Full wwPDB EM Validation Report

Mar 9, 2026 – 08:19 AM UTC

PDB ID	:	9CD3 / pdb_00009cd3
EMDB ID	:	EMD-45461
Title	:	Cryo-EM structure of Candidatus Saccharibacterium phosphoketolase complexed with thiamine diphosphate
Authors	:	Singal, B.; Landwehr, G.; Jewett, M.C.
Deposited on	:	2024-06-24
Resolution	:	2.18 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 (i) 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 (i)) were used in the production of this report:

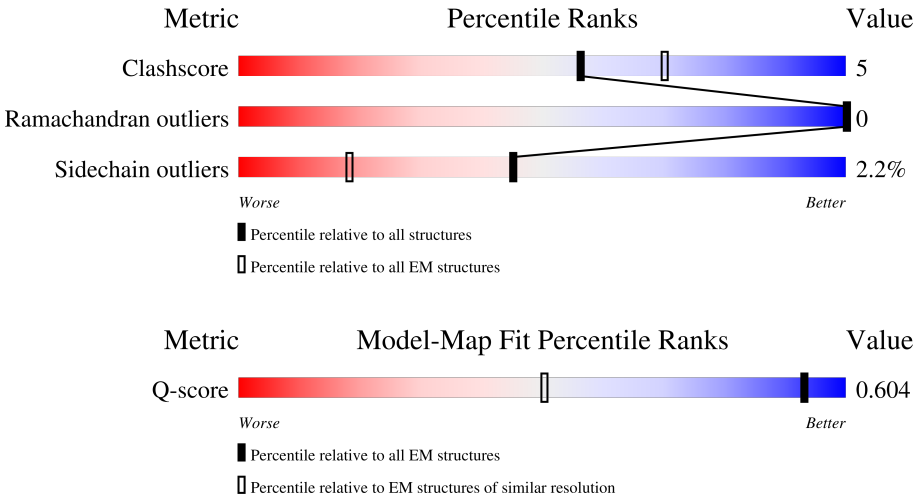
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.18 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	2701 (1.70 - 2.68)

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	799	85% 12%
1	B	799	84% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12592 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 Phosphoketolase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	785	Total	C	N	O	S	0	0
			6270	4022	1057	1176	15		
1	B	785	Total	C	N	O	S	0	0
			6270	4022	1057	1176	15		

There are 34 discrepancies between the modelled and reference sequences:

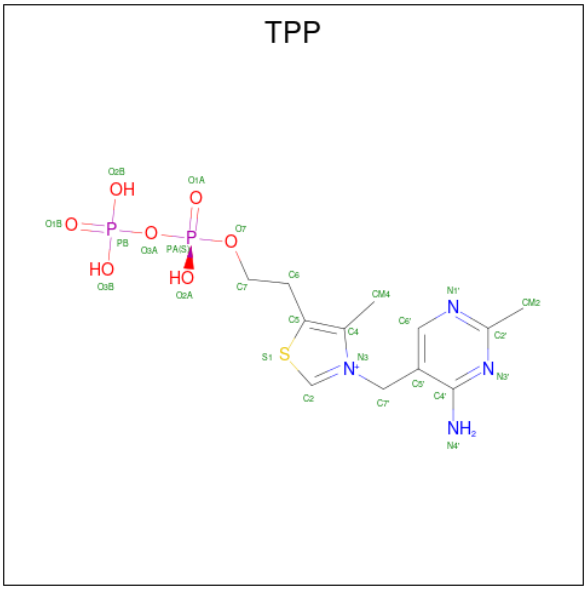
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7W4E7R7
A	2	TRP	-	expression tag	UNP A0A7W4E7R7
A	3	SER	-	expression tag	UNP A0A7W4E7R7
A	4	HIS	-	expression tag	UNP A0A7W4E7R7
A	5	PRO	-	expression tag	UNP A0A7W4E7R7
A	6	GLN	-	expression tag	UNP A0A7W4E7R7
A	7	PHE	-	expression tag	UNP A0A7W4E7R7
A	8	GLU	-	expression tag	UNP A0A7W4E7R7
A	9	LYS	-	expression tag	UNP A0A7W4E7R7
A	10	GLY	-	expression tag	UNP A0A7W4E7R7
A	11	GLY	-	expression tag	UNP A0A7W4E7R7
A	12	SER	-	expression tag	UNP A0A7W4E7R7
A	13	GLY	-	expression tag	UNP A0A7W4E7R7
A	70	TRP	HIS	conflict	UNP A0A7W4E7R7
A	144	SER	HIS	conflict	UNP A0A7W4E7R7
A	491	VAL	ILE	conflict	UNP A0A7W4E7R7
A	535	ASN	SER	conflict	UNP A0A7W4E7R7
B	1	MET	-	initiating methionine	UNP A0A7W4E7R7
B	2	TRP	-	expression tag	UNP A0A7W4E7R7
B	3	SER	-	expression tag	UNP A0A7W4E7R7
B	4	HIS	-	expression tag	UNP A0A7W4E7R7
B	5	PRO	-	expression tag	UNP A0A7W4E7R7
B	6	GLN	-	expression tag	UNP A0A7W4E7R7
B	7	PHE	-	expression tag	UNP A0A7W4E7R7
B	8	GLU	-	expression tag	UNP A0A7W4E7R7
B	9	LYS	-	expression tag	UNP A0A7W4E7R7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLY	-	expression tag	UNP A0A7W4E7R7
B	11	GLY	-	expression tag	UNP A0A7W4E7R7
B	12	SER	-	expression tag	UNP A0A7W4E7R7
B	13	GLY	-	expression tag	UNP A0A7W4E7R7
B	70	TRP	HIS	conflict	UNP A0A7W4E7R7
B	144	SER	HIS	conflict	UNP A0A7W4E7R7
B	491	VAL	ILE	conflict	UNP A0A7W4E7R7
B	535	ASN	SER	conflict	UNP A0A7W4E7R7

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	B	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	

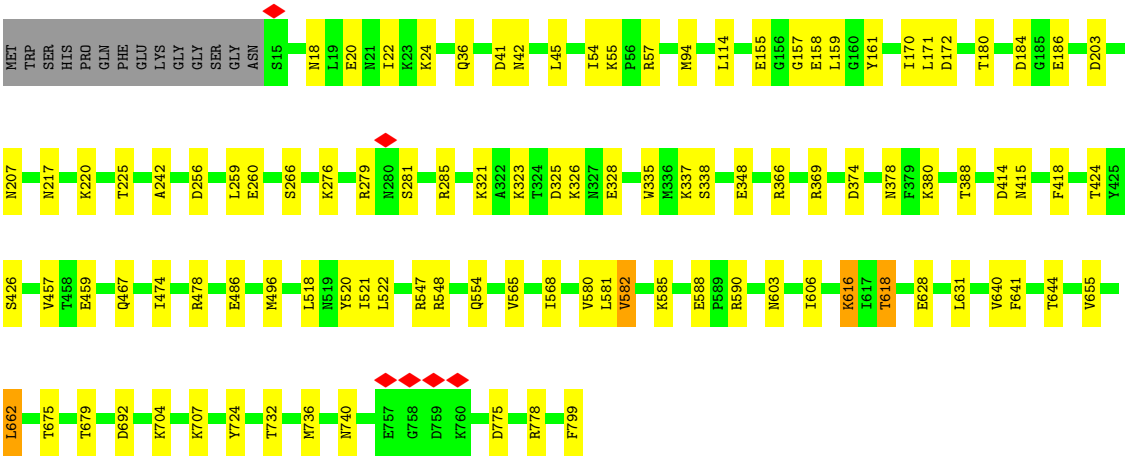
3 Residue-property plots (i)

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: Phosphoketolase family protein

Chain A:

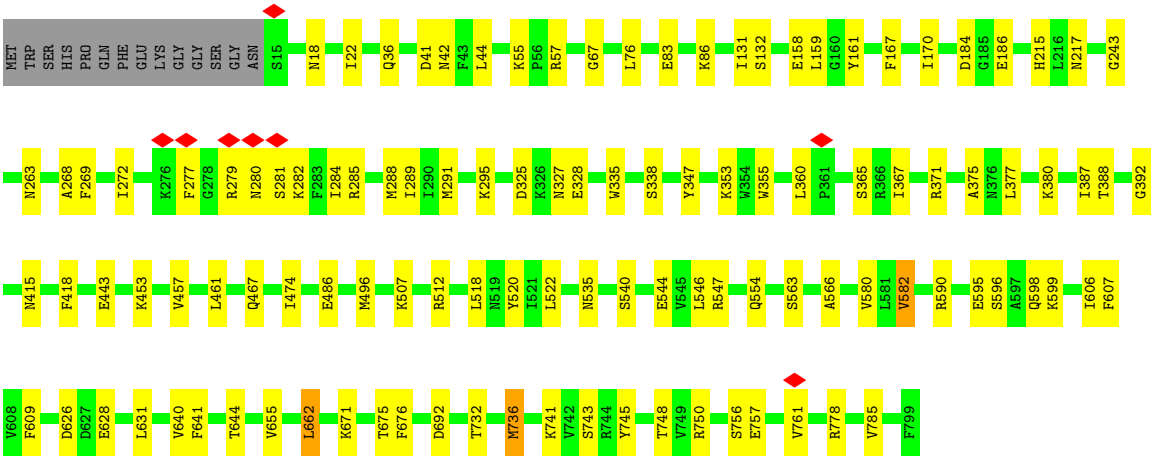




• Molecule 1: Phosphoketolase family protein

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	485609	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.485	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.0947	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.12	0/6417	0.32	1/8668 (0.0%)
1	B	0.12	0/6417	0.32	1/8668 (0.0%)
All	All	0.12	0/12834	0.32	2/17336 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	761	VAL	N-CA-C	-6.12	107.90	113.71
1	A	170	ILE	N-CA-C	5.79	112.40	106.21

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	6270	0	6189	62	0
1	B	6270	0	6189	64	0
2	A	26	0	16	1	0
2	B	26	0	16	3	0
All	All	12592	0	12410	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 5.

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:B:566:ALA:HB3	1:B:598:GLN:HE22	1.33	0.90
1:B:83:GLU:OE2	1:B:365:SER:OG	2.01	0.77
1:A:724:TYR:O	1:A:740:ASN:ND2	2.20	0.74
1:A:20:GLU:N	1:A:20:GLU:OE1	2.21	0.73
1:B:36:GLN:O	1:B:55:LYS:NZ	2.21	0.73
1:A:547:ARG:HB3	1:A:548:ARG:HH21	1.58	0.66
1:B:392:GLY:O	1:B:590:ARG:NH2	2.29	0.65
1:A:418:PHE:HB3	1:A:457:VAL:HG22	1.79	0.65
1:A:57:ARG:HH12	1:B:732:THR:HG22	1.62	0.64
1:B:418:PHE:HB3	1:B:457:VAL:HG22	1.80	0.63
1:A:220:LYS:HG3	1:A:225:THR:HG22	1.79	0.63
1:B:544:GLU:OE1	1:B:547:ARG:NH2	2.32	0.63
1:A:474:ILE:HD12	1:A:518:LEU:HD12	1.80	0.62
1:A:159:LEU:HB3	1:A:186:GLU:HG3	1.81	0.62
1:B:741:LYS:O	1:B:750:ARG:NH2	2.33	0.61
1:A:36:GLN:O	1:A:55:LYS:NZ	2.33	0.60
1:A:603:ASN:ND2	1:A:618:THR:O	2.35	0.60
1:A:279:ARG:HH21	1:A:281:SER:H	1.50	0.59
1:A:374:ASP:O	1:A:378:ASN:ND2	2.36	0.58
1:A:424:THR:OG1	1:A:459:GLU:OE2	2.20	0.57
1:A:217:ASN:ND2	2:A:801:TPP:O1B	2.38	0.56
1:B:281:SER:O	1:B:453:LYS:NZ	2.34	0.56
1:A:590:ARG:HG2	1:A:799:PHE:HE2	1.71	0.56
1:B:566:ALA:HB3	1:B:598:GLN:NE2	2.13	0.56
1:A:54:ILE:HB	1:A:323:LYS:HG3	1.88	0.55
1:A:414:ASP:OD2	1:A:414:ASP:N	2.38	0.55
1:B:474:ILE:HD12	1:B:518:LEU:HD12	1.88	0.55
1:B:335:TRP:O	1:B:338:SER:OG	2.23	0.55
1:A:158:GLU:OE2	1:A:161:TYR:OH	2.19	0.54
1:B:671:LYS:HD3	1:B:676:PHE:HE1	1.72	0.54
1:A:732:THR:HG22	1:B:57:ARG:HH12	1.74	0.53
1:B:41:ASP:OD1	1:B:42:ASN:N	2.41	0.53
1:B:387:ILE:HD12	1:B:599:LYS:HZ1	1.75	0.52
1:B:745:TYR:HA	1:B:748:THR:HG22	1.92	0.51
1:A:426:SER:O	1:A:585:LYS:NZ	2.39	0.51
1:B:159:LEU:HB3	1:B:186:GLU:HG3	1.93	0.51
1:B:628:GLU:N	1:B:628:GLU:OE2	2.44	0.51
1:A:184:ASP:N	1:A:184:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLN:HE22	1:A:675:THR:HA	1.76	0.51
1:B:554:GLN:HE22	1:B:675:THR:HA	1.75	0.50
1:A:256:ASP:HB3	1:A:259:LEU:HB3	1.93	0.50
1:A:41:ASP:OD1	1:A:42:ASN:N	2.42	0.50
1:A:335:TRP:O	1:A:338:SER:OG	2.28	0.49
1:A:547:ARG:HG2	1:A:547:ARG:HH11	1.77	0.49
1:A:547:ARG:HH12	1:B:540:SER:HB2	1.77	0.49
1:B:641:PHE:HE1	1:B:662:LEU:HD11	1.77	0.49
1:A:94:MET:HB3	1:A:180:THR:HA	1.94	0.49
1:A:520:TYR:HB2	1:A:580:VAL:HG22	1.93	0.49
1:A:775:ASP:OD1	1:A:778:ARG:NH2	2.45	0.49
1:B:217:ASN:HD21	2:B:801:TPP:PB	2.36	0.48
1:A:45:LEU:HD13	1:A:337:LYS:HE3	1.95	0.48
1:A:641:PHE:HE1	1:A:662:LEU:HD11	1.78	0.48
1:B:467:GLN:OE1	1:B:520:TYR:OH	2.29	0.48
1:A:616:LYS:HE2	1:A:616:LYS:HB2	1.60	0.48
1:A:172:ASP:HB2	1:A:478:ARG:HH11	1.79	0.47
1:B:280:ASN:HD21	1:B:282:LYS:HG2	1.79	0.47
1:A:325:ASP:HB3	1:A:328:GLU:HB2	1.97	0.47
1:A:704:LYS:HA	1:A:707:LYS:HD2	1.96	0.47
1:A:692:ASP:OD2	1:A:692:ASP:N	2.47	0.47
1:B:563:SER:HA	1:B:598:GLN:HE21	1.80	0.47
1:A:415:ASN:N	1:A:415:ASN:OD1	2.48	0.47
1:B:375:ALA:C	1:B:377:LEU:H	2.23	0.46
1:B:496:MET:HE3	1:B:496:MET:HB3	1.78	0.46
1:A:256:ASP:O	1:A:260:GLU:HG2	2.15	0.46
1:B:277:PHE:HB3	1:B:279:ARG:HG3	1.97	0.46
1:A:565:VAL:HA	1:A:568:ILE:HG22	1.97	0.46
1:A:521:ILE:HD13	1:A:581:LEU:HB3	1.96	0.46
1:B:158:GLU:OE2	1:B:161:TYR:OH	2.22	0.46
1:B:380:LYS:HB2	1:B:380:LYS:HE2	1.71	0.45
1:A:242:ALA:O	1:A:285:ARG:NH2	2.49	0.45
1:B:353:LYS:HB2	1:B:355:TRP:HD1	1.81	0.45
1:A:547:ARG:HB3	1:A:548:ARG:NH2	2.28	0.45
1:B:18:ASN:O	1:B:22:ILE:HG13	2.16	0.45
1:A:157:GLY:HA3	1:B:535:ASN:HD22	1.81	0.45
1:B:756:SER:OG	1:B:757:GLU:N	2.50	0.45
1:B:86:LYS:HB3	1:B:86:LYS:HE3	1.71	0.44
1:A:496:MET:HE3	1:A:496:MET:HB3	1.79	0.44
1:A:628:GLU:N	1:A:628:GLU:OE2	2.50	0.44
1:B:184:ASP:OD1	1:B:184:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASN:N	1:B:415:ASN:OD1	2.51	0.44
1:B:76:LEU:HD23	1:B:367:ILE:HD13	1.99	0.44
1:B:295:LYS:NZ	2:B:801:TPP:O1B	2.48	0.43
1:A:20:GLU:O	1:A:24:LYS:HG3	2.19	0.43
1:A:18:ASN:O	1:A:22:ILE:HG13	2.18	0.43
1:B:269:PHE:C	1:B:269:PHE:CD1	2.96	0.43
1:A:326:LYS:HE2	1:A:326:LYS:H	1.81	0.43
1:B:243:GLY:HA2	1:B:285:ARG:HH12	1.83	0.43
1:B:640:VAL:O	1:B:644:THR:OG1	2.35	0.43
1:B:263:ASN:HD21	1:B:289:ILE:HG23	1.84	0.43
1:A:522:LEU:HB2	1:A:582:VAL:HG12	2.00	0.42
1:B:44:LEU:HB3	1:B:347:TYR:CE2	2.54	0.42
1:B:284:ILE:HD12	1:B:284:ILE:O	2.19	0.42
1:B:288:MET:HE3	1:B:288:MET:HB2	1.86	0.42
1:A:467:GLN:OE1	1:A:520:TYR:OH	2.30	0.42
1:A:736:MET:HE2	1:A:736:MET:HB2	1.71	0.42
1:B:325:ASP:HB3	1:B:328:GLU:HB2	2.00	0.42
1:B:607:PHE:CZ	1:B:609:PHE:HB2	2.55	0.42
1:A:348:GLU:H	1:A:348:GLU:CD	2.28	0.42
1:A:380:LYS:HB2	1:A:380:LYS:HE2	1.72	0.42
1:B:268:ALA:O	1:B:272:ILE:HG23	2.19	0.42
1:B:507:LYS:HB2	1:B:507:LYS:HE3	1.80	0.42
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.84	0.42
1:B:167:PHE:O	1:B:170:ILE:HG22	2.19	0.42
1:B:520:TYR:HB2	1:B:580:VAL:HG22	2.01	0.41
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.93	0.41
1:A:276:LYS:HE2	1:A:276:LYS:HB2	1.82	0.41
1:B:131:ILE:HG13	1:B:132:SER:N	2.36	0.41
1:A:640:VAL:O	1:A:644:THR:OG1	2.37	0.41
2:B:801:TPP:HN42	2:B:801:TPP:C2	2.34	0.41
1:A:203:ASP:O	1:A:207:ASN:ND2	2.31	0.41
1:B:626:ASP:OD2	1:B:626:ASP:N	2.53	0.41
1:B:595:GLU:HG3	1:B:596:SER:H	1.85	0.41
1:B:692:ASP:OD2	1:B:692:ASP:N	2.53	0.41
1:A:321:LYS:HB2	1:A:328:GLU:OE2	2.21	0.41
1:A:675:THR:O	1:A:679:THR:OG1	2.34	0.41
1:B:67:GLY:HA3	1:B:215:HIS:CE1	2.56	0.41
1:A:704:LYS:NZ	1:B:546:LEU:O	2.53	0.41
1:B:325:ASP:OD1	1:B:327:ASN:N	2.51	0.40
1:B:512:ARG:HD3	1:B:512:ARG:HA	1.89	0.40
1:B:736:MET:HE2	1:B:736:MET:HB2	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:LEU:O	1:B:582:VAL:HA	2.22	0.40
1:B:778:ARG:HH11	1:B:778:ARG:HG3	1.86	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	783/799 (98%)	754 (96%)	29 (4%)	0	100	100
1	B	783/799 (98%)	761 (97%)	22 (3%)	0	100	100
All	All	1566/1598 (98%)	1515 (97%)	51 (3%)	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	674/685 (98%)	660 (98%)	14 (2%)	47	59
1	B	674/685 (98%)	659 (98%)	15 (2%)	45	58
All	All	1348/1370 (98%)	1319 (98%)	29 (2%)	45	58

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	GLU
1	A	266	SER
1	A	366	ARG
1	A	369	ARG
1	A	388	THR
1	A	486	GLU
1	A	582	VAL
1	A	588	GLU
1	A	606	ILE
1	A	616	LYS
1	A	618	THR
1	A	631	LEU
1	A	655	VAL
1	A	662	LEU
1	B	291	MET
1	B	360	LEU
1	B	371	ARG
1	B	388	THR
1	B	443	GLU
1	B	461	LEU
1	B	486	GLU
1	B	582	VAL
1	B	606	ILE
1	B	631	LEU
1	B	655	VAL
1	B	662	LEU
1	B	736	MET
1	B	743	SER
1	B	785	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	240	HIS
1	A	454	ASN
1	A	464	ASN
1	A	505	GLN
1	A	554	GLN
1	A	598	GLN
1	A	657	GLN
1	A	666	GLN
1	B	36	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	69	ASN
1	B	77	ASN
1	B	107	ASN
1	B	327	ASN
1	B	370	ASN
1	B	378	ASN
1	B	535	ASN
1	B	554	GLN
1	B	598	GLN
1	B	720	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	TPP	A	801	-	26,27,27	0.31	0	38,40,40	0.29	0
2	TPP	B	801	-	26,27,27	0.32	0	38,40,40	0.28	0

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	TPP	A	801	-	-	2/17/17/17	0/2/2/2
2	TPP	B	801	-	-	2/17/17/17	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	TPP	PB-O3A-PA-O1A
2	A	801	TPP	C7-O7-PA-O3A
2	B	801	TPP	PB-O3A-PA-O2A
2	A	801	TPP	PB-O3A-PA-O2A

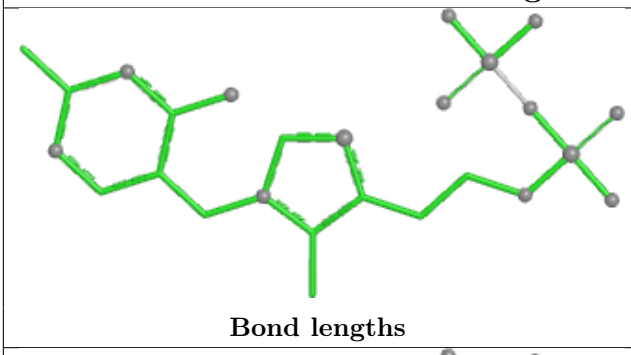
There are no ring outliers.

2 monomers are involved in 4 short contacts:

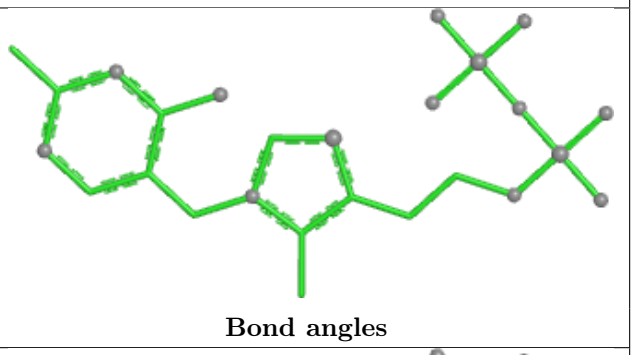
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	TPP	1	0
2	B	801	TPP	3	0

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

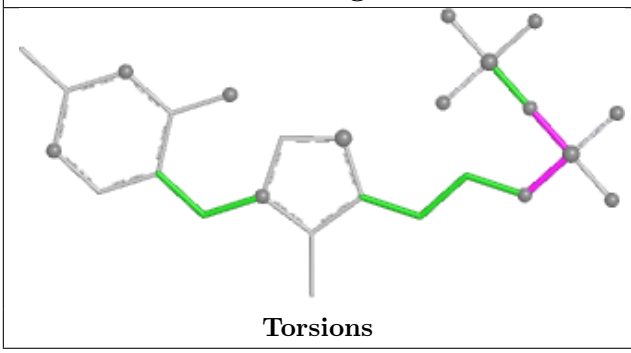
Ligand TPP A 801



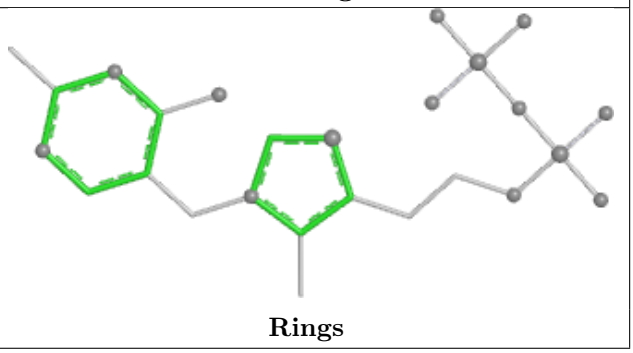
Bond lengths



Bond angles

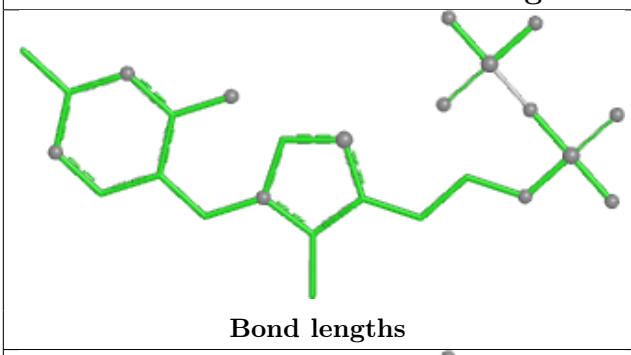


Torsions

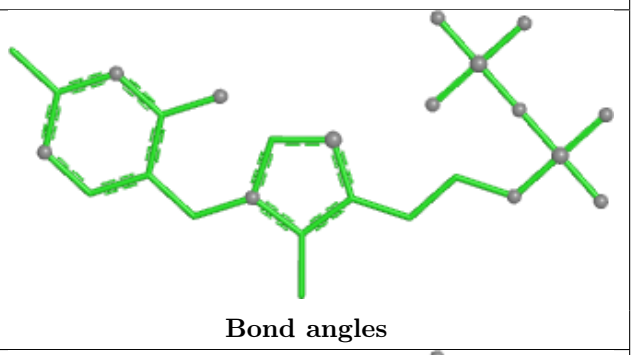


Rings

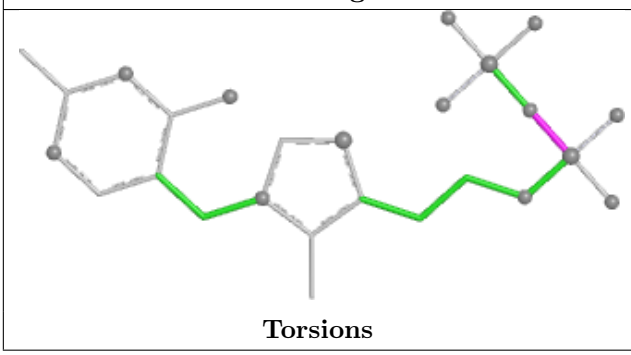
Ligand TPP B 801



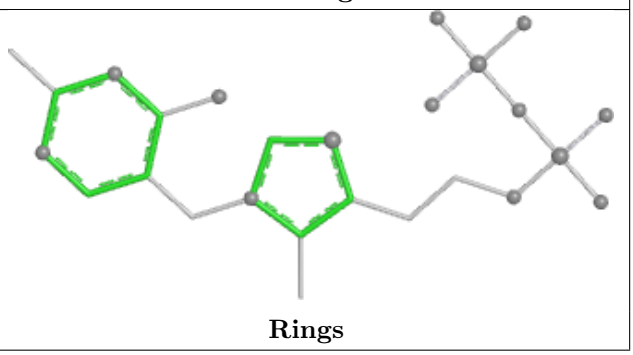
Bond lengths



Bond angles



Torsions



Rings

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.

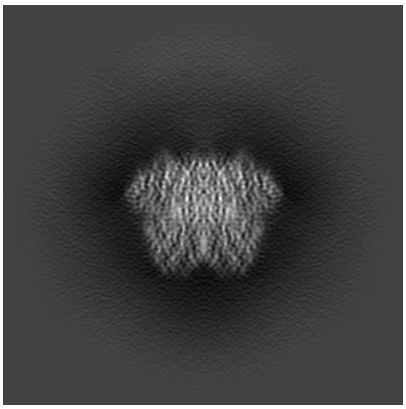
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45461. These allow visual inspection of the internal detail of the map and identification of artifacts.

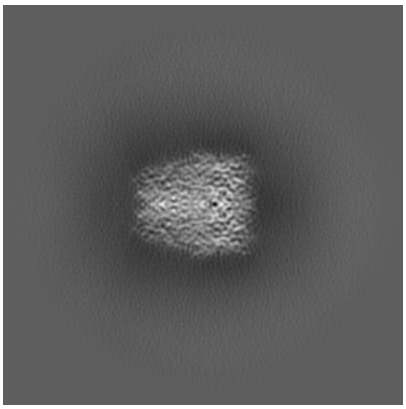
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

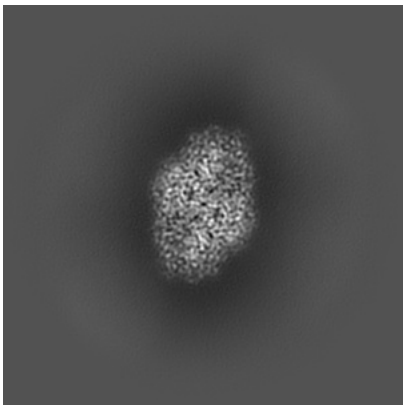
6.1.1 Primary map



X

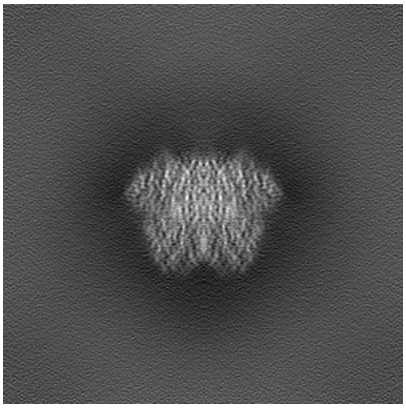


Y

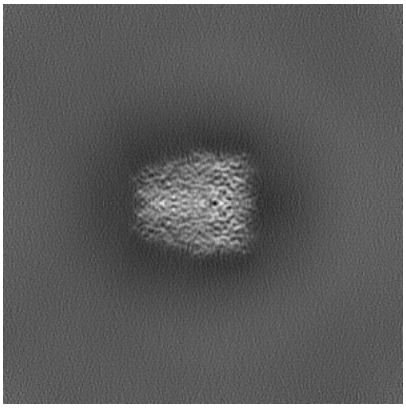


Z

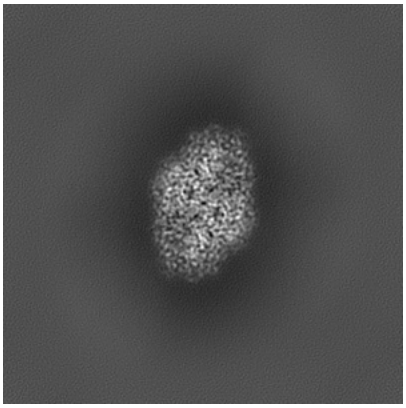
6.1.2 Raw map



X



Y

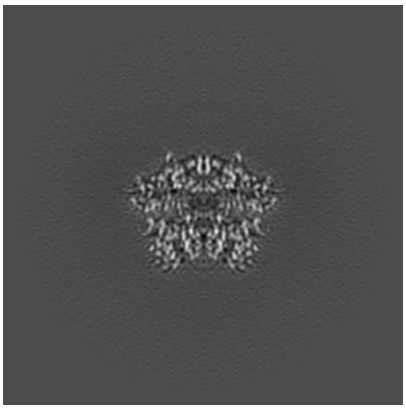


Z

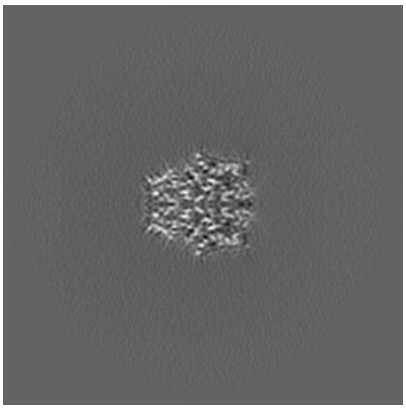
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

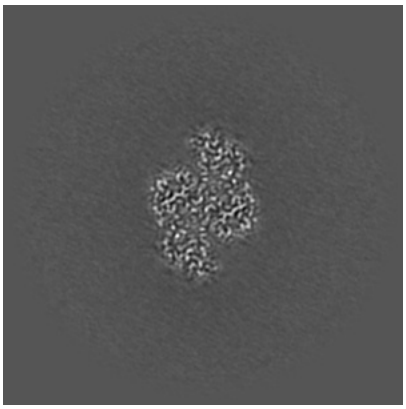
6.2.1 Primary map



X Index: 140

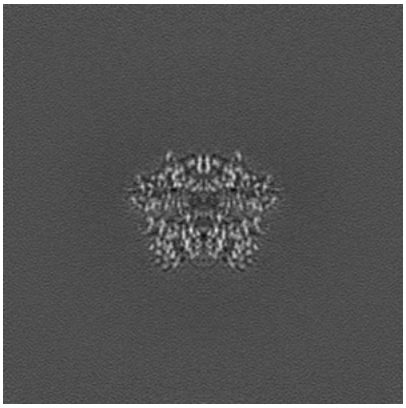


Y Index: 140

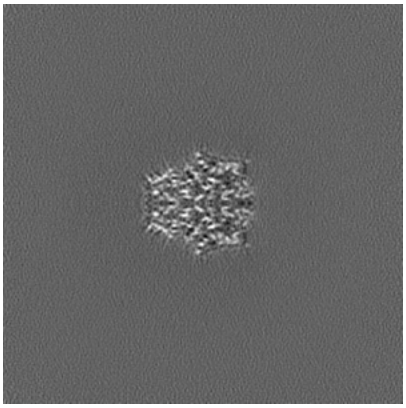


Z Index: 140

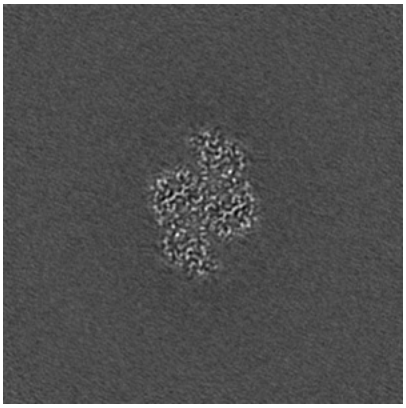
6.2.2 Raw map



X Index: 140



Y Index: 140

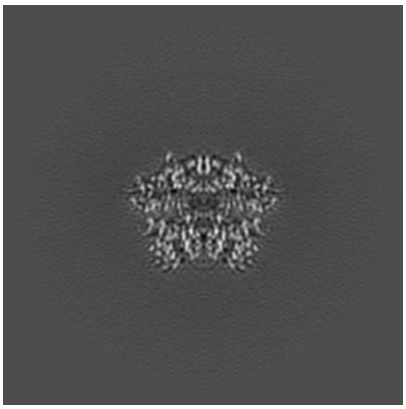


Z Index: 140

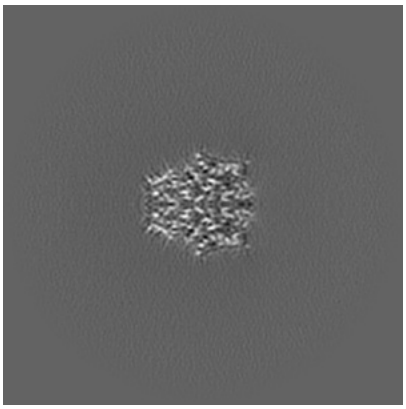
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

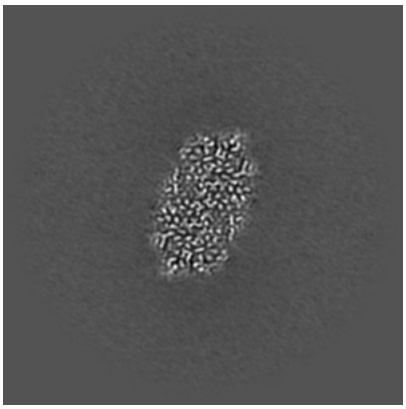
6.3.1 Primary map



X Index: 140

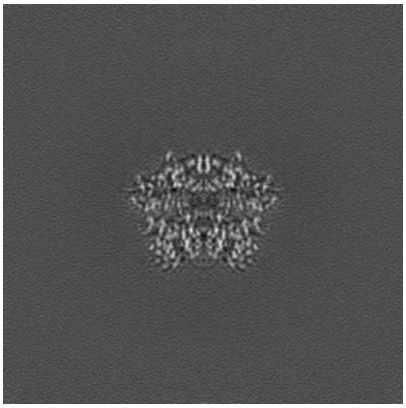


Y Index: 140

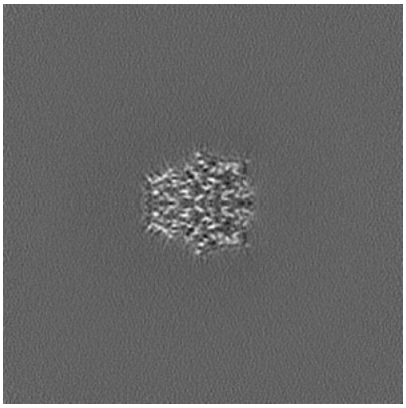


Z Index: 155

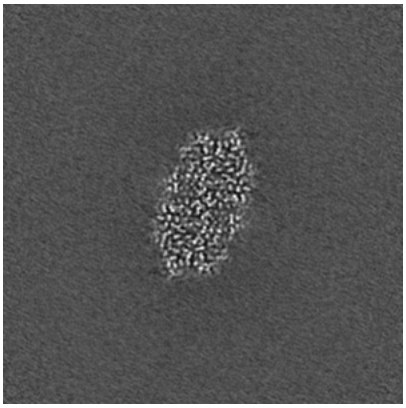
6.3.2 Raw map



X Index: 140



Y Index: 140

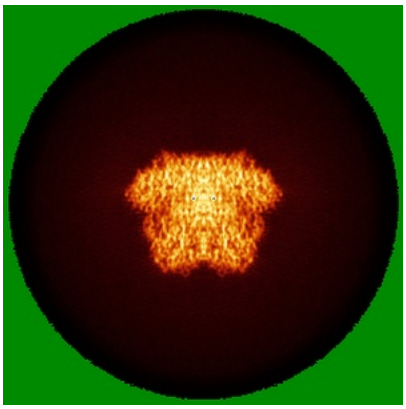


Z Index: 154

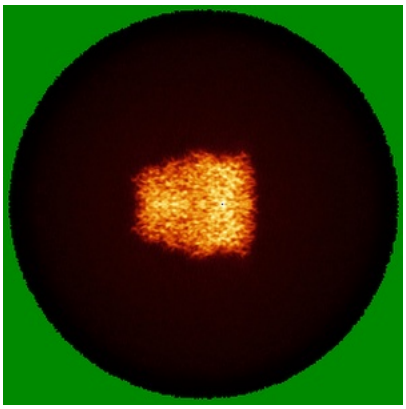
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

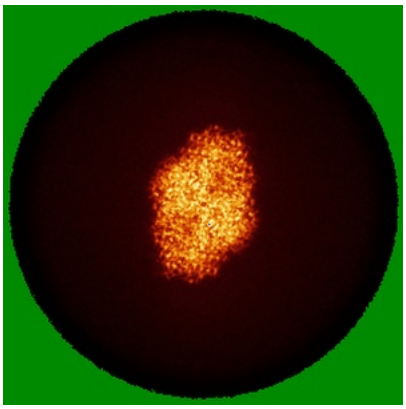
6.4.1 Primary map



X

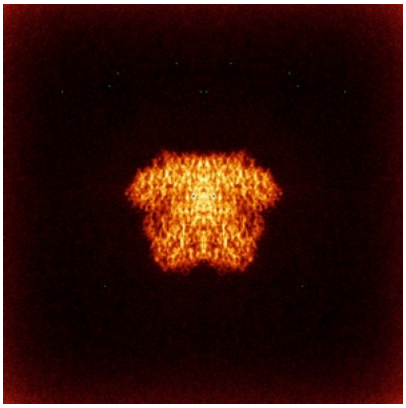


Y

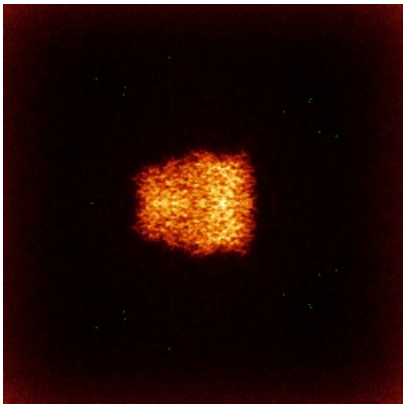


Z

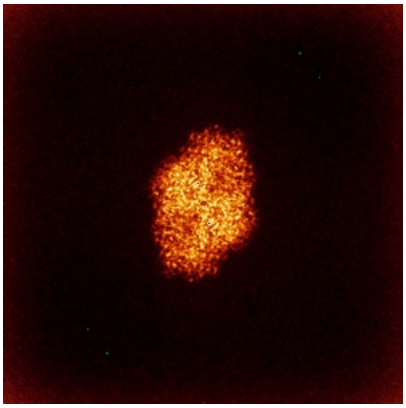
6.4.2 Raw map



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 0.0947. 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.

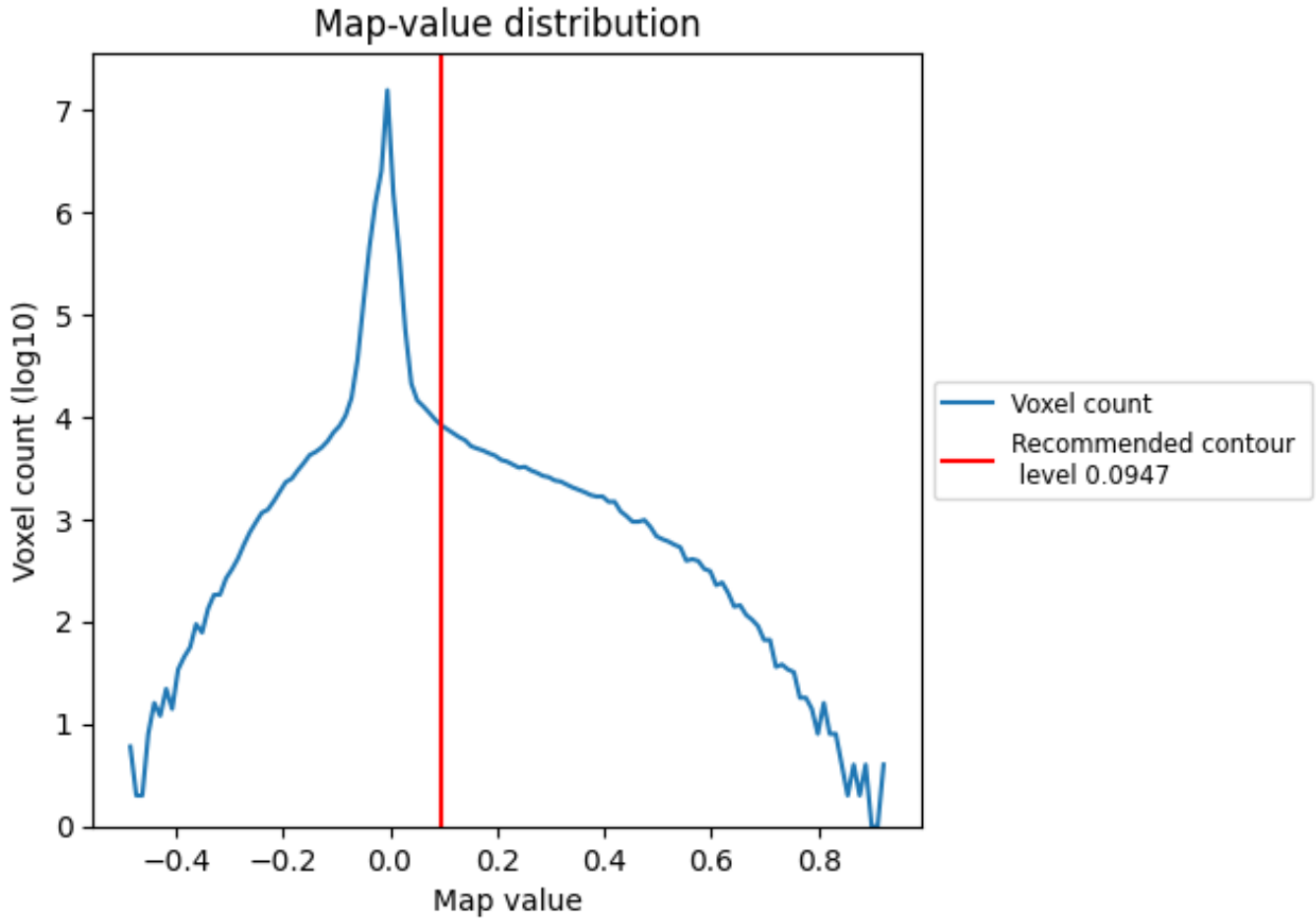
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

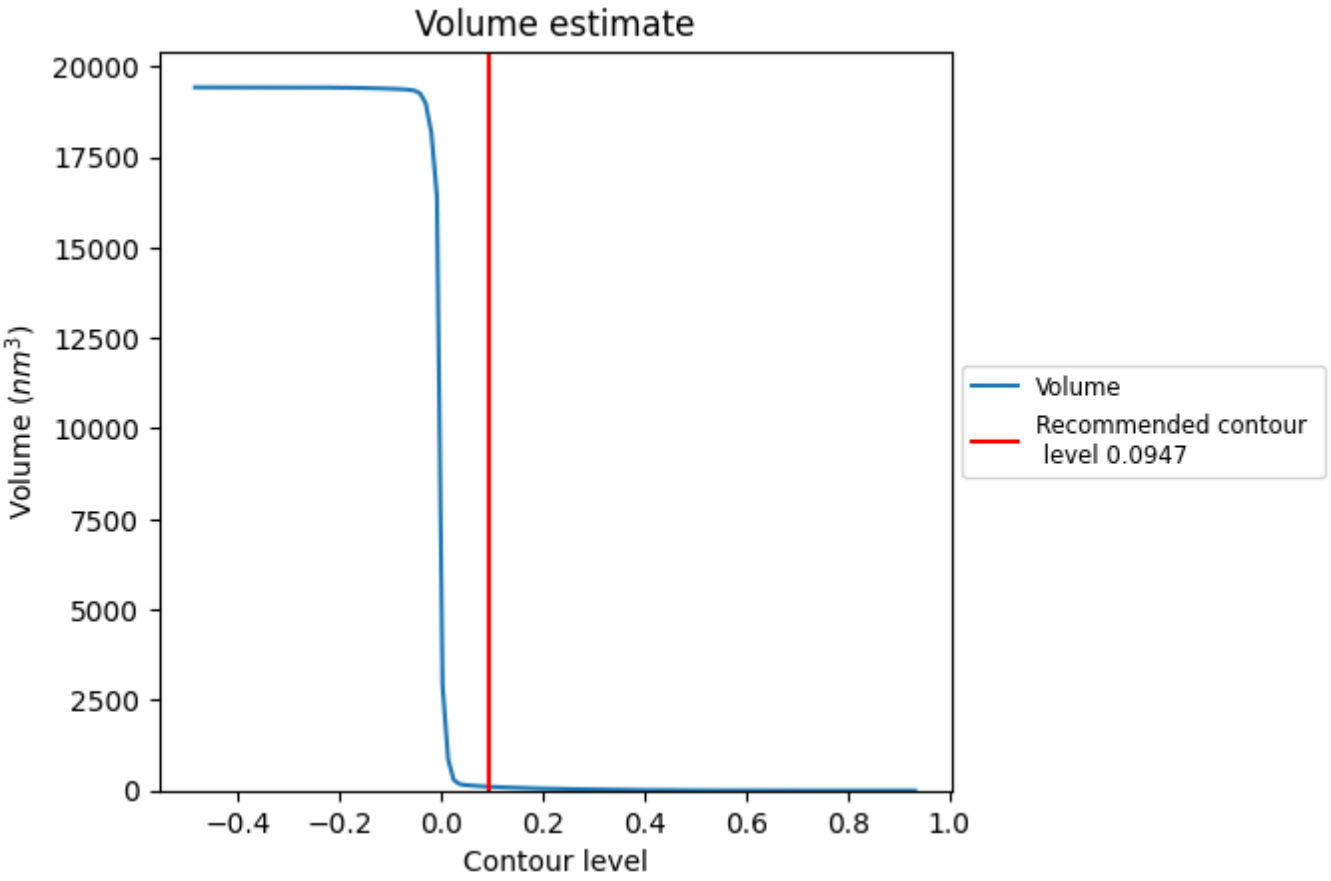
This section contains the results of statistical analysis of the map.

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.

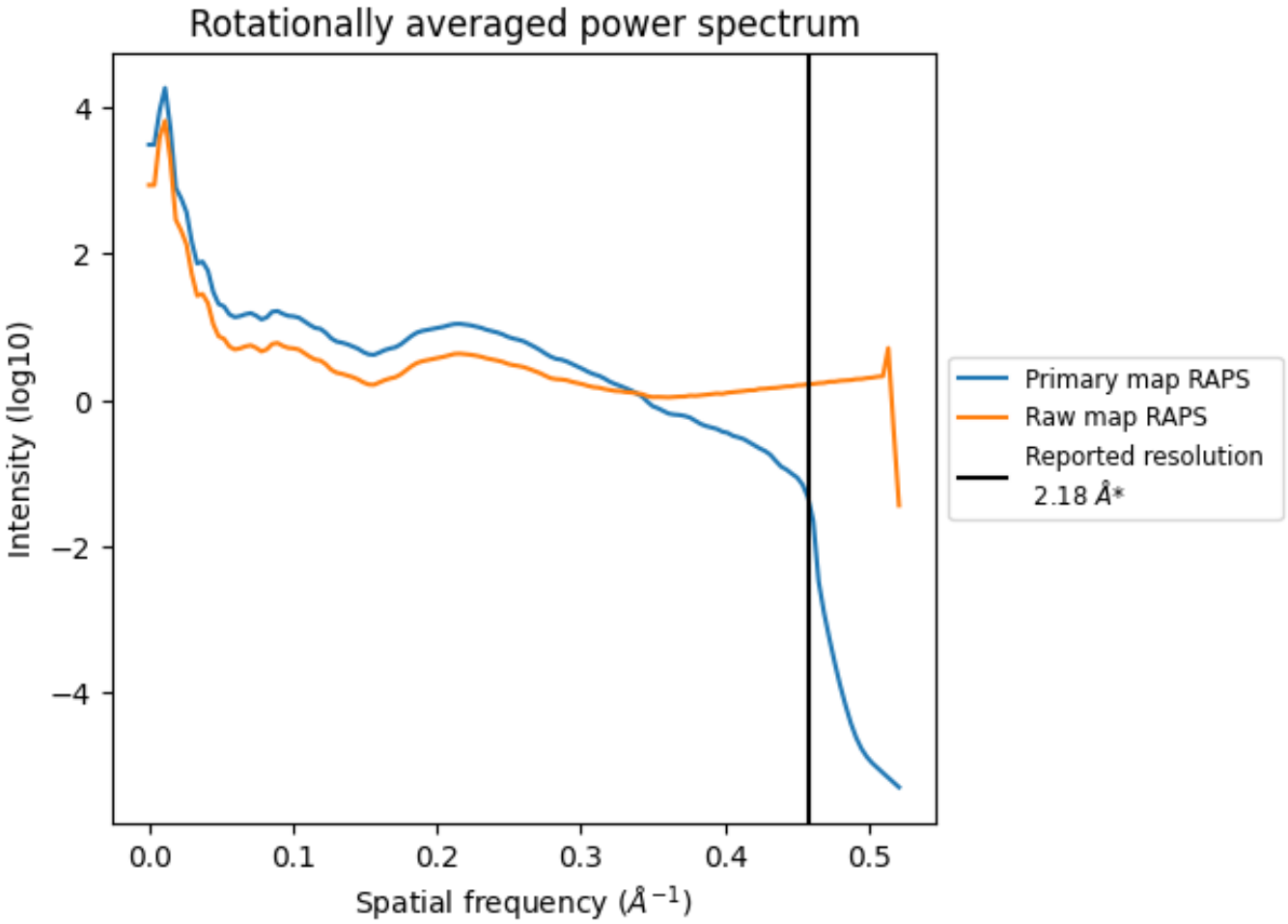
7.2 Volume estimate



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 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)

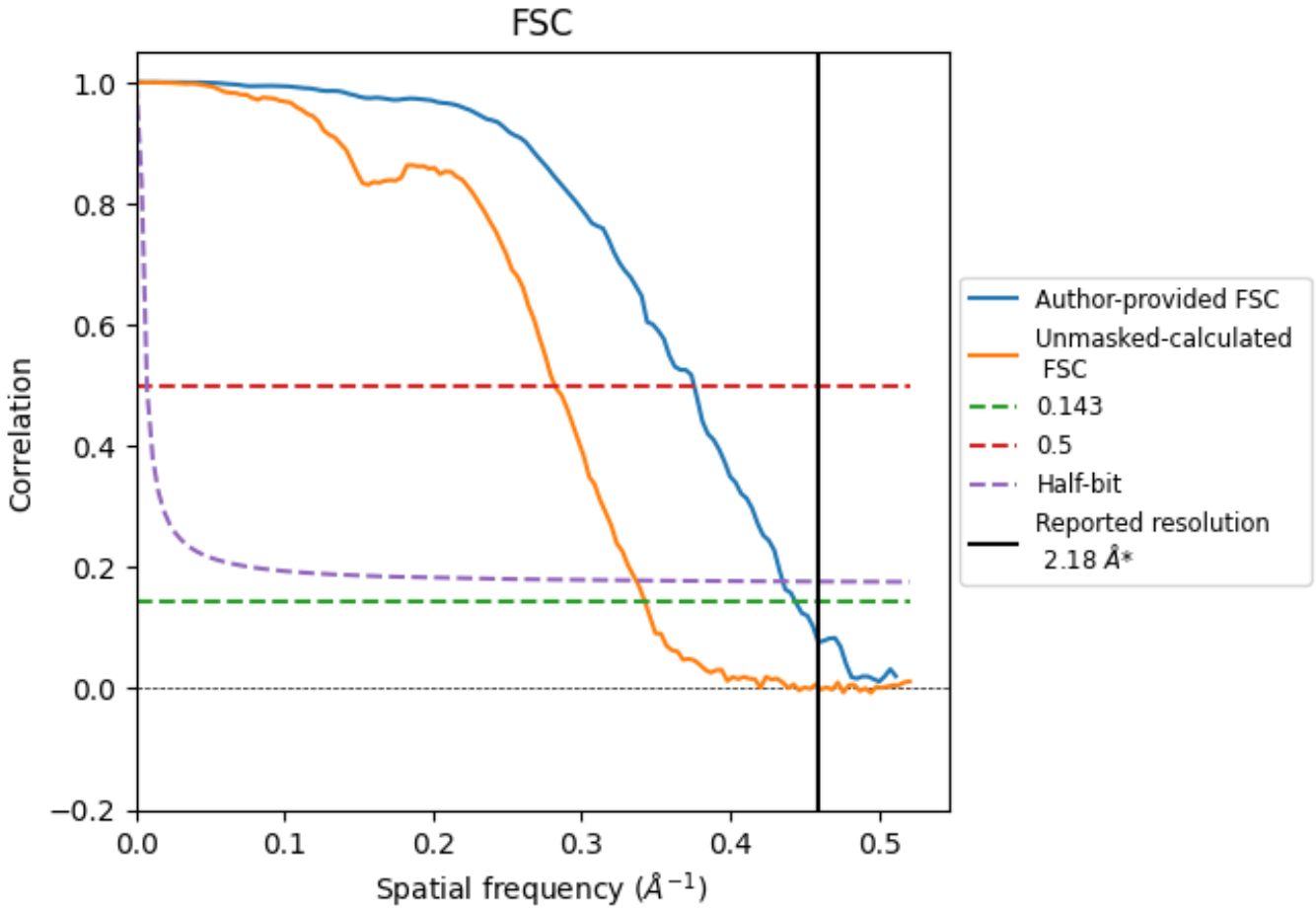


*Reported resolution corresponds to spatial frequency of 0.459 Å^{-1}

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 0.459 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.25	2.66	2.30
Unmasked-calculated*	2.92	3.55	2.97

*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 2.92 differs from the reported value 2.18 by more than 10 %

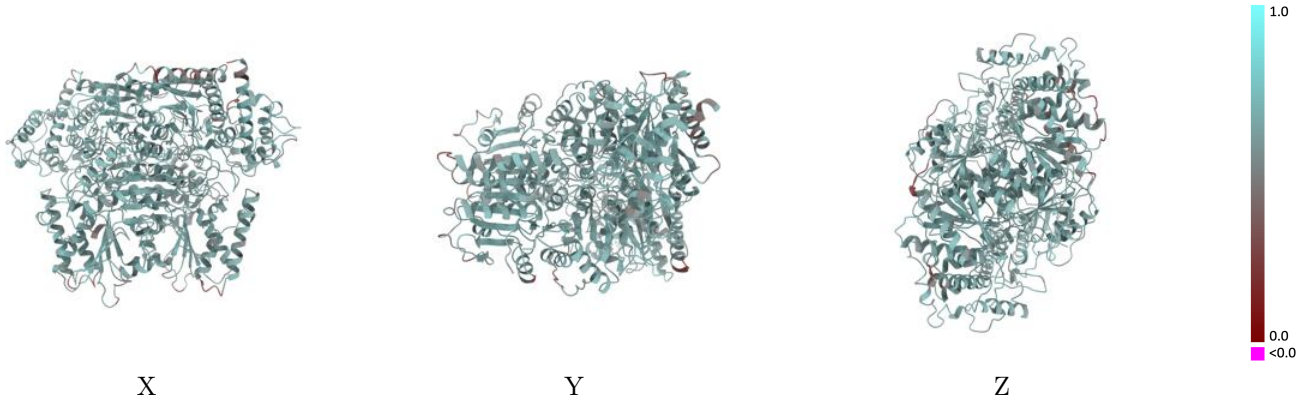
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45461 and PDB model 9CD3. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay

This section was not generated.

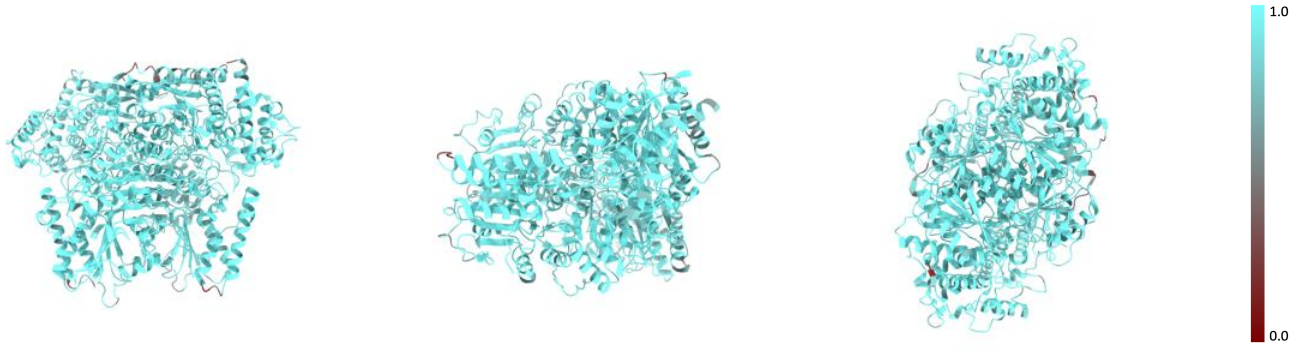
9.2 Q-score mapped to coordinate model



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.

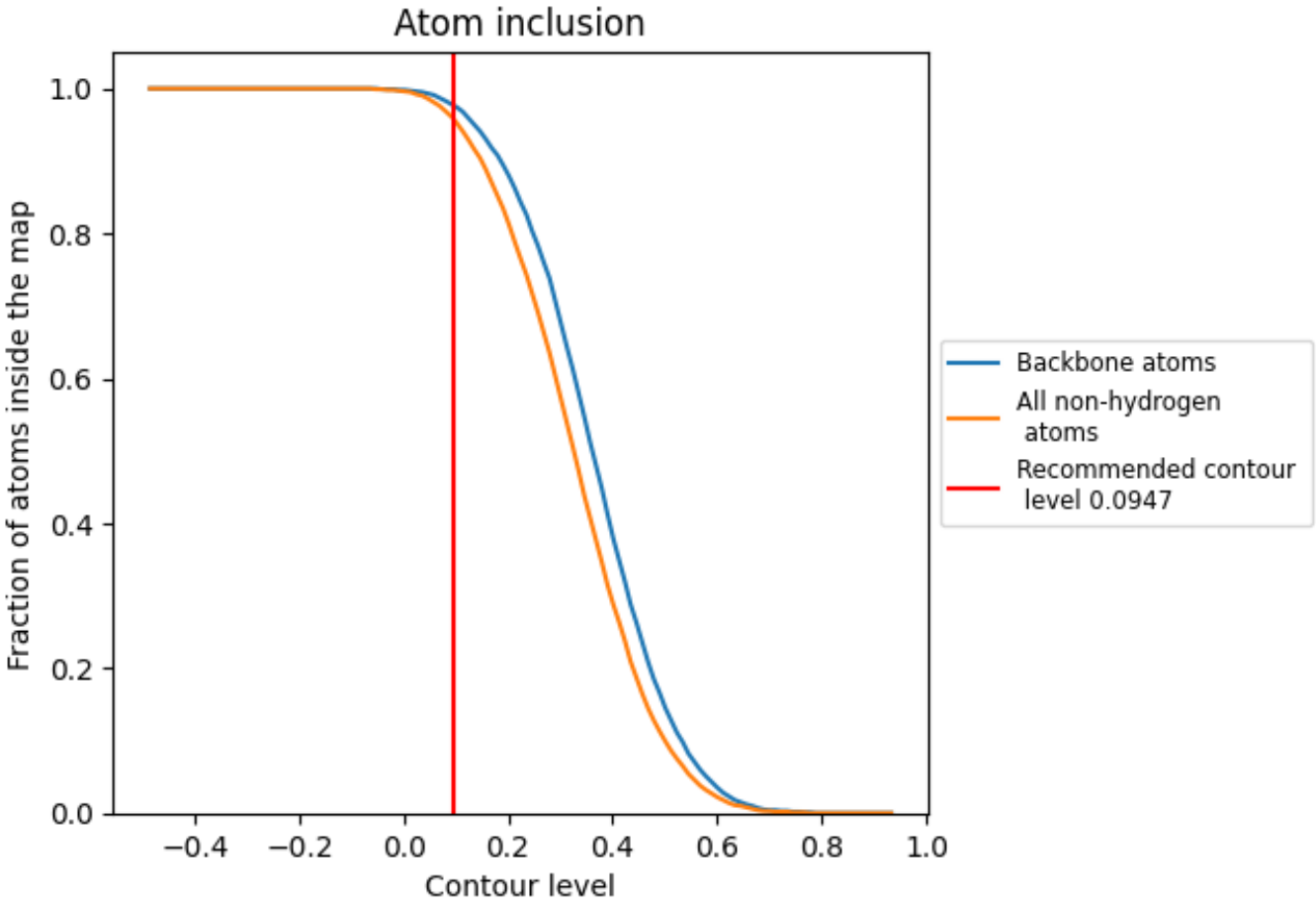
9.3 Atom inclusion mapped to coordinate model



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 (0.0947).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0947) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9590	0.6040
A	0.9610	0.6060
B	0.9570	0.6030