WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Nov 8, 2021 – 04:09 pm GMT

PDB ID	:	7PPO
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)

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

|		
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4 (270009), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2
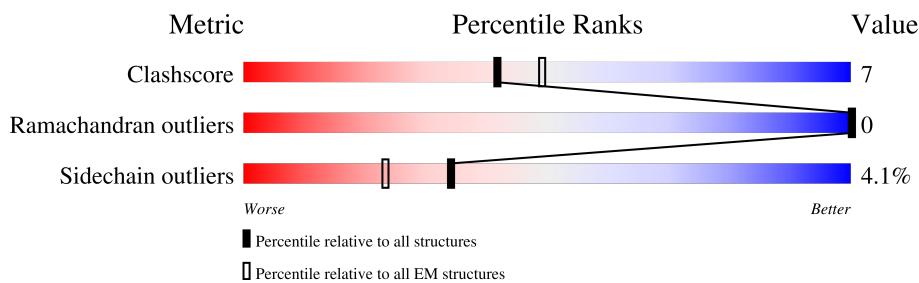
# 1	Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
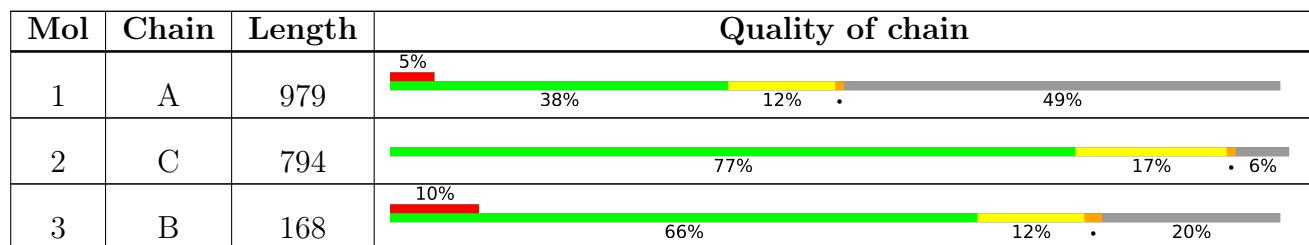
The reported resolution of this entry is 2.91 Å.

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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		4.1%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% — 66% 12% • 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
3	B	134	Total 886	C 549	N 147	O 184	S 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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total 1	Mg 1	0
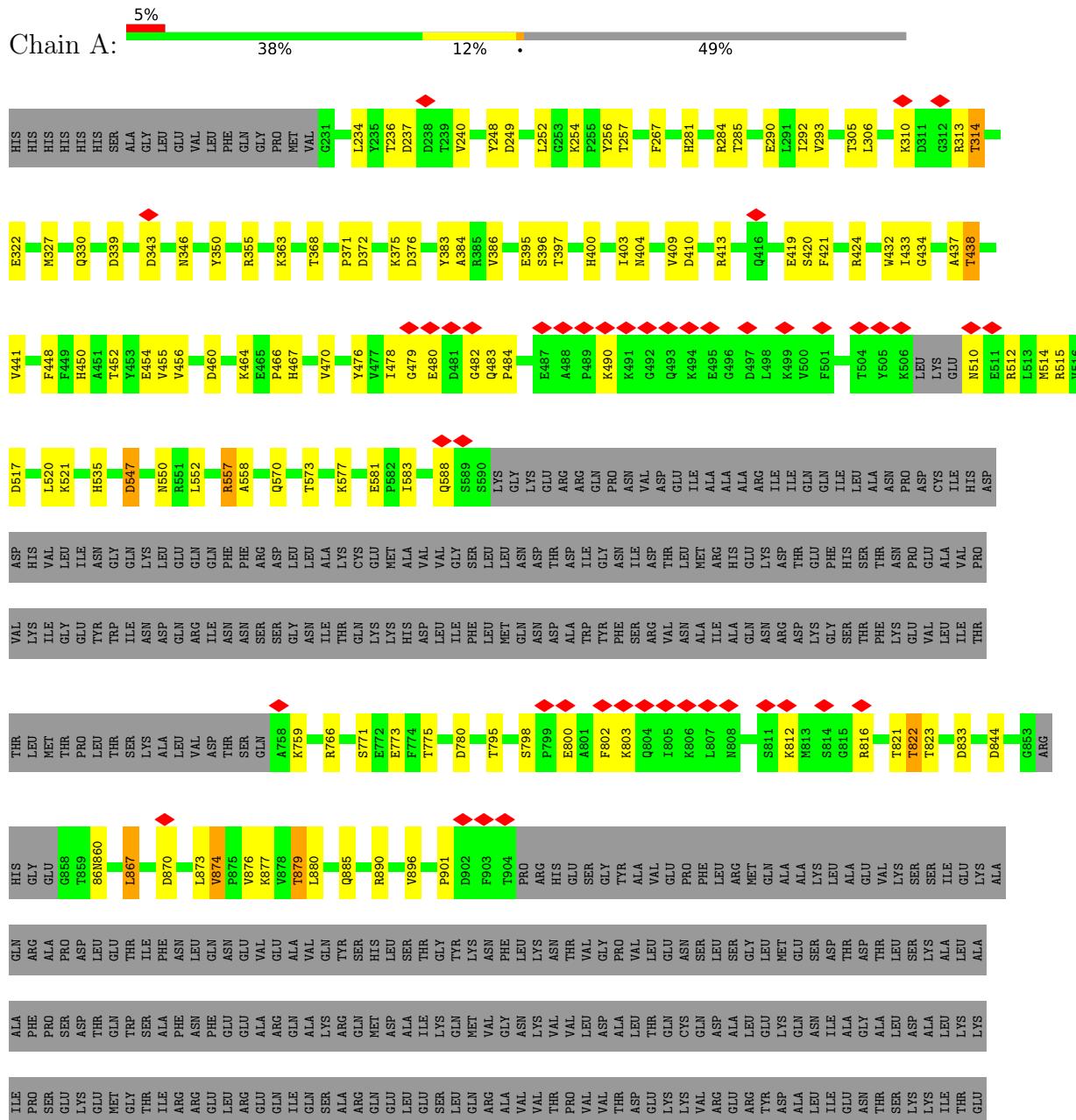
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).
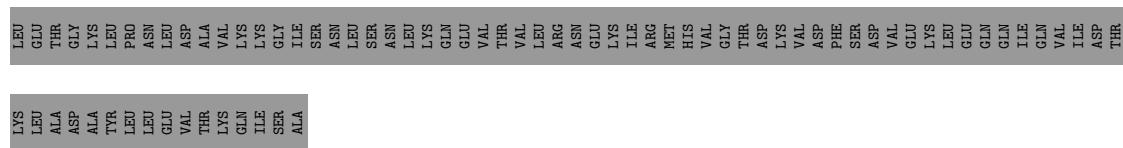
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total 1	Ca 1	0

3   Residue-property plots ⓘ

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: Ubiquitinating/deubiquitinating enzyme SdeA

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

LYS LEU ALA ASP ALA TYR LEU GLU VAL THR LYS GLN ILE SER ALA

• Molecule 2: Calmodulin-dependent glutamylase SidJ

Chain C:

HIS HIS HIS HIS HIS SER ALA GLY LEU GLU VAL LEU PHE GLN GLY PRO MET VAL K100 Q101 Y102 E109 L117 V123 E137 R140 N141 Q145 I146 Y147 H171 Y172 L173 R176 S177 N180 G185 N189 K196 P197 S204 K205 E206 V209

I213 N214 E215 S220 E221 Y222 P223 H234 S235 N236 E248 D263 S264 S265 D285 N289 P290 M291 F292 R293 E294 R295 L296 S297 T298 N299 F300 Y301 T306 L310 E314 G331 D334 S335 R338 Y339 Q340 L347 S357 T358 P359 Q360 V366 K367 V368

R371 L389 R394 V397 Y398 S399 Q403 K412 L416 D424 R427 T430 D434 V440 Y441 V442 L447 L453 Q458 D459 T464 V467 D473 L474 F475 H492 T493 D502 Y506 V510 V515 L520 G521 R522 I523 D524

L552 F553 T554 S555 S556 D557 G595 L598 V599 L600 N601 T602 I603 A604 E605 T613 L614 G615 S616 V617 V621 M626 E632 R636 E637 V641 R660 L665 N670 K673 H674 F675 M682 T683 P684 S687 D692 T693 L694 Q695 M696 E697 Q698

I701 E705 P706 F710 T711 R739 Q757 E761 D780 Q790 L791 L792 D793 V806 L807 E811 E812 A837 T840 I841 W845 R846 E847 T848 ARG LYS ASN LEU SER GLU ASN SER ASP ILE GLU SER GLU LYS PRO GLU SER GLU ARG THR THR ASP LYS ARG

LEU LYS

• Molecule 3: Calmodulin

Chain B:

HIS HIS HIS HIS HIS SER GLY LEU GLU VAL LEU PHE GLN GLY PRO HIS MET ALA D3 Q4 L5 T6 E7 E8 E15 T27 I28 T29 E32 R38 Q42 N43 P44 T45 E46 A47 V56 D57 A58 D59 G60 T63 D79 T80 D81 S82 E83 D94

LYS ASP G97 A104 E105 L106 M110 T111 E115 K116 L117 T118 D119 E120 R127 E128 A129 ASP ILE ASP GLY ASP GLN VAL N138 M145 M146 THR ALA LYS

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 $(e^-/\text{Å}^2)$	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 (Å)	282.24, 282.24, 282.24	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.008, 1.008, 1.008	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.28	0/4055	0.43	0/5469
2	C	0.37	0/6239	0.45	0/8439
3	B	0.28	0/892	0.42	0/1211
All	All	0.33	0/11186	0.44	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 ⓘ

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	81	0
3	B	886	0	723	12	0
4	C	1	0	0	0	0
5	B	1	0	0	0	0
All	All	10990	0	10665	159	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 (159) 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
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
3:B:6:THR:OG1	3:B:7:GLU:N	2.38	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
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
1:A:547:ASP:HA	1:A:550:ASN:HD21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:557:ASP:N	2:C:557:ASP:OD1	2.39	0.53
1:A:547:ASP:OD2	1:A:547:ASP:N	2.42	0.53
1:A:771:SER:O	1:A:775:THR:OG1	2.22	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:234:HIS:HD1	2:C:301:TYR:HH	1.55	0.52
2:C:502:ASP:OD1	2:C:502:ASP:N	2.42	0.52
3:B:27:THR:HB	3:B:63:THR:HB	1.92	0.52
2:C:340:GLN:H	2:C:340:GLN:CD	2.14	0.51
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
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
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
2:C:335:SER:HG	2:C:338:ARG:HE	1.58	0.47
2:C:366:VAL:HG22	2:C:442:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:234:HIS:CE1	2:C:301:TYR:HH	2.34	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
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
1:A:466:PRO:HA	1:A:515:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:684:PRO:O	2:C:687:SER:OG	2.26	0.41
1:A:822:THR:OG1	1:A:823:THR:N	2.54	0.41
2:C:147:TYR:OH	2:C:171:HIS:ND1	2.38	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: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%)	405 (95%)	22 (5%)	23	54
2	C	677/721 (94%)	659 (97%)	18 (3%)	44	75
3	B	69/144 (48%)	61 (88%)	8 (12%)	5	16
All	All	1173/1716 (68%)	1125 (96%)	48 (4%)	34	63

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	TYR
1	A	257	THR
1	A	305	THR
1	A	314	THR
1	A	368	THR

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Mol	Chain	Res	Type
1	A	409	VAL
1	A	413	ARG
1	A	438	THR
1	A	490	LYS
1	A	547	ASP
1	A	557	ARG
1	A	581	GLU
1	A	773	GLU
1	A	780	ASP
1	A	795	THR
1	A	802	PHE
1	A	812	LYS
1	A	822	THR
1	A	867	LEU
1	A	874	VAL
1	A	879	THR
1	A	885	GLN
2	C	123	VAL
2	C	177	SER
2	C	204	SER
2	C	215	GLU
2	C	285	ASP
2	C	296	LEU
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	605	GLU
2	C	621	VAL
2	C	626	MET
2	C	675	PHE
2	C	845	TRP
3	B	7	GLU
3	B	29	THR
3	B	32	GLU
3	B	45	THR
3	B	94	ASP
3	B	111	THR
3	B	115	GLU

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Mol	Chain	Res	Type
3	B	118	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	423	GLN
1	A	537	GLN
1	A	550	ASN
1	A	588	GLN
1	A	818	ASN
2	C	153	GLN
2	C	167	GLN
2	C	454	HIS
3	B	9	GLN
3	B	42	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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.

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry　ⓘ

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　ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues　ⓘ

There are no chain breaks in this entry.
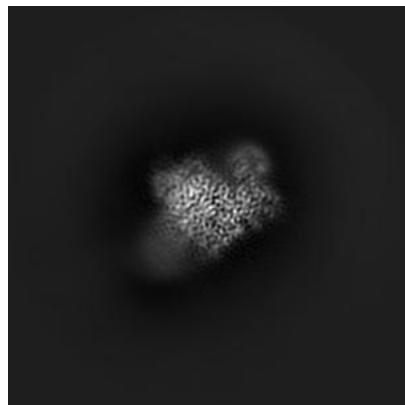
6 Map visualisation ⓘ

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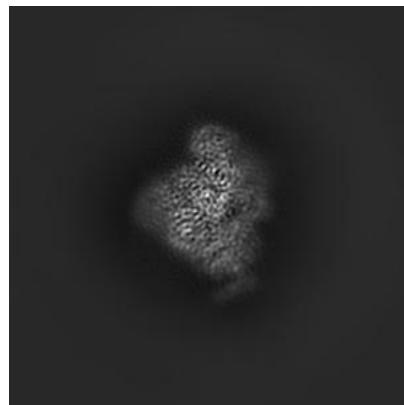
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ
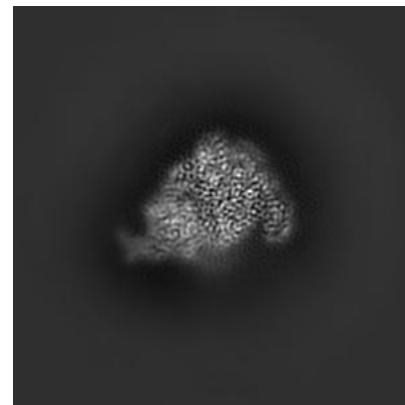
6.1.1 Primary map

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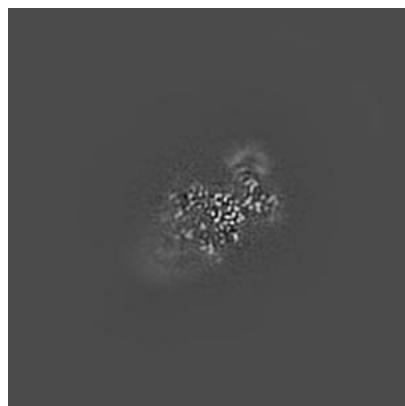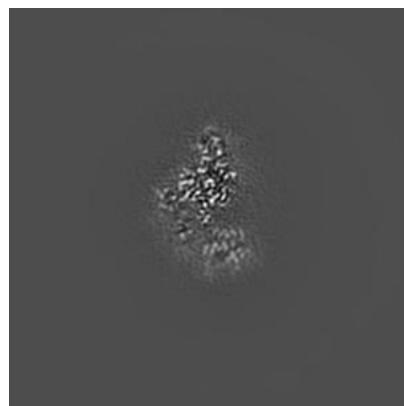
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
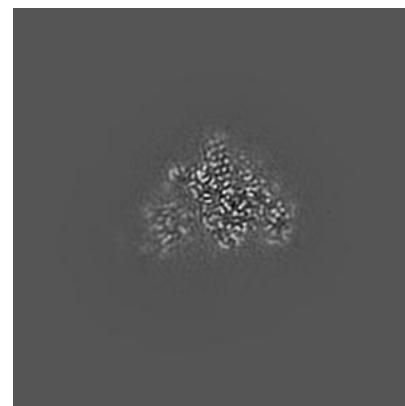
6.2.1 Primary map

X Index: 140	Y Index: 140	Z Index: 140
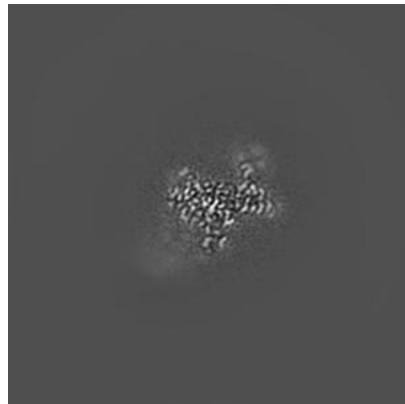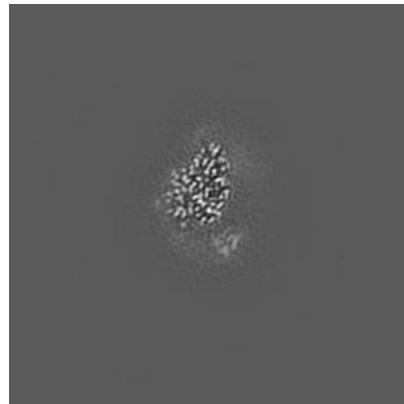
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
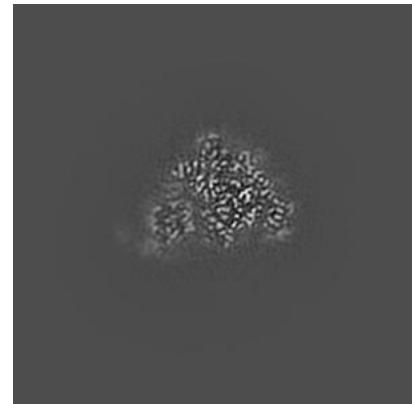
6.3.1 Primary map

| X Index: 146 | Y Index: 148 | Z Index: 143 |
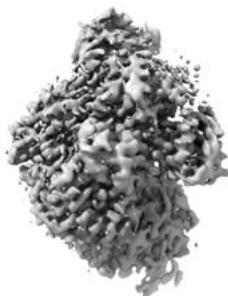
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |

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.
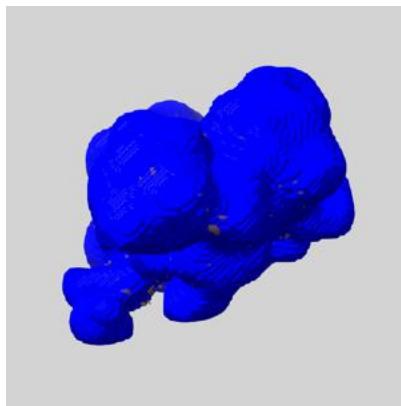
6.5　Mask visualisation ⓘ

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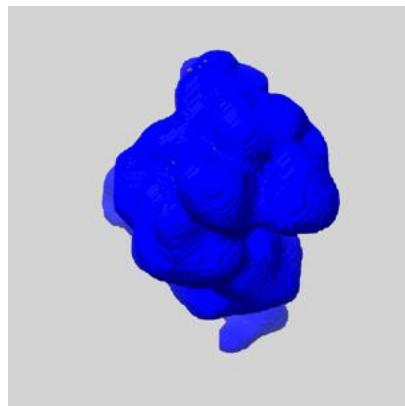
A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure
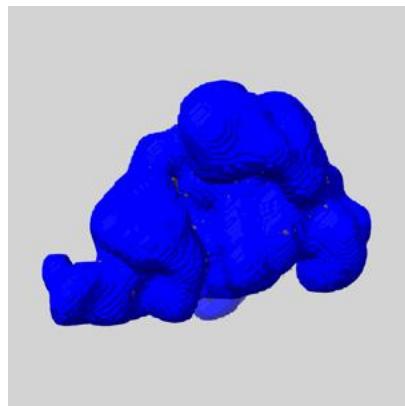
6.5.1　emd_13583_msk_1.map ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
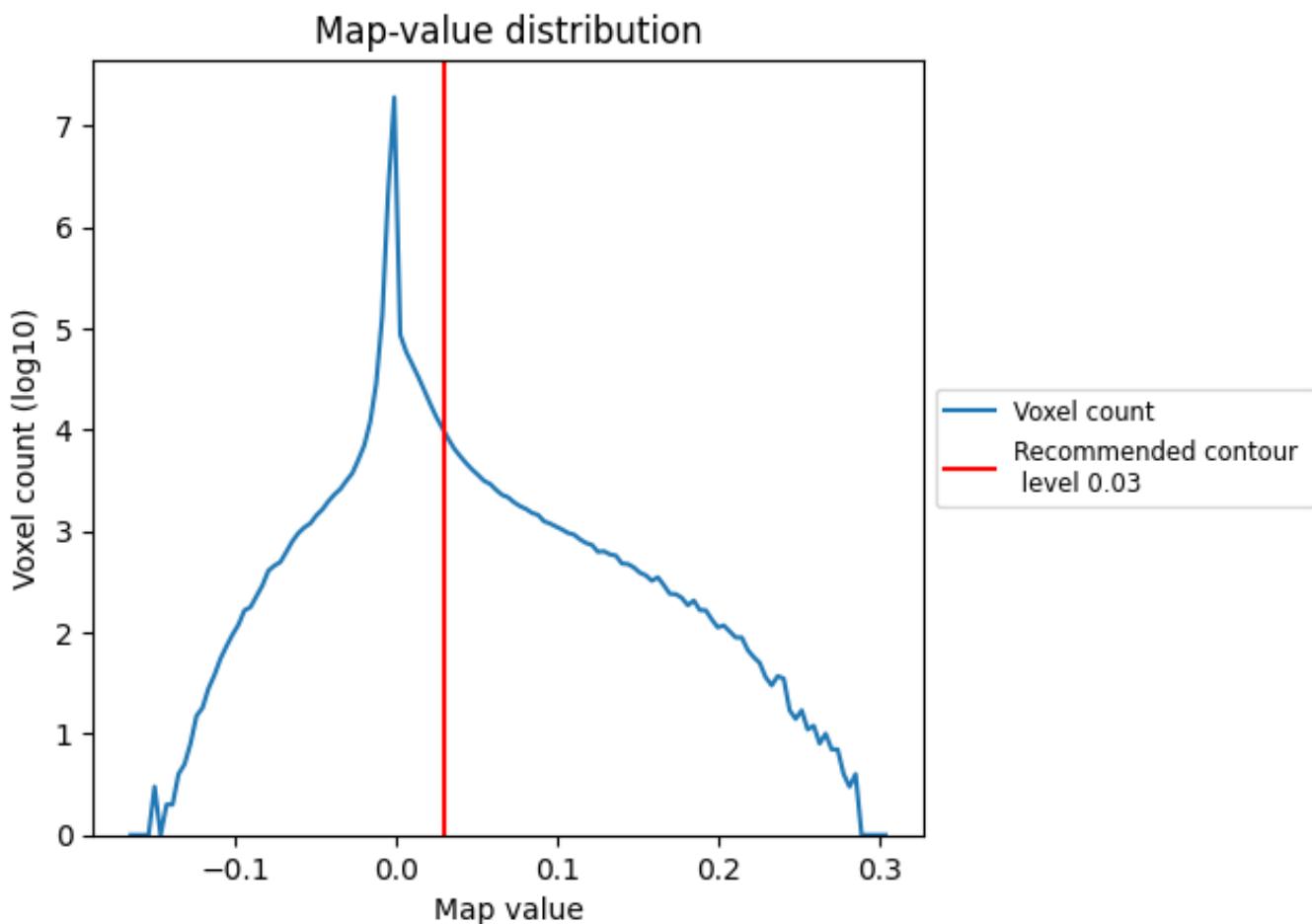
7　Map analysis ⓘ
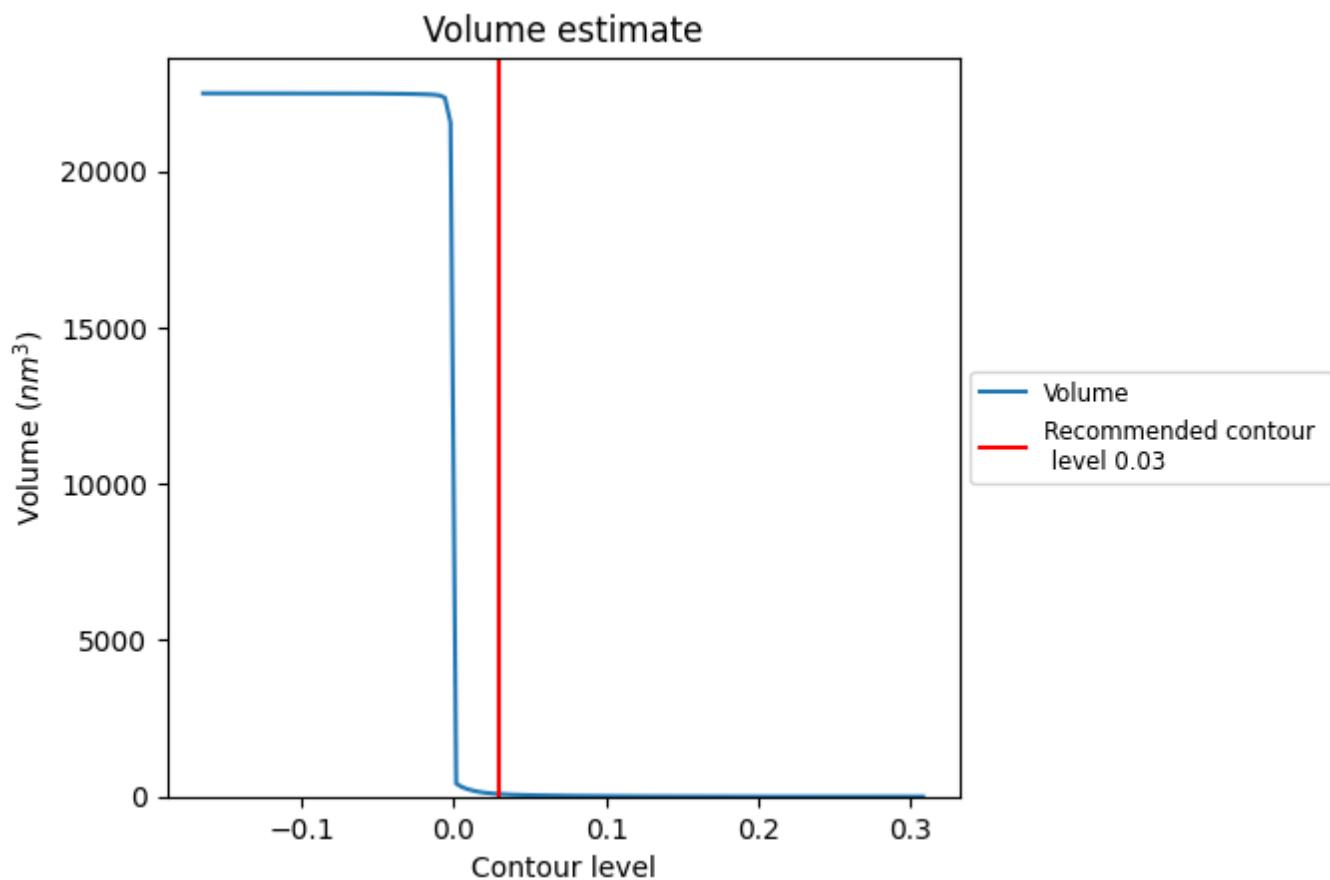
This section contains the results of statistical analysis of the map.

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.
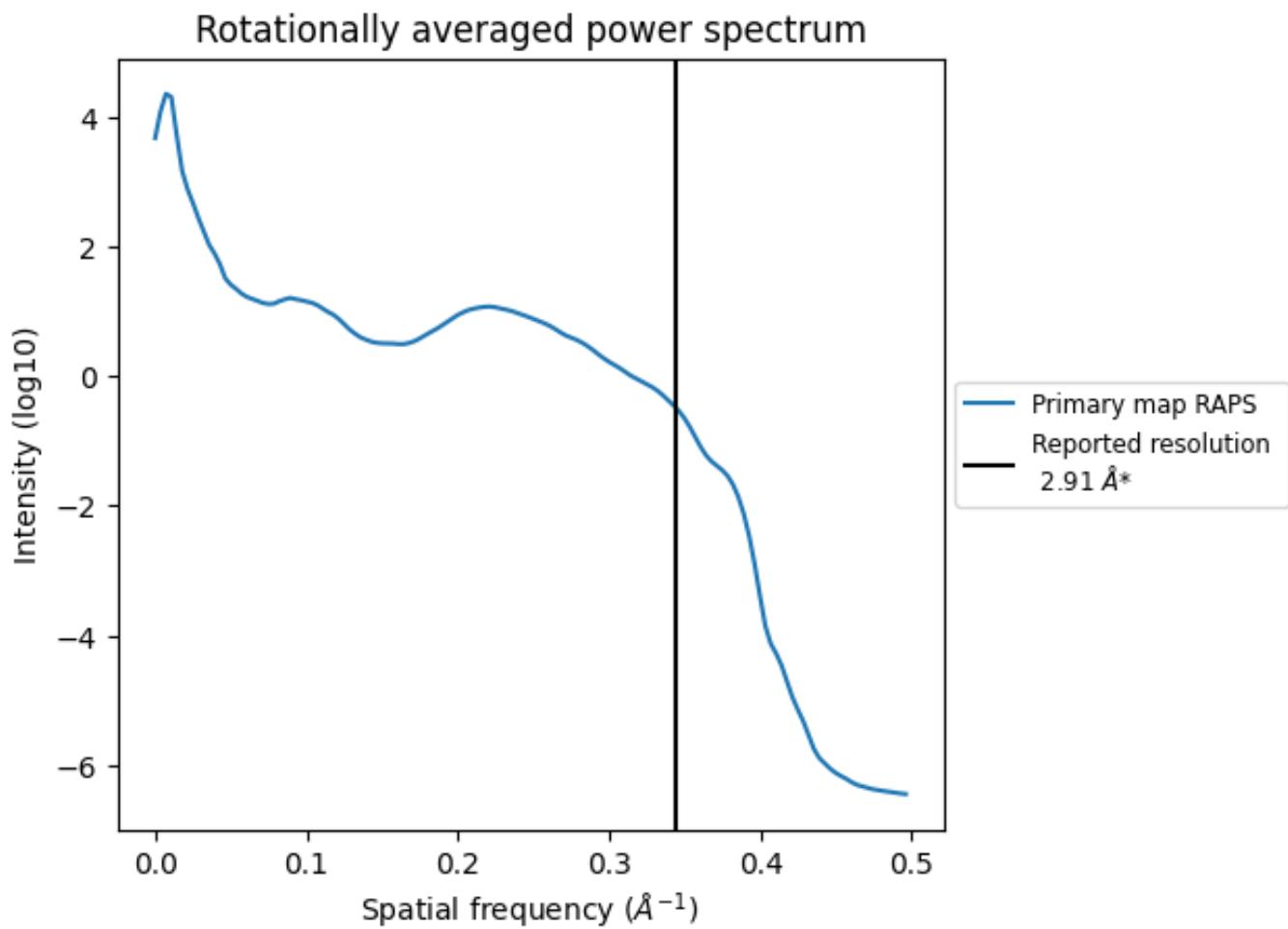
7.2 Volume estimate ⓘ

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

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

7.3　Rotationally averaged power spectrum ⓘ
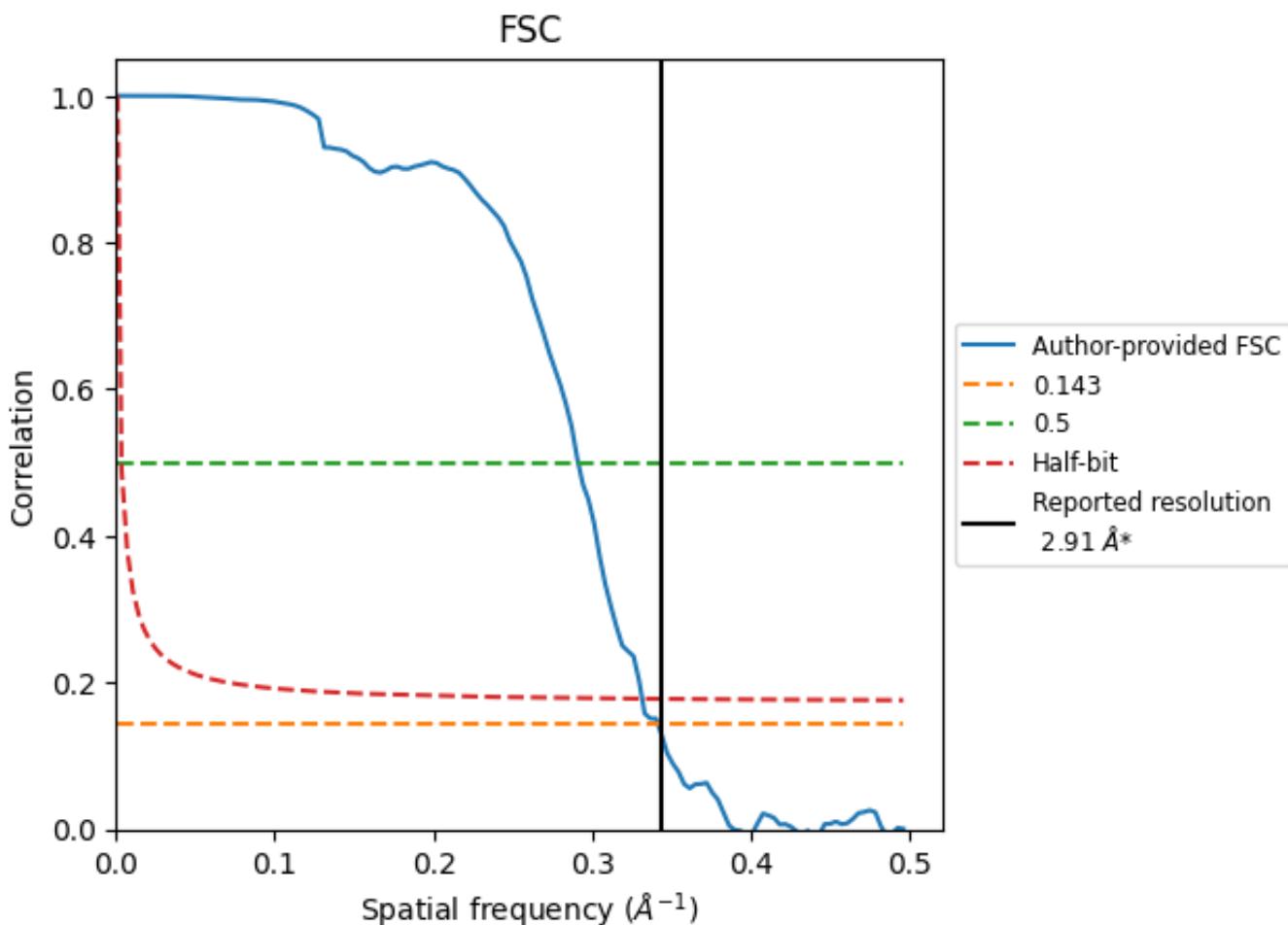
*Reported resolution corresponds to spatial frequency of 0.344 Å^{-1}

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 0.344 Å^{-1}

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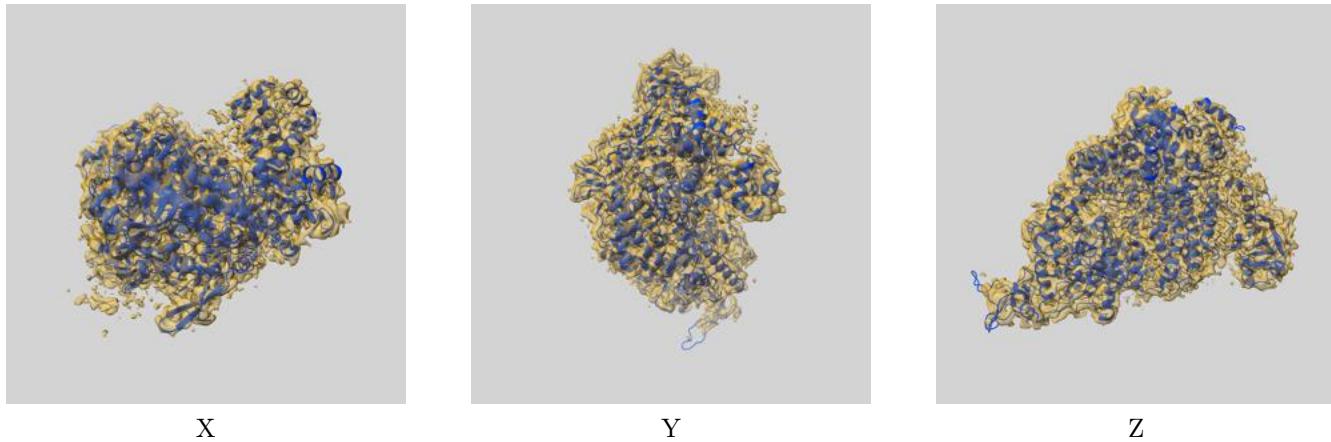
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.93	3.44	3.02
Unmasked-calculated*	-	-	-

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

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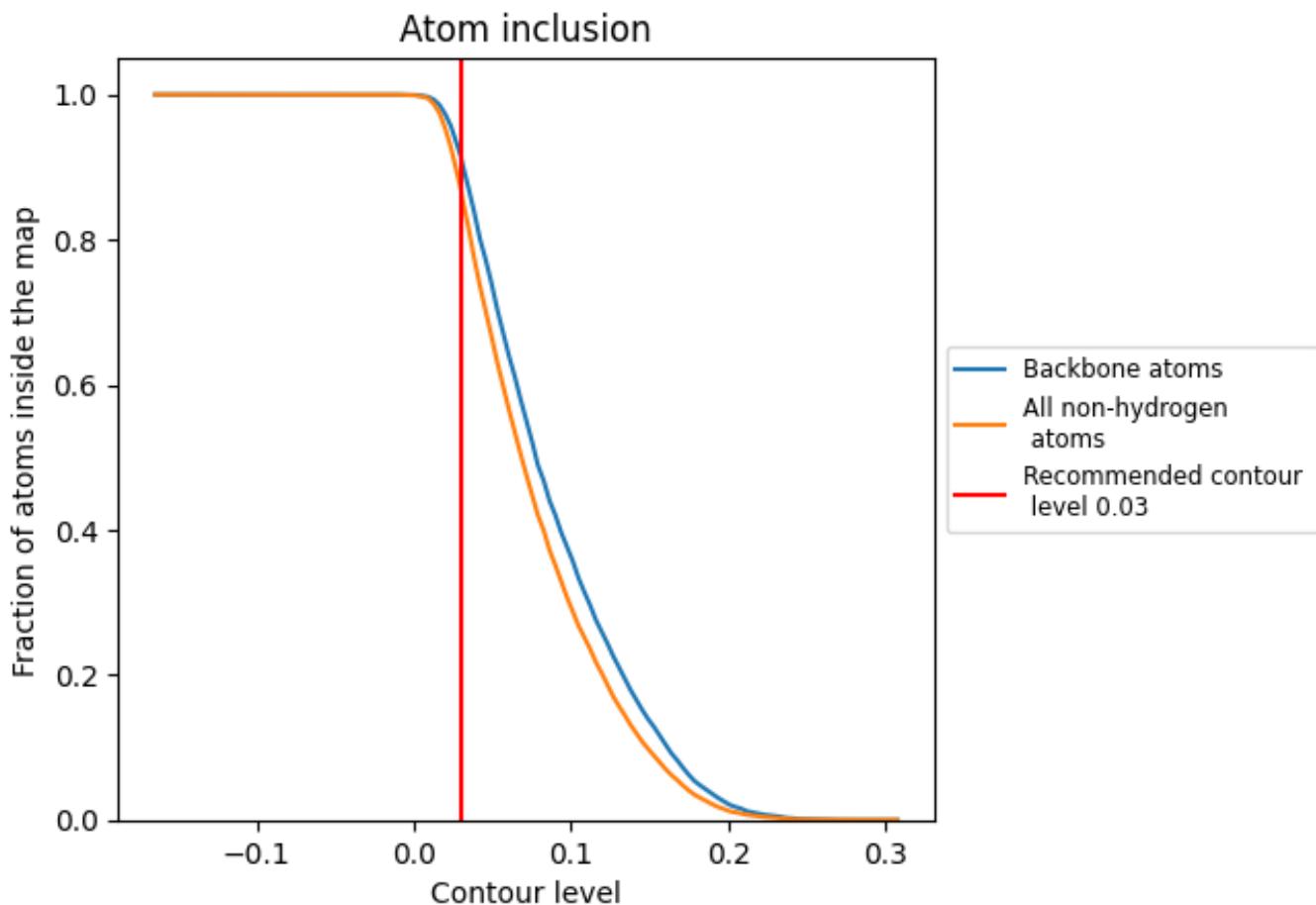
This section contains information regarding the fit between EMDB map EMD-13583 and PDB model 7PPO. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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　Atom inclusion ⓘ

At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.