



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 11:31 PM UTC

PDB ID : 6V1Q / pdb_00006v1q
EMDB ID : EMD-21015
Title : Two-pore channel 3
Authors : Dickinson, M.S.; Stroud, R.M.
Deposited on : 2019-11-20
Resolution : 3.11 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
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

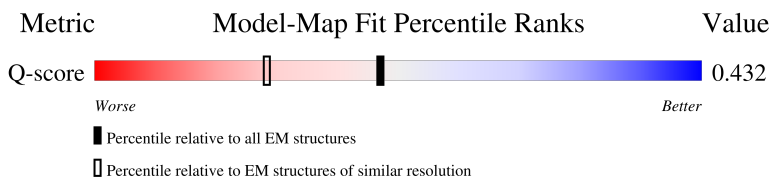
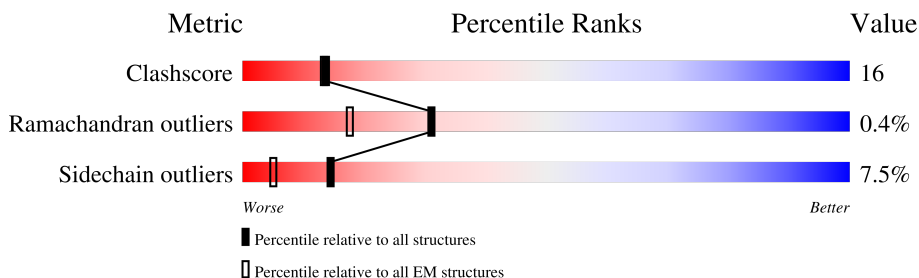
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	773	11% 43% 24% 30%
1	B	773	12% 43% 24% 30%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8825 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 Two pore channel 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	538	Total	C	N	O	S	0	0
			4412	2960	701	732	19		
1	B	538	Total	C	N	O	S	0	0
			4412	2960	701	732	19		

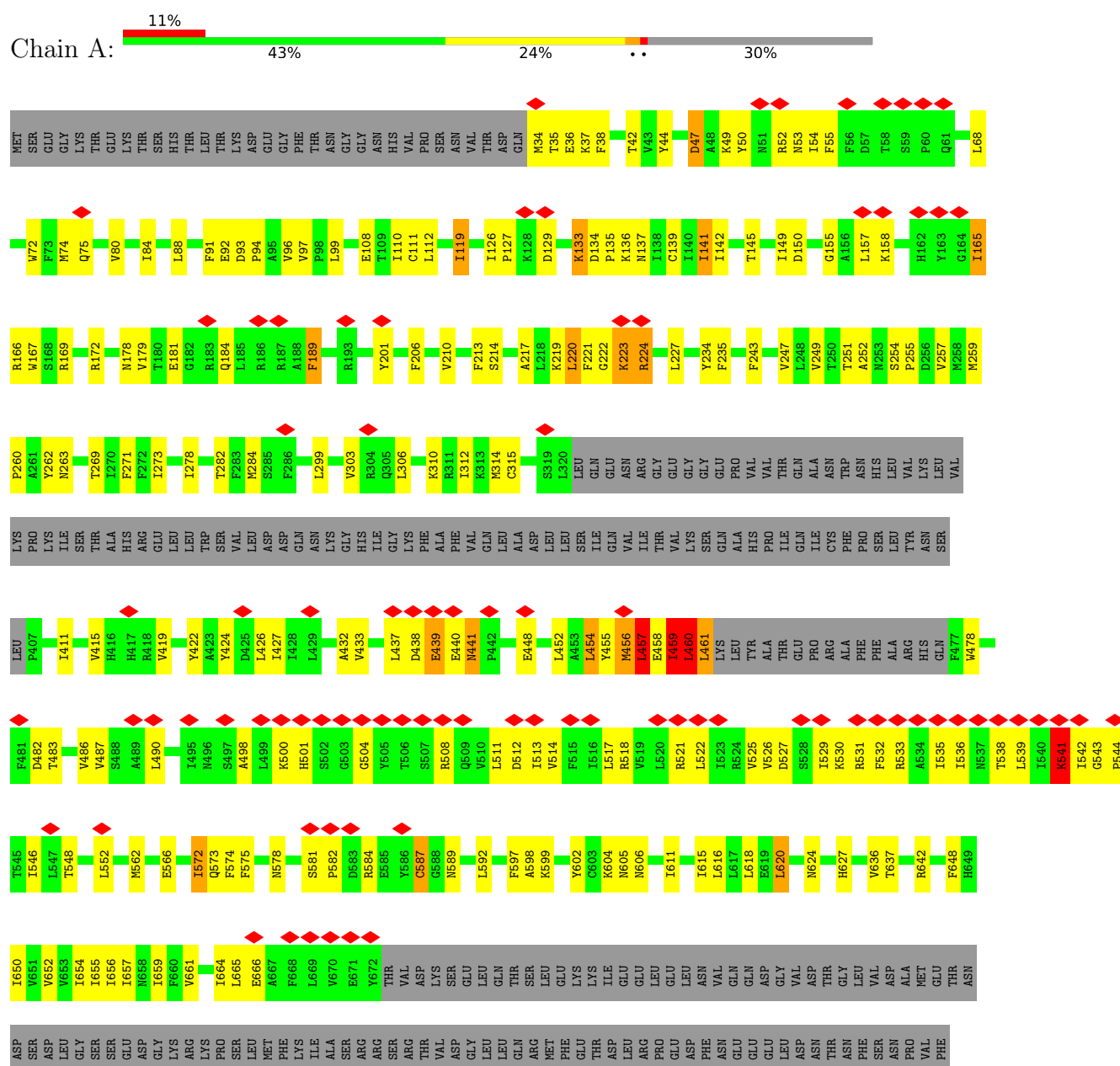
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

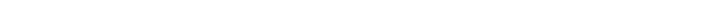
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Na	0
			1	1	

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: Two pore channel 3



Chain B:  12% 43% 24% 30%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	213328	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	92	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.344	Depositor
Minimum map value	-0.642	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.863	Depositor
Map size (Å)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.256, 1.256, 1.256	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.45	4/4528 (0.1%)	0.61	8/6155 (0.1%)
1	B	0.45	4/4528 (0.1%)	0.61	8/6155 (0.1%)
All	All	0.45	8/9056 (0.1%)	0.61	16/12310 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	PRO	CA-C	-7.42	1.41	1.52
1	B	135	PRO	CA-C	-7.40	1.41	1.52
1	B	134	ASP	C-O	-7.37	1.14	1.24
1	A	134	ASP	C-O	-7.33	1.14	1.24
1	B	133	LYS	N-CA	-6.96	1.36	1.46
1	A	133	LYS	N-CA	-6.93	1.36	1.46
1	B	133	LYS	C-O	-5.71	1.16	1.24
1	A	133	LYS	C-O	-5.65	1.16	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ILE	CA-C-N	9.30	135.59	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ILE	C-N-CA	9.30	135.59	121.83
1	B	459	ILE	CA-C-N	9.29	135.58	121.83
1	B	459	ILE	C-N-CA	9.29	135.58	121.83
1	B	262	TYR	N-CA-C	-7.56	105.22	114.75
1	A	262	TYR	N-CA-C	-7.54	105.25	114.75
1	B	460	LEU	N-CA-C	-6.69	99.47	109.83
1	A	460	LEU	N-CA-C	-6.68	99.47	109.83
1	B	457	LEU	CA-C-O	6.34	127.18	119.38
1	A	457	LEU	CA-C-O	6.32	127.15	119.38
1	B	433	VAL	N-CA-C	-6.18	106.19	113.42
1	B	135	PRO	CB-CA-C	-6.17	103.30	112.55
1	A	135	PRO	CB-CA-C	-6.16	103.31	112.55
1	A	433	VAL	N-CA-C	-6.12	106.26	113.42
1	B	135	PRO	N-CA-C	-5.30	106.30	113.40
1	A	135	PRO	N-CA-C	-5.26	106.34	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	456	MET	Mainchain
1	A	541	LYS	Peptide
1	B	224	ARG	Sidechain
1	B	456	MET	Mainchain
1	B	541	LYS	Peptide

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	4412	0	4566	155	0
1	B	4412	0	4566	158	0
2	A	1	0	0	0	0
All	All	8825	0	9132	285	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 16.

All (285) 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:219:LYS:NZ	1:B:438:ASP:OD1	1.78	1.16
1:A:438:ASP:OD1	1:B:219:LYS:NZ	1.79	1.15
1:A:223:LYS:NZ	1:B:439:GLU:OE2	1.85	1.08
1:A:439:GLU:OE2	1:B:223:LYS:NZ	1.90	1.03
1:B:439:GLU:O	1:B:440:GLU:HG2	1.57	1.03
1:A:439:GLU:O	1:A:440:GLU:HG2	1.57	1.02
1:A:129:ASP:O	1:A:133:LYS:HE2	1.64	0.97
1:B:129:ASP:O	1:B:133:LYS:HE2	1.64	0.96
1:A:219:LYS:NZ	1:B:438:ASP:CG	2.26	0.92
1:A:440:GLU:OE1	1:B:224:ARG:NH2	2.04	0.90
1:A:224:ARG:NH2	1:B:440:GLU:OE1	2.05	0.89
1:A:438:ASP:CG	1:B:219:LYS:NZ	2.31	0.88
1:A:247:VAL:HG21	1:A:627:HIS:HB3	1.57	0.86
1:B:247:VAL:HG21	1:B:627:HIS:HB3	1.57	0.86
1:A:438:ASP:CG	1:B:219:LYS:HZ1	1.84	0.84
1:B:169:ARG:NH1	1:B:562:MET:SD	2.53	0.82
1:A:169:ARG:NH1	1:A:562:MET:SD	2.53	0.81
1:B:457:LEU:O	1:B:460:LEU:HB3	1.81	0.80
1:A:457:LEU:O	1:A:460:LEU:HB3	1.81	0.80
1:A:93:ASP:HB2	1:A:94:PRO:HD3	1.67	0.77
1:B:93:ASP:HB2	1:B:94:PRO:HD3	1.66	0.76
1:B:457:LEU:C	1:B:459:ILE:H	1.91	0.76
1:A:219:LYS:HZ3	1:B:438:ASP:CG	1.94	0.76
1:A:584:ARG:NE	1:A:587:CYS:SG	2.59	0.75
1:B:455:TYR:O	1:B:458:GLU:HB2	1.87	0.75
1:A:455:TYR:O	1:A:458:GLU:HB2	1.87	0.75
1:A:457:LEU:C	1:A:459:ILE:H	1.91	0.75
1:B:584:ARG:NE	1:B:587:CYS:SG	2.59	0.73
1:A:273:ILE:HD13	1:B:618:LEU:HD22	1.71	0.72
1:A:618:LEU:HD22	1:B:273:ILE:HD13	1.71	0.72
1:A:624:ASN:HB3	1:B:254:SER:HB3	1.72	0.71
1:A:254:SER:HB3	1:B:624:ASN:HB3	1.72	0.71
1:A:487:VAL:HA	1:A:490:LEU:HD12	1.73	0.70
1:A:224:ARG:CZ	1:B:440:GLU:OE1	2.33	0.70
1:B:487:VAL:HA	1:B:490:LEU:HD12	1.73	0.70
1:B:133:LYS:HD3	1:B:133:LYS:N	2.06	0.69
1:A:133:LYS:HD3	1:A:133:LYS:N	2.06	0.69
1:A:531:ARG:NH1	1:B:201:TYR:O	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HD22	1:A:461:LEU:N	2.09	0.68
1:A:573:GLN:HG3	1:A:575:PHE:HE1	1.59	0.68
1:A:508:ARG:NH1	1:A:512:ASP:OD2	2.26	0.68
1:B:457:LEU:C	1:B:459:ILE:N	2.49	0.68
1:B:508:ARG:NH1	1:B:512:ASP:OD2	2.26	0.68
1:B:573:GLN:HG3	1:B:575:PHE:HE1	1.59	0.67
1:B:461:LEU:N	1:B:461:LEU:HD22	2.09	0.67
1:A:96:VAL:HG23	1:A:97:VAL:HG23	1.77	0.67
1:B:458:GLU:HA	1:B:458:GLU:OE1	1.94	0.67
1:B:459:ILE:O	1:B:459:ILE:HG22	1.95	0.66
1:A:457:LEU:C	1:A:459:ILE:N	2.49	0.66
1:B:460:LEU:HD23	1:B:460:LEU:O	1.96	0.66
1:A:460:LEU:HD23	1:A:460:LEU:O	1.96	0.66
1:A:259:MET:O	1:A:263:ASN:ND2	2.29	0.65
1:A:459:ILE:HG22	1:A:459:ILE:O	1.95	0.65
1:A:438:ASP:CG	1:B:219:LYS:HZ3	2.04	0.65
1:B:259:MET:O	1:B:263:ASN:ND2	2.29	0.65
1:A:47:ASP:OD1	1:A:47:ASP:N	2.30	0.65
1:A:458:GLU:OE1	1:A:458:GLU:HA	1.94	0.65
1:B:96:VAL:HG23	1:B:97:VAL:HG23	1.77	0.65
1:A:201:TYR:O	1:B:531:ARG:NH1	2.27	0.64
1:B:482:ASP:OD1	1:B:521:ARG:NH1	2.31	0.63
1:A:482:ASP:OD1	1:A:521:ARG:NH1	2.31	0.63
1:A:234:TYR:OH	1:A:257:VAL:O	2.12	0.63
1:B:544:PRO:O	1:B:548:THR:N	2.31	0.63
1:B:536:ILE:HA	1:B:539:LEU:HB3	1.82	0.61
1:B:47:ASP:N	1:B:47:ASP:OD1	2.30	0.61
1:A:165:ILE:HG22	1:A:166:ARG:H	1.66	0.61
1:A:129:ASP:O	1:A:133:LYS:CE	2.45	0.61
1:A:535:ILE:O	1:A:539:LEU:N	2.34	0.61
1:A:544:PRO:O	1:A:548:THR:N	2.31	0.60
1:B:530:LYS:HG3	1:B:533:ARG:HH22	1.66	0.60
1:B:129:ASP:O	1:B:133:LYS:CE	2.45	0.60
1:A:536:ILE:HA	1:A:539:LEU:HB3	1.82	0.60
1:A:530:LYS:HG3	1:A:533:ARG:HH22	1.66	0.59
1:B:165:ILE:HG22	1:B:166:ARG:H	1.66	0.59
1:A:535:ILE:HD12	1:A:538:THR:HB	1.85	0.59
1:A:38:PHE:O	1:A:42:THR:HG23	2.03	0.58
1:B:38:PHE:O	1:B:42:THR:HG23	2.03	0.58
1:B:91:PHE:HB3	1:B:99:LEU:HB2	1.86	0.58
1:B:49:LYS:HZ2	1:B:50:TYR:HE1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:TYR:HE1	1:B:54:ILE:HG12	1.69	0.57
1:B:452:LEU:HD21	1:B:490:LEU:HA	1.86	0.57
1:B:535:ILE:HD12	1:B:538:THR:HB	1.85	0.57
1:A:456:MET:O	1:A:459:ILE:HB	2.04	0.57
1:B:456:MET:O	1:B:459:ILE:HB	2.04	0.57
1:B:222:GLY:HA2	1:B:235:PHE:O	2.05	0.56
1:A:219:LYS:NZ	1:B:438:ASP:OD2	2.33	0.56
1:A:222:GLY:HA2	1:A:235:PHE:O	2.05	0.56
1:A:587:CYS:HB3	1:A:598:ALA:HB2	1.87	0.56
1:A:44:TYR:HE1	1:A:54:ILE:HG12	1.69	0.56
1:A:452:LEU:HD21	1:A:490:LEU:HA	1.86	0.56
1:A:91:PHE:HB3	1:A:99:LEU:HB2	1.86	0.56
1:A:49:LYS:HZ2	1:A:50:TYR:HE1	1.53	0.56
1:A:137:ASN:O	1:A:141:ILE:HG23	2.06	0.56
1:A:541:LYS:O	1:A:543:GLY:N	2.40	0.55
1:B:541:LYS:O	1:B:543:GLY:N	2.40	0.55
1:B:535:ILE:O	1:B:539:LEU:N	2.34	0.55
1:B:605:ASN:HB3	1:B:616:LEU:HD13	1.88	0.55
1:A:605:ASN:HB3	1:A:616:LEU:HD13	1.88	0.55
1:B:137:ASN:O	1:B:141:ILE:HG23	2.06	0.55
1:A:92:GLU:CD	1:A:172:ARG:HH22	2.15	0.54
1:B:587:CYS:HB3	1:B:598:ALA:HB2	1.87	0.54
1:A:166:ARG:HB3	1:A:169:ARG:HG3	1.89	0.54
1:B:243:PHE:CG	1:B:642:ARG:HD3	2.43	0.54
1:A:243:PHE:CG	1:A:642:ARG:HD3	2.43	0.54
1:A:461:LEU:HD22	1:A:461:LEU:H	1.73	0.54
1:B:284:MET:HE1	1:B:654:ILE:HG12	1.90	0.54
1:B:52:ARG:HH22	1:B:126:ILE:HD11	1.74	0.53
1:B:92:GLU:CD	1:B:172:ARG:HH22	2.15	0.53
1:B:656:ILE:O	1:B:659:ILE:HG22	2.08	0.53
1:A:55:PHE:HB2	1:A:127:PRO:HD3	1.89	0.53
1:B:52:ARG:NH1	1:B:53:ASN:O	2.42	0.53
1:A:52:ARG:HH22	1:A:126:ILE:HD11	1.74	0.53
1:A:52:ARG:NH1	1:A:53:ASN:O	2.42	0.53
1:A:68:LEU:HD11	1:A:74:MET:HE2	1.91	0.53
1:B:55:PHE:HB2	1:B:127:PRO:HD3	1.89	0.53
1:A:656:ILE:O	1:A:659:ILE:HG22	2.08	0.53
1:B:166:ARG:HB3	1:B:169:ARG:HG3	1.89	0.53
1:B:461:LEU:HD22	1:B:461:LEU:H	1.73	0.52
1:A:284:MET:HE1	1:A:654:ILE:HG12	1.90	0.52
1:A:441:ASN:OD1	1:A:441:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:O	1:B:145:THR:OG1	2.22	0.52
1:A:133:LYS:N	1:A:133:LYS:CD	2.72	0.52
1:B:251:THR:O	1:B:251:THR:OG1	2.24	0.52
1:B:133:LYS:N	1:B:133:LYS:CD	2.72	0.52
1:B:511:LEU:HA	1:B:514:VAL:HG12	1.92	0.52
1:B:35:THR:OG1	1:B:36:GLU:OE1	2.16	0.52
1:B:636:VAL:HG23	1:B:637:THR:HG23	1.91	0.51
1:A:636:VAL:HG23	1:A:637:THR:HG23	1.91	0.51
1:B:441:ASN:OD1	1:B:441:ASN:N	2.42	0.51
1:A:606:ASN:OD1	1:A:606:ASN:N	2.43	0.51
1:B:68:LEU:HD11	1:B:74:MET:HE2	1.91	0.51
1:B:411:ILE:O	1:B:415:VAL:HG23	2.11	0.51
1:A:529:ILE:HG21	1:A:531:ARG:HH21	1.76	0.51
1:B:210:VAL:O	1:B:214:SER:OG	2.26	0.51
1:B:448:GLU:HB2	1:B:518:ARG:HH12	1.76	0.51
1:A:511:LEU:HA	1:A:514:VAL:HG12	1.92	0.50
1:A:448:GLU:HB2	1:A:518:ARG:HH12	1.76	0.50
1:A:35:THR:OG1	1:A:36:GLU:OE1	2.16	0.50
1:A:427:ILE:HD13	1:A:454:LEU:HG	1.94	0.50
1:B:461:LEU:N	1:B:461:LEU:CD2	2.73	0.50
1:B:529:ILE:HG21	1:B:531:ARG:HH21	1.76	0.50
1:A:411:ILE:O	1:A:415:VAL:HG23	2.11	0.50
1:B:234:TYR:OH	1:B:257:VAL:O	2.12	0.50
1:A:589:ASN:HD21	1:A:636:VAL:HG12	1.76	0.50
1:A:217:ALA:HB2	1:A:271:PHE:CZ	2.47	0.50
1:B:34:MET:N	1:B:37:LYS:HB2	2.27	0.50
1:A:34:MET:N	1:A:37:LYS:HB2	2.27	0.50
1:B:427:ILE:HD13	1:B:454:LEU:HG	1.94	0.50
1:B:589:ASN:HD21	1:B:636:VAL:HG12	1.76	0.50
1:A:167:TRP:CD1	1:A:167:TRP:H	2.30	0.50
1:A:572:ILE:HD12	1:A:597:PHE:CE2	2.47	0.50
1:B:529:ILE:HG21	1:B:531:ARG:NH2	2.27	0.50
1:B:217:ALA:HB2	1:B:271:PHE:CZ	2.47	0.49
1:A:529:ILE:HG21	1:A:531:ARG:NH2	2.27	0.49
1:B:606:ASN:OD1	1:B:606:ASN:N	2.43	0.49
1:A:531:ARG:HH12	1:B:201:TYR:C	2.18	0.49
1:B:572:ILE:HD12	1:B:597:PHE:CE2	2.47	0.49
1:B:167:TRP:CD1	1:B:167:TRP:H	2.30	0.49
1:A:514:VAL:O	1:A:518:ARG:HG2	2.12	0.49
1:B:514:VAL:O	1:B:518:ARG:HG2	2.12	0.49
1:A:251:THR:O	1:A:251:THR:OG1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HH11	1:A:54:ILE:HG22	1.78	0.48
1:B:52:ARG:HH11	1:B:54:ILE:HG22	1.78	0.48
1:A:461:LEU:N	1:A:461:LEU:CD2	2.73	0.48
1:A:598:ALA:O	1:A:599:LYS:HG3	2.13	0.48
1:B:598:ALA:O	1:B:599:LYS:HG3	2.13	0.48
1:A:210:VAL:O	1:A:214:SER:OG	2.26	0.48
1:B:654:ILE:HG22	1:B:655:ILE:HG23	1.95	0.48
1:A:150:ASP:OD2	1:A:166:ARG:NE	2.47	0.48
1:B:661:VAL:O	1:B:665:LEU:HB2	2.14	0.48
1:B:150:ASP:OD2	1:B:166:ARG:NE	2.47	0.47
1:A:652:VAL:HA	1:A:656:ILE:HB	1.95	0.47
1:A:531:ARG:HD3	1:B:201:TYR:CE2	2.48	0.47
1:A:654:ILE:HG22	1:A:655:ILE:HG23	1.95	0.47
1:B:652:VAL:HA	1:B:656:ILE:HB	1.95	0.47
1:B:37:LYS:HB3	1:B:37:LYS:HE2	1.77	0.47
1:A:661:VAL:O	1:A:665:LEU:HB2	2.14	0.47
1:B:133:LYS:HD3	1:B:133:LYS:H	1.79	0.47
1:A:201:TYR:CE2	1:B:531:ARG:HD3	2.51	0.46
1:B:139:CYS:CB	1:B:178:ASN:HD22	2.28	0.46
1:A:483:THR:O	1:A:487:VAL:HG22	2.15	0.46
1:B:500:LYS:HG3	1:B:501:HIS:CD2	2.51	0.46
1:A:141:ILE:O	1:A:145:THR:OG1	2.22	0.46
1:A:615:ILE:HD12	1:B:269:THR:HG21	1.98	0.46
1:B:483:THR:O	1:B:487:VAL:HG22	2.15	0.46
1:A:189:PHE:HE1	1:A:552:LEU:HD13	1.81	0.46
1:A:139:CYS:CB	1:A:178:ASN:HD22	2.28	0.46
1:A:80:VAL:O	1:A:84:ILE:HG12	2.16	0.46
1:B:80:VAL:O	1:B:84:ILE:HG12	2.16	0.46
1:B:99:LEU:HD12	1:B:99:LEU:HA	1.77	0.46
1:B:581:SER:N	1:B:582:PRO:HD2	2.31	0.46
1:B:562:MET:O	1:B:566:GLU:HG2	2.16	0.46
1:A:581:SER:N	1:A:582:PRO:HD2	2.31	0.45
1:A:424:TYR:OH	1:A:457:LEU:HD11	2.17	0.45
1:A:213:PHE:HD1	1:A:271:PHE:HE1	1.64	0.45
1:A:650:ILE:O	1:A:654:ILE:HB	2.17	0.45
1:B:213:PHE:HD1	1:B:271:PHE:HE1	1.64	0.45
1:B:605:ASN:O	1:B:616:LEU:HD22	2.17	0.45
1:A:299:LEU:HD12	1:A:666:GLU:HG2	1.99	0.45
1:A:500:LYS:HG3	1:A:501:HIS:CD2	2.51	0.45
1:B:299:LEU:HD12	1:B:666:GLU:HG2	1.99	0.45
1:B:578:ASN:OD1	1:B:578:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HD3	1:A:133:LYS:H	1.79	0.45
1:A:562:MET:O	1:A:566:GLU:HG2	2.16	0.45
1:A:75:GLN:HG3	1:A:181:GLU:HG2	1.99	0.45
1:A:439:GLU:O	1:A:440:GLU:CG	2.47	0.45
1:A:605:ASN:O	1:A:616:LEU:HD22	2.17	0.45
1:B:189:PHE:HE1	1:B:552:LEU:HD13	1.81	0.45
1:B:439:GLU:C	1:B:440:GLU:HG2	2.39	0.45
1:B:75:GLN:HG3	1:B:181:GLU:HG2	1.99	0.44
1:A:574:PHE:CD2	1:A:604:LYS:HD2	2.52	0.44
1:B:424:TYR:OH	1:B:457:LEU:HD11	2.16	0.44
1:B:650:ILE:O	1:B:654:ILE:HB	2.17	0.44
1:A:478:TRP:NE1	1:A:527:ASP:OD1	2.51	0.44
1:B:108:GLU:HA	1:B:111:CYS:HB2	1.99	0.44
1:A:92:GLU:OE1	1:A:172:ARG:NH2	2.49	0.44
1:A:141:ILE:HG13	1:A:142:ILE:N	2.32	0.44
1:B:278:ILE:O	1:B:282:THR:HB	2.18	0.44
1:B:478:TRP:O	1:B:482:ASP:N	2.35	0.44
1:B:574:PHE:CD2	1:B:604:LYS:HD2	2.52	0.44
1:A:166:ARG:HA	1:A:166:ARG:HD2	1.74	0.44
1:A:88:LEU:CD2	1:A:108:GLU:HB3	2.48	0.44
1:A:278:ILE:O	1:A:282:THR:HB	2.18	0.44
1:B:93:ASP:HB2	1:B:94:PRO:CD	2.45	0.44
1:B:478:TRP:NE1	1:B:527:ASP:OD1	2.51	0.44
1:A:419:VAL:HG23	1:A:422:TYR:HB2	2.00	0.43
1:B:141:ILE:HG13	1:B:142:ILE:N	2.32	0.43
1:A:108:GLU:HA	1:A:111:CYS:HB2	1.99	0.43
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.70	0.43
1:A:432:ALA:HB2	1:A:522:LEU:HD21	2.01	0.43
1:B:88:LEU:CD2	1:B:108:GLU:HB3	2.48	0.43
1:A:438:ASP:OD2	1:B:219:LYS:NZ	2.39	0.43
1:A:611:ILE:HD13	1:A:611:ILE:HA	1.83	0.43
1:B:419:VAL:HG23	1:B:422:TYR:HB2	2.00	0.43
1:A:657:ILE:O	1:A:661:VAL:HG23	2.19	0.42
1:A:234:TYR:CE1	1:A:260:PRO:HG2	2.54	0.42
1:A:255:PRO:HG2	1:B:602:TYR:OH	2.19	0.42
1:B:108:GLU:O	1:B:112:LEU:HG	2.19	0.42
1:B:432:ALA:HB2	1:B:522:LEU:HD21	2.01	0.42
1:B:581:SER:OG	1:B:585:GLU:OE2	2.36	0.42
1:B:166:ARG:HD2	1:B:166:ARG:HA	1.74	0.42
1:B:234:TYR:CE1	1:B:260:PRO:HG2	2.54	0.42
1:A:108:GLU:O	1:A:112:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLN:HG3	1:A:548:THR:OG1	2.19	0.42
1:A:530:LYS:HB3	1:A:530:LYS:HE3	1.72	0.42
1:A:158:LYS:HE2	1:A:158:LYS:HB2	1.86	0.42
1:A:119:ILE:HD12	1:A:119:ILE:HA	1.81	0.42
1:A:220:LEU:O	1:A:221:PHE:C	2.63	0.42
1:A:513:ILE:HD12	1:A:513:ILE:HA	1.87	0.42
1:B:184:GLN:HG3	1:B:548:THR:OG1	2.19	0.42
1:B:220:LEU:O	1:B:221:PHE:C	2.63	0.42
1:B:482:ASP:O	1:B:486:VAL:HG23	2.19	0.42
1:B:657:ILE:O	1:B:661:VAL:HG23	2.19	0.42
1:A:269:THR:HG21	1:B:615:ILE:HD12	2.02	0.41
1:A:155:GLY:O	1:A:157:LEU:N	2.53	0.41
1:A:206:PHE:CE1	1:A:249:VAL:HG11	2.55	0.41
1:A:52:ARG:NH1	1:A:54:ILE:HG22	2.35	0.41
1:B:155:GLY:O	1:B:157:LEU:N	2.53	0.41
1:A:439:GLU:C	1:A:440:GLU:HG2	2.39	0.41
1:A:482:ASP:O	1:A:486:VAL:HG23	2.19	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.70	0.41
1:B:584:ARG:HA	1:B:584:ARG:HD2	1.88	0.41
1:B:530:LYS:HE3	1:B:530:LYS:HB3	1.72	0.41
1:B:92:GLU:OE1	1:B:172:ARG:NH2	2.49	0.41
1:B:206:PHE:CE1	1:B:249:VAL:HG11	2.55	0.41
1:A:602:TYR:OH	1:B:255:PRO:HG2	2.21	0.41
1:B:573:GLN:HA	1:B:606:ASN:HD22	1.85	0.41
1:B:57:ASP:HB2	1:B:63:VAL:HB	2.03	0.41
1:B:119:ILE:HD12	1:B:119:ILE:HA	1.81	0.41
1:A:573:GLN:HA	1:A:606:ASN:HD22	1.85	0.41
1:B:52:ARG:NH1	1:B:54:ILE:HG22	2.35	0.40
1:B:498:ALA:O	1:B:504:GLY:HA2	2.21	0.40
1:A:460:LEU:O	1:A:460:LEU:CD2	2.68	0.40
1:A:498:ALA:O	1:A:504:GLY:HA2	2.21	0.40
1:A:201:TYR:C	1:B:531:ARG:HH12	2.22	0.40
1:A:247:VAL:HG22	1:A:252:ALA:HB3	2.04	0.40
1:B:419:VAL:HG23	1:B:422:TYR:HD2	1.87	0.40
1:B:589:ASN:OD1	1:B:592:LEU:HD12	2.22	0.40
1:A:578:ASN:OD1	1:A:578:ASN:N	2.48	0.40
1:A:589:ASN:OD1	1:A:592:LEU:HD12	2.22	0.40
1:A:620:LEU:HB3	1:A:648:PHE:CE2	2.57	0.40
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.85	0.40
1:B:460:LEU:O	1:B:460:LEU:CD2	2.68	0.40
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:VAL:HG22	1:B:252:ALA:HB3	2.04	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	532/773 (69%)	480 (90%)	50 (9%)	2 (0%)	30	60
1	B	532/773 (69%)	480 (90%)	50 (9%)	2 (0%)	30	60
All	All	1064/1546 (69%)	960 (90%)	100 (9%)	4 (0%)	31	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	LEU
1	A	542	ILE
1	B	220	LEU
1	B	542	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/699 (70%)	451 (92%)	37 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	488/699 (70%)	452 (93%)	36 (7%)	13	38
All	All	976/1398 (70%)	903 (92%)	73 (8%)	14	38

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	72	TRP
1	A	110	ILE
1	A	119	ILE
1	A	136	LYS
1	A	141	ILE
1	A	149	ILE
1	A	165	ILE
1	A	179	VAL
1	A	189	PHE
1	A	223	LYS
1	A	227	LEU
1	A	303	VAL
1	A	306	LEU
1	A	310	LYS
1	A	312	ILE
1	A	314	MET
1	A	315	CYS
1	A	426	LEU
1	A	437	LEU
1	A	439	GLU
1	A	441	ASN
1	A	454	LEU
1	A	457	LEU
1	A	459	ILE
1	A	460	LEU
1	A	461	LEU
1	A	517	LEU
1	A	525	VAL
1	A	526	VAL
1	A	532	PHE
1	A	541	LYS
1	A	546	ILE
1	A	572	ILE
1	A	587	CYS
1	A	620	LEU

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Mol	Chain	Res	Type
1	A	664	ILE
1	B	72	TRP
1	B	110	ILE
1	B	119	ILE
1	B	136	LYS
1	B	141	ILE
1	B	149	ILE
1	B	165	ILE
1	B	179	VAL
1	B	189	PHE
1	B	223	LYS
1	B	227	LEU
1	B	303	VAL
1	B	306	LEU
1	B	310	LYS
1	B	312	ILE
1	B	314	MET
1	B	315	CYS
1	B	426	LEU
1	B	437	LEU
1	B	439	GLU
1	B	441	ASN
1	B	454	LEU
1	B	457	LEU
1	B	459	ILE
1	B	460	LEU
1	B	461	LEU
1	B	517	LEU
1	B	525	VAL
1	B	526	VAL
1	B	532	PHE
1	B	541	LYS
1	B	546	ILE
1	B	572	ILE
1	B	587	CYS
1	B	620	LEU
1	B	664	ILE

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	194	ASN

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Mol	Chain	Res	Type
1	A	263	ASN
1	A	279	ASN
1	A	294	ASN
1	A	658	ASN
1	B	194	ASN
1	B	263	ASN
1	B	279	ASN
1	B	294	ASN
1	B	431	ASN
1	B	658	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

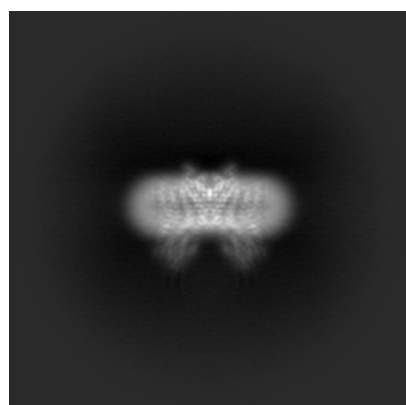
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21015. These allow visual inspection of the internal detail of the map and identification of artifacts.

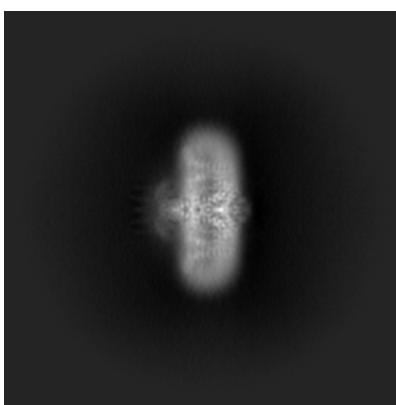
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

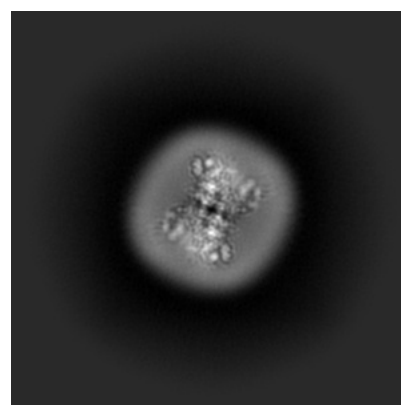
6.1.1 Primary map



X



Y

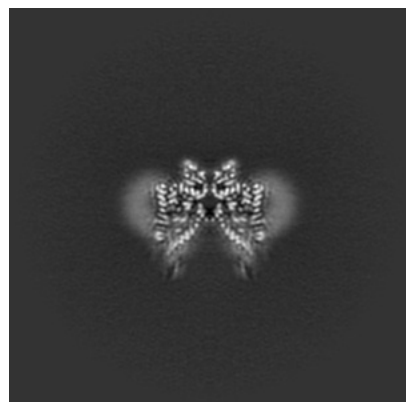


Z

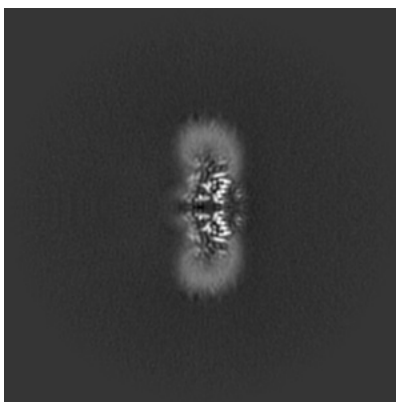
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

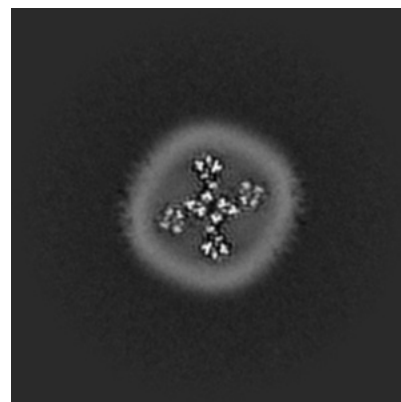
6.2.1 Primary map



X Index: 140



Y Index: 140

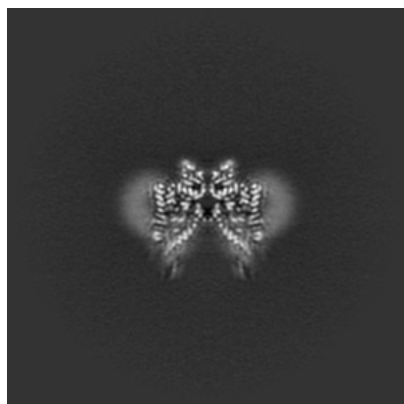


Z Index: 140

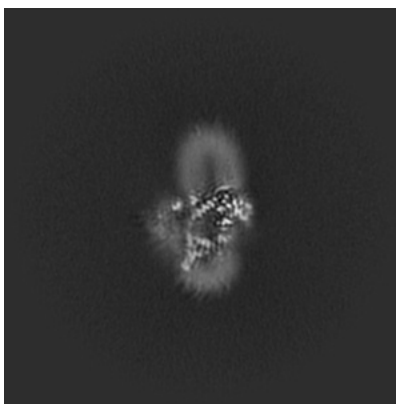
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

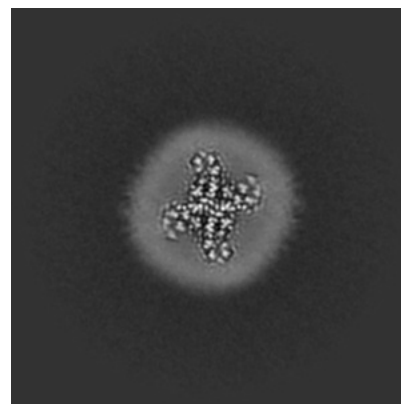
6.3.1 Primary map



X Index: 140



Y Index: 125

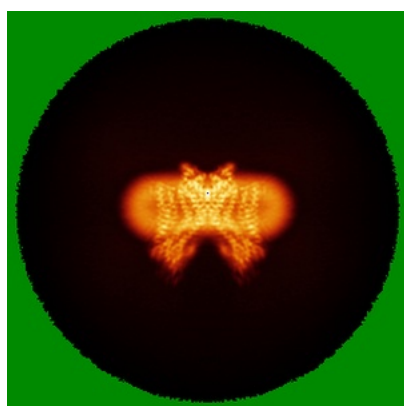


Z Index: 151

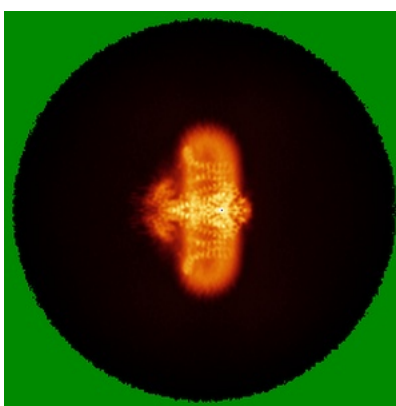
The images above show the largest variance slices of the map in three orthogonal directions.

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

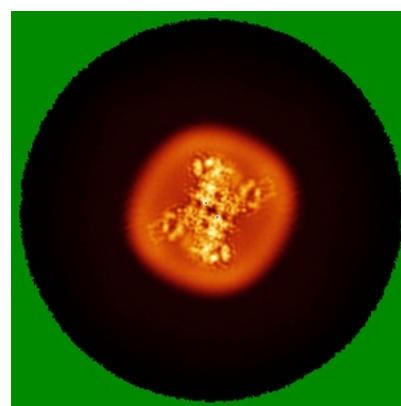
6.4.1 Primary map



X



Y

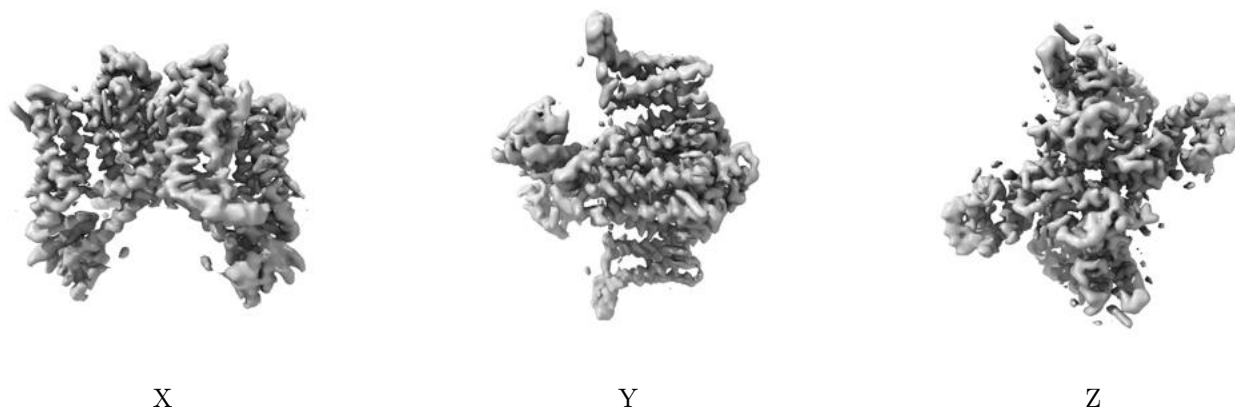


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.863. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

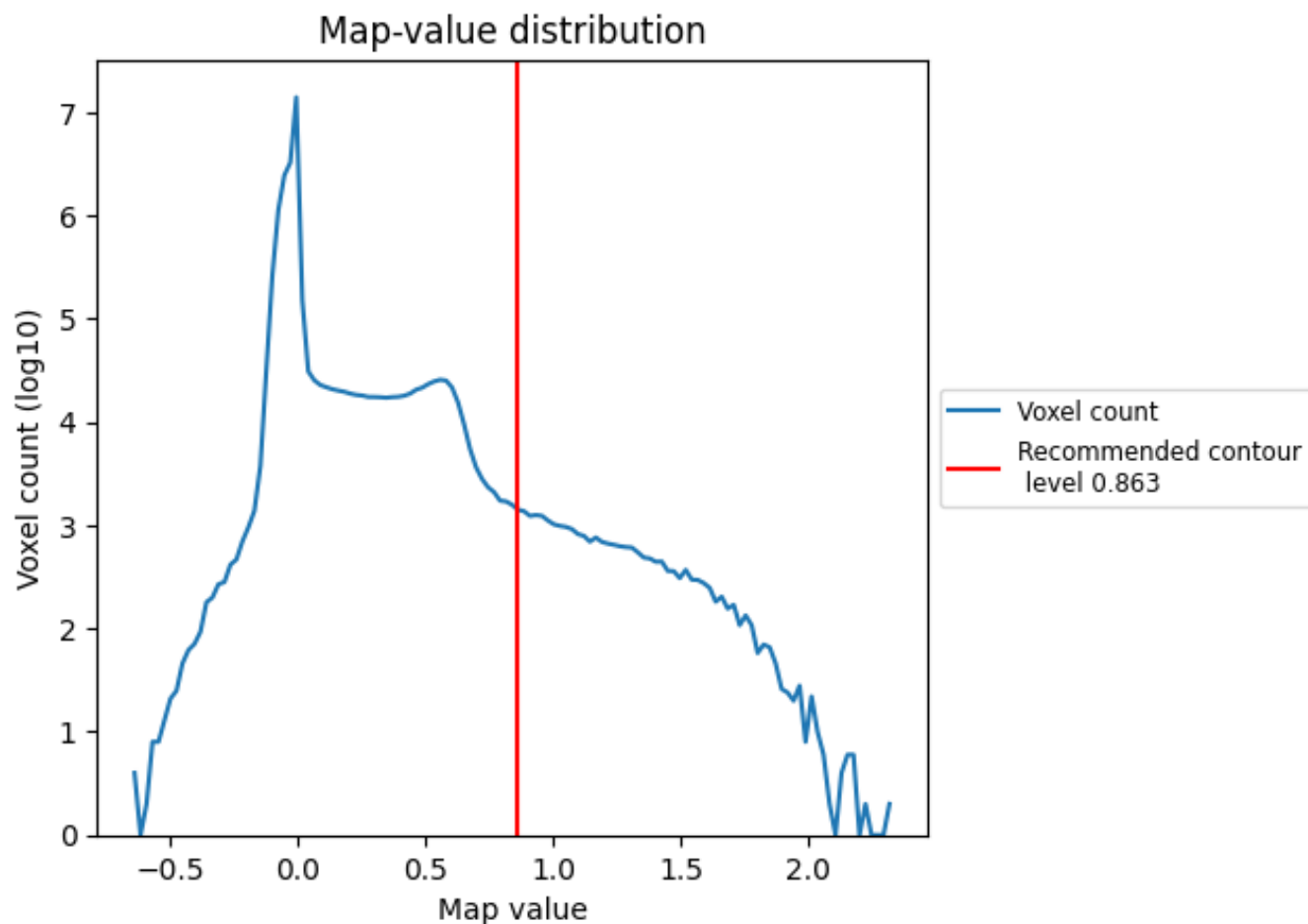
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

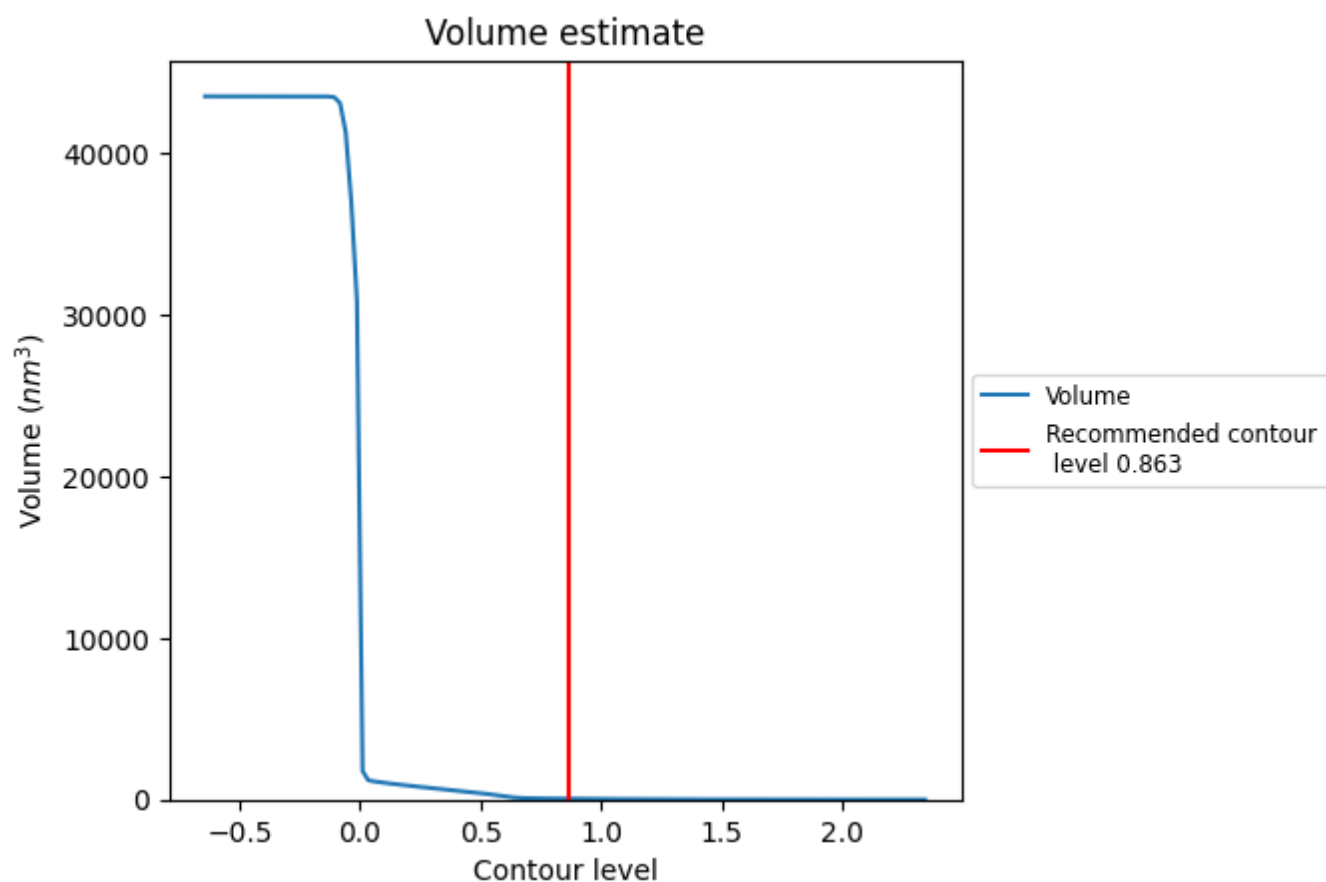
This section contains the results of statistical analysis of the map.

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.

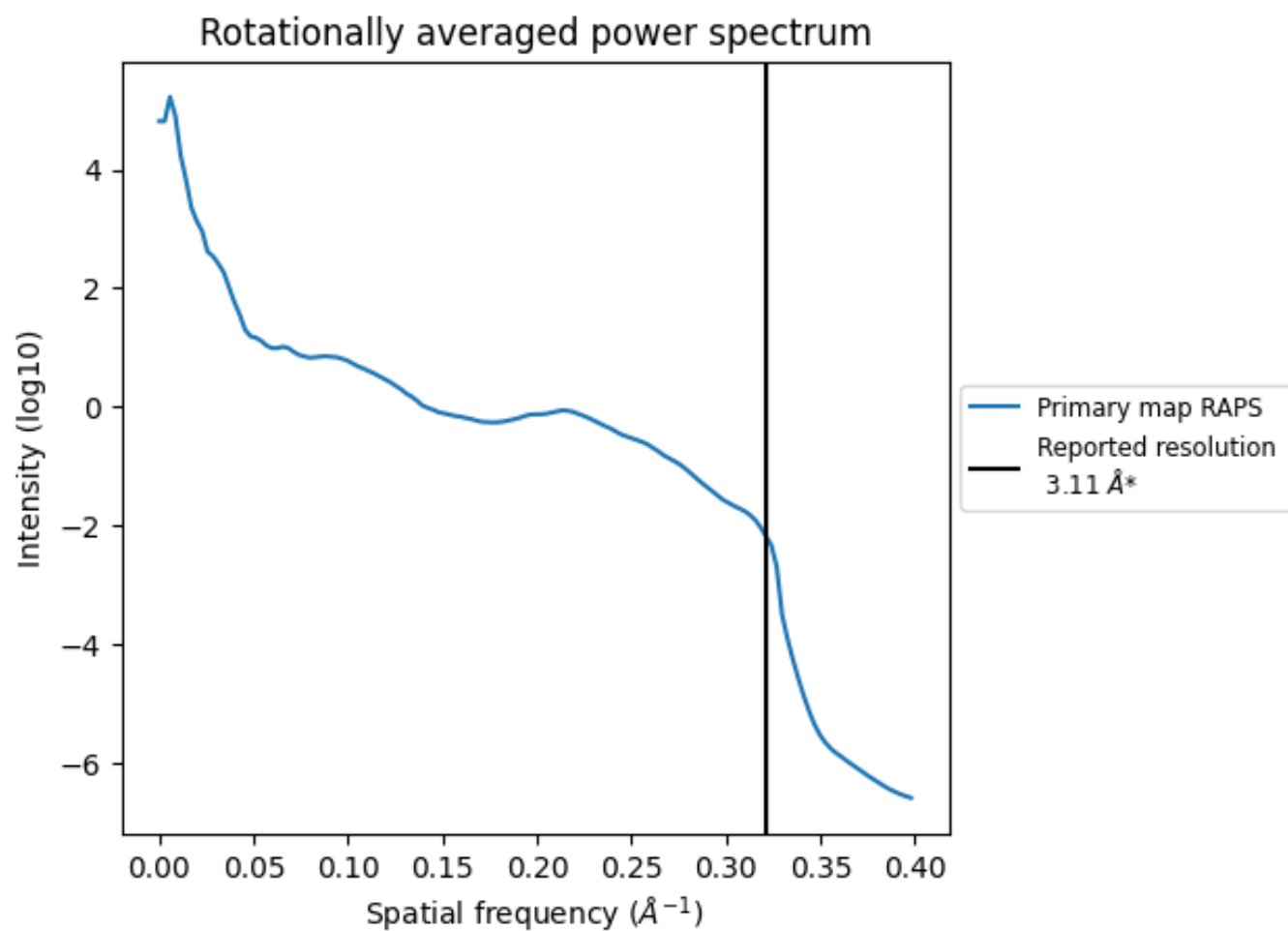
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm³; this corresponds to an approximate mass of 45 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 0.322 $\text{\AA}^{-1}$

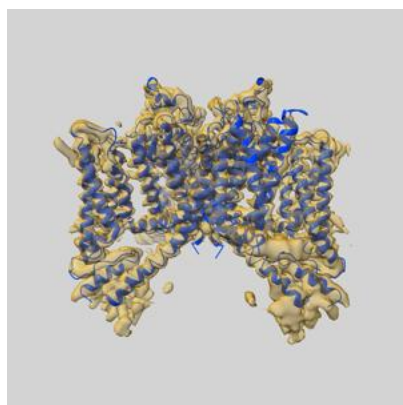
8 Fourier-Shell correlation

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

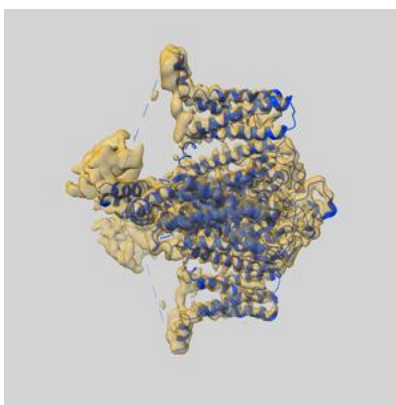
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21015 and PDB model 6V1Q. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

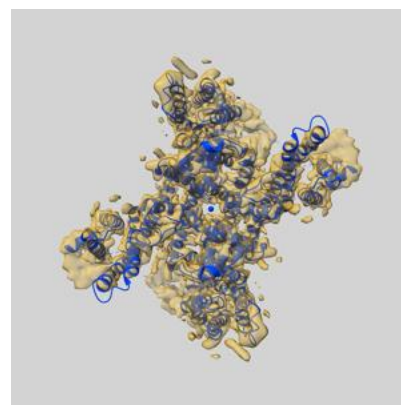
9.1 Map-model overlay [i](#)



X



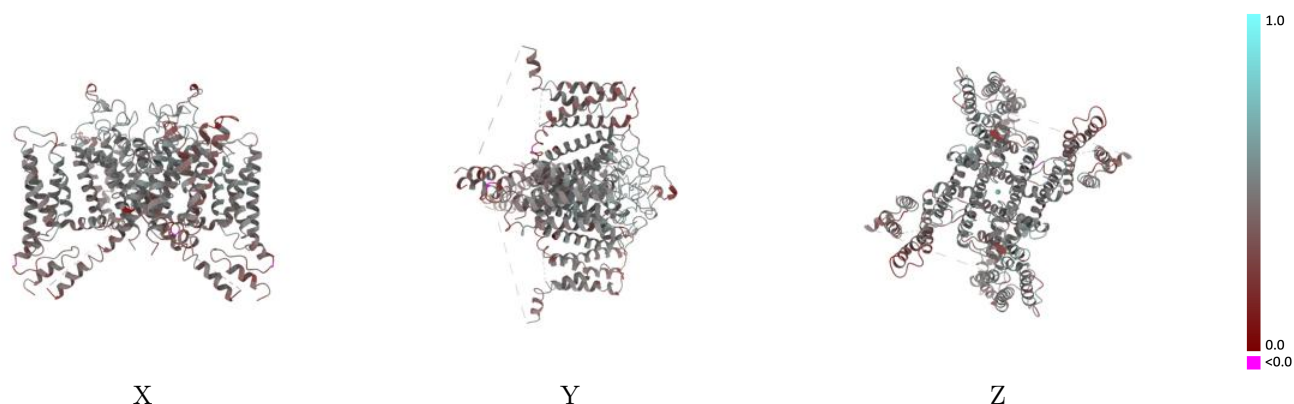
Y



Z

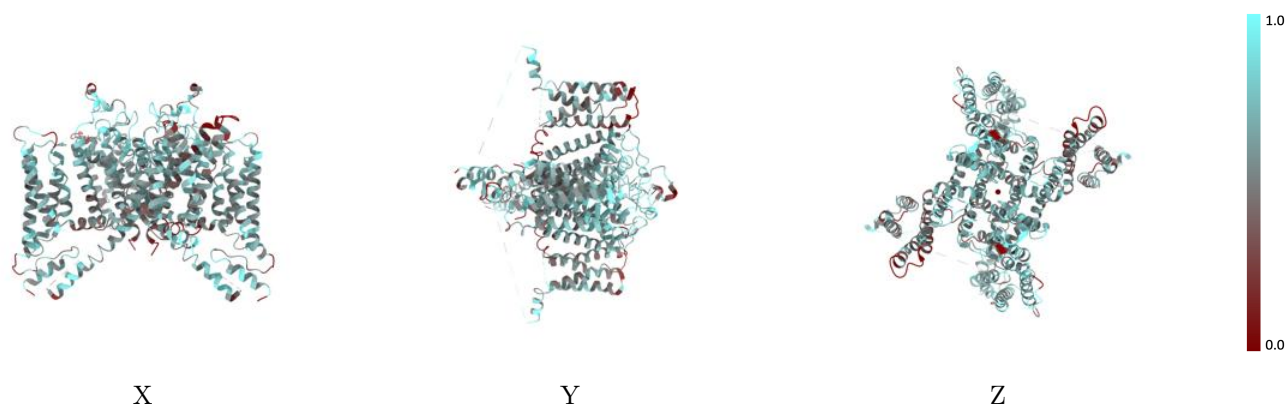
The images above show the 3D surface view of the map at the recommended contour level 0.863 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



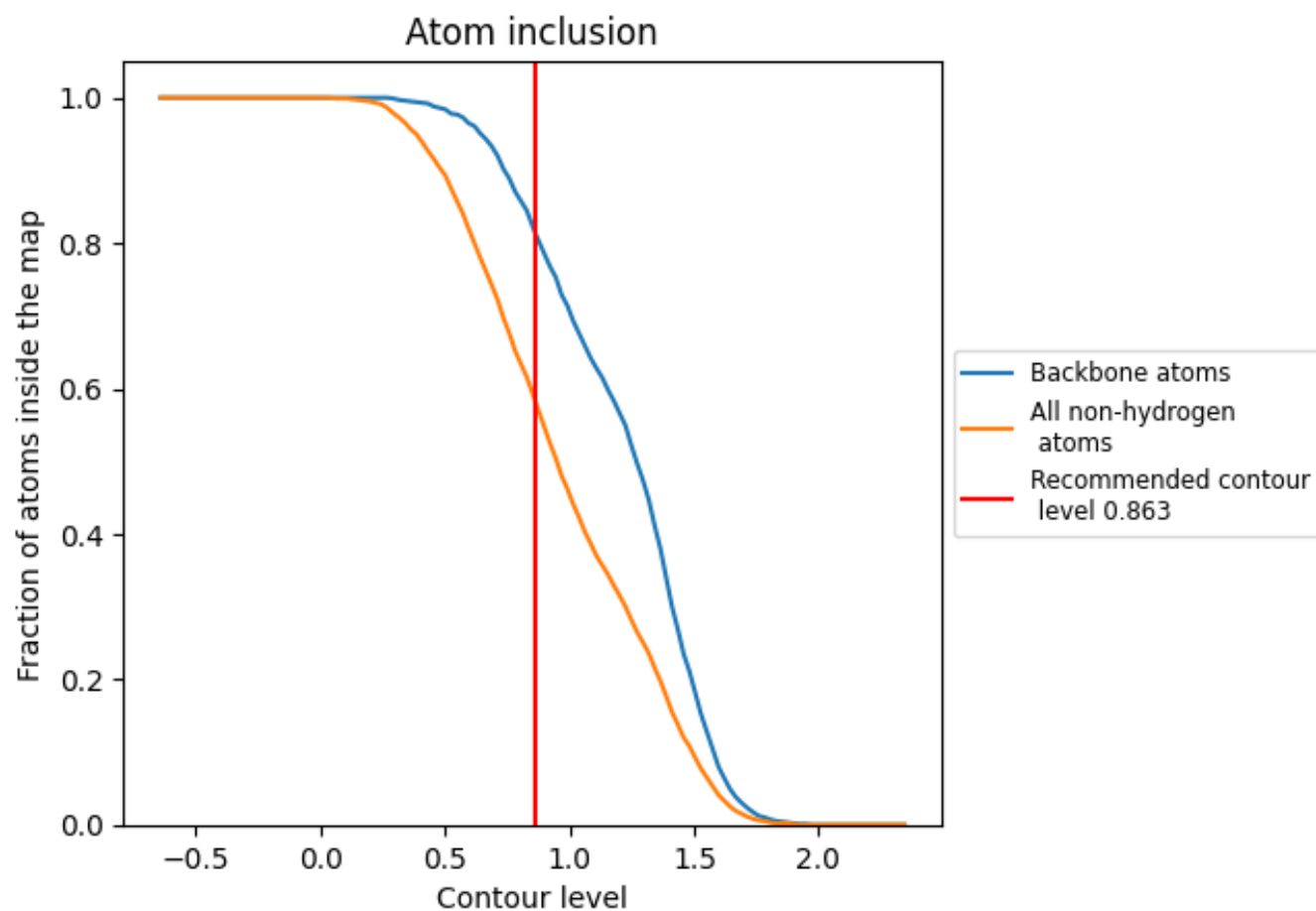
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.863).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 58% 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 (0.863) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5820	0.4320
A	0.5830	0.4320
B	0.5820	0.4310

