Full wwPDB EM Validation Report (i)

Mar 28, 2023 – 10:12 AM EDT

PDB ID	:	8F7C
EMDB ID	:	EMD-28902
Title	:	Cryo-EM structure of human pannexin 2
Authors	:	He, Z.; Yuan, P.
Deposited on	:	2022-11-18
Resolution	:	3.92 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 (i) symbol.

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

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

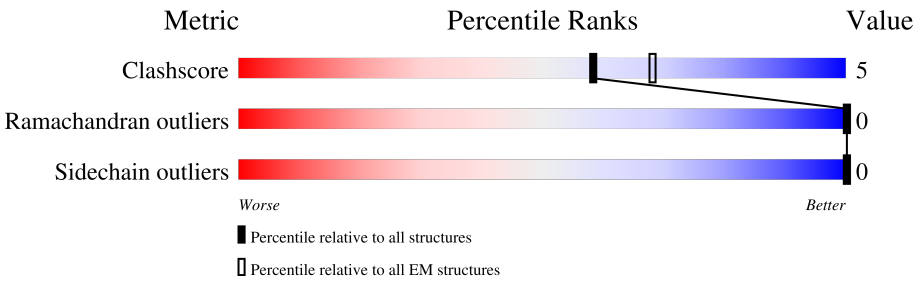
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.92 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 of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	13% 53% 6% 41%
1	B	487	13% 51% 8% 41%
1	C	487	13% 52% 7% 41%
1	D	487	13% 52% 7% 41%
1	E	487	13% 53% 6% 41%
1	F	487	13% 53% 6% 41%
1	G	487	13% 53% 6% 41%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15925 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 Pannexin-2, Soluble cytochrome b562 fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	287	2275	1489	388	387	11	0	0
1	B	287	2275	1489	388	387	11	0	0
1	C	287	2275	1489	388	387	11	0	0
1	D	287	2275	1489	388	387	11	0	0
1	E	287	2275	1489	388	387	11	0	0
1	F	287	2275	1489	388	387	11	0	0
1	G	287	2275	1489	388	387	11	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	TRP	MET	conflict	UNP P0ABE7
A	474	ILE	HIS	conflict	UNP P0ABE7
A	478	LEU	-	expression tag	UNP P0ABE7
A	479	SER	-	expression tag	UNP P0ABE7
A	480	ASN	-	expression tag	UNP P0ABE7
A	481	SER	-	expression tag	UNP P0ABE7
A	482	LEU	-	expression tag	UNP P0ABE7
A	483	GLU	-	expression tag	UNP P0ABE7
A	484	VAL	-	expression tag	UNP P0ABE7
A	485	LEU	-	expression tag	UNP P0ABE7
A	486	PHE	-	expression tag	UNP P0ABE7
A	487	GLN	-	expression tag	UNP P0ABE7
B	379	TRP	MET	conflict	UNP P0ABE7
B	474	ILE	HIS	conflict	UNP P0ABE7
B	478	LEU	-	expression tag	UNP P0ABE7
B	479	SER	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	480	ASN	-	expression tag	UNP P0ABE7
B	481	SER	-	expression tag	UNP P0ABE7
B	482	LEU	-	expression tag	UNP P0ABE7
B	483	GLU	-	expression tag	UNP P0ABE7
B	484	VAL	-	expression tag	UNP P0ABE7
B	485	LEU	-	expression tag	UNP P0ABE7
B	486	PHE	-	expression tag	UNP P0ABE7
B	487	GLN	-	expression tag	UNP P0ABE7
C	379	TRP	MET	conflict	UNP P0ABE7
C	474	ILE	HIS	conflict	UNP P0ABE7
C	478	LEU	-	expression tag	UNP P0ABE7
C	479	SER	-	expression tag	UNP P0ABE7
C	480	ASN	-	expression tag	UNP P0ABE7
C	481	SER	-	expression tag	UNP P0ABE7
C	482	LEU	-	expression tag	UNP P0ABE7
C	483	GLU	-	expression tag	UNP P0ABE7
C	484	VAL	-	expression tag	UNP P0ABE7
C	485	LEU	-	expression tag	UNP P0ABE7
C	486	PHE	-	expression tag	UNP P0ABE7
C	487	GLN	-	expression tag	UNP P0ABE7
D	379	TRP	MET	conflict	UNP P0ABE7
D	474	ILE	HIS	conflict	UNP P0ABE7
D	478	LEU	-	expression tag	UNP P0ABE7
D	479	SER	-	expression tag	UNP P0ABE7
D	480	ASN	-	expression tag	UNP P0ABE7
D	481	SER	-	expression tag	UNP P0ABE7
D	482	LEU	-	expression tag	UNP P0ABE7
D	483	GLU	-	expression tag	UNP P0ABE7
D	484	VAL	-	expression tag	UNP P0ABE7
D	485	LEU	-	expression tag	UNP P0ABE7
D	486	PHE	-	expression tag	UNP P0ABE7
D	487	GLN	-	expression tag	UNP P0ABE7
E	379	TRP	MET	conflict	UNP P0ABE7
E	474	ILE	HIS	conflict	UNP P0ABE7
E	478	LEU	-	expression tag	UNP P0ABE7
E	479	SER	-	expression tag	UNP P0ABE7
E	480	ASN	-	expression tag	UNP P0ABE7
E	481	SER	-	expression tag	UNP P0ABE7
E	482	LEU	-	expression tag	UNP P0ABE7
E	483	GLU	-	expression tag	UNP P0ABE7
E	484	VAL	-	expression tag	UNP P0ABE7
E	485	LEU	-	expression tag	UNP P0ABE7

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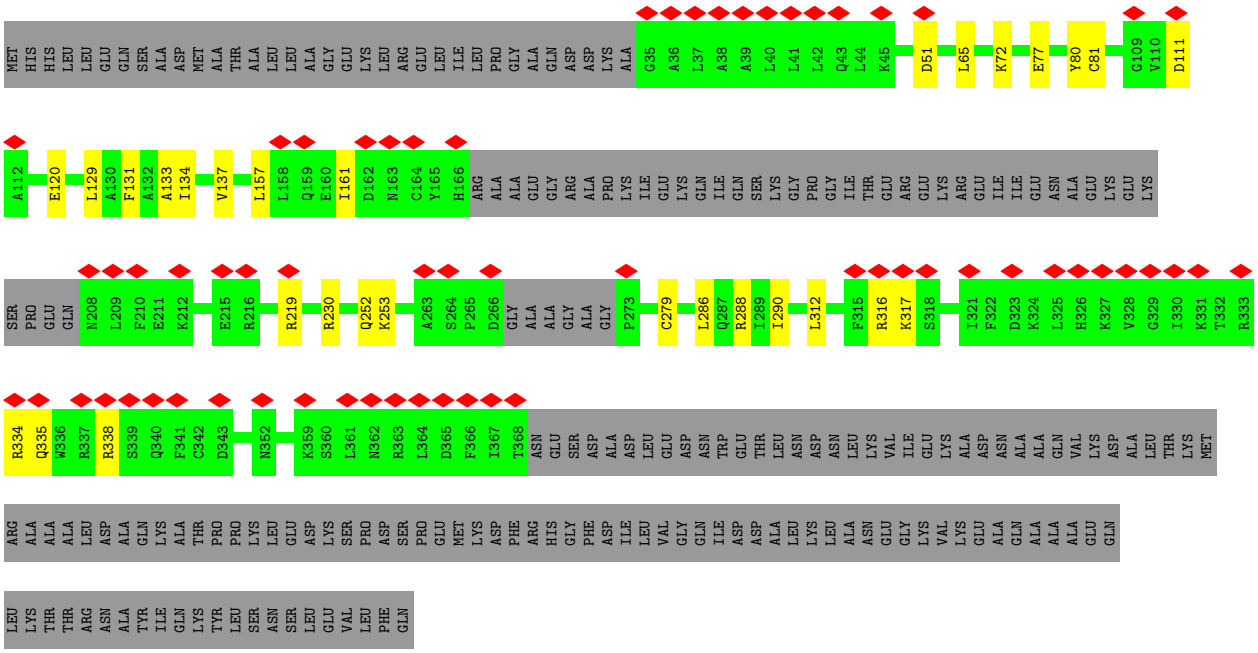
Chain	Residue	Modelled	Actual	Comment	Reference
E	486	PHE	-	expression tag	UNP P0ABE7
E	487	GLN	-	expression tag	UNP P0ABE7
F	379	TRP	MET	conflict	UNP P0ABE7
F	474	ILE	HIS	conflict	UNP P0ABE7
F	478	LEU	-	expression tag	UNP P0ABE7
F	479	SER	-	expression tag	UNP P0ABE7
F	480	ASN	-	expression tag	UNP P0ABE7
F	481	SER	-	expression tag	UNP P0ABE7
F	482	LEU	-	expression tag	UNP P0ABE7
F	483	GLU	-	expression tag	UNP P0ABE7
F	484	VAL	-	expression tag	UNP P0ABE7
F	485	LEU	-	expression tag	UNP P0ABE7
F	486	PHE	-	expression tag	UNP P0ABE7
F	487	GLN	-	expression tag	UNP P0ABE7
G	379	TRP	MET	conflict	UNP P0ABE7
G	474	ILE	HIS	conflict	UNP P0ABE7
G	478	LEU	-	expression tag	UNP P0ABE7
G	479	SER	-	expression tag	UNP P0ABE7
G	480	ASN	-	expression tag	UNP P0ABE7
G	481	SER	-	expression tag	UNP P0ABE7
G	482	LEU	-	expression tag	UNP P0ABE7
G	483	GLU	-	expression tag	UNP P0ABE7
G	484	VAL	-	expression tag	UNP P0ABE7
G	485	LEU	-	expression tag	UNP P0ABE7
G	486	PHE	-	expression tag	UNP P0ABE7
G	487	GLN	-	expression tag	UNP P0ABE7

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

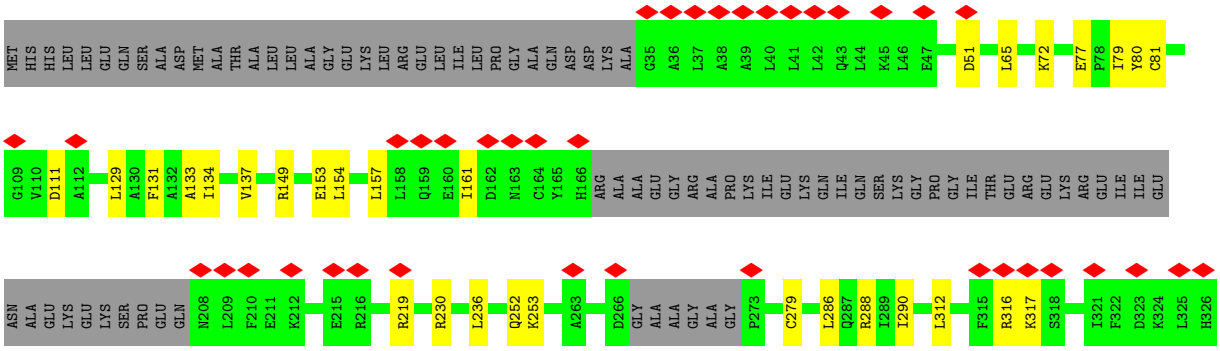
• Molecule 1: Pannexin-2, Soluble cytochrome b562 fusion

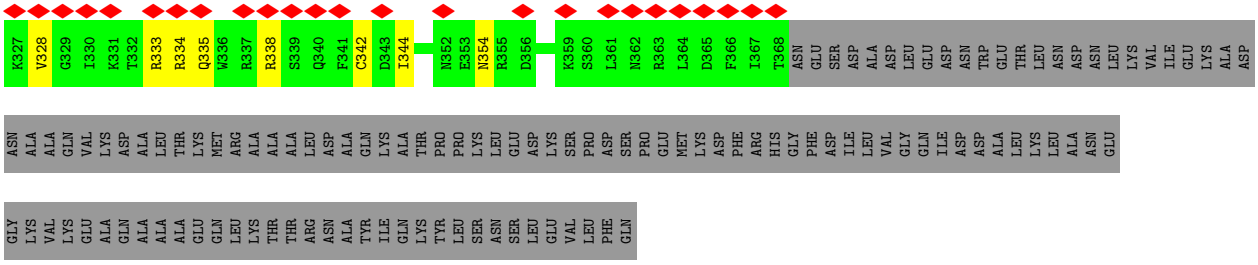
Chain A:



• Molecule 1: Pannexin-2, Soluble cytochrome b562 fusion

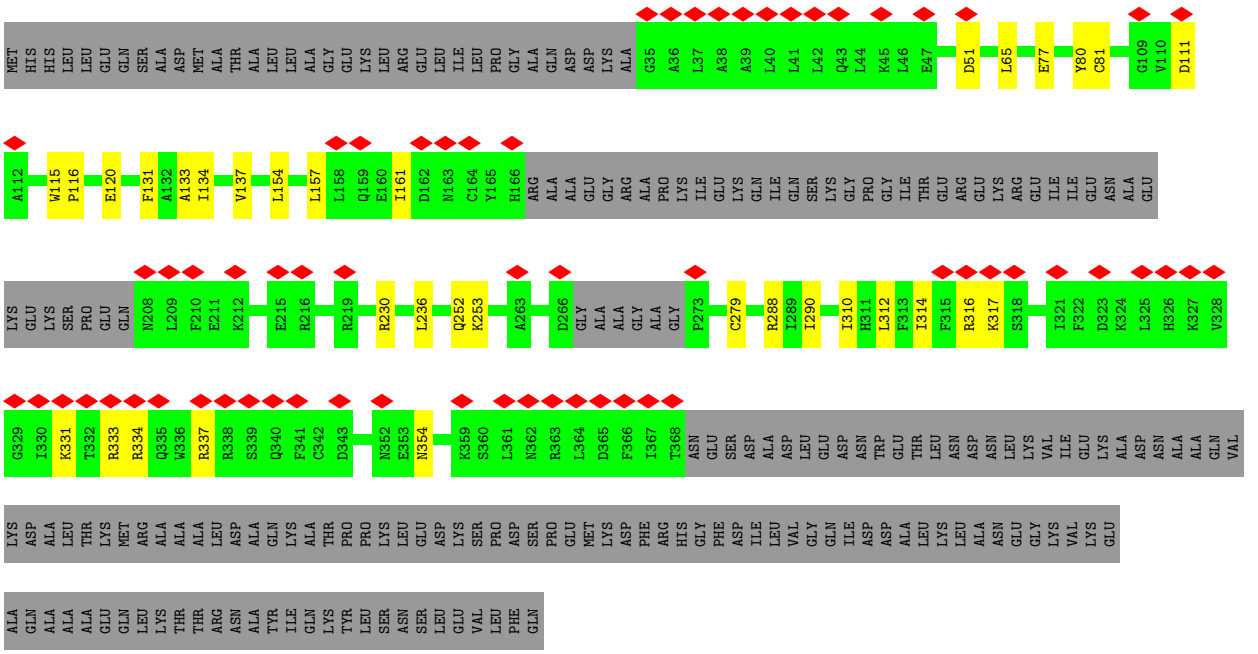
Chain B:





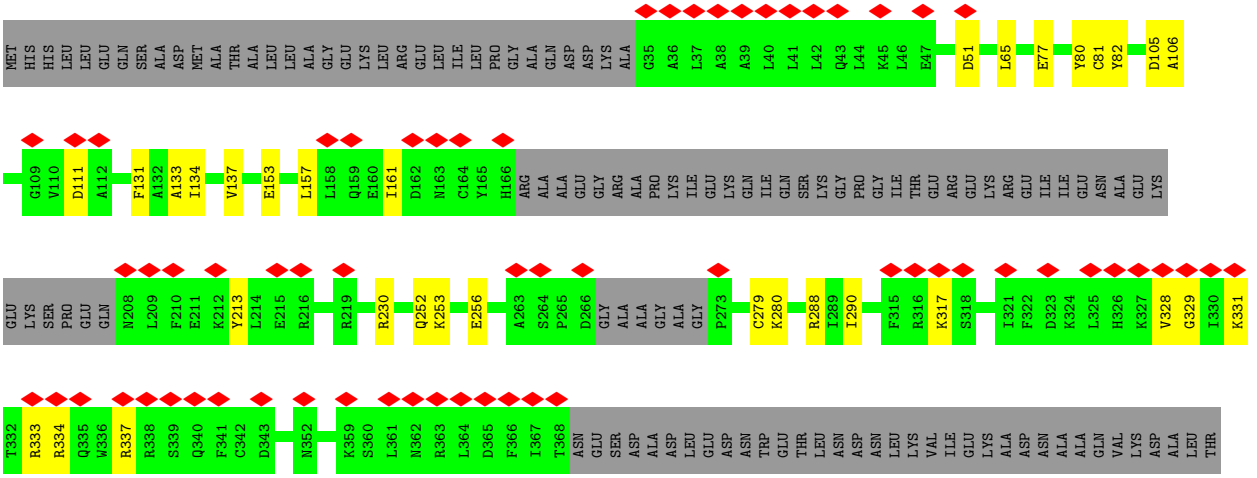
• Molecule 1: Pannexin-2, Soluble cytochrome b562 fusion

Chain C:



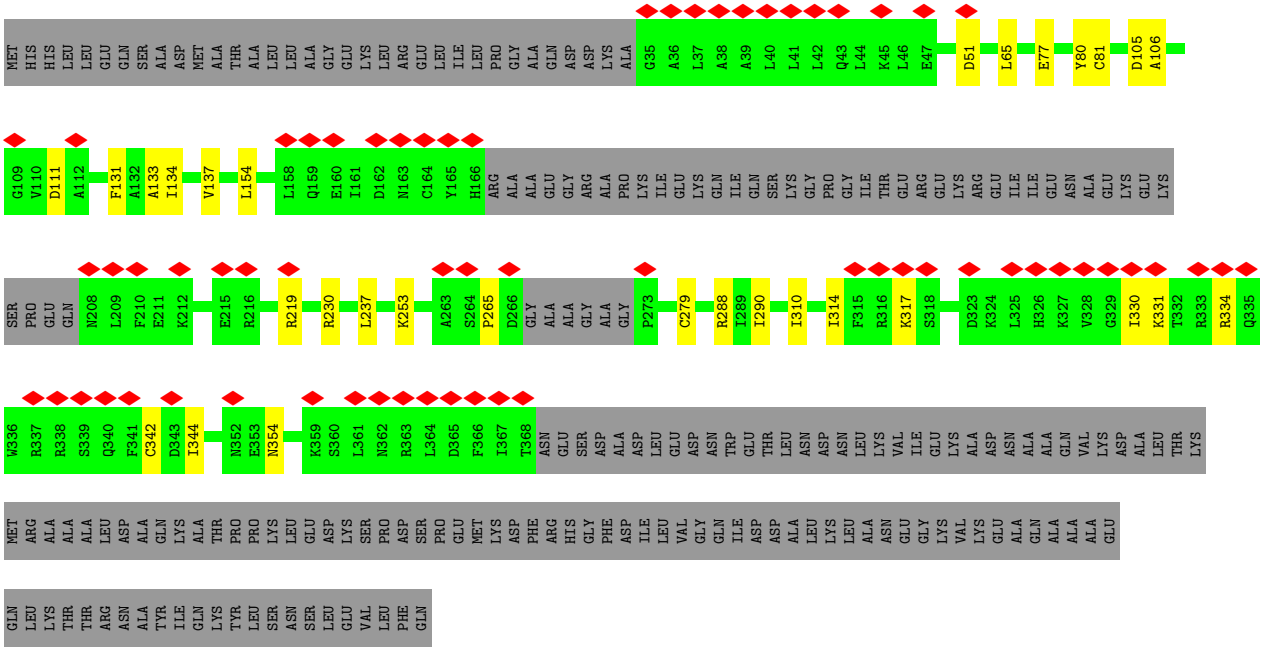
• Molecule 1: Pannexin-2, Soluble cytochrome b562 fusion

Chain D:



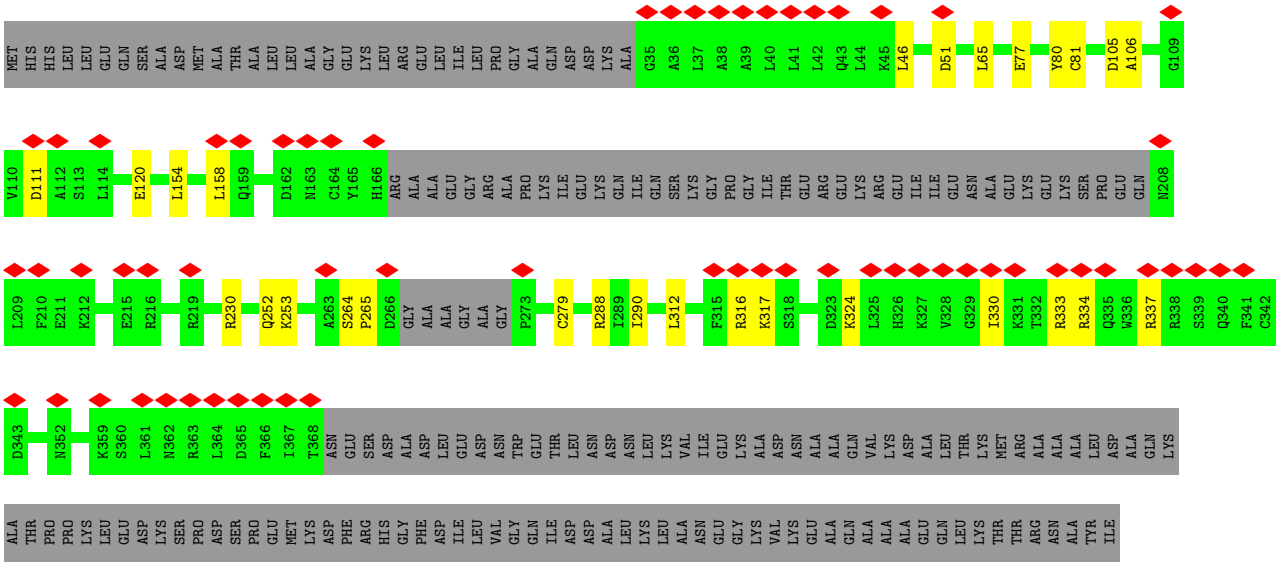
• Molecule 1: Pannexin-2, Soluble cytochrome b562 fusion

Chain E:



• Molecule 1: Pannexin-2, Soluble cytochrome b562 fusion

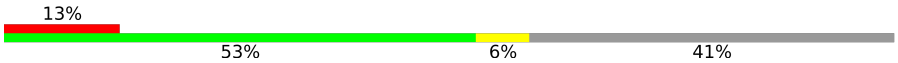
Chain F:



GLN LYS TYR LEU SER ASN SER LEU GLU VAL LEU PHE GLN

- Molecule 1: Pannexin-2, Soluble cytochrome b562 fusion

Chain G:



MET HIS HIS LEU LEU GLU GLN SER ALA ASP MET ALA THR ALA LEU LEU ALA GLY GLU LYS LEU ARG GLU LEU ILE LEU PRO GLY ALA GLN ASP ASP LYS ALA G35 A36 L37 A38 A39 L40 L41 L42 Q43 L44 K45 L46 E47 D51 L65 K72 D105 A106 G109 V110 D111

A112 F131 A132 A133 I134 V137 L154 L157 L158 Q159 E160 I161 D162 N163 C164 Y165 H166 ARG ALA ALA GLU GLY ARG ALA PRO LYS ILE GLU LYS GLN ILE GLN SER LYS GLY PRO GLY ILE THR GLU ARG GLU LYS ARG GLU ILE ILE GLU ASN ALA GLU LYS GLU LYS SER PRO

GLU GLN N208 L209 F210 E211 K212 E215 R216 R219 R230 L236 K253 A263 D266 GLY ALA ALA GLY ALA GLY P273 L286 Q287 R288 I289 I290 L312 F315 R316 K317 S318 I321 F322 D323 K324 L325 H326 K327 V328 G329 I330 K331 T332 R333 R334 Q335 W336 R337

R338 S339 Q340 F341 C342 D343 N352 E353 N354 R355 D356 K359 S360 L361 N362 R363 L364 D365 F366 I367 T368 ASN GLU SER ASP ALA ASP LEU GLU ASP ASN TRP GLU THR LEU ASN ASP ASN LEU LYS VAL ILE GLU LYS ALA ASP ASN ALA ALA GLN VAL LYS ASP ALA LEU THR LYS MET

ARG ALA ALA ALA LEU ASP ALA GLN LYS ALA THR PRO PRO LYS LEU GLU ASP LYS SER PRO ASP SER PRO GLU MET LYS ASP PHE ARG HIS GLY PHE ASP ILE LEU VAL GLY GLN ILE ASP ASP ALA LEU LYS LEU ALA ASN GLU GLY LYS VAL LYS GLU ALA GLN ALA ALA ALA GLU GLN

LEU LYS THR THR ARG ASN ALA TYR ILE GLN LYS TYR LEU SER ASN SER LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	25191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.438	Depositor
Minimum map value	-2.889	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.154	Depositor
Recommended contour level	0.86	Depositor
Map size (Å)	252.0, 252.0, 252.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	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	0/2327	0.47	0/3164
1	B	0.25	0/2327	0.47	0/3164
1	C	0.25	0/2327	0.47	0/3164
1	D	0.25	0/2327	0.48	0/3164
1	E	0.25	0/2327	0.47	0/3164
1	F	0.24	0/2327	0.48	0/3164
1	G	0.24	0/2327	0.45	0/3164
All	All	0.25	0/16289	0.47	0/22148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2275	0	2284	32	0
1	B	2275	0	2285	28	0
1	C	2275	0	2285	22	0
1	D	2275	0	2285	20	0
1	E	2275	0	2285	21	0
1	F	2275	0	2285	19	0
1	G	2275	0	2285	15	0
All	All	15925	0	15994	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (156) 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:335:GLN:CB	1:A:338:ARG:NH2	1.68	1.56
1:A:335:GLN:HB3	1:A:338:ARG:NH2	1.11	1.38
1:A:335:GLN:HA	1:A:338:ARG:NE	1.45	1.29
1:A:335:GLN:CA	1:A:338:ARG:HE	1.69	1.05
1:B:334:ARG:HD2	1:B:338:ARG:NH1	1.69	1.05
1:A:334:ARG:O	1:A:338:ARG:HG3	1.58	1.03
1:A:335:GLN:HB2	1:A:338:ARG:NH2	1.74	0.98
1:A:335:GLN:HB3	1:A:338:ARG:HH22	1.35	0.92
1:A:335:GLN:CA	1:A:338:ARG:NE	2.32	0.90
1:B:334:ARG:HD2	1:B:338:ARG:HH12	1.33	0.89
1:A:335:GLN:CA	1:A:338:ARG:NH2	2.36	0.88
1:A:81:CYS:HB3	1:A:279:CYS:HA	1.60	0.84
1:B:334:ARG:CD	1:B:338:ARG:NH1	2.42	0.82
1:A:335:GLN:HA	1:A:338:ARG:CZ	2.11	0.80
1:C:81:CYS:HB3	1:C:279:CYS:HA	1.65	0.77
1:A:335:GLN:HA	1:A:338:ARG:HE	0.74	0.76
1:F:81:CYS:HB3	1:F:279:CYS:HA	1.66	0.76
1:E:81:CYS:HB3	1:E:279:CYS:HA	1.68	0.76
1:D:77:GLU:HB2	1:D:80:TYR:HE1	1.50	0.75
1:F:77:GLU:HB2	1:F:80:TYR:HE1	1.50	0.74
1:A:335:GLN:CA	1:A:338:ARG:CZ	2.66	0.71
1:E:77:GLU:HB2	1:E:80:TYR:HE1	1.53	0.71
1:B:81:CYS:HB3	1:B:279:CYS:HA	1.72	0.71
1:B:77:GLU:HB2	1:B:80:TYR:HE1	1.57	0.70
1:D:81:CYS:HB3	1:D:279:CYS:HA	1.74	0.70
1:B:334:ARG:CD	1:B:338:ARG:HH12	2.03	0.66
1:C:77:GLU:HB2	1:C:80:TYR:HE1	1.61	0.66
1:D:253:LYS:HA	1:D:288:ARG:HH22	1.61	0.65
1:F:253:LYS:HA	1:F:288:ARG:HH22	1.60	0.65
1:F:333:ARG:HB3	1:F:337:ARG:HH22	1.63	0.64
1:B:252:GLN:O	1:B:288:ARG:NH2	2.31	0.64
1:E:253:LYS:HA	1:E:288:ARG:HH22	1.64	0.62
1:G:253:LYS:HA	1:G:288:ARG:HH22	1.64	0.62
1:D:329:GLY:O	1:D:333:ARG:NH1	2.33	0.61
1:D:65:LEU:HD23	1:D:290:ILE:HG23	1.83	0.60
1:B:334:ARG:HD2	1:B:338:ARG:CZ	2.31	0.60
1:C:65:LEU:HD23	1:C:290:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:HA	1:C:288:ARG:HH22	1.67	0.60
1:F:120:GLU:OE2	1:F:252:GLN:NE2	2.33	0.60
1:A:65:LEU:HD23	1:A:290:ILE:HG23	1.85	0.59
1:A:335:GLN:CB	1:A:338:ARG:CZ	2.70	0.59
1:C:252:GLN:O	1:C:288:ARG:NH2	2.35	0.59
1:A:253:LYS:HA	1:A:288:ARG:HH22	1.67	0.59
1:F:330:ILE:O	1:F:334:ARG:NH1	2.36	0.58
1:C:120:GLU:OE1	1:C:252:GLN:NE2	2.36	0.58
1:E:65:LEU:HD23	1:E:290:ILE:HG23	1.85	0.58
1:A:77:GLU:HB2	1:A:80:TYR:HE1	1.69	0.57
1:G:219:ARG:NH1	1:G:335:GLN:OE1	2.36	0.57
1:F:65:LEU:HD23	1:F:290:ILE:HG23	1.85	0.57
1:A:252:GLN:O	1:A:288:ARG:NH2	2.37	0.57
1:B:253:LYS:HA	1:B:288:ARG:HH22	1.68	0.57
1:A:131:PHE:HA	1:A:134:ILE:HG22	1.86	0.57
1:E:331:LYS:HA	1:E:334:ARG:HH12	1.70	0.56
1:G:65:LEU:HD23	1:G:290:ILE:HG23	1.85	0.56
1:D:131:PHE:HA	1:D:134:ILE:HG22	1.86	0.56
1:B:77:GLU:HB2	1:B:80:TYR:CE1	2.40	0.56
1:A:219:ARG:NH1	1:A:335:GLN:OE1	2.39	0.56
1:E:51:ASP:OD1	1:E:230:ARG:NH1	2.39	0.56
1:D:333:ARG:HB3	1:D:337:ARG:HH22	1.71	0.55
1:D:51:ASP:OD1	1:D:230:ARG:NH1	2.39	0.55
1:E:131:PHE:HA	1:E:134:ILE:HG22	1.88	0.55
1:B:157:LEU:O	1:B:161:ILE:HG12	2.06	0.55
1:C:131:PHE:HA	1:C:134:ILE:HG22	1.87	0.55
1:G:331:LYS:HA	1:G:334:ARG:HH12	1.72	0.54
1:E:342:CYS:SG	1:E:344:ILE:HG22	2.48	0.54
1:B:65:LEU:HD23	1:B:290:ILE:HG23	1.89	0.54
1:A:77:GLU:HB2	1:A:80:TYR:CE1	2.43	0.54
1:G:131:PHE:HA	1:G:134:ILE:HG22	1.90	0.54
1:A:120:GLU:OE1	1:A:252:GLN:NE2	2.42	0.53
1:B:131:PHE:HA	1:B:134:ILE:HG22	1.88	0.53
1:E:81:CYS:CB	1:E:279:CYS:HA	2.38	0.53
1:B:219:ARG:NH1	1:B:335:GLN:OE1	2.41	0.53
1:B:51:ASP:OD1	1:B:230:ARG:NH1	2.41	0.52
1:F:154:LEU:HG	1:F:158:LEU:HD13	1.92	0.52
1:E:154:LEU:HD21	1:E:354:ASN:HD22	1.75	0.52
1:B:81:CYS:CB	1:B:279:CYS:HA	2.39	0.52
1:A:51:ASP:OD1	1:A:230:ARG:NH1	2.42	0.52
1:C:51:ASP:OD1	1:C:230:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:GLN:O	1:F:288:ARG:NH2	2.42	0.52
1:A:157:LEU:O	1:A:161:ILE:HG12	2.10	0.51
1:G:51:ASP:OD2	1:G:230:ARG:NH1	2.43	0.51
1:D:153:GLU:OE2	1:D:213:TYR:OH	2.24	0.51
1:D:157:LEU:O	1:D:161:ILE:HG12	2.11	0.51
1:C:157:LEU:O	1:C:161:ILE:HG12	2.10	0.51
1:F:51:ASP:OD1	1:F:230:ARG:NH1	2.43	0.50
1:D:81:CYS:CB	1:D:279:CYS:HA	2.40	0.50
1:C:331:LYS:HA	1:C:334:ARG:NH1	2.28	0.49
1:G:157:LEU:O	1:G:161:ILE:HG12	2.12	0.49
1:A:133:ALA:O	1:A:137:VAL:HG23	2.12	0.49
1:A:81:CYS:CB	1:A:279:CYS:HA	2.38	0.49
1:B:133:ALA:O	1:B:137:VAL:HG23	2.13	0.48
1:G:133:ALA:O	1:G:137:VAL:HG23	2.13	0.48
1:C:77:GLU:HB2	1:C:80:TYR:CE1	2.44	0.48
1:B:342:CYS:SG	1:B:344:ILE:HG22	2.52	0.48
1:D:133:ALA:O	1:D:137:VAL:HG23	2.13	0.48
1:E:105:ASP:OD1	1:E:106:ALA:N	2.44	0.48
1:E:77:GLU:HB2	1:E:80:TYR:CE1	2.42	0.48
1:G:105:ASP:OD1	1:G:106:ALA:N	2.44	0.48
1:B:149:ARG:O	1:B:153:GLU:HG2	2.14	0.48
1:E:133:ALA:O	1:E:137:VAL:HG23	2.14	0.48
1:C:133:ALA:O	1:C:137:VAL:HG23	2.14	0.47
1:G:72:LYS:HG2	1:G:286:LEU:HD22	1.96	0.47
1:C:331:LYS:HA	1:C:334:ARG:HH12	1.80	0.47
1:B:154:LEU:HD21	1:B:354:ASN:HD22	1.79	0.47
1:D:252:GLN:O	1:D:288:ARG:NH2	2.48	0.46
1:F:330:ILE:HB	1:F:334:ARG:HH12	1.81	0.45
1:D:328:VAL:HG23	1:D:333:ARG:NH1	2.32	0.45
1:F:105:ASP:OD1	1:F:106:ALA:N	2.45	0.45
1:D:331:LYS:HA	1:D:334:ARG:HH22	1.82	0.45
1:E:219:ARG:NE	1:E:219:ARG:HA	2.32	0.45
1:F:81:CYS:CB	1:F:279:CYS:HA	2.40	0.45
1:C:154:LEU:HD21	1:C:354:ASN:HD22	1.81	0.45
1:B:317:LYS:HA	1:B:317:LYS:HE2	1.99	0.45
1:D:111:ASP:N	1:D:111:ASP:OD1	2.50	0.45
1:A:111:ASP:N	1:A:111:ASP:OD1	2.50	0.45
1:B:72:LYS:HG2	1:B:286:LEU:HD22	1.99	0.45
1:B:111:ASP:OD1	1:B:111:ASP:N	2.50	0.44
1:C:111:ASP:N	1:C:111:ASP:OD1	2.50	0.44
1:A:72:LYS:HG2	1:A:286:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HA	1:A:317:LYS:HE2	2.00	0.44
1:A:334:ARG:O	1:A:338:ARG:CG	2.46	0.44
1:F:324:LYS:HD3	1:F:324:LYS:HA	1.77	0.44
1:G:312:LEU:HD12	1:G:316:ARG:HE	1.83	0.44
1:G:317:LYS:HA	1:G:317:LYS:HE2	1.99	0.44
1:C:81:CYS:CB	1:C:279:CYS:HA	2.41	0.44
1:C:317:LYS:HA	1:C:317:LYS:HE2	2.00	0.44
1:G:111:ASP:N	1:G:111:ASP:OD1	2.50	0.44
1:G:236:LEU:HD23	1:G:236:LEU:HA	1.86	0.44
1:D:82:TYR:CE2	1:E:265:PRO:HG2	2.53	0.43
1:F:111:ASP:OD1	1:F:111:ASP:N	2.50	0.43
1:F:317:LYS:HA	1:F:317:LYS:HE2	1.99	0.43
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.90	0.43
1:C:333:ARG:O	1:C:337:ARG:NH1	2.52	0.43
1:B:79:ILE:HD11	1:B:279:CYS:HB3	2.01	0.43
1:D:256:GLU:HG2	1:D:280:LYS:HD2	2.01	0.43
1:A:312:LEU:HD12	1:A:316:ARG:HE	1.83	0.43
1:B:328:VAL:HB	1:B:333:ARG:HH22	1.84	0.43
1:E:310:ILE:HG23	1:E:314:ILE:HD12	2.01	0.42
1:E:317:LYS:HA	1:E:317:LYS:HE2	2.00	0.42
1:D:317:LYS:HE2	1:D:317:LYS:HA	2.00	0.42
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.86	0.42
1:B:312:LEU:HD12	1:B:316:ARG:HE	1.85	0.42
1:G:154:LEU:HD21	1:G:354:ASN:HD22	1.84	0.42
1:A:129:LEU:HD12	1:A:129:LEU:HA	1.90	0.42
1:C:312:LEU:HD12	1:C:316:ARG:HE	1.85	0.42
1:F:312:LEU:HD12	1:F:316:ARG:HE	1.85	0.41
1:C:236:LEU:HD23	1:C:236:LEU:HA	1.87	0.41
1:E:331:LYS:HA	1:E:334:ARG:NH1	2.33	0.41
1:F:264:SER:N	1:F:265:PRO:HD3	2.36	0.41
1:C:310:ILE:HG23	1:C:314:ILE:HD12	2.02	0.41
1:E:111:ASP:N	1:E:111:ASP:OD1	2.50	0.41
1:C:115:TRP:HA	1:C:116:PRO:HD3	1.98	0.41
1:E:237:LEU:HD23	1:E:237:LEU:HA	1.91	0.41
1:F:46:LEU:HG	1:F:46:LEU:O	2.21	0.40
1:E:330:ILE:O	1:E:334:ARG:NH2	2.54	0.40
1:D:105:ASP:OD1	1:D:106:ALA:N	2.43	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	281/487 (58%)	272 (97%)	9 (3%)	0	100	100
1	B	281/487 (58%)	271 (96%)	10 (4%)	0	100	100
1	C	281/487 (58%)	273 (97%)	8 (3%)	0	100	100
1	D	281/487 (58%)	270 (96%)	11 (4%)	0	100	100
1	E	281/487 (58%)	271 (96%)	10 (4%)	0	100	100
1	F	281/487 (58%)	273 (97%)	8 (3%)	0	100	100
1	G	281/487 (58%)	274 (98%)	7 (2%)	0	100	100
All	All	1967/3409 (58%)	1904 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/414 (58%)	239 (100%)	0	100	100
1	B	239/414 (58%)	239 (100%)	0	100	100
1	C	239/414 (58%)	239 (100%)	0	100	100
1	D	239/414 (58%)	239 (100%)	0	100	100
1	E	239/414 (58%)	239 (100%)	0	100	100
1	F	239/414 (58%)	239 (100%)	0	100	100
1	G	239/414 (58%)	239 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1673/2898 (58%)	1673 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

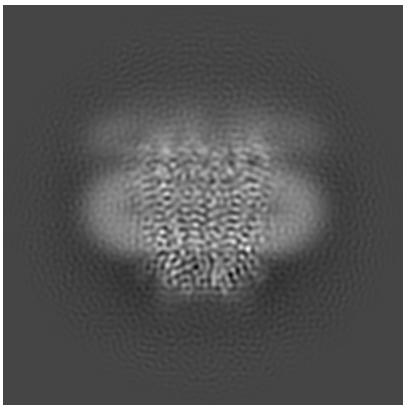
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-28902. These allow visual inspection of the internal detail of the map and identification of artifacts.

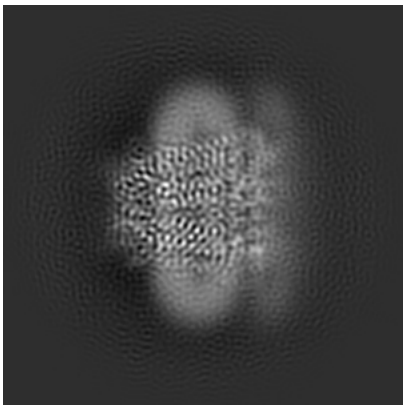
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

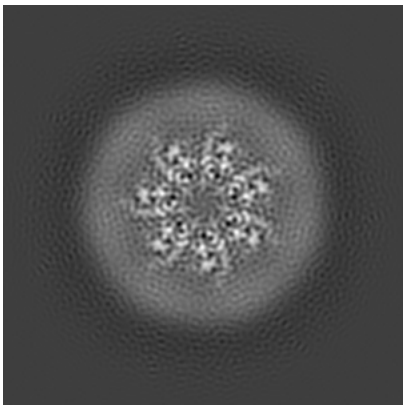
6.1.1 Primary map



X

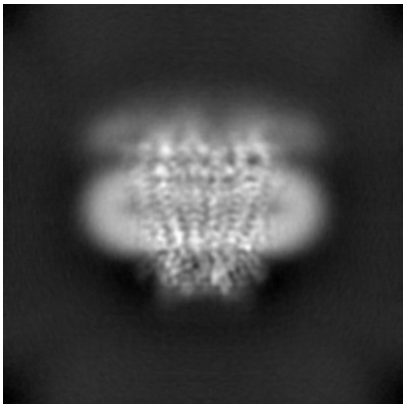


Y

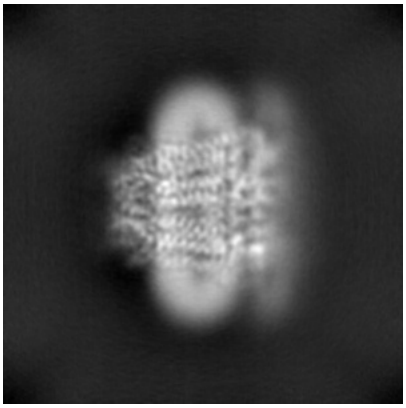


Z

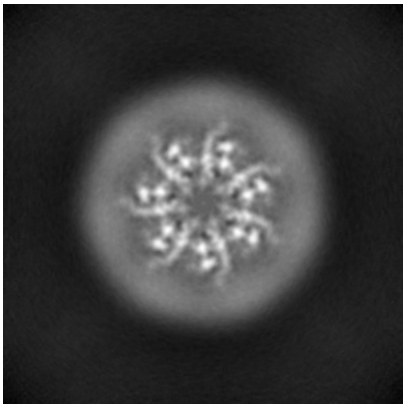
6.1.2 Raw map



X



Y

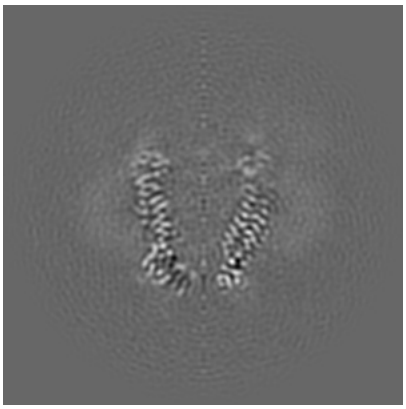


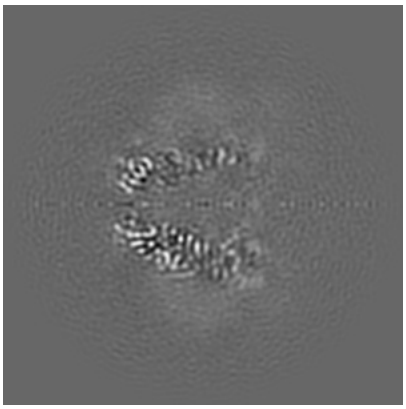
Z

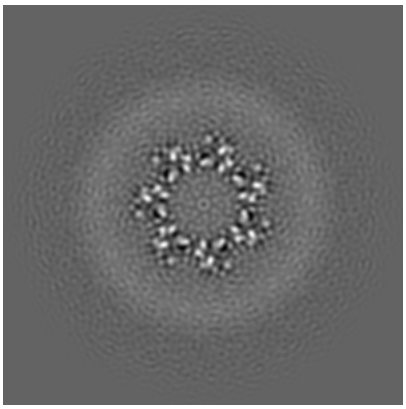
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

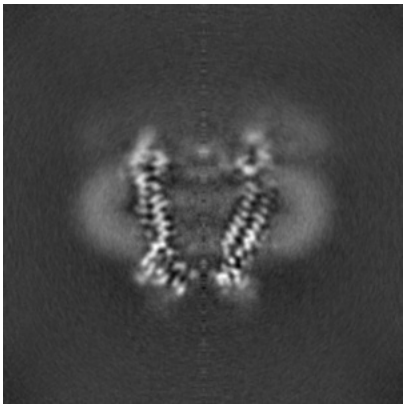
6.2.1 Primary map

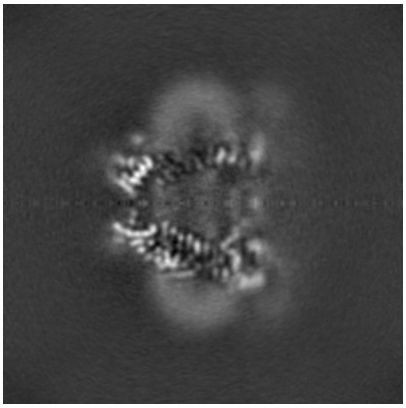

X Index: 140

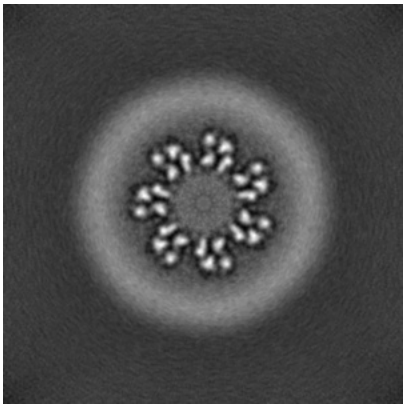

Y Index: 140


Z Index: 140

6.2.2 Raw map


X Index: 140

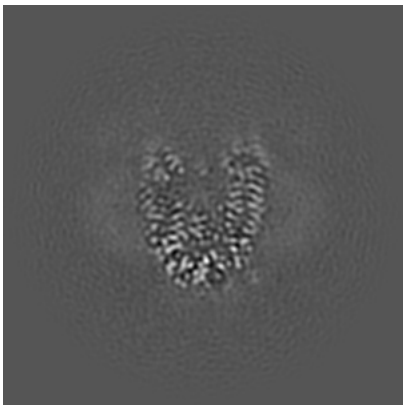

Y Index: 140

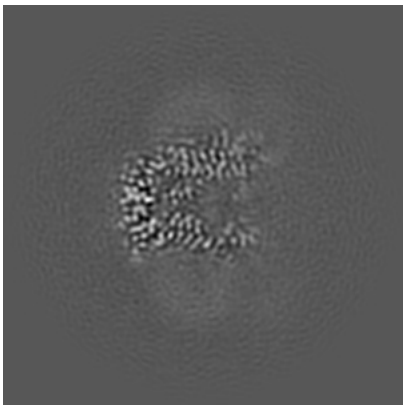

Z Index: 140

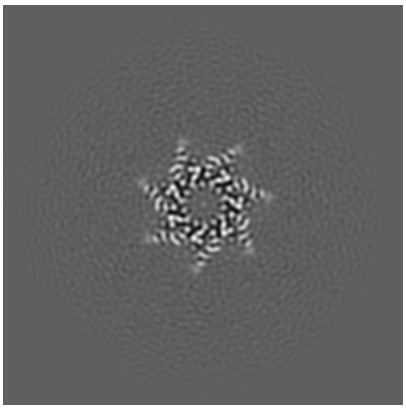
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

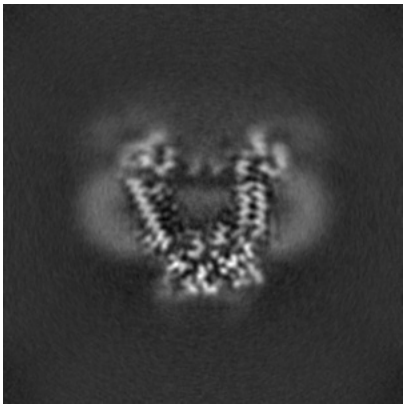
6.3.1 Primary map

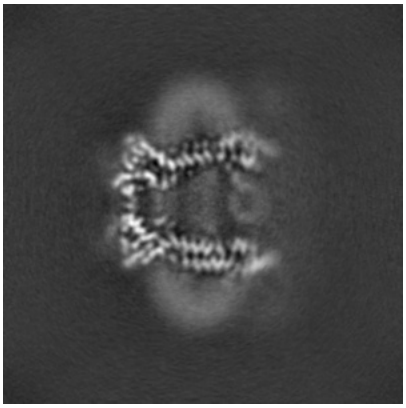

X Index: 118

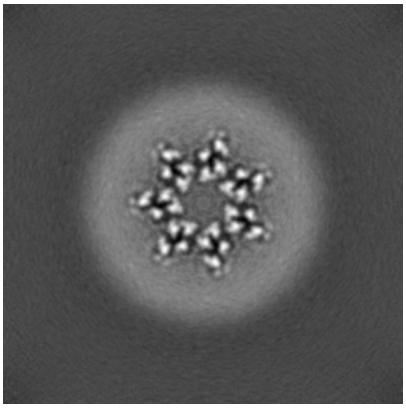

Y Index: 119


Z Index: 97

6.3.2 Raw map


X Index: 155

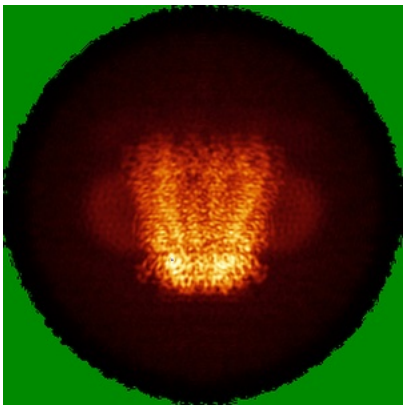

Y Index: 148

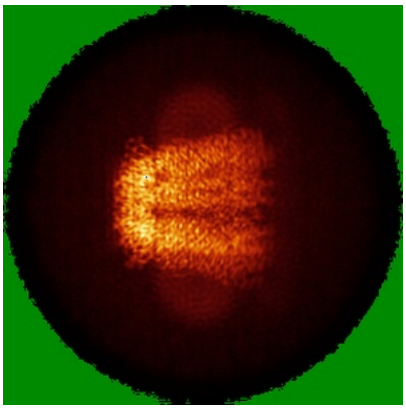

Z Index: 119

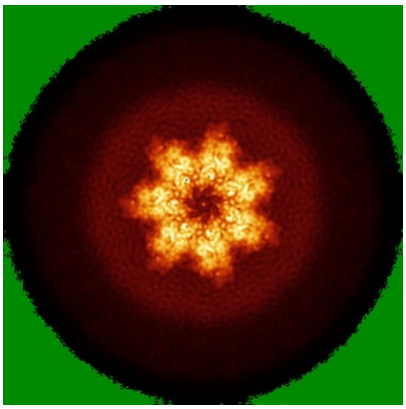
The images above show the largest variance slices of the map in three orthogonal directions.

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

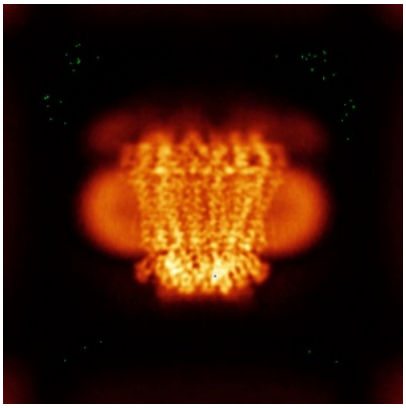
6.4.1 Primary map

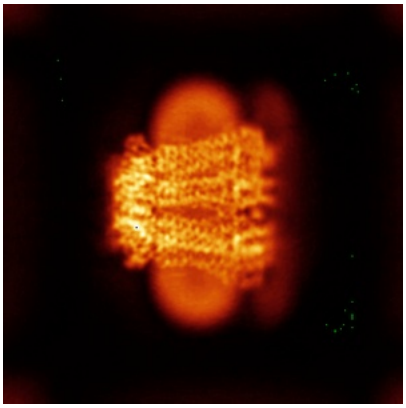

X

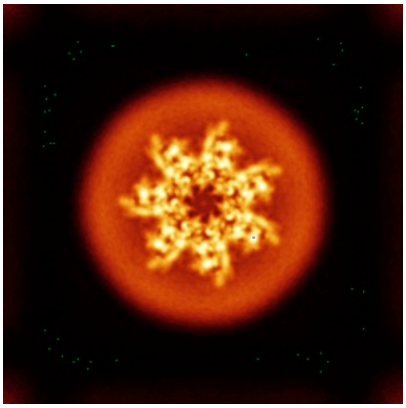

Y


Z

6.4.2 Raw map


X

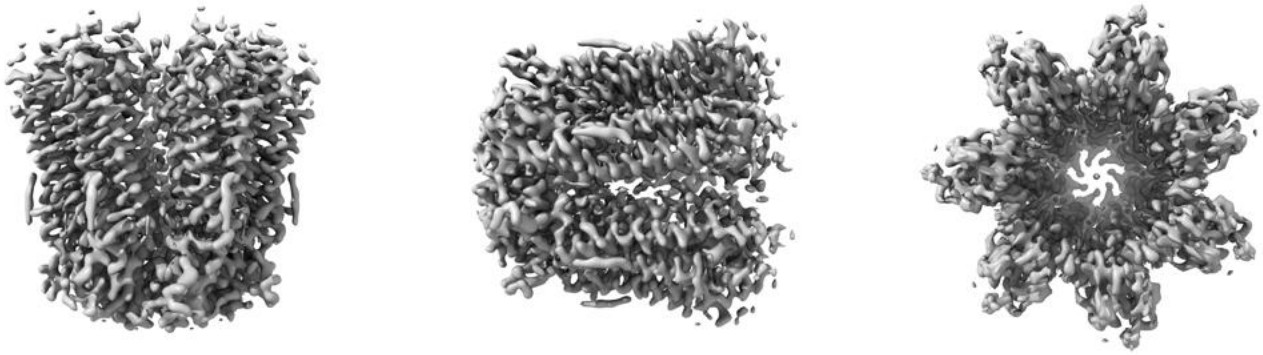

Y


Z

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

6.5 Orthogonal surface views (i)

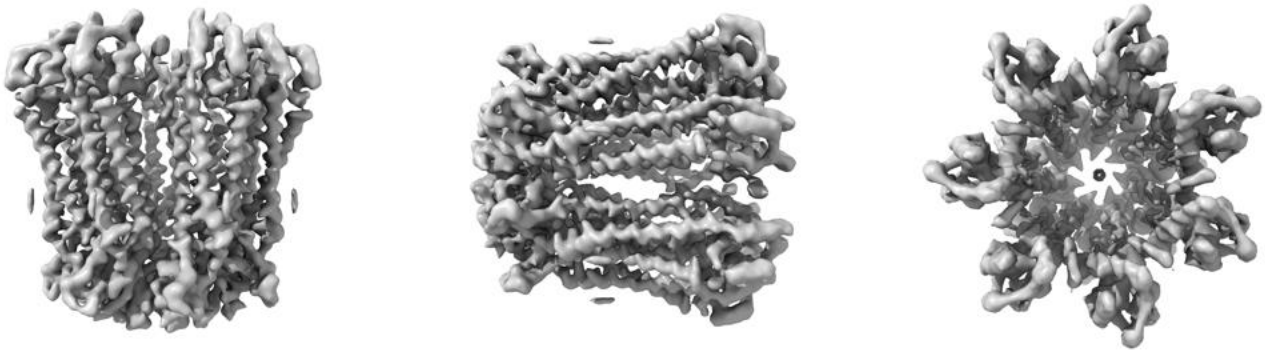
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.86. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

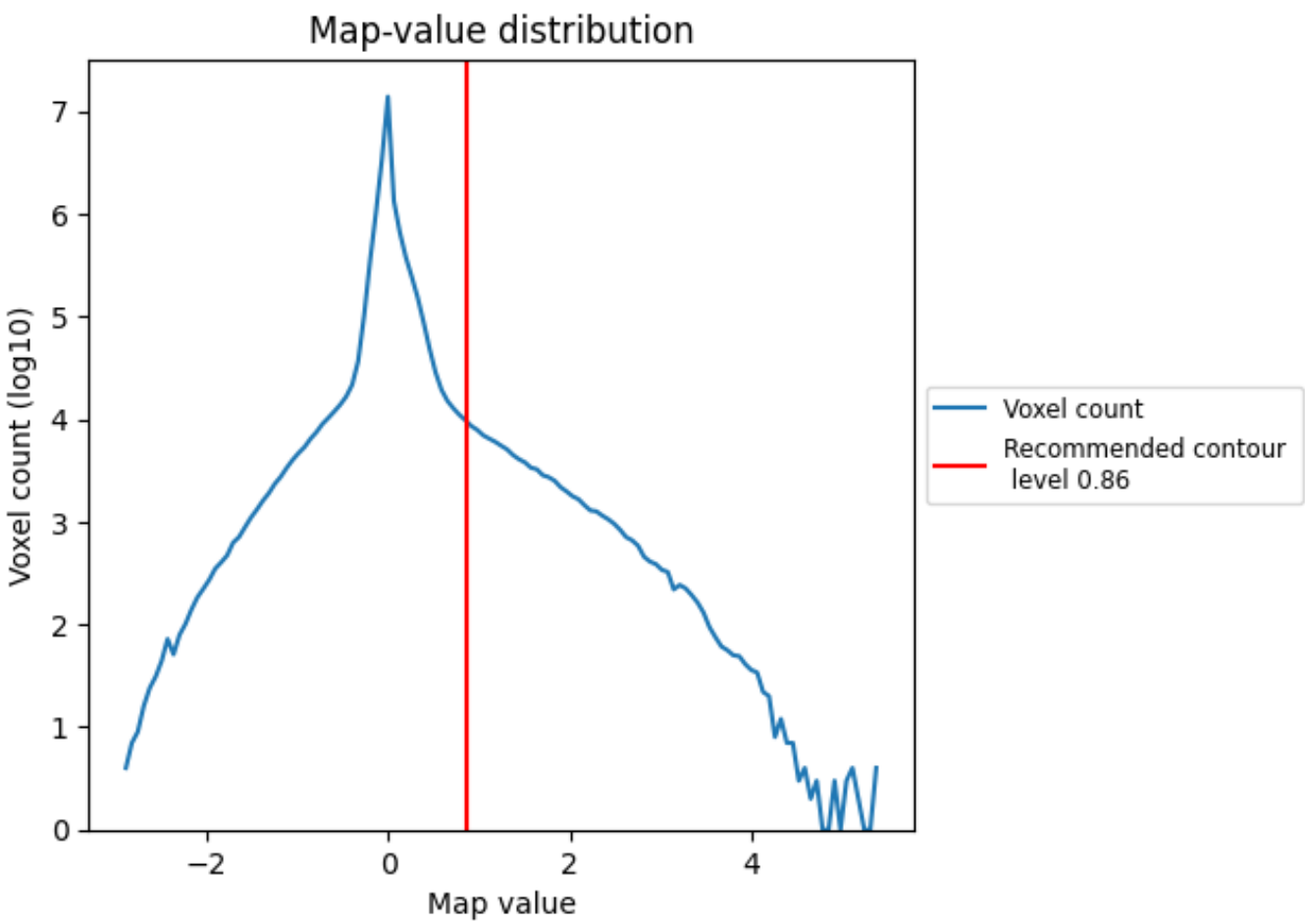
6.6 Mask visualisation (i)

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

7 Map analysis (i)

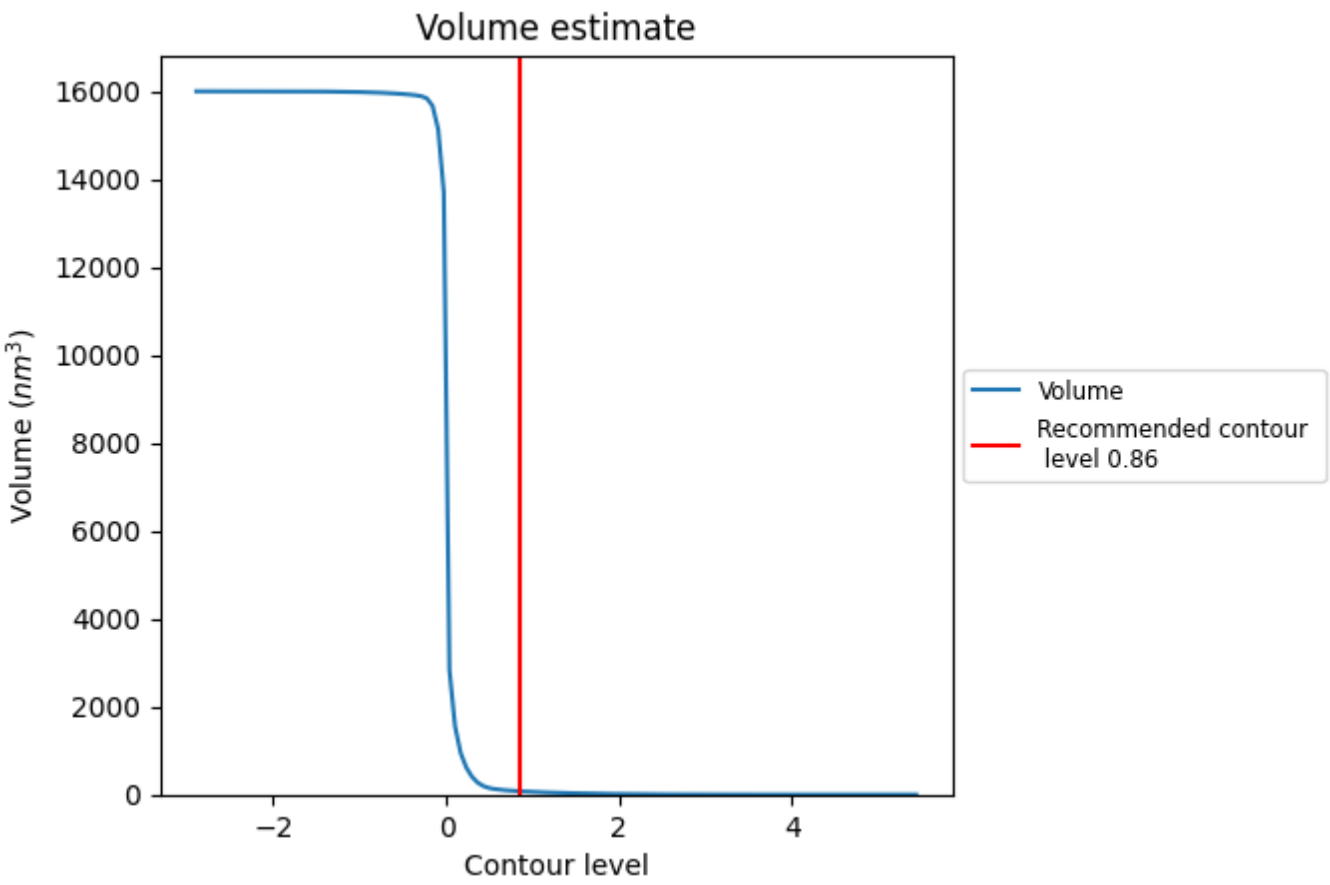
This section contains the results of statistical analysis of the map.

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.

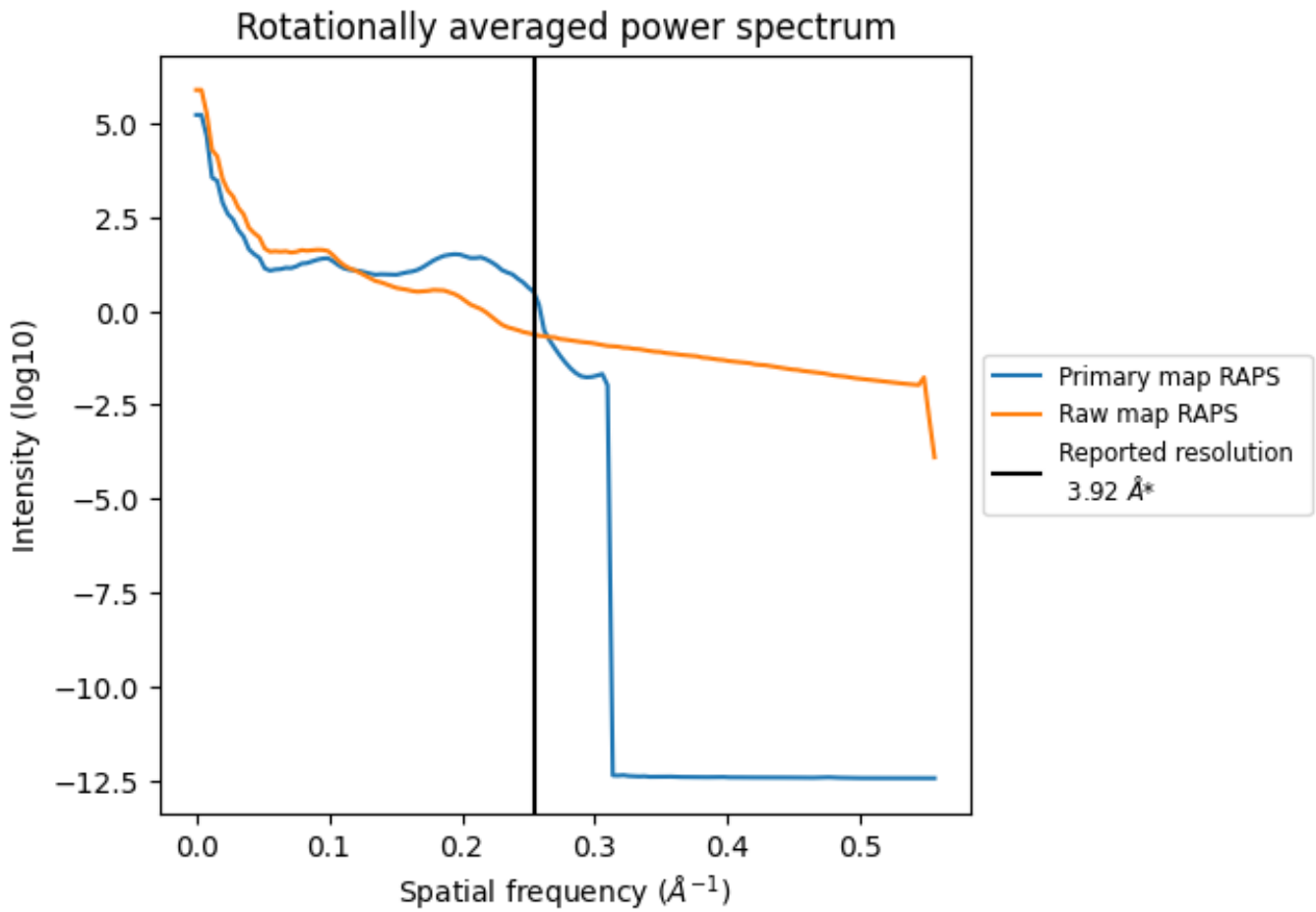
7.2 Volume estimate (i)



The volume at the recommended contour level is 75 nm^3; this corresponds to an approximate mass of 68 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

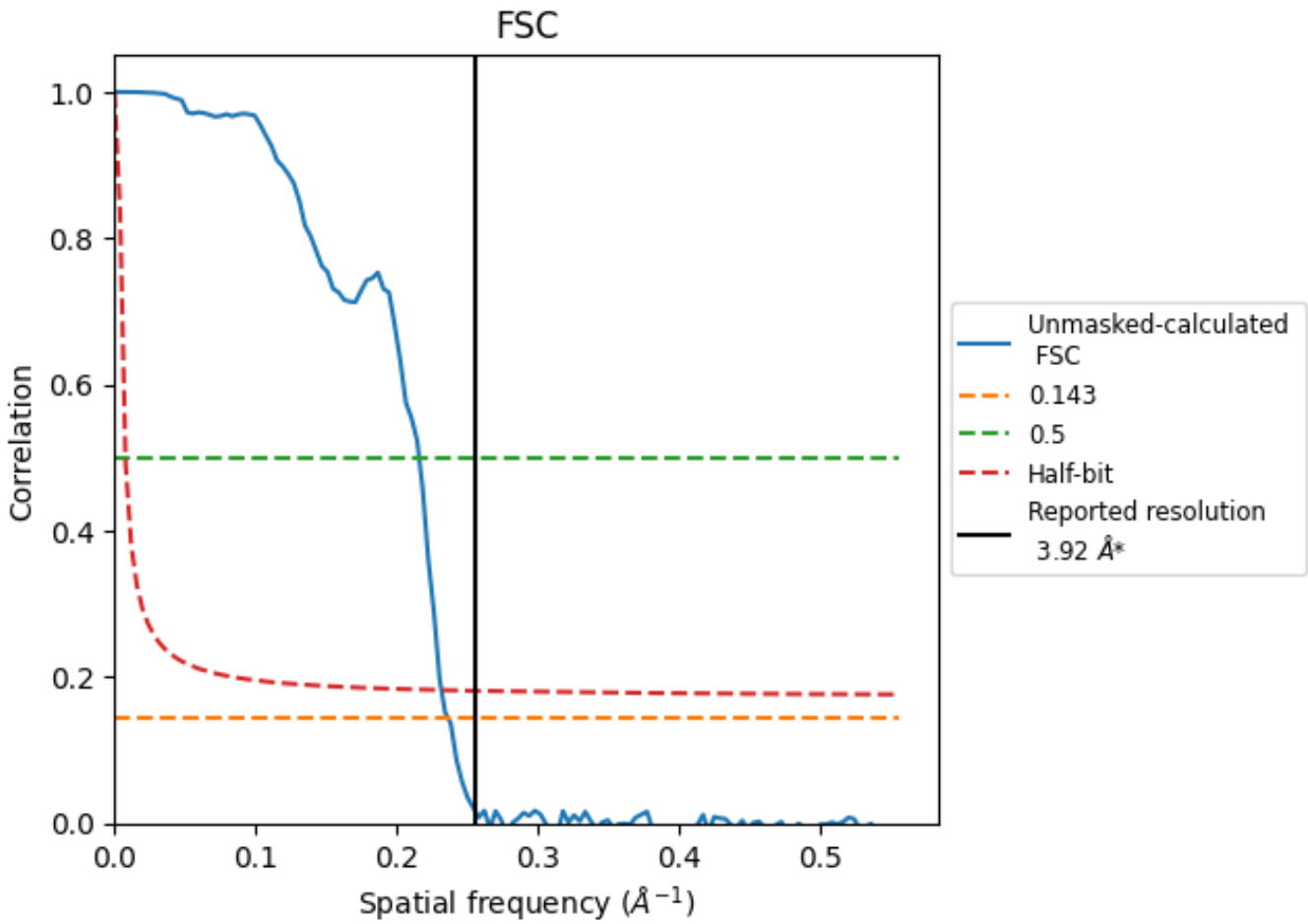


*Reported resolution corresponds to spatial frequency of 0.255 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.255 Å^{-1}

8.2 Resolution estimates (i)

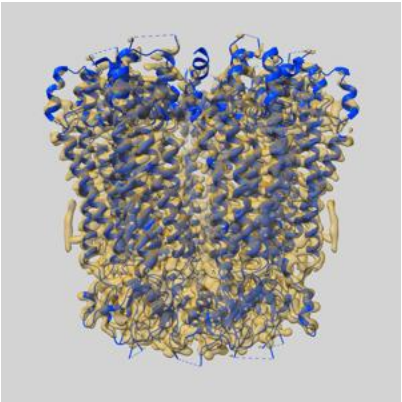
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.23	4.64	4.32

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

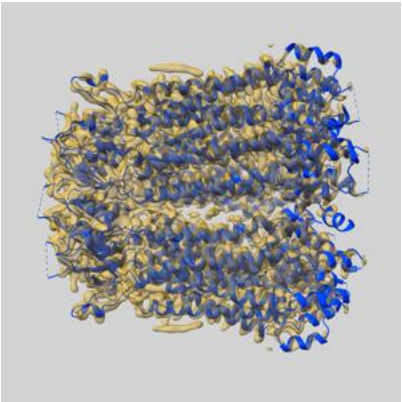
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-28902 and PDB model 8F7C. Per-residue inclusion information can be found in section 3 on page 6.

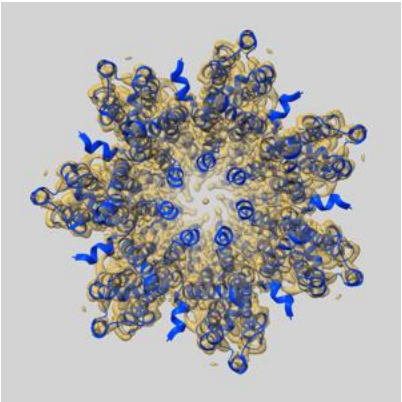
9.1 Map-model overlay (i)



X



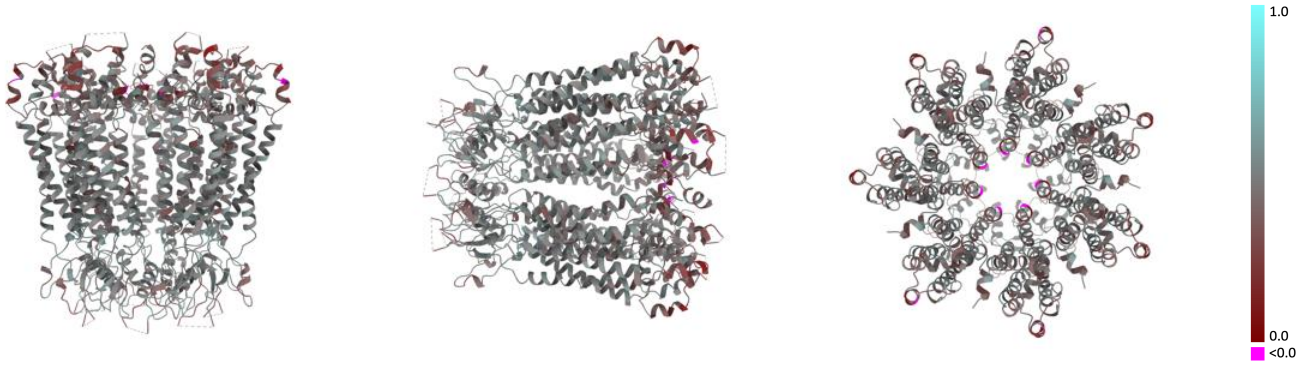
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.86 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.

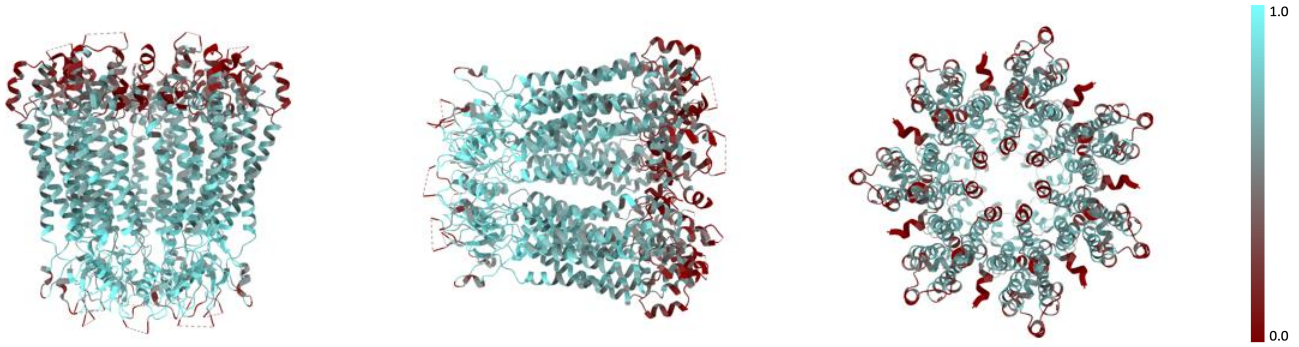
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

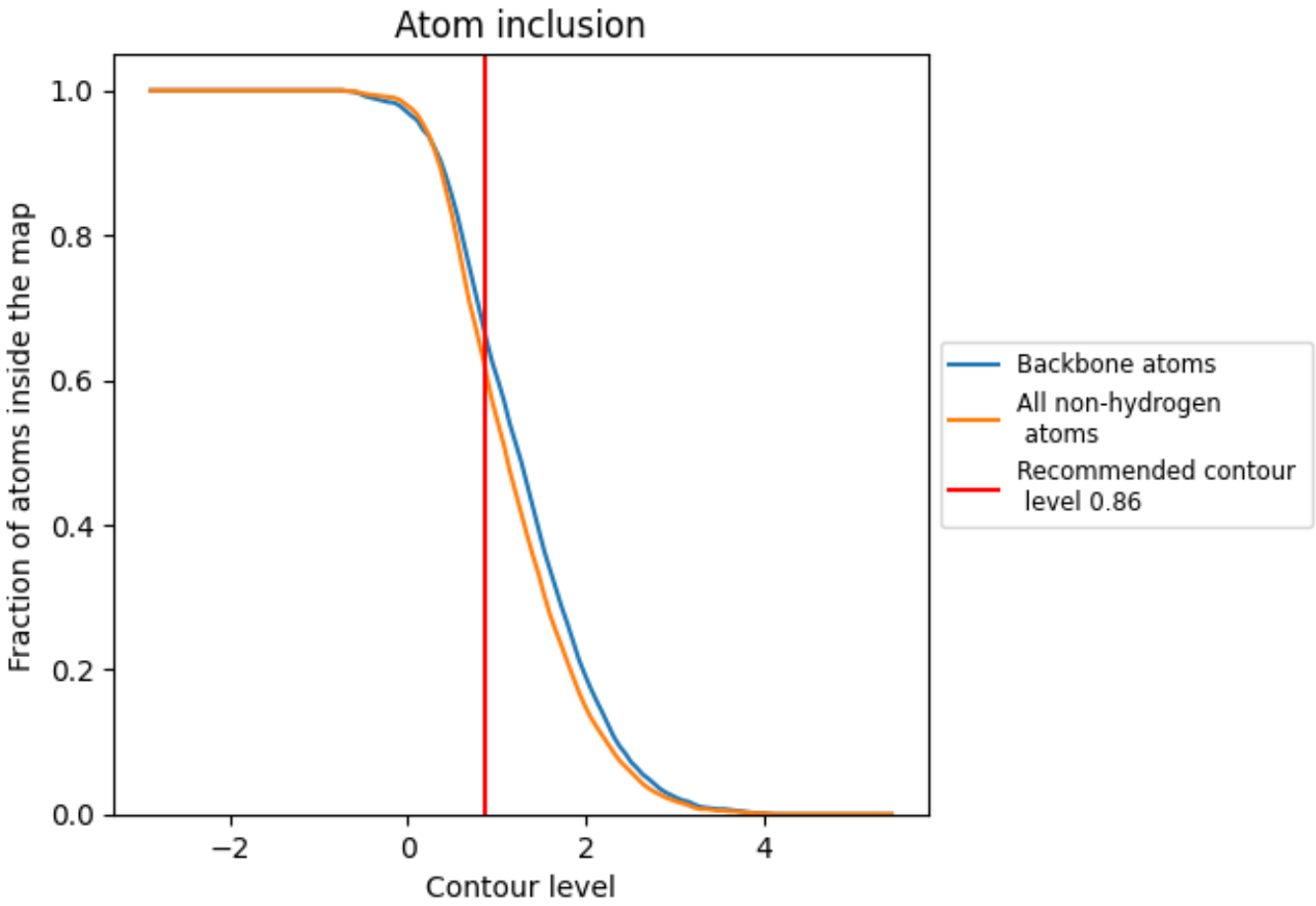
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.86).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.86) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.4580
A	0.6210	0.4580
B	0.6210	0.4570
C	0.6180	0.4600
D	0.6210	0.4580
E	0.6250	0.4570
F	0.6280	0.4620
G	0.6210	0.4580