Full wwPDB EM Map/Model Validation Report ⓘ

Sep 14, 2020 – 02:43 PM BST

PDB ID	:	6WU1
EMDB ID	:	EMD-21902
Title	:	Structure of apo LaINDY
Authors	:	Sauer, D.B.; Marden, J.J.; Cocco, N.C.; Song, J.M.; Wang, D.N.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on	:	2020-05-04
Resolution	:	3.09 Å(reported)

This is a Full wwPDB EM Map/Model 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 following versions of software and data (see references ⓘ) were used in the production of this report:

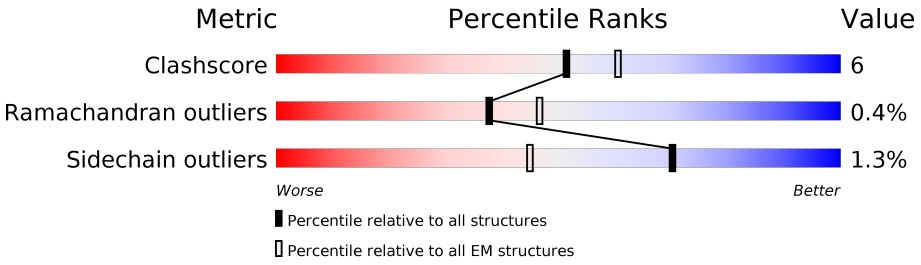
EMDB validation analysis	:	0.0.0.dev33
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 3.09 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on 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	516	19% 80% 14% • 5%
1	B	516	19% 79% 15% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15958 atoms, of which 8250 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 DASS family sodium-coupled anion symporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	489	Total	C	H	N	O	S	0	0
			7673	2517	3913	588	630	25		
1	B	489	Total	C	H	N	O	S	0	0
			7673	2517	3913	588	630	25		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP A0A3A9Y7Q2
A	-26	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-25	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-24	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-23	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-22	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-21	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-20	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-19	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-18	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-17	HIS	-	expression tag	UNP A0A3A9Y7Q2
A	-16	SER	-	expression tag	UNP A0A3A9Y7Q2
A	-15	SER	-	expression tag	UNP A0A3A9Y7Q2
A	-14	GLY	-	expression tag	UNP A0A3A9Y7Q2
A	-13	VAL	-	expression tag	UNP A0A3A9Y7Q2
A	-12	ASP	-	expression tag	UNP A0A3A9Y7Q2
A	-11	LEU	-	expression tag	UNP A0A3A9Y7Q2
A	-10	GLY	-	expression tag	UNP A0A3A9Y7Q2
A	-9	THR	-	expression tag	UNP A0A3A9Y7Q2
A	-8	GLU	-	expression tag	UNP A0A3A9Y7Q2
A	-7	ASN	-	expression tag	UNP A0A3A9Y7Q2
A	-6	LEU	-	expression tag	UNP A0A3A9Y7Q2
A	-5	TYR	-	expression tag	UNP A0A3A9Y7Q2
A	-4	PHE	-	expression tag	UNP A0A3A9Y7Q2
A	-3	GLN	-	expression tag	UNP A0A3A9Y7Q2
A	-2	SER	-	expression tag	UNP A0A3A9Y7Q2

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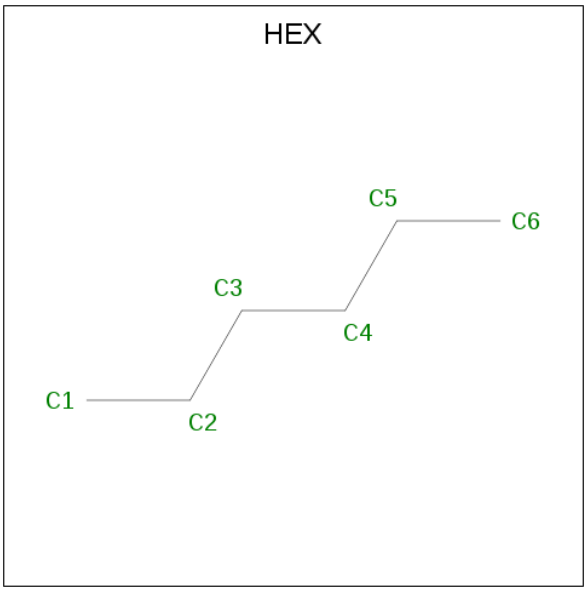
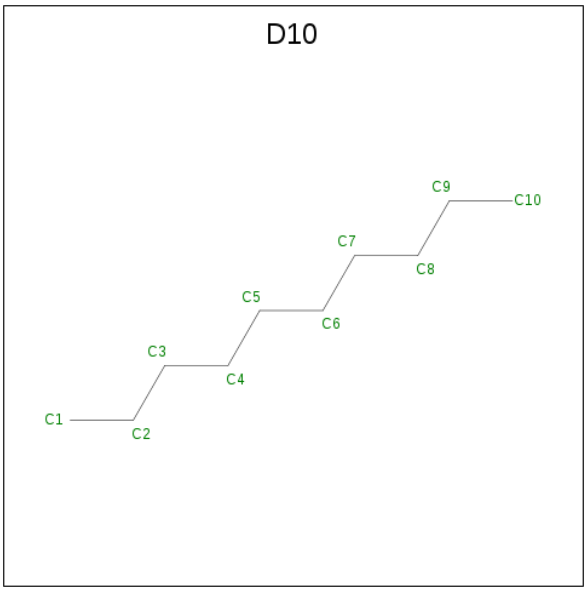
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP A0A3A9Y7Q2
A	0	ALA	-	expression tag	UNP A0A3A9Y7Q2
B	-27	MET	-	initiating methionine	UNP A0A3A9Y7Q2
B	-26	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-25	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-24	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-23	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-22	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-21	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-20	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-19	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-18	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-17	HIS	-	expression tag	UNP A0A3A9Y7Q2
B	-16	SER	-	expression tag	UNP A0A3A9Y7Q2
B	-15	SER	-	expression tag	UNP A0A3A9Y7Q2
B	-14	GLY	-	expression tag	UNP A0A3A9Y7Q2
B	-13	VAL	-	expression tag	UNP A0A3A9Y7Q2
B	-12	ASP	-	expression tag	UNP A0A3A9Y7Q2
B	-11	LEU	-	expression tag	UNP A0A3A9Y7Q2
B	-10	GLY	-	expression tag	UNP A0A3A9Y7Q2
B	-9	THR	-	expression tag	UNP A0A3A9Y7Q2
B	-8	GLU	-	expression tag	UNP A0A3A9Y7Q2
B	-7	ASN	-	expression tag	UNP A0A3A9Y7Q2
B	-6	LEU	-	expression tag	UNP A0A3A9Y7Q2
B	-5	TYR	-	expression tag	UNP A0A3A9Y7Q2
B	-4	PHE	-	expression tag	UNP A0A3A9Y7Q2
B	-3	GLN	-	expression tag	UNP A0A3A9Y7Q2
B	-2	SER	-	expression tag	UNP A0A3A9Y7Q2
B	-1	ASN	-	expression tag	UNP A0A3A9Y7Q2
B	0	ALA	-	expression tag	UNP A0A3A9Y7Q2

- Molecule 2 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



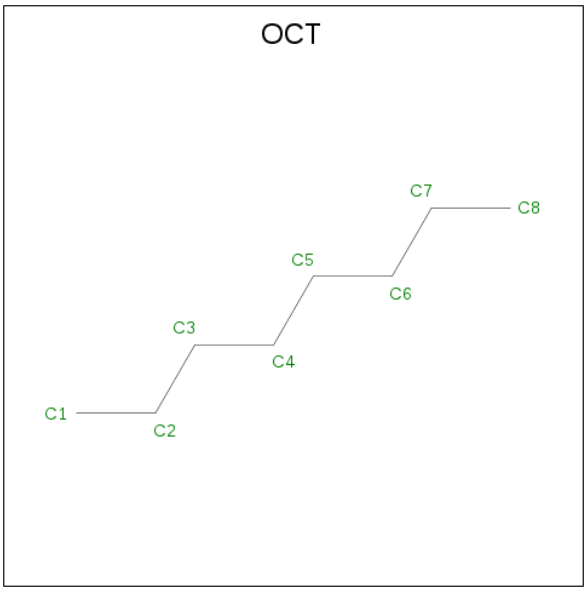
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C H 120 36 84	0
2	A	1	Total C H 120 36 84	0
2	A	1	Total C H 120 36 84	0
2	A	1	Total C H 120 36 84	0
2	A	1	Total C H 120 36 84	0
2	A	1	Total C H 120 36 84	0
2	B	1	Total C H 80 24 56	0
2	B	1	Total C H 80 24 56	0
2	B	1	Total C H 80 24 56	0
2	B	1	Total C H 80 24 56	0

- Molecule 3 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 160	C 50	H 110	0
3	A	1	Total 160	C 50	H 110	0
3	A	1	Total 160	C 50	H 110	0
3	A	1	Total 160	C 50	H 110	0
3	A	1	Total 160	C 50	H 110	0
3	B	1	Total 96	C 30	H 66	0
3	B	1	Total 96	C 30	H 66	0
3	B	1	Total 96	C 30	H 66	0

- Molecule 4 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



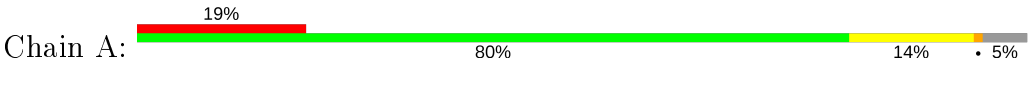
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	H	0
			78	24	54	
4	A	1	Total	C	H	0
			78	24	54	
4	A	1	Total	C	H	0
			78	24	54	
4	B	1	Total	C	H	0
			78	24	54	
4	B	1	Total	C	H	0
			78	24	54	
4	B	1	Total	C	H	0
			78	24	54	

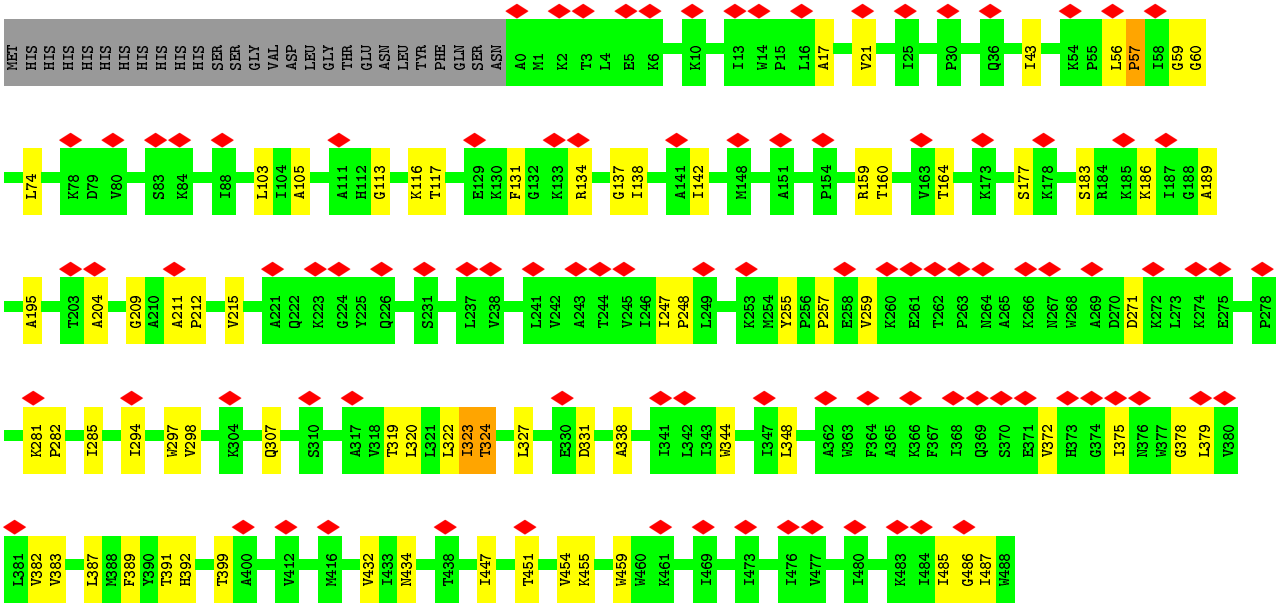
3 Residue-property plots

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: DASS family sodium-coupled anion symporter

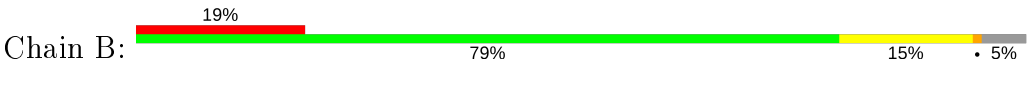
Chain A:

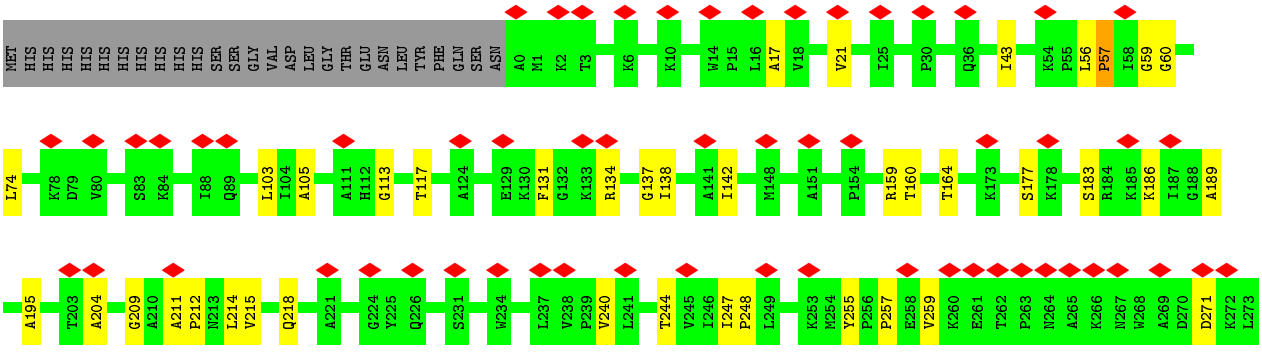


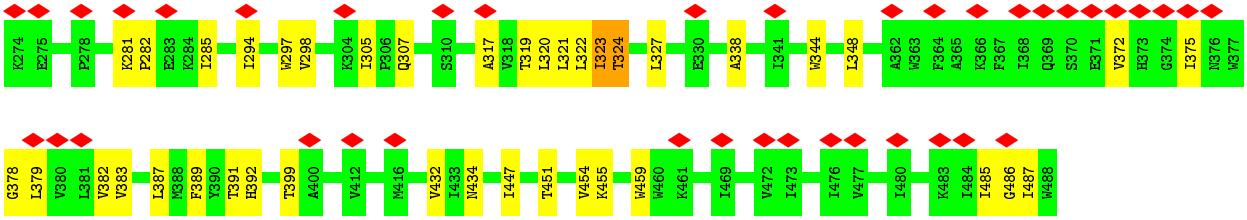


- Molecule 1: DASS family sodium-coupled anion symporter

Chain B:






K274 E275 P278 K281 P282 E283 K284 I285 I294 W297 V298 K304 I305 P306 Q307 S310 A317 V318 T319 I320 L321 I322 I323 T324 I327 E330 A338 I341 W344 I348 A362 M363 F364 A365 K366 F367 I368 Q369 S370 E371 V372 H373 G374 I375 N376 W377
G378 I379 V380 L381 V382 V383 L387 M388 F389 Y390 T391 H392 T399 A400 V412 M416 V432 I433 N434 I447 T451 V454 K455 W459 W460 K461 I469 V472 I473 I476 V477 I480 K483 I484 I485 G486 I487 W488

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	278663	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 ($e^-/Å^2$)	75.05	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	27.396	Depositor
Minimum map value	-18.327	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.48	Depositor
Map size (Å)	209.59999, 209.59999, 209.59999	Depositor
Map dimensions	200, 200, 200	Depositor
Map angles (°)	90.0, 90.0, 90.0	Depositor
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D10, HEX, OCT

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	0.34	0/3867	0.42	0/5275
1	B	0.34	0/3867	0.42	0/5275
All	All	0.34	0/7734	0.42	0/10550

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3760	3913	3915	47	0
1	B	3760	3913	3915	49	0
2	A	36	84	84	0	0
2	B	24	56	56	0	0
3	A	50	110	110	0	0
3	B	30	66	66	0	0
4	A	24	54	54	0	0
4	B	24	54	54	0	0
All	All	7708	8250	8254	92	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 6.

All (92) 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:320:LEU:O	1:A:324:THR:OG1	1.91	0.89
1:B:320:LEU:O	1:B:324:THR:OG1	1.91	0.87
1:A:159:ARG:NH2	1:A:209:GLY:O	2.19	0.75
1:B:159:ARG:NH2	1:B:209:GLY:O	2.19	0.74
1:A:134:ARG:O	1:A:137:GLY:N	2.22	0.70
1:B:17:ALA:O	1:B:21:VAL:HG23	1.92	0.70
1:B:294:ILE:O	1:B:298:VAL:HG13	1.93	0.69
1:A:17:ALA:O	1:A:21:VAL:HG23	1.92	0.69
1:B:319:THR:O	1:B:323:ILE:HG23	1.94	0.68
1:A:294:ILE:O	1:A:298:VAL:HG13	1.93	0.68
1:A:319:THR:O	1:A:323:ILE:HG23	1.94	0.68
1:B:134:ARG:O	1:B:137:GLY:N	2.22	0.64
1:B:387:LEU:O	1:B:391:THR:HG23	2.01	0.61
1:A:387:LEU:O	1:A:391:THR:HG23	2.01	0.59
1:A:56:LEU:HD11	1:B:323:ILE:HG22	1.86	0.57
1:A:56:LEU:CD1	1:B:323:ILE:HG22	2.35	0.57
1:A:57:PRO:O	1:A:60:GLY:N	2.38	0.57
1:B:57:PRO:O	1:B:60:GLY:N	2.38	0.55
1:B:485:ILE:O	1:B:487:ILE:N	2.39	0.54
1:A:323:ILE:HG22	1:B:56:LEU:HD11	1.89	0.54
1:A:485:ILE:O	1:A:487:ILE:N	2.39	0.54
1:A:447:ILE:O	1:A:451:THR:HG23	2.07	0.54
1:A:323:ILE:HG22	1:B:56:LEU:CD1	2.38	0.54
1:B:447:ILE:O	1:B:451:THR:HG23	2.07	0.54
1:A:43:ILE:HD12	1:A:74:LEU:HD12	1.90	0.53
1:A:160:THR:HA	1:A:164:THR:HG22	1.91	0.53
1:B:43:ILE:HD12	1:B:74:LEU:HD12	1.90	0.53
1:B:372:VAL:HG23	1:B:375:ILE:HD12	1.91	0.53
1:B:160:THR:HA	1:B:164:THR:HG22	1.91	0.53
1:A:322:LEU:HD23	1:A:327:LEU:O	2.09	0.52
1:B:322:LEU:HD23	1:B:327:LEU:O	2.09	0.52
1:A:372:VAL:HG23	1:A:375:ILE:HD12	1.91	0.52
1:B:307:GLN:N	1:B:307:GLN:OE1	2.42	0.52
1:B:372:VAL:HG23	1:B:375:ILE:CD1	2.40	0.52
1:A:307:GLN:OE1	1:A:307:GLN:N	2.43	0.52
1:A:372:VAL:HG23	1:A:375:ILE:CD1	2.40	0.51
1:A:186:LYS:O	1:A:259:VAL:HG12	2.11	0.50
1:A:57:PRO:O	1:A:59:GLY:N	2.44	0.50
1:B:186:LYS:O	1:B:259:VAL:HG12	2.11	0.50
1:B:57:PRO:O	1:B:59:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:O	1:A:117:THR:HG23	2.12	0.49
1:B:285:ILE:HG21	1:B:324:THR:HG21	1.96	0.48
1:B:113:GLY:O	1:B:117:THR:HG23	2.12	0.48
1:A:204:ALA:HB2	1:A:432:VAL:HG11	1.96	0.48
1:B:204:ALA:HB2	1:B:432:VAL:HG11	1.96	0.47
1:B:183:SER:O	1:B:183:SER:OG	2.33	0.47
1:A:285:ILE:HG21	1:A:324:THR:HG21	1.96	0.47
1:A:454:VAL:HG11	1:A:459:TRP:HE3	1.80	0.46
1:B:378:GLY:O	1:B:382:VAL:HG23	2.15	0.46
1:A:211:ALA:N	1:A:212:PRO:HD2	2.31	0.46
1:B:211:ALA:N	1:B:212:PRO:HD2	2.31	0.46
1:A:392:HIS:HB2	1:A:434:ASN:ND2	2.31	0.46
1:B:454:VAL:HG11	1:B:459:TRP:HE3	1.80	0.46
1:A:247:ILE:HB	1:A:248:PRO:HD3	1.98	0.46
1:A:378:GLY:O	1:A:382:VAL:HG23	2.15	0.45
1:A:379:LEU:O	1:A:383:VAL:HG23	2.16	0.45
1:A:183:SER:OG	1:A:183:SER:O	2.33	0.45
1:B:247:ILE:HB	1:B:248:PRO:HD3	1.98	0.45
1:B:379:LEU:O	1:B:383:VAL:HG23	2.16	0.45
1:B:392:HIS:HB2	1:B:434:ASN:ND2	2.31	0.45
1:A:116:LYS:NZ	1:A:331:ASP:OD2	2.48	0.44
1:B:389:PHE:HA	1:B:434:ASN:ND2	2.33	0.44
1:B:105:ALA:HB1	1:B:338:ALA:HB1	1.99	0.43
1:A:105:ALA:HB1	1:A:338:ALA:HB1	1.99	0.43
1:A:344:TRP:CE3	1:A:348:LEU:HD12	2.54	0.43
1:A:389:PHE:HA	1:A:434:ASN:ND2	2.33	0.43
1:B:344:TRP:CE3	1:B:348:LEU:HD12	2.54	0.43
1:A:142:ILE:HD11	1:A:195:ALA:HB2	2.02	0.42
1:B:138:ILE:O	1:B:142:ILE:HG22	2.19	0.42
1:B:142:ILE:HD11	1:B:195:ALA:HB2	2.02	0.42
1:A:138:ILE:O	1:A:142:ILE:HG22	2.19	0.42
1:A:189:ALA:HB1	1:A:255:TYR:HE2	1.85	0.41
1:A:259:VAL:HG13	1:A:259:VAL:O	2.20	0.41
1:B:189:ALA:HB1	1:B:255:TYR:HE2	1.85	0.41
1:B:259:VAL:HG13	1:B:259:VAL:O	2.20	0.41
1:B:294:ILE:HD13	1:B:297:TRP:HE3	1.85	0.41
1:A:389:PHE:HA	1:A:434:ASN:HD21	1.86	0.41
1:B:281:LYS:N	1:B:282:PRO:HD2	2.35	0.41
1:A:294:ILE:HD13	1:A:297:TRP:HE3	1.85	0.41
1:B:215:VAL:HG21	1:B:399:THR:HG23	2.03	0.41
1:A:103:LEU:HD12	1:A:103:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:VAL:HG12	1:A:455:LYS:O	2.21	0.41
1:B:454:VAL:HG12	1:B:455:LYS:O	2.21	0.41
1:B:317:ALA:O	1:B:321:LEU:HG	2.21	0.41
1:B:103:LEU:O	1:B:103:LEU:HD12	2.20	0.41
1:B:240:VAL:O	1:B:244:THR:OG1	2.35	0.41
1:B:305:ILE:HG22	1:B:307:GLN:H	1.86	0.41
1:A:281:LYS:N	1:A:282:PRO:HD2	2.35	0.40
1:A:257:PRO:O	1:A:259:VAL:N	2.55	0.40
1:B:257:PRO:O	1:B:259:VAL:N	2.54	0.40
1:A:215:VAL:HG21	1:A:399:THR:HG23	2.03	0.40
1:B:214:LEU:O	1:B:218:GLN:HG2	2.21	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	487/516 (94%)	458 (94%)	27 (6%)	2 (0%)	34 69
1	B	487/516 (94%)	459 (94%)	26 (5%)	2 (0%)	34 69
All	All	974/1032 (94%)	917 (94%)	53 (5%)	4 (0%)	38 69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLY
1	B	486	GLY
1	A	57	PRO
1	B	57	PRO

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	395/420 (94%)	390 (99%)	5 (1%)	69 87
1	B	395/420 (94%)	390 (99%)	5 (1%)	69 87
All	All	790/840 (94%)	780 (99%)	10 (1%)	70 87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	PHE
1	A	177	SER
1	A	271	ASP
1	A	323	ILE
1	A	324	THR
1	B	131	PHE
1	B	177	SER
1	B	271	ASP
1	B	323	ILE
1	B	324	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	121	ASN
1	A	264	ASN
1	A	392	HIS
1	A	401	HIS
1	B	98	ASN
1	B	121	ASN
1	B	264	ASN
1	B	392	HIS
1	B	401	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 monosaccharides in this entry.

5.6 Ligand geometry

24 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	$\#\|Z\| > 2$
4	OCT	A	508	-	7,7,7	0.18	0	6,6,6	0.52	0
2	HEX	B	509	-	5,5,5	0.17	0	4,4,4	0.64	0
3	D10	B	506	-	9,9,9	0.15	0	8,8,8	1.08	0
4	OCT	A	510	-	7,7,7	0.22	0	6,6,6	0.54	0
4	OCT	A	509	-	7,7,7	0.24	0	6,6,6	0.48	0
2	HEX	A	504	-	5,5,5	0.16	0	4,4,4	0.66	0
3	D10	A	505	-	9,9,9	0.09	0	8,8,8	1.02	0
2	HEX	A	503	-	5,5,5	0.17	0	4,4,4	0.64	0
4	OCT	B	503	-	7,7,7	0.18	0	6,6,6	0.56	0
3	D10	A	506	-	9,9,9	0.11	0	8,8,8	1.02	0
2	HEX	A	501	-	5,5,5	0.13	0	4,4,4	0.69	0
2	HEX	B	502	-	5,5,5	0.10	0	4,4,4	0.67	0
2	HEX	B	508	-	5,5,5	0.13	0	4,4,4	0.70	0
3	D10	B	501	-	9,9,9	0.10	0	8,8,8	1.00	0
2	HEX	A	513	-	5,5,5	0.09	0	4,4,4	0.68	0
3	D10	A	512	-	9,9,9	0.10	0	8,8,8	1.05	0
4	OCT	B	504	-	7,7,7	0.14	0	6,6,6	0.57	0
2	HEX	A	514	-	5,5,5	0.14	0	4,4,4	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEX	B	510	-	5,5,5	0.13	0	4,4,4	0.65	0
2	HEX	A	502	-	5,5,5	0.15	0	4,4,4	0.66	0
3	D10	A	511	-	9,9,9	0.11	0	8,8,8	1.07	0
3	D10	A	507	-	9,9,9	0.12	0	8,8,8	1.10	0
3	D10	B	507	-	9,9,9	0.12	0	8,8,8	1.09	0
4	OCT	B	505	-	7,7,7	0.23	0	6,6,6	0.54	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
4	OCT	A	508	-	-	1/5/5/5	-
2	HEX	B	509	-	-	1/3/3/3	-
3	D10	B	506	-	-	2/7/7/7	-
4	OCT	A	510	-	-	3/5/5/5	-
4	OCT	A	509	-	-	2/5/5/5	-
2	HEX	A	504	-	-	2/3/3/3	-
3	D10	A	505	-	-	2/7/7/7	-
2	HEX	A	503	-	-	1/3/3/3	-
4	OCT	B	503	-	-	2/5/5/5	-
3	D10	A	506	-	-	2/7/7/7	-
2	HEX	A	501	-	-	1/3/3/3	-
2	HEX	B	502	-	-	0/3/3/3	-
2	HEX	B	508	-	-	1/3/3/3	-
3	D10	B	501	-	-	1/7/7/7	-
2	HEX	A	513	-	-	0/3/3/3	-
3	D10	A	512	-	-	1/7/7/7	-
4	OCT	B	504	-	-	0/5/5/5	-
2	HEX	A	514	-	-	0/3/3/3	-
2	HEX	B	510	-	-	1/3/3/3	-
2	HEX	A	502	-	-	1/3/3/3	-
3	D10	A	511	-	-	2/7/7/7	-
3	D10	A	507	-	-	0/7/7/7	-
3	D10	B	507	-	-	0/7/7/7	-
4	OCT	B	505	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	506	D10	C2-C3-C4-C5
3	A	506	D10	C3-C4-C5-C6
2	A	504	HEX	C2-C3-C4-C5
3	A	505	D10	C5-C6-C7-C8
2	A	502	HEX	C2-C3-C4-C5
4	A	509	OCT	C2-C3-C4-C5
2	A	503	HEX	C2-C3-C4-C5
4	B	503	OCT	C4-C5-C6-C7
4	B	503	OCT	C1-C2-C3-C4
3	B	506	D10	C6-C7-C8-C9
2	B	510	HEX	C1-C2-C3-C4
2	B	508	HEX	C3-C4-C5-C6
4	A	510	OCT	C3-C4-C5-C6
3	A	511	D10	C5-C6-C7-C8
3	A	512	D10	C2-C3-C4-C5
3	A	511	D10	C7-C8-C9-C10
4	A	510	OCT	C5-C6-C7-C8
2	A	504	HEX	C3-C4-C5-C6
4	A	510	OCT	C1-C2-C3-C4
4	A	509	OCT	C1-C2-C3-C4
2	A	501	HEX	C3-C4-C5-C6
3	B	501	D10	C2-C3-C4-C5
4	A	508	OCT	C3-C4-C5-C6
3	A	506	D10	C6-C7-C8-C9
3	A	505	D10	C6-C7-C8-C9
2	B	509	HEX	C2-C3-C4-C5

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.

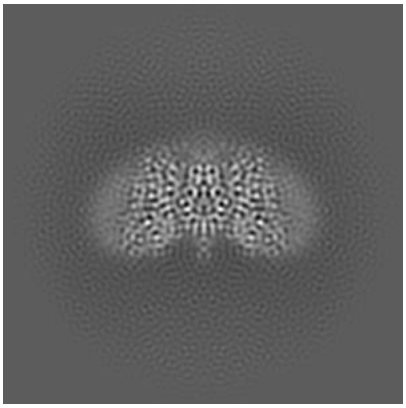
5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

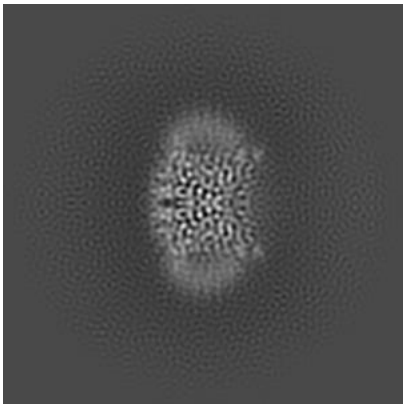
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21902. These are intended to permit visual inspection of the internal detail of the map and identification of artifacts.

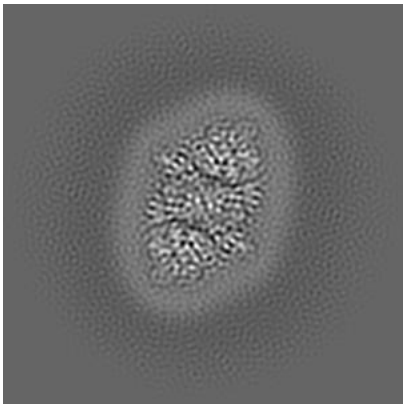
6.1 Orthogonal projections



X



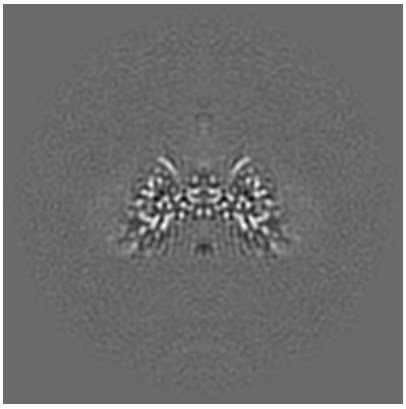
Y



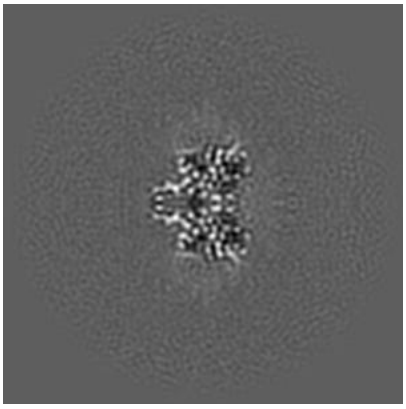
Z

The images above show the map projected in three orthogonal projections, in greyscale.

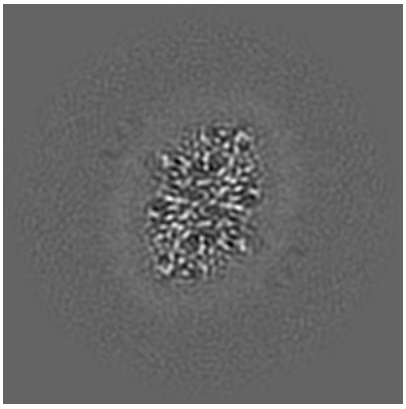
6.2 Central slices



X



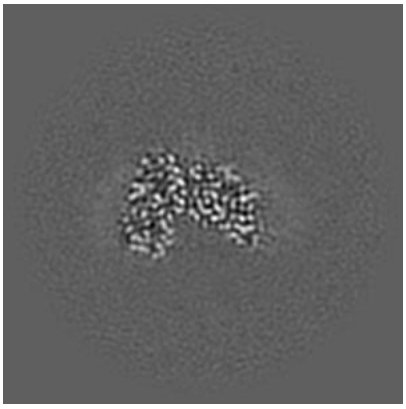
Y



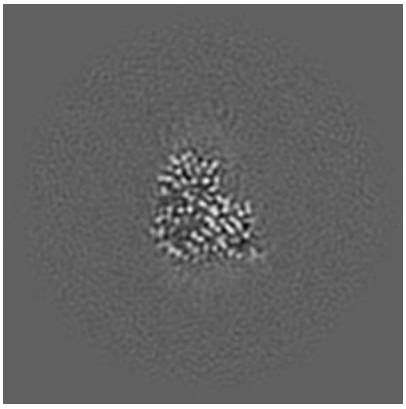
Z

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

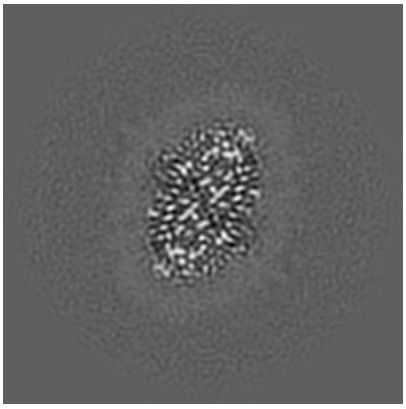
6.3 Largest variance slices (i)



X Index: 85



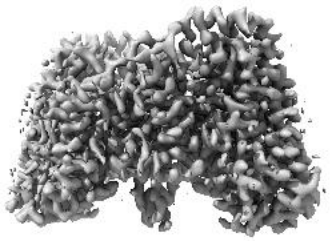
Y Index: 78



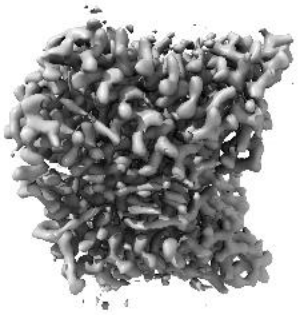
Z Index: 99

The images above show the highest variance slices of the map in three orthogonal directions, in greyscale.

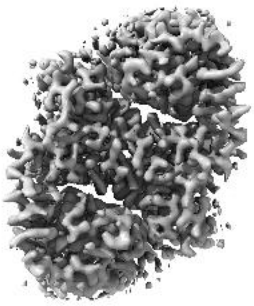
6.4 Orthogonal surface views (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.48. This in conjunction with the slice images can indicate whether an appropriate contour level has been selected.

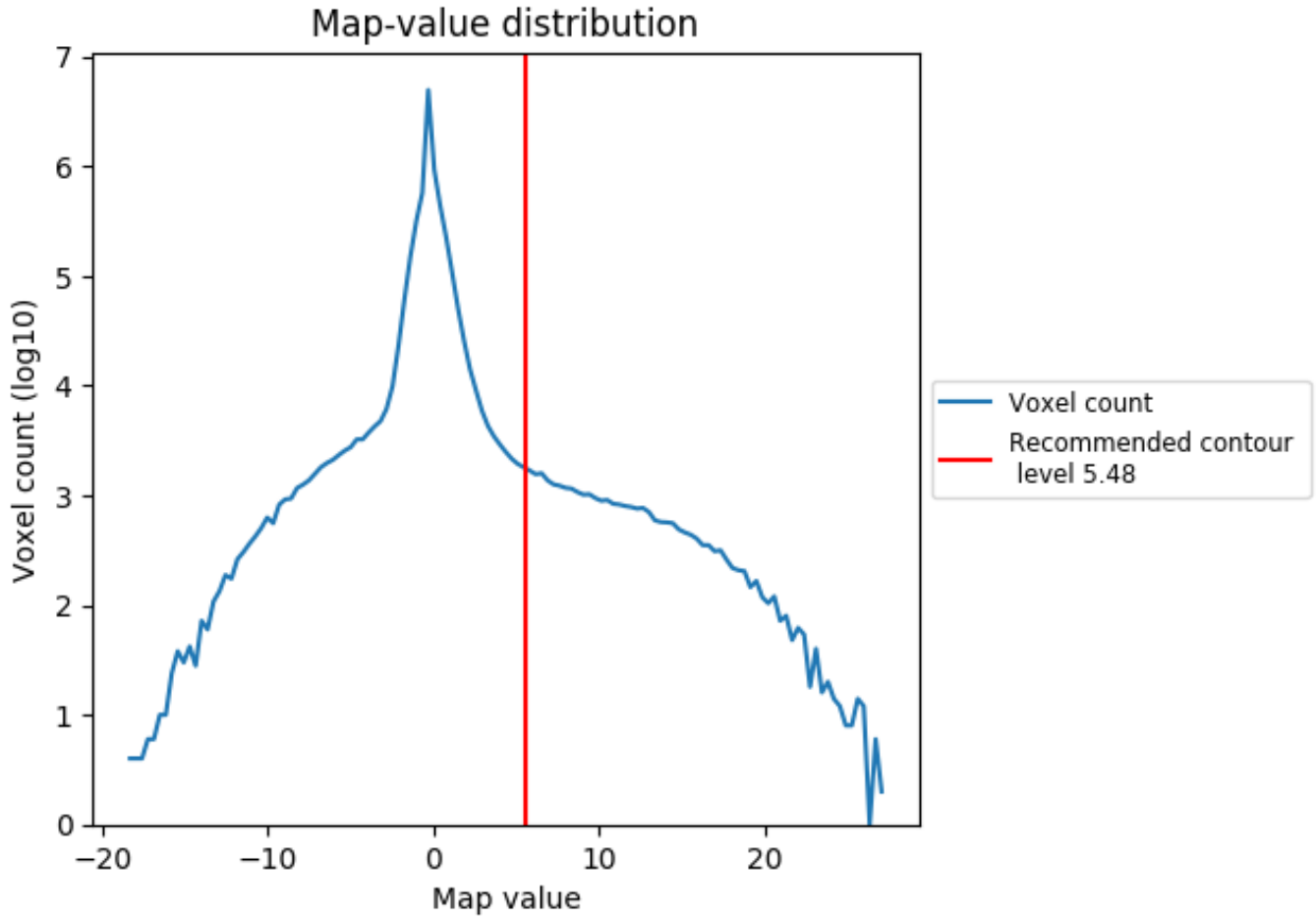
6.5 Mask visualisation (i)

This section was not generated. No masks were provided.

7 Map analysis

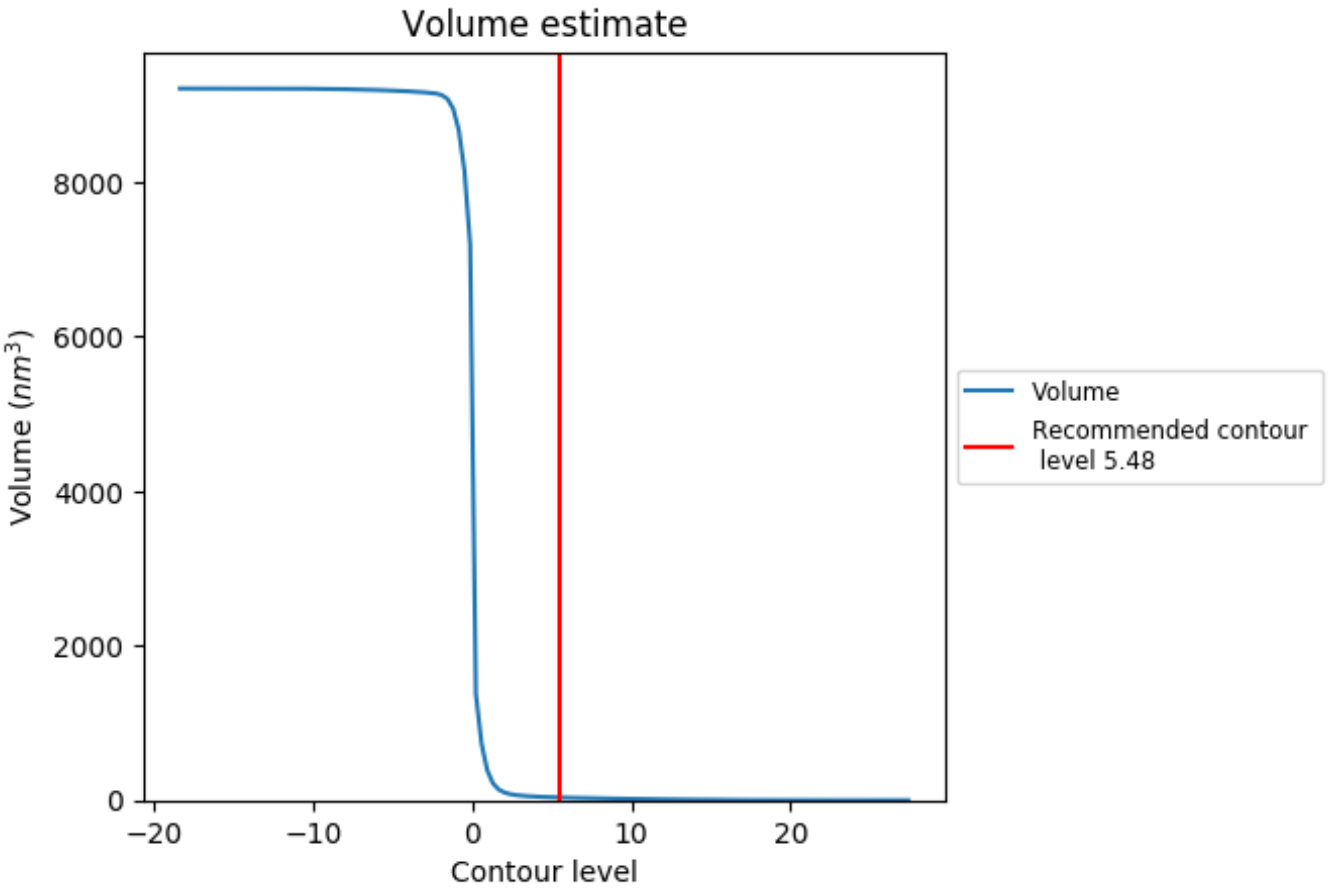
This section contains the results of statistical analysis of the map.

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.

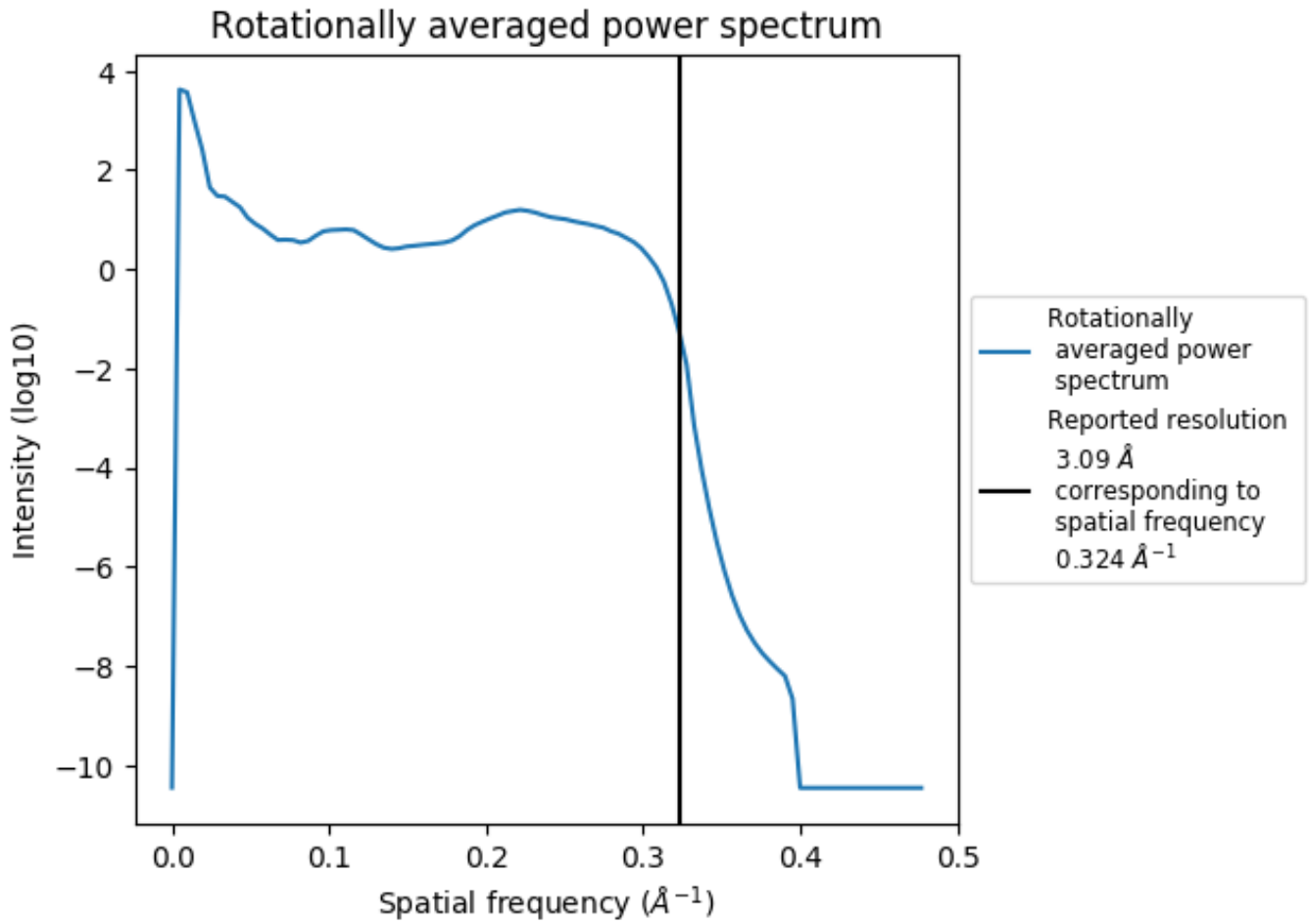
7.2 Volume estimate



The volume at the recommended contour level is 36 nm^3; this corresponds to an approximate mass of 33 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)



8 Fourier-Shell correlation

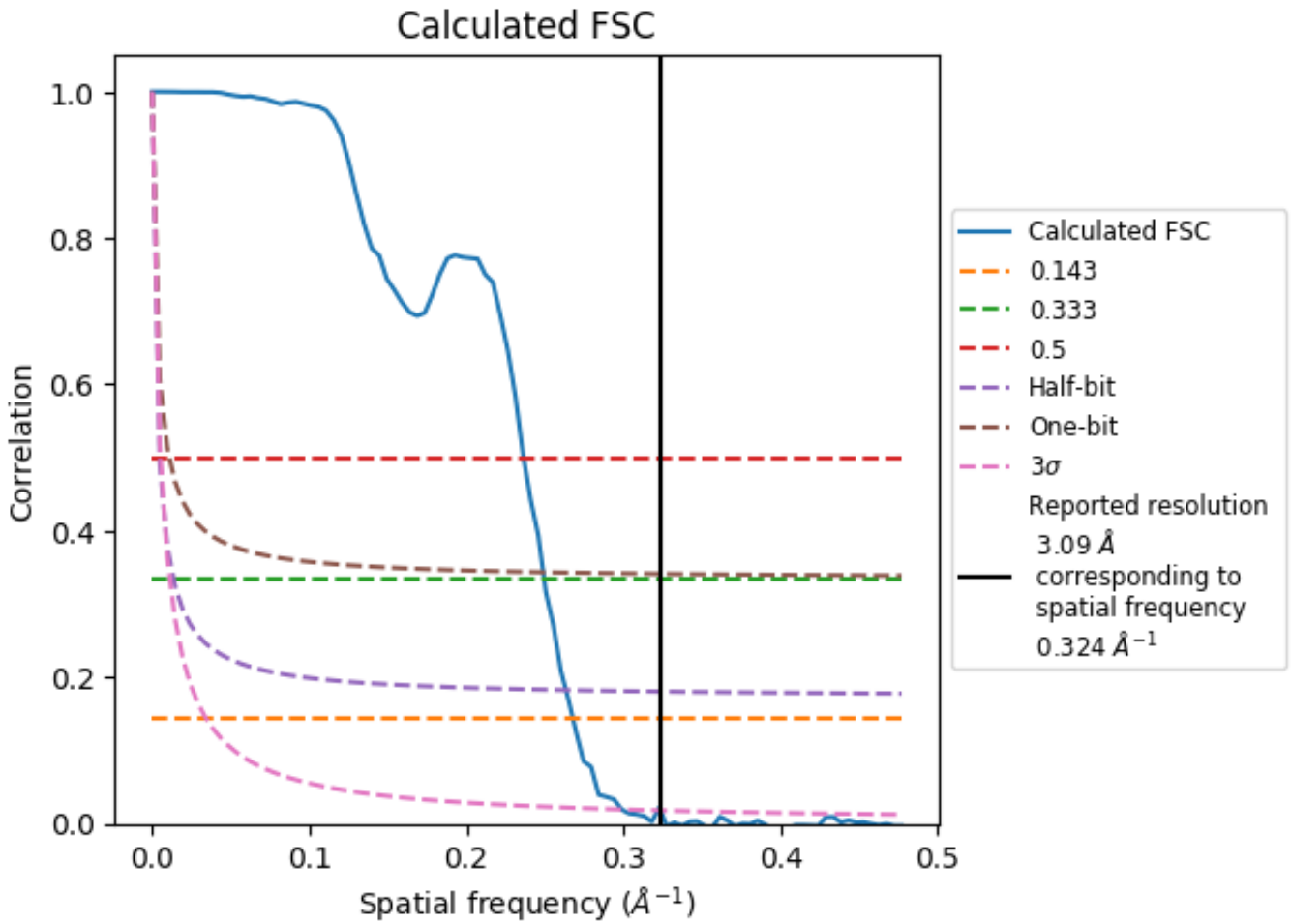
Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution for single-particle and subtomogram-averaging methods. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. Curves are displayed for 3σ, 1-bit and 1/2-bit in addition to lines showing the 0.143 gold standard cut-off, 0.333 cut-off and legacy 0.5 cut-off.

8.1 Resolution estimates

These are global values for the map.

Source	Criterion	Resolution estimate (Å)
Reported value	FSC 0.143 CUT-OFF	3.09
Calculated FSC	FSC 0.5 CUT-OFF	4.23
Calculated FSC	FSC 1 BIT CUT-OFF	4.10
Calculated FSC	FSC 0.33 CUT-OFF	4.01
Calculated FSC	FSC 1/2 BIT CUT-OFF	3.87
Calculated FSC	FSC 0.143 CUT-OFF	3.73
Calculated FSC	FSC 3 SIGMA CUT-OFF	3.40

8.2 Calculated FSC (i)



This FSC information has been calculated from the half-maps provided by the depositor. As we request un-masked, un-processed half-maps the curve may be significantly different to the author-provided FSC.

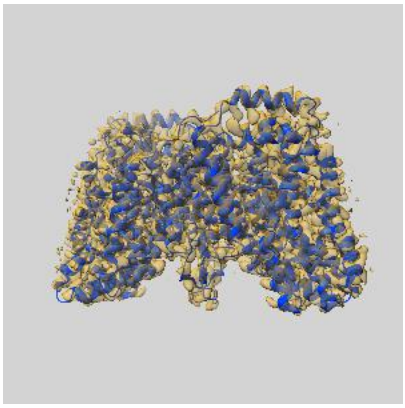
8.3 Author-provided FSC (i)

This section was not generated. The author did not provide an FSC file.

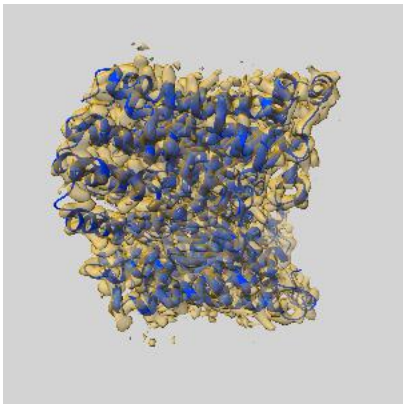
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21902 and PDB model 6WU1. Per-residue inclusion information can be found in section 3 on page 8.

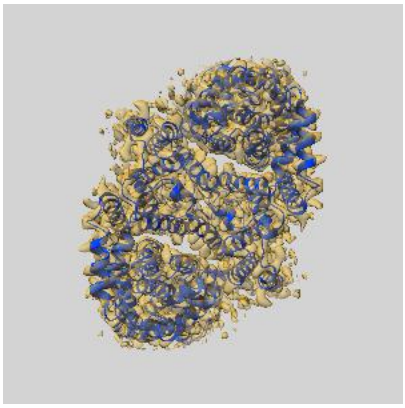
9.1 Map-model overlay



X



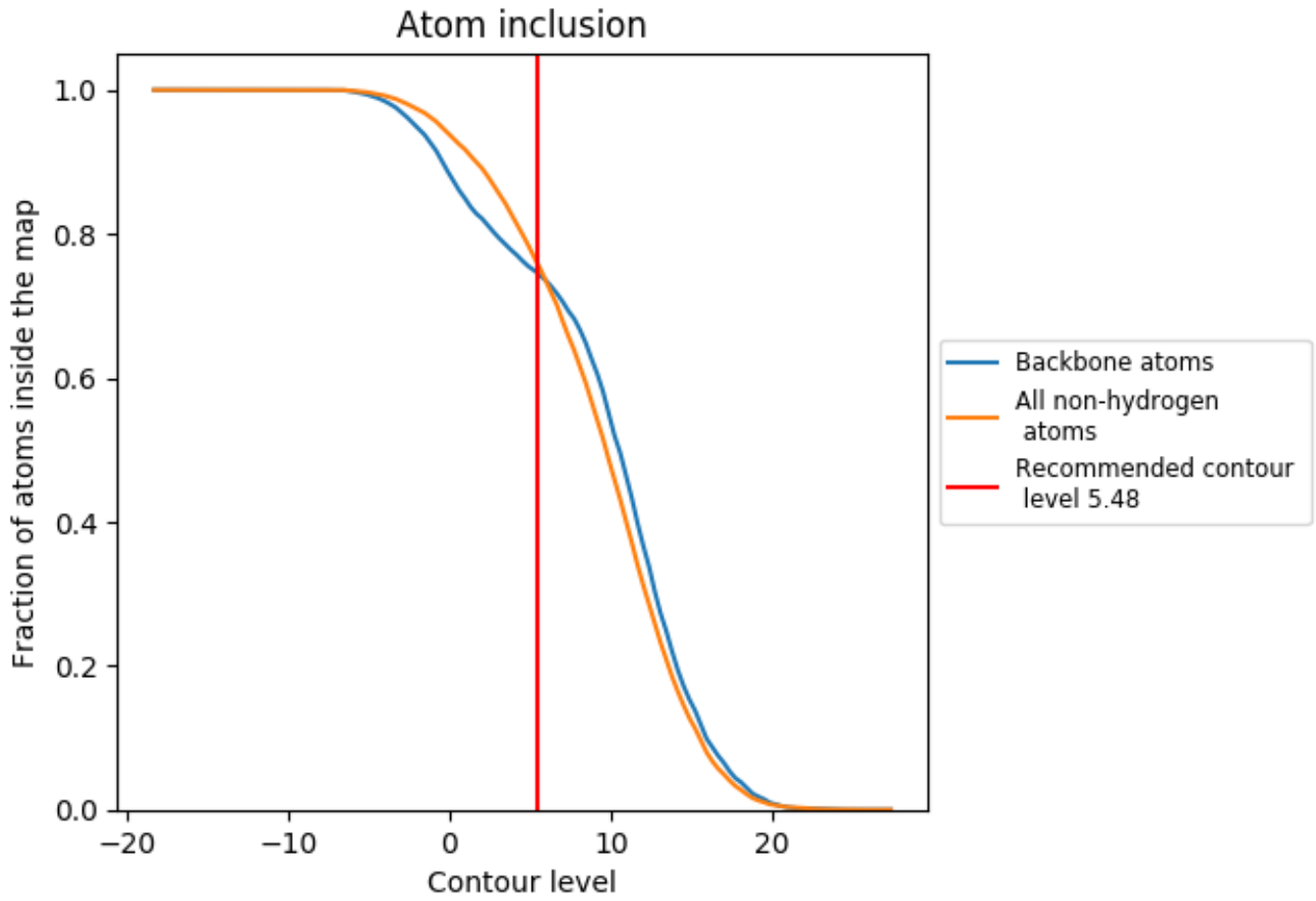
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.48 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.