wwPDB EM Validation Summary Report (i)

Mar 3, 2024 – 10:45 AM EST

PDB ID	:	6ANU
EMDB ID	:	EMD-8886
Title	:	Cryo-EM structure of F-actin complexed with the beta-III-spectrin actin-binding domain
Authors	:	Wang, F.; Orlova, A.; Avery, A.W.; Hays, T.S.; Egelman, E.H.
Deposited on	:	2017-08-14
Resolution	:	7.00 Å(reported)

This is a wwPDB EM Validation Summary 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:

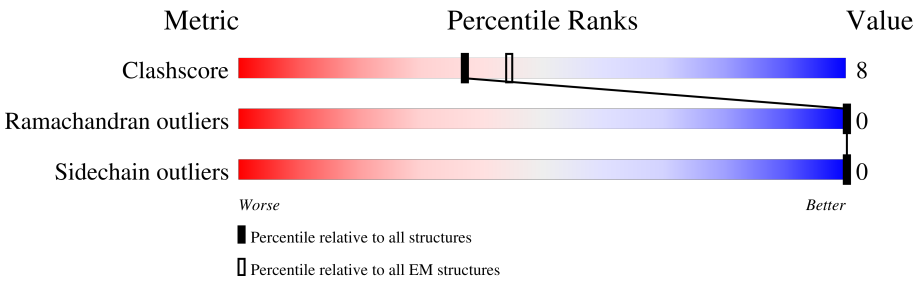
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.00 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	375	81% 19%
1	B	375	79% 21%
1	C	375	81% 19%
1	D	375	80% 20%
1	E	375	79% 21%
1	F	375	80% 20%
2	a	284	10% 47% 53%
2	b	284	10% 47% 53%

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Mol	Chain	Length	Quality of chain
2	c	284	10% 47% 53%
2	d	284	10% 47% 53%
2	e	284	10% 47% 53%
2	f	284	11% 47% 53%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24012 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 Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	375	2925	1850	491	561	23	0	0
1	A	375	2925	1850	491	561	23	0	0
1	B	375	2925	1850	491	561	23	0	0
1	C	375	2925	1850	491	561	23	0	0
1	D	375	2925	1850	491	561	23	0	0
1	E	375	2925	1850	491	561	23	0	0

- Molecule 2 is a protein called Spectrin beta chain, non-erythrocytic 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	f	133	1077	675	204	194	4	0	0
2	a	133	1077	675	204	194	4	0	0
2	b	133	1077	675	204	194	4	0	0
2	c	133	1077	675	204	194	4	0	0
2	d	133	1077	675	204	194	4	0	0
2	e	133	1077	675	204	194	4	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	1253	PRO	LEU	engineered mutation	UNP O15020
a	1253	PRO	LEU	engineered mutation	UNP O15020

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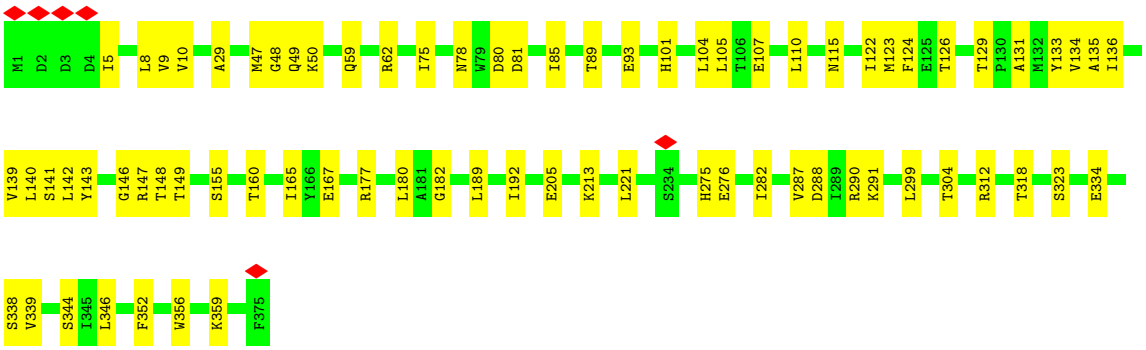
Chain	Residue	Modelled	Actual	Comment	Reference
b	1253	PRO	LEU	engineered mutation	UNP O15020
c	1253	PRO	LEU	engineered mutation	UNP O15020
d	1253	PRO	LEU	engineered mutation	UNP O15020
e	1253	PRO	LEU	engineered mutation	UNP O15020

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.

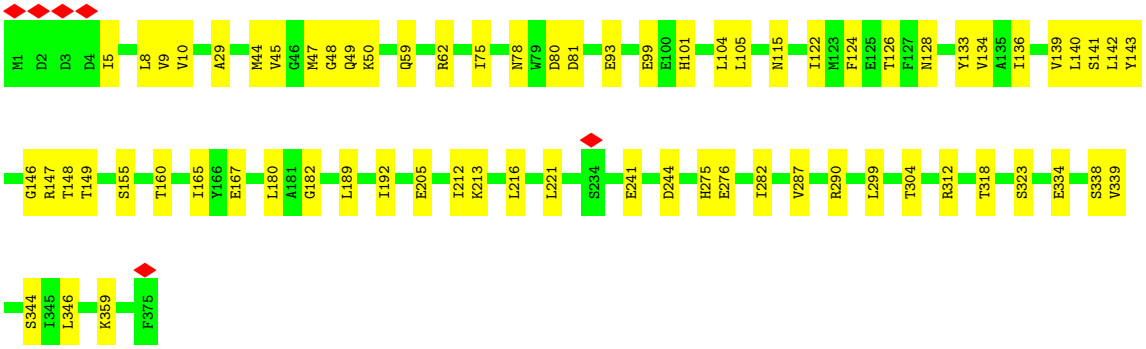
• Molecule 1: Actin, cytoplasmic 1

Chain F: 80% 20%



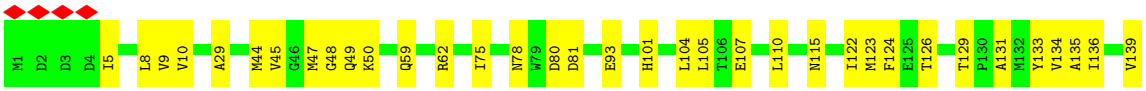
• Molecule 1: Actin, cytoplasmic 1

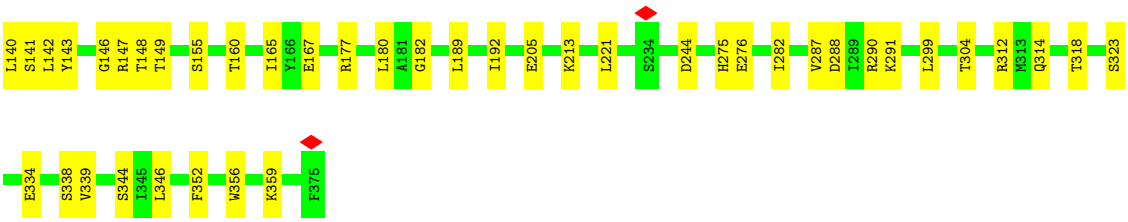
Chain A: 81% 19%



• Molecule 1: Actin, cytoplasmic 1

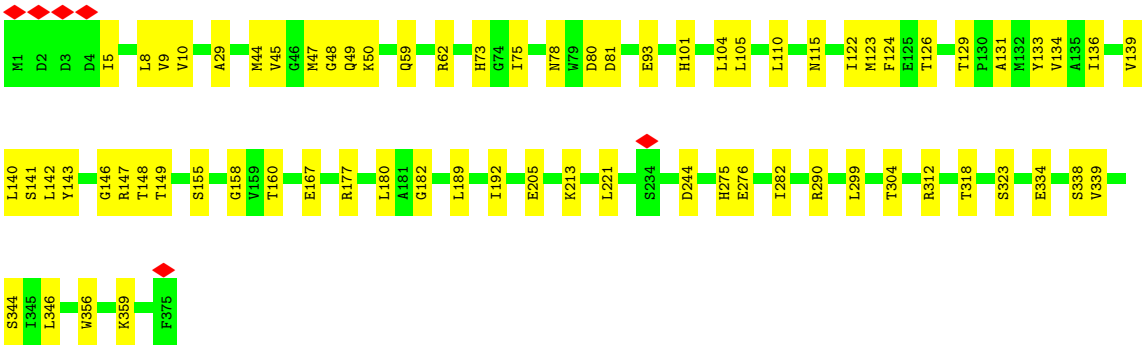
Chain B: 79% 21%





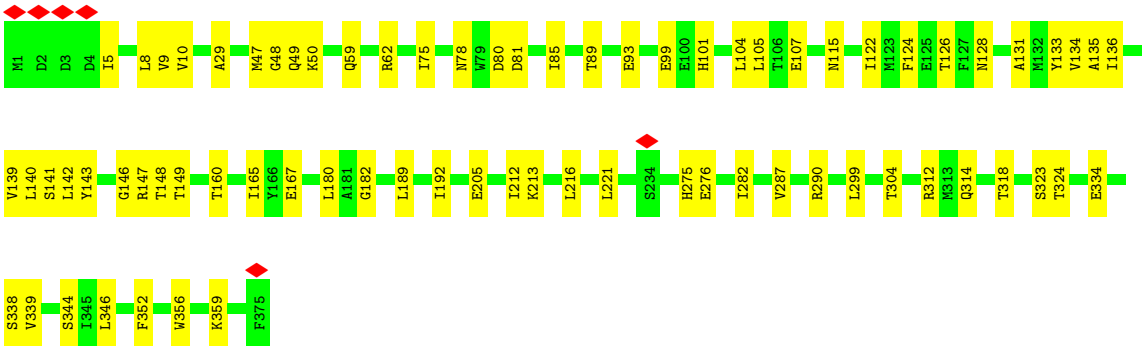
• Molecule 1: Actin, cytoplasmic 1

Chain C:



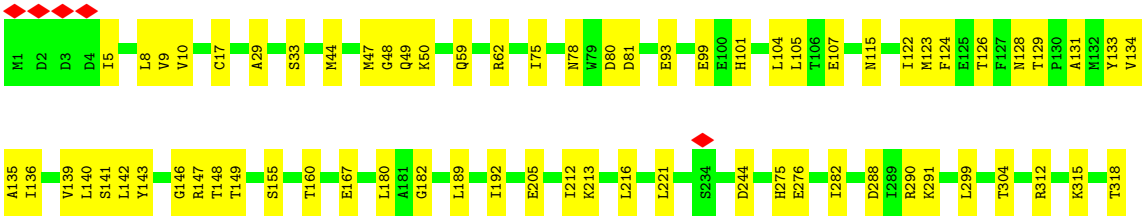
• Molecule 1: Actin, cytoplasmic 1

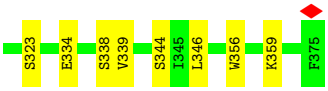
Chain D:



• Molecule 1: Actin, cytoplasmic 1

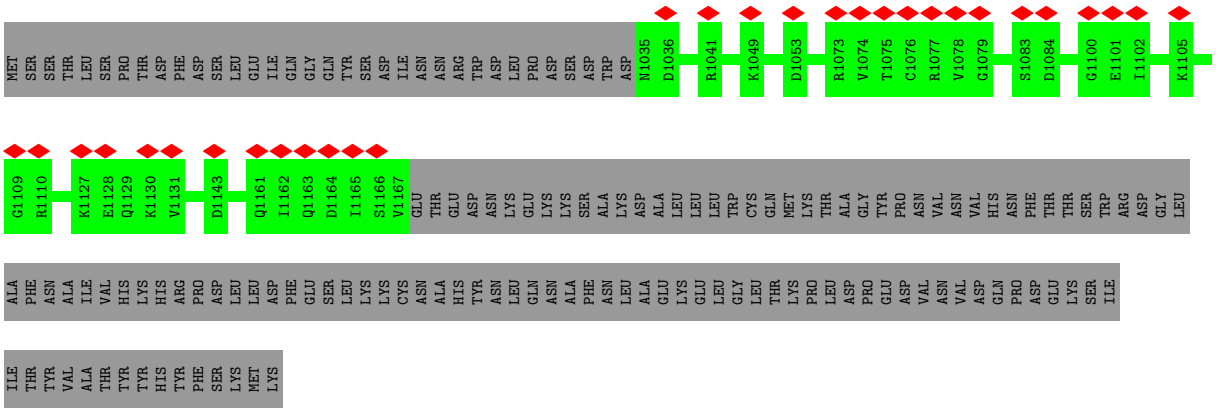
Chain E:





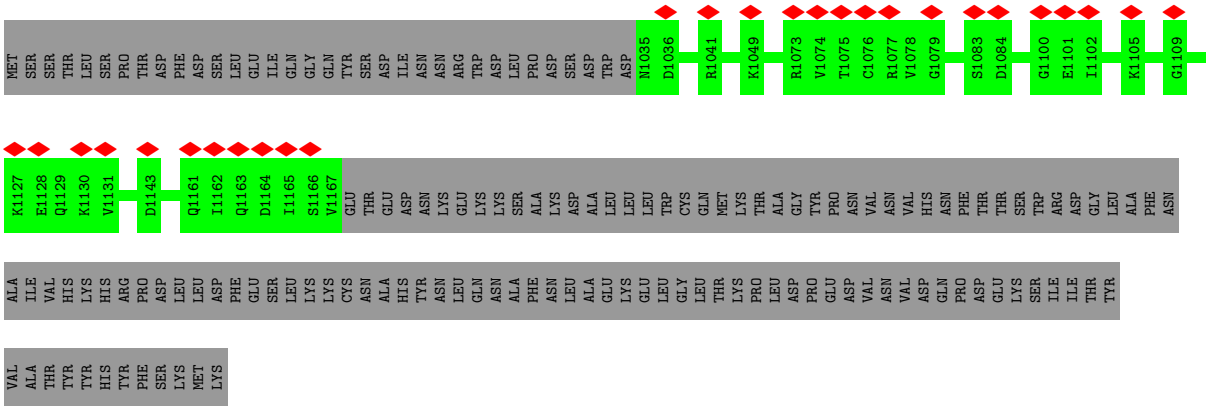
- Molecule 2: Spectrin beta chain, non-erythrocytic 2

Chain f:



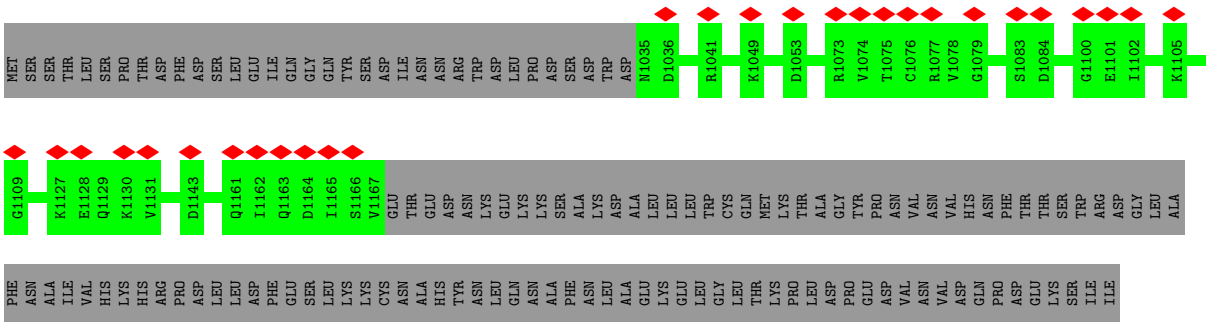
- Molecule 2: Spectrin beta chain, non-erythrocytic 2

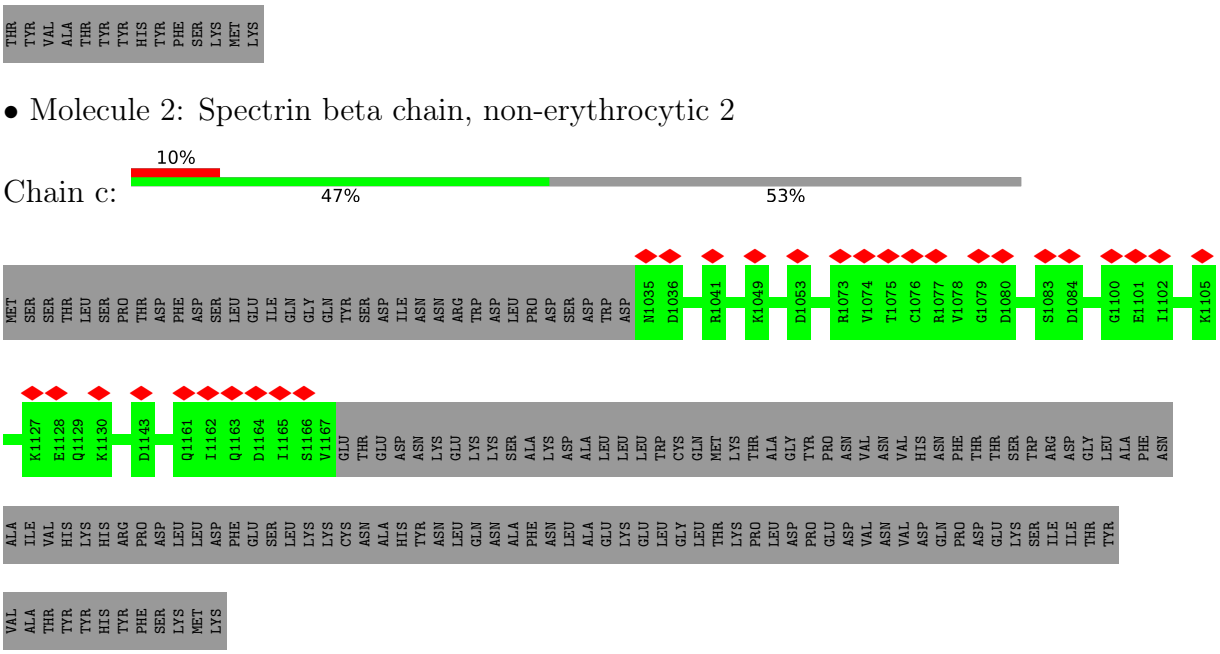
Chain a:

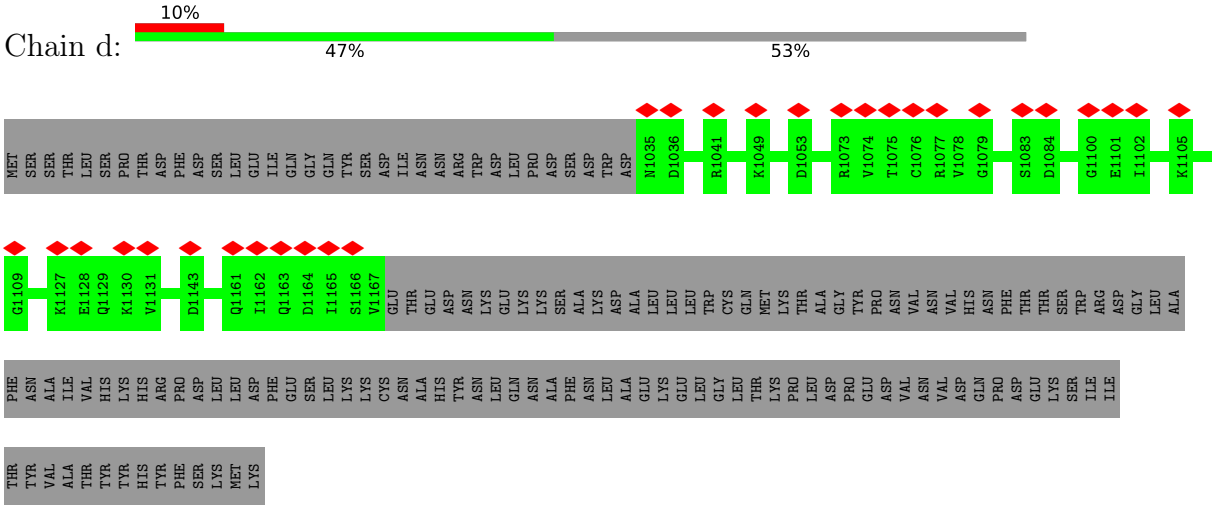


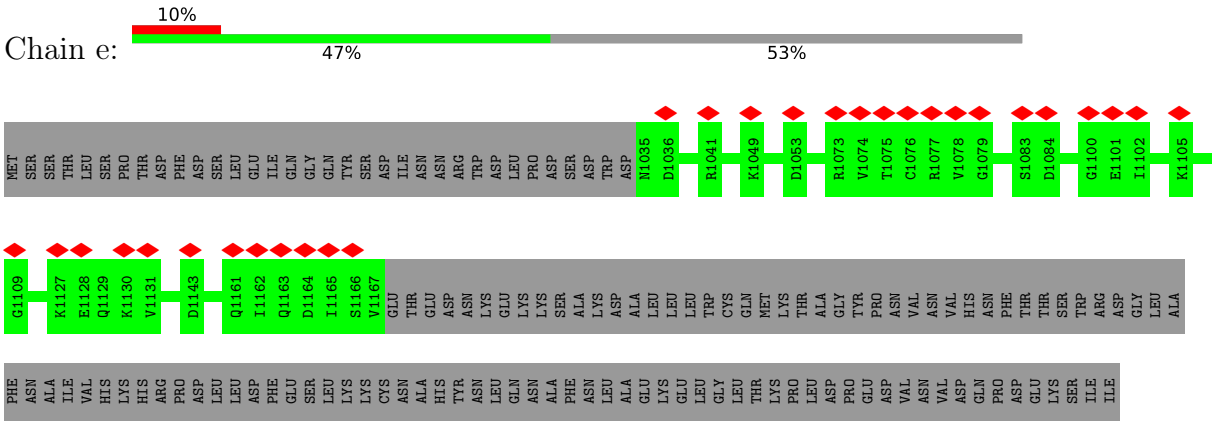
- Molecule 2: Spectrin beta chain, non-erythrocytic 2

Chain b:




THR TYR VAL ALA THR TYR TYR HIS TYR PHE SER LYS MET LYS
• Molecule 2: Spectrin beta chain, non-erythrocytic 2
Chain c:
10%
47%
53%
MET SER SER THR LEU SER PRO THR ASP PHE ASP SER LEU GLU ILE GLN GLY GLN TYR SER ASP ILE ASN ASN ARG TRP ASP LEU PRO ASP SER ASP TRP ASP N1035 D1036 R1041 K1049 D1053 R1073 V1074 T1075 C1076 R1077 V1078 G1079 D1080 S1083 D1084 G1100 E1101 I1102 K1105
K1127 E1128 Q1129 K1130 D1143 Q1161 I1162 Q1163 D1164 I1165 S1166 V1167 GLU THR GLU ASP ASN LYS GLU LYS LYS SER ALA LYS ASP ALA LEU LEU LEU TRP CYS GLN MET LYS THR ALA GLY TYR PRO ASN VAL ASN VAL HIS ASN PHE THR THR SER TRP ARG ASP GLY LEU ALA PHE ASN
ALA ILE VAL HIS LYS HIS ARG PRO ASP LEU LEU ASP PHE GLU SER LEU LYS LYS CYS ASN ALA HIS TYR ASN LEU GLN ASN ALA PHE ASN LEU ALA GLU LYS GLU LEU GLY LEU THR LYS PRO LEU ASP PRO GLU ASP VAL ASN VAL ASP GLN PRO ASP GLU LYS SER ILE ILE THR TYR
VAL ALA THR TYR TYR HIS TYR PHE SER LYS MET LYS


• Molecule 2: Spectrin beta chain, non-erythrocytic 2
Chain d:
10%
47%
53%
MET SER SER THR LEU SER PRO THR ASP PHE ASP SER LEU GLU ILE GLN GLY GLN TYR SER ASP ILE ASN ASN ARG TRP ASP LEU PRO ASP SER ASP TRP ASP N1035 D1036 R1041 K1049 D1053 R1073 V1074 T1075 C1076 R1077 V1078 G1079 S1083 D1084 G1100 E1101 I1102 K1105
G1109 K1127 E1128 Q1129 K1130 V1131 D1143 Q1161 I1162 Q1163 D1164 I1165 S1166 V1167 GLU THR GLU ASP ASN LYS GLU LYS LYS SER ALA LYS ASP ALA LEU LEU LEU TRP CYS GLN MET LYS THR ALA GLY TYR PRO ASN VAL ASN VAL HIS ASN PHE THR THR SER TRP ARG ASP GLY LEU ALA
PHE ASN ALA ILE VAL HIS LYS HIS ARG PRO ASP LEU LEU ASP PHE GLU SER LEU LYS LYS CYS ASN ALA HIS TYR ASN LEU GLN ASN ALA PHE ASN LEU ALA GLU LYS GLU LEU GLY LEU THR LYS PRO LEU ASP PRO GLU ASP VAL ASN VAL ASP GLN PRO ASP GLU LYS SER ILE ILE
THR TYR VAL ALA THR TYR TYR HIS TYR PHE SER LYS MET LYS


• Molecule 2: Spectrin beta chain, non-erythrocytic 2
Chain e:
10%
47%
53%
MET SER SER THR LEU SER PRO THR ASP PHE ASP SER LEU GLU ILE GLN GLY GLN TYR SER ASP ILE ASN ASN ARG TRP ASP LEU PRO ASP SER ASP TRP ASP N1035 D1036 R1041 K1049 D1053 R1073 V1074 T1075 C1076 R1077 V1078 G1079 S1083 D1084 G1100 E1101 I1102 K1105
G1109 K1127 E1128 Q1129 K1130 V1131 D1143 Q1161 I1162 Q1163 D1164 I1165 S1166 V1167 GLU THR GLU ASP ASN LYS GLU LYS LYS SER ALA LYS ASP ALA LEU LEU LEU TRP CYS GLN MET LYS THR ALA GLY TYR PRO ASN VAL ASN VAL HIS ASN PHE THR THR SER TRP ARG ASP GLY LEU ALA
PHE ASN ALA ILE VAL HIS LYS HIS ARG PRO ASP LEU LEU ASP PHE GLU SER LEU LYS LYS CYS ASN ALA HIS TYR ASN LEU GLN ASN ALA PHE ASN LEU ALA GLU LYS GLU LEU GLY LEU THR LYS PRO LEU ASP PRO GLU ASP VAL ASN VAL ASP GLN PRO ASP GLU LYS SER ILE ILE

THR
TYR
VAL
ALA
THR
TYR
TYR
HIS
TYR
PHE
SER
LYS
MET
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.87°, rise=27.25 Å, axial sym=C1	Depositor
Number of segments used	12443	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.429	Depositor
Minimum map value	-0.622	Depositor
Average map value	0.121	Depositor
Map value standard deviation	0.327	Depositor
Recommended contour level	0.95	Depositor
Map size (Å)	209.99998, 209.99998, 209.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.38	0/2988	0.63	0/4045
1	B	0.38	0/2988	0.63	0/4045
1	C	0.38	0/2988	0.63	0/4045
1	D	0.38	0/2988	0.63	0/4045
1	E	0.38	0/2988	0.63	0/4045
1	F	0.38	0/2988	0.63	0/4045
2	a	0.33	0/1092	0.63	0/1468
2	b	0.33	0/1092	0.63	0/1468
2	c	0.33	0/1092	0.63	0/1468
2	d	0.33	0/1092	0.63	0/1468
2	e	0.33	0/1092	0.63	0/1468
2	f	0.33	0/1092	0.63	0/1468
All	All	0.37	0/24480	0.63	0/33078

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	2925	0	2891	46	0
1	B	2925	0	2891	50	0
1	C	2925	0	2891	43	0
1	D	2925	0	2891	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2925	0	2891	47	0
1	F	2925	0	2891	46	0
2	a	1077	0	1112	0	0
2	b	1077	0	1112	0	0
2	c	1077	0	1112	0	0
2	d	1077	0	1112	0	0
2	e	1077	0	1112	0	0
2	f	1077	0	1112	0	0
All	All	24012	0	24018	262	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 8.

The worst 5 of 262 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:124:PHE:O	1:B:359:LYS:NZ	2.15	0.80
1:F:124:PHE:O	1:F:359:LYS:NZ	2.15	0.80
1:A:124:PHE:O	1:A:359:LYS:NZ	2.15	0.80
1:C:124:PHE:O	1:C:359:LYS:NZ	2.15	0.80
1:D:124:PHE:O	1:D:359:LYS:NZ	2.15	0.80

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	373/375 (100%)	342 (92%)	31 (8%)	0	100	100
1	B	373/375 (100%)	342 (92%)	31 (8%)	0	100	100
1	C	373/375 (100%)	342 (92%)	31 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	373/375 (100%)	342 (92%)	31 (8%)	0	100	100
1	E	373/375 (100%)	342 (92%)	31 (8%)	0	100	100
1	F	373/375 (100%)	342 (92%)	31 (8%)	0	100	100
2	a	131/284 (46%)	125 (95%)	6 (5%)	0	100	100
2	b	131/284 (46%)	125 (95%)	6 (5%)	0	100	100
2	c	131/284 (46%)	125 (95%)	6 (5%)	0	100	100
2	d	131/284 (46%)	125 (95%)	6 (5%)	0	100	100
2	e	131/284 (46%)	125 (95%)	6 (5%)	0	100	100
2	f	131/284 (46%)	125 (95%)	6 (5%)	0	100	100
All	All	3024/3954 (76%)	2802 (93%)	222 (7%)	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	318/318 (100%)	318 (100%)	0	100	100
1	B	318/318 (100%)	318 (100%)	0	100	100
1	C	318/318 (100%)	318 (100%)	0	100	100
1	D	318/318 (100%)	318 (100%)	0	100	100
1	E	318/318 (100%)	318 (100%)	0	100	100
1	F	318/318 (100%)	318 (100%)	0	100	100
2	a	120/258 (46%)	120 (100%)	0	100	100
2	b	120/258 (46%)	120 (100%)	0	100	100
2	c	120/258 (46%)	120 (100%)	0	100	100
2	d	120/258 (46%)	120 (100%)	0	100	100
2	e	120/258 (46%)	120 (100%)	0	100	100
2	f	120/258 (46%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2628/3456 (76%)	2628 (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. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	296	ASN
2	d	1118	ASN
1	D	115	ASN
2	a	1118	ASN
1	D	40	HIS

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.

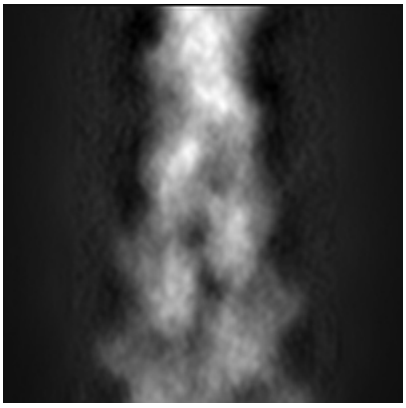
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8886. These allow visual inspection of the internal detail of the map and identification of artifacts.

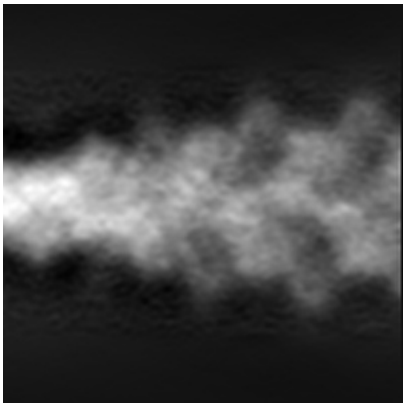
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

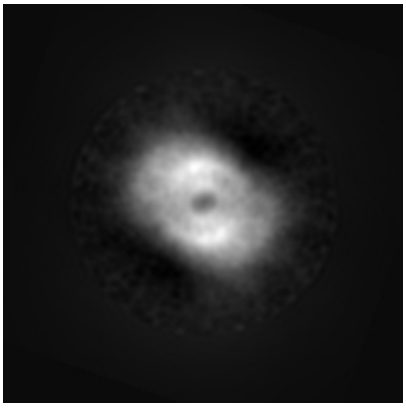
6.1.1 Primary map



X



Y

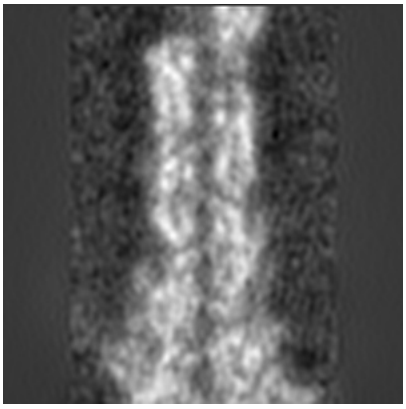


Z

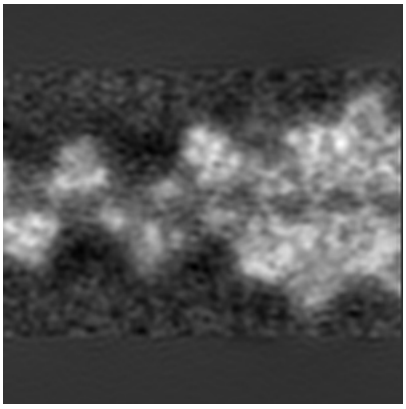
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

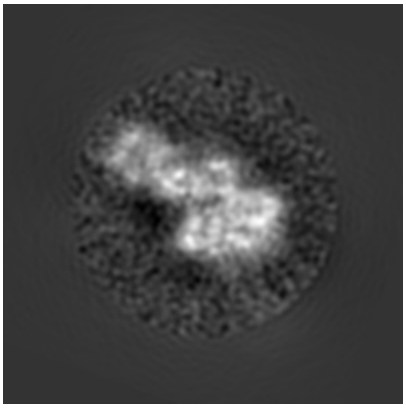
6.2.1 Primary map



X Index: 100



Y Index: 100

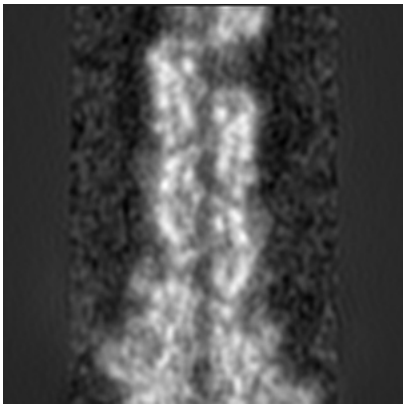


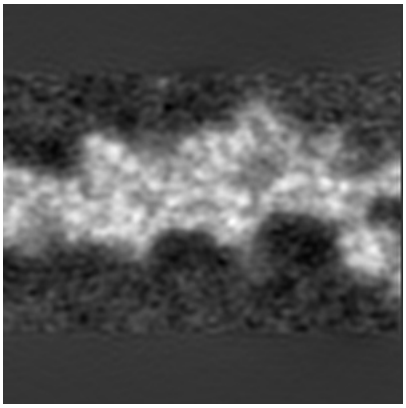
Z Index: 100

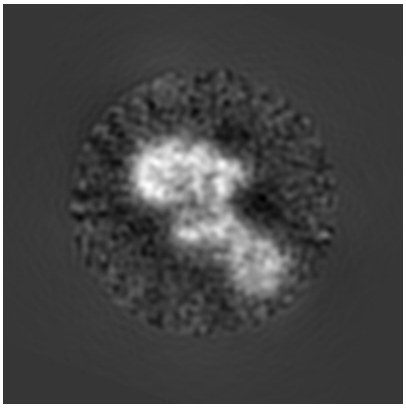
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 102

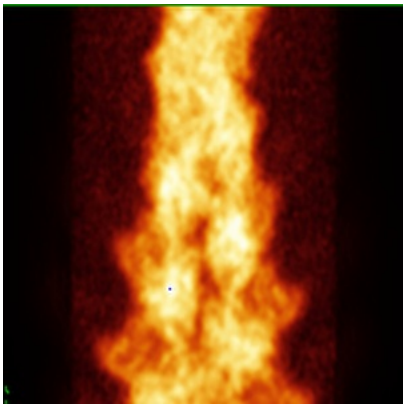

Y Index: 84

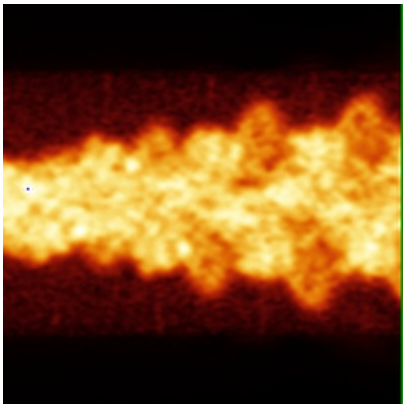

Z Index: 79

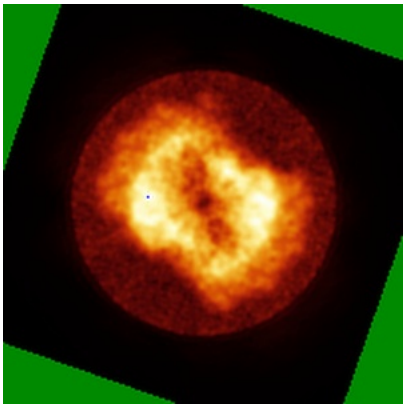
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

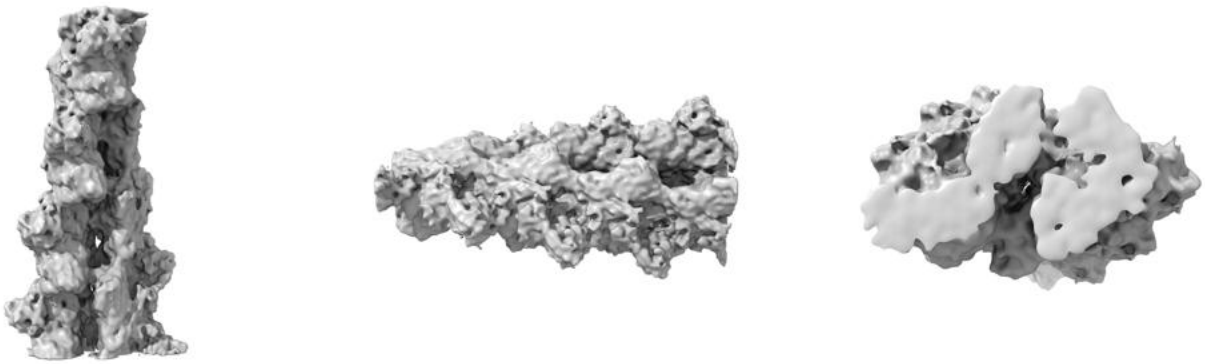

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.95. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

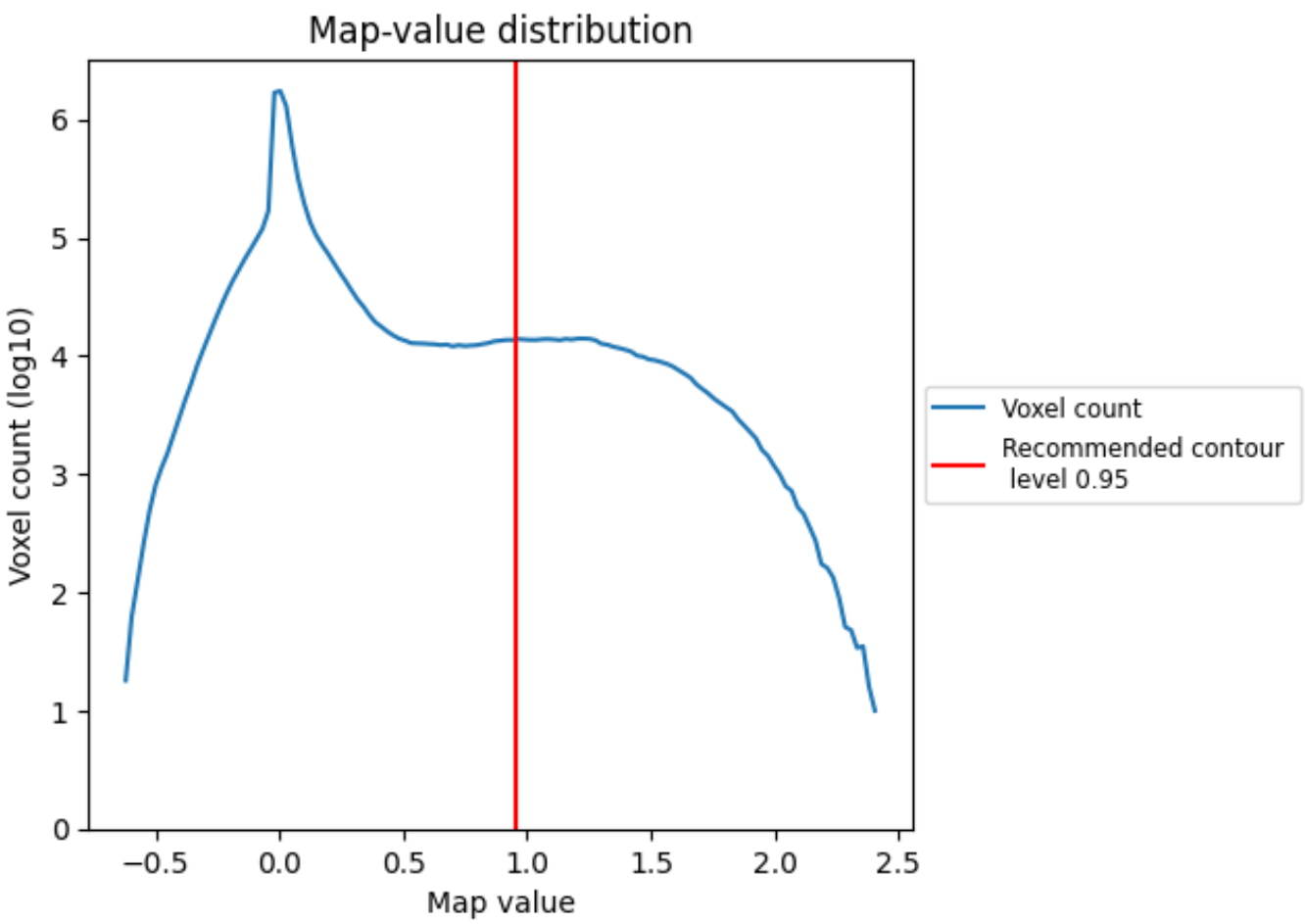
6.6 Mask visualisation (i)

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

7 Map analysis (i)

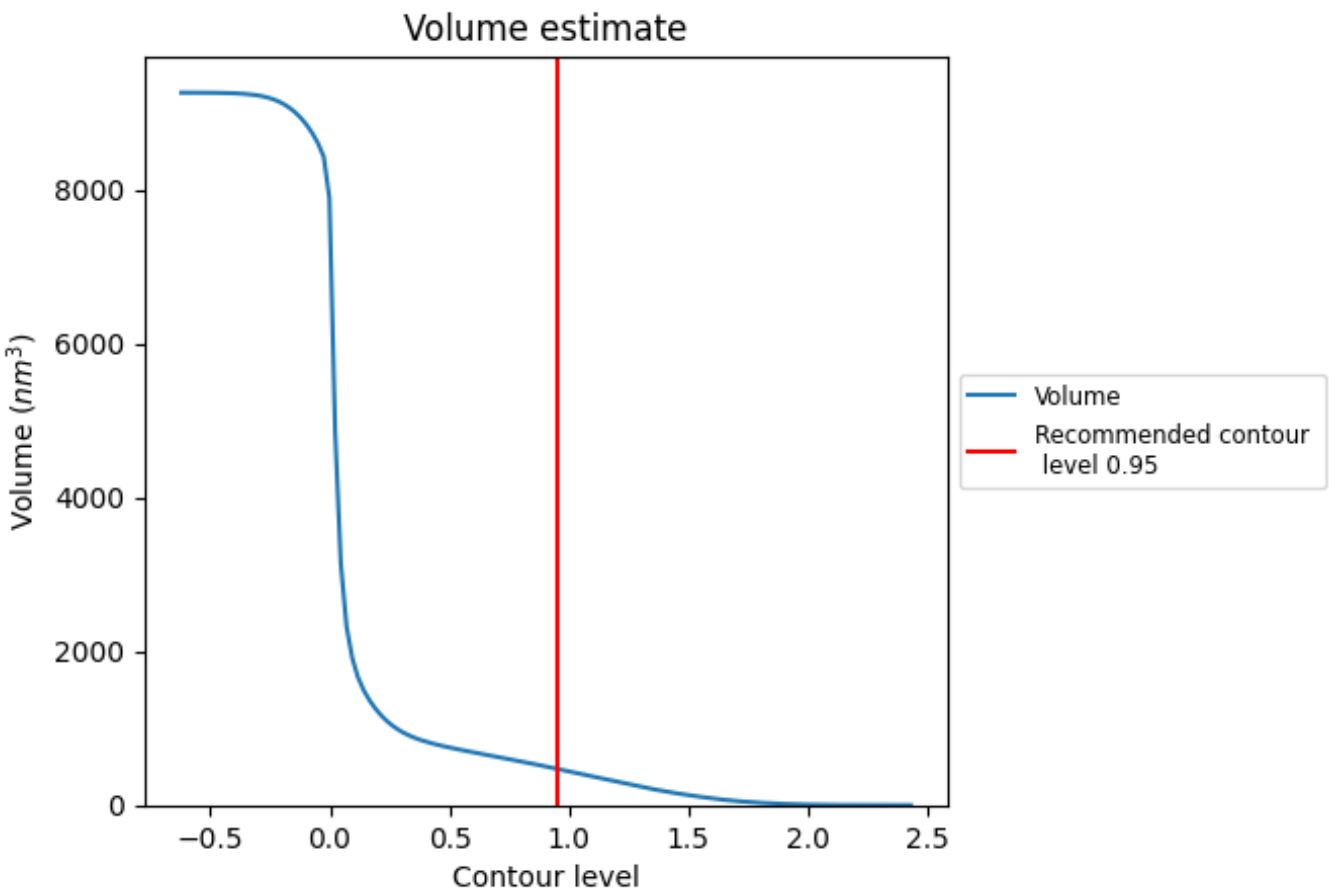
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

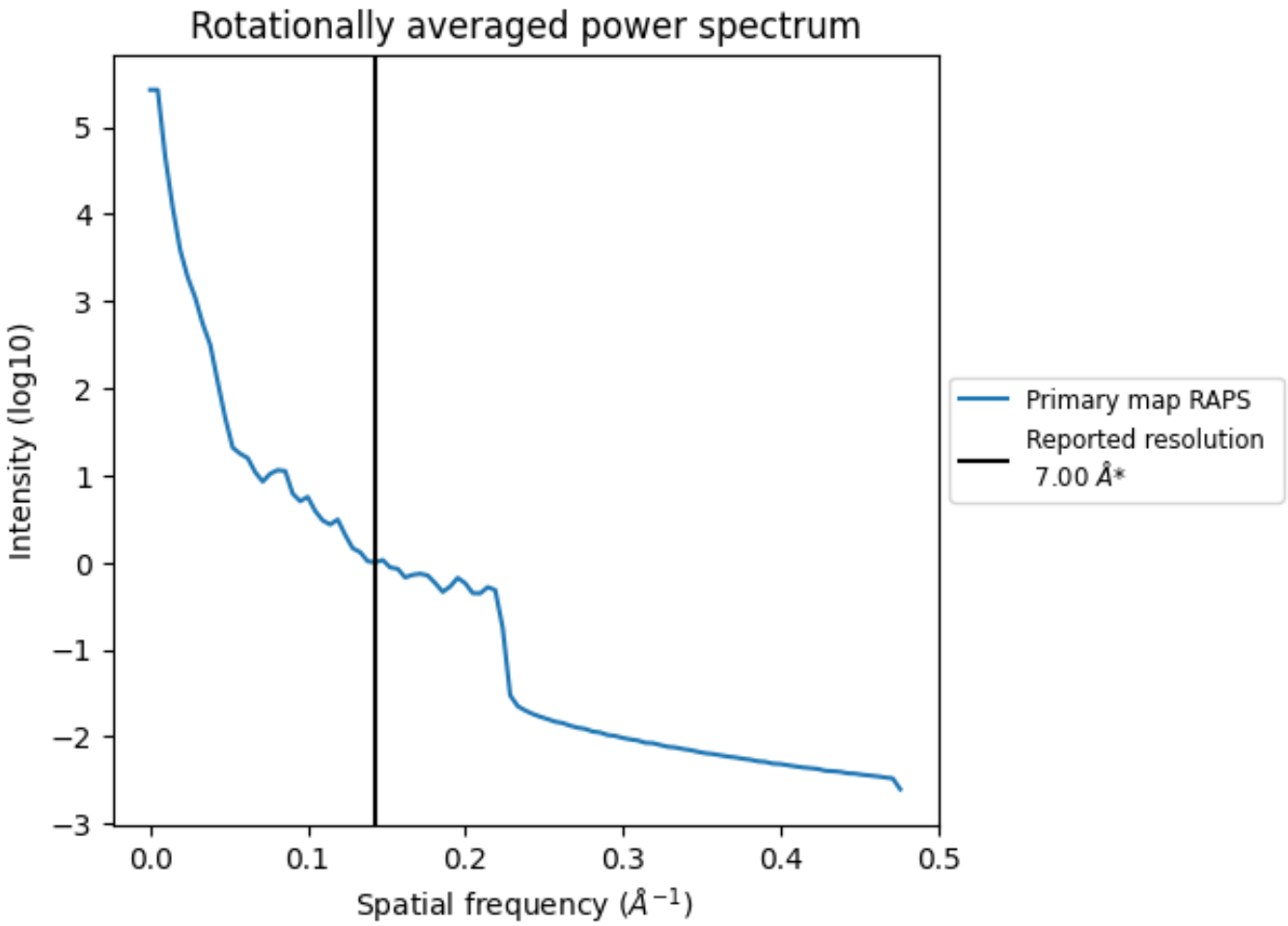
7.2 Volume estimate (i)



The volume at the recommended contour level is 472 nm^3; this corresponds to an approximate mass of 426 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 0.143 Å^{-1}

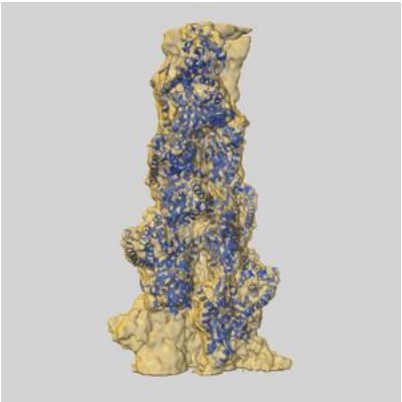
8 Fourier-Shell correlation (i)

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

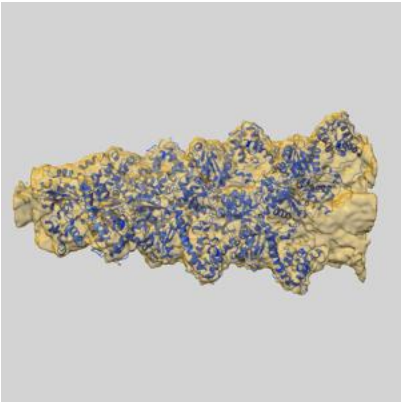
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8886 and PDB model 6ANU. Per-residue inclusion information can be found in section 3 on page 6.

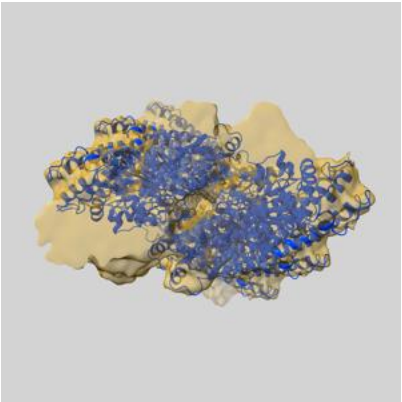
9.1 Map-model overlay (i)



X



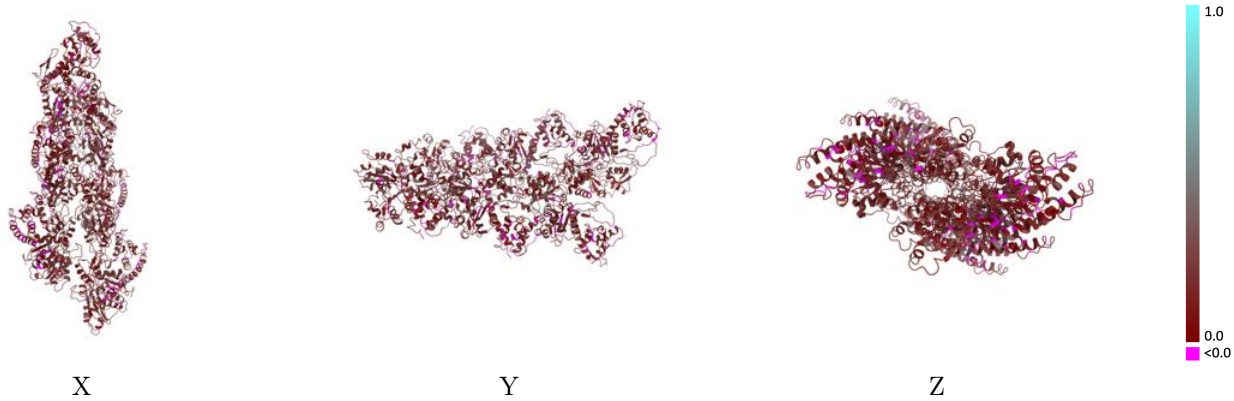
Y



Z

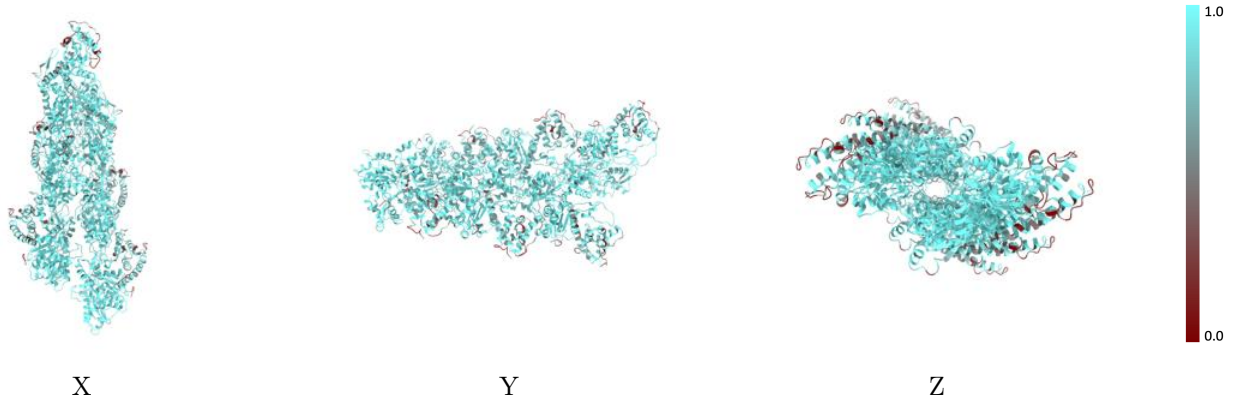
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



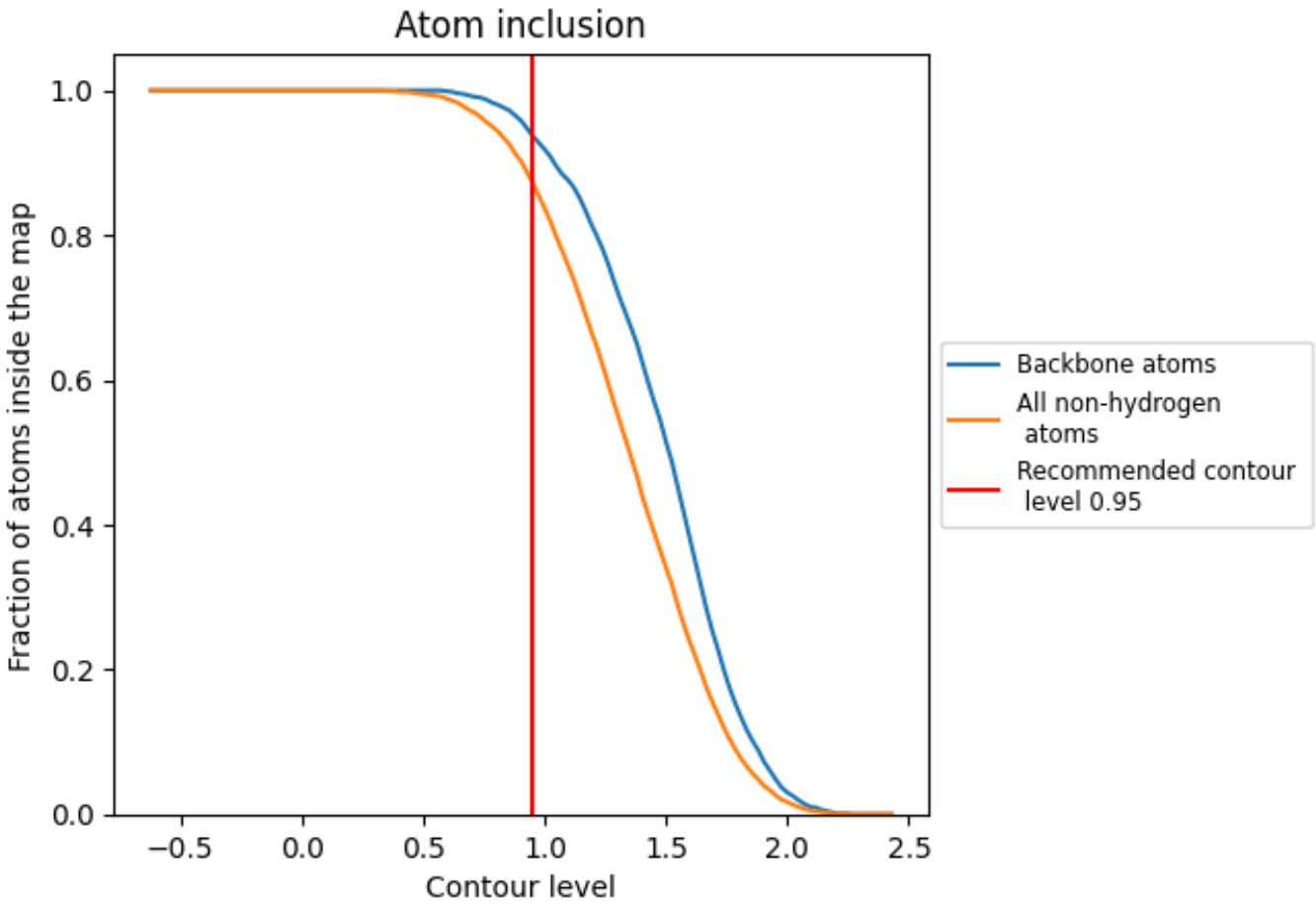
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.95).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.1720
A	0.9340	0.1880
B	0.9360	0.1870
C	0.9350	0.1860
D	0.9330	0.1880
E	0.9340	0.1880
F	0.9350	0.1870
a	0.7050	0.1300
b	0.7090	0.1330
c	0.7160	0.1310
d	0.7020	0.1320
e	0.7090	0.1280
f	0.6920	0.1280