



## wwPDB EM Validation Summary Report ⓘ

May 28, 2026 – 10:15 am BST

PDB ID : 9HC6 / pdb\_00009hc6  
EMDB ID : EMD-52038  
Title : The L2A-I alpha-synuclein fibril in the presence of MODAG-005 (short incubation)  
Authors : Frieg, B.; Kim, M.; Griesinger, C.; Schroeder, G.F.  
Deposited on : 2024-11-08  
Resolution : 2.79 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

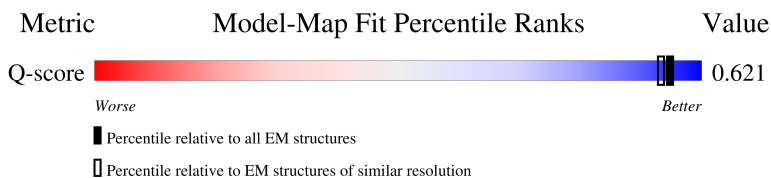
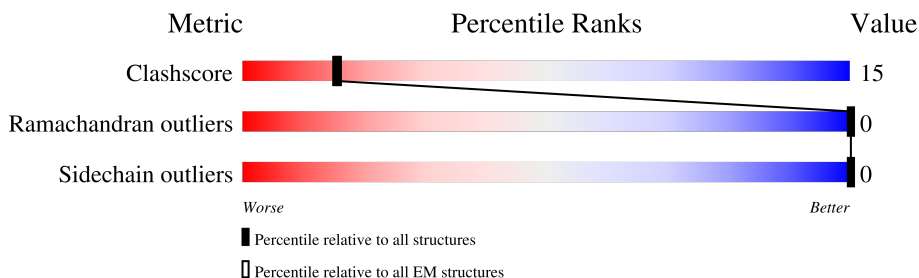
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.79 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.



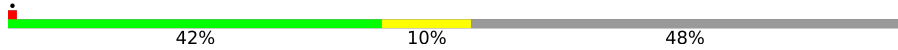
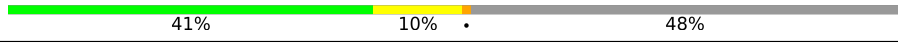
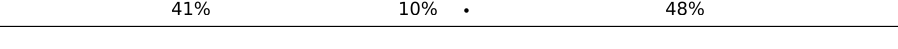
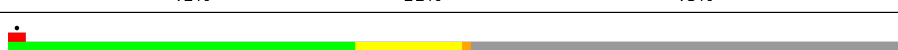
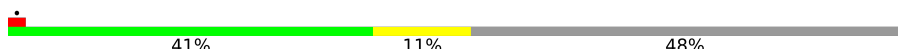
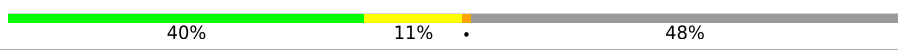
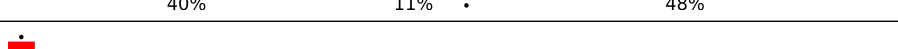
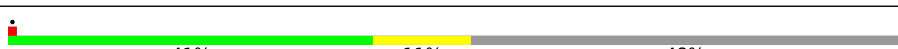
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10811 ( 2.29 - 3.29 )                                    |

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  $\geq 3$ , 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    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 140    |    |
| 1   | F     | 140    |    |
| 1   | G     | 140    |    |
| 1   | H     | 140    |    |
| 1   | I     | 140    |    |
| 1   | J     | 140    |    |
| 1   | K     | 140    |    |
| 1   | L     | 140    |    |
| 1   | M     | 140    |    |
| 1   | N     | 140    |   |
| 1   | O     | 140    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7560 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.

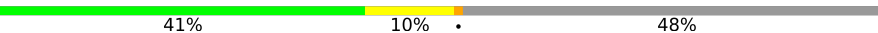
- Molecule 1 is a protein called Alpha-synuclein.

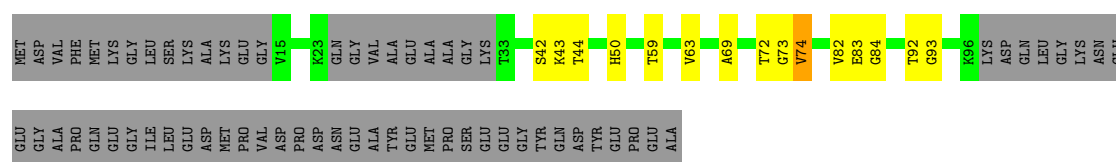
| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 1   | A     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | B     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | C     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | D     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | E     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | F     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | G     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | H     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | I     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | J     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | K     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | L     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | M     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | N     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |
| 1   | O     | 73       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 504   | 316 | 87 | 101 |         |       |

### 3 Residue-property plots

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

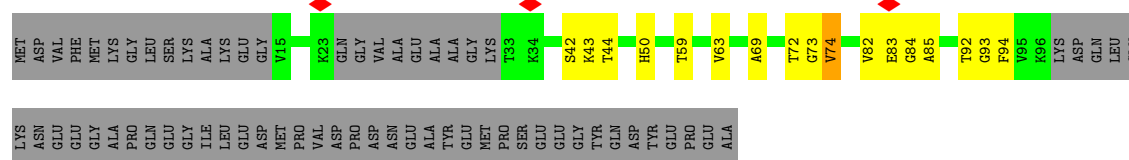
#### • Molecule 1: Alpha-synuclein

Chain A: 



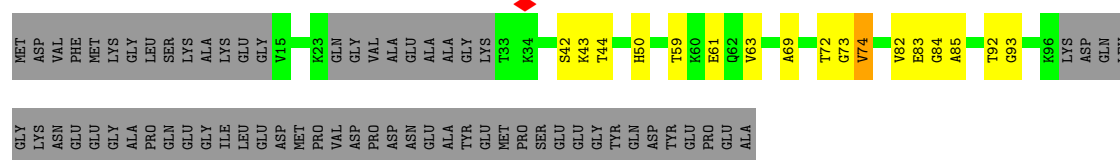
#### • Molecule 1: Alpha-synuclein

Chain B: 

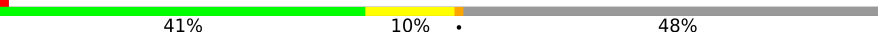


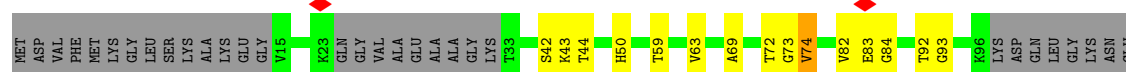
#### • Molecule 1: Alpha-synuclein

Chain C: 



#### • Molecule 1: Alpha-synuclein

Chain D: 



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

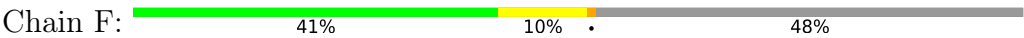
● Molecule 1: Alpha-synuclein



MET  
ASP  
VAL  
PHE  
MET  
LYS  
GLY  
LEU  
SER  
GLU  
ASP  
ALA  
LYS  
GLY  
VAL  
ASP  
K23  
GLN  
GLY  
VAL  
ALA  
TYR  
GLU  
MET  
ALA  
TYR  
GLU  
SER  
GLY  
LYS  
T33  
S42  
K43  
T44  
H50  
T59  
V63  
A69  
T72  
G73  
V74  
V82  
E83  
G84  
T92  
G93  
K96  
LYS  
ASP  
GLN  
LEU  
GLY  
LYS  
ASN  
GLU

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

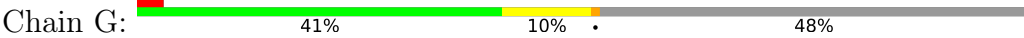
● Molecule 1: Alpha-synuclein



MET  
ASP  
VAL  
PHE  
MET  
LYS  
GLY  
LEU  
SER  
GLU  
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ALA  
LYS  
GLY  
VAL  
ASP  
K23  
GLN  
GLY  
VAL  
ALA  
TYR  
GLU  
MET  
ALA  
TYR  
GLU  
SER  
GLY  
LYS  
T33  
S42  
K43  
T44  
H50  
T59  
V63  
A69  
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G73  
V74  
V82  
E83  
G84  
T92  
G93  
K96  
LYS  
ASP  
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ALA  
PRO  
PHE  
GLN  
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ILE  
LEU  
SER  
GLU  
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VAL  
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ASN  
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ASN  
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GLY  
ALA  
TYR  
GLU  
MET  
MET  
PRO  
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GLU  
ALA

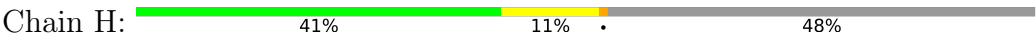
● Molecule 1: Alpha-synuclein



MET  
ASP  
VAL  
PHE  
MET  
LYS  
GLY  
LEU  
SER  
GLU  
ASP  
ALA  
LYS  
GLY  
VAL  
ASP  
K23  
GLN  
GLY  
VAL  
ALA  
TYR  
GLU  
MET  
ALA  
TYR  
GLU  
SER  
GLY  
LYS  
T33  
K34  
S42  
K43  
T44  
H50  
T59  
V63  
A69  
T72  
G73  
V74  
V82  
E83  
G84  
T92  
G93  
K96  
LYS  
ASP  
GLN  
LEU  
GLY  
LYS

ASN  
GLU  
GLY  
ALA  
PRO  
PHE  
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GLU  
GLY  
ILE  
LEU  
SER  
GLU  
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TYR  
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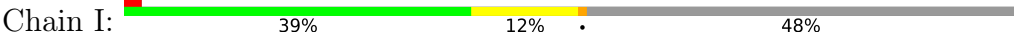
● Molecule 1: Alpha-synuclein



MET  
ASP  
VAL  
PHE  
MET  
LYS  
GLY  
LEU  
SER  
GLU  
ASP  
ALA  
LYS  
GLY  
VAL  
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V82  
E83  
G84  
T92  
G93  
F94  
V95  
K96  
LYS  
ASP  
GLN  
LEU  
GLY  
LYS  
ASN

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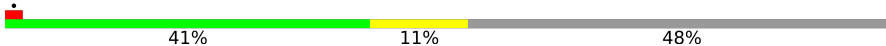
● Molecule 1: Alpha-synuclein



MET  
ASP  
VAL  
PHE  
MET  
LYS  
GLY  
LEU  
SER  
GLU  
ASP  
ALA  
LYS  
GLY  
VAL  
ASP  
K23  
GLN  
GLY  
VAL  
ALA  
TYR  
GLU  
MET  
ALA  
TYR  
GLU  
LYS  
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K34  
S42  
K43  
T44  
K45  
H50  
T59  
K60  
E61  
G62  
V63  
A69  
T72  
G73  
V74  
V82  
E83  
G84  
T92  
G93  
F94  
V95  
K96  
LYS  
ASP  
GLN

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

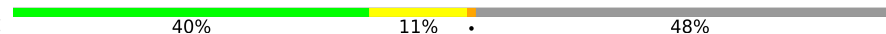
• Molecule 1: Alpha-synuclein

Chain J:  41% 11% 48%

MET ASP VAL PHE MET LYS GLY LEU SER LYS ALA GLY ILE LEU GLU ASP V15 K23 GLN GLY VAL ASP ALA ASP ASN GLU ALA TYR MET T33 K34 S42 K43 T44 K45 H50 T59 K60 E61 Q62 V63 A69 T72 G73 V74 V82 E83 G84 T92 G93 K96 LYS ASP GLN LEU

GLY LYS ASN GLU GLY MET PRO VAL ASP PRO ASP ASN GLU ALA TYR MET T33 K34 S42 K43 T44 K45 H50 T59 K60 E61 Q62 V63 A69 T72 G73 V74 V82 E83 G84 T92 G93 K96 LYS ASP GLN LEU

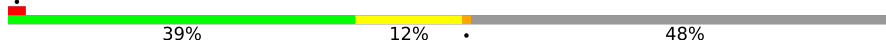
• Molecule 1: Alpha-synuclein

Chain K:  40% 11% 48%

MET ASP VAL PHE MET LYS GLY LEU SER LYS ALA GLY ILE LEU GLU ASP V15 K23 GLN GLY VAL ASP ALA ASP ASN GLU ALA TYR MET T33 K34 S42 K43 T44 K45 H50 T59 K60 E61 Q62 V63 A69 T72 G73 V74 V82 E83 G84 T92 G93 K96 LYS ASP GLN LEU LYS

ASN GLU GLY VAL PHE MET LYS GLY LEU SER LYS ALA GLY ILE LEU GLU ASP V15 K23 GLN GLY VAL ASP ALA ASP ASN GLU ALA TYR MET T33 K34 S42 K43 T44 K45 H50 T59 K60 E61 Q62 V63 A69 T72 G73 V74 V82 E83 G84 T92 G93 K96 LYS ASP GLN LEU LYS

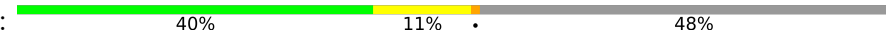
• Molecule 1: Alpha-synuclein

Chain L:  39% 12% 48%

MET ASP VAL PHE MET LYS GLY LEU SER LYS ALA GLY ILE LEU GLU ASP V15 K23 GLN GLY VAL ASP ALA ASP ASN GLU ALA TYR MET T33 K34 S42 K43 T44 K45 H50 T59 K60 E61 Q62 V63 A69 T72 G73 V74 V82 E83 G84 T92 G93 K96 LYS ASP GLN LEU

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

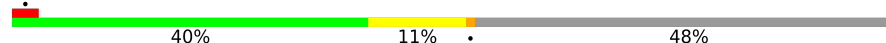
• Molecule 1: Alpha-synuclein

Chain M:  40% 11% 48%

MET ASP VAL PHE MET LYS GLY LEU SER LYS ALA GLY ILE LEU GLU ASP V15 K23 GLN GLY VAL ASP ALA ASP ASN GLU ALA TYR MET T33 K34 S42 K43 T44 K45 H50 T59 K60 E61 Q62 V63 A69 T72 G73 V74 V82 E83 G84 T92 G93 K96 LYS ASP GLN LEU GLY

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

• Molecule 1: Alpha-synuclein

Chain N:  40% 11% 48%

MET ASP VAL PHE MET LYS GLY LEU SER LYS ALA GLY ILE LEU GLU ASP V15 K23 GLN GLY VAL ASP ALA ASP ASN GLU ALA TYR MET T33 K34 S42 K43 T44 K45 H50 T59 K60 E61 Q62 V63 A69 T72 G73 V74 V82 E83 G84 T92 G93 K96 LYS ASP GLN LEU GLN

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

● Molecule 1: Alpha-synuclein



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ASP | VAL | PHE | MET | LYS | GLY | LEU | SER | LYS | ALA | LYS | GLU | GLY | V15 | K23 | GLN | GLY | VAL | ALA | GLU | ALA | ALA | GLY | LYS | T33 | S42 | K43 | T44 | H50 | T59 | K60 | E61 | Q62 | V63 | A69 | T72 | G73 | V74 | V82 | E83 | G84 | T92 | G93 | K96 | LYS | ASP | GLN | LEU | GLY | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASN | GLU | GLY | GLY | ALA | PRO | GLN | GLY | GLU | ILE | LEU | GLU | ASP | MET | PRO | VAL | ASP | PRO | ASN | ASP | 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=-0.74°, rise=4.69 Å, axial sym=C3 | Depositor |
| Number of segments used            | 200200                                           | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                                | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION          | Depositor |
| Microscope                         | TFS KRIOS                                        | Depositor |
| Voltage (kV)                       | 300                                              | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 40                                               | Depositor |
| Minimum defocus (nm)               | 600                                              | Depositor |
| Maximum defocus (nm)               | 2300                                             | Depositor |
| Magnification                      | Not provided                                     |           |
| Image detector                     | GATAN K3 (6k x 4k)                               | Depositor |
| Maximum map value                  | 0.209                                            | Depositor |
| Minimum map value                  | -0.106                                           | Depositor |
| Average map value                  | 0.001                                            | Depositor |
| Map value standard deviation       | 0.014                                            | Depositor |
| Recommended contour level          | 0.06                                             | Depositor |
| Map size (Å)                       | 262.5, 262.5, 262.5                              | wwPDB     |
| Map dimensions                     | 250, 250, 250                                    | 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     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | B     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | C     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | D     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | E     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | F     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | G     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | H     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | I     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | J     | 1.12         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | K     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | L     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | M     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | N     | 1.12         | 0/505       | 1.42        | 3/681 (0.4%)    |
| 1   | O     | 1.11         | 0/505       | 1.42        | 3/681 (0.4%)    |
| All | All   | 1.11         | 0/7575      | 1.42        | 45/10215 (0.4%) |

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 74  | VAL  | N-CA-C | -9.63 | 100.80      | 110.62   |
| 1   | I     | 74  | VAL  | N-CA-C | -9.61 | 100.81      | 110.62   |
| 1   | D     | 74  | VAL  | N-CA-C | -9.61 | 100.82      | 110.62   |
| 1   | O     | 74  | VAL  | N-CA-C | -9.61 | 100.82      | 110.62   |
| 1   | F     | 74  | VAL  | N-CA-C | -9.60 | 100.83      | 110.62   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 504   | 0        | 534      | 17      | 0            |
| 1   | B     | 504   | 0        | 534      | 32      | 0            |
| 1   | C     | 504   | 0        | 534      | 32      | 0            |
| 1   | D     | 504   | 0        | 534      | 30      | 0            |
| 1   | E     | 504   | 0        | 534      | 17      | 0            |
| 1   | F     | 504   | 0        | 534      | 17      | 0            |
| 1   | G     | 504   | 0        | 534      | 30      | 0            |
| 1   | H     | 504   | 0        | 534      | 31      | 0            |
| 1   | I     | 504   | 0        | 534      | 33      | 0            |
| 1   | J     | 504   | 0        | 534      | 19      | 0            |
| 1   | K     | 504   | 0        | 534      | 19      | 0            |
| 1   | L     | 504   | 0        | 534      | 33      | 0            |
| 1   | M     | 504   | 0        | 534      | 32      | 0            |
| 1   | N     | 504   | 0        | 534      | 32      | 0            |
| 1   | O     | 504   | 0        | 534      | 18      | 0            |
| All | All   | 7560  | 0        | 8010     | 228     | 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 15.

The worst 5 of 228 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:C:74:VAL:CG1 | 1:D:44:THR:HG21 | 2.13                     | 0.79              |
| 1:L:74:VAL:CG1 | 1:M:44:THR:HG21 | 2.13                     | 0.79              |
| 1:D:74:VAL:CG1 | 1:E:44:THR:HG21 | 2.13                     | 0.79              |
| 1:K:74:VAL:CG1 | 1:L:44:THR:HG21 | 2.13                     | 0.79              |
| 1:M:74:VAL:CG1 | 1:N:44:THR:HG21 | 2.13                     | 0.79              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | B     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | C     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | D     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | E     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | F     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | G     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | H     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | I     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | J     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | K     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | L     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | M     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | N     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 1   | O     | 69/140 (49%)    | 67 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| All | All   | 1035/2100 (49%) | 1005 (97%) | 30 (3%) | 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     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | B     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | C     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | D     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | E     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | F     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | G     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | H     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | I     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | J     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | K     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | L     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | M     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | N     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| 1   | O     | 51/103 (50%)   | 51 (100%)  | 0        | 100         | 100 |
| All | All   | 765/1545 (50%) | 765 (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 12 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 50  | HIS  |
| 1   | K     | 50  | HIS  |
| 1   | O     | 50  | HIS  |
| 1   | K     | 79  | GLN  |
| 1   | E     | 50  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

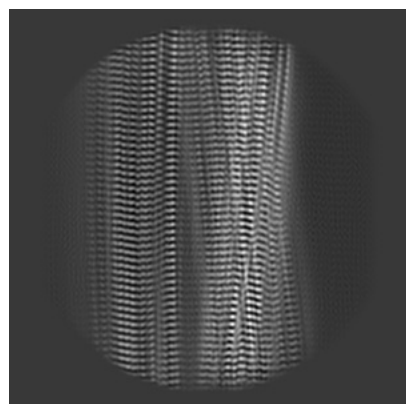
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52038. These allow visual inspection of the internal detail of the map and identification of artifacts.

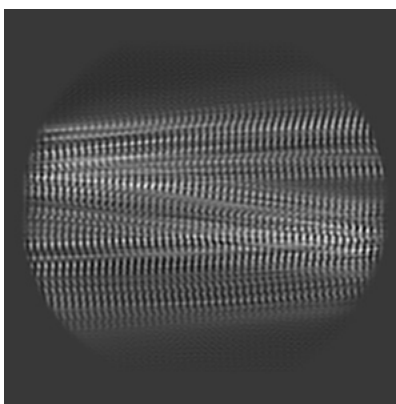
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

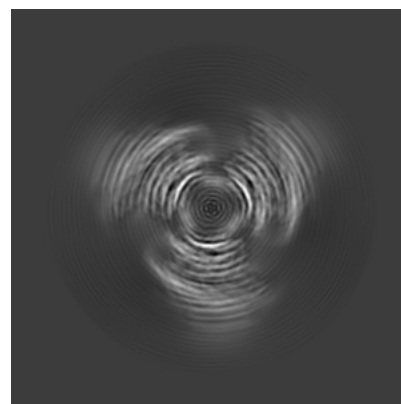
#### 6.1.1 Primary map



X

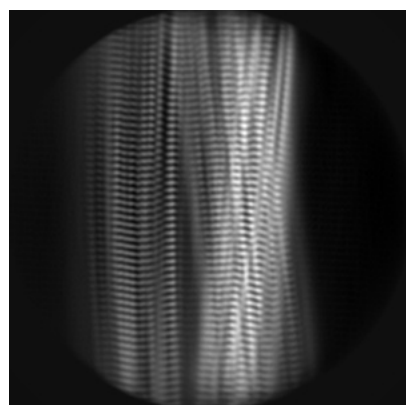


Y

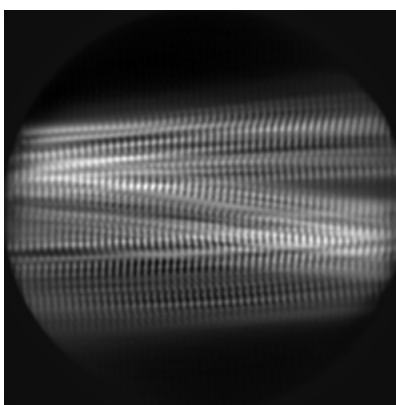


Z

#### 6.1.2 Raw map



X



Y

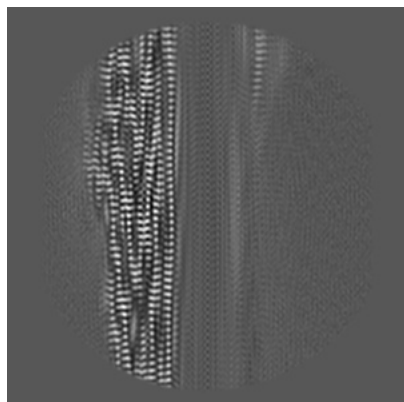


Z

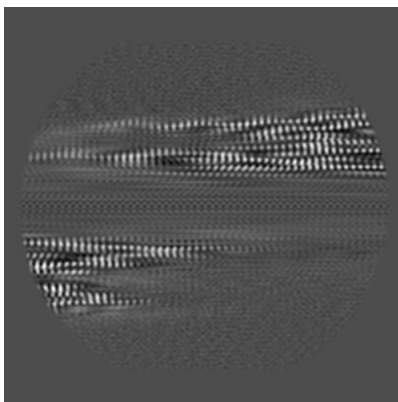
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

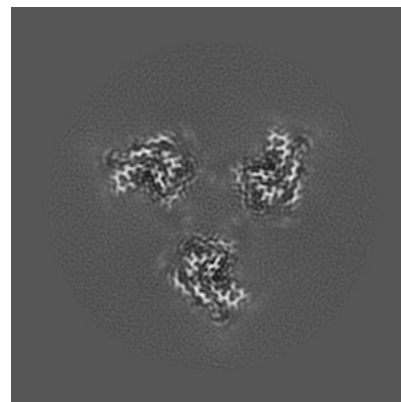
### 6.2.1 Primary map



X Index: 125

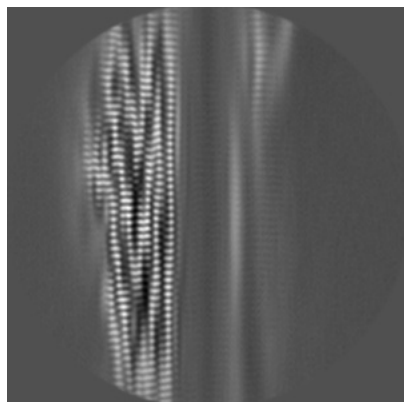


Y Index: 125

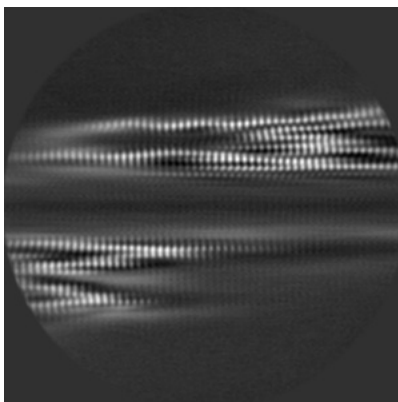


Z Index: 125

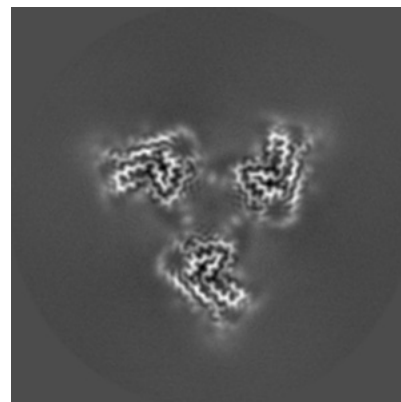
### 6.2.2 Raw map



X Index: 125



Y Index: 125

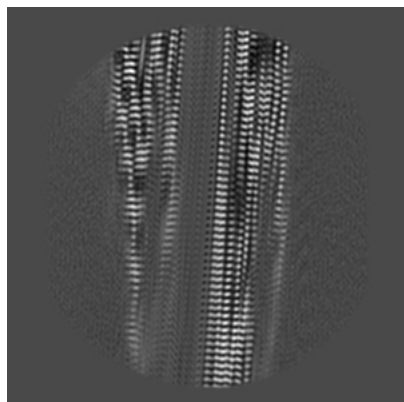


Z Index: 125

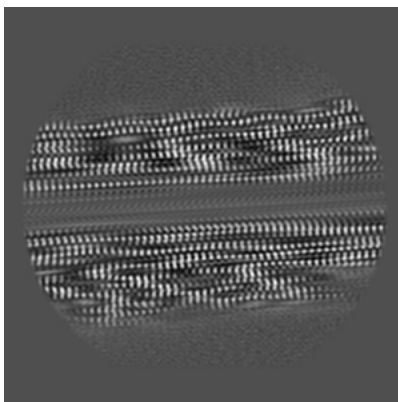
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

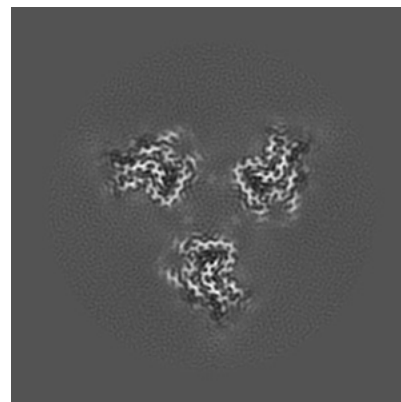
### 6.3.1 Primary map



X Index: 103

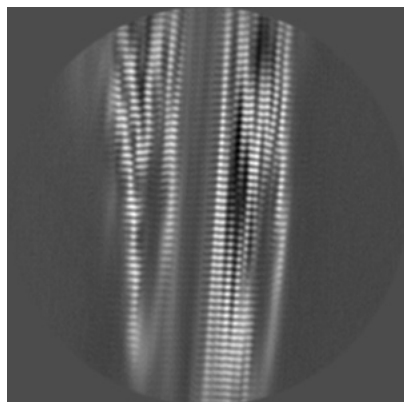


Y Index: 145

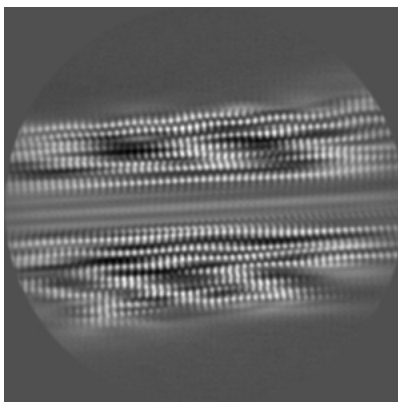


Z Index: 124

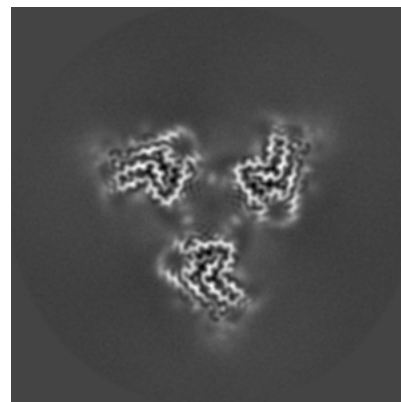
### 6.3.2 Raw map



X Index: 103



Y Index: 144

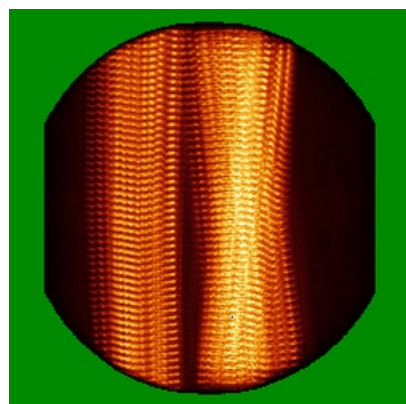


Z Index: 124

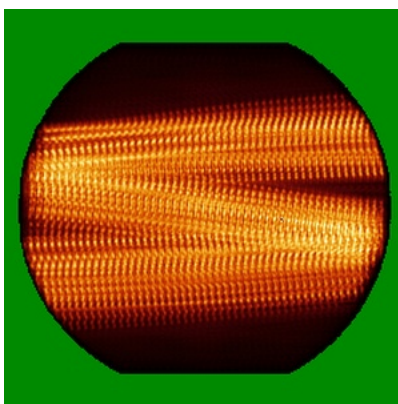
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

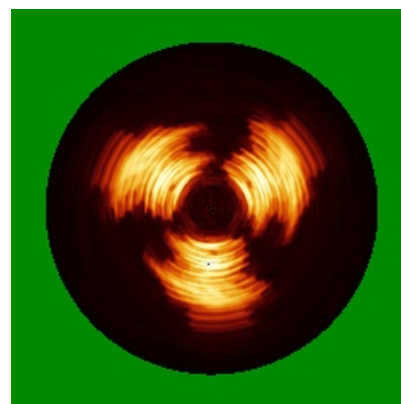
### 6.4.1 Primary map



X

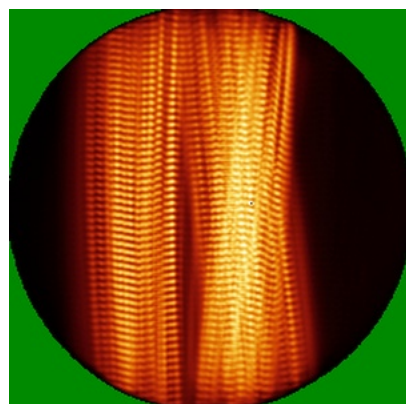


Y

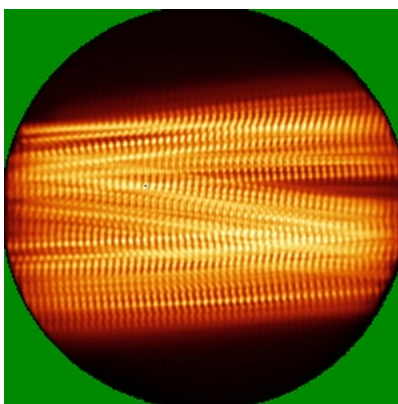


Z

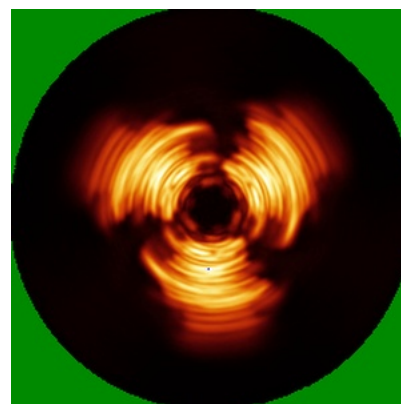
### 6.4.2 Raw map



X



Y

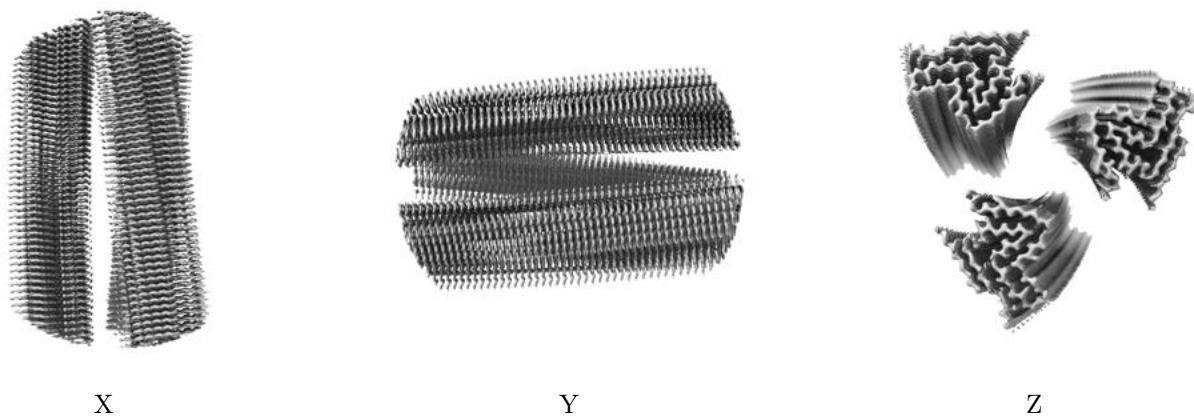


Z

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.

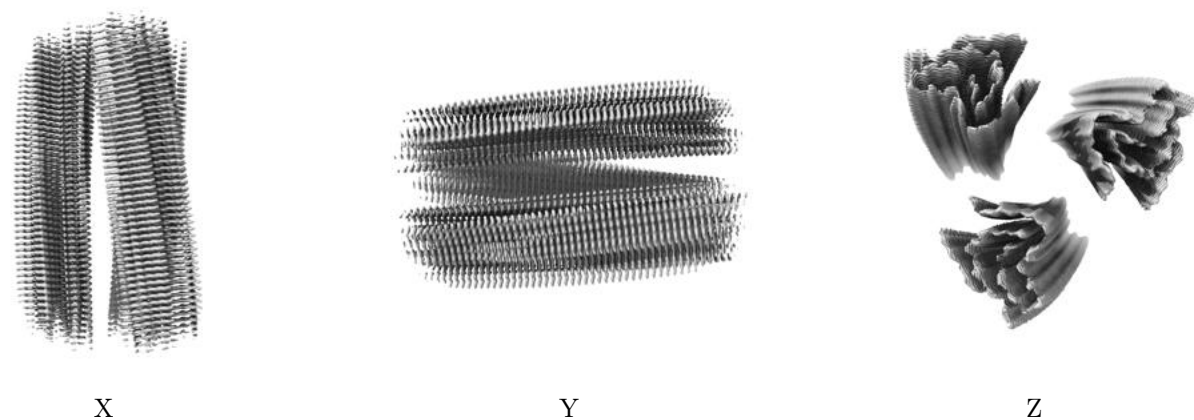
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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



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.

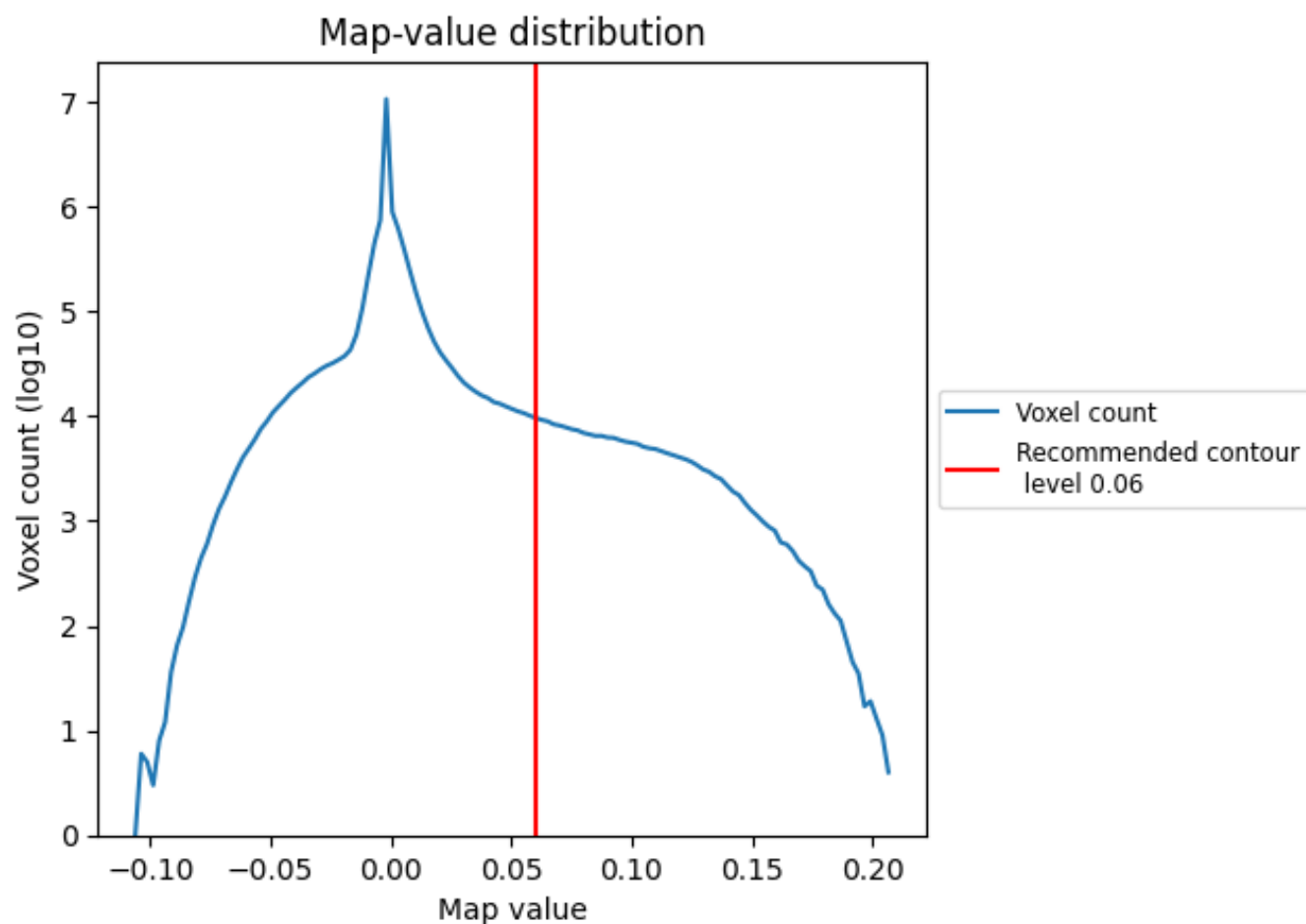
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

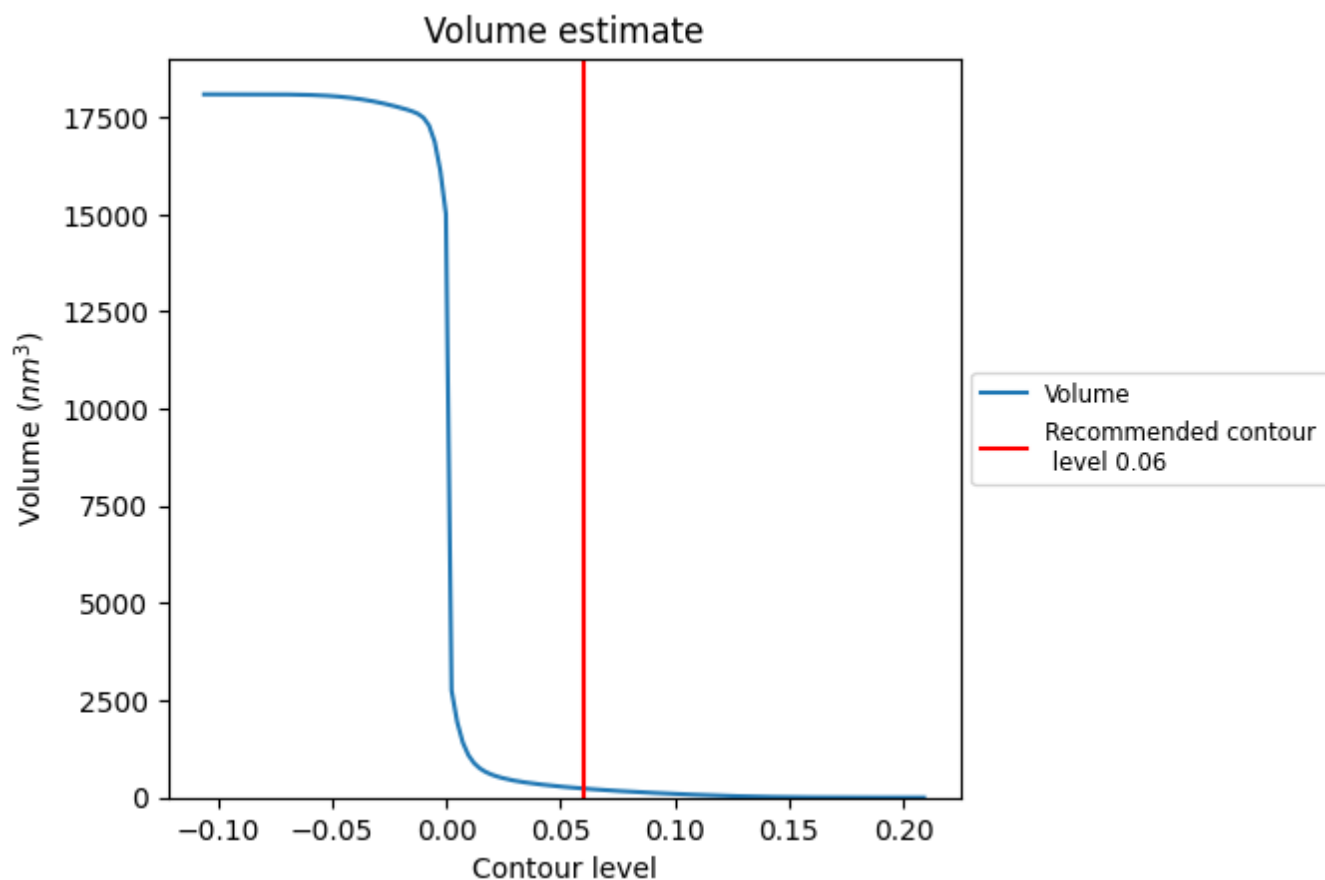
This section contains the results of statistical analysis of the map.

### 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.

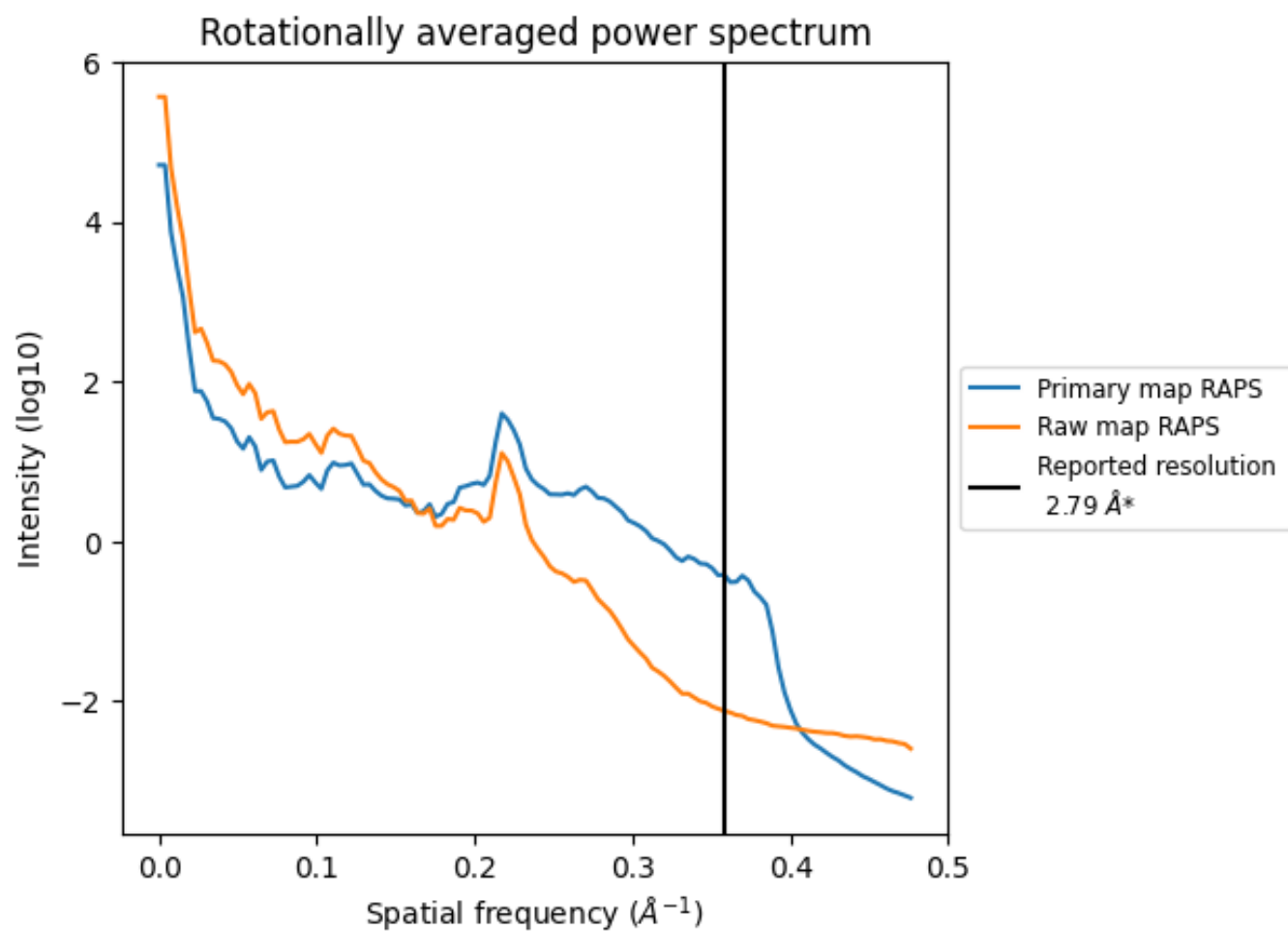
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 232 nm<sup>3</sup>; this corresponds to an approximate mass of 210 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 ⓘ

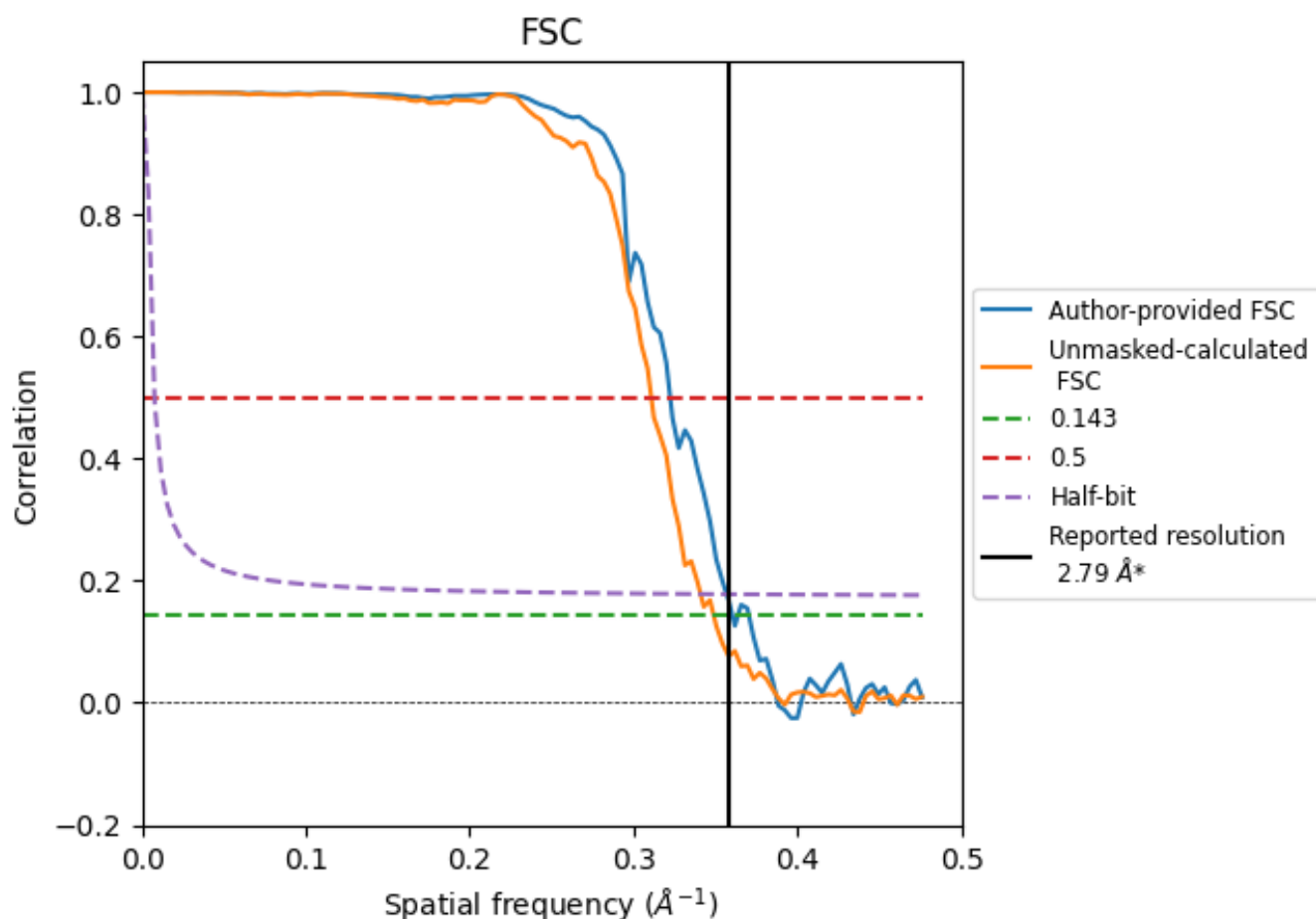


\*Reported resolution corresponds to spatial frequency of 0.358 Å<sup>-1</sup>

## 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  $0.358 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

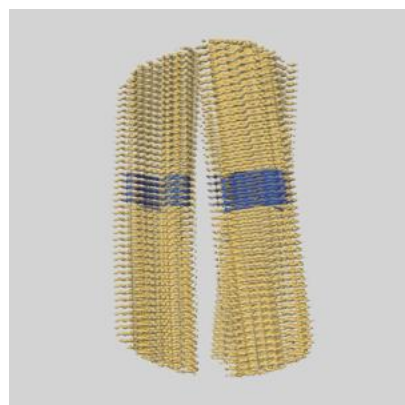
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.79                               | -    | -        |
| Author-provided FSC curve | 2.77                               | 3.10 | 2.80     |
| Unmasked-calculated*      | 2.87                               | 3.22 | 2.93     |

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

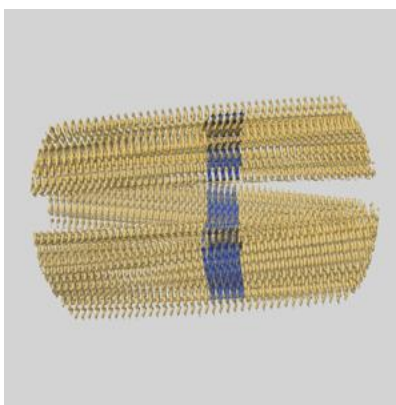
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52038 and PDB model 9HC6. Per-residue inclusion information can be found in section [3](#) on page [5](#).

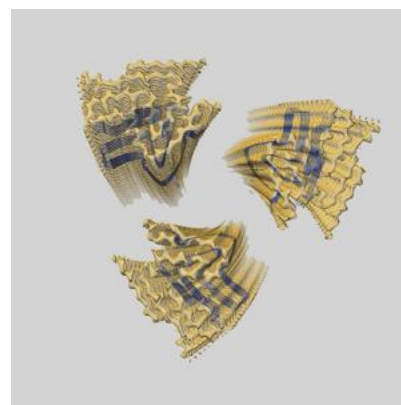
### 9.1 Map-model overlay [i](#)



X



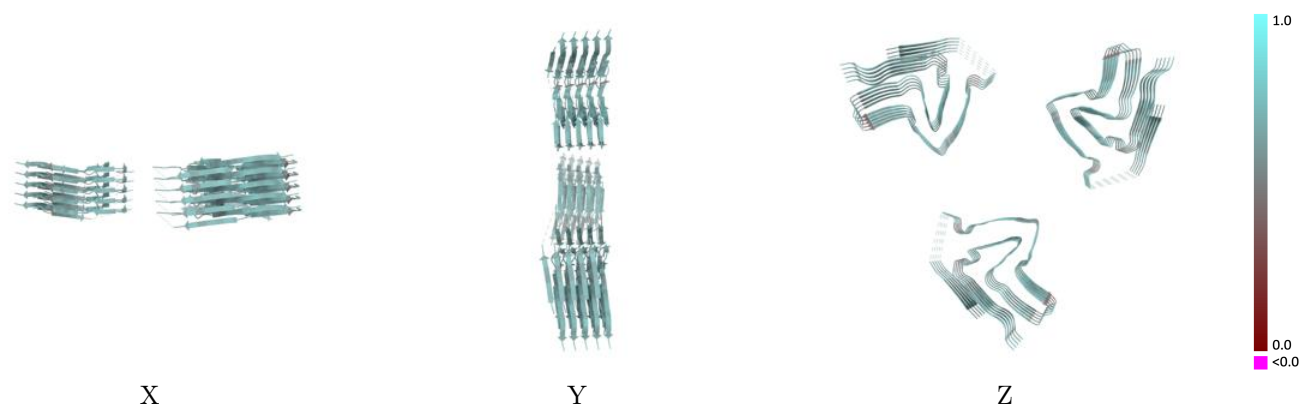
Y



Z

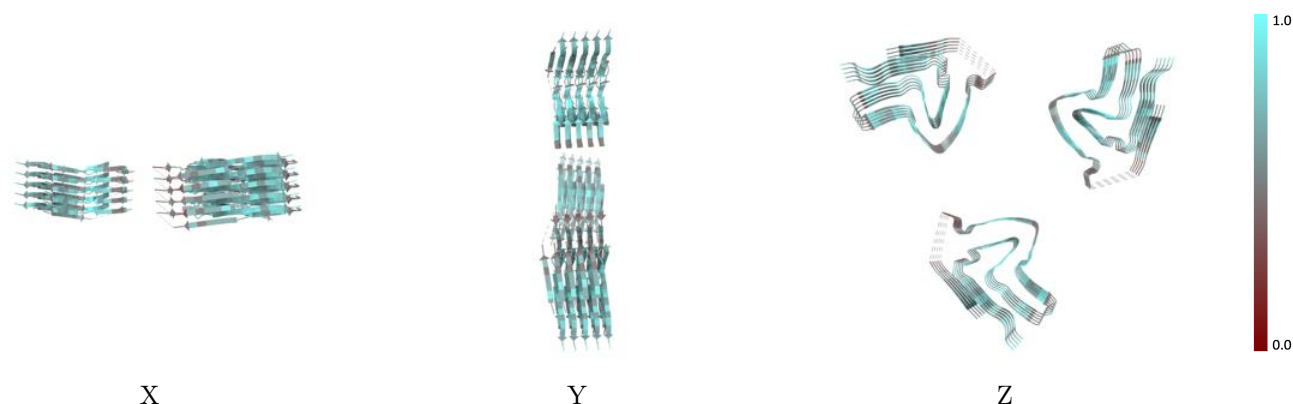
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



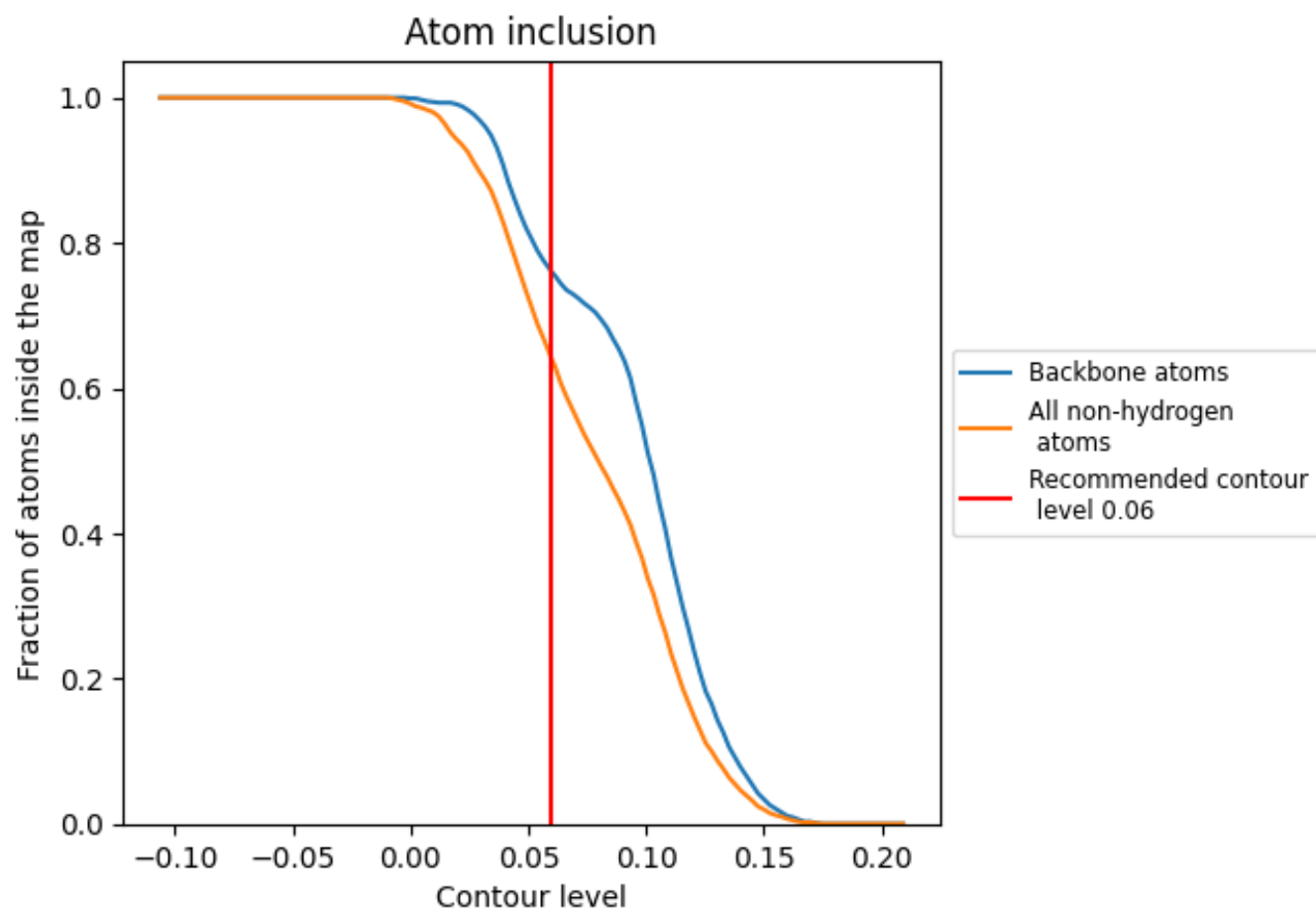
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 64% 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 (0.06) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6400 | <div></div> 0.6210 |
| A     | <div></div> 0.6460 | <div></div> 0.6250 |
| B     | <div></div> 0.6300 | <div></div> 0.6170 |
| C     | <div></div> 0.6380 | <div></div> 0.6240 |
| D     | <div></div> 0.6340 | <div></div> 0.6170 |
| E     | <div></div> 0.6260 | <div></div> 0.6220 |
| F     | <div></div> 0.6520 | <div></div> 0.6230 |
| G     | <div></div> 0.6500 | <div></div> 0.6170 |
| H     | <div></div> 0.6460 | <div></div> 0.6210 |
| I     | <div></div> 0.6340 | <div></div> 0.6150 |
| J     | <div></div> 0.6240 | <div></div> 0.6190 |
| K     | <div></div> 0.6560 | <div></div> 0.6240 |
| L     | <div></div> 0.6500 | <div></div> 0.6210 |
| M     | <div></div> 0.6420 | <div></div> 0.6260 |
| N     | <div></div> 0.6300 | <div></div> 0.6200 |
| O     | <div></div> 0.6340 | <div></div> 0.6230 |

1.0

0.0

<0.0