



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:15 PM UTC

PDB ID : 6XWN / pdb_00006xwn
EMDB ID : EMD-10632
Title : Structure of glutamate transporter homologue GltTk in the presence of TBOA inhibitor
Authors : Arkhipova, V.; Slotboom, D.J.; Guskov, A.
Deposited on : 2020-01-24
Resolution : 3.47 Å(reported)

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

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

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

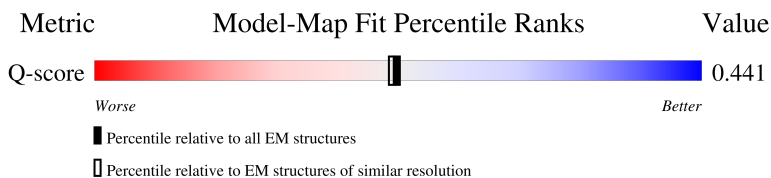
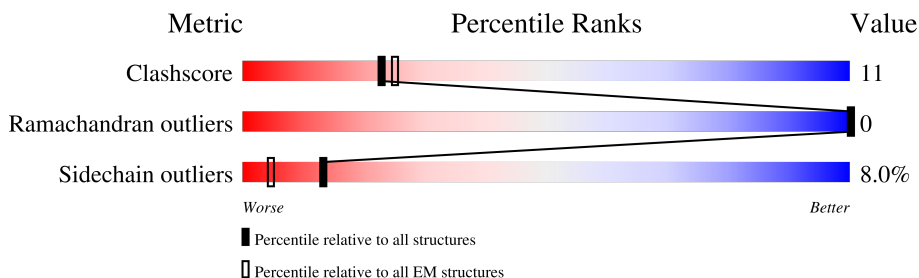
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 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	13733 (2.97 - 3.97)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	
1	B	430	
1	C	430	

2 Entry composition [i](#)

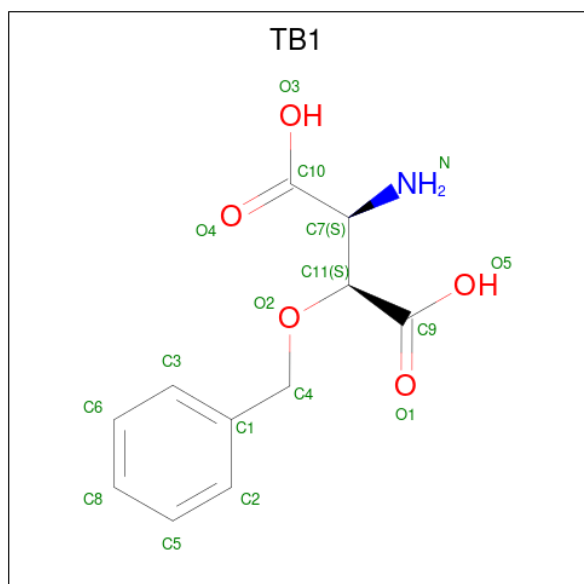
There are 2 unique types of molecules in this entry. The entry contains 9547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proton/glutamate symporter, SDF family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	427	Total	C	N	O	S	0	0
			3184	2100	515	553	16		
1	B	426	Total	C	N	O	S	0	0
			3178	2097	514	551	16		
1	C	423	Total	C	N	O	S	0	0
			3151	2079	508	548	16		

- Molecule 2 is (3S)-3-(BENZYLOXY)-L-ASPARTIC ACID (CCD ID: TB1) (formula: C₁₁H₁₃NO₅).

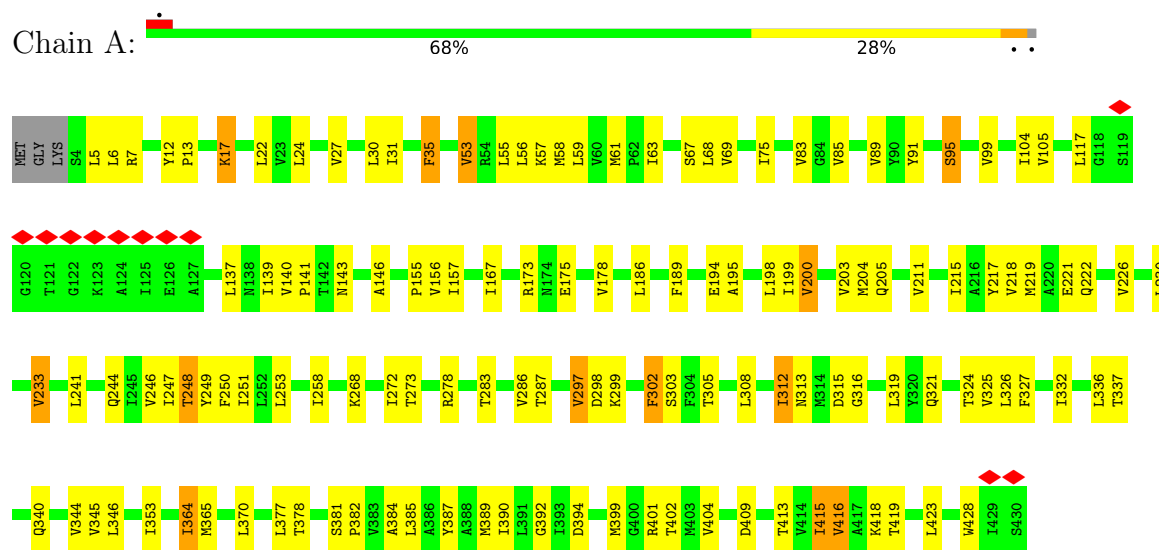


Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			17	11	1	5	
2	C	1	Total	C	N	O	0
			17	11	1	5	

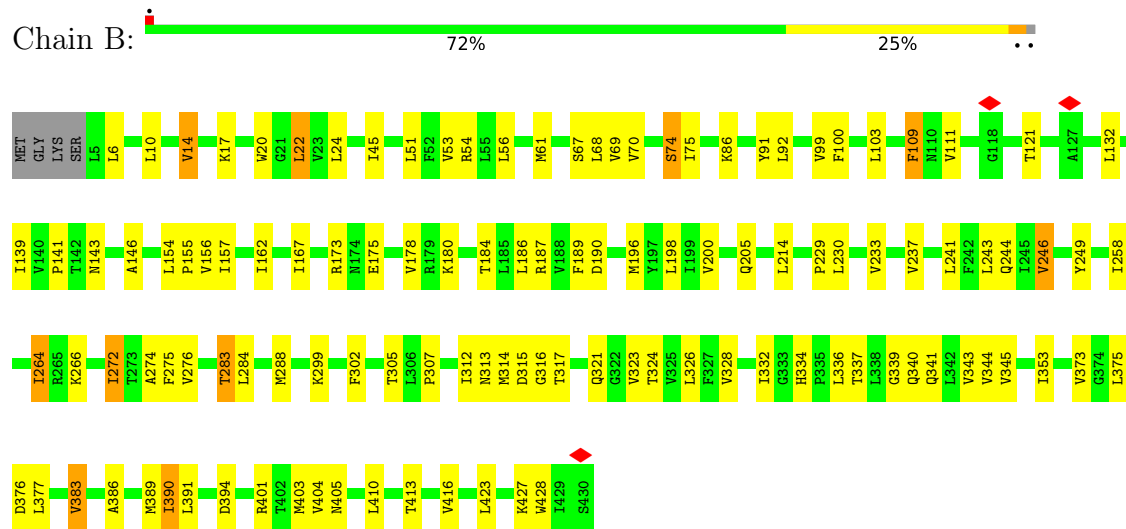
3 Residue-property plots

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: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family

Chain C:

70%

26%

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132917	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.442	Depositor
Minimum map value	-0.171	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.102	Depositor
Map size ($\text{\AA}$)	259.072, 259.072, 259.072	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.012, 1.012, 1.012	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: TB1

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	0.18	0/3243	0.36	0/4414
1	B	0.17	0/3237	0.32	0/4406
1	C	0.18	0/3210	0.33	0/4370
All	All	0.17	0/9690	0.34	0/13190

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	3184	0	3393	78	0
1	B	3178	0	3388	65	0
1	C	3151	0	3353	82	0
2	B	17	0	11	0	0
2	C	17	0	11	3	0
All	All	9547	0	10156	220	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 11.

All (220) 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:246:VAL:O	1:A:250:PHE:HB2	1.88	0.74
1:A:278:ARG:HA	1:A:402:THR:HG21	1.72	0.72
1:B:157:ILE:HD11	1:B:307:PRO:HB2	1.73	0.71
1:A:233:VAL:HG11	1:A:390:ILE:HD11	1.73	0.69
1:C:299:LYS:O	1:C:303:SER:OG	2.12	0.67
1:C:314:MET:HB3	1:C:317:THR:HB	1.78	0.66
1:A:75:ILE:HG22	1:A:308:LEU:HD11	1.77	0.66
1:A:12:TYR:HD2	1:A:17:LYS:HG3	1.60	0.65
1:C:123:LYS:H	1:C:388:ALA:HB2	1.61	0.65
1:C:67:SER:HG	1:C:197:TYR:HH	1.38	0.64
1:B:423:LEU:HD11	1:B:428:TRP:HE1	1.62	0.64
1:B:337:THR:H	1:B:340:GLN:HE21	1.44	0.64
1:C:314:MET:SD	1:C:405:ASN:ND2	2.71	0.63
1:C:12:TYR:HB3	1:C:17:LYS:HE2	1.81	0.63
1:B:314:MET:SD	1:B:405:ASN:ND2	2.72	0.63
1:B:274:ALA:HA	1:B:283:THR:HG21	1.81	0.63
1:C:211:VAL:HG13	1:C:276:VAL:HG11	1.80	0.62
1:B:332:ILE:HD13	1:B:375:LEU:HD21	1.79	0.62
1:C:211:VAL:HG22	1:C:276:VAL:HG21	1.81	0.61
1:C:233:VAL:HG21	1:C:390:ILE:HD11	1.81	0.61
1:B:167:ILE:HG21	1:B:186:LEU:HD13	1.80	0.61
1:A:418:LYS:HD3	1:A:423:LEU:HD22	1.83	0.61
1:A:321:GLN:NE2	1:A:365:MET:O	2.34	0.61
1:A:241:LEU:HD23	1:A:319:LEU:HD13	1.82	0.60
1:B:332:ILE:HG21	1:B:383:VAL:HG12	1.83	0.60
1:A:258:ILE:HD11	1:A:418:LYS:HG3	1.83	0.60
1:C:368:MET:O	1:C:372:SER:OG	2.19	0.60
1:C:175:GLU:HB3	1:C:178:VAL:HG12	1.82	0.60
1:A:17:LYS:NZ	1:A:205:GLN:OE1	2.35	0.59
1:A:175:GLU:HB3	1:A:178:VAL:HG12	1.85	0.59
1:C:221:GLU:OE2	1:C:222:GLN:NE2	2.36	0.58
1:A:137:LEU:HD22	1:B:51:LEU:HB2	1.83	0.58
1:A:167:ILE:HG21	1:A:186:LEU:HD13	1.85	0.58
1:A:141:PRO:HB3	1:A:155:PRO:HB3	1.86	0.58
1:A:12:TYR:HB3	1:A:17:LYS:HD3	1.85	0.57
1:A:22:LEU:HD13	1:A:392:GLY:HA3	1.86	0.57
1:C:401:ARG:NE	2:C:501:TB1:O1	2.36	0.57
1:C:401:ARG:HE	2:C:501:TB1:C9	2.18	0.56
1:B:314:MET:HB3	1:B:317:THR:HB	1.87	0.56
1:C:173:ARG:HD2	1:C:178:VAL:HG11	1.87	0.56
1:B:266:LYS:NZ	1:B:427:LYS:O	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:THR:O	1:A:381:SER:OG	2.22	0.56
1:A:57:LYS:HD3	1:A:377:LEU:HB3	1.89	0.56
1:C:343:VAL:O	1:C:347:THR:OG1	2.23	0.56
1:B:69:VAL:HG11	1:B:189:PHE:CD2	2.42	0.55
1:A:313:ASN:ND2	1:A:409:ASP:OD2	2.39	0.55
1:C:278:ARG:HH21	1:C:395:ALA:HA	1.71	0.55
1:C:378:THR:O	1:C:381:SER:OG	2.20	0.55
1:A:137:LEU:O	1:B:54:ARG:NE	2.40	0.54
1:A:299:LYS:O	1:A:303:SER:HB3	2.06	0.54
1:A:305:THR:OG1	1:A:413:THR:OG1	2.23	0.54
1:C:241:LEU:HD23	1:C:319:LEU:HD13	1.89	0.54
1:C:423:LEU:HD11	1:C:428:TRP:HE1	1.71	0.54
1:A:139:ILE:HD11	1:A:346:LEU:HD13	1.90	0.54
1:C:63:ILE:O	1:C:67:SER:HB2	2.08	0.54
1:C:365:MET:O	1:C:369:VAL:HG23	2.08	0.54
1:B:10:LEU:O	1:B:205:GLN:NE2	2.40	0.54
1:A:336:LEU:HA	1:A:340:GLN:HE21	1.73	0.54
1:B:244:GLN:NE2	1:B:315:ASP:OD2	2.42	0.53
1:C:398:ASP:HA	1:C:401:ARG:HG2	1.90	0.53
1:A:249:TYR:OH	1:A:315:ASP:OD2	2.26	0.53
1:C:75:ILE:HG21	1:C:80:LEU:HD13	1.91	0.53
1:A:316:GLY:HA3	1:A:401:ARG:HB2	1.91	0.53
1:A:59:LEU:HD13	1:A:200:VAL:HG23	1.88	0.53
1:A:61:MET:HE1	1:A:156:VAL:HG11	1.90	0.53
1:C:141:PRO:HB3	1:C:155:PRO:HB3	1.91	0.53
1:C:153:VAL:O	1:C:157:ILE:HG12	2.09	0.53
1:C:273:THR:HG21	1:C:286:VAL:HG11	1.90	0.53
1:A:244:GLN:O	1:A:248:THR:OG1	2.24	0.53
1:C:321:GLN:HE22	1:C:366:LEU:HB2	1.74	0.53
1:C:17:LYS:HD2	1:C:208:PRO:HG2	1.89	0.53
1:A:173:ARG:HH12	1:B:198:LEU:HD11	1.75	0.52
1:C:364:ILE:HG22	1:C:368:MET:HE3	1.90	0.52
1:A:219:MET:HE2	1:A:226:VAL:HG23	1.91	0.52
1:C:10:LEU:HD12	1:C:10:LEU:H	1.75	0.52
1:A:143:ASN:HB3	1:A:146:ALA:HB3	1.92	0.51
1:A:423:LEU:HD21	1:A:428:TRP:CD1	2.46	0.51
1:C:225:ARG:NH1	1:C:392:GLY:O	2.44	0.51
1:A:69:VAL:HG11	1:A:189:PHE:CD2	2.46	0.51
1:B:337:THR:H	1:B:340:GLN:NE2	2.09	0.51
1:B:328:VAL:HG23	1:B:386:ALA:HB3	1.92	0.50
1:B:299:LYS:HA	1:B:302:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HB	1:A:353:ILE:HA	1.94	0.49
1:B:180:LYS:NZ	1:B:187:ARG:HH12	2.09	0.49
1:C:318:ALA:HA	1:C:321:GLN:HG2	1.94	0.49
1:C:69:VAL:HG11	1:C:189:PHE:CD2	2.48	0.49
1:A:253:LEU:HD22	1:A:258:ILE:HG21	1.94	0.49
1:B:14:VAL:HA	1:B:17:LYS:HB3	1.94	0.49
1:A:12:TYR:CD1	1:A:13:PRO:HD2	2.48	0.49
1:A:247:ILE:O	1:A:251:ILE:HG12	2.13	0.49
1:A:325:VAL:HG23	1:A:370:LEU:HD23	1.93	0.49
1:B:339:GLY:O	1:B:343:VAL:HG23	2.13	0.49
1:C:375:LEU:HB3	1:C:383:VAL:HG21	1.94	0.49
1:C:317:THR:O	1:C:321:GLN:HG2	2.13	0.48
1:C:90:TYR:O	1:C:94:THR:HG23	2.14	0.48
1:A:268:LYS:HG3	1:A:272:ILE:HD11	1.95	0.48
1:A:253:LEU:HD23	1:A:415:ILE:HD11	1.95	0.48
1:B:196:MET:O	1:B:200:VAL:HG23	2.14	0.48
1:C:119:SER:HA	1:C:385:LEU:HD13	1.96	0.48
1:A:241:LEU:HD22	1:A:404:VAL:HG11	1.96	0.48
1:B:61:MET:HE1	1:B:156:VAL:HG11	1.95	0.48
1:B:121:THR:O	1:B:121:THR:OG1	2.29	0.48
1:C:271:MET:SD	1:C:407:THR:OG1	2.71	0.47
1:B:332:ILE:HG13	1:B:334:HIS:H	1.78	0.47
1:C:19:LEU:O	1:C:23:VAL:HG23	2.13	0.47
1:C:317:THR:OG1	2:C:501:TB1:O1	2.26	0.47
1:C:278:ARG:HG2	1:C:399:MET:HG2	1.96	0.47
1:C:238:TYR:HE1	1:C:400:GLY:HA3	1.79	0.47
1:B:237:VAL:HG22	1:B:323:VAL:HG11	1.95	0.47
1:A:324:THR:HG23	1:A:390:ILE:HG12	1.96	0.47
1:B:143:ASN:HB3	1:B:146:ALA:HB3	1.97	0.47
1:B:237:VAL:O	1:B:241:LEU:HG	2.15	0.47
1:C:317:THR:HA	1:C:401:ARG:HD2	1.96	0.47
1:A:27:VAL:O	1:A:31:ILE:HG13	2.15	0.47
1:B:241:LEU:HB3	1:B:404:VAL:HG21	1.97	0.47
1:C:387:TYR:CZ	1:C:391:LEU:HD12	2.49	0.47
1:A:117:LEU:HG	1:A:382:PRO:HB3	1.95	0.47
1:C:56:LEU:HA	1:C:56:LEU:HD23	1.76	0.47
1:C:60:VAL:HG22	1:C:285:PRO:HD3	1.97	0.47
1:A:91:TYR:O	1:A:95:SER:OG	2.30	0.46
1:A:385:LEU:O	1:A:389:MET:HG3	2.15	0.46
1:A:91:TYR:CG	1:A:313:ASN:HB2	2.50	0.46
1:C:157:ILE:HD11	1:C:307:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:O	1:A:99:VAL:HG23	2.16	0.46
1:B:175:GLU:HB2	1:B:178:VAL:HG12	1.97	0.46
1:B:377:LEU:HD12	1:B:383:VAL:HG23	1.97	0.46
1:B:391:LEU:HA	1:B:394:ASP:HB2	1.98	0.46
1:B:141:PRO:HB3	1:B:155:PRO:HB3	1.96	0.46
1:C:270:ALA:HA	1:C:273:THR:HG22	1.96	0.46
1:C:46:LYS:NZ	1:C:50:ASP:OD2	2.34	0.45
1:A:58:MET:HB2	1:C:141:PRO:O	2.16	0.45
1:A:200:VAL:HG21	1:A:364:ILE:HG13	1.99	0.45
1:C:8:ARG:N	1:C:11:ASP:OD2	2.49	0.45
1:C:68:LEU:HD21	1:C:161:ILE:HG12	1.98	0.45
1:C:273:THR:O	1:C:277:THR:OG1	2.30	0.45
1:A:217:TYR:CE1	1:A:221:GLU:HG3	2.51	0.45
1:B:139:ILE:HG12	1:B:154:LEU:HD13	1.97	0.45
1:C:59:LEU:HD13	1:C:200:VAL:HG22	1.97	0.45
1:A:117:LEU:HB2	1:A:222:GLN:HE22	1.82	0.45
1:B:229:PRO:O	1:B:233:VAL:HG23	2.17	0.45
1:C:84:GLY:O	1:C:88:VAL:HG23	2.16	0.45
1:C:299:LYS:HA	1:C:302:PHE:CE1	2.52	0.45
1:A:5:LEU:HG	1:A:7:ARG:H	1.81	0.45
1:B:67:SER:OG	1:B:288:MET:HE1	2.17	0.45
1:C:423:LEU:HD11	1:C:428:TRP:NE1	2.32	0.45
1:B:53:VAL:HG23	1:B:214:LEU:HD11	1.99	0.44
1:C:221:GLU:HG3	1:C:222:GLN:HG2	1.98	0.44
1:C:177:ARG:HE	1:C:177:ARG:HB3	1.64	0.44
1:B:344:VAL:HG22	1:B:373:VAL:HG21	1.99	0.44
1:C:325:VAL:HG21	1:C:369:VAL:HG12	1.99	0.44
1:A:194:GLU:HG3	1:C:178:VAL:HG23	1.99	0.44
1:A:297:VAL:HG22	1:A:423:LEU:HD12	1.99	0.44
1:B:249:TYR:OH	1:B:315:ASP:OD2	2.32	0.44
1:B:316:GLY:C	1:B:401:ARG:HB2	2.42	0.44
1:C:22:LEU:HD13	1:C:272:ILE:HG23	1.98	0.44
1:A:283:THR:O	1:A:287:THR:HG22	2.17	0.44
1:C:347:THR:HG21	1:C:372:SER:HB3	1.98	0.44
1:B:173:ARG:HD3	1:B:173:ARG:HA	1.75	0.44
1:C:326:LEU:HD12	1:C:326:LEU:HA	1.88	0.44
1:A:218:VAL:HG22	1:A:385:LEU:HD13	2.01	0.43
1:A:12:TYR:CG	1:A:13:PRO:HD2	2.53	0.43
1:B:258:ILE:HD12	1:B:258:ILE:H	1.83	0.43
1:A:273:THR:HG21	1:A:286:VAL:HG11	2.00	0.43
1:C:267:ALA:O	1:C:271:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:O	1:A:204:MET:HG2	2.18	0.43
1:A:218:VAL:HG21	1:A:385:LEU:HB3	2.00	0.43
1:B:70:VAL:HG21	1:B:190:ASP:HA	2.01	0.43
1:B:243:LEU:HA	1:B:246:VAL:HG12	2.01	0.43
1:B:321:GLN:HA	1:B:324:THR:HG22	2.01	0.43
1:B:91:TYR:OH	1:B:305:THR:O	2.34	0.43
1:A:56:LEU:HD23	1:A:387:TYR:HE1	1.84	0.42
1:C:186:LEU:HA	1:C:186:LEU:HD12	1.80	0.42
1:A:99:VAL:HG11	1:A:345:VAL:HA	2.00	0.42
1:B:86:LYS:HG3	1:B:416:VAL:HG22	2.01	0.42
1:C:332:ILE:HD11	1:C:375:LEU:HD22	2.01	0.42
1:B:109:PHE:HD1	1:B:109:PHE:HA	1.72	0.42
1:A:75:ILE:HG21	1:A:312:ILE:HG21	2.01	0.42
1:A:415:ILE:HD13	1:A:415:ILE:HA	1.79	0.42
1:B:91:TYR:CG	1:B:313:ASN:HB2	2.54	0.42
1:C:222:GLN:HG3	1:C:395:ALA:HB3	2.02	0.42
1:C:306:LEU:HD23	1:C:306:LEU:HA	1.77	0.42
1:C:397:LEU:HD12	1:C:397:LEU:HA	1.77	0.42
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.84	0.42
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.73	0.42
1:B:92:LEU:HD21	1:B:353:ILE:HD11	2.02	0.42
1:B:390:ILE:HD13	1:B:390:ILE:HA	1.76	0.42
1:C:268:LYS:HD3	1:C:268:LYS:HA	1.84	0.42
1:C:321:GLN:NE2	1:C:366:LEU:HB2	2.34	0.42
1:C:67:SER:OG	1:C:197:TYR:OH	2.14	0.42
1:A:53:VAL:HG21	1:A:384:ALA:HB1	2.01	0.41
1:B:74:SER:O	1:B:74:SER:OG	2.32	0.41
1:B:410:LEU:HD23	1:B:410:LEU:HA	1.90	0.41
1:A:327:PHE:CD2	1:A:390:ILE:HD13	2.54	0.41
1:B:241:LEU:HD22	1:B:404:VAL:HG21	2.01	0.41
1:A:83:VAL:HG13	1:A:416:VAL:HG11	2.02	0.41
1:A:299:LYS:HA	1:A:302:PHE:CE1	2.54	0.41
1:A:63:ILE:O	1:A:67:SER:HB3	2.21	0.41
1:A:85:VAL:O	1:A:89:VAL:HG12	2.20	0.41
1:A:415:ILE:O	1:A:419:THR:HG22	2.20	0.41
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.91	0.41
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.70	0.41
1:A:59:LEU:HD11	1:A:203:VAL:HG21	2.03	0.41
1:B:22:LEU:HD13	1:B:272:ILE:HG22	2.02	0.41
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.80	0.41
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ARG:HB3	1:C:9:TYR:H	1.60	0.41
1:C:15:LEU:HD12	1:C:16:TRP:HB3	2.03	0.41
1:C:68:LEU:HD23	1:C:160:ALA:HB3	2.03	0.41
1:C:90:TYR:CZ	1:C:94:THR:HG21	2.56	0.41
1:A:195:ALA:O	1:A:199:ILE:HG13	2.20	0.41
1:B:275:PHE:HB2	1:B:403:MET:HB2	2.02	0.41
1:C:87:ILE:HG13	1:C:91:TYR:CE2	2.56	0.41
1:C:226:VAL:HG13	1:C:226:VAL:O	2.21	0.41
1:B:6:LEU:O	1:B:6:LEU:HD23	2.21	0.40
1:B:99:VAL:HG11	1:B:345:VAL:HA	2.02	0.40
1:B:230:LEU:HD21	1:B:389:MET:HG2	2.03	0.40
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.90	0.40
1:B:264:ILE:HD13	1:B:264:ILE:HA	1.81	0.40
1:C:391:LEU:O	1:C:391:LEU:HD23	2.21	0.40
1:B:103:LEU:HD13	1:B:341:GLN:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	425/430 (99%)	410 (96%)	15 (4%)	0	100	100
1	B	424/430 (99%)	409 (96%)	15 (4%)	0	100	100
1	C	421/430 (98%)	409 (97%)	12 (3%)	0	100	100
All	All	1270/1290 (98%)	1228 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/337 (99%)	304 (91%)	31 (9%)	8	31
1	B	334/337 (99%)	309 (92%)	25 (8%)	12	38
1	C	331/337 (98%)	307 (93%)	24 (7%)	13	38
All	All	1000/1011 (99%)	920 (92%)	80 (8%)	13	36

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	17	LYS
1	A	30	LEU
1	A	35	PHE
1	A	53	VAL
1	A	68	LEU
1	A	95	SER
1	A	104	ILE
1	A	105	VAL
1	A	140	VAL
1	A	157	ILE
1	A	198	LEU
1	A	200	VAL
1	A	211	VAL
1	A	215	ILE
1	A	230	LEU
1	A	233	VAL
1	A	248	THR
1	A	297	VAL
1	A	298	ASP
1	A	302	PHE
1	A	312	ILE
1	A	326	LEU
1	A	332	ILE
1	A	337	THR
1	A	344	VAL

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Mol	Chain	Res	Type
1	A	364	ILE
1	A	394	ASP
1	A	399	MET
1	A	415	ILE
1	A	416	VAL
1	B	14	VAL
1	B	20	TRP
1	B	22	LEU
1	B	24	LEU
1	B	45	ILE
1	B	68	LEU
1	B	74	SER
1	B	75	ILE
1	B	100	PHE
1	B	109	PHE
1	B	111	VAL
1	B	132	LEU
1	B	162	ILE
1	B	184	THR
1	B	246	VAL
1	B	264	ILE
1	B	272	ILE
1	B	276	VAL
1	B	283	THR
1	B	312	ILE
1	B	326	LEU
1	B	376	ASP
1	B	383	VAL
1	B	390	ILE
1	B	413	THR
1	C	31	ILE
1	C	45	ILE
1	C	59	LEU
1	C	75	ILE
1	C	105	VAL
1	C	156	VAL
1	C	168	THR
1	C	184	THR
1	C	215	ILE
1	C	221	GLU
1	C	243	LEU
1	C	276	VAL

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Mol	Chain	Res	Type
1	C	281	SER
1	C	290	VAL
1	C	312	ILE
1	C	317	THR
1	C	342	LEU
1	C	347	THR
1	C	352	SER
1	C	372	SER
1	C	373	VAL
1	C	375	LEU
1	C	378	THR
1	C	413	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	172	ASN
1	A	222	GLN
1	A	340	GLN
1	B	134	GLN
1	B	330	ASN
1	B	340	GLN
1	C	174	ASN
1	C	340	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

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	TB1	B	501	-	16,17,17	0.87	0	19,22,22	0.93	0
2	TB1	C	501	-	16,17,17	0.88	0	19,22,22	1.04	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TB1	B	501	-	-	9/17/17/17	0/1/1/1
2	TB1	C	501	-	-	8/17/17/17	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	TB1	O2-C11-C9	-2.14	109.06	112.26

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	TB1	C9-C11-O2-C4
2	B	501	TB1	O2-C11-C9-O5
2	B	501	TB1	O2-C11-C9-O1
2	B	501	TB1	O2-C11-C7-C10
2	B	501	TB1	O2-C11-C7-N
2	B	501	TB1	C9-C11-C7-C10
2	B	501	TB1	C9-C11-C7-N

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Mol	Chain	Res	Type	Atoms
2	C	501	TB1	O2-C11-C7-N
2	C	501	TB1	C9-C11-C7-C10
2	C	501	TB1	O2-C11-C9-O1
2	C	501	TB1	O2-C11-C9-O5
2	B	501	TB1	C1-C4-O2-C11
2	C	501	TB1	C9-C11-C7-N
2	C	501	TB1	C1-C4-O2-C11
2	C	501	TB1	O3-C10-C7-N
2	B	501	TB1	O4-C10-C7-N
2	C	501	TB1	O4-C10-C7-N

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	TB1	3	0

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.

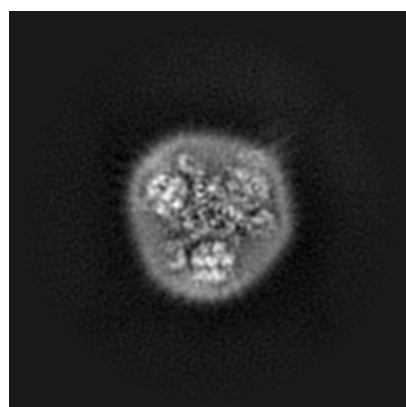
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10632. These allow visual inspection of the internal detail of the map and identification of artifacts.

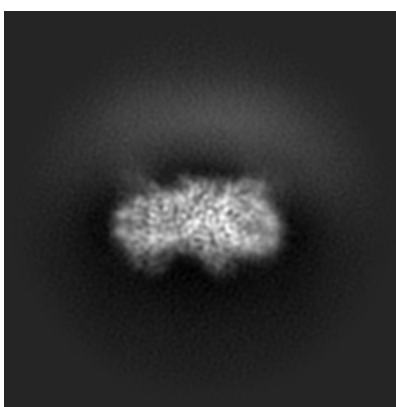
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

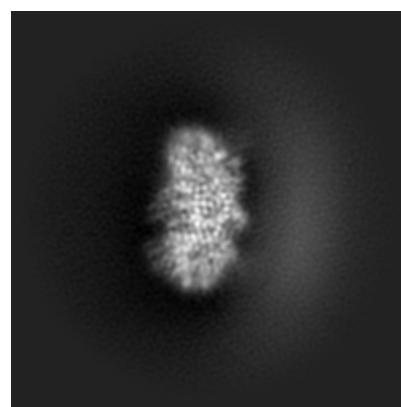
6.1.1 Primary map



X



Y

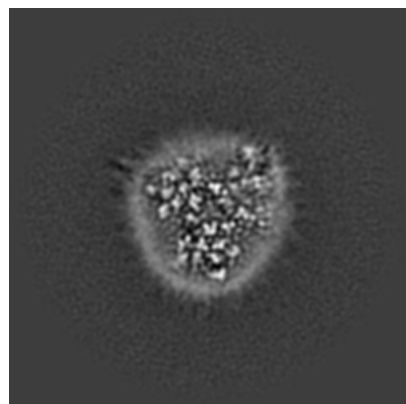


Z

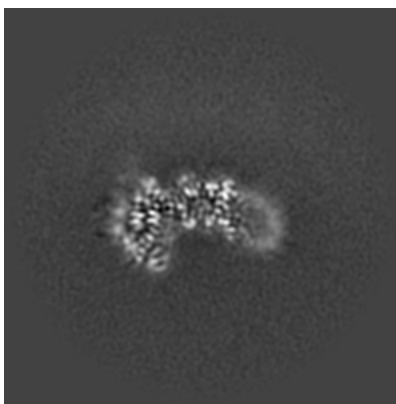
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

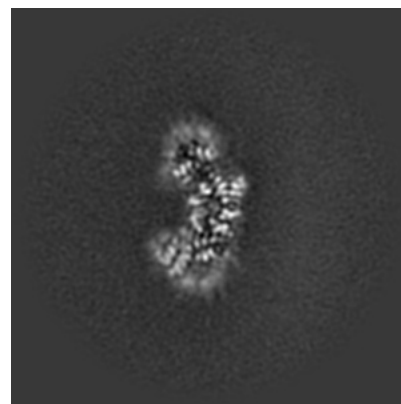
6.2.1 Primary map



X Index: 128



Y Index: 128

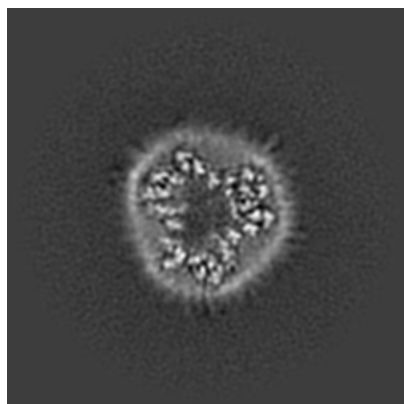


Z Index: 128

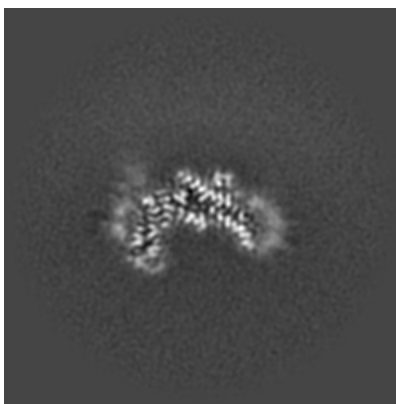
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

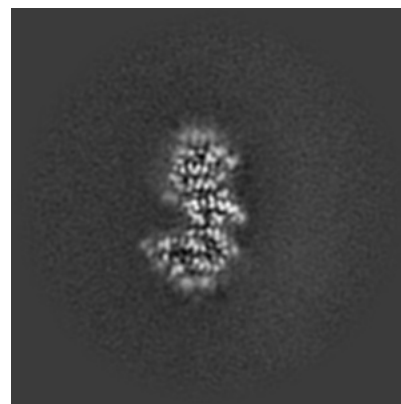
6.3.1 Primary map



X Index: 111



Y Index: 122

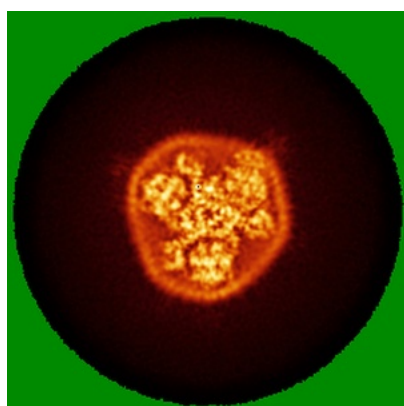


Z Index: 142

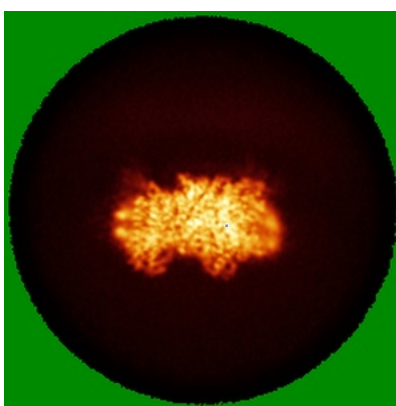
The images above show the largest variance slices of the map in three orthogonal directions.

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

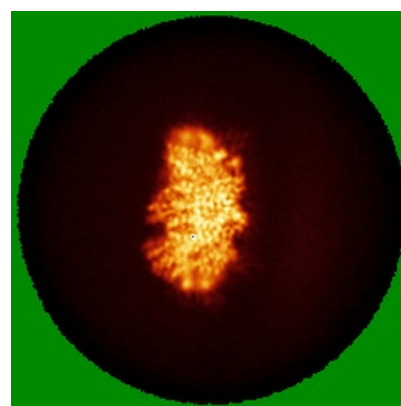
6.4.1 Primary map



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

This section was not generated.

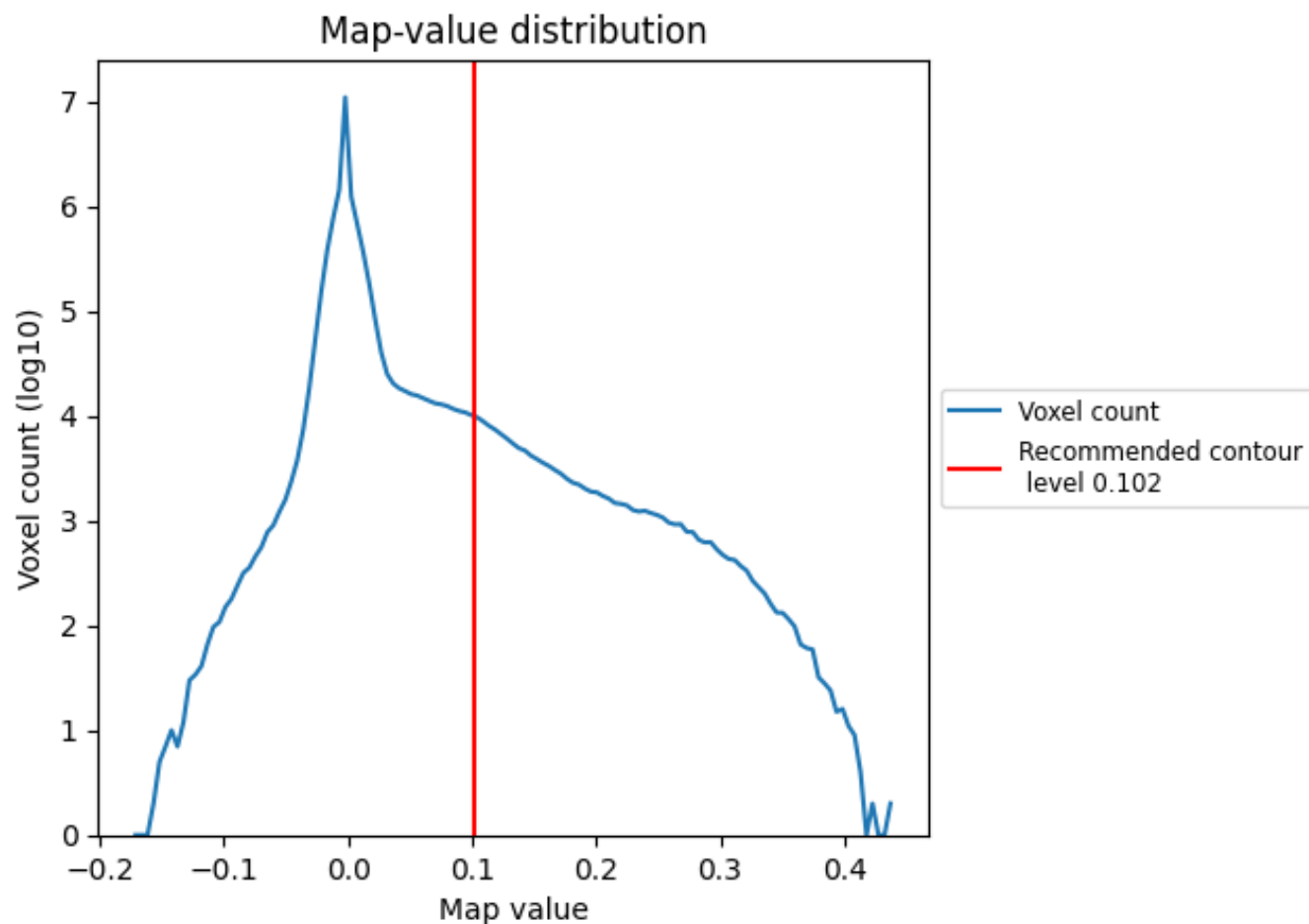
6.6 Mask visualisation

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

7 Map analysis [i](#)

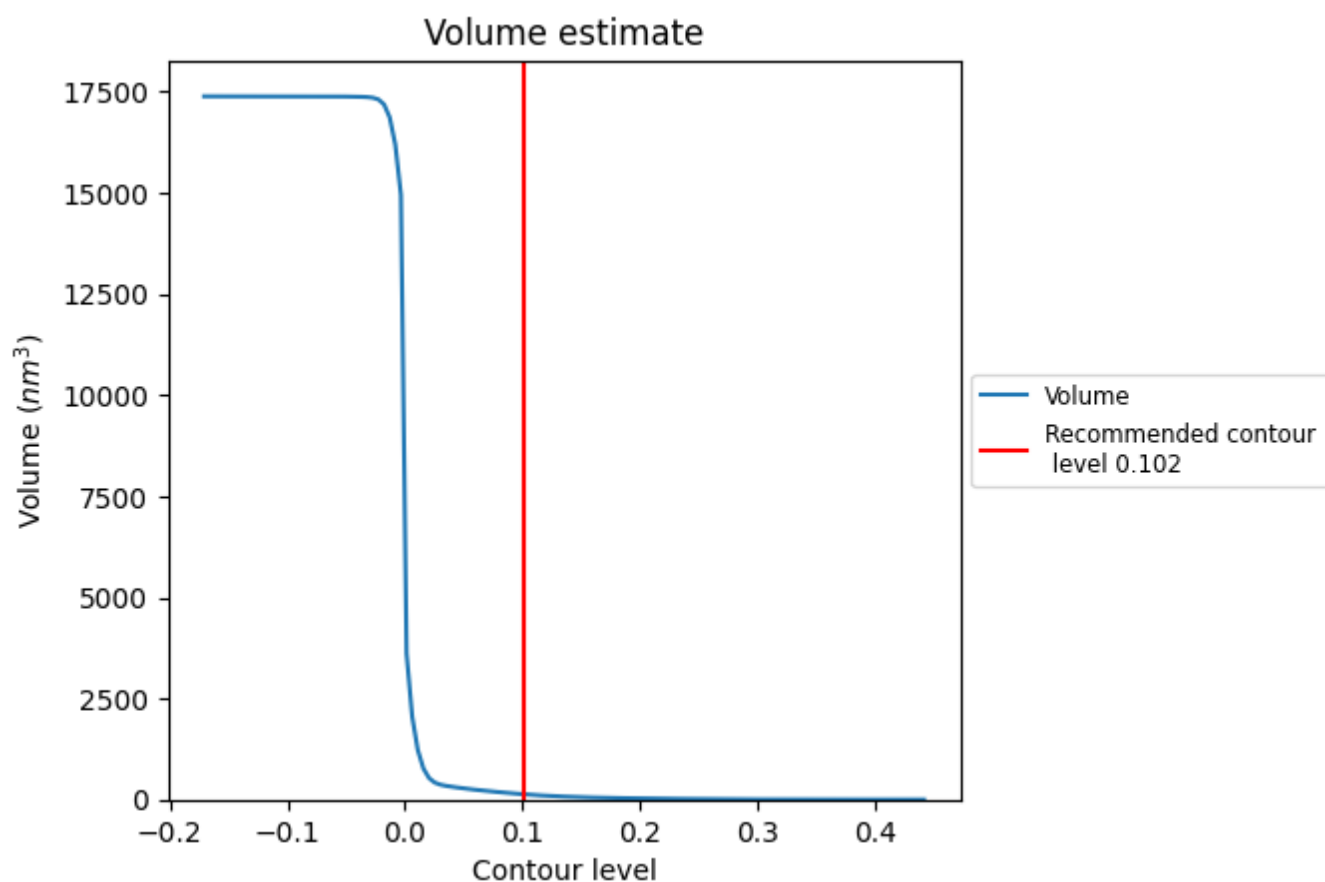
This section contains the results of statistical analysis of the map.

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.

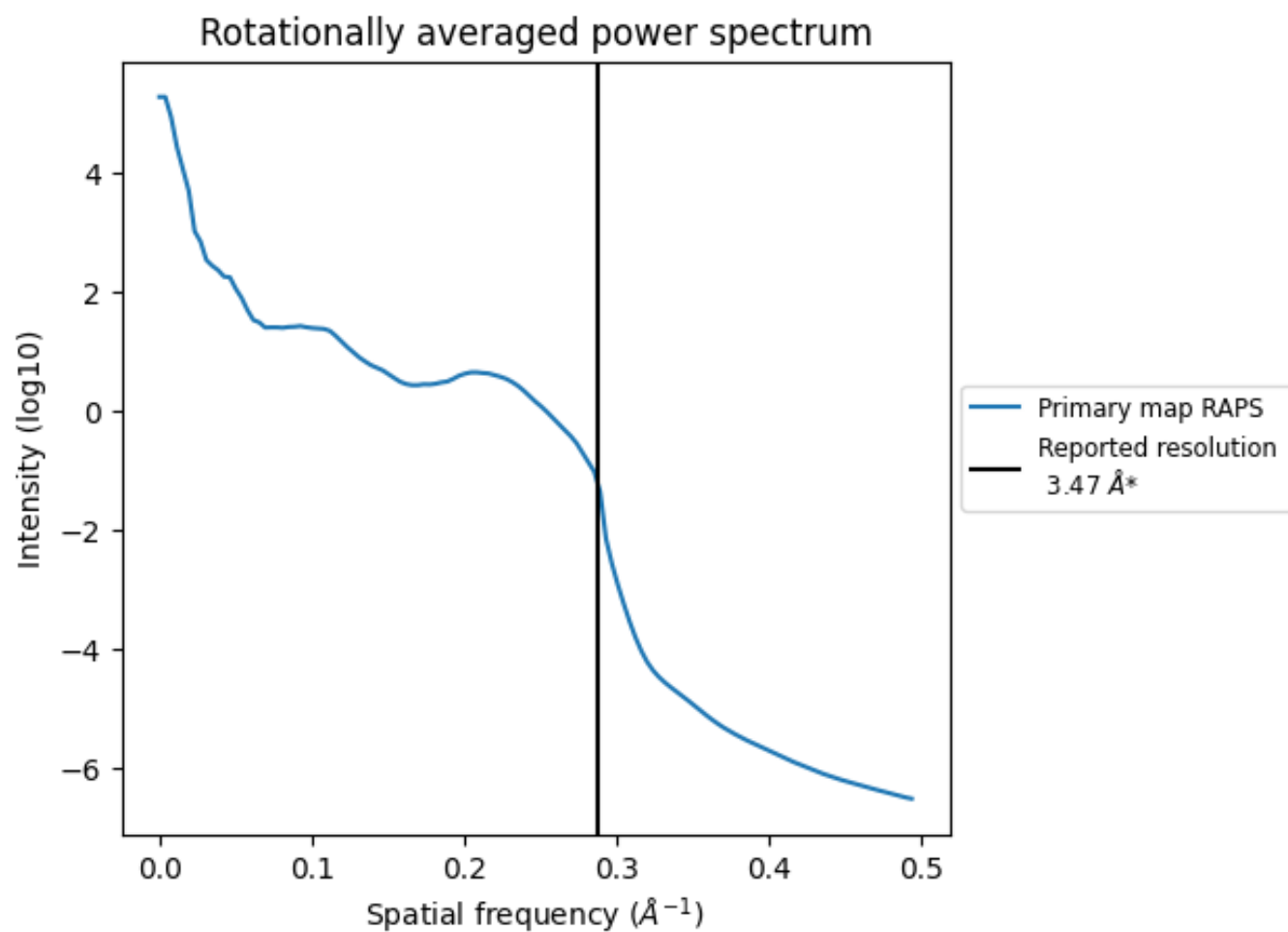
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 117 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 0.288 Å⁻¹

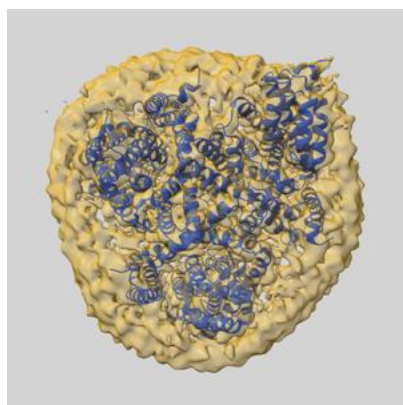
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

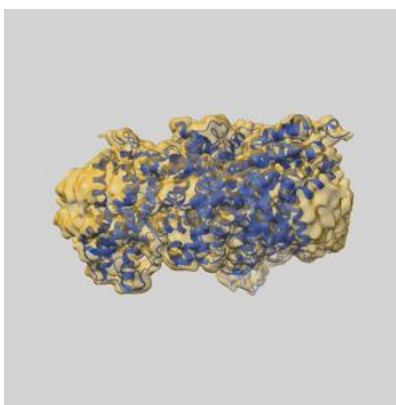
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10632 and PDB model 6XWN. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

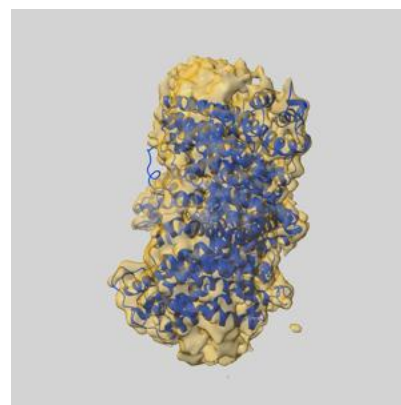
9.1 Map-model overlay [i](#)



X



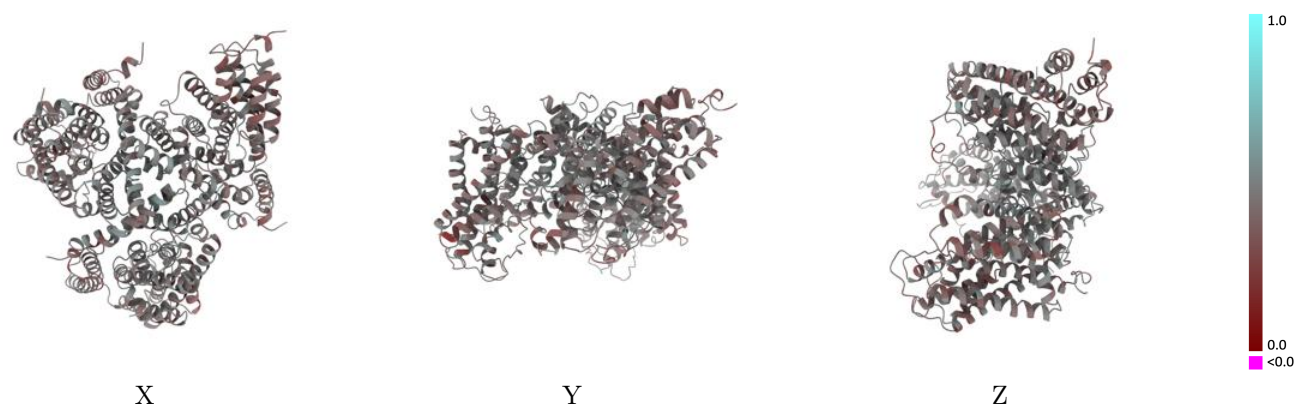
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

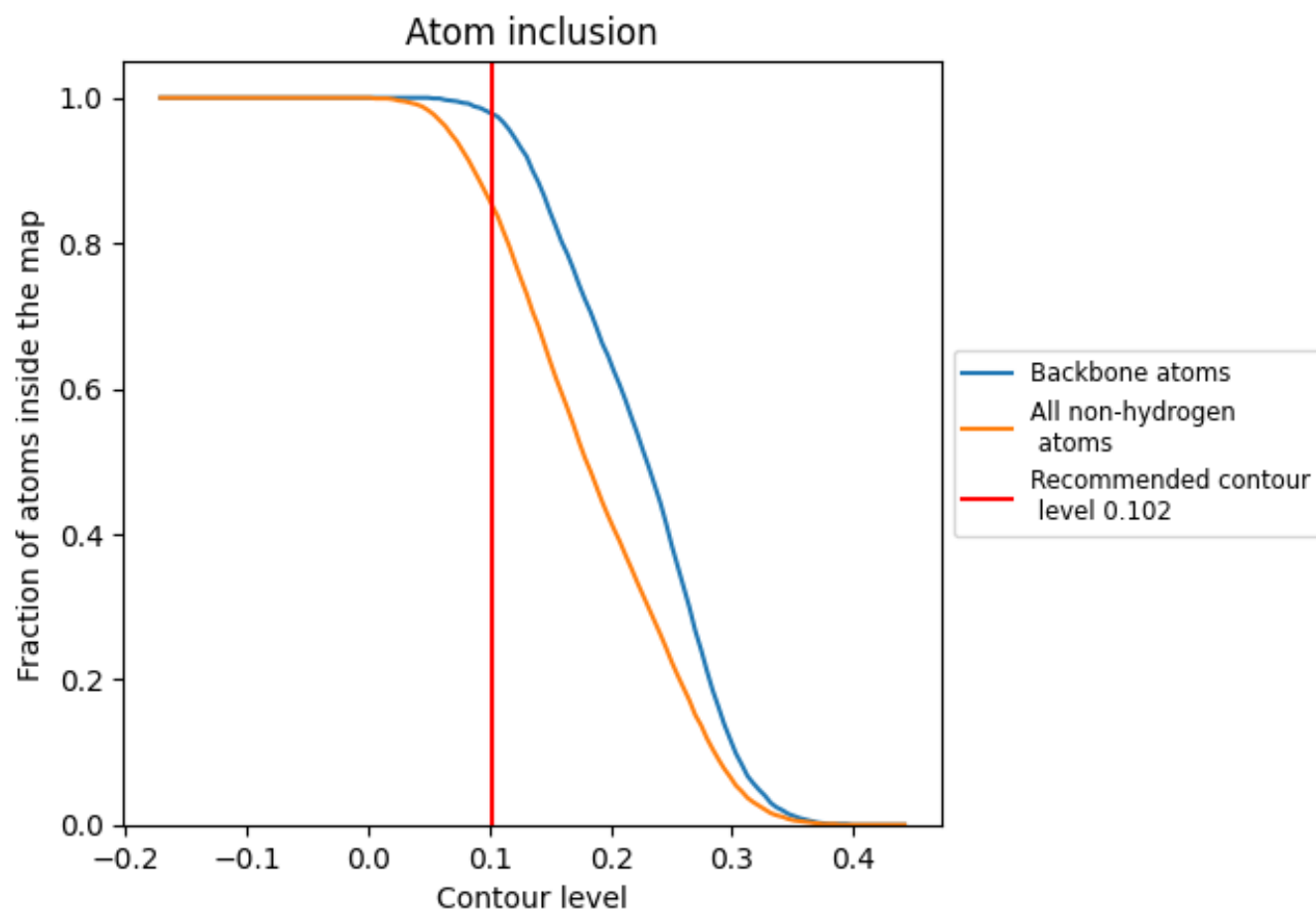


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 85% 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 (0.102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.4410
A	0.8460	0.4390
B	0.8550	0.4380
C	0.8590	0.4470

