WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 07:04 pm GMT

PDB ID	:	7AU3
EMDB ID	:	EMD-11924
Title	:	Cytochrome c oxidase structure in F-state
Authors	:	Kolbe, F.; Safarian, S.; Michel, H.
Deposited on	:	2020-11-02
Resolution	:	2.56 Å(reported)
Based on initial model	:	3HB3

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 ⓘ 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
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
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)	:	2.31.3

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 2.56 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.
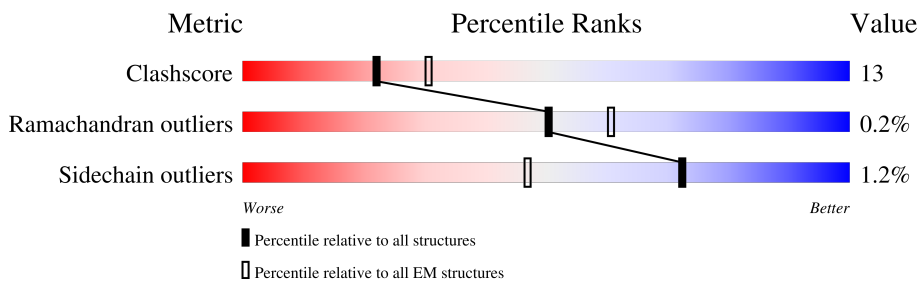
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	558	74% 21%
2	B	298	6% 65% 18% 16%
3	C	274	9% 68% 29%
4	D	50	30% 72% 10% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	2FK	A	607	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	PGV	C	301	X	-	-	-
6	HEA	A	602	X	-	-	-
6	HEA	A	603	X	-	-	-
9	O	A	606	-	-	X	-

2   Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 9012 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 Cytochrome c oxidase subunit 1-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	537	Total	C	N	O	S	0	0
			4257	2854	667	703	33		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	250	Total	C	N	O	S	0	0
			1959	1286	316	349	8		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	268	Total	C	N	O	S	0	0
			2138	1457	328	342	11		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	41	Total	C	N	O	S	0	0
			317	206	56	54	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mn	0
			1	1	

- Molecule 6 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).

HEA
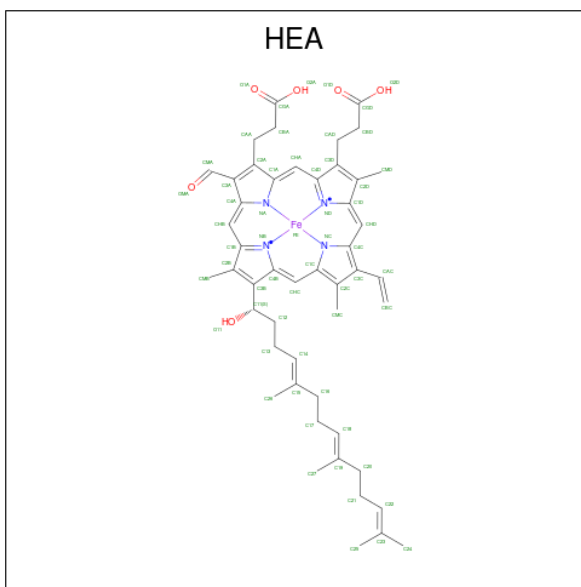
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
6	A	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Cu	0
			1	1	

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Ca	0
			1	1	

- Molecule 9 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	O	0
			1	1	

- Molecule 10 is SUPEROXO ION (three-letter code: 2FK) (formula: O_2).

2FK

O1 O^- ═══ O O2
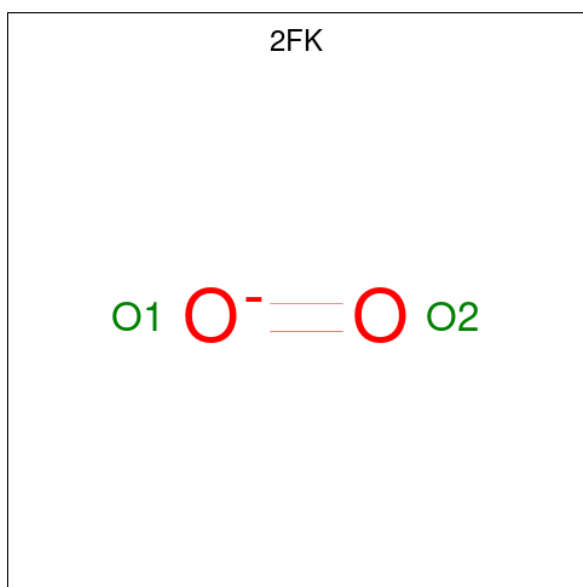
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total 2	O 2	0

- Molecule 11 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).

CUA

CU1 Cu — Cu CU2
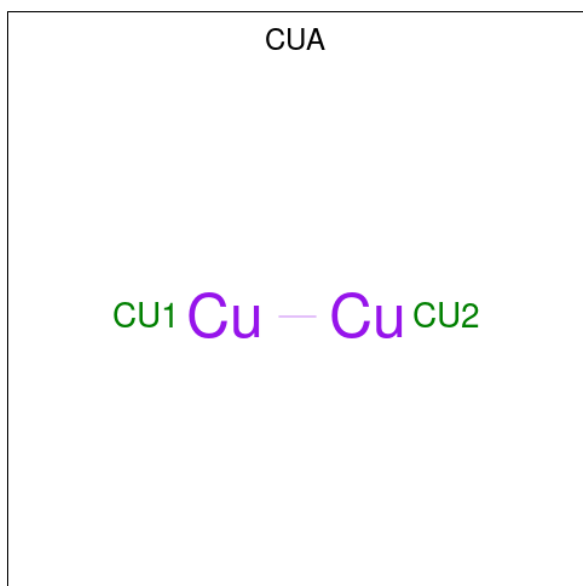
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total 2	Cu 2	0

- Molecule 12 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPH ORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).

PGV
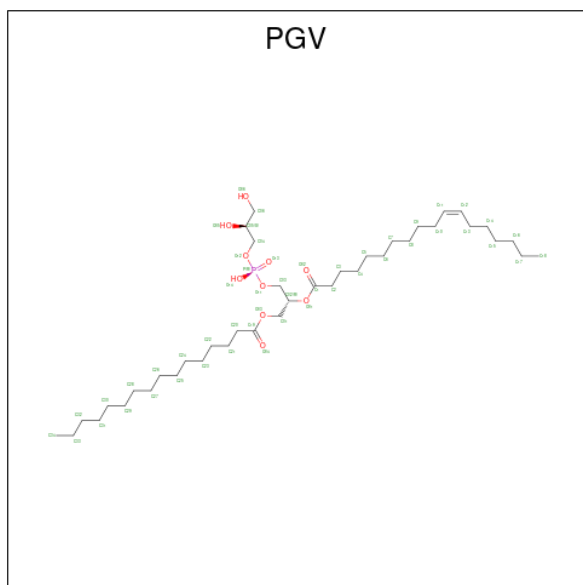
Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	104	Total	O	0
			104	104	
13	B	44	Total	O	0
			44	44	
13	C	14	Total	O	0
			14	14	

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: Cytochrome c oxidase subunit 1-beta
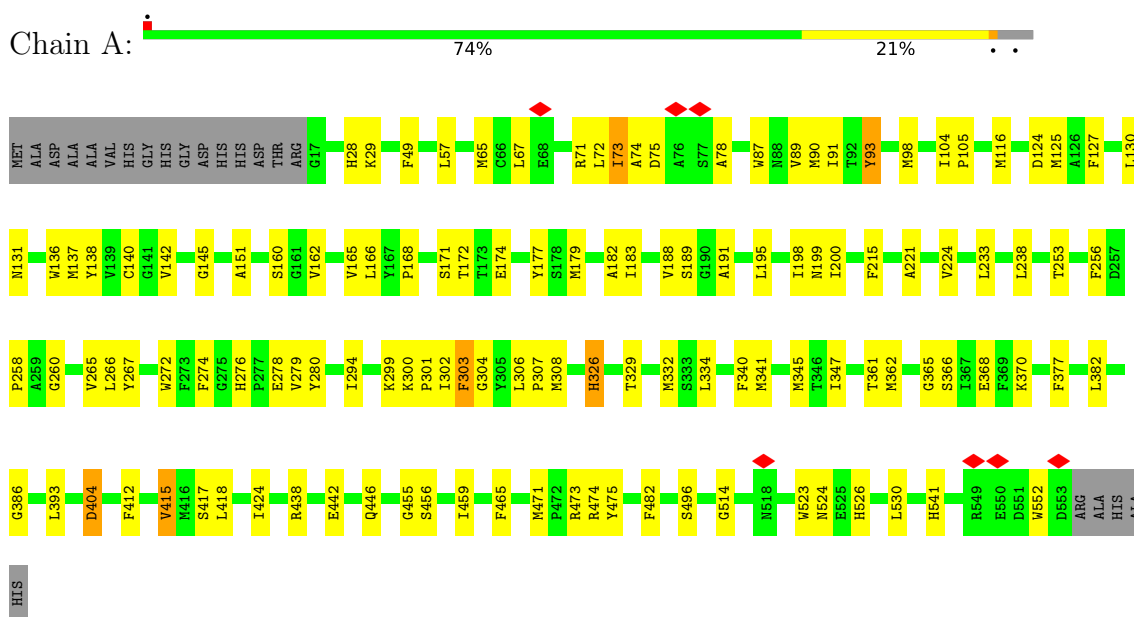
Chain A:

- Molecule 2: Cytochrome c oxidase subunit 2
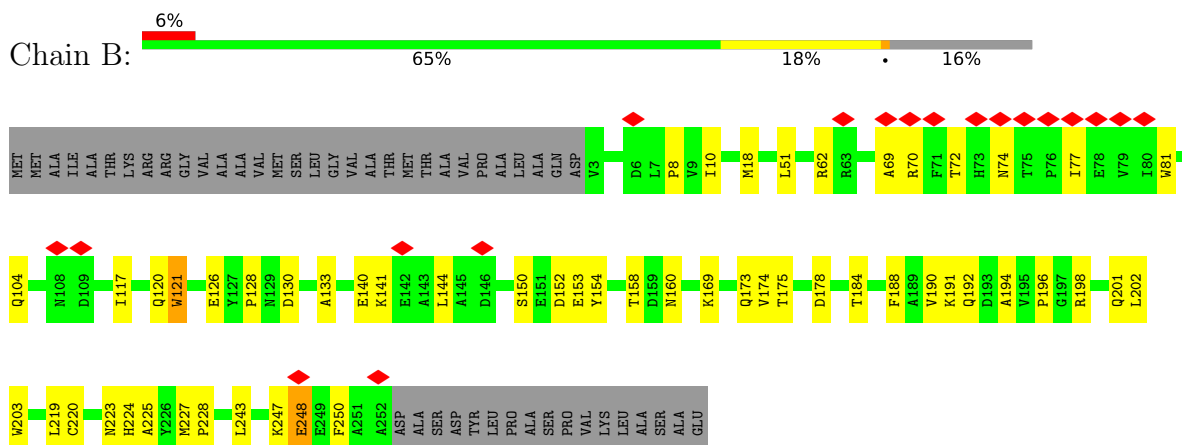
Chain B:

- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:

9%

68%   29%

MET ALA HIS VAL LYS N5 Q9 W16 P17 F18 A21 I22 G23 A24 F25 T29 A33 G37 I38 T39 F40 F41 G42 L43 W49 M50 V58 L59 M62 W66 V70 P80 R83 Q87 F90 M99 V102 A107 F108 A112 L113

Y114 P115 M116 D119 I122 K123 D124 W127 P128 P129 E130 G131 F135 D136 P137 W138 H139 I140 P141 L142 I143 N144 L148 W157 F162 V163 L164 E165 G166 D167 R168 K169 T170 T171 I172 I176 V179 I180 F185 L188 E192 H195 A196 A197 L200 A201

D202 T203 V204 G207 M211 A212 T213 H216 V220 T224 I225 F226 L227 F228 I232 R233 L234 L235 K236 G237 Q238 M239 K242 Q243 H244 F256 V259 V260 W261 L262 I268 G272 ARG

• Molecule 4: Cytochrome c oxidase subunit 4

Chain D:

30%

72%   10%   18%

MET ALA SER HIS GLU ILE THR ASP H9 K10 I16 R17 A30 T31 W32 V33 S34 I35 L36 S37 I38 A39 V40 F43 L44 A45 L46 A47 N48 S49
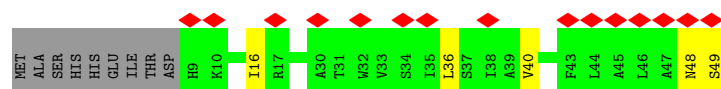
4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	373069	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	25.567	Depositor
Minimum map value	-17.402	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.406	Depositor
Recommended contour level	1.26	Depositor
Map size (Å)	102.459, 122.451004, 139.11101	wwPDB
Map dimensions	123, 147, 167	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.83300006	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: O, CUA, MN, 2FK, PGV, CU, CA, HEA

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	0.86	13/4416 (0.3%)	0.90	9/6028 (0.1%)
2	B	0.66	0/2016	0.92	6/2764 (0.2%)
3	C	0.64	1/2223 (0.0%)	0.85	4/3046 (0.1%)
4	D	0.54	0/324	0.74	0/436
All	All	0.75	14/8979 (0.2%)	0.89	19/12274 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	415	VAL	C-O	-14.52	0.95	1.23
1	A	75	ASP	C-O	-12.78	0.99	1.23
1	A	73	ILE	C-O	-12.54	0.99	1.23
1	A	301	PRO	C-O	-12.25	0.98	1.23
1	A	417	SER	CB-OG	-11.10	1.27	1.42

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
2	B	69	ALA	N-CA-C	12.37	144.39	111.00
2	B	69	ALA	CB-CA-C	-9.74	95.48	110.10
3	C	139	HIS	O-C-N	-8.77	108.67	122.70
1	A	523	TRP	N-CA-C	-7.46	90.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	524	ASN	N-CA-CB	-7.24	97.57	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	139	HIS	Mainchain

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	4257	0	4171	113	0
2	B	1959	0	1948	41	0
3	C	2138	0	2100	80	0
4	D	317	0	320	3	0
5	A	1	0	0	0	0
6	A	120	0	108	14	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	5	0
10	A	2	0	0	2	0
11	B	2	0	0	0	0
12	C	51	0	76	11	0
13	A	104	0	0	24	0
13	B	44	0	0	2	0
13	C	14	0	0	7	0
All	All	9012	0	8723	224	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 13.

The worst 5 of 224 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:HB	13:A:736:HOH:O	1.38	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:HIS:O	3:C:143:ILE:HD12	1.61	1.00
1:A:182:ALA:HB3	13:A:786:HOH:O	1.65	0.97
3:C:213:THR:HB	13:C:408:HOH:O	1.66	0.95
1:A:332:MET:HG3	13:A:769:HOH:O	1.68	0.94

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	535/558 (96%)	522 (98%)	12 (2%)	1 (0%)	47	58
2	B	248/298 (83%)	244 (98%)	4 (2%)	0	100	100
3	C	266/274 (97%)	259 (97%)	6 (2%)	1 (0%)	34	45
4	D	39/50 (78%)	38 (97%)	1 (3%)	0	100	100
All	All	1088/1180 (92%)	1063 (98%)	23 (2%)	2 (0%)	50	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	PHE
3	C	140	LEU

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	440/454 (97%)	438 (100%)	2 (0%)	88	93
2	B	209/243 (86%)	205 (98%)	4 (2%)	57	71
3	C	216/221 (98%)	211 (98%)	5 (2%)	50	64
4	D	32/40 (80%)	32 (100%)	0	100	100
All	All	897/958 (94%)	886 (99%)	11 (1%)	72	81

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	140	LEU
3	C	148	LEU
3	C	256	PHE
3	C	226	PHE
2	B	178	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
11	CUA	B	301	2	0,1,1	-	-	-		
12	PGV	C	301	-	50,50,50	0.31	0	53,56,56	0.71	3 (5%)
6	HEA	A	602	1	57,67,67	1.54	10 (17%)	61,103,103	2.40	20 (32%)
10	2FK	A	607	-	1,1,1	0.40	0	-		
6	HEA	A	603	1	57,67,67	1.44	9 (15%)	61,103,103	2.26	25 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGV	C	301	-	1/1/5/7	14/55/55/55	-
6	HEA	A	602	1	3/3/7/16	4/32/76/76	-
6	HEA	A	603	1	3/3/7/16	11/32/76/76	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HEA	C3A-C2A	-4.29	1.34	1.40
6	A	602	HEA	C3A-C2A	-4.22	1.34	1.40
6	A	603	HEA	FE-NB	4.12	2.17	1.96
6	A	602	HEA	C3C-C2C	-3.90	1.35	1.40
6	A	602	HEA	FE-NB	3.70	2.15	1.96

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	HEA	C4B-NB-C1B	7.26	112.57	105.07
6	A	602	HEA	C1D-ND-C4D	6.53	111.82	105.07
6	A	603	HEA	C4B-NB-C1B	6.04	111.31	105.07
6	A	603	HEA	C4A-CHB-C1B	5.46	129.76	122.56
6	A	602	HEA	C4A-CHB-C1B	5.37	129.65	122.56

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	602	HEA	NB
6	A	602	HEA	NA
6	A	602	HEA	ND
6	A	603	HEA	NB
6	A	603	HEA	NA

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	HEA	C2D-C3D-CAD-CBD
6	A	603	HEA	C4D-C3D-CAD-CBD
6	A	603	HEA	C19-C20-C21-C22
12	C	301	PGV	C10-C11-C12-C13
12	C	301	PGV	O04-C19-O03-C01

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	301	PGV	11	0
6	A	602	HEA	3	0
10	A	607	2FK	2	0
6	A	603	HEA	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PGV C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand HEA A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand HEA A 603

Bond lengths

Bond angles

Torsions

Rings
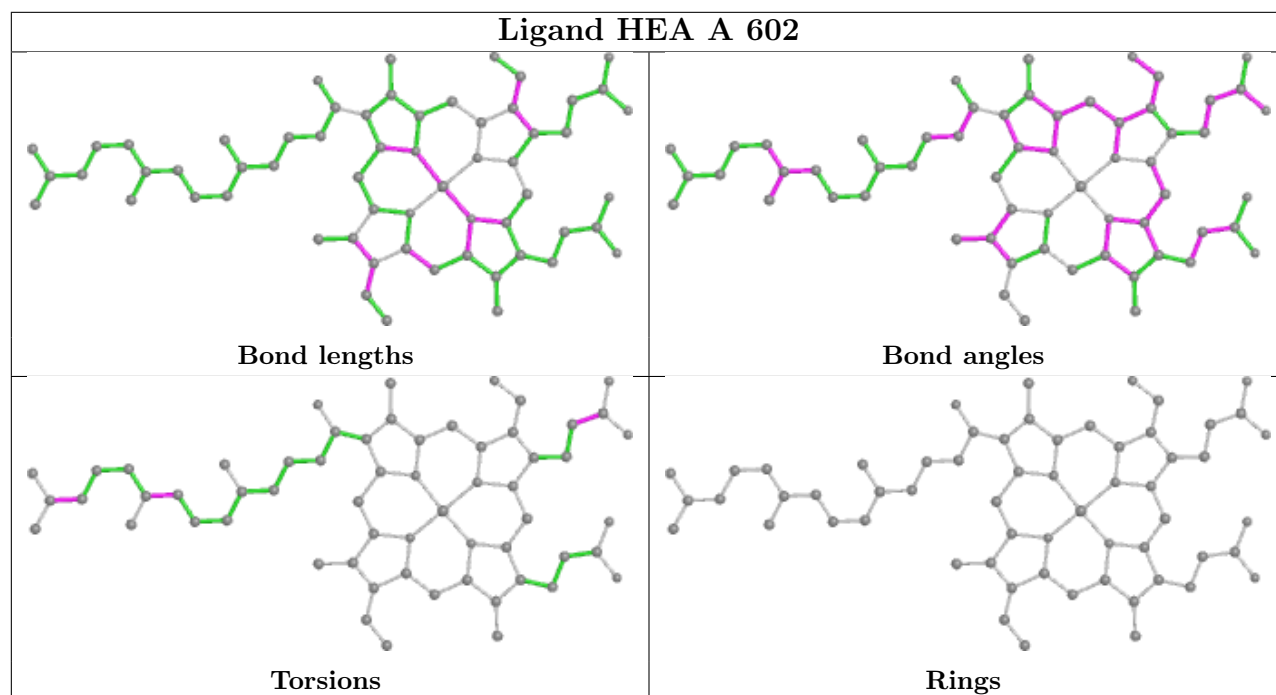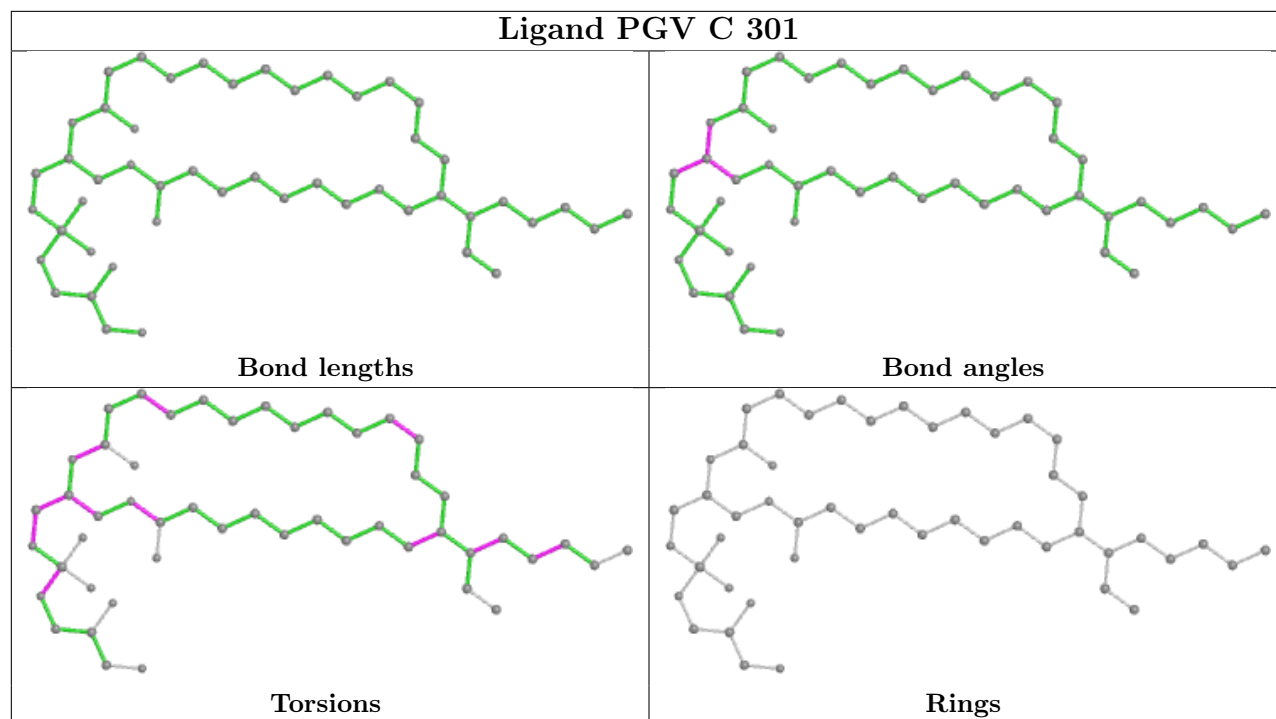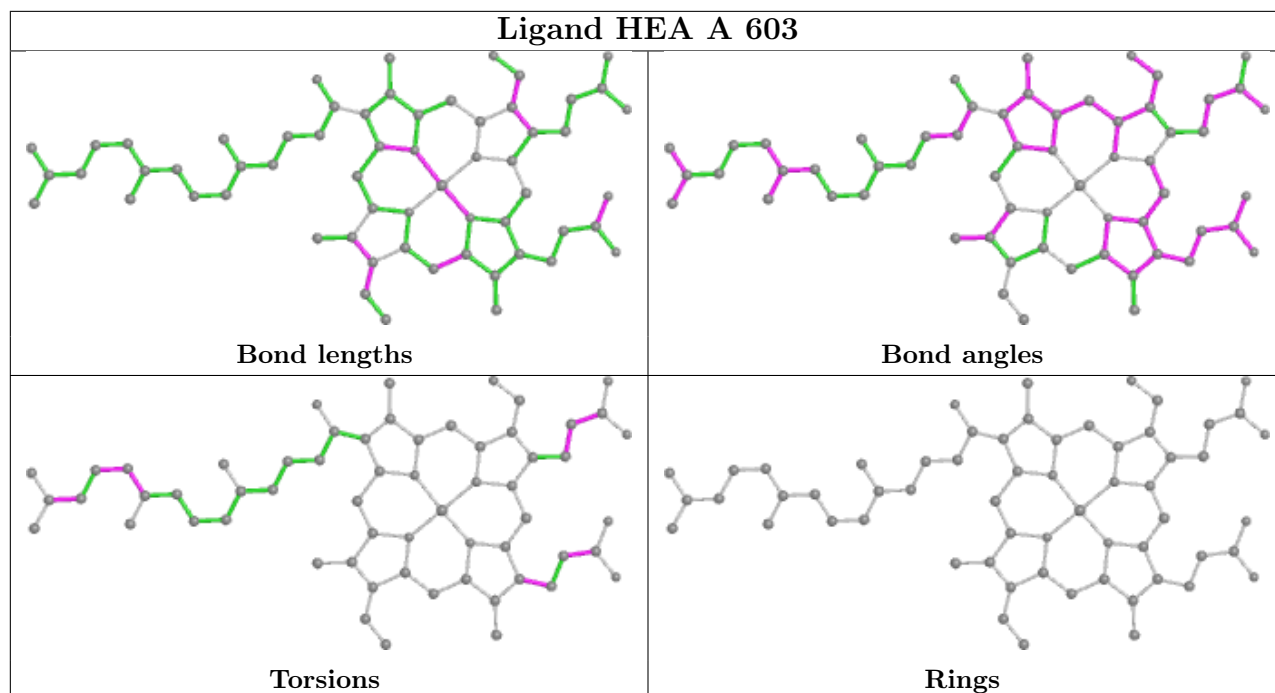
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	139:HIS	C	140:LEU	N	1.18

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-11924. 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 ⓘ
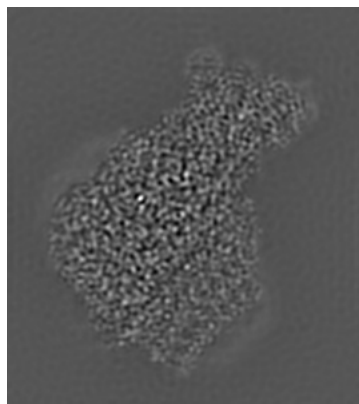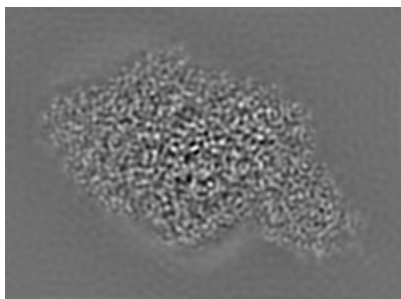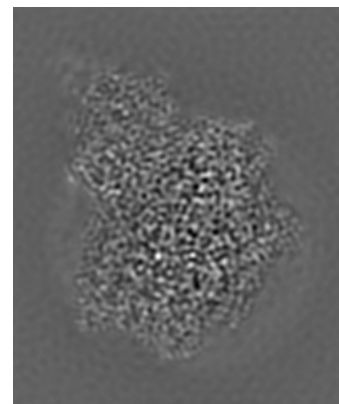
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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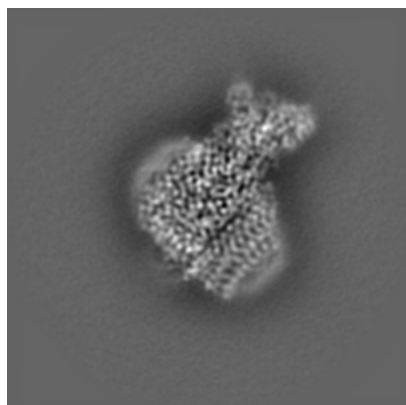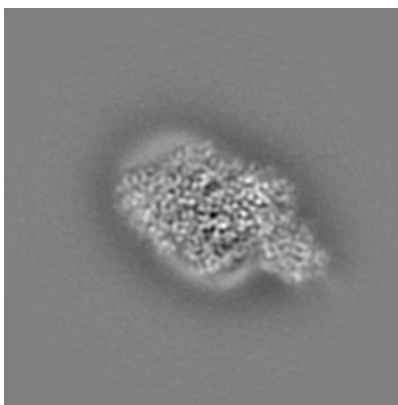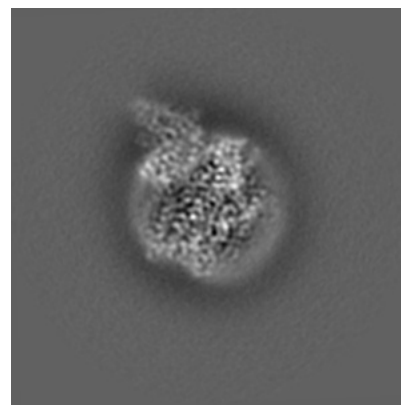
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
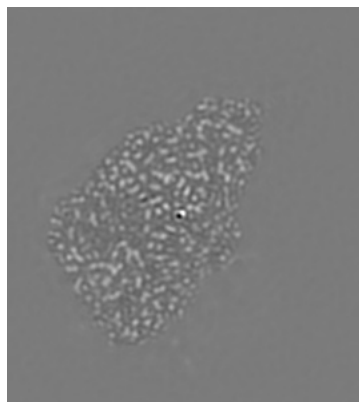
6.2.1 Primary map

X Index: 61
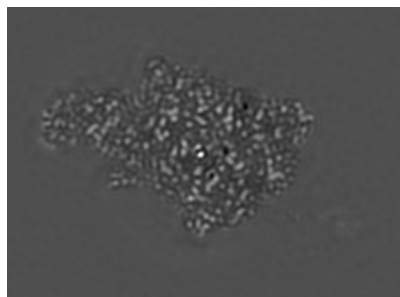
Y Index: 73
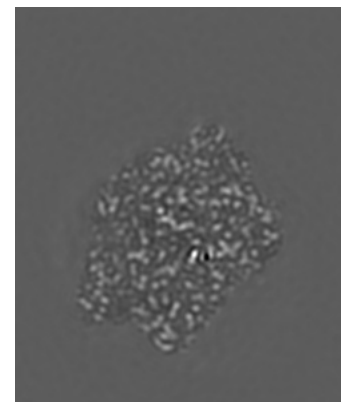
Z Index: 83

6.2.2 Raw map
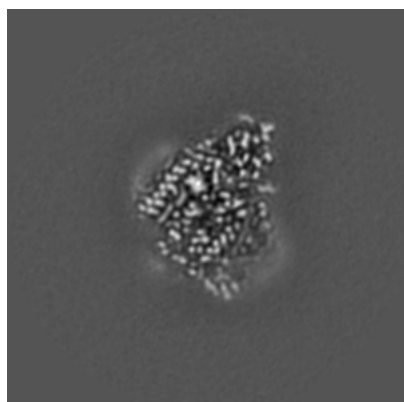
X Index: 128
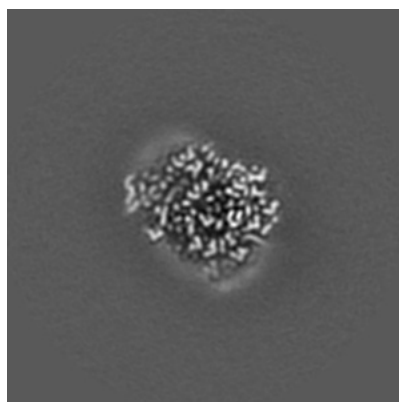
Y Index: 128
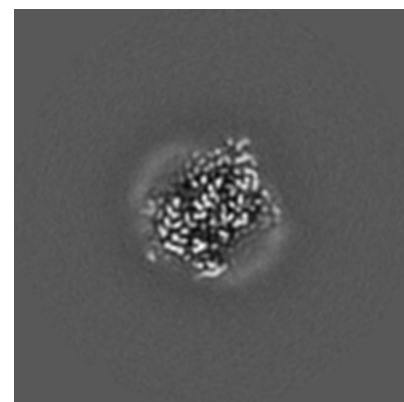
Z Index: 128

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

6.3 Largest variance slices (i)

6.3.1 Primary map
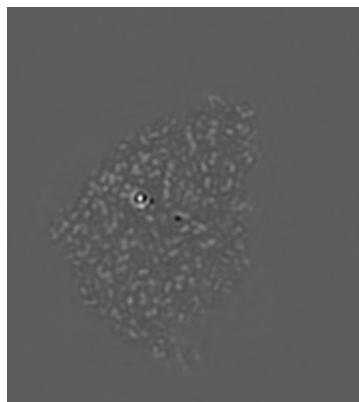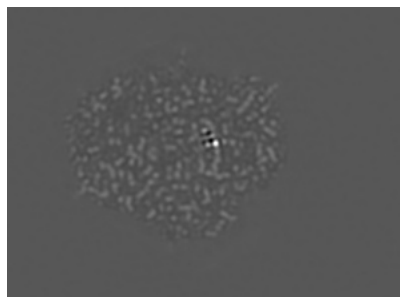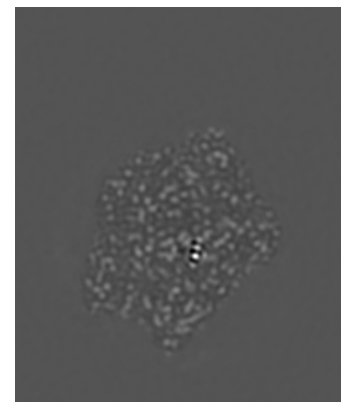
| X Index: 65 | Y Index: 55 | Z Index: 86 |

6.3.2 Raw map
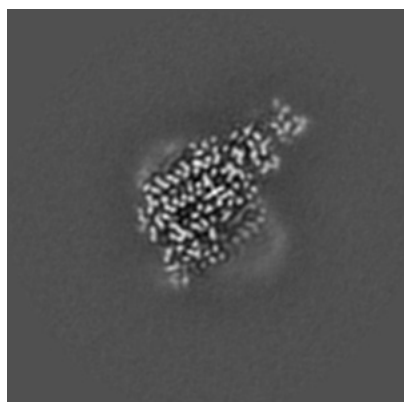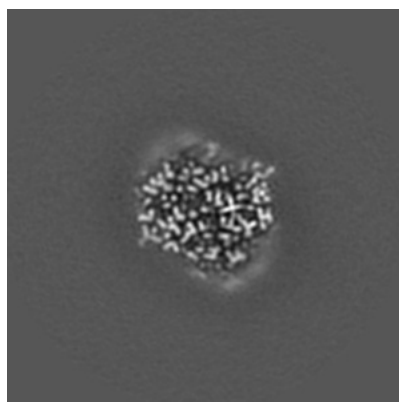
| X Index: 118 | Y Index: 121 | Z Index: 131 |
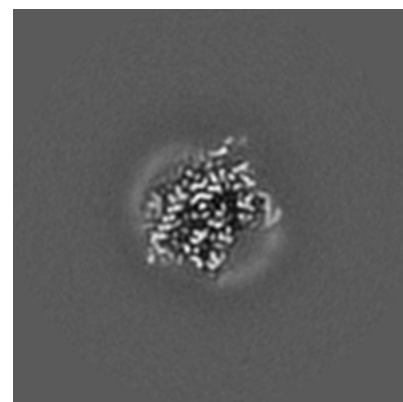
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
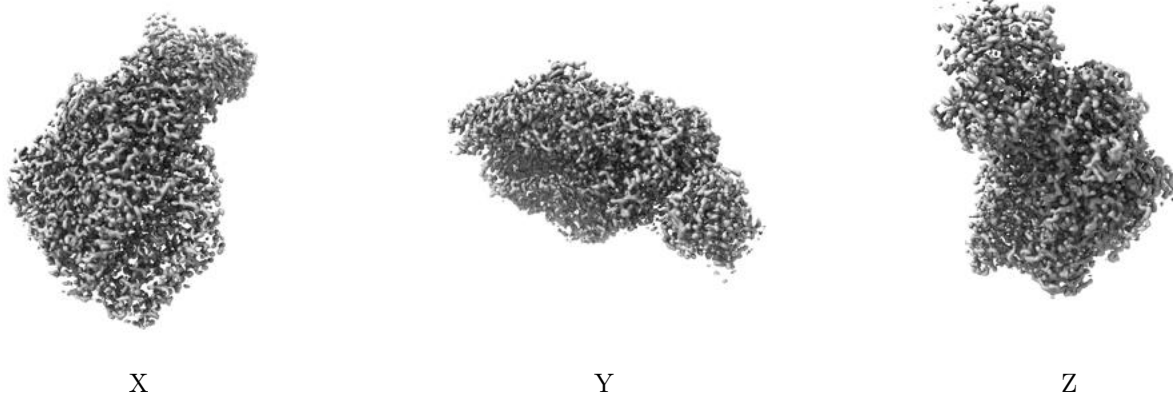
The images above show the 3D surface view of the map at the recommended contour level 1.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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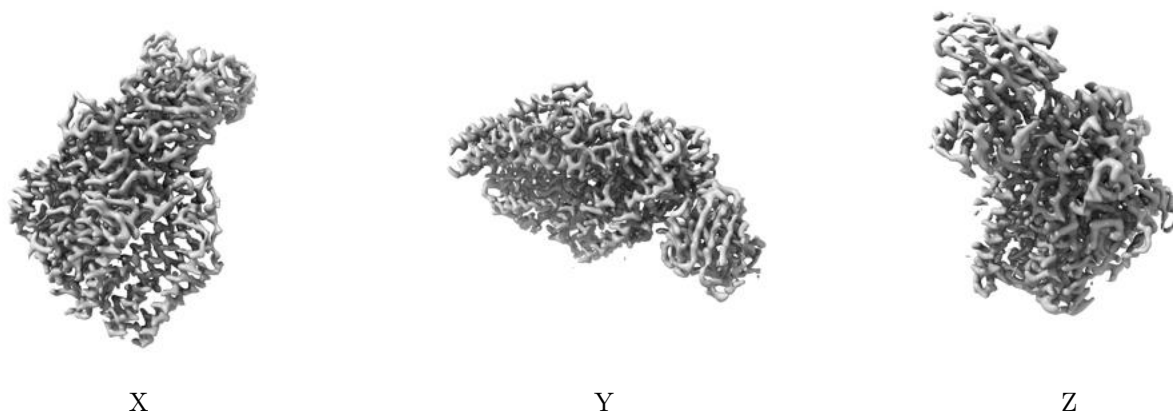
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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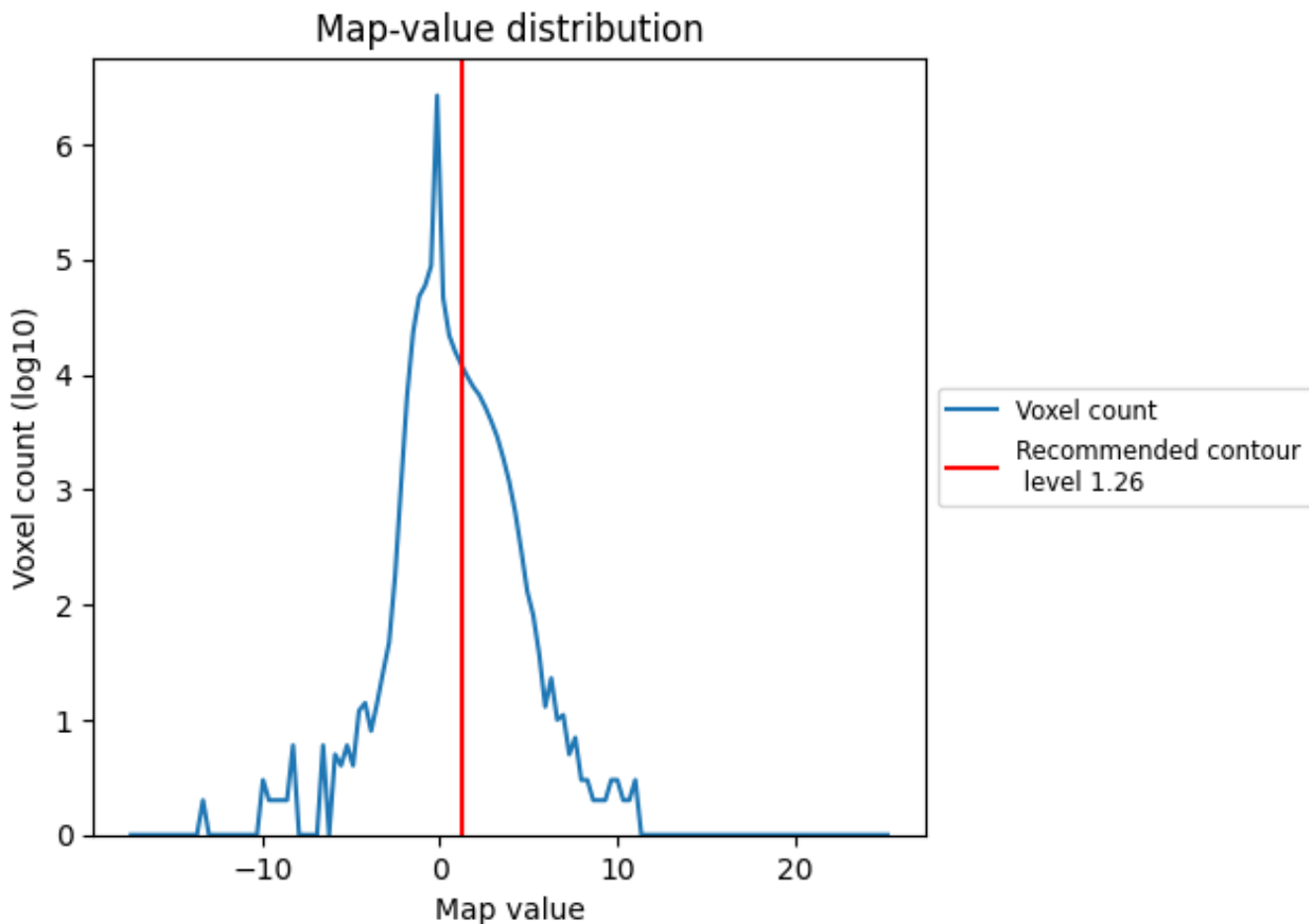
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
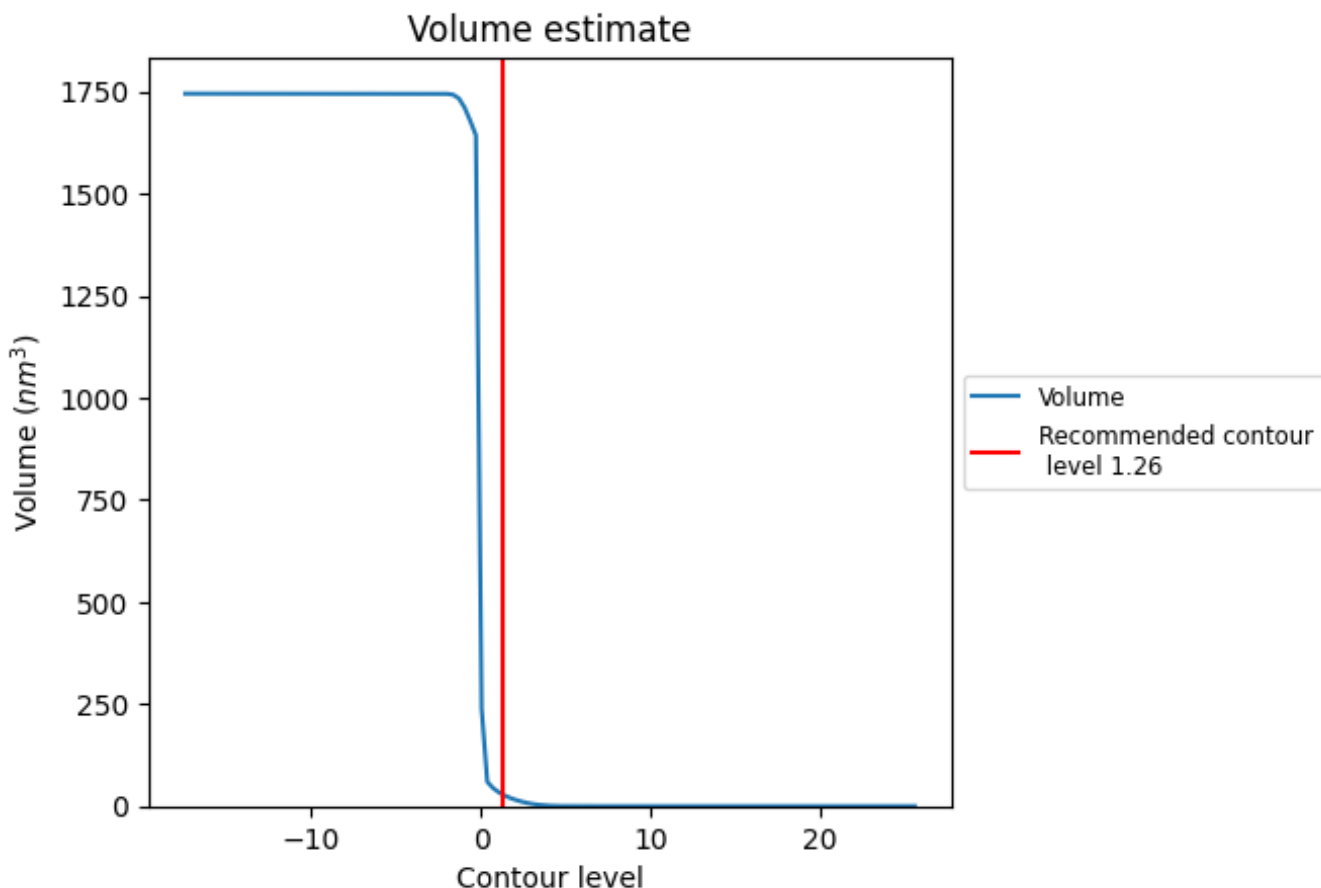
The volume at the recommended contour level is 30 nm^3; this corresponds to an approximate mass of 27 kDa.

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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

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 ⓘ
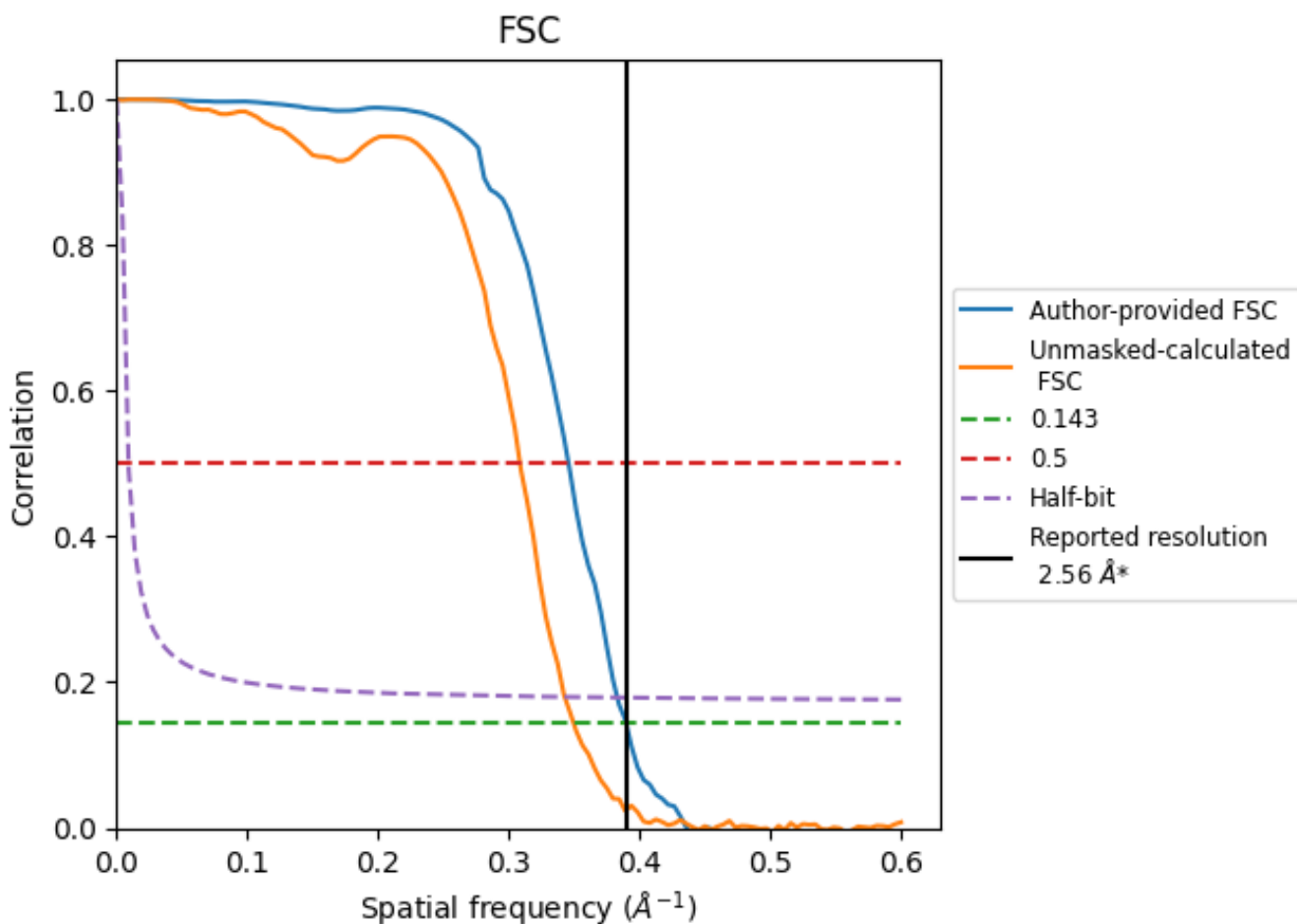
*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.56	2.89	2.61
Unmasked-calculated*	2.86	3.24	2.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.86 differs from the reported value 2.56 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11924 and PDB model 7AU3. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ

| X | Y | Z |
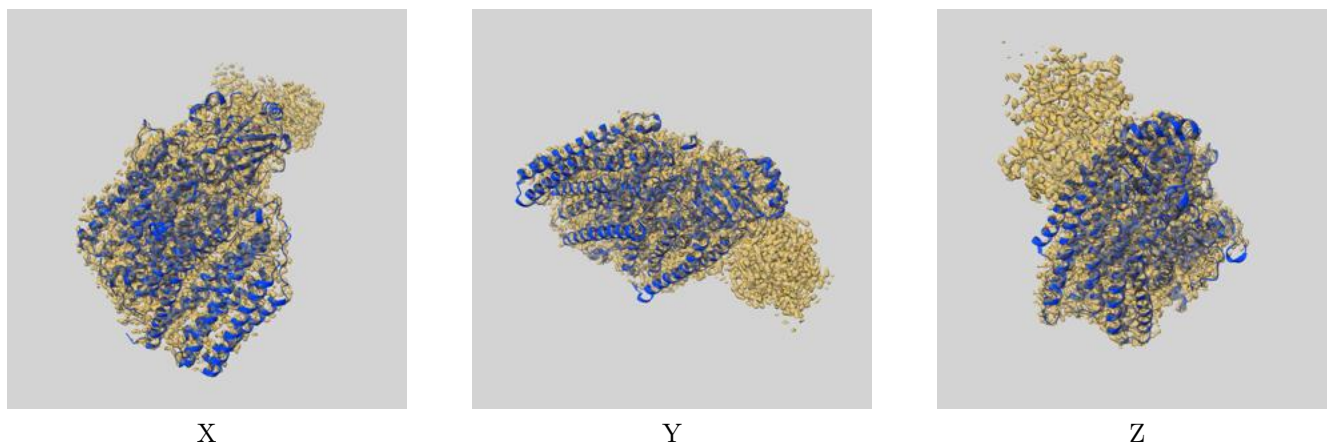
The images above show the 3D surface view of the map at the recommended contour level 1.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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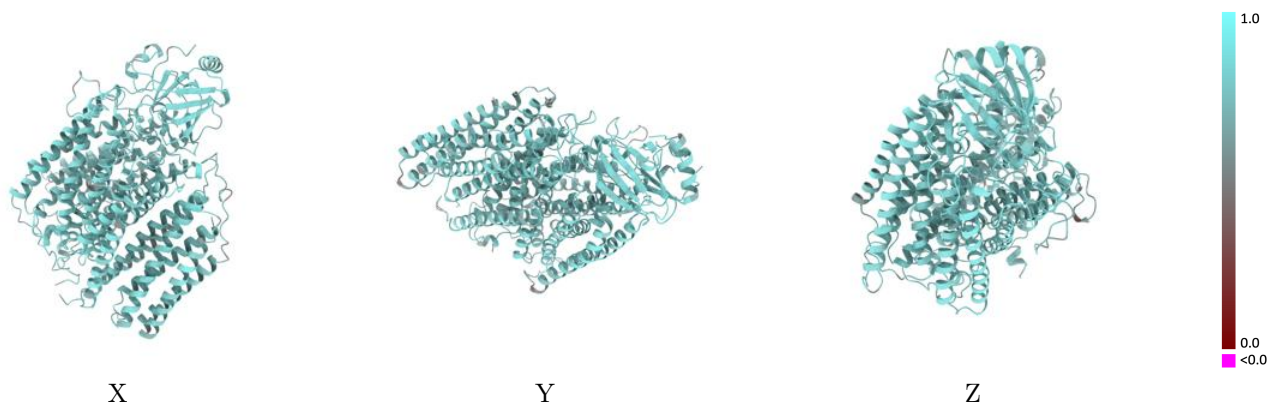
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
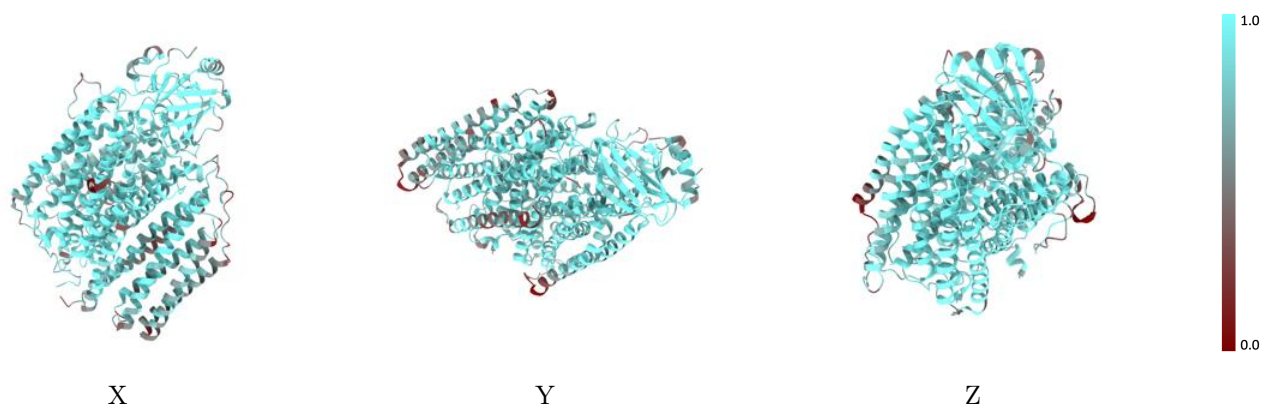
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.26).

9.4 Atom inclusion ⓘ
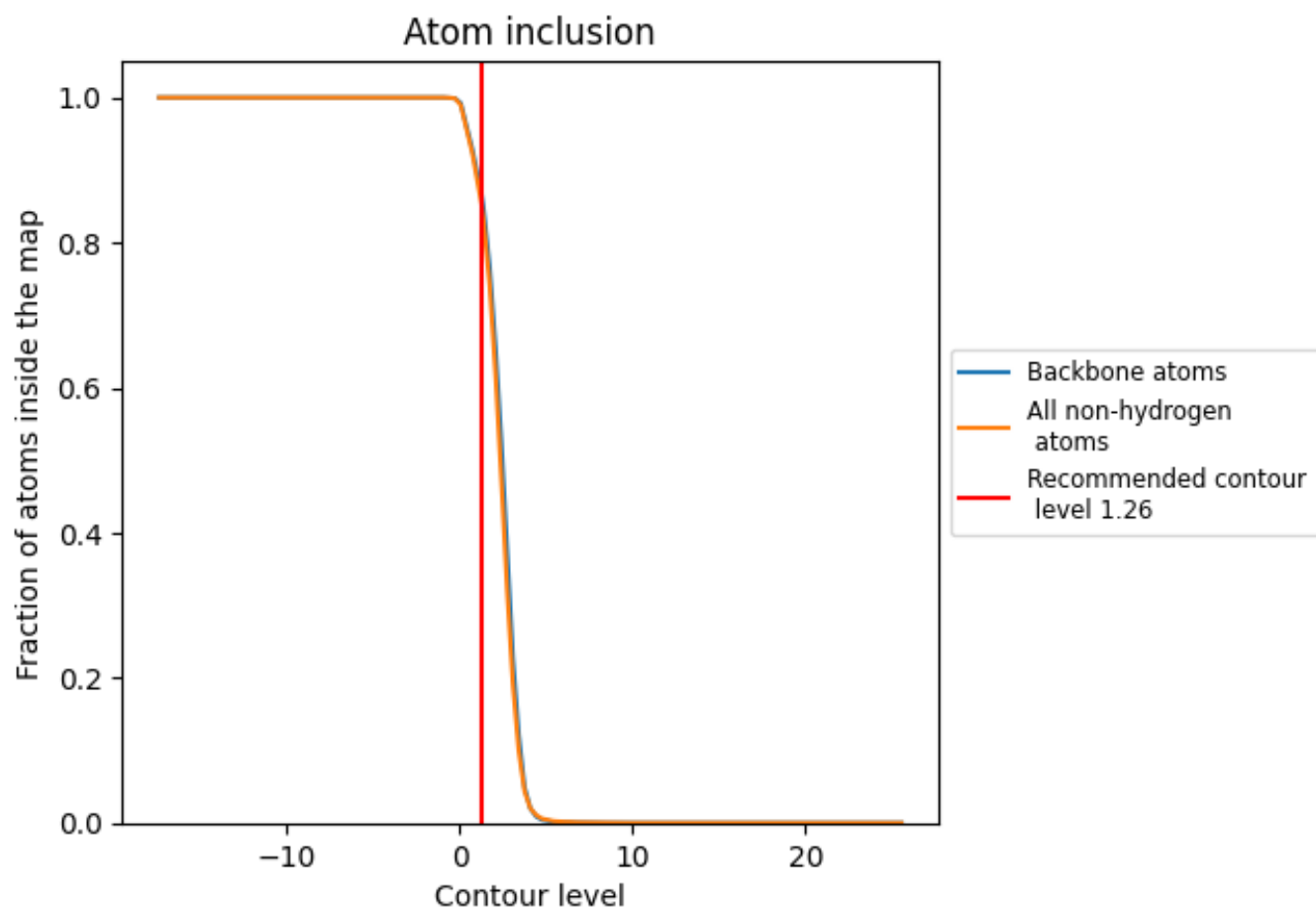
At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8528	0.7440
A	0.9375	0.7600
B	0.8381	0.7440
C	0.7443	0.7180
D	0.5541	0.7000

1.0

0.0
<0.0