wwPDB EM Validation Summary Report

Dec 29, 2024 – 01:19 PM EST

PDB ID	:	7QRU
EMDB ID	:	EMD-14124
Title	:	Structure of Bacillus pseudofirmus Mrp antiporter complex, monomer
Authors	:	Lee, Y.
Deposited on	:	2022-01-12
Resolution	:	2.24 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

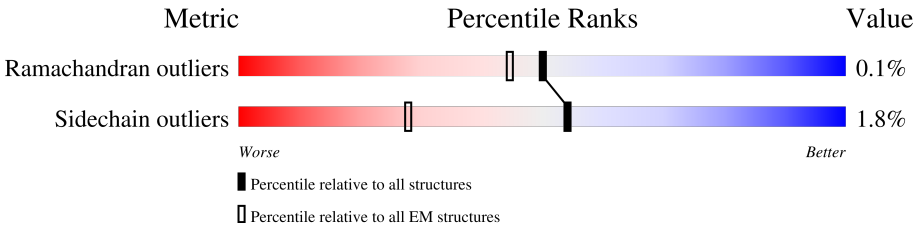
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.24 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	D	493	97%
2	A	805	97%
3	B	144	10% 93%
4	C	112	96%
5	E	158	31% 92% 8%
5	e	158	10% 28% 70%
6	F	91	96%
7	G	133	5% 81% 15%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16100 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 Na+/H+ antiporter subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	491	3906	2652	589	642	23	7	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	49	MET	VAL	conflict	UNP A0A1Q9PMS5
D	180	ILE	LEU	conflict	UNP A0A1Q9PMS5
D	183	VAL	ILE	conflict	UNP A0A1Q9PMS5
D	189	MET	LEU	conflict	UNP A0A1Q9PMS5
D	198	GLN	GLU	conflict	UNP A0A1Q9PMS5
D	349	ARG	LYS	conflict	UNP A0A1Q9PMS5

- Molecule 2 is a protein called Na+/H+ antiporter subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	805	6440	4322	983	1096	39	16	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ARG	GLN	conflict	UNP A0A1Q9PN15
A	51	VAL	ILE	conflict	UNP A0A1Q9PN15
A	423	THR	VAL	conflict	UNP A0A1Q9PN15
A	461	LYS	GLN	conflict	UNP A0A1Q9PN15
A	509	ILE	VAL	conflict	UNP A0A1Q9PN15
A	513	LEU	VAL	conflict	UNP A0A1Q9PN15
A	519	VAL	LEU	conflict	UNP A0A1Q9PN15
A	603	THR	ALA	conflict	UNP A0A1Q9PN15

- Molecule 3 is a protein called Na(+)/H(+) antiporter subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	140	Total	C	N	O	S	1	0
			1089	734	158	192	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	84	ILE	VAL	conflict	UNP A0A1Q9PN06

- Molecule 4 is a protein called Na(+)/H(+) antiporter subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	112	Total	C	N	O	S	0	0
			859	562	138	155	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	ALA	conflict	UNP Q9RGZ3

- Molecule 5 is a protein called Na+/H+ antiporter subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	158	Total	C	N	O	S	1	0
			1305	872	207	220	6		
5	e	47	Total	C	N	O	S	0	0
			395	274	62	58	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	62	VAL	SER	conflict	UNP A0A1Q9PMT4
E	158	ASN	LYS	conflict	UNP A0A1Q9PMT4
e	62	VAL	SER	conflict	UNP A0A1Q9PMT4
e	158	ASN	LYS	conflict	UNP A0A1Q9PMT4

- Molecule 6 is a protein called Na(+)/H(+) antiporter subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	91	Total	C	N	O	S	3	0
			723	481	110	124	8		

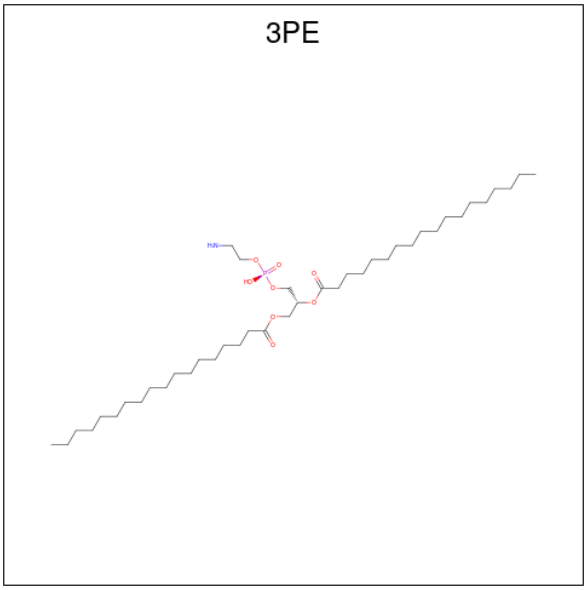
- Molecule 7 is a protein called Na+/H+ antiporter subunit G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	113	Total	C	N	O	S	1	0
			888	598	138	146	6		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	120	HIS	-	expression tag	UNP A0A1Q9PMU8
G	121	HIS	-	expression tag	UNP A0A1Q9PMU8
G	122	HIS	-	expression tag	UNP A0A1Q9PMU8
G	123	HIS	-	expression tag	UNP A0A1Q9PMU8
G	124	HIS	-	expression tag	UNP A0A1Q9PMU8
G	125	HIS	-	expression tag	UNP A0A1Q9PMU8
G	126	ASP	-	expression tag	UNP A0A1Q9PMU8
G	127	TYR	-	expression tag	UNP A0A1Q9PMU8
G	128	LYS	-	expression tag	UNP A0A1Q9PMU8
G	129	ASP	-	expression tag	UNP A0A1Q9PMU8
G	130	ASP	-	expression tag	UNP A0A1Q9PMU8
G	131	ASP	-	expression tag	UNP A0A1Q9PMU8
G	132	ASP	-	expression tag	UNP A0A1Q9PMU8
G	133	LYS	-	expression tag	UNP A0A1Q9PMU8

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			49	39	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
8	E	1	Total 37	C 27	N 1	O 8	P 1	0
8	E	1	Total 49	C 39	N 1	O 8	P 1	0

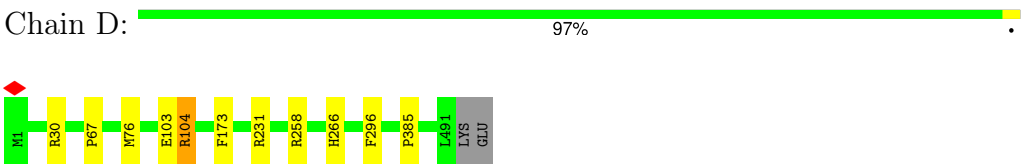
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	D	113	Total 113	O 113	0
9	A	140	Total 140	O 140	0
9	B	24	Total 24	O 24	0
9	C	36	Total 36	O 36	0
9	E	11	Total 11	O 11	0
9	F	19	Total 19	O 19	0
9	G	15	Total 15	O 15	0
9	e	2	Total 2	O 2	0

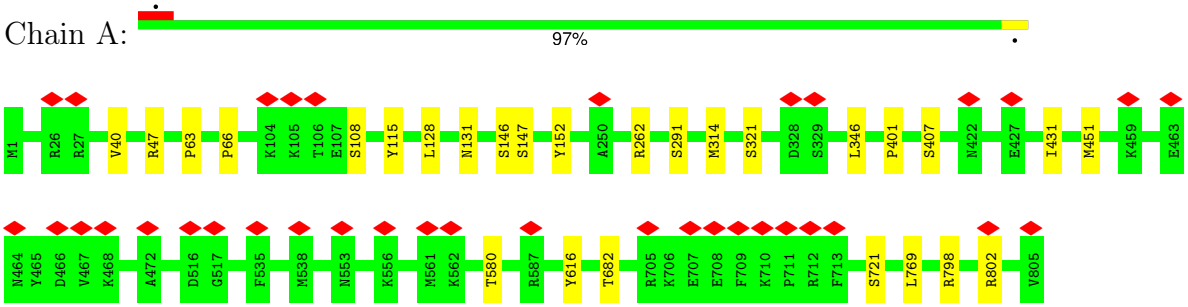
3 Residue-property plots (i)

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

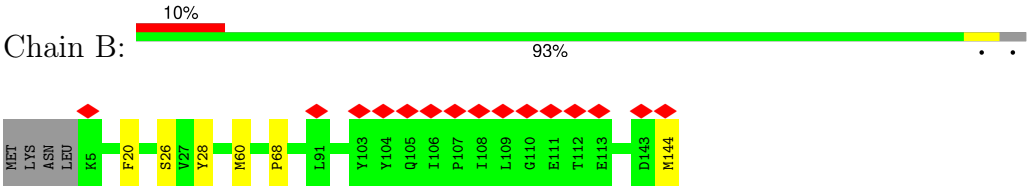
• Molecule 1: Na+/H+ antiporter subunit D



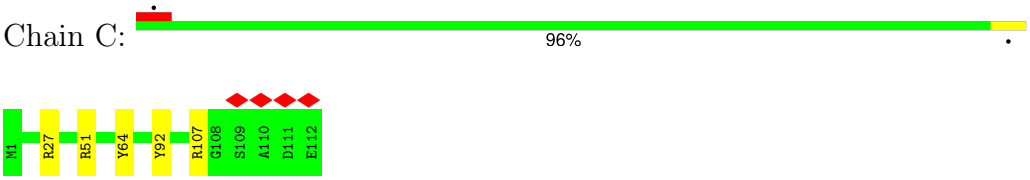
• Molecule 2: Na+/H+ antiporter subunit A



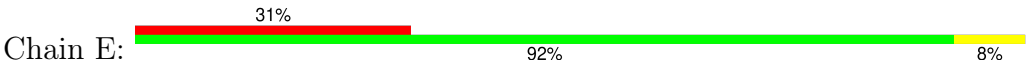
• Molecule 3: Na(+)/H(+) antiporter subunit B

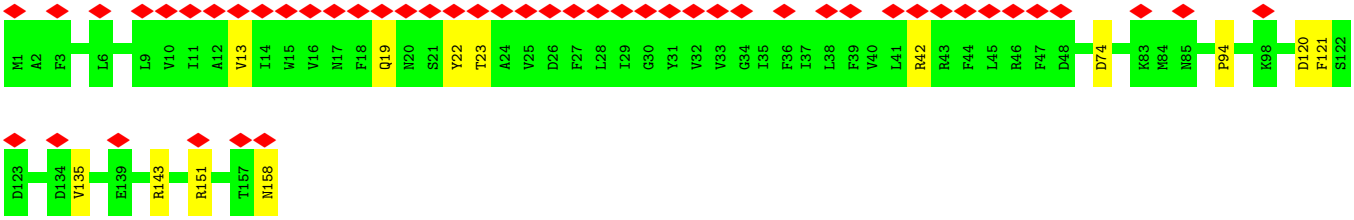


• Molecule 4: Na(+)/H(+) antiporter subunit C



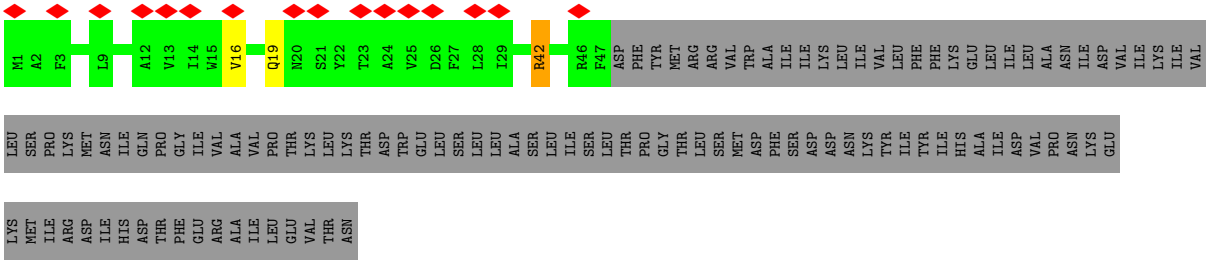
• Molecule 5: Na+/H+ antiporter subunit E





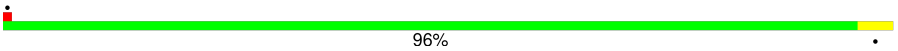
• Molecule 5: Na+/H+ antiporter subunit E

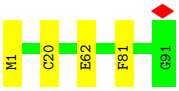
Chain e:



• Molecule 6: Na(+)/H(+) antiporter subunit F

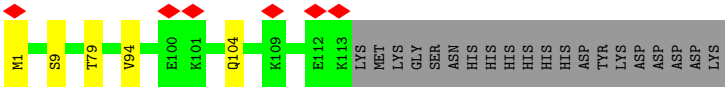
Chain F:





• Molecule 7: Na+/H+ antiporter subunit G1

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	513743	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07136, 1.07136, 1.07136	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE

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	D	0.96	1/4009 (0.0%)	1.20	5/5452 (0.1%)
2	A	0.88	3/6609 (0.0%)	1.13	10/8998 (0.1%)
3	B	0.81	1/1115 (0.1%)	1.07	4/1514 (0.3%)
4	C	0.92	0/873	1.17	1/1187 (0.1%)
5	E	0.68	0/1334	1.01	5/1810 (0.3%)
5	e	0.87	0/405	1.24	3/550 (0.5%)
6	F	0.94	1/732 (0.1%)	1.16	1/986 (0.1%)
7	G	0.93	1/908 (0.1%)	1.15	0/1225
All	All	0.89	7/15985 (0.0%)	1.14	29/21722 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
2	A	0	4
3	B	0	1
4	C	0	3
5	E	0	1
6	F	0	1
All	All	0	12

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	62	GLU	CD-OE1	8.36	1.34	1.25
2	A	721	SER	CA-CB	-7.14	1.42	1.52
7	G	9	SER	CA-CB	-5.78	1.44	1.52
1	D	266	HIS	CE1-NE2	5.62	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	146	SER	CA-CB	-5.60	1.44	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	258	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	D	258	ARG	NE-CZ-NH1	9.23	124.92	120.30
5	e	42	ARG	NE-CZ-NH1	8.67	124.64	120.30
2	A	798	ARG	NE-CZ-NH1	-8.67	115.97	120.30
5	E	22	TYR	CB-CA-C	6.39	123.19	110.40

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	128	LEU	Mainchain
2	A	291	SER	Mainchain
2	A	47	ARG	Sidechain
1	D	104	ARG	Sidechain
1	D	231	ARG	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	D	496/493 (101%)	486 (98%)	10 (2%)	0	100	100
2	A	819/805 (102%)	795 (97%)	24 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	139/144 (96%)	133 (96%)	6 (4%)	0	100	100
4	C	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
5	E	157/158 (99%)	151 (96%)	6 (4%)	0	100	100
5	e	45/158 (28%)	44 (98%)	1 (2%)	0	100	100
6	F	92/91 (101%)	90 (98%)	2 (2%)	0	100	100
7	G	112/133 (84%)	108 (96%)	3 (3%)	1 (1%)	14	11
All	All	1970/2094 (94%)	1916 (97%)	53 (3%)	1 (0%)	50	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	104	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	411/406 (101%)	406 (99%)	5 (1%)	67	75
2	A	693/678 (102%)	682 (98%)	11 (2%)	58	66
3	B	116/119 (98%)	115 (99%)	1 (1%)	75	82
4	C	96/96 (100%)	95 (99%)	1 (1%)	73	79
5	E	146/145 (101%)	139 (95%)	7 (5%)	21	21
5	e	42/145 (29%)	40 (95%)	2 (5%)	21	21
6	F	83/80 (104%)	82 (99%)	1 (1%)	67	75
7	G	95/113 (84%)	92 (97%)	3 (3%)	34	39
All	All	1682/1782 (94%)	1651 (98%)	31 (2%)	54	61

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	580	THR

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Mol	Chain	Res	Type
7	G	79	THR
4	C	92	TYR
5	e	19	GLN
5	E	158	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	43	ASN
5	e	8	ASN
5	e	19	GLN
2	A	365	HIS
2	A	111	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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	$\#\|Z\|>2$
8	3PE	E	201	-	36,36,50	0.63	1 (2%)	39,41,55	0.74	1 (2%)
8	3PE	A	901	-	48,48,50	1.16	5 (10%)	51,53,55	0.84	2 (3%)
8	3PE	E	202	-	48,48,50	0.84	1 (2%)	51,53,55	0.77	2 (3%)

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
8	3PE	E	201	-	-	11/40/40/54	-
8	3PE	A	901	-	-	23/52/52/54	-
8	3PE	E	202	-	-	26/52/52/54	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	901	3PE	C2A-C29	-4.44	1.29	1.51
8	E	202	3PE	C2A-C29	-3.55	1.34	1.51
8	A	901	3PE	C22-C21	-3.05	1.41	1.50
8	E	201	3PE	C2A-C29	-2.93	1.33	1.51
8	A	901	3PE	C24-C23	-2.34	1.40	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	901	3PE	O21-C2-C3	-2.82	98.23	108.34
8	A	901	3PE	C3-C2-C1	2.38	117.33	111.78
8	E	201	3PE	O21-C21-O22	-2.21	118.54	123.70
8	E	202	3PE	C2B-C2A-C29	2.19	125.44	114.37
8	E	202	3PE	O11-P-O14	2.00	116.87	108.94

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	901	3PE	C1-O11-P-O12
8	A	901	3PE	C1-O11-P-O13
8	A	901	3PE	C1-O11-P-O14
8	A	901	3PE	O13-C11-C12-N

Continued on next page...

Continued from previous page...

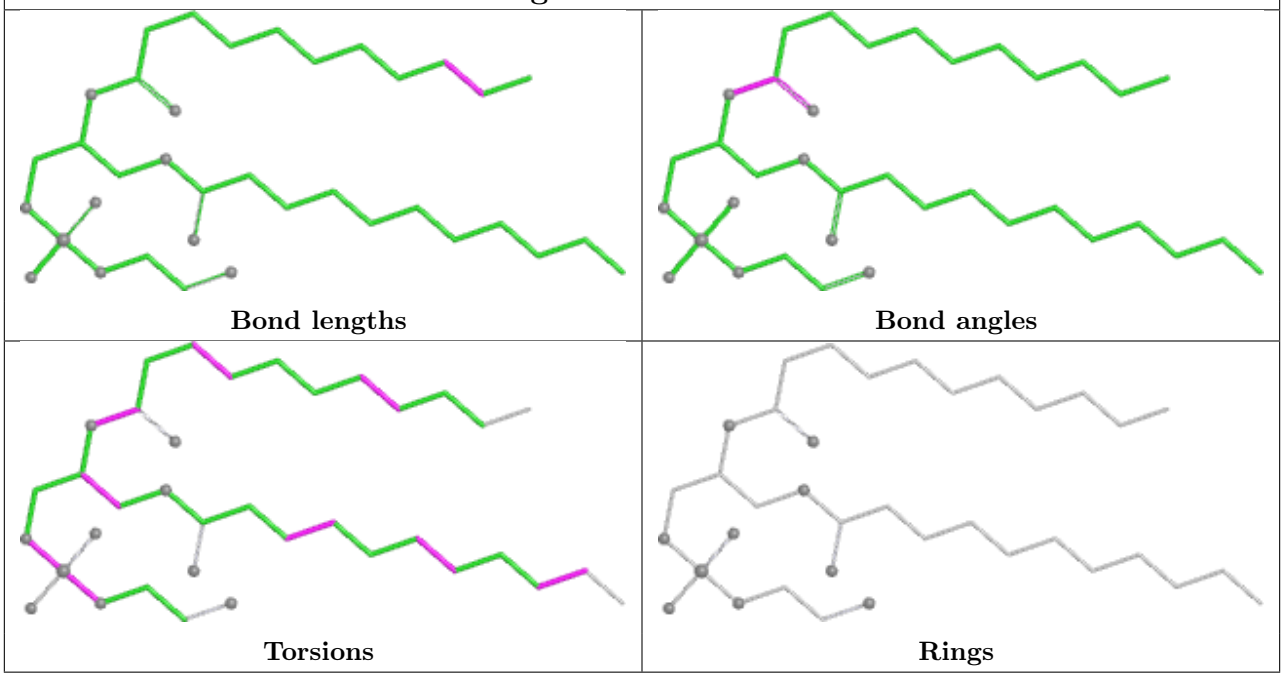
Mol	Chain	Res	Type	Atoms
8	E	201	3PE	C1-O11-P-O13

There are no ring outliers.

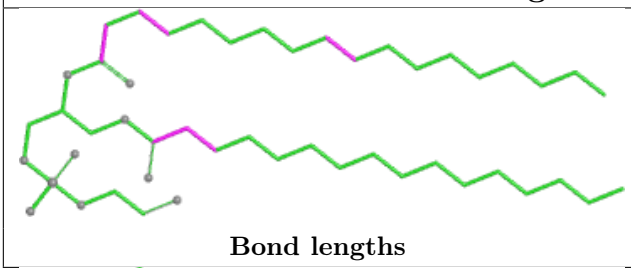
No monomer is involved in short contacts.

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.

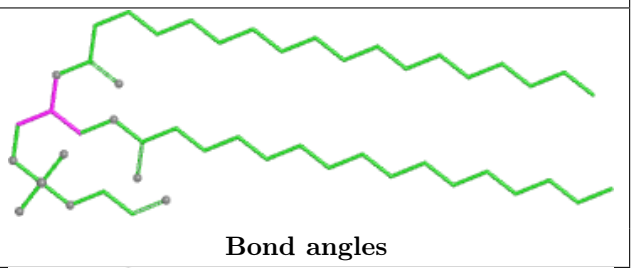
Ligand 3PE E 201



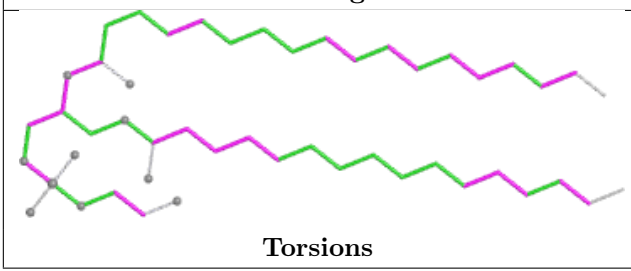
Ligand 3PE A 901



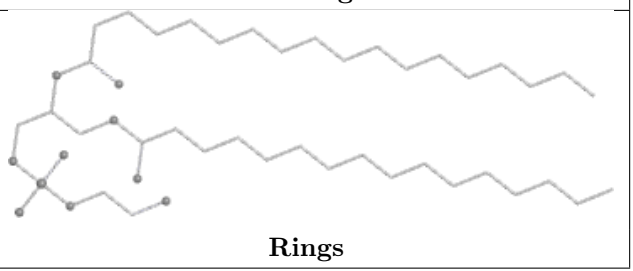
Bond lengths



Bond angles

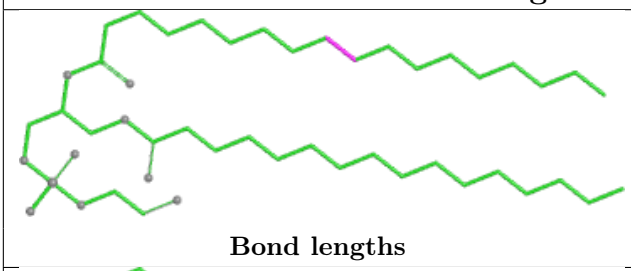


Torsions

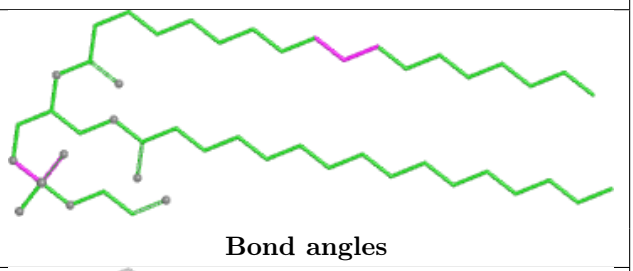


Rings

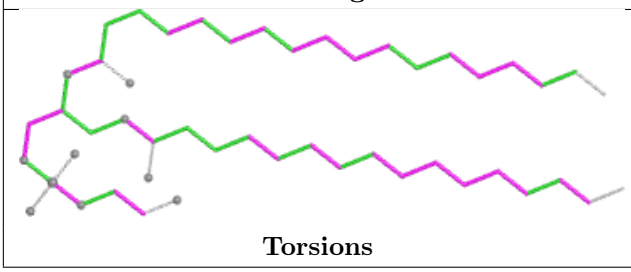
Ligand 3PE E 202



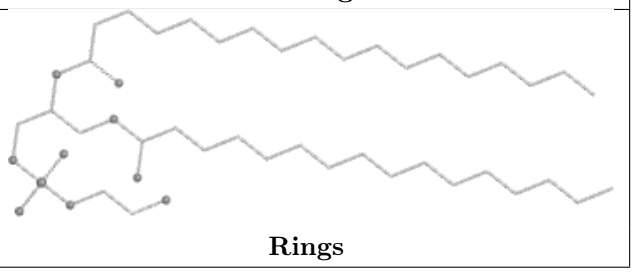
Bond lengths



Bond angles



Torsions



Rings

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.

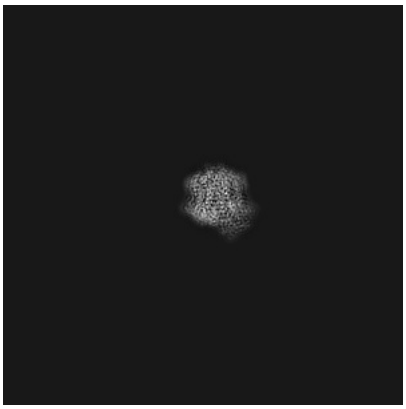
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14124. 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.

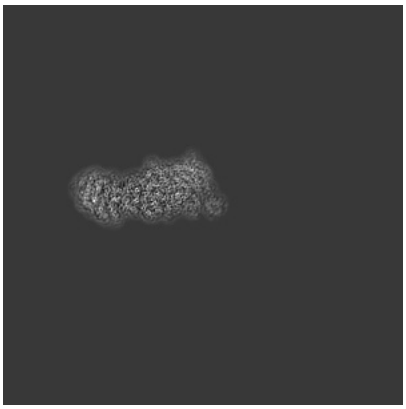
6.1 Orthogonal projections

6.1.1 Primary map



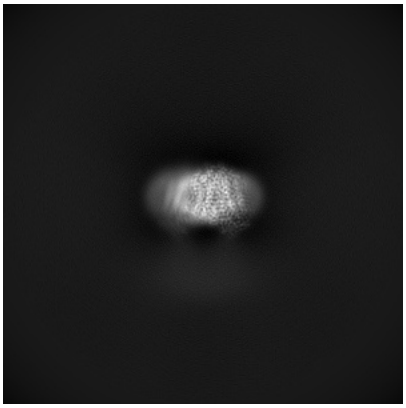
X

Y

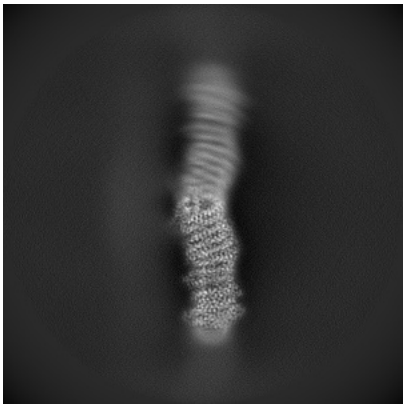


Z

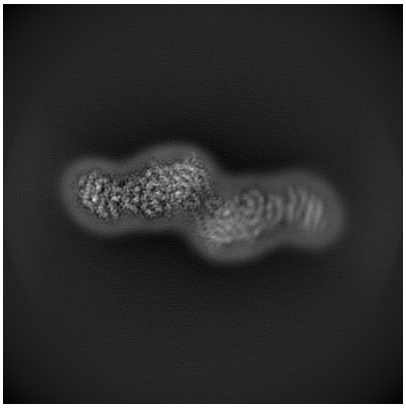
6.1.2 Raw map



X



Y

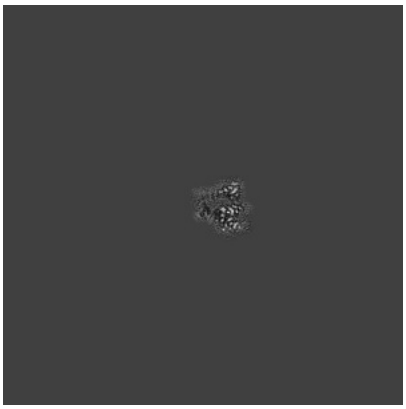


Z

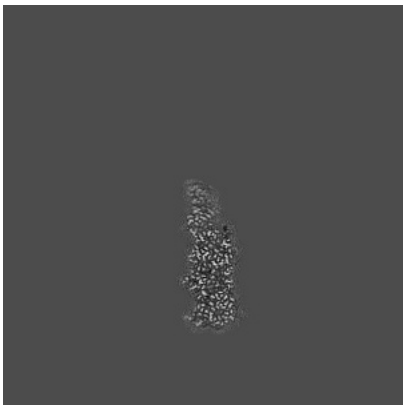
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



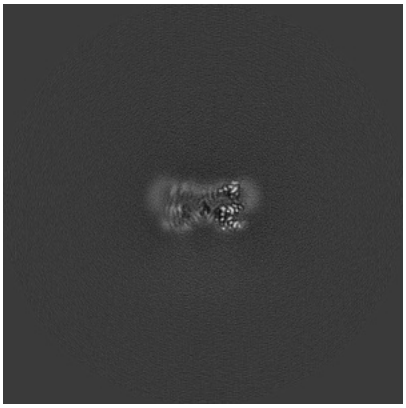
X Index: 200



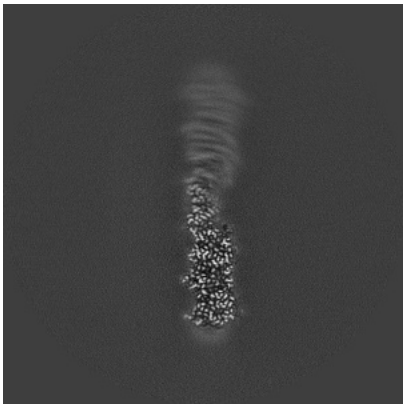
Y Index: 200

Z Index: 200

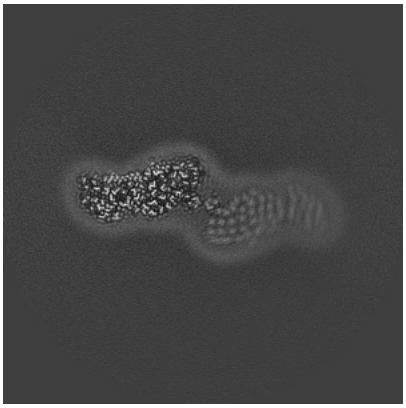
6.2.2 Raw map



X Index: 200



Y Index: 200

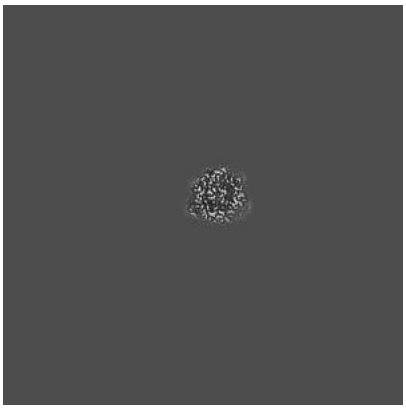


Z Index: 200

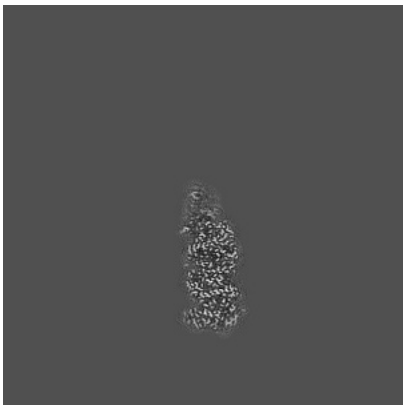
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

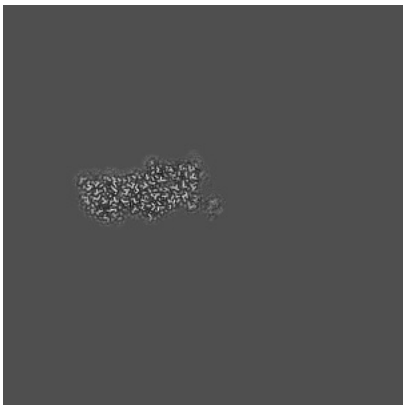
6.3.1 Primary map



X Index: 154

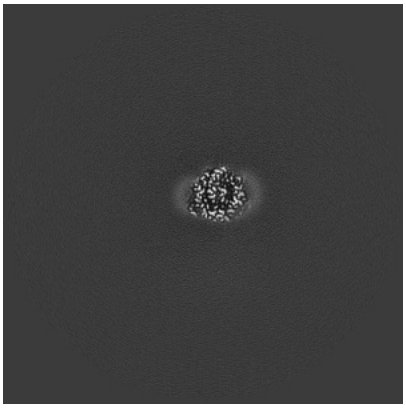


Y Index: 206

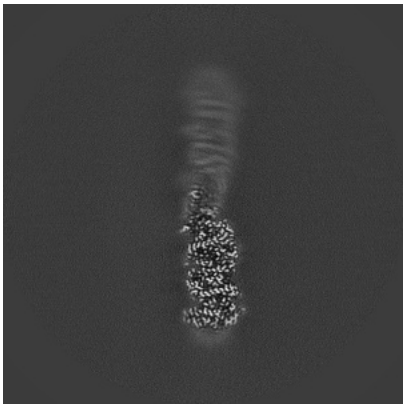


Z Index: 202

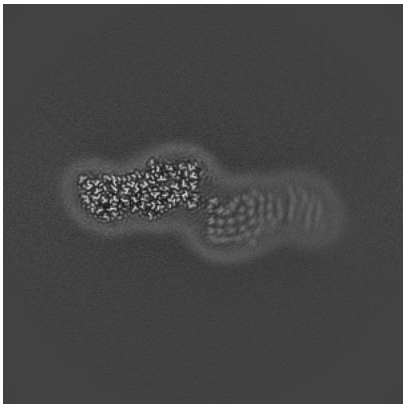
6.3.2 Raw map



X Index: 154



Y Index: 206

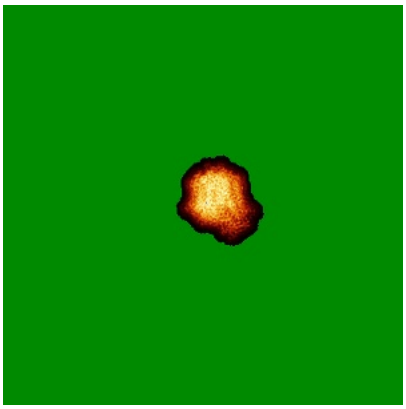


Z Index: 202

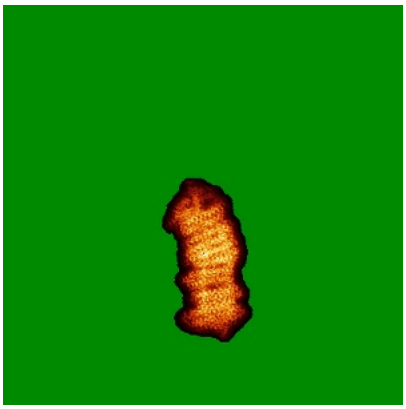
The images above show the largest variance slices of the map in three orthogonal directions.

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

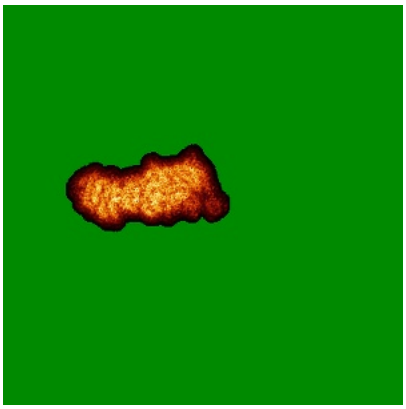
6.4.1 Primary map



X

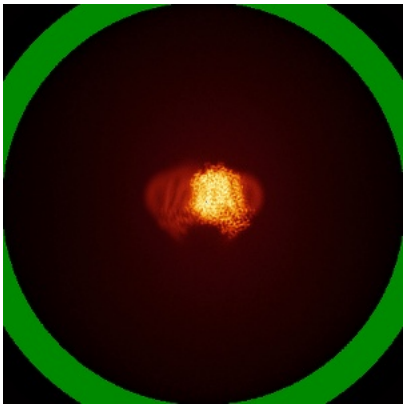


Y

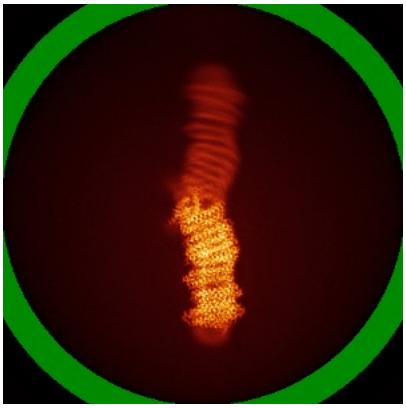


Z

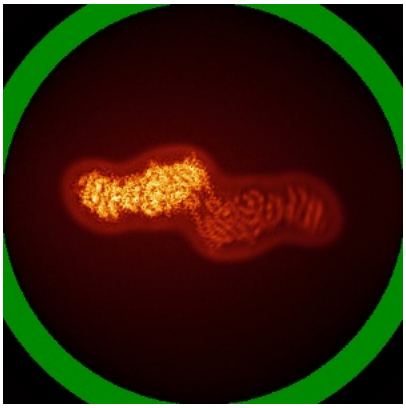
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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

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.

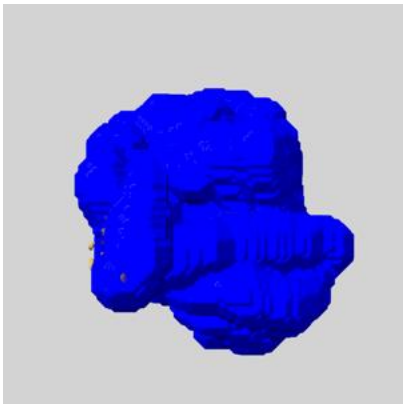
6.6 Mask visualisation (i)

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

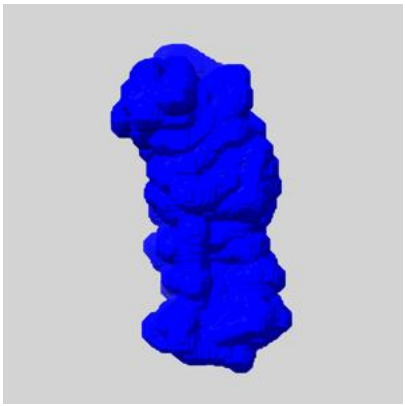
A mask typically either:

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

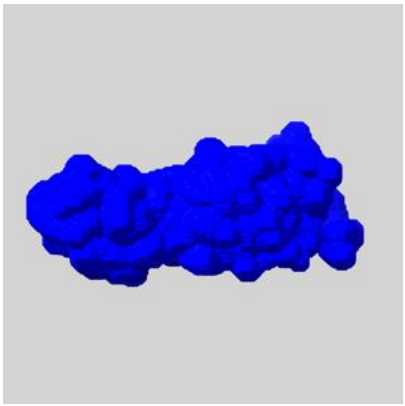
6.6.1 emd_14124_msk_1.map (i)



X



Y

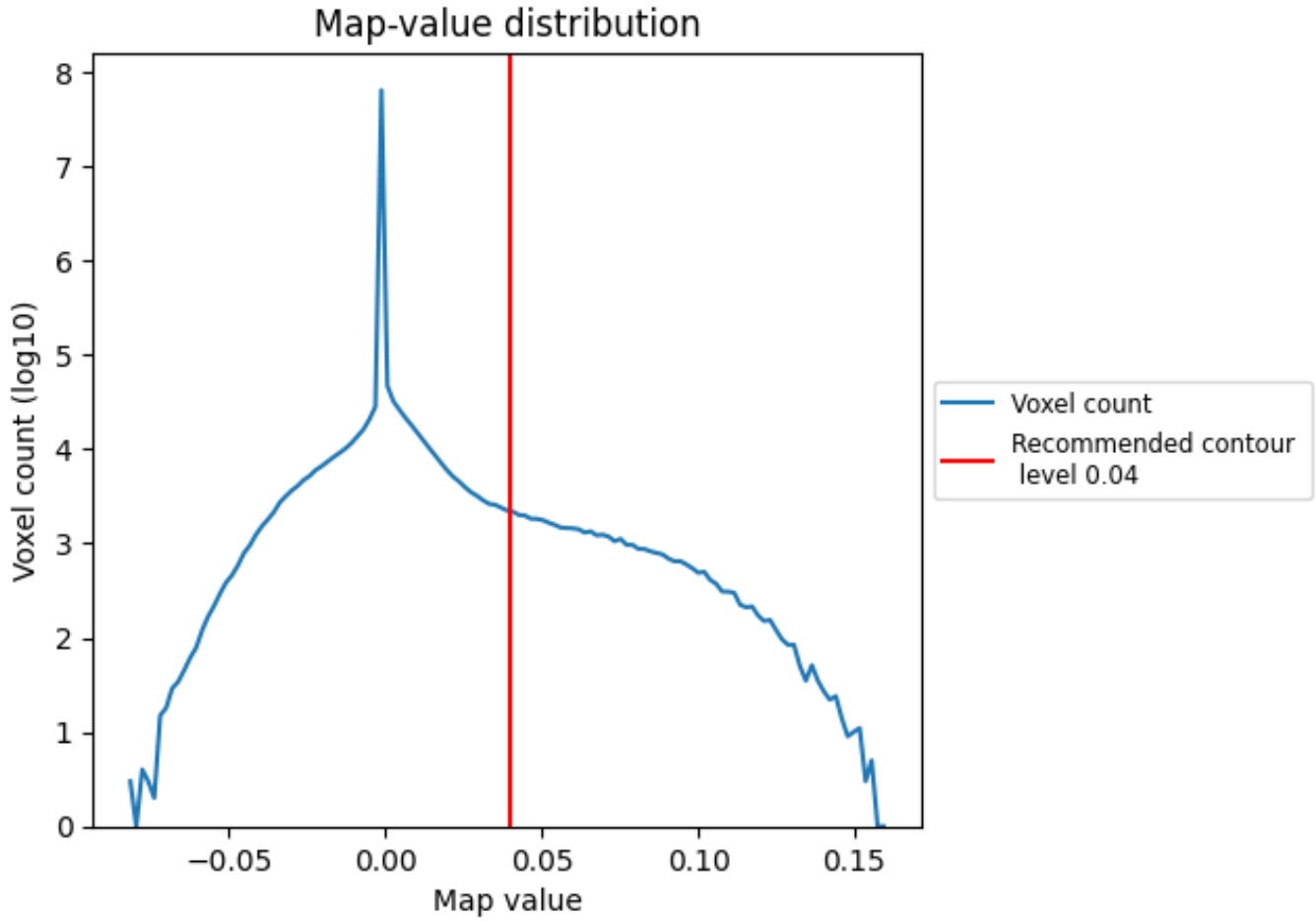


Z

7 Map analysis

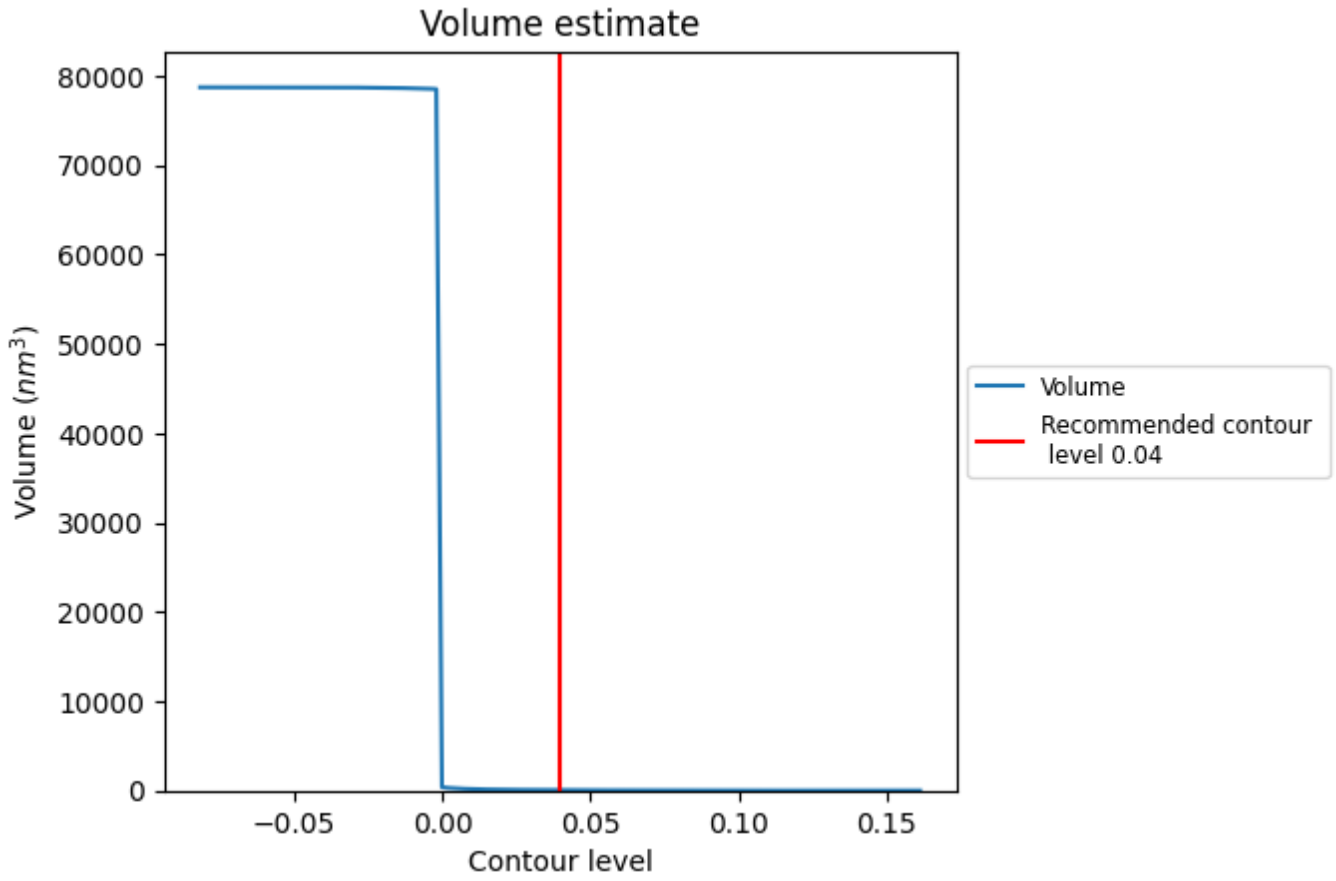
This section contains the results of statistical analysis of the map.

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.

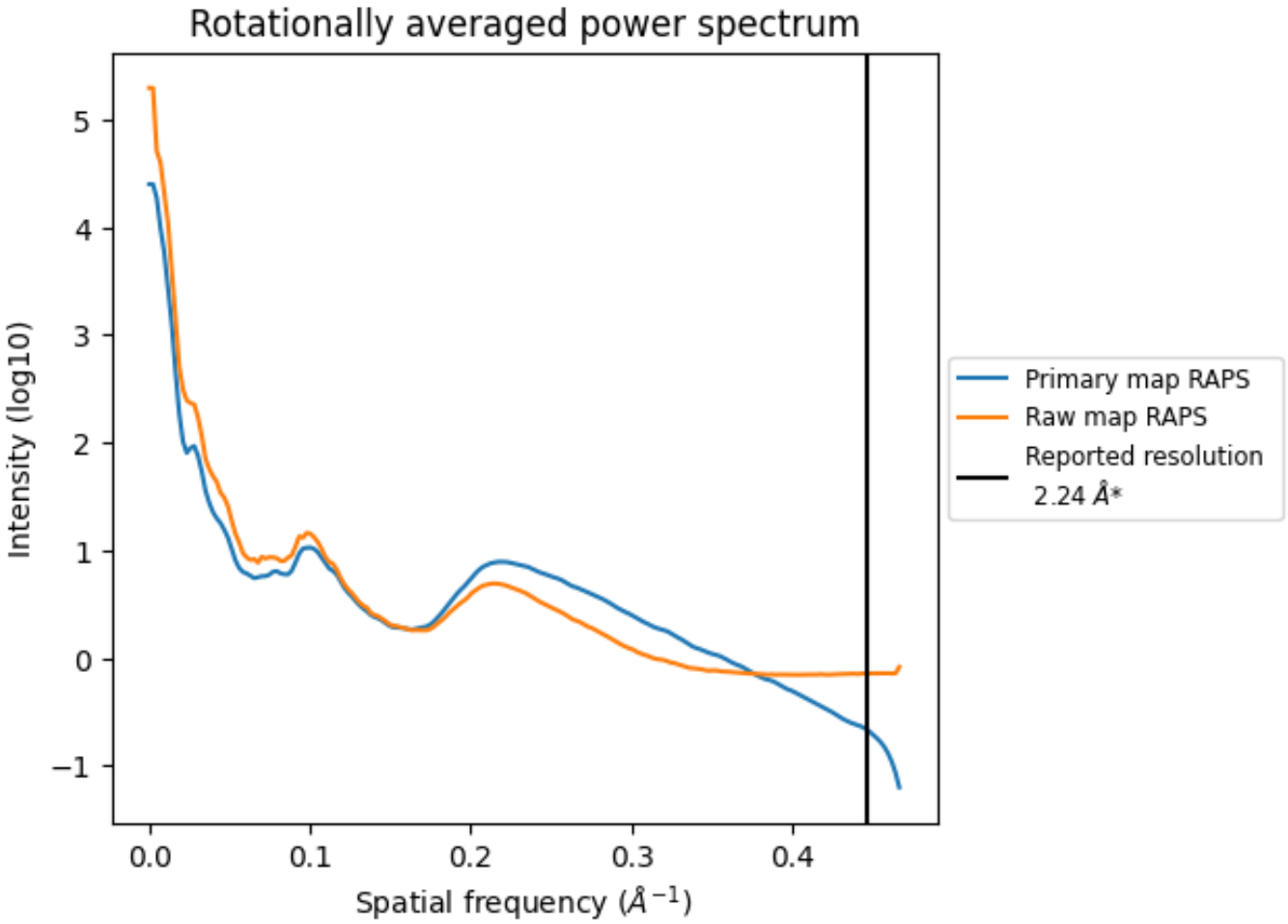
7.2 Volume estimate (i)



The volume at the recommended contour level is 54 nm^3; this corresponds to an approximate mass of 48 kDa.

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

7.3 Rotationally averaged power spectrum (i)

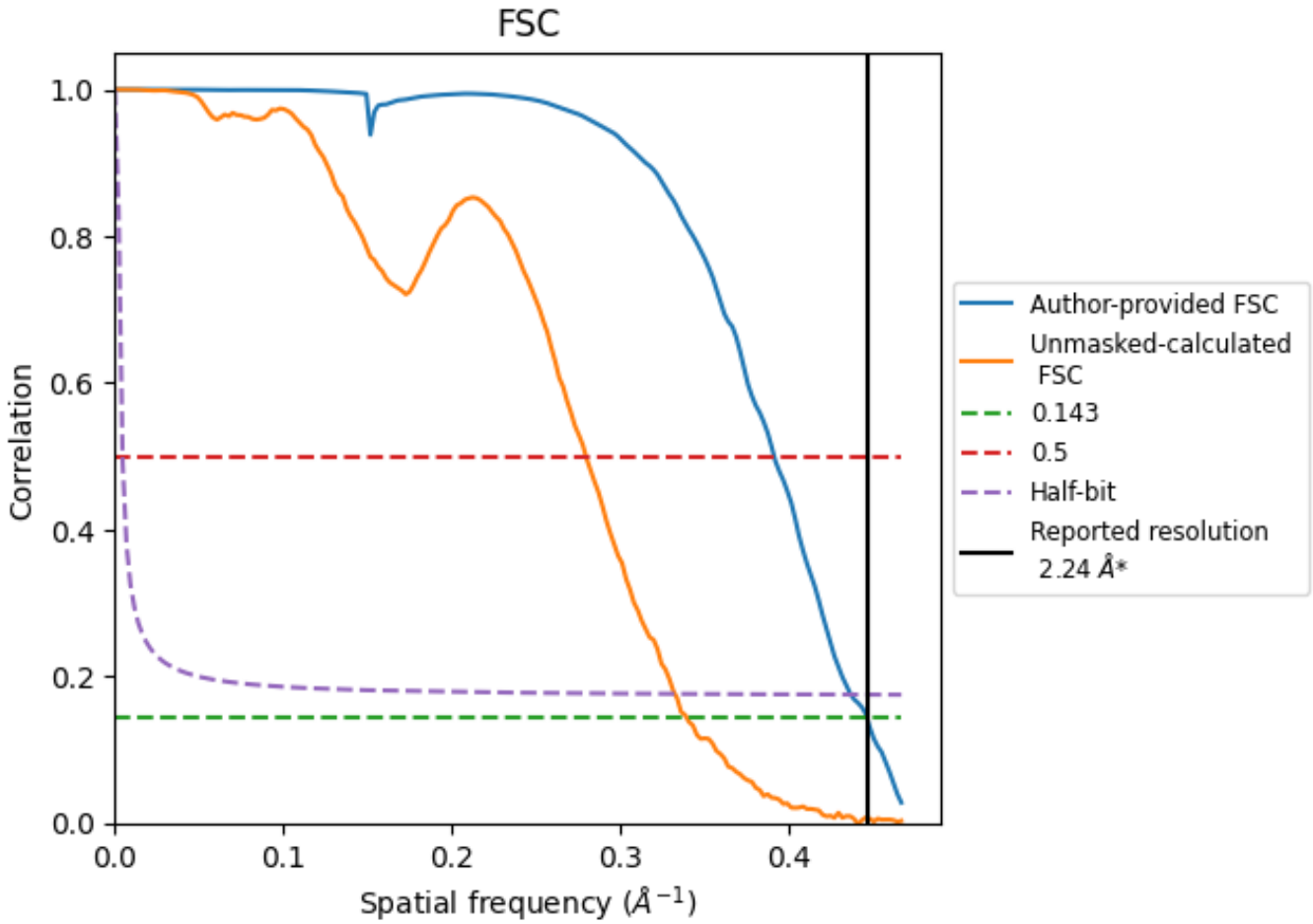


*Reported resolution corresponds to spatial frequency of 0.446 $Å^{-1}$

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 0.446 Å^{-1}

8.2 Resolution estimates (i)

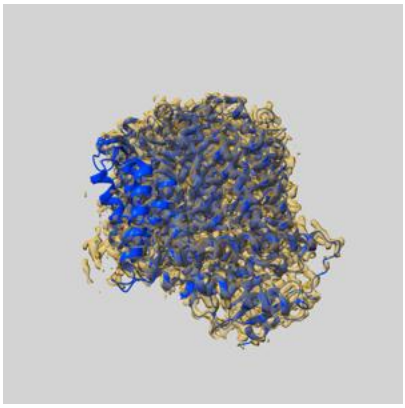
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.56	2.29
Unmasked-calculated*	2.95	3.58	3.01

*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 2.95 differs from the reported value 2.24 by more than 10 %

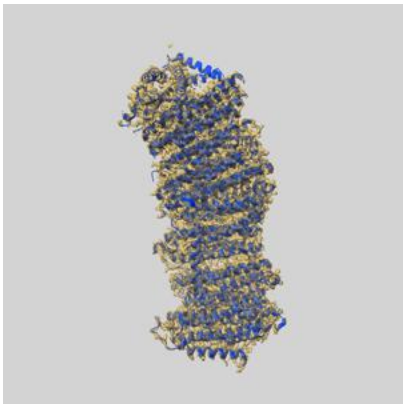
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14124 and PDB model 7QRU. Per-residue inclusion information can be found in section 3 on page 7.

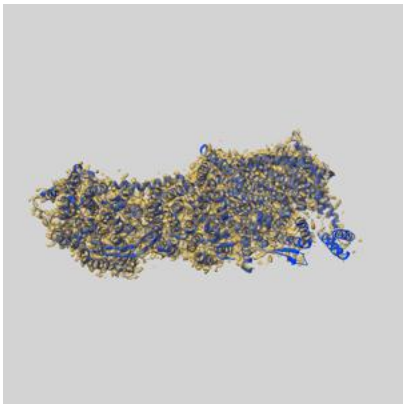
9.1 Map-model overlay



X



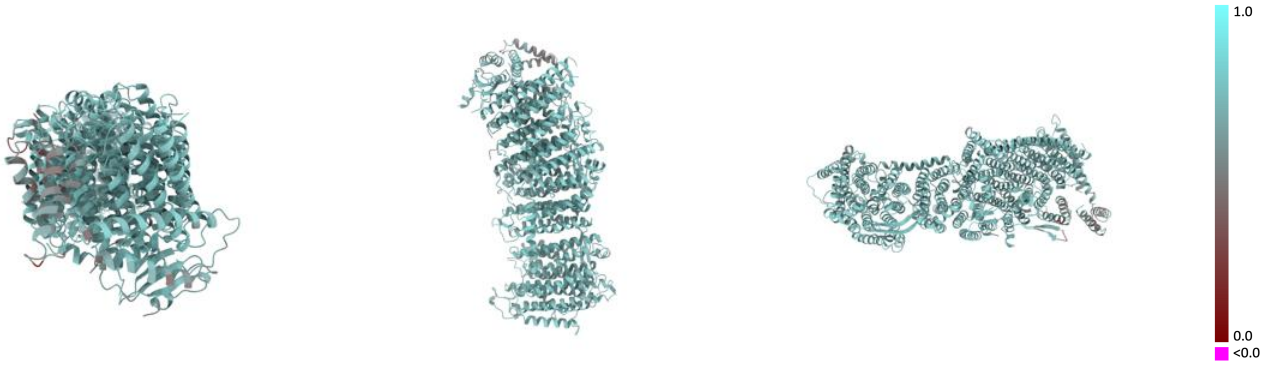
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

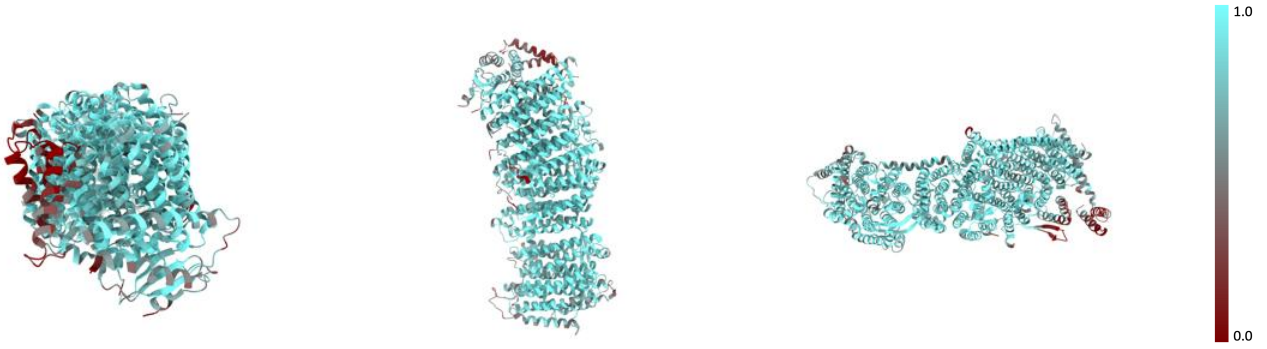
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

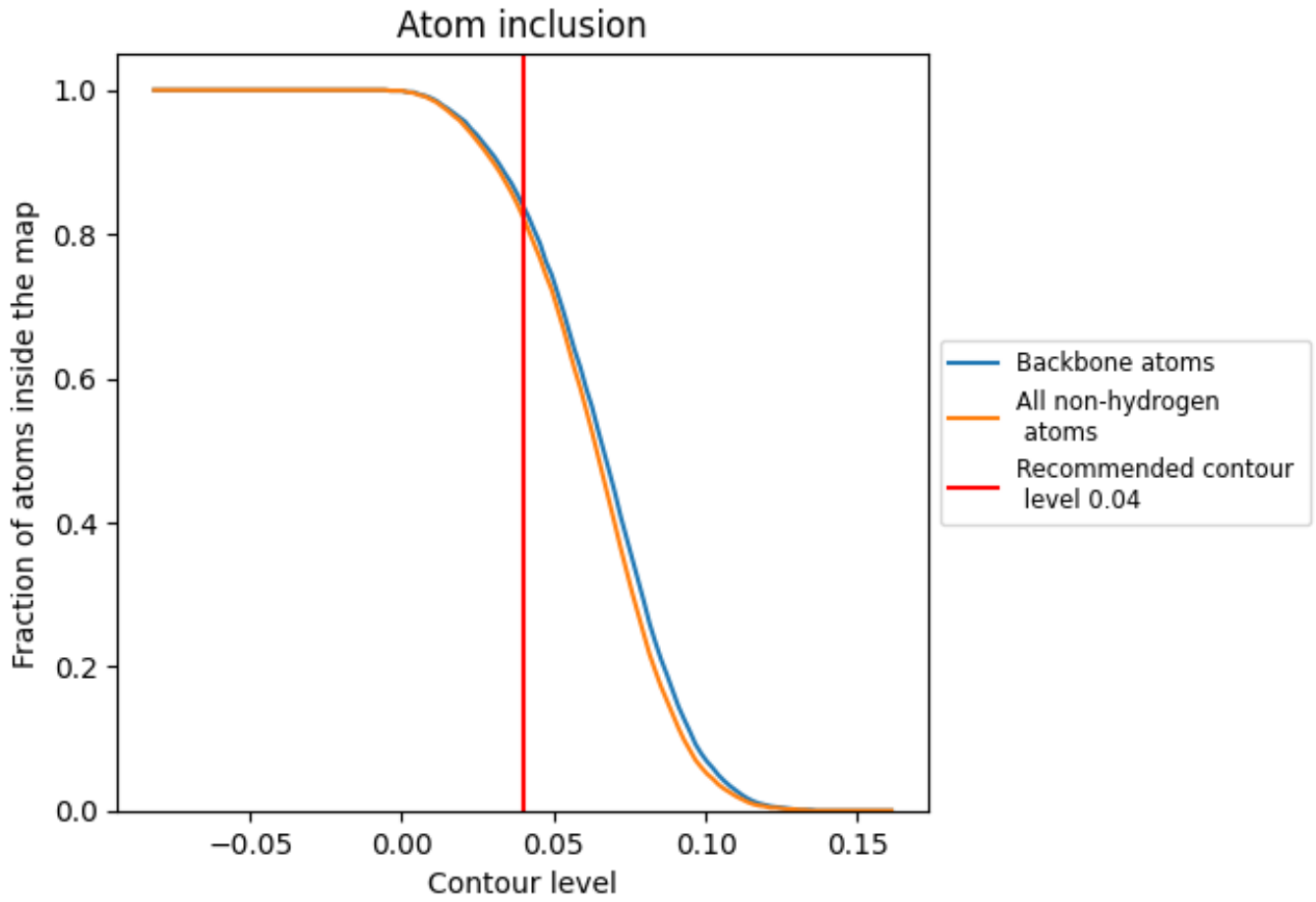
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.6920
A	0.8420	0.6960
B	0.7760	0.6850
C	0.8850	0.7040
D	0.9360	0.7210
E	0.5150	0.6100
F	0.8580	0.6990
G	0.8250	0.6930
e	0.5780	0.5980