



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 02:12 PM EST

PDB ID : 6CU8
EMDB ID : EMD-7619
Title : Alpha Synuclein fibril formed by full length protein - Twister Polymorph
Authors : Li, B.; Hatami, A.; Ge, P.; Murray, K.A.; Sheth, P.; Zhang, M.; Nair, G.; Sawaya, M.R.; Zhu, C.; Broad, M.; Shin, W.S.; Ye, S.; John, V.; Eisenberg, D.S.; Zhou, Z.H.; Jiang, L.
Deposited on : 2018-03-23
Resolution : 3.60 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

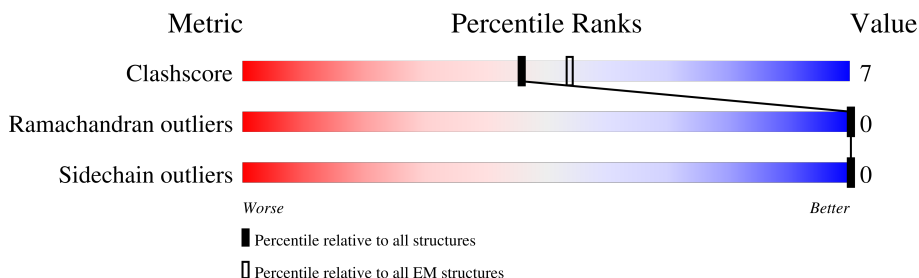
1 Overall quality at a glance

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	140	
1	B	140	
1	C	140	
1	D	140	
1	E	140	
1	F	140	
1	G	140	
1	H	140	

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Mol	Chain	Length	Quality of chain
1	I	140	 27%71%
1	J	140	 28%71%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2880 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 Alpha-synuclein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	41	Total	C	N	O	0	0
			288	178	51	59		
1	A	41	Total	C	N	O	0	0
			288	178	51	59		
1	B	41	Total	C	N	O	0	0
			288	178	51	59		
1	C	41	Total	C	N	O	0	0
			288	178	51	59		
1	D	41	Total	C	N	O	0	0
			288	178	51	59		
1	F	41	Total	C	N	O	0	0
			288	178	51	59		
1	G	41	Total	C	N	O	0	0
			288	178	51	59		
1	H	41	Total	C	N	O	0	0
			288	178	51	59		
1	I	41	Total	C	N	O	0	0
			288	178	51	59		
1	J	41	Total	C	N	O	0	0
			288	178	51	59		

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

• Molecule 1: Alpha-synuclein

Chain D:  26% 71%

MET
ASP
VAL
PHE
MET
GLY
LEU
SER
LYS
LYS
ALA
GLN
LEU
GLY
LYS
VAL
GLU
VAL
ALA
ALA
GLU
LYS
THR
GLY
GLN
GLY
VAL
ALA
ASP
MET
GLU
PRO
ALA
ALA
GLY
LYS
THR
ASN
GLY
GLY
VAL
LEU
GLU
ASP
MET
PRO
VAL
ASP
PRO
ASN
GLY
GLY
VAL
LEU
TYR
GLU
MET
VAL
TYR
GLY
SER
GLY
SER
K43
E57
K58
N65
V66
T72
G73
V74
E83
GLY
ALA
GLY
SER
ILE

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

• Molecule 1: Alpha-synuclein

Chain F:  25% 71%

MET
ASP
VAL
PHE
MET
GLY
LEU
SER
LYS
LYS
ALA
GLN
LEU
GLY
LYS
VAL
GLU
VAL
ALA
ALA
GLU
LYS
THR
GLY
GLN
GLY
VAL
LEU
GLU
ASP
MET
GLU
PRO
ALA
ALA
GLY
LYS
THR
ASN
GLY
GLY
VAL
LEU
TYR
GLU
MET
VAL
TYR
GLY
SER
GLY
SER
K43
T44
E57
K58
T59
K60
N65
V66
T72
G73
V74
E83
GLY
ALA
GLY
SER

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

• Molecule 1: Alpha-synuclein

Chain G:  25% 71%

MET
ASP
VAL
PHE
MET
GLY
LEU
SER
LYS
LYS
ALA
GLN
LEU
GLY
LYS
VAL
GLU
VAL
ALA
ALA
GLU
LYS
THR
GLY
GLN
GLY
VAL
LEU
GLU
ASP
MET
GLU
PRO
ALA
ALA
GLY
LYS
THR
ASN
GLY
GLY
VAL
LEU
TYR
GLU
MET
VAL
TYR
GLY
SER
SER
K43
T44
E46
E57
K58
T59
K60
N65
T72
G73
V74
E83
GLY
ALA
GLY

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

• Molecule 1: Alpha-synuclein

Chain H:  26% 71%

MET
ASP
VAL
PHE
MET
GLY
LEU
SER
LYS
LYS
ALA
GLN
LEU
GLY
LYS
VAL
GLU
VAL
ALA
ALA
GLU
LYS
THR
GLY
GLN
GLY
VAL
LEU
GLU
ASP
MET
GLU
PRO
ALA
ALA
GLY
LYS
THR
ASN
GLY
GLY
VAL
LEU
TYR
GLU
MET
VAL
TYR
GLY
SER
SER
K43
E57
K58
T59
K60
N65
T72
G73
V74
E83
GLY
ALA
GLY
SER

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

• Molecule 1: Alpha-synuclein

Chain I:  27% 71%

MET
ASP
VAL
PHE
MET
GLY
LEU
SER
LYS
LYS
ALA
GLN
LEU
GLY
LYS
VAL
GLU
VAL
ALA
ALA
GLU
LYS
THR
GLY
GLN
GLY
VAL
LEU
GLU
ASP
MET
GLU
PRO
ALA
ALA
GLY
LYS
THR
ASN
GLY
GLY
VAL
LEU
TYR
GLU
MET
VAL
TYR
GLY
SER
SER
K43
T44
K45
E46
E57
K58
N65
E83
GLY
ALA
GLY
SER
ILE
ALA
ALA

ALA	THR	GLY	PHE	VAL	LYS	ASP	GLN	GLY	LYS	ASN	GLU	GLY	ALA	PRO	GLN	GLY	ILE	LEU	GLU	ASP	MET	PRO	VAL	ASP	PRO	ASP	ASN	GLU	ALA	TYR	GLU	MET	PRO	SER	GLU	GLY	TYR	GLN	ASP	TYR	GLU	PRO	GLU	ALA
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● Molecule 1: Alpha-synuclein



MET	ASP	VAL	PHE	LYS	MET	GLY	LEU	SER	LYS	ALA	LYS	GLU	GLY	VAL	ALA	GLN	ALA	GLY	GLU	LYS	THR	LYS	GLN	GLY	VAL	ALA	GLU	LYS	THR	LYS	GLU	TYR	GLY	VAL	LEU	TYR	VAL	GLY	SER	K43	T44	E57	K58	I72	E83	GLY	ALA	GLY	SER	ILE	ALA	ALA	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY	PHE	VAL	LYS	ASP	GLN	LEU	GLY	LYS	ASN	GLU	GLY	ALA	PRO	GLN	GLY	ILE	LEU	GLU	ASP	MET	PRO	VAL	ASP	PRO	ASP	ASN	GLU	ALA	TYR	GLU	MET	PRO	SER	GLU	GLY	TYR	GLN	ASP	TYR	GLU	PRO	GLU	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=179.06°, rise=2.4 Å, axial sym=C1	Depositor
Number of segments used	34091	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0085	Depositor
Map size (Å)	205.44, 205.44, 205.44	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.27	0/288	0.61	0/390
1	B	0.26	0/288	0.61	0/390
1	C	0.27	0/288	0.61	0/390
1	D	0.27	0/288	0.61	0/390
1	E	0.27	0/288	0.61	0/390
1	F	0.26	0/288	0.61	0/390
1	G	0.27	0/288	0.61	0/390
1	H	0.27	0/288	0.61	0/390
1	I	0.26	0/288	0.61	0/390
1	J	0.27	0/288	0.61	0/390
All	All	0.27	0/2880	0.61	0/3900

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	288	0	305	4	0
1	B	288	0	305	5	0
1	C	288	0	305	5	0
1	D	288	0	305	7	0
1	E	288	0	305	8	0
1	F	288	0	305	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	288	0	305	6	0
1	H	288	0	305	6	0
1	I	288	0	305	3	0
1	J	288	0	305	2	0
All	All	2880	0	3050	39	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 7.

The worst 5 of 39 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:E:65:ASN:OD1	1:E:65:ASN:N	2.41	0.53
1:H:65:ASN:OD1	1:H:65:ASN:N	2.41	0.53
1:B:57:GLU:HG2	1:B:58:LYS:HG3	1.96	0.47
1:D:57:GLU:HG2	1:D:58:LYS:HG3	1.96	0.47
1:I:57:GLU:HG2	1:I:58:LYS:HG3	1.96	0.47

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	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	B	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	C	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	D	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	E	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	F	39/140 (28%)	37 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	H	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	I	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
1	J	39/140 (28%)	37 (95%)	2 (5%)	0	100	100
All	All	390/1400 (28%)	370 (95%)	20 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	31/103 (30%)	31 (100%)	0	100	100
1	B	31/103 (30%)	31 (100%)	0	100	100
1	C	31/103 (30%)	31 (100%)	0	100	100
1	D	31/103 (30%)	31 (100%)	0	100	100
1	E	31/103 (30%)	31 (100%)	0	100	100
1	F	31/103 (30%)	31 (100%)	0	100	100
1	G	31/103 (30%)	31 (100%)	0	100	100
1	H	31/103 (30%)	31 (100%)	0	100	100
1	I	31/103 (30%)	31 (100%)	0	100	100
1	J	31/103 (30%)	31 (100%)	0	100	100
All	All	310/1030 (30%)	310 (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.

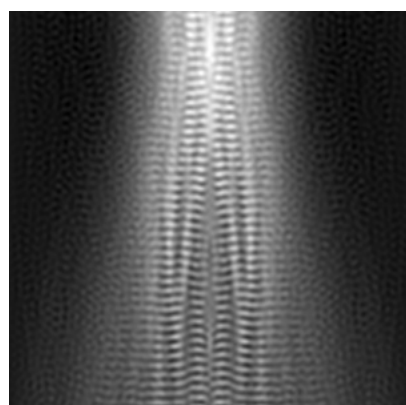
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7619. These allow visual inspection of the internal detail of the map and identification of artifacts.

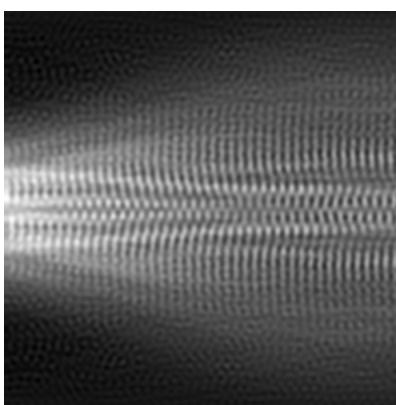
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

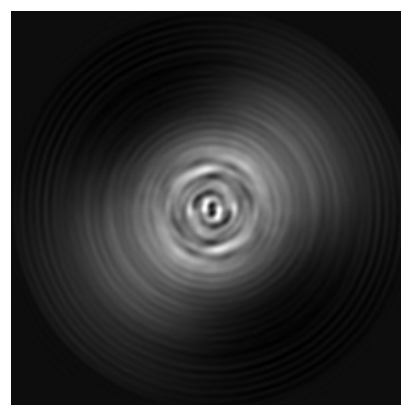
6.1.1 Primary map



X



Y

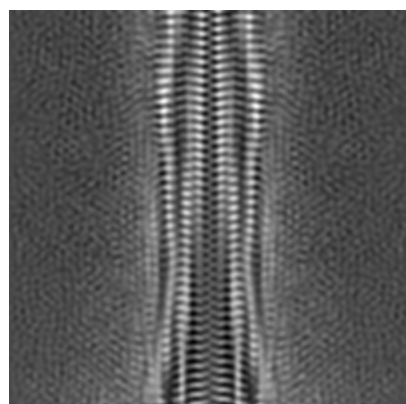


Z

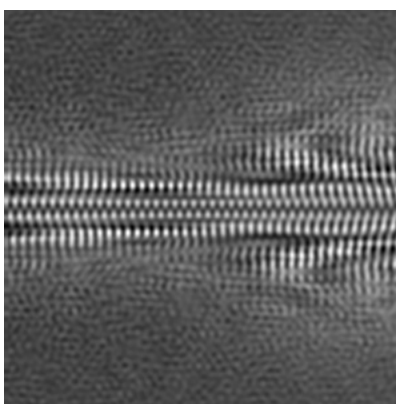
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

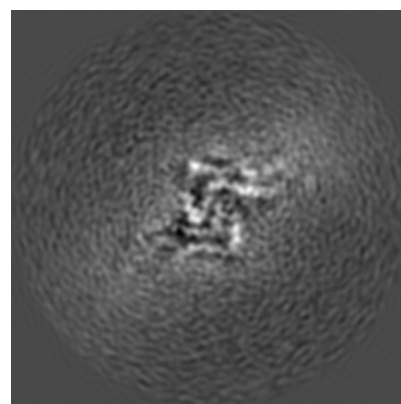
6.2.1 Primary map



X Index: 96



Y Index: 96

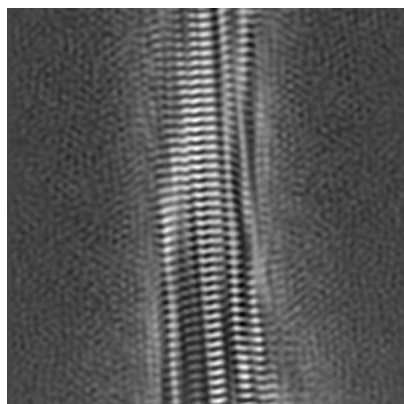


Z Index: 96

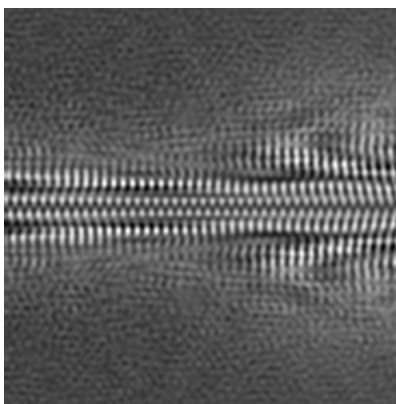
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

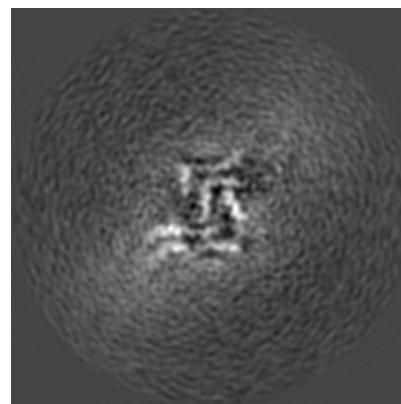
6.3.1 Primary map



X Index: 106



Y Index: 96



Z Index: 75

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 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

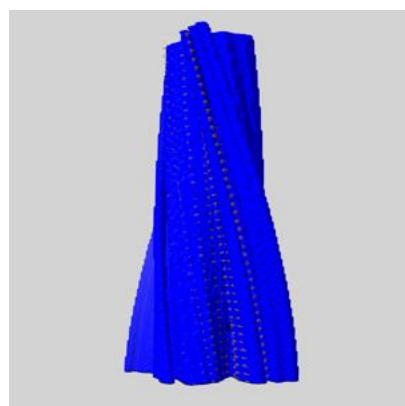
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

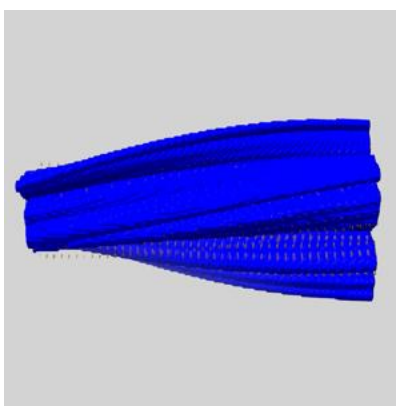
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

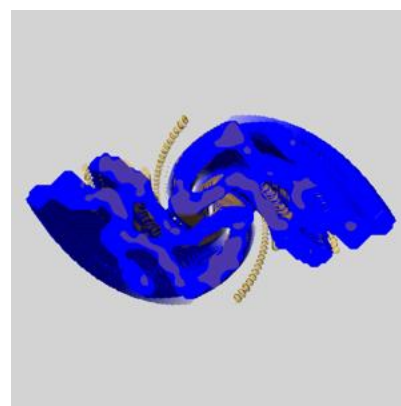
6.5.1 emd_7619_msk_1.map [i](#)



X



Y

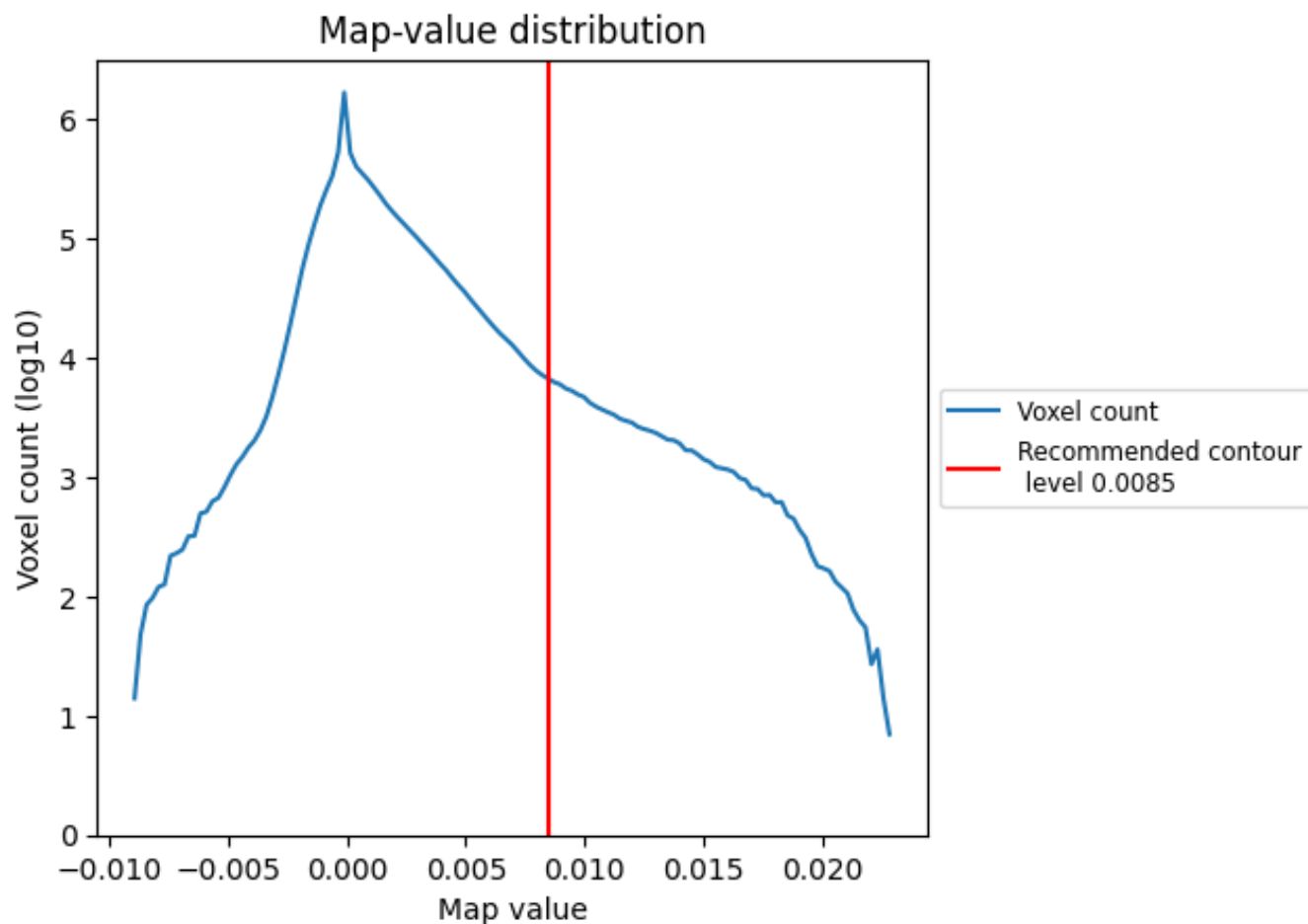


Z

7 Map analysis [i](#)

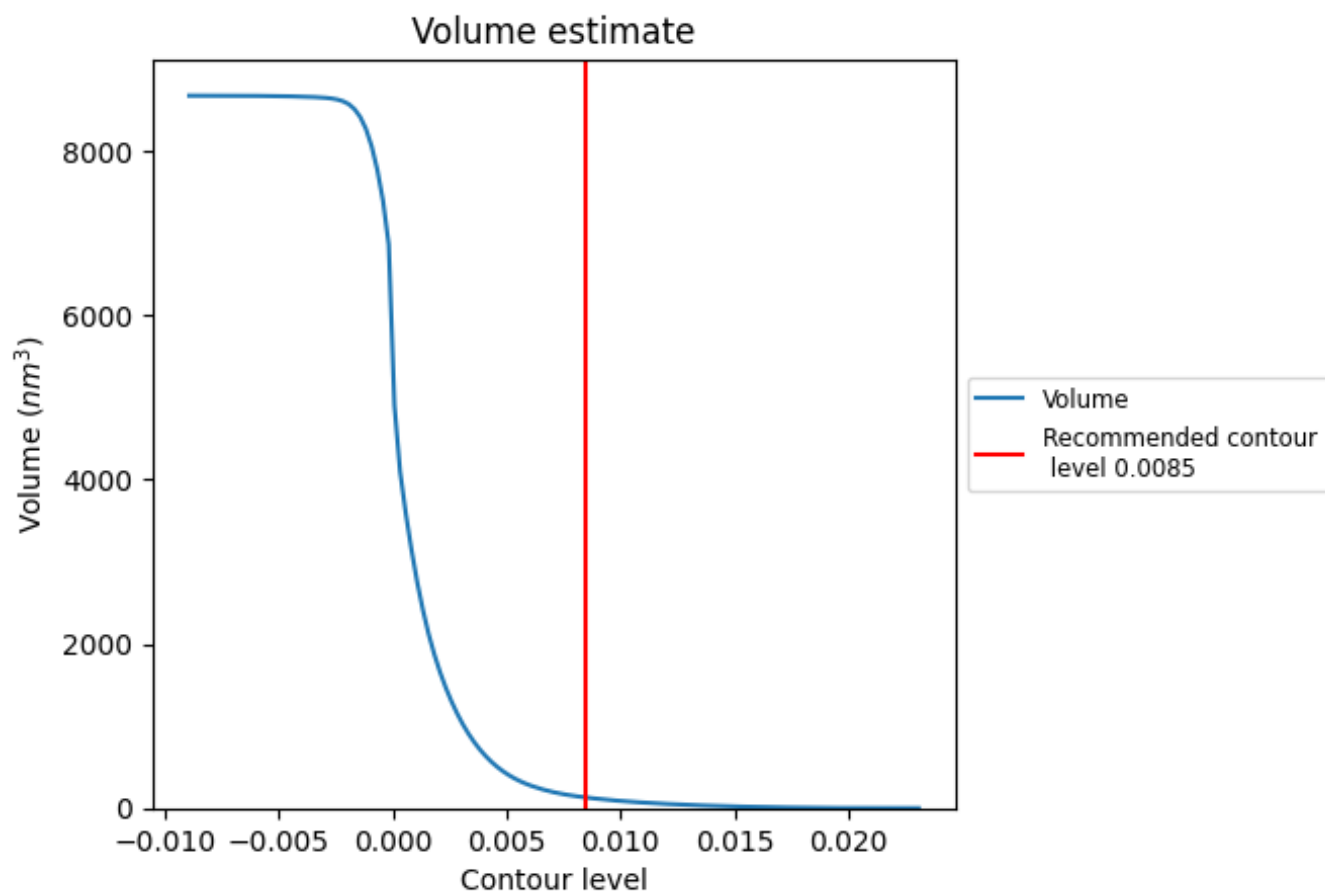
This section contains the results of statistical analysis of the map.

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.

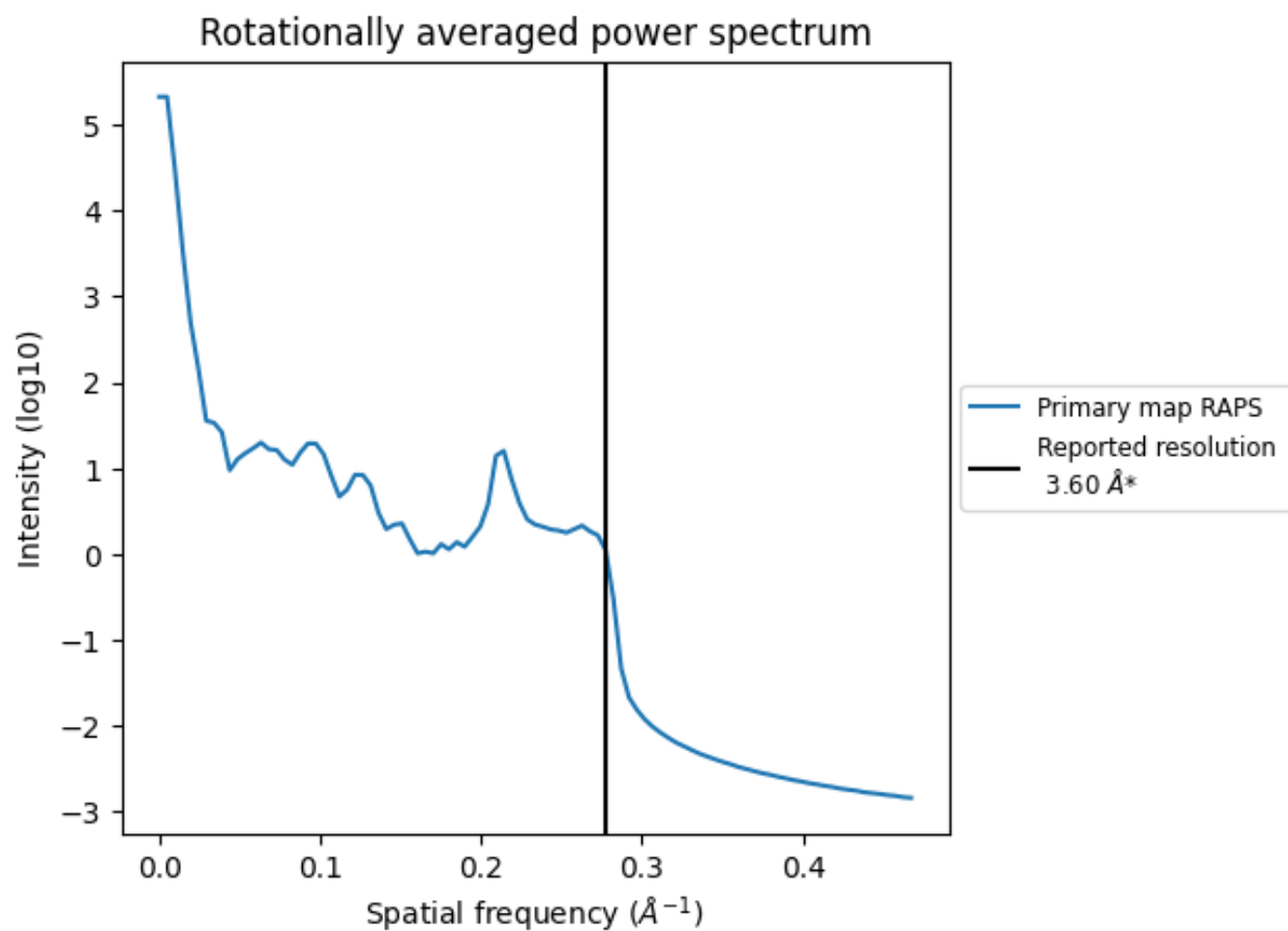
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm³; this corresponds to an approximate mass of 117 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation

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

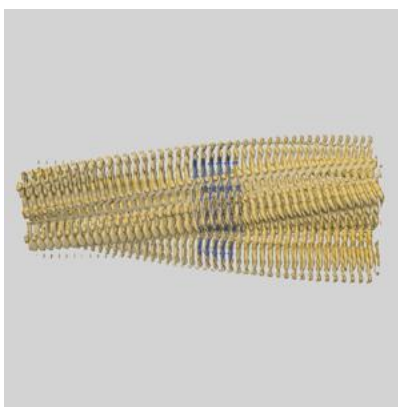
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7619 and PDB model 6CU8. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



X



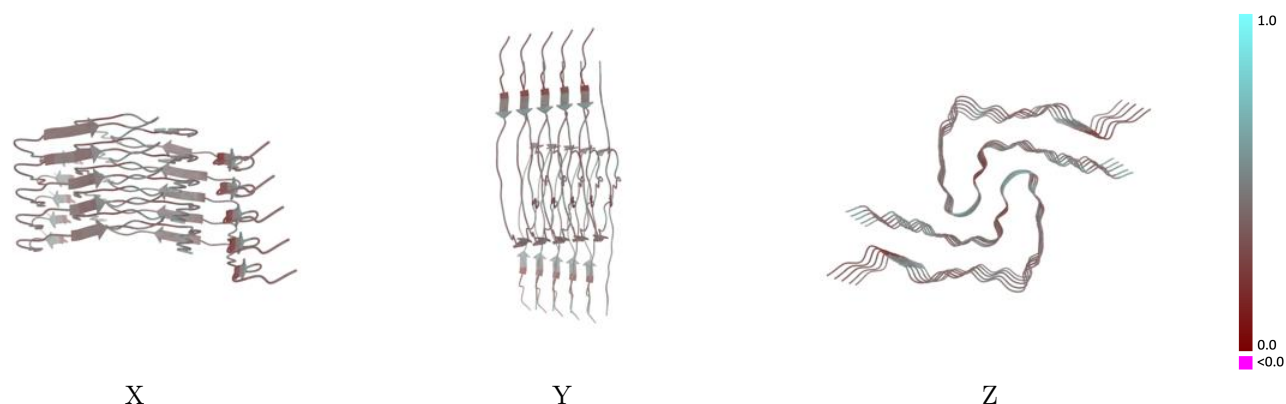
Y



Z

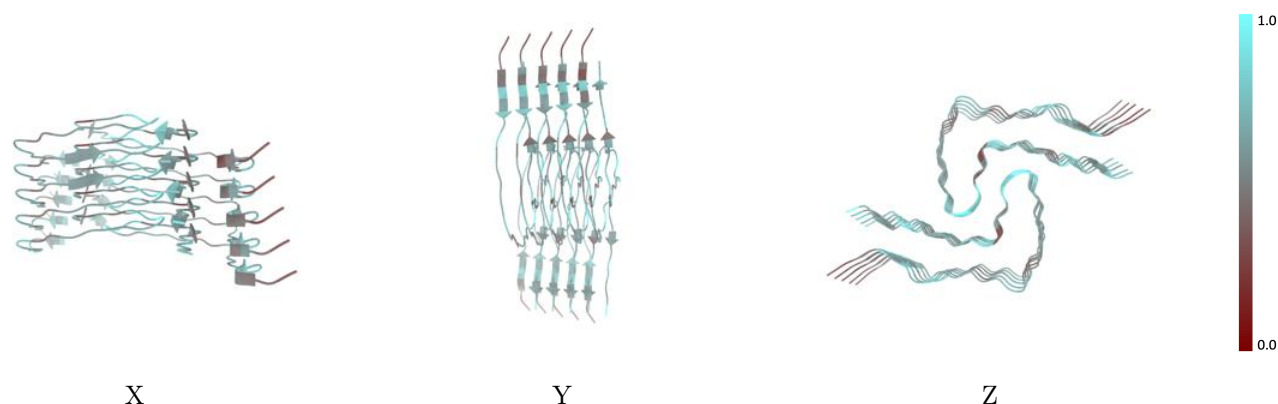
The images above show the 3D surface view of the map at the recommended contour level 0.0085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



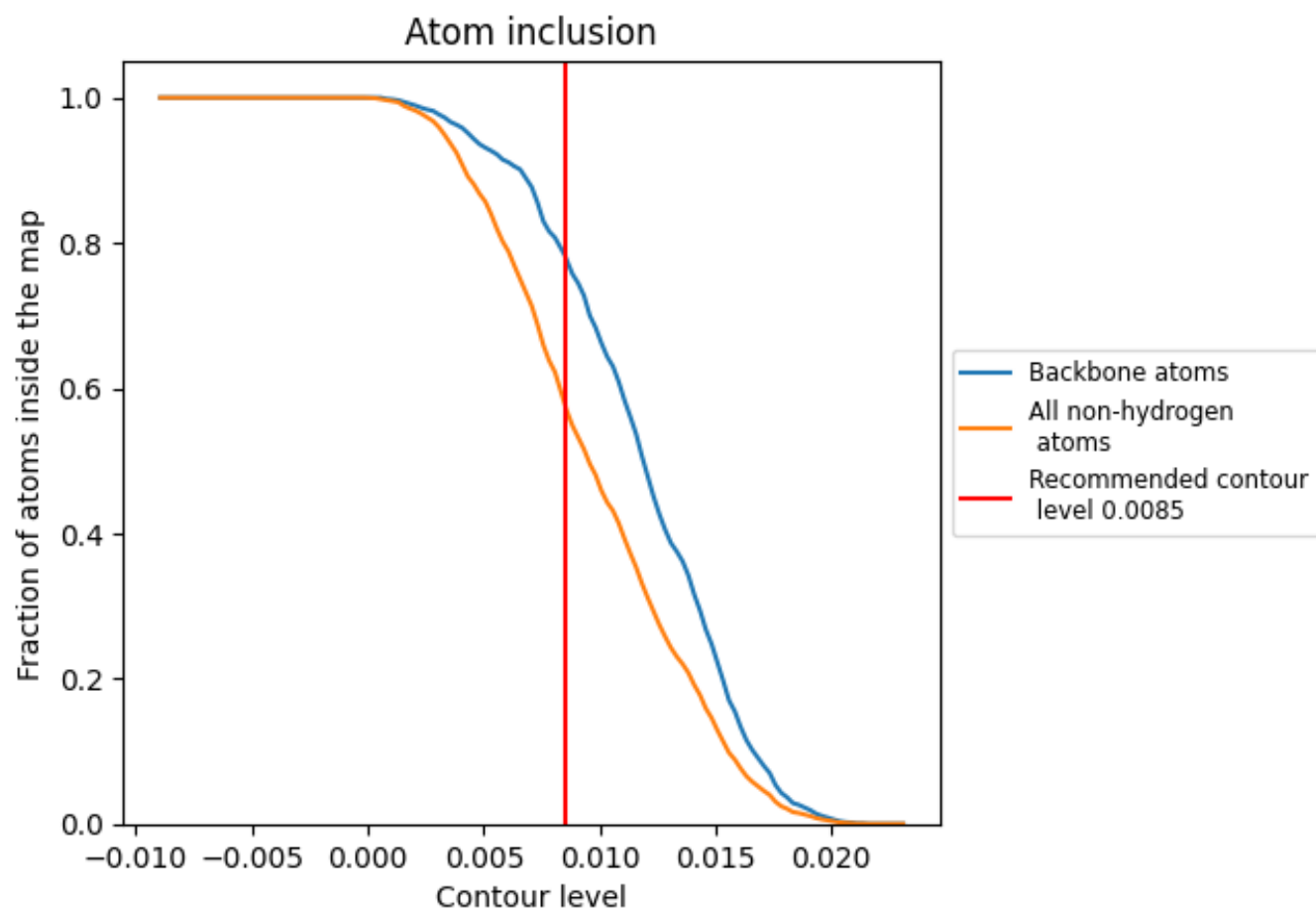
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5774	<div></div> 0.4230
A	<div></div> 0.5833	<div></div> 0.4220
B	<div></div> 0.5833	<div></div> 0.4230
C	<div></div> 0.5764	<div></div> 0.4230
D	<div></div> 0.5694	<div></div> 0.4200
E	<div></div> 0.5729	<div></div> 0.4250
F	<div></div> 0.5833	<div></div> 0.4240
G	<div></div> 0.5660	<div></div> 0.4200
H	<div></div> 0.5799	<div></div> 0.4230
I	<div></div> 0.5694	<div></div> 0.4210
J	<div></div> 0.5903	<div></div> 0.4250

