



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:23 AM UTC

PDB ID : 7WIU / pdb_00007wiu
EMDB ID : EMD-32536
Title : Cryo-EM structure of Mycobacterium tuberculosis irtAB in inward-facing state
Authors : Zhang, B.; Sun, S.; Yang, H.; Rao, Z.
Deposited on : 2022-01-05
Resolution : 3.48 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

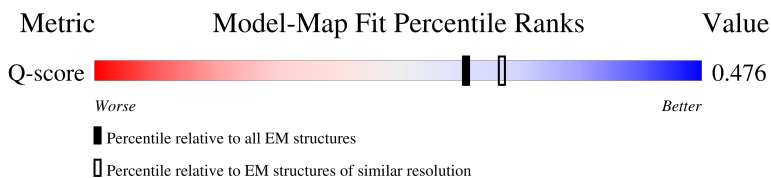
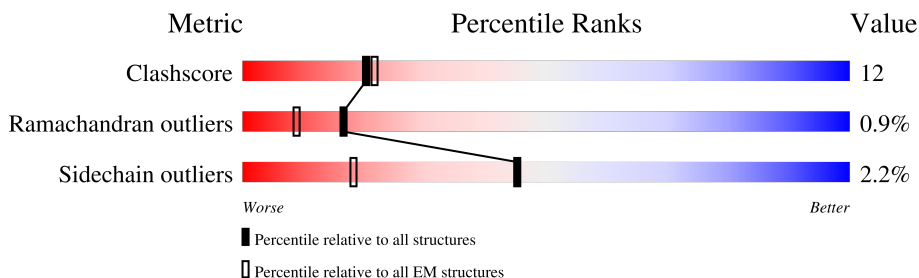
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.48 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	13672 (2.98 - 3.98)

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	859	 51% 14% 34%
2	B	579	 74% 24% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8615 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 Mycobactin import ATP-binding/permease protein IrtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	571	Total	C	N	O	S	0	0
			4344	2785	783	771	5		

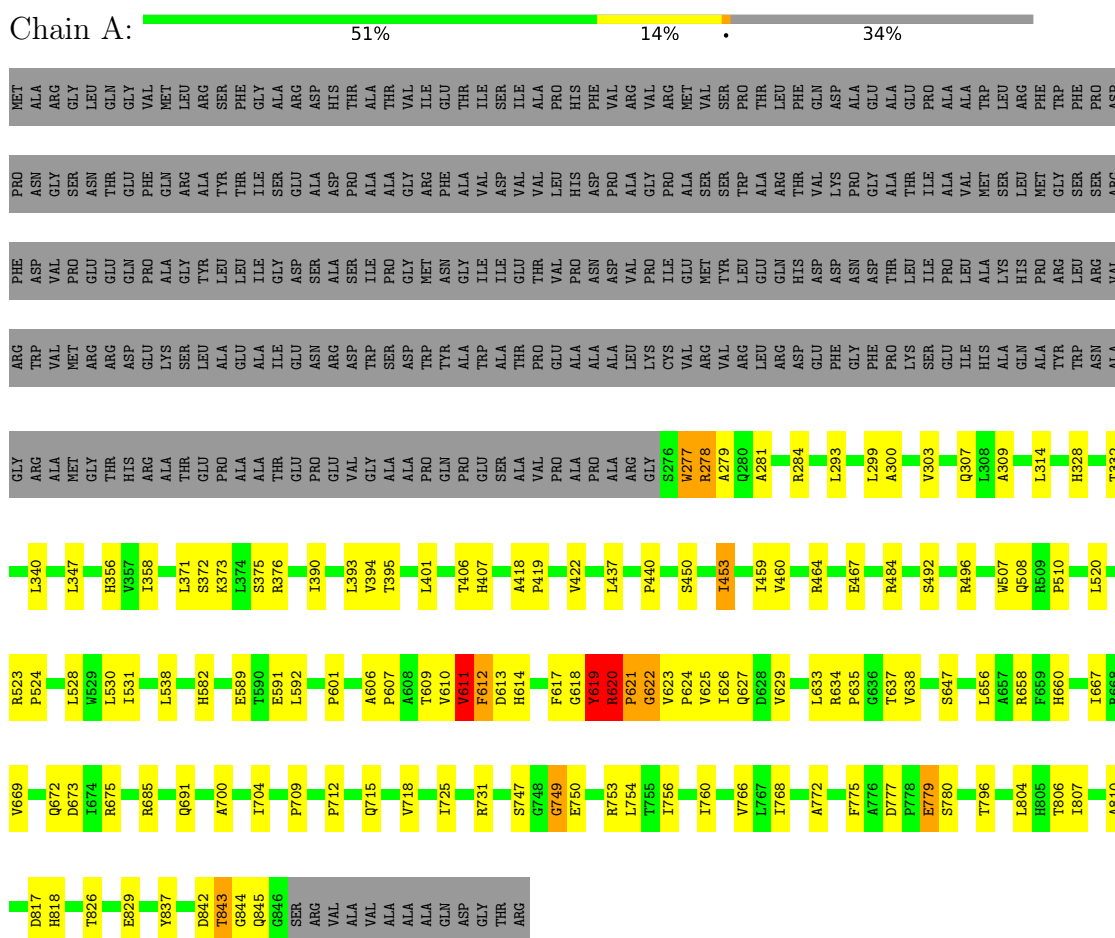
- Molecule 2 is a protein called Mycobactin import ATP-binding/permease protein IrtB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	576	Total	C	N	O	S	0	0
			4271	2716	764	782	9		

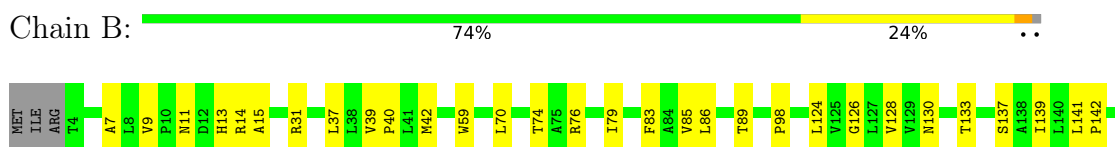
3 Residue-property plots

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: Mycobactin import ATP-binding/permease protein IrtA



• Molecule 2: Mycobactin import ATP-binding/permease protein IrtB



L150	L276	T386	A525
S153	I277	R387	L528
L156	V278	G388	I531
G157	V279	R389	D548
L161	R282	V390	G549
L161	L391	I392	F564
V164	F287	D393	E579
P165	T288	G394	
	E292	T395	
R179	D396		
	S289	L400	
T183		D401	
D186	T303	A402	
K187	L304	R403	
	A318	A404	
E194		V408	
I197	G321	H420	
R211	T322		
V212	W323	L445	
E213	R324	A446	
P214	D325	R447	
A215	G326	V448	
R216	A327		
	V328	L451	
A279	V329	V453	
T230	P330	G464	
M231	R331		
R232	I332	L470	
L233	E333	E474	
L234	F334	R477	
G235	D335	V478	
M236	D336		
Q237	V337	L484	
	A338	L485	
Q241	F339	K486	
	G340	A487	
L253		A488	
V254	S345	F489	
L255	G346	V490	
T258	P347	E495	
T259	V348	D501	
A260	L349	N504	
A261	D350	E505	
	G351	V509	
T265	Q357	R517	
	P358	I523	
L268	T374	V524	
T269	L378		
V270	G381		
P271	L382		
E272	H383		
	Q384		
A275	P385		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.715	Depositor
Minimum map value	-0.559	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/4429	0.61	4/6041 (0.1%)
2	B	0.29	0/4349	0.61	3/5950 (0.1%)
All	All	0.27	0/8778	0.61	7/11991 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	326	GLY	N-CA-C	-6.27	106.77	114.92
1	A	620	ARG	CA-C-N	6.14	127.52	119.84
1	A	620	ARG	C-N-CA	6.14	127.52	119.84
2	B	385	PRO	N-CA-C	-5.74	102.14	110.80
1	A	278	ARG	N-CA-C	5.55	117.01	111.07
2	B	395	THR	CB-CA-C	-5.49	102.59	113.45
1	A	453	ILE	N-CA-C	-5.45	108.53	113.71

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	4344	0	4498	105	0
2	B	4271	0	4369	120	0
All	All	8615	0	8867	214	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 12.

All (214) 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:620:ARG:NH1	1:A:622:GLY:H	1.50	1.08
1:A:620:ARG:NH1	1:A:622:GLY:N	2.23	0.85
2:B:395:THR:OG1	2:B:396:ASP:N	2.07	0.84
2:B:334:PHE:HE1	2:B:390:VAL:HG13	1.44	0.81
2:B:334:PHE:CE1	2:B:390:VAL:HG13	2.16	0.81
2:B:387:ARG:HG3	2:B:387:ARG:HH11	1.44	0.81
1:A:842:ASP:C	1:A:844:GLY:H	1.93	0.76
2:B:39:VAL:HG22	2:B:279:VAL:HG21	1.68	0.76
2:B:382:LEU:HD23	2:B:382:LEU:N	2.00	0.74
1:A:620:ARG:NE	1:A:620:ARG:O	2.20	0.74
2:B:336:ASP:O	2:B:387:ARG:NH1	2.22	0.73
1:A:658:ARG:HH11	1:A:675:ARG:HA	1.55	0.72
2:B:389:ARG:HG2	2:B:389:ARG:HH11	1.57	0.69
1:A:625:VAL:HG13	1:A:626:ILE:HG12	1.75	0.69
2:B:321:GLY:H	2:B:401:ASP:HB2	1.56	0.69
2:B:326:GLY:O	2:B:327:ALA:HB3	1.91	0.68
1:A:484:ARG:NH1	2:B:98:PRO:O	2.25	0.68
1:A:621:PRO:O	1:A:623:VAL:N	2.27	0.68
2:B:323:TRP:CZ2	2:B:392:ILE:HD11	2.30	0.67
2:B:13:HIS:O	2:B:15:ALA:N	2.28	0.67
1:A:621:PRO:O	1:A:622:GLY:C	2.41	0.64
2:B:323:TRP:HZ2	2:B:392:ILE:HD11	1.63	0.63
1:A:437:LEU:HD12	1:A:531:ILE:HD11	1.83	0.61
2:B:528:LEU:HA	2:B:531:ILE:HG12	1.82	0.61
2:B:448:VAL:HG23	2:B:451:LEU:HD12	1.83	0.61
1:A:618:GLY:HA2	1:A:624:PRO:HA	1.83	0.60
1:A:620:ARG:HH12	1:A:622:GLY:H	1.47	0.60
2:B:42:MET:HB2	2:B:275:ALA:HB2	1.84	0.59
1:A:528:LEU:HD13	2:B:282:ARG:HH11	1.66	0.59
1:A:826:THR:OG1	1:A:829:GLU:OE1	2.21	0.59
1:A:691:GLN:NE2	1:A:772:ALA:O	2.35	0.59
1:A:779:GLU:HA	1:A:779:GLU:OE1	2.01	0.59
1:A:756:ILE:O	1:A:760:ILE:HG13	2.04	0.58
2:B:389:ARG:HH11	2:B:389:ARG:CG	2.15	0.58
2:B:382:LEU:HD23	2:B:382:LEU:H	1.69	0.58
1:A:842:ASP:C	1:A:844:GLY:N	2.58	0.57
2:B:486:LYS:HE2	2:B:488:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:HA	2:B:197:ILE:HD12	1.87	0.56
1:A:393:LEU:HD12	1:A:582:HIS:HE1	1.70	0.56
1:A:299:LEU:HD11	1:A:347:LEU:HD22	1.86	0.56
2:B:321:GLY:HA3	2:B:401:ASP:H	1.69	0.56
2:B:548:ASP:OD2	2:B:549:GLY:N	2.39	0.56
2:B:348:VAL:O	2:B:349:LEU:HB2	2.04	0.56
2:B:495:GLU:HG3	2:B:525:ALA:HA	1.88	0.56
1:A:620:ARG:HH11	1:A:622:GLY:N	2.04	0.55
1:A:656:LEU:HD23	1:A:768:ILE:HD11	1.87	0.55
2:B:9:VAL:HB	2:B:85:VAL:HG23	1.88	0.55
1:A:328:HIS:O	1:A:332:THR:HG23	2.06	0.55
2:B:392:ILE:HD13	2:B:392:ILE:O	2.07	0.55
1:A:673:ASP:OD1	1:A:673:ASP:N	2.38	0.55
1:A:601:PRO:HB3	1:A:672:GLN:HG3	1.89	0.55
2:B:328:VAL:HG23	2:B:329:VAL:H	1.72	0.54
1:A:619:TYR:CD1	1:A:619:TYR:C	2.85	0.54
1:A:806:THR:HG23	1:A:807:ILE:HG23	1.90	0.54
2:B:326:GLY:O	2:B:327:ALA:CB	2.56	0.54
2:B:387:ARG:HH11	2:B:387:ARG:CG	2.14	0.54
1:A:373:LYS:NZ	1:A:589:GLU:O	2.40	0.54
2:B:389:ARG:CZ	2:B:389:ARG:CB	2.85	0.54
1:A:635:PRO:O	1:A:796:THR:OG1	2.26	0.53
1:A:777:ASP:OD1	1:A:780:SER:OG	2.23	0.53
1:A:309:ALA:HB3	1:A:340:LEU:HD21	1.90	0.53
2:B:487:ALA:O	2:B:517:ARG:NH2	2.39	0.53
2:B:463:VAL:HG13	2:B:464:GLY:H	1.74	0.53
2:B:447:ARG:O	2:B:477:ARG:NE	2.39	0.52
1:A:372:SER:O	1:A:376:ARG:NE	2.42	0.52
2:B:268:LEU:HB2	2:B:272:GLU:OE2	2.10	0.52
2:B:164:VAL:HG23	2:B:287:PHE:HZ	1.75	0.52
2:B:186:ASP:OD1	2:B:187:LYS:N	2.43	0.51
2:B:387:ARG:HG3	2:B:387:ARG:NH1	2.19	0.51
2:B:213:GLU:HB3	2:B:214:PRO:HD3	1.92	0.51
2:B:348:VAL:CG1	2:B:349:LEU:N	2.73	0.51
2:B:179:ARG:O	2:B:183:THR:HG23	2.11	0.51
1:A:638:VAL:HB	1:A:810:ALA:HB1	1.93	0.50
2:B:505:GLU:O	2:B:509:VAL:HG23	2.12	0.50
1:A:523:ARG:HH11	2:B:31:ARG:HH11	1.59	0.50
1:A:373:LYS:NZ	1:A:591:GLU:OE2	2.39	0.49
2:B:334:PHE:HE1	2:B:390:VAL:CG1	2.22	0.49
1:A:626:ILE:HG22	1:A:627:GLN:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:TRP:HD1	2:B:404:ALA:HB1	1.77	0.49
2:B:378:LEU:HD23	2:B:383:HIS:HB2	1.94	0.49
2:B:339:PHE:N	2:B:348:VAL:O	2.46	0.49
2:B:150:LEU:HD23	2:B:157:GLY:HA3	1.95	0.49
2:B:37:LEU:HD21	2:B:59:TRP:HB3	1.95	0.49
2:B:347:PRO:O	2:B:349:LEU:N	2.46	0.49
2:B:357:GLN:HB3	2:B:358:PRO:HD2	1.94	0.49
1:A:592:LEU:HD12	1:A:658:ARG:HH21	1.77	0.48
2:B:385:PRO:O	2:B:385:PRO:HG2	2.13	0.48
1:A:647:SER:HB2	1:A:818:HIS:H	1.79	0.48
1:A:777:ASP:C	1:A:779:GLU:H	2.21	0.48
2:B:347:PRO:HG2	2:B:374:THR:HG21	1.95	0.48
2:B:389:ARG:CG	2:B:389:ARG:NH1	2.72	0.48
2:B:86:LEU:HA	2:B:124:LEU:HD22	1.96	0.48
1:A:300:ALA:HA	1:A:303:VAL:HG12	1.96	0.47
1:A:612:PHE:O	1:A:613:ASP:HB2	2.12	0.47
2:B:288:THR:O	2:B:292:GLU:HG2	2.14	0.47
2:B:401:ASP:OD2	2:B:402:ALA:N	2.48	0.47
1:A:371:LEU:HD21	2:B:216:ARG:HG3	1.95	0.47
1:A:715:GLN:HA	1:A:718:VAL:HG12	1.97	0.47
1:A:419:PRO:HA	1:A:422:VAL:HG12	1.96	0.47
1:A:747:SER:OG	1:A:750:GLU:OE2	2.27	0.47
2:B:338:ALA:HB3	2:B:387:ARG:HG3	1.96	0.47
1:A:749:GLY:O	1:A:753:ARG:NH1	2.47	0.47
2:B:85:VAL:O	2:B:89:THR:HG22	2.14	0.47
1:A:817:ASP:OD1	1:A:817:ASP:N	2.48	0.47
2:B:420:HIS:HA	2:B:464:GLY:HA2	1.96	0.47
1:A:610:VAL:HG22	1:A:669:VAL:HG13	1.97	0.47
2:B:387:ARG:NH1	2:B:387:ARG:CG	2.73	0.47
2:B:445:LEU:HD23	2:B:484:LEU:HD11	1.96	0.47
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.78	0.47
2:B:474:GLU:O	2:B:478:VAL:HG23	2.15	0.47
1:A:777:ASP:O	1:A:779:GLU:N	2.48	0.46
2:B:37:LEU:O	2:B:40:PRO:HD2	2.15	0.46
1:A:464:ARG:O	1:A:467:GLU:HG3	2.15	0.46
2:B:501:ASP:HB3	2:B:504:ASN:HB2	1.98	0.46
2:B:139:ILE:O	2:B:142:PRO:HD2	2.16	0.46
1:A:749:GLY:O	1:A:753:ARG:HG3	2.15	0.46
2:B:270:VAL:N	2:B:271:PRO:HD2	2.31	0.46
2:B:13:HIS:C	2:B:15:ALA:H	2.24	0.46
2:B:348:VAL:HG12	2:B:349:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:THR:HB	2:B:271:PRO:HD2	1.98	0.45
2:B:470:LEU:HA	2:B:474:GLU:HB2	1.97	0.45
1:A:394:VAL:HG13	1:A:395:THR:N	2.32	0.45
1:A:700:ALA:O	1:A:704:ILE:HG13	2.16	0.45
1:A:620:ARG:NE	1:A:620:ARG:C	2.75	0.45
1:A:437:LEU:O	1:A:440:PRO:HD2	2.17	0.45
2:B:70:LEU:O	2:B:74:THR:HG23	2.16	0.45
1:A:845:GLN:CD	1:A:845:GLN:N	2.73	0.45
1:A:606:ALA:HB1	1:A:607:PRO:HD2	1.99	0.45
1:A:617:PHE:CZ	1:A:660:HIS:HB3	2.52	0.45
1:A:437:LEU:HA	1:A:530:LEU:HD21	1.99	0.44
1:A:508:GLN:HB2	2:B:83:PHE:HZ	1.83	0.44
1:A:667:ILE:O	1:A:673:ASP:HA	2.17	0.44
2:B:325:ASP:HB3	2:B:327:ALA:H	1.83	0.44
1:A:507:TRP:O	1:A:510:PRO:HD2	2.18	0.44
1:A:804:LEU:HD12	1:A:837:TYR:HE1	1.82	0.44
2:B:133:THR:O	2:B:137:SER:OG	2.31	0.44
1:A:610:VAL:C	1:A:611:VAL:O	2.60	0.44
1:A:277:TRP:HB3	1:A:278:ARG:H	1.67	0.44
1:A:356:HIS:HB3	2:B:234:LEU:HD22	2.00	0.44
1:A:358:ILE:HD12	1:A:358:ILE:HA	1.87	0.44
1:A:390:ILE:O	1:A:394:VAL:HG12	2.16	0.44
2:B:408:VAL:O	2:B:490:VAL:HG12	2.17	0.44
2:B:153:SER:OG	2:B:156:LEU:HB2	2.17	0.44
1:A:609:THR:HA	1:A:633:LEU:O	2.18	0.44
2:B:141:LEU:HB3	2:B:142:PRO:HD3	1.98	0.44
1:A:524:PRO:HB2	2:B:282:ARG:HH22	1.82	0.44
2:B:39:VAL:HB	2:B:40:PRO:HD3	2.00	0.44
1:A:303:VAL:O	1:A:307:GLN:HG2	2.18	0.43
1:A:685:ARG:O	1:A:766:VAL:HB	2.18	0.43
1:A:418:ALA:HB3	1:A:419:PRO:HD3	1.98	0.43
1:A:375:SER:HB3	2:B:216:ARG:HH11	1.82	0.43
2:B:340:GLY:HA2	2:B:348:VAL:H	1.83	0.43
1:A:376:ARG:HB3	1:A:591:GLU:HG2	2.00	0.43
2:B:128:VAL:O	2:B:133:THR:HG23	2.18	0.43
1:A:592:LEU:HD12	1:A:658:ARG:NH2	2.34	0.43
1:A:843:THR:HG23	1:A:843:THR:O	2.17	0.43
2:B:389:ARG:NH1	2:B:389:ARG:HB3	2.33	0.43
2:B:76:ARG:O	2:B:79:ILE:HG22	2.19	0.43
2:B:331:ARG:O	2:B:393:ASP:N	2.37	0.43
1:A:731:ARG:HD2	1:A:731:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:SER:OG	1:A:780:SER:O	2.34	0.43
2:B:261:ALA:O	2:B:265:THR:HG23	2.19	0.43
1:A:459:ILE:HG13	1:A:460:VAL:N	2.34	0.43
2:B:523:ILE:HG12	2:B:525:ALA:HB2	2.01	0.43
2:B:7:ALA:HB2	2:B:304:LEU:HD11	2.01	0.42
2:B:161:LEU:HD12	2:B:161:LEU:HA	1.94	0.42
2:B:332:ILE:HG22	2:B:333:GLU:H	1.82	0.42
2:B:463:VAL:HG13	2:B:464:GLY:N	2.33	0.42
1:A:281:ALA:HA	1:A:284:ARG:HB3	2.01	0.42
1:A:450:SER:O	1:A:453:ILE:HG12	2.20	0.42
1:A:406:THR:OG1	1:A:407:HIS:ND1	2.48	0.42
1:A:620:ARG:HA	1:A:620:ARG:HD2	1.79	0.42
2:B:348:VAL:HG12	2:B:349:LEU:N	2.35	0.42
1:A:401:LEU:HD23	1:A:401:LEU:HA	1.90	0.42
1:A:617:PHE:CZ	1:A:660:HIS:CB	3.03	0.42
1:A:754:LEU:HD12	1:A:754:LEU:HA	1.89	0.42
2:B:408:VAL:O	2:B:488:ALA:HB1	2.20	0.42
1:A:508:GLN:HB2	2:B:83:PHE:CZ	2.55	0.42
1:A:709:PRO:HG3	2:B:211:ARG:HD2	2.02	0.41
2:B:126:GLY:O	2:B:130:ASN:ND2	2.45	0.41
2:B:164:VAL:CG1	2:B:165:PRO:HD3	2.49	0.41
2:B:400:LEU:HD23	2:B:401:ASP:N	2.34	0.41
1:A:626:ILE:HG22	1:A:627:GLN:N	2.36	0.41
1:A:712:PRO:HD2	1:A:715:GLN:HG2	2.02	0.41
2:B:259:THR:HG21	2:B:277:ILE:HG13	2.03	0.41
1:A:725:ILE:HD12	1:A:725:ILE:HA	1.92	0.41
2:B:150:LEU:HD23	2:B:150:LEU:HA	1.88	0.41
1:A:394:VAL:HG13	1:A:395:THR:HG23	2.02	0.41
1:A:492:SER:O	1:A:496:ARG:HG2	2.21	0.41
2:B:229:ALA:O	2:B:231:MET:N	2.53	0.41
2:B:299:SER:O	2:B:303:THR:HG23	2.20	0.41
2:B:318:ALA:HB1	2:B:400:LEU:O	2.21	0.41
2:B:232:ARG:HD2	2:B:232:ARG:HA	1.68	0.41
2:B:328:VAL:HG23	2:B:329:VAL:N	2.36	0.41
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.87	0.41
1:A:634:ARG:HB2	1:A:637:THR:OG1	2.20	0.41
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.90	0.41
1:A:620:ARG:C	1:A:620:ARG:CD	2.93	0.41
1:A:772:ALA:HA	1:A:775:PHE:CE1	2.56	0.41
1:A:845:GLN:OE1	1:A:845:GLN:CA	2.69	0.41
2:B:230:THR:O	2:B:234:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:LEU:O	2:B:258:THR:HG22	2.20	0.41
2:B:336:ASP:OD1	2:B:351:GLY:HA2	2.21	0.41
2:B:445:LEU:HD12	2:B:445:LEU:HA	1.90	0.41
1:A:779:GLU:OE2	2:B:564:PHE:HE1	2.04	0.41
2:B:213:GLU:OE1	2:B:216:ARG:NH2	2.54	0.41
2:B:392:ILE:O	2:B:392:ILE:CD1	2.70	0.41
1:A:278:ARG:HG3	1:A:279:ALA:N	2.36	0.40
2:B:237:GLN:HE21	2:B:241:GLN:HG2	1.86	0.40
2:B:392:ILE:O	2:B:392:ILE:CG1	2.68	0.40
2:B:233:LEU:HA	2:B:236:MET:HG2	2.04	0.40
1:A:520:LEU:HD23	1:A:520:LEU:HA	1.94	0.40
1:A:627:GLN:O	1:A:629:VAL:HG13	2.21	0.40
2:B:7:ALA:O	2:B:9:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/859 (66%)	495 (87%)	67 (12%)	7 (1%)	10	41
2	B	574/579 (99%)	504 (88%)	67 (12%)	3 (0%)	24	58
All	All	1143/1438 (80%)	999 (87%)	134 (12%)	10 (1%)	16	47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	611	VAL
1	A	614	HIS
1	A	621	PRO
1	A	622	GLY
2	B	14	ARG

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Mol	Chain	Res	Type
1	A	843	THR
2	B	11	ASN
1	A	619	TYR
1	A	749	GLY
2	B	381	GLY

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	448/674 (66%)	442 (99%)	6 (1%)	61	72
2	B	432/435 (99%)	419 (97%)	13 (3%)	36	60
All	All	880/1109 (79%)	861 (98%)	19 (2%)	45	65

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	TRP
1	A	611	VAL
1	A	612	PHE
1	A	619	TYR
1	A	620	ARG
1	A	779	GLU
2	B	253	ILE
2	B	329	VAL
2	B	345	SER
2	B	348	VAL
2	B	382	LEU
2	B	386	THR
2	B	387	ARG
2	B	389	ARG
2	B	390	VAL
2	B	391	LEU
2	B	392	ILE
2	B	393	ASP

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Mol	Chain	Res	Type
2	B	395	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	470	ASN
1	A	480	GLN
1	A	548	ASN
1	A	582	HIS
1	A	597	HIS
1	A	614	HIS
1	A	627	GLN
1	A	805	HIS
1	A	812	GLN
2	B	109	ASN
2	B	204	GLN
2	B	237	GLN
2	B	241	GLN
2	B	415	HIS
2	B	420	HIS
2	B	526	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

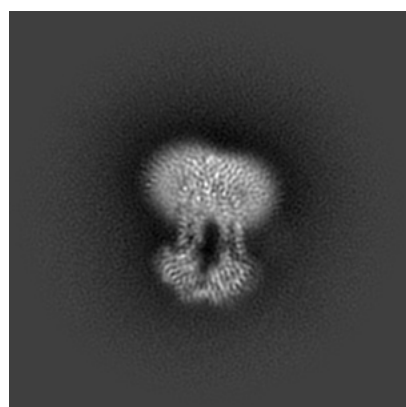
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32536. These allow visual inspection of the internal detail of the map and identification of artifacts.

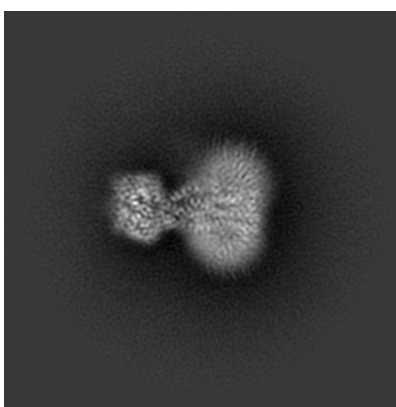
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

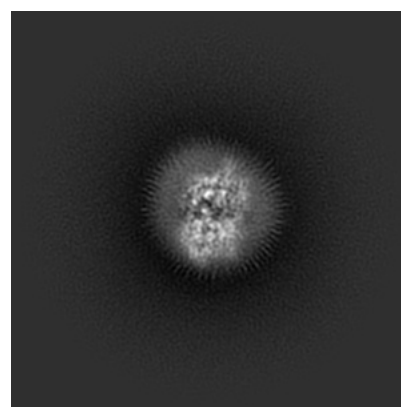
6.1.1 Primary map



X



Y

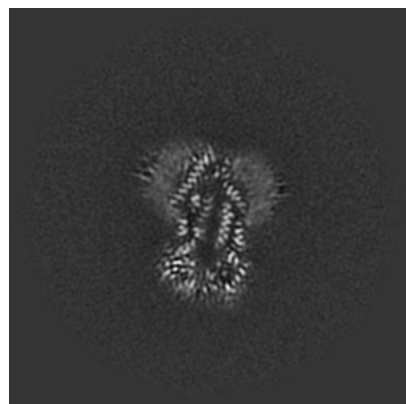


Z

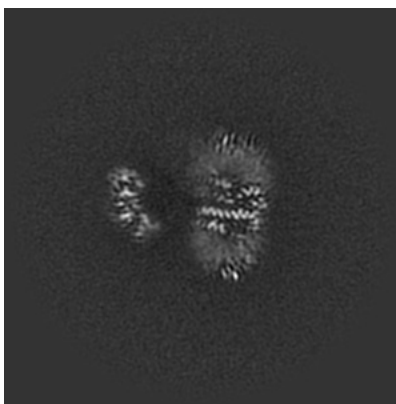
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

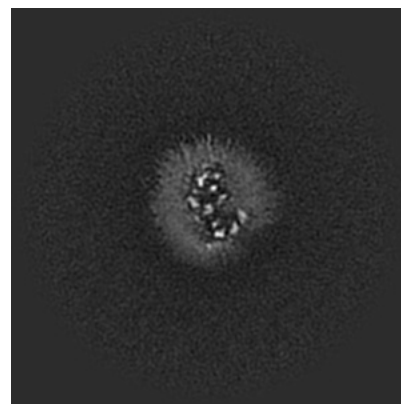
6.2.1 Primary map



X Index: 192



Y Index: 192

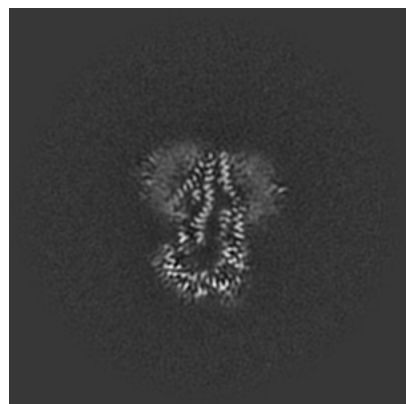


Z Index: 192

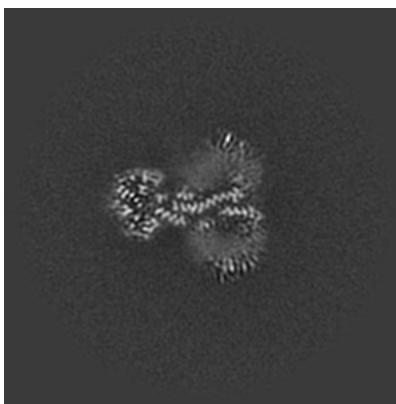
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

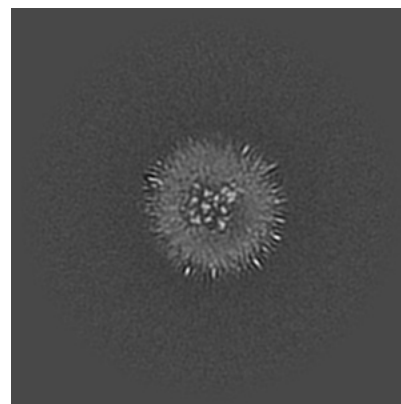
6.3.1 Primary map



X Index: 188



Y Index: 208

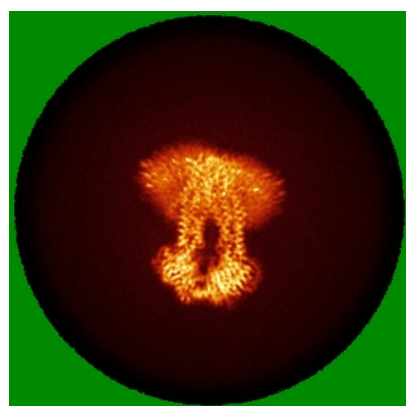


Z Index: 227

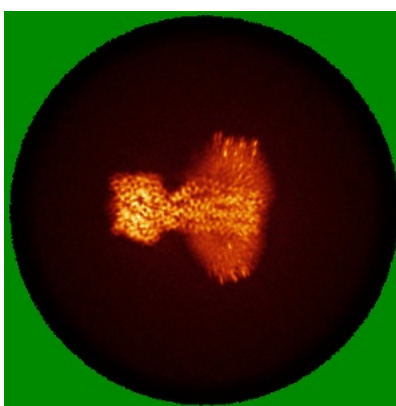
The images above show the largest variance slices of the map in three orthogonal directions.

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

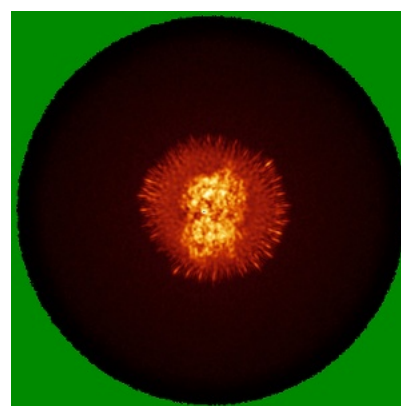
6.4.1 Primary map



X



Y

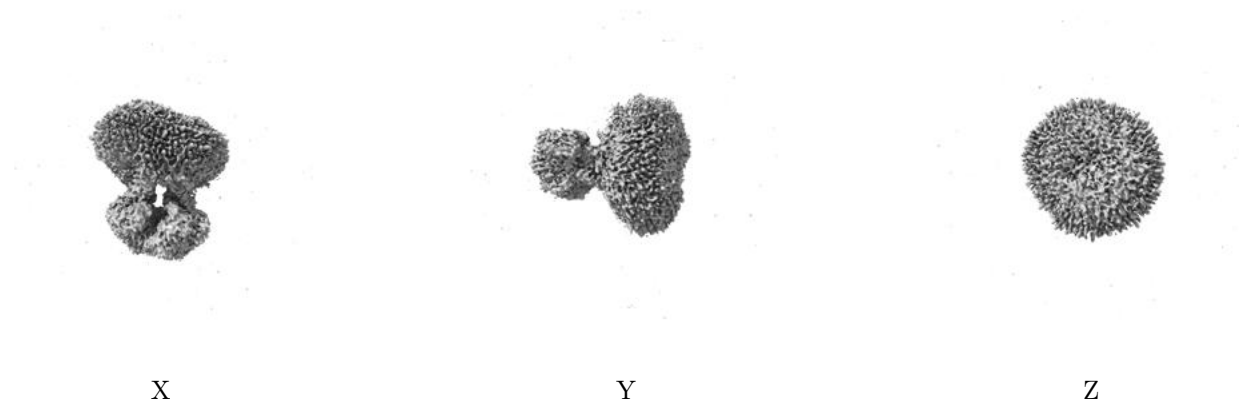


Z

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

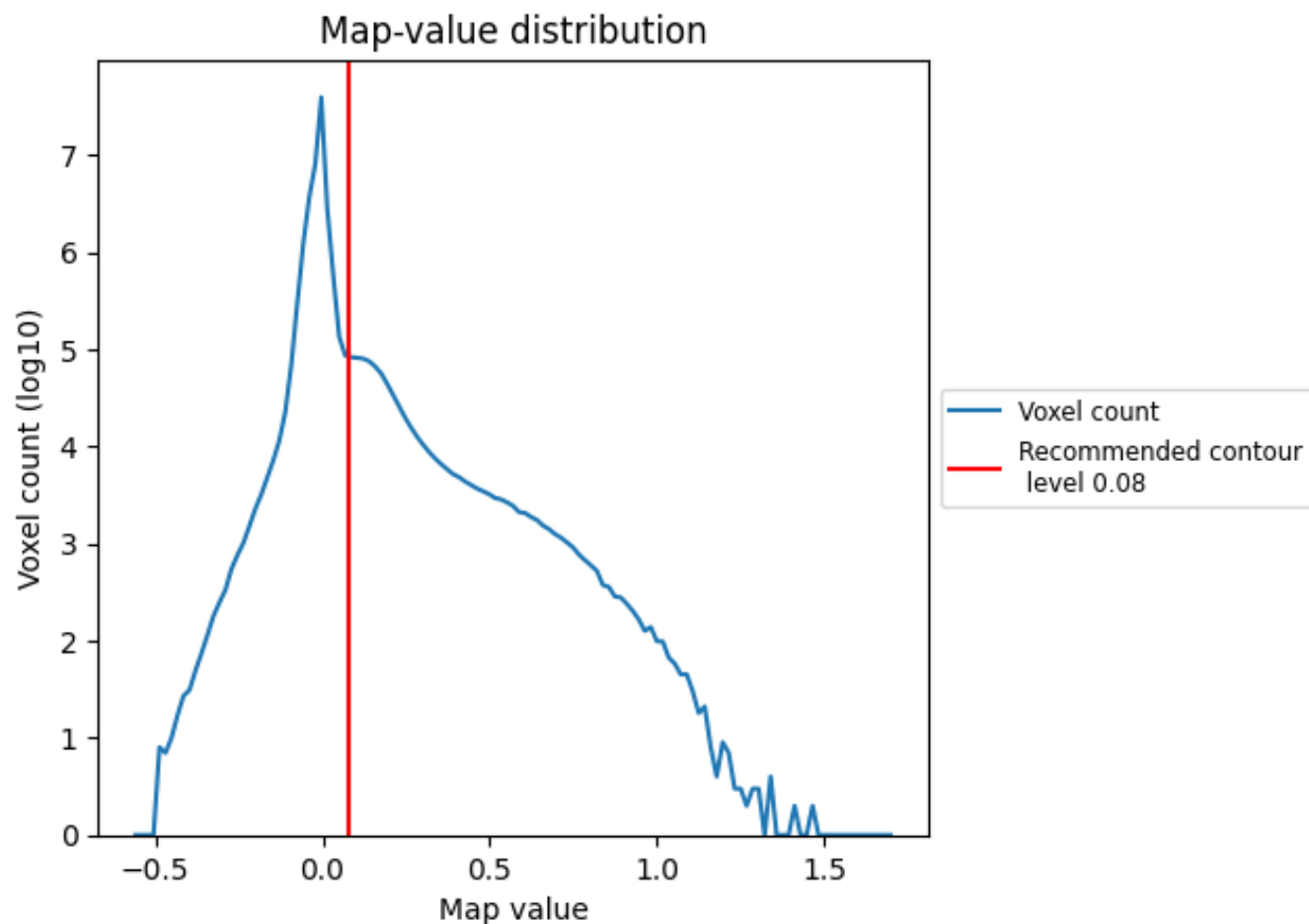
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

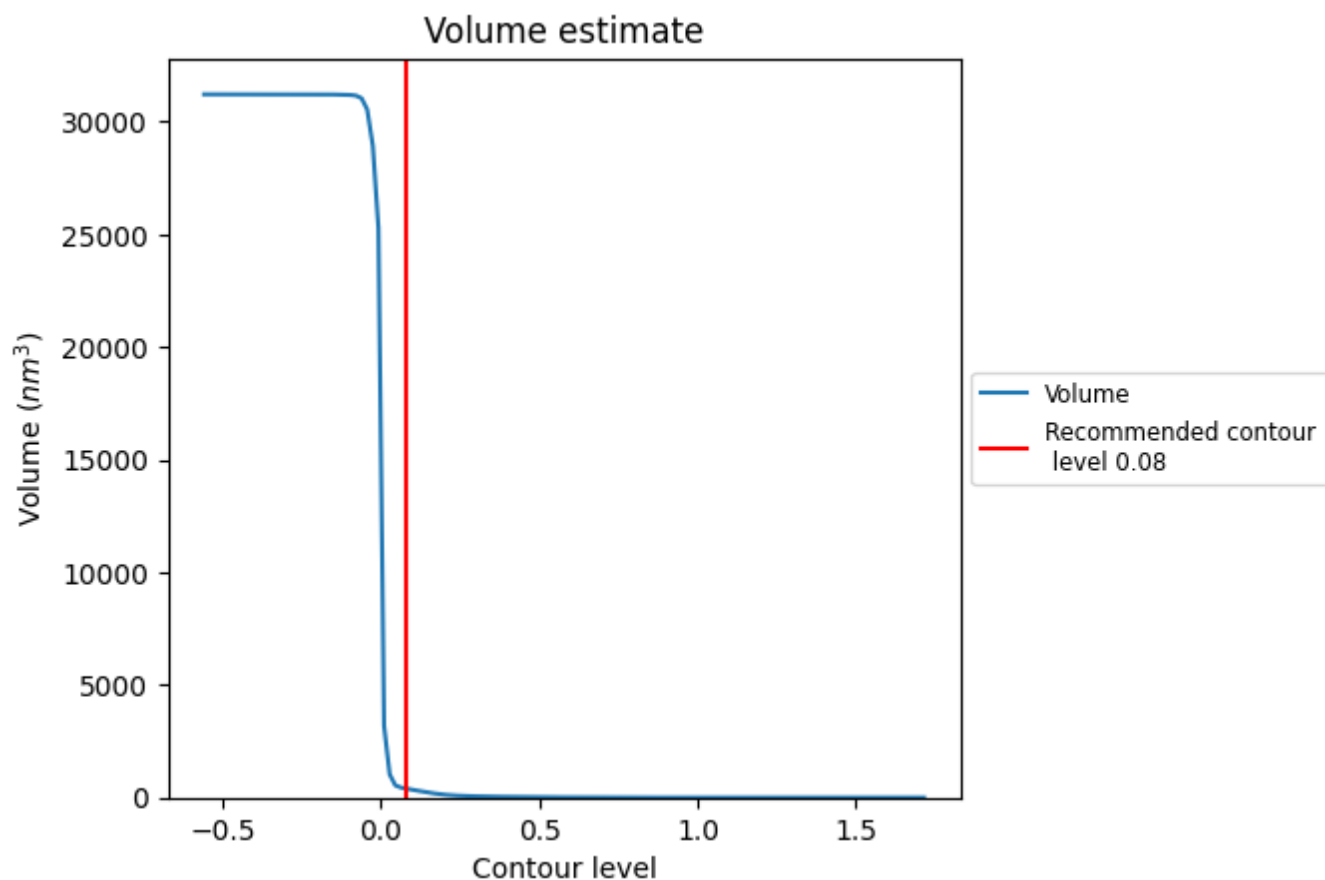
This section contains the results of statistical analysis of the map.

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.

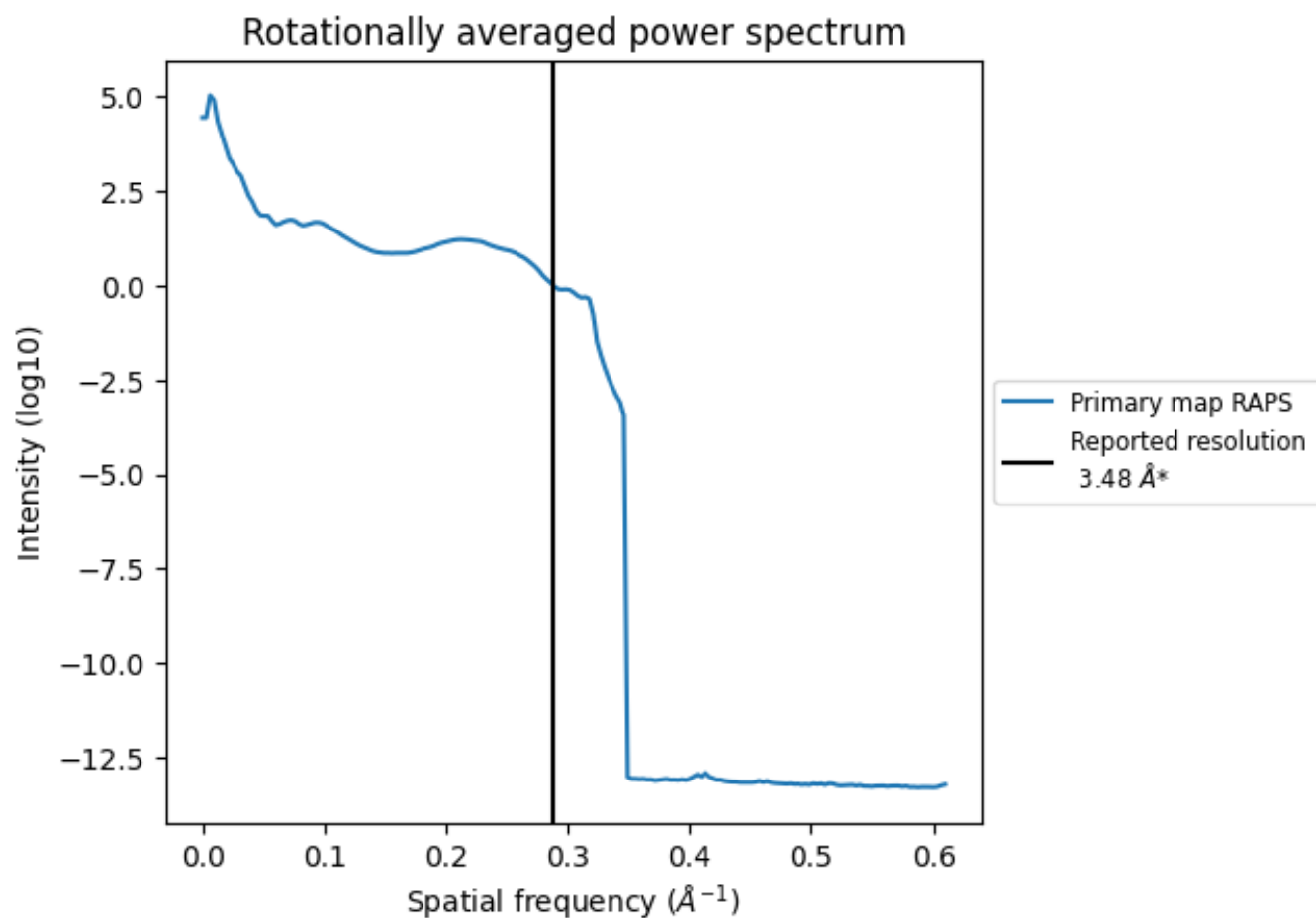
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 396 nm^3 ; this corresponds to an approximate mass of 358 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 0.287 Å⁻¹

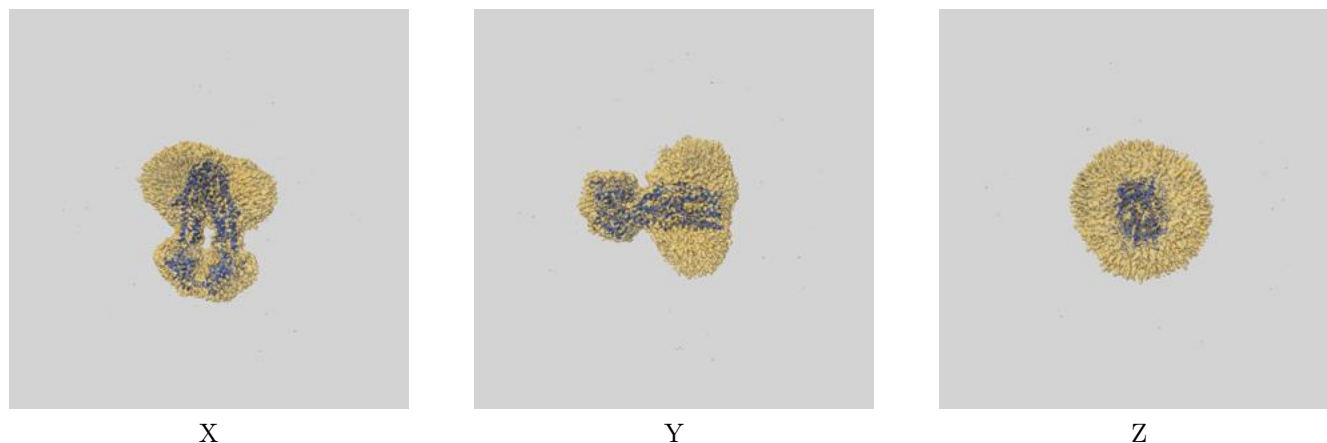
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

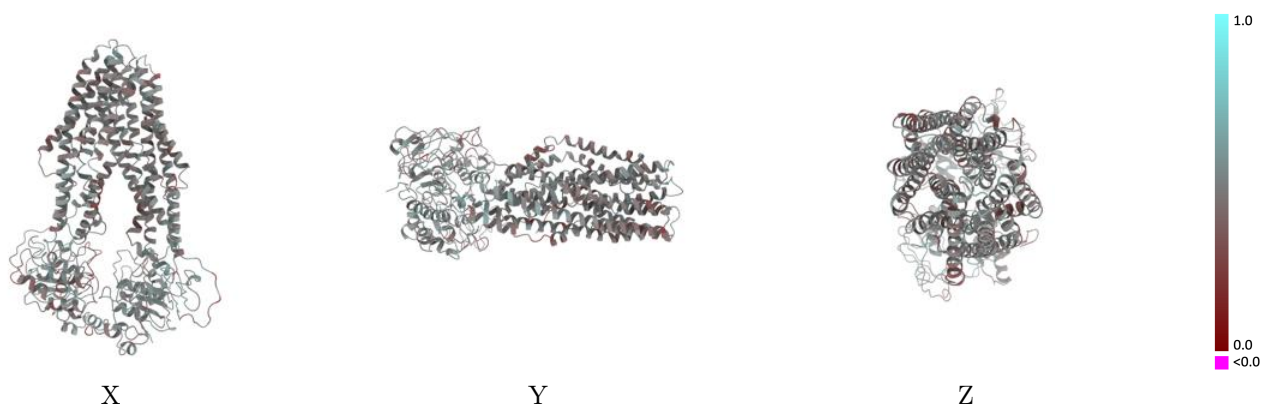
This section contains information regarding the fit between EMDB map EMD-32536 and PDB model 7WIU. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



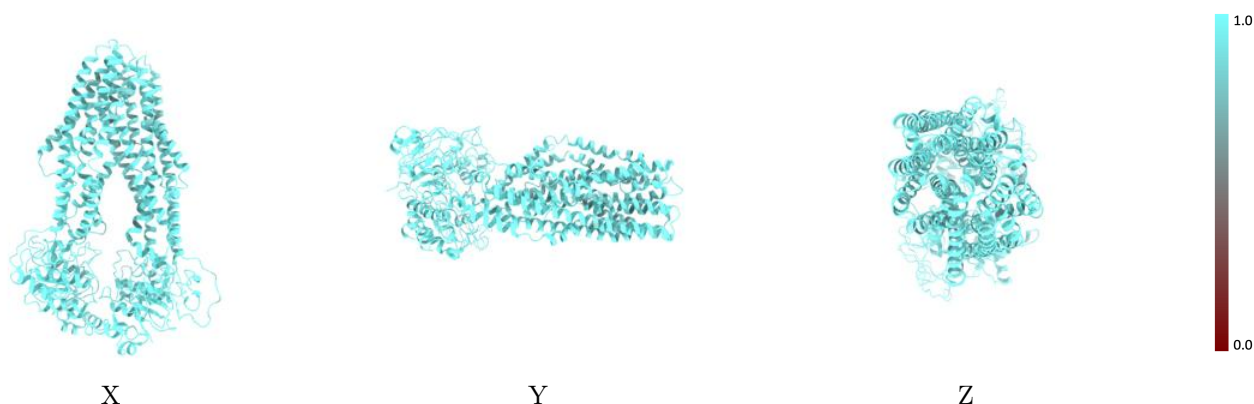
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



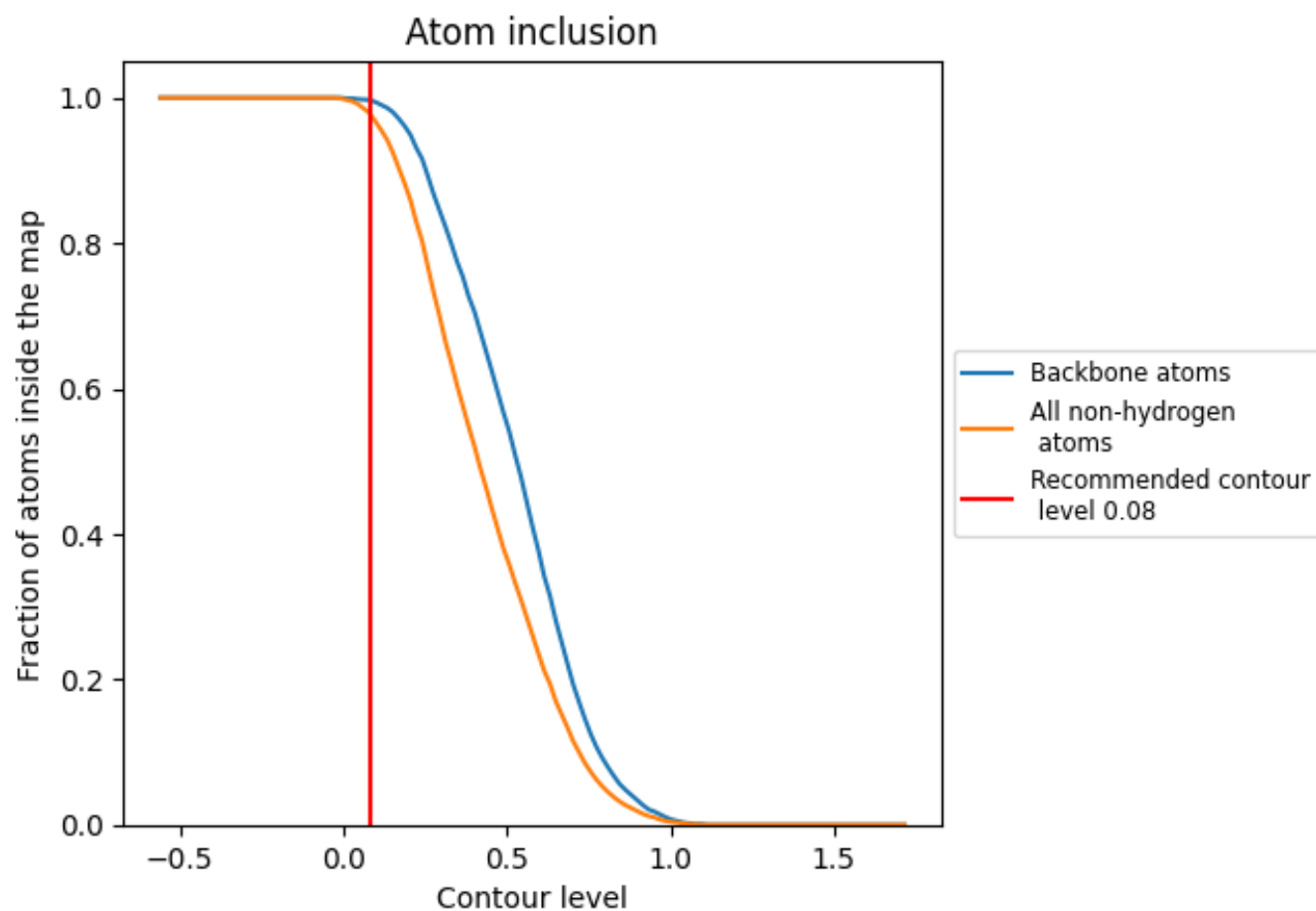
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9790	0.4760
A	0.9790	0.4780
B	0.9780	0.4740

