Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 11:35 AM EST

PDB ID	:	6N4Q
EMDB ID	:	EMD-0341
Title	:	CryoEM structure of Nav1.7 VSD2 (actived state) in complex with the gating modifier toxin ProTx2
Authors	:	Xu, H.; Rohou, A.; Arthur, C.P.; Estevez, A.; Ciferri, C.; Payandeh, J.; Koth, C.M.
Deposited on	:	2018-11-20
Resolution	:	3.60 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:

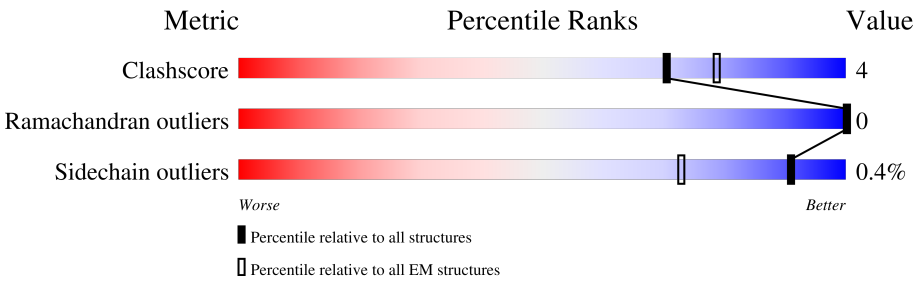
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 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	288	• 82% 8% 9%
1	B	288	5% 82% 9% 9%
1	C	288	• 81% 10% 9%
1	D	288	6% 82% 9% 9%
2	E	30	37% 87% 13%
2	F	30	33% 87% 13%
2	G	30	27% 87% 13%
2	H	30	33% 83% 17%

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Mol	Chain	Length	Quality of chain
3	I	215	26% 88% 12%
3	K	215	27% 89% 10%
4	J	228	34% 88% 12%
4	L	228	34% 88% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16358 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 Nav1.7 VSD2-NavAb chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	261	2136	1430	328	364	14	0	0
1	B	262	2150	1439	332	365	14	0	0
1	C	261	2136	1430	328	364	14	0	0
1	D	262	2150	1439	332	365	14	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	MET	-	initiating methionine	UNP A8EVM5
A	705	ASP	-	expression tag	UNP A8EVM5
A	706	TYR	-	expression tag	UNP A8EVM5
A	707	LYS	-	expression tag	UNP A8EVM5
A	708	ASP	-	expression tag	UNP A8EVM5
A	709	ASP	-	expression tag	UNP A8EVM5
A	710	ASP	-	expression tag	UNP A8EVM5
A	711	ASP	-	expression tag	UNP A8EVM5
A	712	LYS	-	expression tag	UNP A8EVM5
A	713	GLY	-	expression tag	UNP A8EVM5
A	714	SER	-	expression tag	UNP A8EVM5
A	715	LEU	-	expression tag	UNP A8EVM5
A	716	VAL	-	expression tag	UNP A8EVM5
A	717	PRO	-	expression tag	UNP A8EVM5
A	718	ARG	-	expression tag	UNP A8EVM5
A	719	GLY	-	expression tag	UNP A8EVM5
A	720	SER	-	expression tag	UNP A8EVM5
A	721	HIS	-	expression tag	UNP A8EVM5
A	941	CYS	ILE	conflict	UNP A8EVM5
B	704	MET	-	initiating methionine	UNP A8EVM5
B	705	ASP	-	expression tag	UNP A8EVM5
B	706	TYR	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	707	LYS	-	expression tag	UNP A8EVM5
B	708	ASP	-	expression tag	UNP A8EVM5
B	709	ASP	-	expression tag	UNP A8EVM5
B	710	ASP	-	expression tag	UNP A8EVM5
B	711	ASP	-	expression tag	UNP A8EVM5
B	712	LYS	-	expression tag	UNP A8EVM5
B	713	GLY	-	expression tag	UNP A8EVM5
B	714	SER	-	expression tag	UNP A8EVM5
B	715	LEU	-	expression tag	UNP A8EVM5
B	716	VAL	-	expression tag	UNP A8EVM5
B	717	PRO	-	expression tag	UNP A8EVM5
B	718	ARG	-	expression tag	UNP A8EVM5
B	719	GLY	-	expression tag	UNP A8EVM5
B	720	SER	-	expression tag	UNP A8EVM5
B	721	HIS	-	expression tag	UNP A8EVM5
B	941	CYS	ILE	conflict	UNP A8EVM5
C	704	MET	-	initiating methionine	UNP A8EVM5
C	705	ASP	-	expression tag	UNP A8EVM5
C	706	TYR	-	expression tag	UNP A8EVM5
C	707	LYS	-	expression tag	UNP A8EVM5
C	708	ASP	-	expression tag	UNP A8EVM5
C	709	ASP	-	expression tag	UNP A8EVM5
C	710	ASP	-	expression tag	UNP A8EVM5
C	711	ASP	-	expression tag	UNP A8EVM5
C	712	LYS	-	expression tag	UNP A8EVM5
C	713	GLY	-	expression tag	UNP A8EVM5
C	714	SER	-	expression tag	UNP A8EVM5
C	715	LEU	-	expression tag	UNP A8EVM5
C	716	VAL	-	expression tag	UNP A8EVM5
C	717	PRO	-	expression tag	UNP A8EVM5
C	718	ARG	-	expression tag	UNP A8EVM5
C	719	GLY	-	expression tag	UNP A8EVM5
C	720	SER	-	expression tag	UNP A8EVM5
C	721	HIS	-	expression tag	UNP A8EVM5
C	941	CYS	ILE	conflict	UNP A8EVM5
D	704	MET	-	initiating methionine	UNP A8EVM5
D	705	ASP	-	expression tag	UNP A8EVM5
D	706	TYR	-	expression tag	UNP A8EVM5
D	707	LYS	-	expression tag	UNP A8EVM5
D	708	ASP	-	expression tag	UNP A8EVM5
D	709	ASP	-	expression tag	UNP A8EVM5
D	710	ASP	-	expression tag	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	711	ASP	-	expression tag	UNP A8EVM5
D	712	LYS	-	expression tag	UNP A8EVM5
D	713	GLY	-	expression tag	UNP A8EVM5
D	714	SER	-	expression tag	UNP A8EVM5
D	715	LEU	-	expression tag	UNP A8EVM5
D	716	VAL	-	expression tag	UNP A8EVM5
D	717	PRO	-	expression tag	UNP A8EVM5
D	718	ARG	-	expression tag	UNP A8EVM5
D	719	GLY	-	expression tag	UNP A8EVM5
D	720	SER	-	expression tag	UNP A8EVM5
D	721	HIS	-	expression tag	UNP A8EVM5
D	941	CYS	ILE	conflict	UNP A8EVM5

- Molecule 2 is a protein called Beta/omega-theraphotoxin-Tp2a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	30	262	168	46	40	8	0	0
2	F	30	262	168	46	40	8	0	0
2	G	30	262	168	46	40	8	0	0
2	H	30	262	168	46	40	8	0	0

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	215	1649	1029	271	341	8	0	0
3	K	215	1649	1029	271	341	8	0	0

- Molecule 4 is a protein called Fab heavy chain.

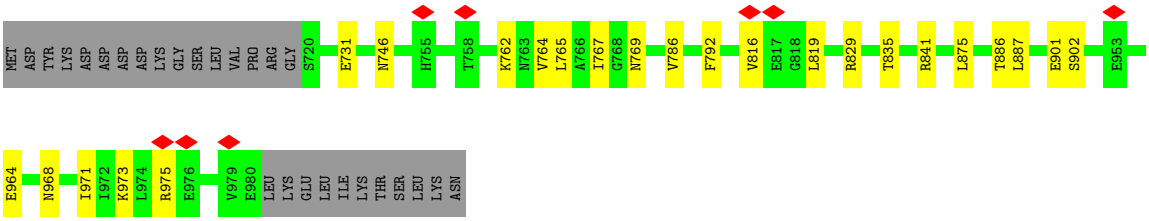
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	228	1720	1085	289	338	8	0	0
4	L	228	1720	1085	289	338	8	0	0

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.

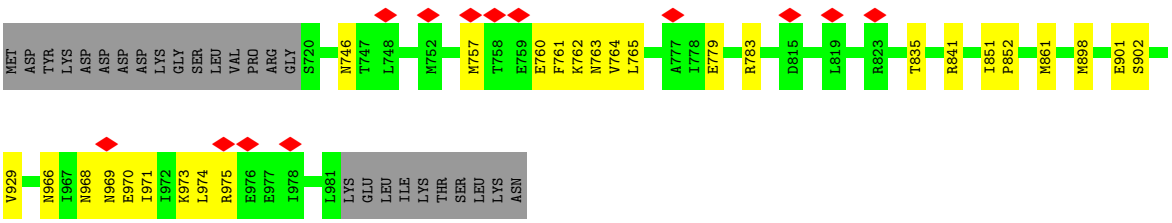
• Molecule 1: Nav1.7 VSD2-NavAb chimera

Chain A:



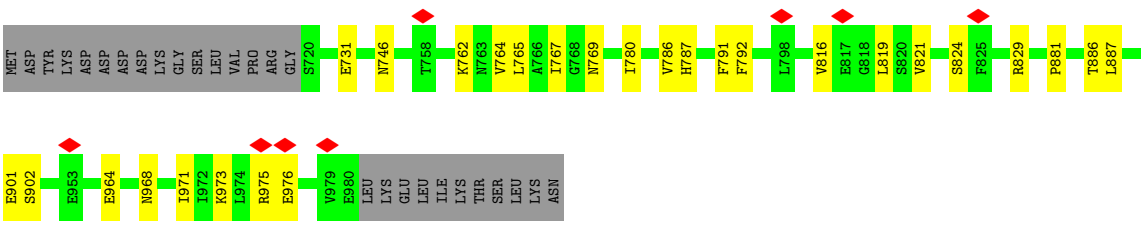
• Molecule 1: Nav1.7 VSD2-NavAb chimera

Chain B:



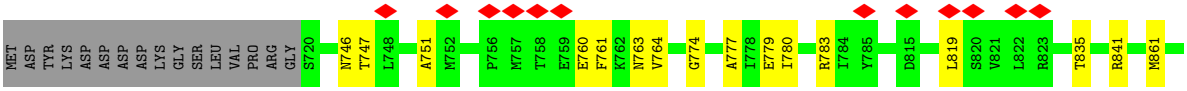
• Molecule 1: Nav1.7 VSD2-NavAb chimera

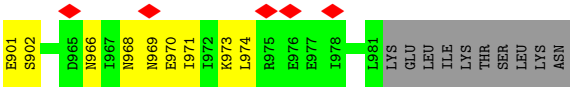
Chain C:



• Molecule 1: Nav1.7 VSD2-NavAb chimera

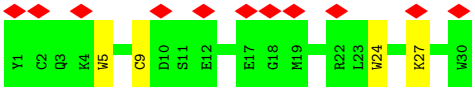
Chain D:





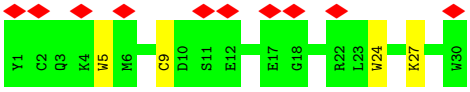
• Molecule 2: Beta/omega-theraphotoxin-Tp2a

Chain E:



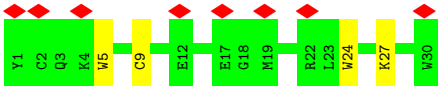
• Molecule 2: Beta/omega-theraphotoxin-Tp2a

Chain F:



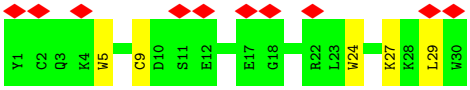
• Molecule 2: Beta/omega-theraphotoxin-Tp2a

Chain G:



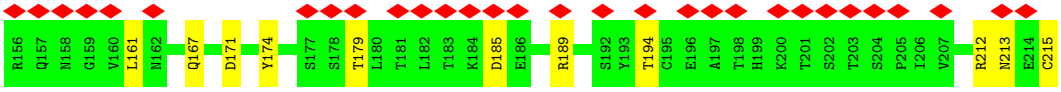
• Molecule 2: Beta/omega-theraphotoxin-Tp2a

Chain H:



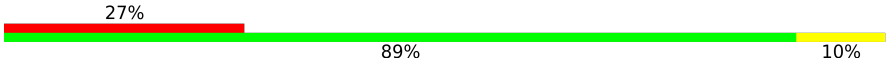
• Molecule 3: Fab light chain

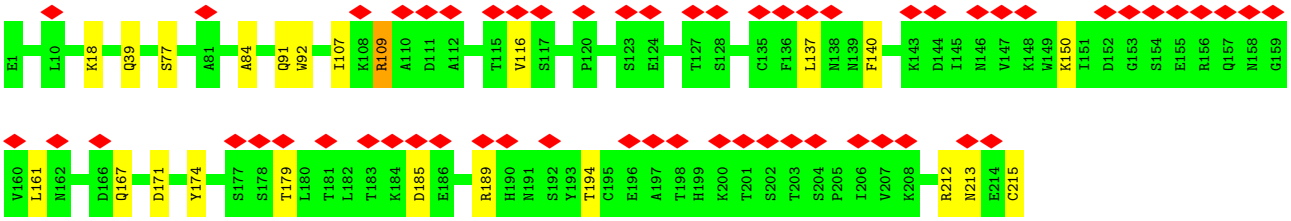
Chain I:



• Molecule 3: Fab light chain

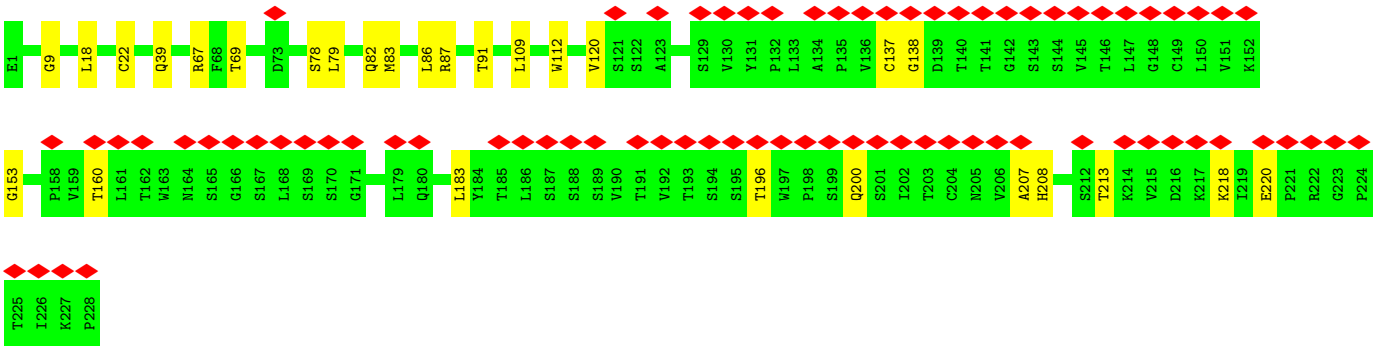
Chain K:





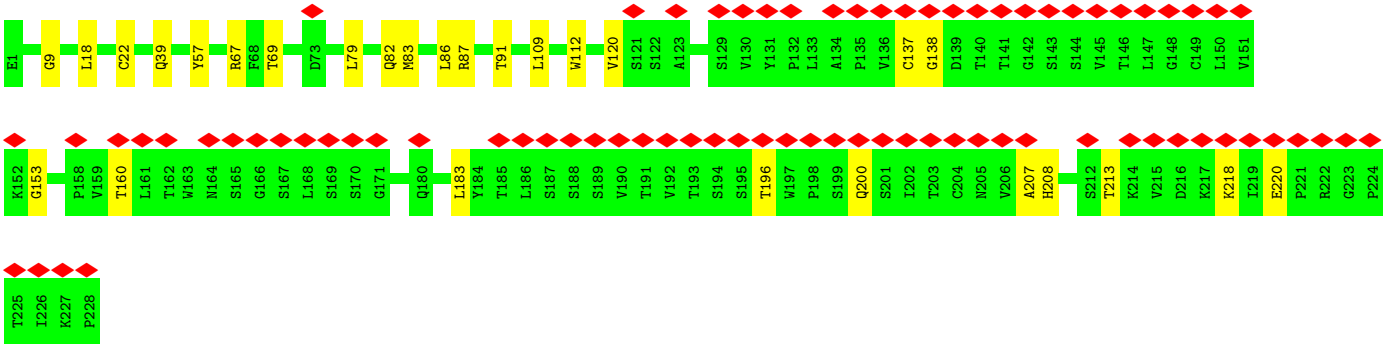
- Molecule 4: Fab heavy chain

Chain J:



- Molecule 4: Fab heavy chain

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	187192	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 ($e^-/Å^2$)	41	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.995	Depositor
Minimum map value	-0.684	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.067	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0.48	0/2190	0.63	0/2975
1	B	0.46	0/2204	0.60	0/2993
1	C	0.48	0/2190	0.63	0/2975
1	D	0.46	0/2204	0.60	0/2993
2	E	0.26	0/270	0.59	0/360
2	F	0.26	0/270	0.59	0/360
2	G	0.26	0/270	0.59	0/360
2	H	0.26	0/270	0.59	0/360
3	I	0.30	0/1688	0.53	0/2292
3	K	0.31	0/1688	0.53	0/2292
4	J	0.37	0/1764	0.58	0/2406
4	L	0.37	0/1764	0.57	0/2406
All	All	0.41	0/16772	0.59	0/22772

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PHE	Peptide
1	C	792	PHE	Peptide

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	2136	0	2186	15	0
1	B	2150	0	2208	17	0
1	C	2136	0	2186	19	0
1	D	2150	0	2208	16	0
2	E	262	0	254	2	0
2	F	262	0	254	2	0
2	G	262	0	254	2	0
2	H	262	0	254	3	0
3	I	1649	0	1577	14	0
3	K	1649	0	1577	12	0
4	J	1720	0	1684	15	0
4	L	1720	0	1684	15	0
All	All	16358	0	16326	119	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 4.

All (119) 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:B:760:GLU:OE2	1:B:763:ASN:ND2	2.29	0.65
4:J:22:CYS:HB3	4:J:79:LEU:HB3	1.78	0.65
4:L:22:CYS:HB3	4:L:79:LEU:HB3	1.78	0.65
3:K:109:ARG:NH1	3:K:171:ASP:O	2.31	0.63
3:I:109:ARG:NH1	3:I:171:ASP:O	2.31	0.63
3:I:150:LYS:HB2	3:I:194:THR:HB	1.81	0.62
3:K:150:LYS:HB2	3:K:194:THR:HB	1.81	0.61
2:G:9:CYS:H	2:G:24:TRP:HA	1.67	0.60
2:E:9:CYS:H	2:E:24:TRP:HA	1.67	0.59
2:H:9:CYS:H	2:H:24:TRP:HA	1.67	0.58
1:A:973:LYS:HE3	1:D:974:LEU:HD22	1.85	0.58
2:F:9:CYS:H	2:F:24:TRP:HA	1.67	0.58
3:K:39:GLN:HE22	4:L:39:GLN:HE22	1.49	0.58
1:D:761:PHE:O	1:D:764:VAL:HB	2.04	0.58
4:J:91:THR:HG22	4:J:120:VAL:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:160:THR:HB	4:L:207:ALA:HB3	1.87	0.57
4:J:9:GLY:HA2	4:J:18:LEU:HD21	1.87	0.56
4:L:91:THR:HG22	4:L:120:VAL:H	1.70	0.56
4:J:160:THR:HB	4:J:207:ALA:HB3	1.87	0.56
1:B:974:LEU:HD22	1:C:973:LYS:HE3	1.87	0.56
1:A:816:VAL:H	1:A:819:LEU:HD11	1.71	0.56
3:I:91:GLN:NE2	3:I:92:TRP:O	2.39	0.56
3:K:91:GLN:NE2	3:K:92:TRP:O	2.39	0.55
4:L:9:GLY:HA2	4:L:18:LEU:HD21	1.87	0.55
1:B:761:PHE:O	1:B:764:VAL:HB	2.06	0.55
3:K:107:ILE:H	3:K:167:GLN:HE22	1.53	0.55
1:A:762:LYS:O	1:A:765:LEU:HB2	2.07	0.55
3:I:185:ASP:OD2	3:I:189:ARG:NH1	2.40	0.55
1:D:760:GLU:OE2	1:D:763:ASN:ND2	2.40	0.54
1:A:886:THR:OG1	1:A:887:LEU:N	2.41	0.54
3:I:161:LEU:HB3	3:I:179:THR:HB	1.89	0.54
1:C:762:LYS:O	1:C:765:LEU:HB2	2.08	0.54
4:J:69:THR:HB	4:J:82:GLN:HB3	1.90	0.54
1:A:769:ASN:OD1	1:A:829:ARG:NH2	2.40	0.54
1:C:764:VAL:HA	1:C:767:ILE:HD12	1.90	0.54
3:I:39:GLN:HE22	4:J:39:GLN:HE22	1.54	0.54
3:I:107:ILE:H	3:I:167:GLN:HE22	1.53	0.54
4:L:69:THR:HB	4:L:82:GLN:HB3	1.89	0.54
3:K:161:LEU:HB3	3:K:179:THR:HB	1.89	0.54
3:K:185:ASP:OD2	3:K:189:ARG:NH1	2.40	0.53
4:L:137:CYS:SG	4:L:138:GLY:N	2.82	0.53
1:A:964:GLU:O	1:A:968:ASN:ND2	2.41	0.53
1:C:769:ASN:OD1	1:C:829:ARG:NH2	2.41	0.53
1:C:964:GLU:O	1:C:968:ASN:ND2	2.41	0.53
1:A:764:VAL:HA	1:A:767:ILE:HD12	1.92	0.52
4:J:137:CYS:SG	4:J:138:GLY:N	2.82	0.52
1:C:886:THR:OG1	1:C:887:LEU:N	2.43	0.51
3:I:116:VAL:HG22	3:I:137:LEU:HG	1.93	0.50
1:C:816:VAL:H	1:C:819:LEU:HD11	1.77	0.50
1:D:779:GLU:OE2	1:D:783:ARG:NE	2.45	0.50
3:K:116:VAL:HG22	3:K:137:LEU:HG	1.93	0.50
4:J:208:HIS:HB3	4:J:213:THR:HB	1.95	0.49
4:J:109:LEU:HB3	4:J:112:TRP:HE1	1.77	0.49
4:J:218:LYS:NZ	4:J:220:GLU:OE2	2.45	0.49
4:L:208:HIS:HB3	4:L:213:THR:HB	1.95	0.49
3:K:212:ARG:HA	3:K:215:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:GLU:OE2	1:B:783:ARG:NE	2.45	0.49
3:I:212:ARG:HA	3:I:215:CYS:HB2	1.94	0.49
4:L:218:LYS:NZ	4:L:220:GLU:OE2	2.45	0.49
4:L:67:ARG:HH12	4:L:87:ARG:HG3	1.78	0.48
4:J:67:ARG:HH12	4:J:87:ARG:HG3	1.78	0.48
4:L:109:LEU:HB3	4:L:112:TRP:HE1	1.78	0.48
1:A:731:GLU:OE2	1:A:786:VAL:HG11	2.13	0.47
1:A:968:ASN:HA	1:A:971:ILE:HD12	1.95	0.47
3:K:18:LYS:HG3	3:K:77:SER:HA	1.97	0.47
1:C:968:ASN:HA	1:C:971:ILE:HD12	1.96	0.47
3:I:18:LYS:HG3	3:I:77:SER:HA	1.97	0.46
1:D:968:ASN:HA	1:D:971:ILE:HD12	1.97	0.46
1:B:968:ASN:HA	1:B:971:ILE:HD12	1.97	0.46
1:D:861:MET:HB3	1:D:861:MET:HE3	1.77	0.45
1:C:731:GLU:OE2	1:C:786:VAL:HG11	2.16	0.45
1:B:970:GLU:O	1:B:973:LYS:HB3	2.17	0.44
1:C:902:SER:HA	1:D:901:GLU:OE2	2.17	0.44
1:D:835:THR:O	1:D:841:ARG:NH2	2.51	0.44
1:A:975:ARG:HA	1:B:973:LYS:HZ3	1.83	0.44
1:A:902:SER:HA	1:B:901:GLU:OE2	2.18	0.43
1:B:762:LYS:HA	1:B:765:LEU:HD12	2.00	0.43
1:B:902:SER:HA	1:C:901:GLU:OE2	2.18	0.43
3:K:140:PHE:O	3:K:174:TYR:N	2.48	0.43
1:B:861:MET:HE2	1:B:861:MET:HB3	1.81	0.43
1:D:747:THR:O	1:D:751:ALA:HB2	2.19	0.43
1:A:816:VAL:HB	1:A:819:LEU:HD21	2.02	0.42
1:B:851:ILE:HG23	1:B:852:PRO:HD3	2.00	0.42
4:L:196:THR:O	4:L:200:GLN:N	2.45	0.42
1:A:901:GLU:OE2	1:D:902:SER:HA	2.19	0.42
1:C:764:VAL:O	1:C:767:ILE:HB	2.19	0.42
2:E:5:TRP:CE2	2:E:27:LYS:HE3	2.55	0.42
1:D:774:GLY:O	1:D:777:ALA:HB3	2.20	0.42
2:F:5:TRP:CE2	2:F:27:LYS:HE3	2.55	0.42
1:C:975:ARG:HA	1:D:973:LYS:HZ3	1.85	0.42
1:B:835:THR:O	1:B:841:ARG:NH2	2.52	0.42
2:H:5:TRP:CE2	2:H:27:LYS:HE3	2.55	0.42
1:D:966:ASN:O	1:D:969:ASN:HB2	2.19	0.41
1:D:970:GLU:O	1:D:973:LYS:HB3	2.20	0.41
1:C:787:HIS:HB2	1:C:791:PHE:HB2	2.02	0.41
1:C:973:LYS:HA	1:C:976:GLU:HG2	2.01	0.41
1:D:780:ILE:HD12	1:D:780:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:TRP:CE2	2:G:27:LYS:HE3	2.55	0.41
3:I:84:ALA:HB2	3:I:107:ILE:HG12	2.01	0.41
1:B:757:MET:SD	1:B:762:LYS:HB3	2.60	0.41
3:I:7:SER:O	3:I:22:THR:OG1	2.29	0.41
3:K:84:ALA:HB2	3:K:107:ILE:HG12	2.01	0.41
1:A:835:THR:O	1:A:841:ARG:NH2	2.54	0.41
1:B:966:ASN:O	1:B:969:ASN:HB2	2.21	0.41
1:D:819:LEU:HD22	2:H:29:LEU:HD22	2.03	0.41
4:L:83:MET:HB3	4:L:86:LEU:HD21	2.03	0.41
4:L:153:GLY:HA2	4:L:183:LEU:HB3	2.03	0.41
1:A:875:LEU:HD23	1:A:875:LEU:HA	1.92	0.41
4:J:22:CYS:O	4:J:78:SER:OG	2.34	0.41
4:J:196:THR:O	4:J:200:GLN:N	2.45	0.41
3:I:33:ASN:OD1	3:I:33:ASN:N	2.54	0.40
1:B:898:MET:HG3	1:B:929:VAL:HG11	2.03	0.40
1:B:975:ARG:HE	1:C:973:LYS:HZ2	1.70	0.40
1:C:821:VAL:O	1:C:824:SER:HB3	2.20	0.40
4:J:153:GLY:HA2	4:J:183:LEU:HB3	2.03	0.40
1:C:881:PRO:HB2	4:L:57:TYR:HD2	1.86	0.40
3:I:140:PHE:O	3:I:174:TYR:N	2.48	0.40
4:J:83:MET:HB3	4:J:86:LEU:HD21	2.03	0.40
1:C:780:ILE:HD12	1:C:780:ILE:HA	1.95	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	259/288 (90%)	240 (93%)	19 (7%)	0	100	100
1	B	260/288 (90%)	243 (94%)	17 (6%)	0	100	100
1	C	259/288 (90%)	239 (92%)	20 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	260/288 (90%)	246 (95%)	14 (5%)	0	100	100
2	E	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
2	F	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
2	G	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
2	H	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
3	I	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
3	K	213/215 (99%)	197 (92%)	16 (8%)	0	100	100
4	J	226/228 (99%)	207 (92%)	19 (8%)	0	100	100
4	L	226/228 (99%)	206 (91%)	20 (9%)	0	100	100
All	All	2028/2158 (94%)	1867 (92%)	161 (8%)	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	239/265 (90%)	238 (100%)	1 (0%)	91	97
1	B	241/265 (91%)	240 (100%)	1 (0%)	91	97
1	C	239/265 (90%)	238 (100%)	1 (0%)	91	97
1	D	241/265 (91%)	240 (100%)	1 (0%)	91	97
2	E	29/29 (100%)	29 (100%)	0	100	100
2	F	29/29 (100%)	29 (100%)	0	100	100
2	G	29/29 (100%)	29 (100%)	0	100	100
2	H	29/29 (100%)	29 (100%)	0	100	100
3	I	190/190 (100%)	188 (99%)	2 (1%)	73	88
3	K	190/190 (100%)	188 (99%)	2 (1%)	73	88
4	J	193/194 (100%)	193 (100%)	0	100	100
4	L	193/194 (100%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1842/1944 (95%)	1834 (100%)	8 (0%)	91 97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	746	ASN
1	B	746	ASN
1	C	746	ASN
1	D	746	ASN
3	I	109	ARG
3	I	213	ASN
3	K	109	ARG
3	K	213	ASN

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	966	ASN
1	B	746	ASN
1	B	963	HIS
1	C	966	ASN
1	D	746	ASN
1	D	963	HIS
1	D	969	ASN
3	I	39	GLN
3	I	167	GLN
3	I	213	ASN
4	J	99	HIS
4	J	164	ASN
3	K	39	GLN
3	K	167	GLN
3	K	213	ASN
4	L	99	HIS
4	L	164	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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-0341. These allow visual inspection of the internal detail of the map and identification of artifacts.

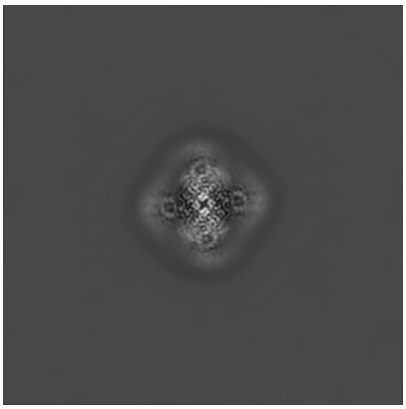
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map

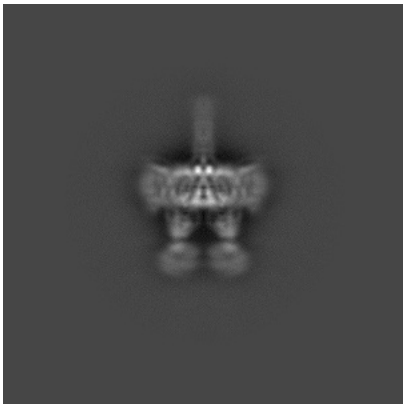
X

Y

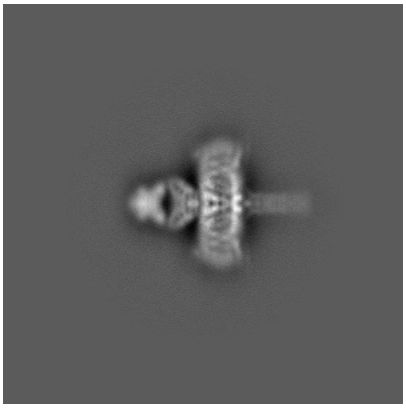


Z

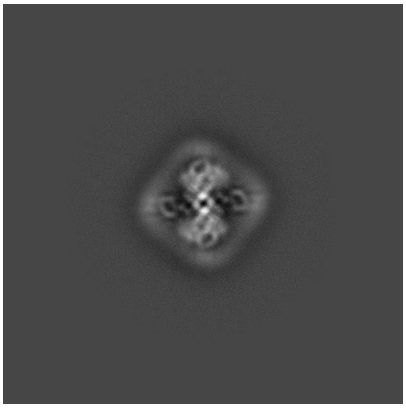
6.1.2 Raw map



X



Y



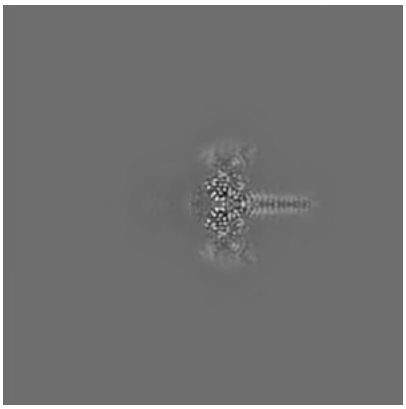
Z

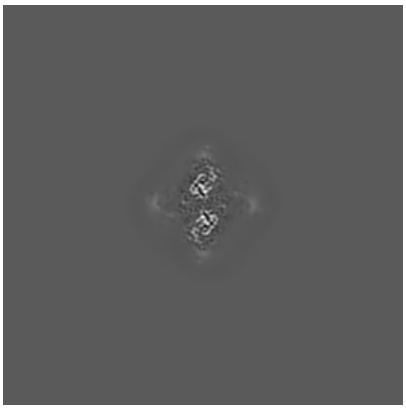
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

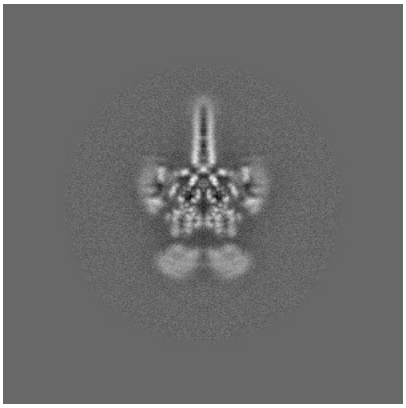
6.2.1 Primary map

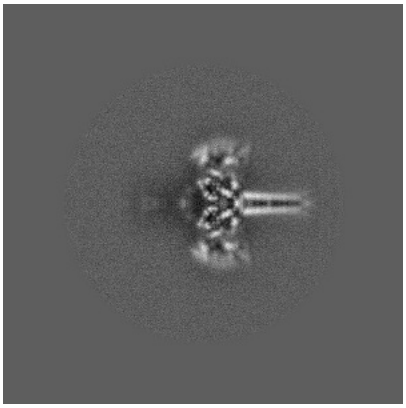
X Index: 180

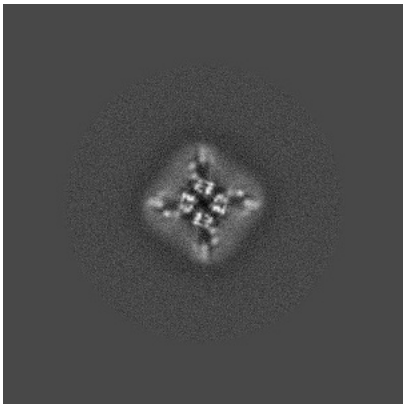

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180


Y Index: 180


Z Index: 180

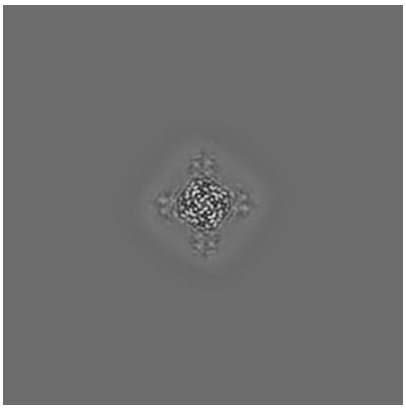
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

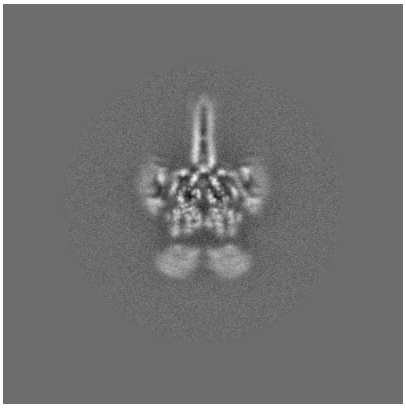
X Index: 184

Y Index: 176

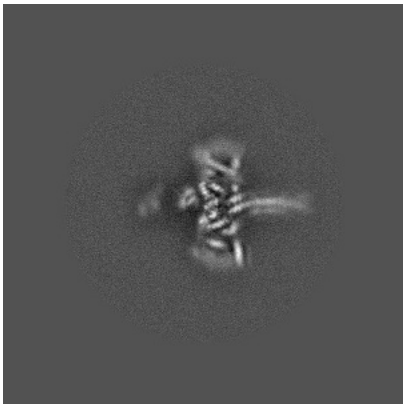


Z Index: 193

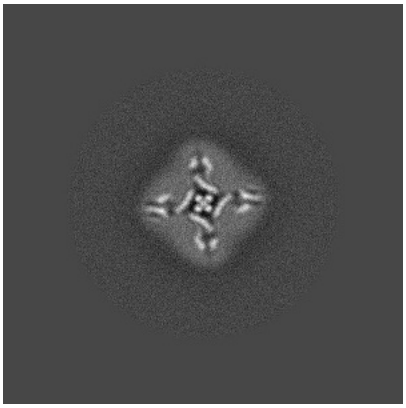
6.3.2 Raw map



X Index: 181



Y Index: 175



Z Index: 209

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.067. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

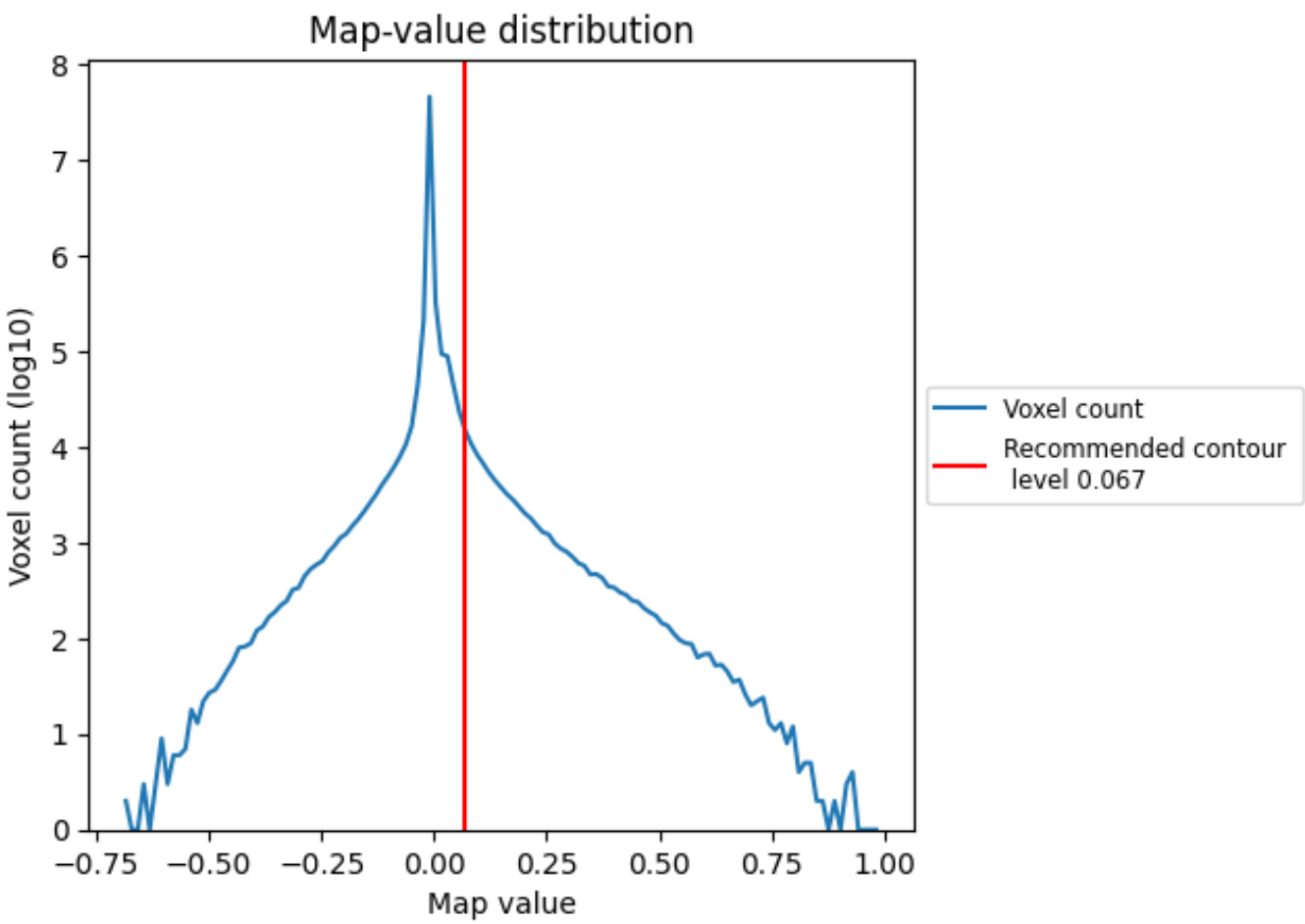
6.5 Mask visualisation (i)

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

7 Map analysis (i)

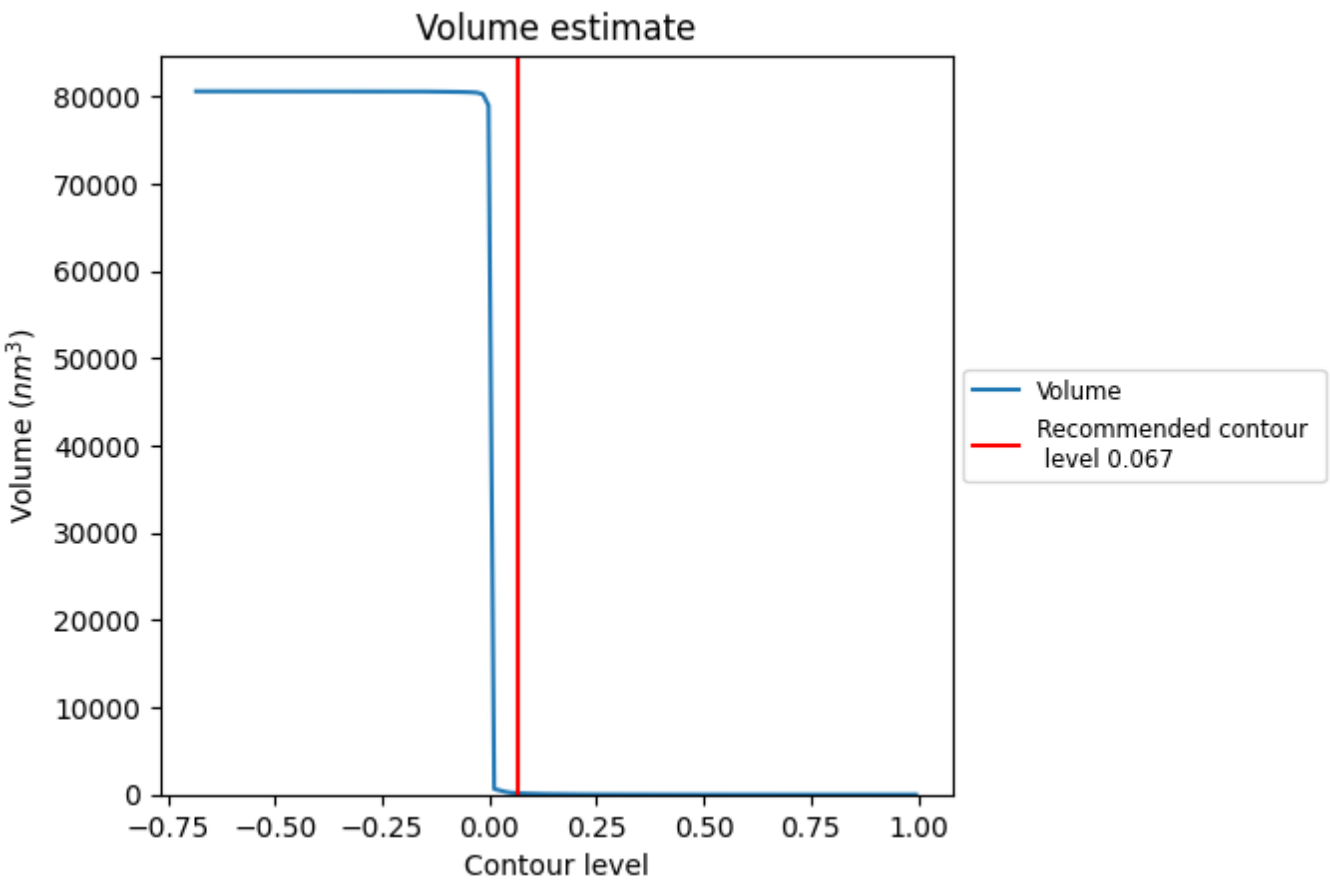
This section contains the results of statistical analysis of the map.

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.

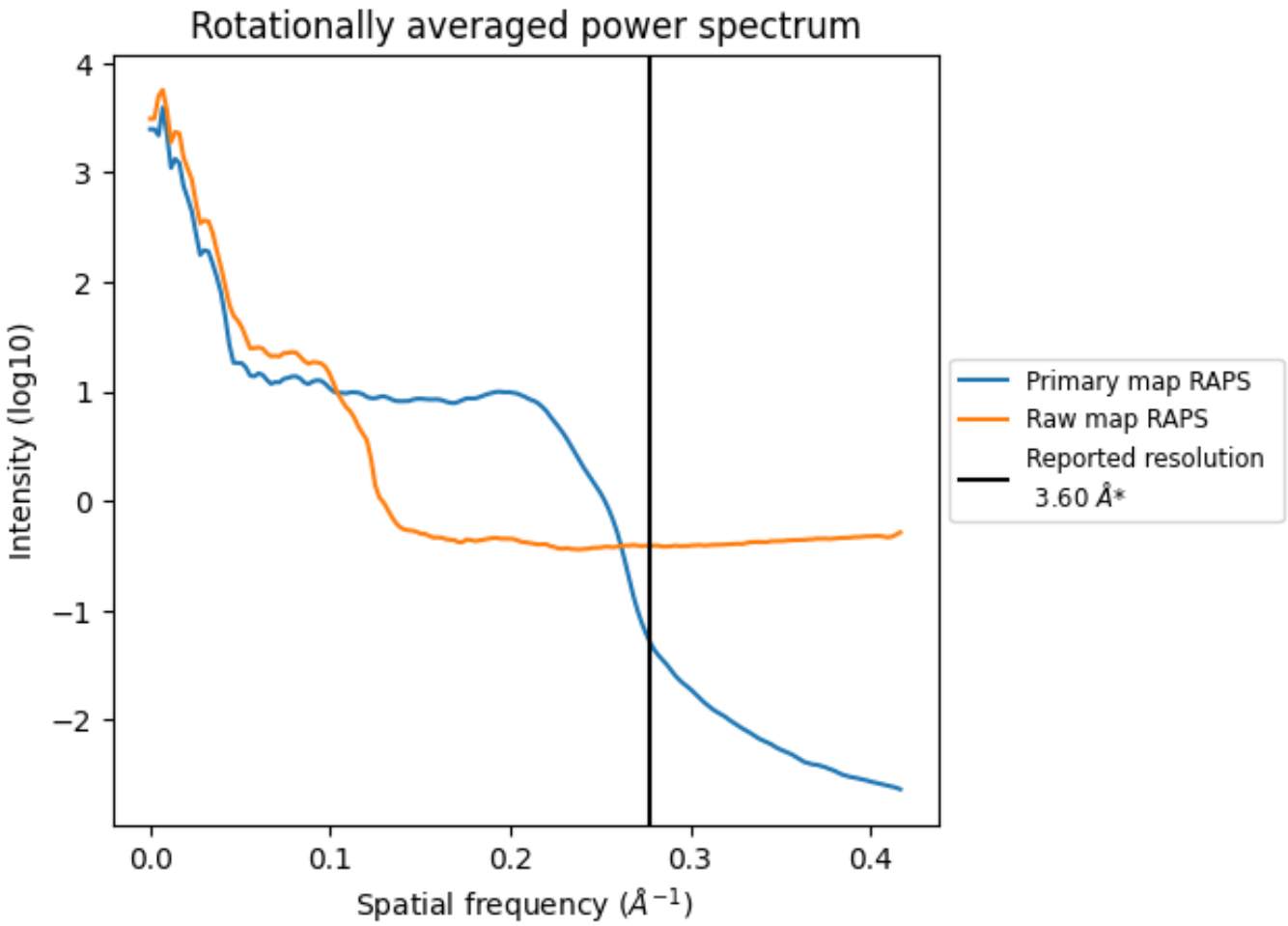
7.2 Volume estimate (i)



The volume at the recommended contour level is 145 nm^3; this corresponds to an approximate mass of 131 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)

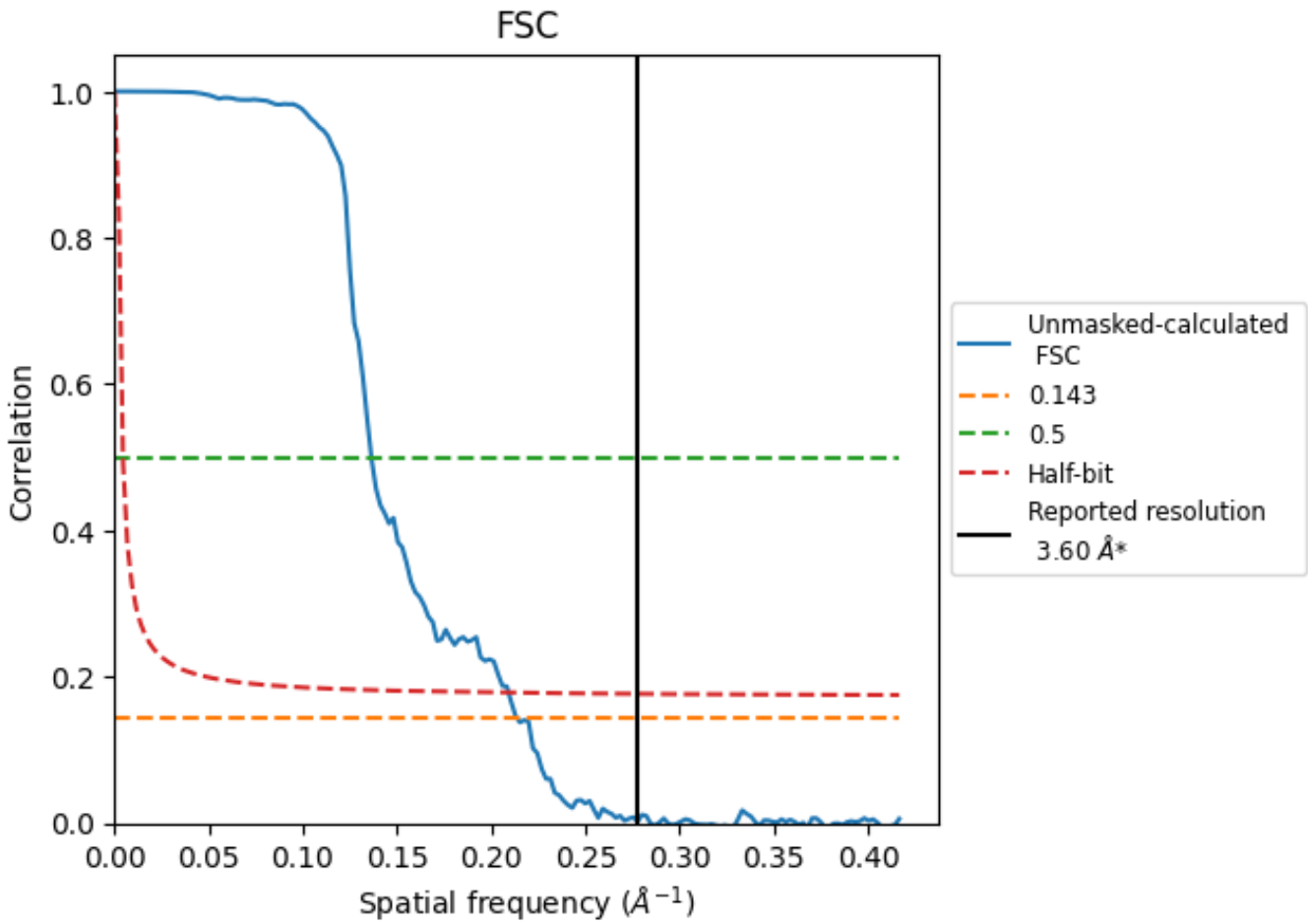


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

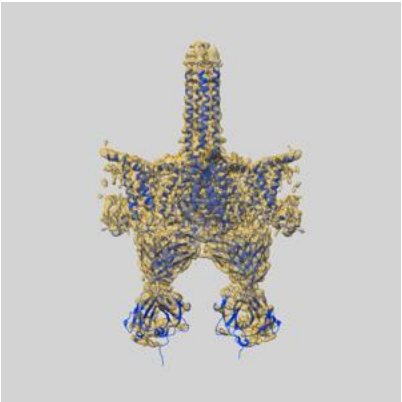
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	7.33	4.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.68 differs from the reported value 3.6 by more than 10 %

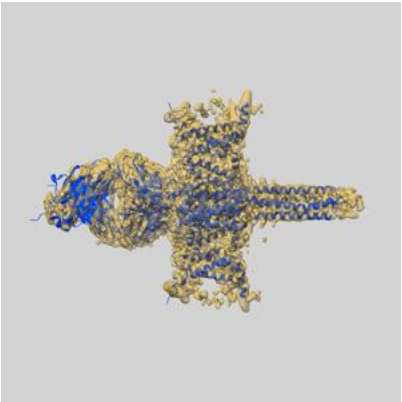
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0341 and PDB model 6N4Q. Per-residue inclusion information can be found in section 3 on page 7.

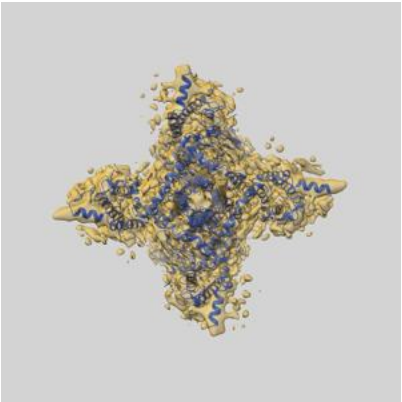
9.1 Map-model overlay (i)



X



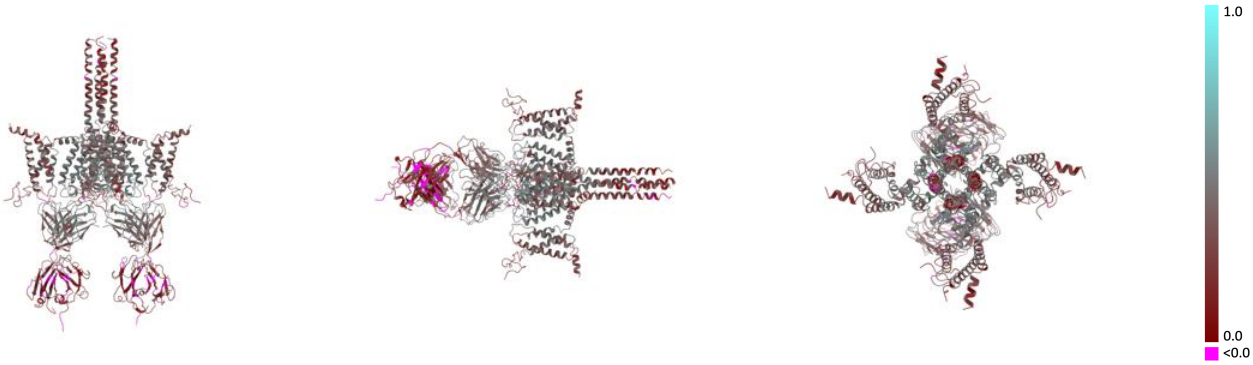
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.067 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.

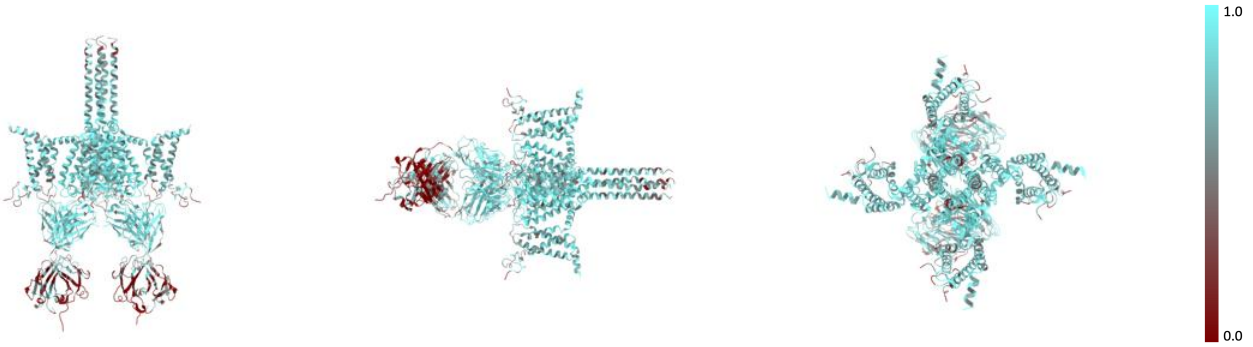
9.2 Q-score mapped to coordinate model (i)



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.

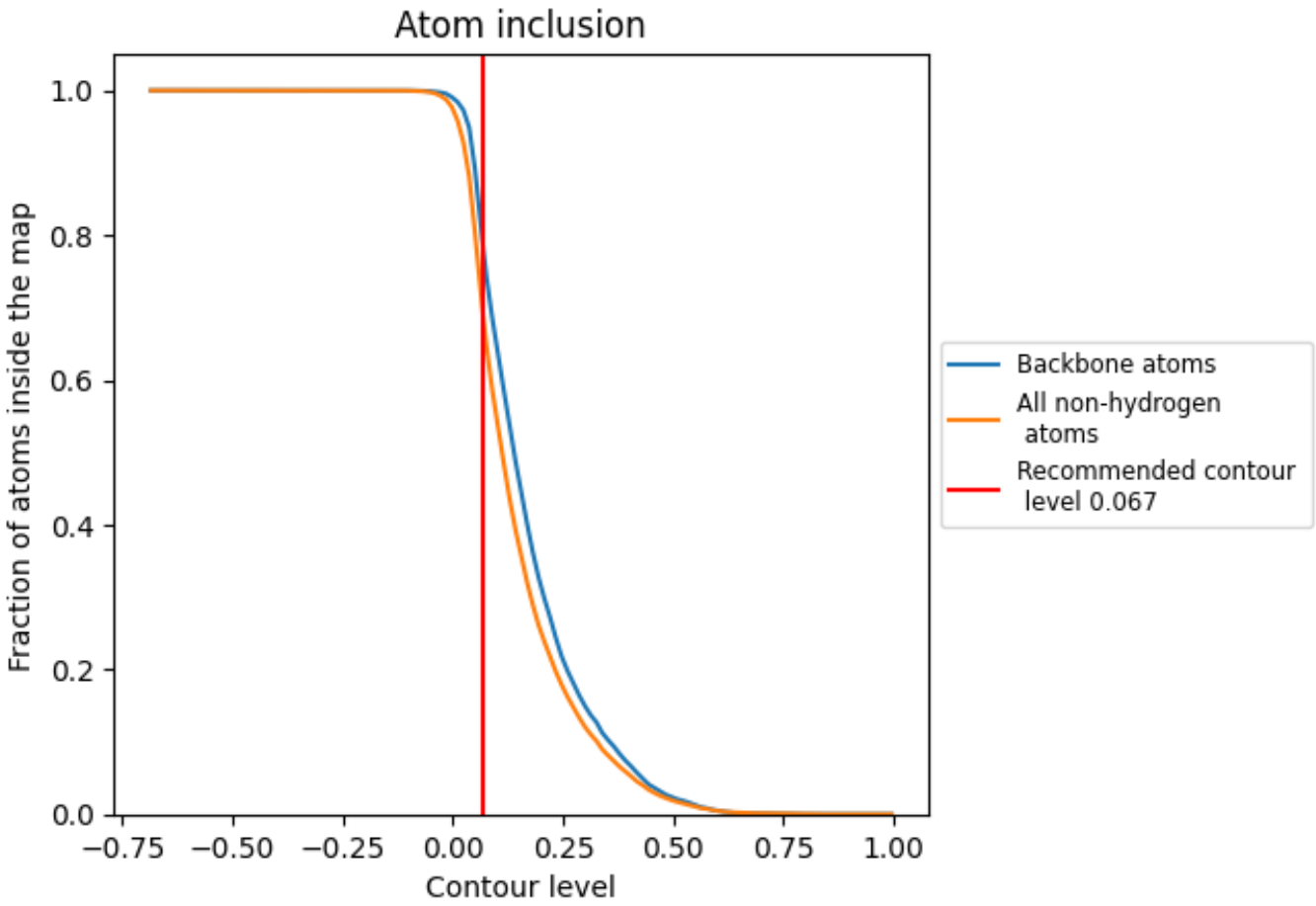
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.067).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.067) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6993	0.3430
A	0.8095	0.4010
B	0.7785	0.3920
C	0.8147	0.4030
D	0.7794	0.3880
E	0.5336	0.1950
F	0.5375	0.2370
G	0.5771	0.2190
H	0.5296	0.2280
I	0.6092	0.2800
J	0.5914	0.3080
K	0.6062	0.2790
L	0.5950	0.3060