LYS:HG3	2:C:206:GLU:HG2	1.93	0.50
3:B:6:THR:OG1	3:B:7:GLU:N	2.38	0.50
1:A:570:GLN:NE2	2:C:696:MET:SD	2.84	0.50
1:A:237:ASP:HB3	1:A:240:VAL:HG22	1.92	0.50
2:C:846:ARG:NH1	3:B:8:GLU:OE1	2.45	0.50
2:C:285:ASP:OD1	2:C:285:ASP:N	2.23	0.50
1:A:547:ASP:HA	1:A:550:ASN:ND2	2.26	0.50
1:A:766:ARG:HB2	1:A:821:THR:HG22	1.94	0.50
1:A:876:VAL:HG12	1:A:877:LYS:HG2	1.94	0.49
2:C:310:LEU:HD11	2:C:600:LEU:HD12	1.94	0.49
1:A:455:VAL:HG22	1:A:552:LEU:HD13	1.93	0.49
1:A:588:GLN:HE21	1:A:901:PRO:HD2	1.78	0.49
1:A:419:GLU:HB3	1:A:520:LEU:HD11	1.94	0.49
2:C:117:LEU:HD23	2:C:555:SER:HB2	1.93	0.49
2:C:341:MET:HE1	2:C:415:ILE:HD13	1.93	0.49
1:A:479:GLY:N	1:A:483:GLN:O	2.29	0.49
1:A:372:ASP:OD1	1:A:372:ASP:N	2.44	0.49
2:C:807:LEU:O	2:C:811:GLU:HG2	2.13	0.48
1:A:450:HIS:CD2	1:A:456:VAL:HG21	2.49	0.48
2:C:358:THR:HG22	2:C:360:GLN:H	1.78	0.48
1:A:249:ASP:O	1:A:254:LYS:NZ	2.44	0.47
1:A:395:GLU:HG3	1:A:432:TRP:HZ2	1.79	0.47
2:C:660:ARG:NH2	3:B:15:GLU:OE2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:VAL:HG22	2:C:442:VAL:HG22	1.96	0.47
1:A:400:HIS:O	1:A:404:ASN:ND2	2.35	0.47
1:A:512:ARG:HH12	1:A:515:ARG:HH12	1.63	0.47
2:C:141:ASN:O	2:C:145:GLN:HG2	2.16	0.46
2:C:173:LEU:HD22	2:C:223:PRO:HB2	1.97	0.46
2:C:427:ARG:NH2	2:C:430:THR:OG1	2.35	0.46
2:C:371:ARG:NH2	2:C:434:ASP:OD1	2.48	0.46
2:C:475:PHE:HE1	2:C:603:ILE:HG23	1.80	0.46
2:C:757:GLN:O	2:C:761:GLU:HG2	2.14	0.46
1:A:420:SER:HG	1:A:467:HIS:CE1	2.31	0.46
1:A:879:THR:HG22	1:A:880:LEU:H	1.80	0.45
1:A:573:THR:HG22	1:A:577:LYS:HE2	1.98	0.45
2:C:792:LEU:HB2	2:C:806:VAL:HG11	1.98	0.45
2:C:602:THR:O	2:C:605:GLU:HG3	2.16	0.45
1:A:460:ASP:OD1	1:A:535:HIS:ND1	2.49	0.45
2:C:522:ARG:NH1	2:C:524:ASP:OD1	2.38	0.45
2:C:698:GLN:HA	2:C:701:ILE:HG12	1.97	0.45
1:A:798:SER:HB2	1:A:800:GLU:OE1	2.17	0.44
2:C:665:LEU:HD23	2:C:665:LEU:HA	1.88	0.44
1:A:339:ASP:OD1	1:A:350:TYR:OH	2.20	0.44
1:A:363:LYS:HE3	1:A:363:LYS:HB3	1.76	0.44
2:C:196:LYS:HB3	2:C:197:PRO:HD3	1.98	0.44
2:C:389:LEU:HD11	2:C:403:GLN:HA	1.99	0.44
1:A:313:ARG:NH2	1:A:322:GLU:OE1	2.50	0.44
2:C:147:TYR:OH	2:C:171:HIS:ND1	2.38	0.44
3:B:4:GLN:HG3	3:B:5:LEU:H	1.82	0.44
2:C:335:SER:OG	2:C:338:ARG:NE	2.44	0.44
2:C:464:THR:HG22	2:C:641:VAL:HG22	2.00	0.44
3:B:42:GLN:O	3:B:44:PRO:HD3	2.17	0.43
2:C:670:ASN:HD22	2:C:673:LYS:HD3	1.84	0.43
1:A:476:TYR:O	1:A:514:MET:N	2.50	0.43
2:C:347:LEU:HD21	2:C:357:SER:HB3	2.01	0.43
2:C:458:GLN:O	2:C:617:TYR:OH	2.26	0.43
2:C:692:ASP:OD1	2:C:693:THR:N	2.51	0.43
1:A:383:TYR:O	1:A:386:VAL:HG12	2.18	0.43
1:A:437:ALA:O	1:A:441:VAL:HG23	2.17	0.43
2:C:173:LEU:HD21	2:C:213:ILE:HG23	2.00	0.43
1:A:480:GLU:OE1	1:A:510:ASN:N	2.51	0.43
2:C:109:GLU:HG3	2:C:314:GLU:HB3	2.01	0.43
1:A:395:GLU:HG3	1:A:432:TRP:CZ2	2.53	0.43
2:C:780:ASP:OD1	2:C:780:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:PRO:HA	1:A:515:ARG:HA	2.01	0.42
1:A:583:ILE:HG21	1:A:874:VAL:HG21	2.00	0.42
1:A:448:PHE:O	1:A:452:THR:HG22	2.19	0.42
1:A:798:SER:HB2	1:A:800:GLU:H	1.83	0.42
1:A:310:LYS:NZ	1:A:396:SER:HA	2.34	0.42
2:C:637:GLU:O	2:C:641:VAL:HG23	2.19	0.42
3:B:106:LEU:O	3:B:110:MET:HG2	2.20	0.42
1:A:284:ARG:HH21	1:A:452:THR:HG21	1.83	0.42
2:C:756:MET:HA	2:C:756:MET:HE2	2.01	0.42
2:C:837:ALA:HA	2:C:840:THR:HG22	2.01	0.42
2:C:510:VAL:HG12	2:C:520:LEU:HD12	2.02	0.42
2:C:553:PHE:HD1	2:C:595:GLY:HA3	1.85	0.42
3:B:42:GLN:HE21	3:B:42:GLN:HB3	1.66	0.42
1:A:375:LYS:HG3	1:A:376:ASP:OD1	2.20	0.41
2:C:697:GLU:O	2:C:701:ILE:HG23	2.19	0.41
2:C:177:SER:HB3	2:C:222:TYR:HA	2.02	0.41
2:C:453:LEU:HB3	2:C:613:THR:HG21	2.03	0.41
1:A:822:THR:OG1	1:A:823:THR:N	2.54	0.41
1:A:290:GLU:O	1:A:293:VAL:HG12	2.21	0.41
1:A:464:LYS:HD2	1:A:515:ARG:HD2	2.02	0.41
1:A:860:86N:O3P	2:C:492:HIS:NE2	2.42	0.41
2:C:611:GLN:HB2	2:C:642:MET:HE2	2.02	0.41
2:C:615:GLY:HA3	2:C:682:MET:SD	2.61	0.41
1:A:234:LEU:HB2	1:A:327:MET:SD	2.60	0.41
1:A:281:HIS:O	1:A:285:THR:HG23	2.21	0.41
2:C:236:ASN:HA	2:C:265:SER:HB2	2.03	0.41
2:C:412:LYS:HG2	2:C:416:LEU:HD23	2.03	0.41
2:C:694:LEU:HD21	2:C:710:PHE:CZ	2.53	0.41
3:B:28:ILE:HB	3:B:32:GLU:OE1	2.21	0.41
2:C:841:ILE:HD13	2:C:841:ILE:HA	1.93	0.41
1:A:588:GLN:H	1:A:588:GLN:HG2	1.68	0.40
2:C:289:ASN:O	2:C:291:MET:N	2.45	0.40
2:C:492:HIS:HB2	2:C:506:TYR:HD1	1.86	0.40
3:B:118:THR:OG1	3:B:119:ASP:N	2.55	0.40
1:A:343:ASP:OD2	1:A:346:ASN:ND2	2.48	0.40
1:A:371:PRO:HG3	2:C:209:VAL:HG22	2.03	0.40
1:A:798:SER:OG	1:A:800:GLU:HB2	2.22	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	491/979 (50%)	451 (92%)	40 (8%)	0	100	100
2	C	747/794 (94%)	714 (96%)	33 (4%)	0	100	100
3	B	128/168 (76%)	125 (98%)	3 (2%)	0	100	100
All	All	1366/1941 (70%)	1290 (94%)	76 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/851 (50%)	409 (96%)	18 (4%)	26	59
2	C	677/721 (94%)	662 (98%)	15 (2%)	45	75
3	B	69/144 (48%)	62 (90%)	7 (10%)	7	23
All	All	1173/1716 (68%)	1133 (97%)	40 (3%)	33	65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	THR
1	A	305	THR
1	A	314	THR
1	A	368	THR
1	A	409	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	413	ARG
1	A	438	THR
1	A	543	MET
1	A	547	ASP
1	A	581	GLU
1	A	773	GLU
1	A	780	ASP
1	A	795	THR
1	A	802	PHE
1	A	822	THR
1	A	867	LEU
1	A	874	VAL
1	A	879	THR
2	C	123	VAL
2	C	177	SER
2	C	204	SER
2	C	215	GLU
2	C	285	ASP
2	C	306	THR
2	C	397	VAL
2	C	424	ASP
2	C	447	LEU
2	C	459	ASP
2	C	502	ASP
2	C	515	VAL
2	C	621	VAL
2	C	675	PHE
2	C	845	TRP
3	B	29	THR
3	B	32	GLU
3	B	45	THR
3	B	94	ASP
3	B	111	THR
3	B	115	GLU
3	B	118	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	330	GLN
1	A	377	GLN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	A	381	ASN
1	A	423	GLN
1	A	430	GLN
1	A	537	GLN
1	A	550	ASN
1	A	572	GLN
1	A	588	GLN
2	C	145	GLN
2	C	153	GLN
2	C	167	GLN
2	C	254	GLN
2	C	289	ASN
2	C	454	HIS
2	C	494	HIS
2	C	561	HIS
2	C	670	ASN
2	C	679	GLN
3	B	9	GLN
3	B	42	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](#)

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
1	86N	A	860	1	29,33,34	3.36	10 (34%)	30,48,50	2.47	7 (23%)

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
1	86N	A	860	1	-	5/16/22/24	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	860	86N	P-OE1	14.13	1.87	1.60
1	A	860	86N	P-O2P	5.43	1.69	1.50
1	A	860	86N	P-O3P	4.66	1.76	1.55
1	A	860	86N	P-O5'	4.49	1.77	1.59
1	A	860	86N	O5'-C5'	-3.68	1.39	1.43
1	A	860	86N	C5'-C4'	2.70	1.52	1.48
1	A	860	86N	C8-N9	2.64	1.41	1.37
1	A	860	86N	O-C	2.46	1.29	1.20
1	A	860	86N	C5-C4	2.46	1.43	1.39
1	A	860	86N	C6-N6	2.10	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	86N	OE1-P-O5'	8.12	127.39	103.00
1	A	860	86N	CB-CG-CD	6.68	132.18	113.21
1	A	860	86N	OE1-P-O2P	-4.60	95.13	109.95
1	A	860	86N	C5-C4-N9	4.32	107.36	105.06
1	A	860	86N	C4'-O4'-C1'	2.81	109.16	106.16
1	A	860	86N	OE2-CD-CG	-2.47	114.14	123.78
1	A	860	86N	O5'-P-O2P	-2.05	100.81	108.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	860	86N	C-CA-CB-CG
1	A	860	86N	C4'-C5'-O5'-P
1	A	860	86N	C5'-O5'-P-O2P
1	A	860	86N	OE1-CD-CG-CB
1	A	860	86N	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	860	86N	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

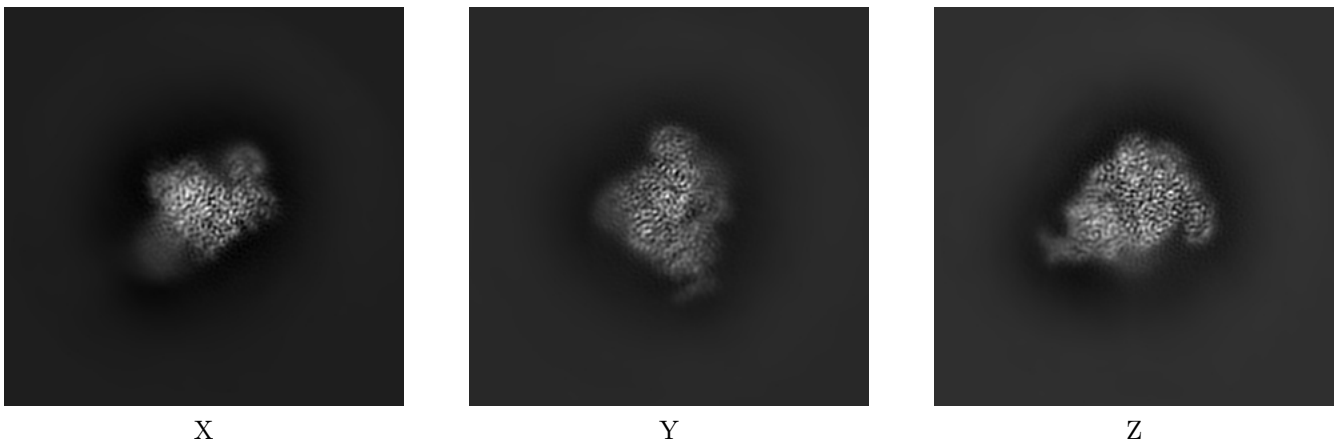
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13583. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

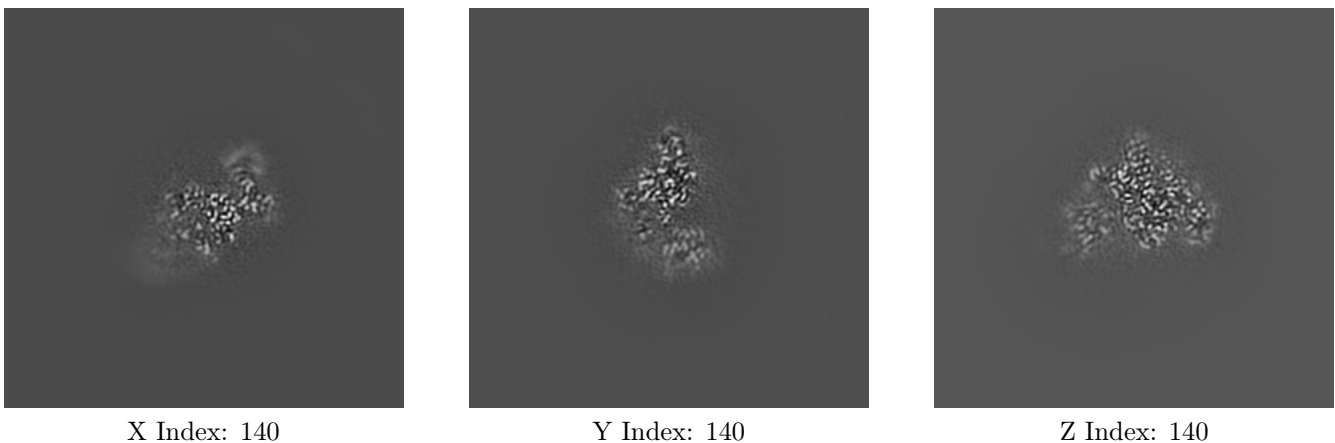
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

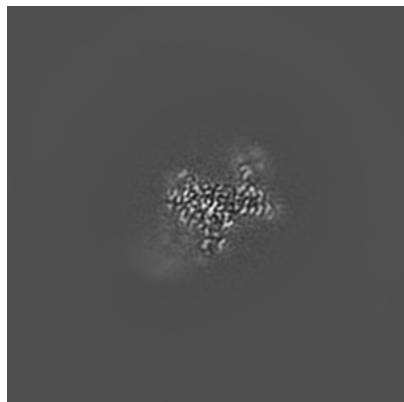
#### 6.2.1 Primary map



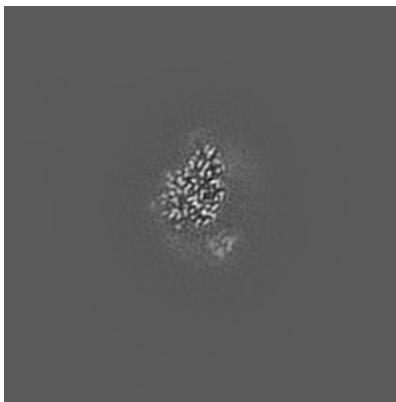
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

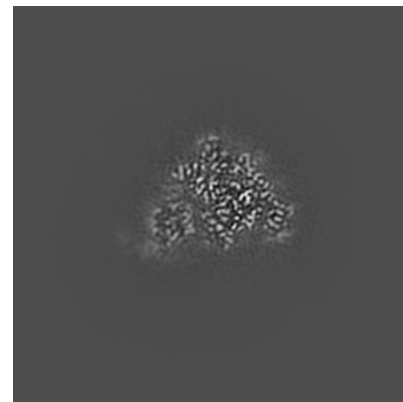
### 6.3.1 Primary map



X Index: 146



Y Index: 148

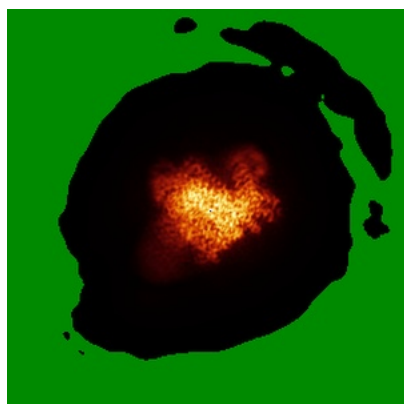


Z Index: 143

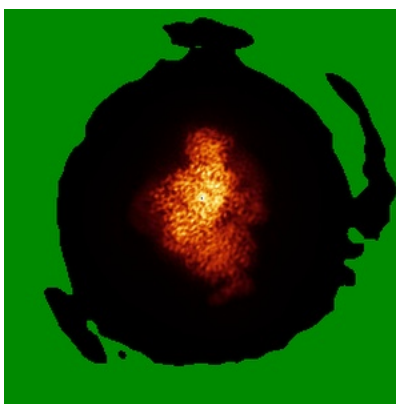
The images above show the largest variance slices of the map in three orthogonal directions.

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

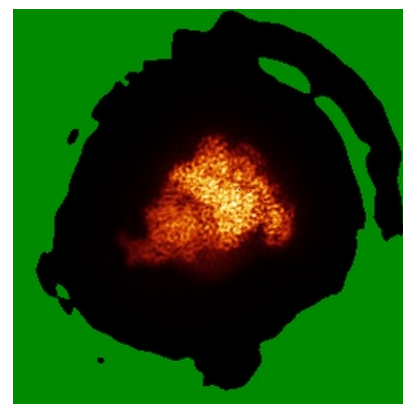
### 6.4.1 Primary map



X



Y

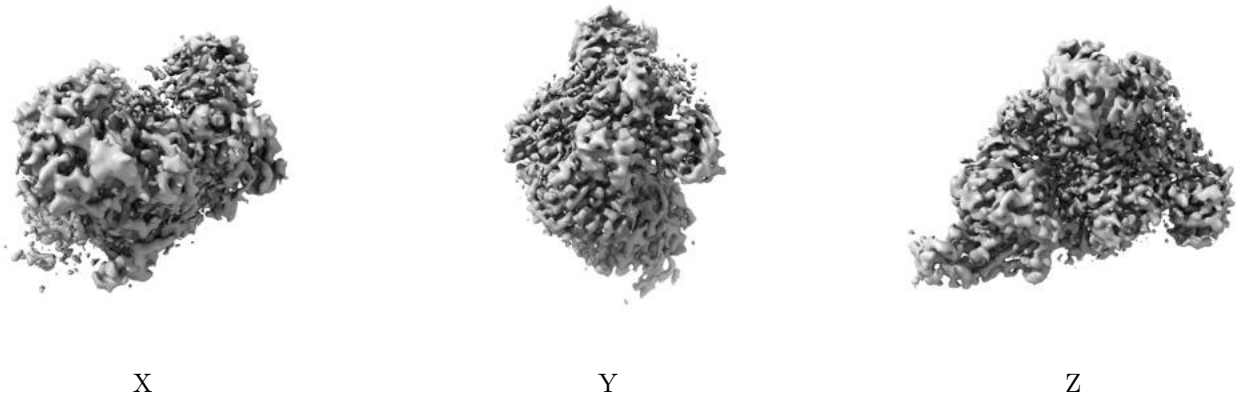


Z

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

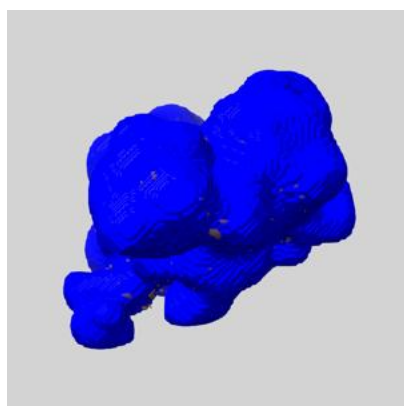
## 6.6 Mask visualisation [i](#)

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

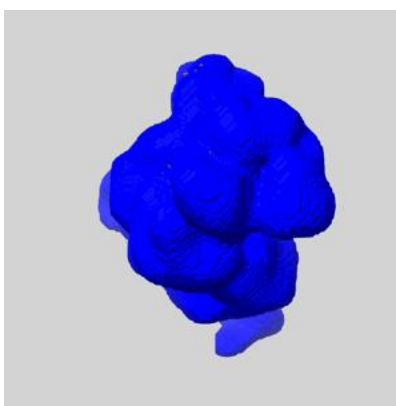
A mask typically either:

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

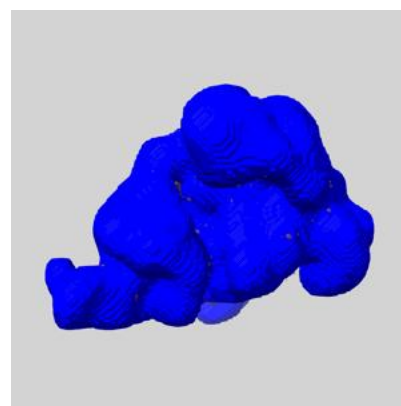
### 6.6.1 emd\_13583\_msk\_1.map [i](#)



X



Y

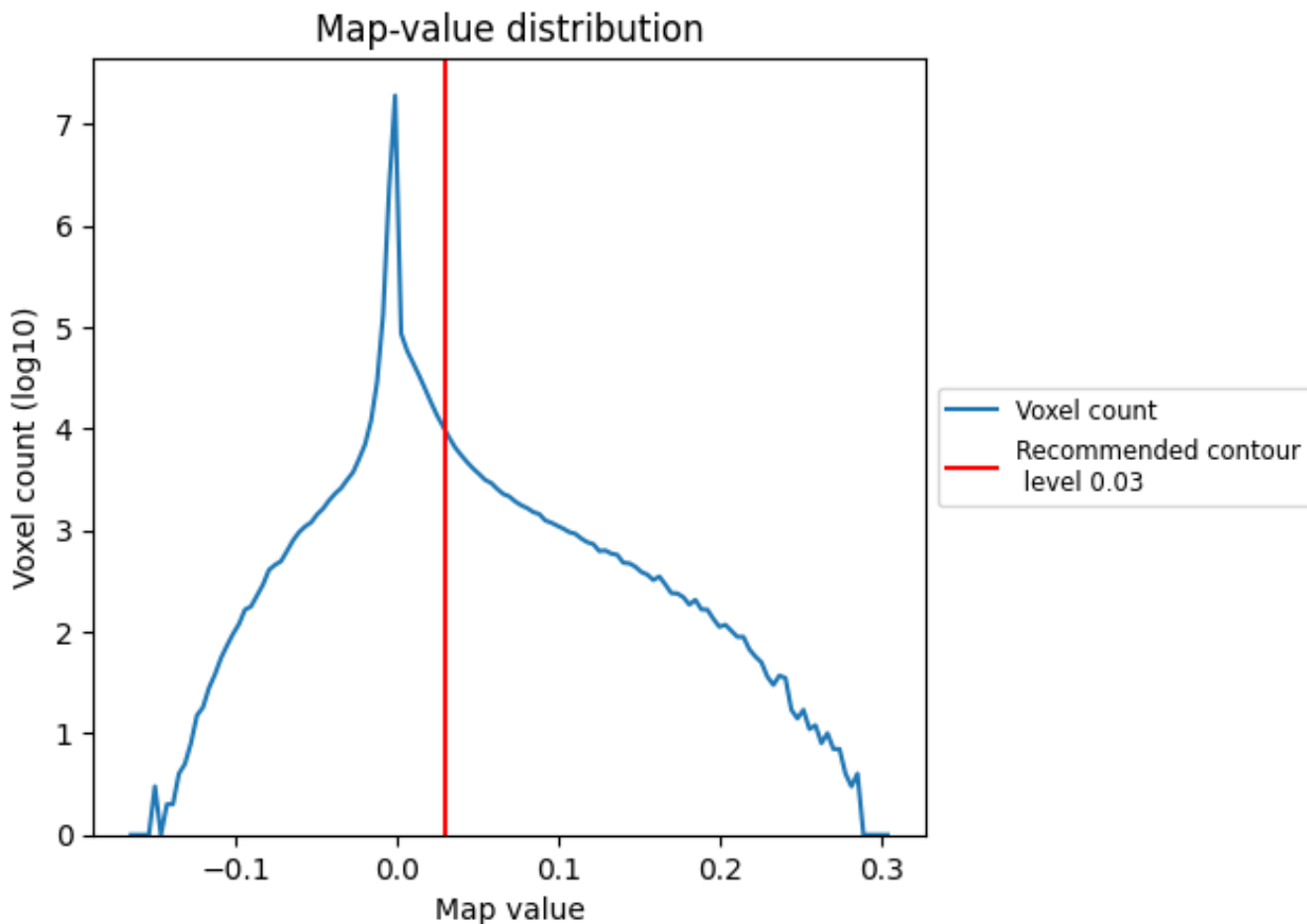


Z

## 7 Map analysis [i](#)

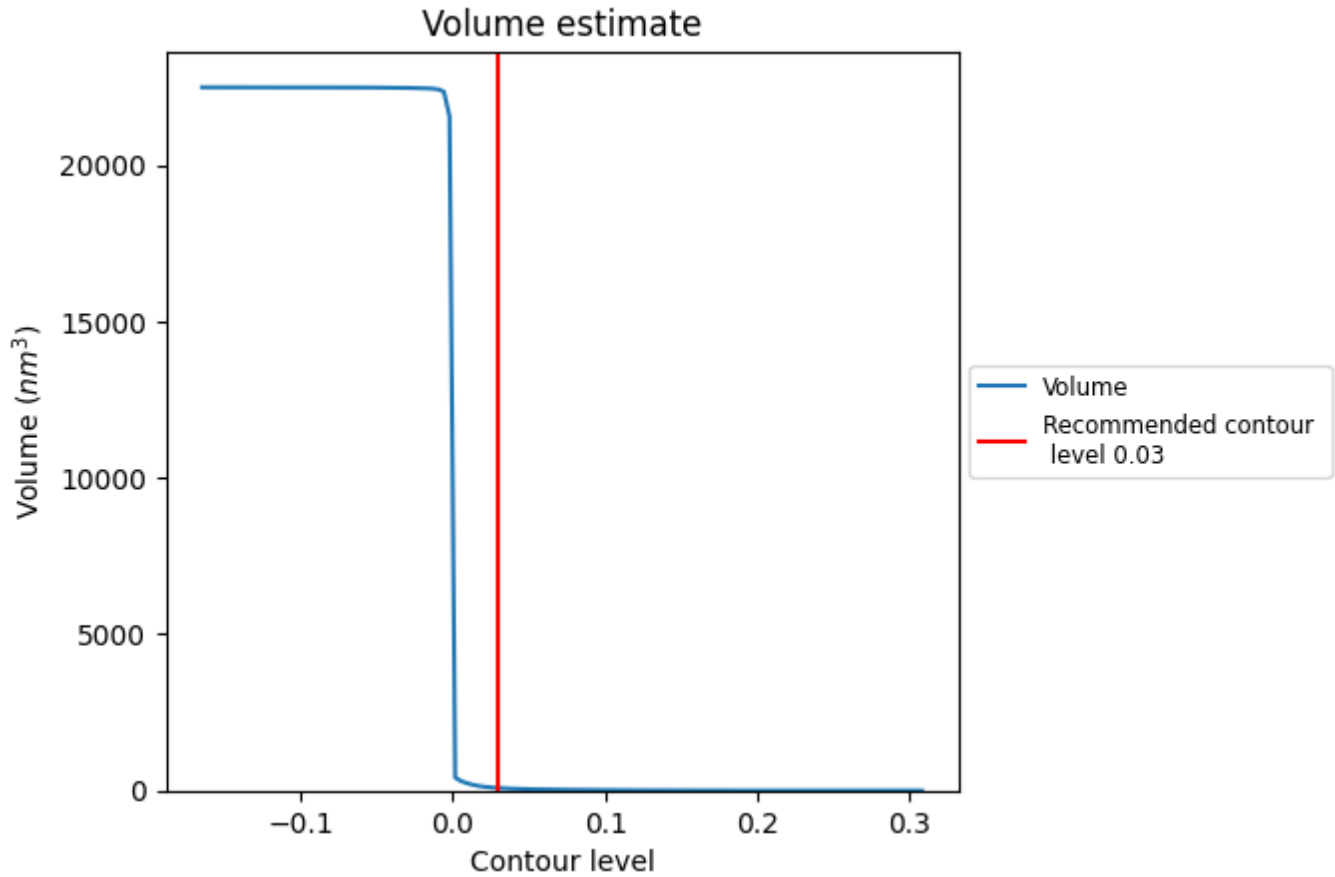
This section contains the results of statistical analysis of the map.

### 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.

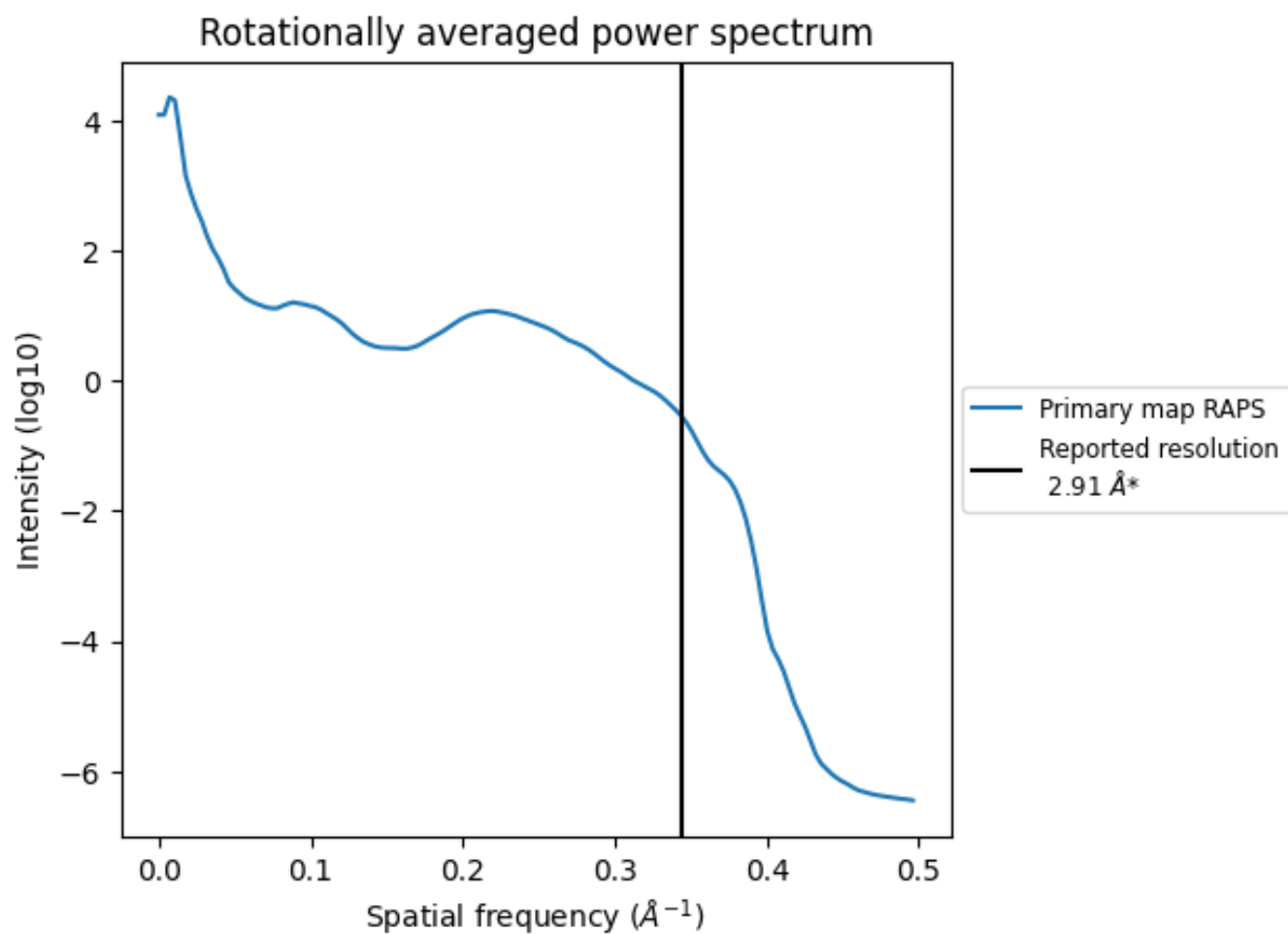
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $80 \text{ nm}^3$ ; this corresponds to an approximate mass of 72 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

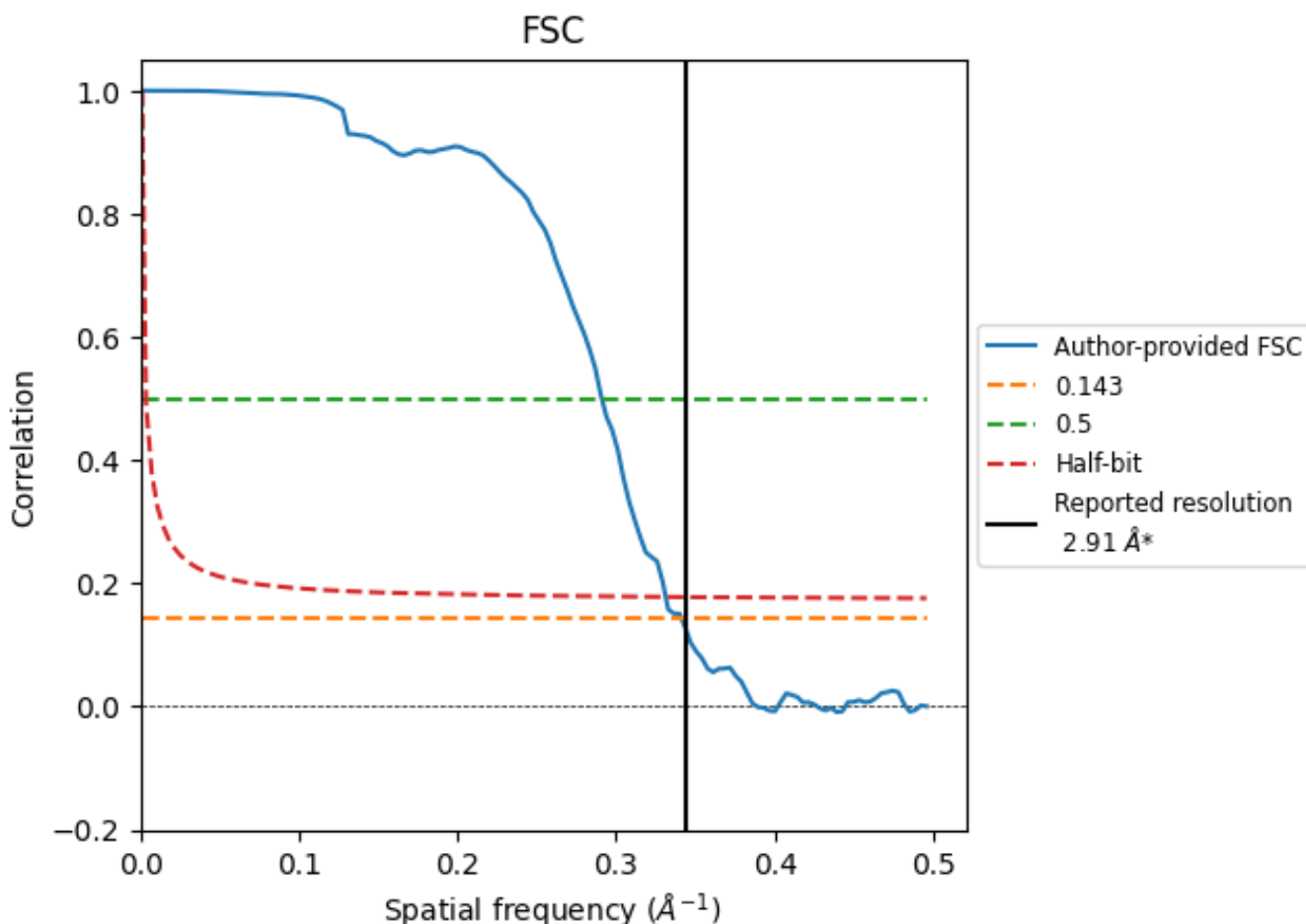


\*Reported resolution corresponds to spatial frequency of  $0.344 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.344 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.93	3.44	3.02
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

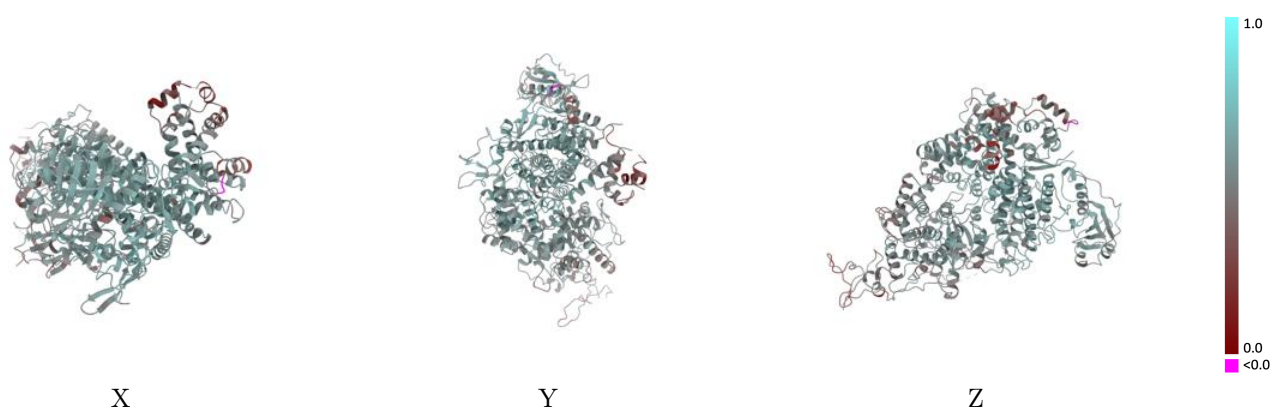
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13583 and PDB model 7PPO. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)

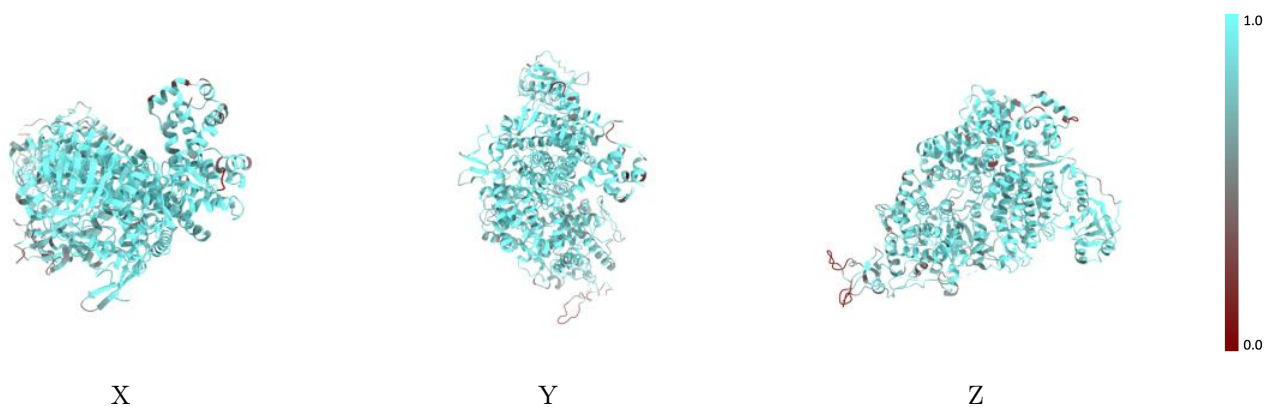
This section was not generated.

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



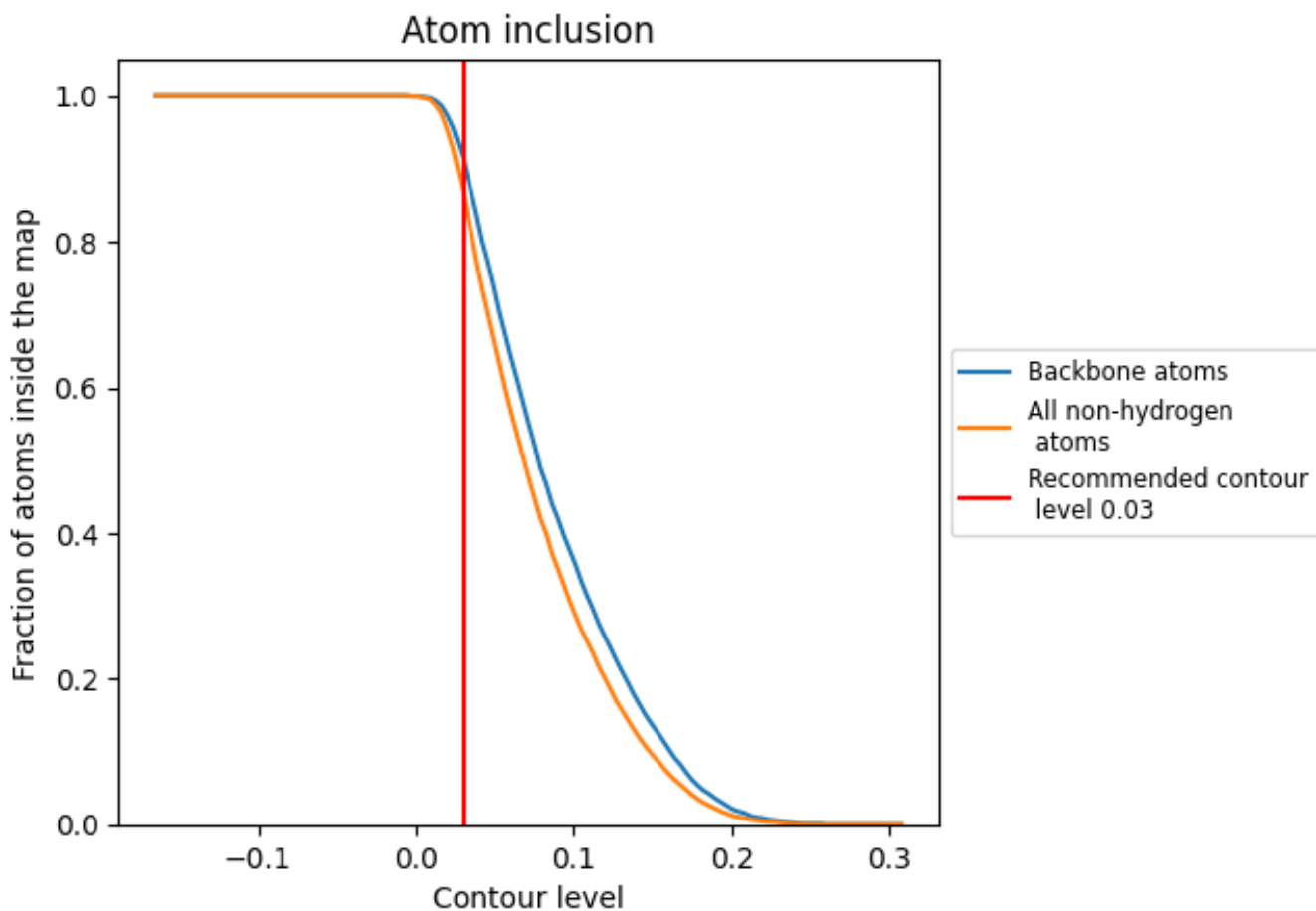
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.5450
A	 0.7840	 0.5010
B	 0.8240	 0.4620
C	 0.9320	 0.5860

