Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 04:27 pm GMT

PDB ID	:	6SRS
EMDB ID	:	EMD-10294
Title	:	Structure of the Fanconi anaemia core subcomplex
Authors	:	Shakeel, S.; Rajendra, E.; Alcon, P.; He, S.; Scheres, S.H.W.; Passmore, L.A.
Deposited on	:	2019-09-05
Resolution	:	4.60 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

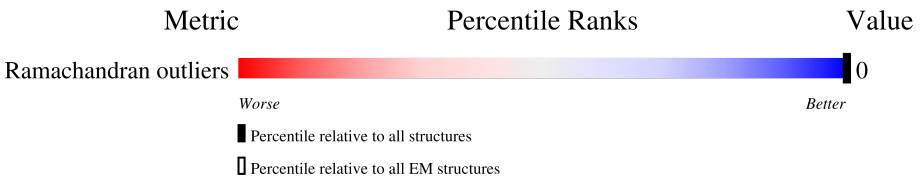
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023

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	76	100%
1	a	76	100%
2	B	25	100%
2	b	25	100%
3	C	30	100%
3	c	30	100%
4	D	23	100%
4	d	23	100%
5	E	9	100%
5	e	9	100%
6	F	15	100%

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Mol	Chain	Length	Quality of chain
6	f	15	100%
7	G	26	100%
7	g	26	100%
8	H	17	6% 100%
8	J	17	6% 94% 6%
8	h	17	6% 100%
8	j	17	94% 6%
9	I	37	100%
9	i	37	100%
10	K	21	100%
10	k	21	100%
11	L	18	94% 6%
11	l	18	94% 6%
12	M	120	100%
12	m	120	100%
13	N	43	9% 100%
13	n	43	5% 100%
14	O	279	100%
14	o	279	100%
15	P	276	100%
15	p	276	100%
16	R	285	5% 100%
16	r	285	100%
17	S	145	100%
17	s	145	100%

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Mol	Chain	Length	Quality of chain
18	Q	91	100%
18	q	91	100%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 12590 atoms, of which 166 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 Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	76	304	152	76	76	0	0
1	a	76	304	152	76	76	0	0

- Molecule 2 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	25	100	50	25	25	0	0
2	b	25	100	50	25	25	0	0

- Molecule 3 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	30	120	60	30	30	0	0
3	c	30	120	60	30	30	0	0

- Molecule 4 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	23	92	46	23	23	0	0
4	d	23	92	46	23	23	0	0

- Molecule 5 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	9	36	18	9	9	0	0
5	e	9	36	18	9	9	0	0

- Molecule 6 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	15	60	30	15	15	0	0
6	f	15	60	30	15	15	0	0

- Molecule 7 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	26	104	52	26	26	0	0
7	g	26	104	52	26	26	0	0

- Molecule 8 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	17	68	34	17	17	0	0
8	J	17	68	34	17	17	0	0
8	h	17	68	34	17	17	0	0
8	j	17	68	34	17	17	0	0

- Molecule 9 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	37	148	74	37	37	0	0
9	i	37	148	74	37	37	0	0

- Molecule 10 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	K	21	84	42	21	21	0	0
10	k	21	84	42	21	21	0	0

- Molecule 11 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	L	18	72	36	18	18	0	0
11	l	18	72	36	18	18	0	0

- Molecule 12 is a protein called Unassigned secondary structure elements (proposed FANCB).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
12	M	120	521	240	41	120	120	0	0
12	m	120	521	240	41	120	120	0	0

- Molecule 13 is a protein called Unassigned secondary structure elements (proposed FAAP100).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
13	N	43	214	86	42	43	43	0	0
13	n	43	214	86	42	43	43	0	0

- Molecule 14 is a protein called Unassigned secondary structure elements (proposed FANCB).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	O	279	1116	558	279	279	0	0
14	o	279	1116	558	279	279	0	0

- Molecule 15 is a protein called Unassigned secondary structure elements (proposed FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	P	276	1104	552	276	276	0	0
15	p	276	1104	552	276	276	0	0

- Molecule 16 is a protein called Unassigned secondary structure elements (proposed FANCG).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	R	285	1140	570	285	285	0	0
16	r	285	1140	570	285	285	0	0

- Molecule 17 is a protein called Unassigned secondary structure elements (proposed FANCG).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	S	145	580	290	145	145	0	0
17	s	145	580	290	145	145	0	0

- Molecule 18 is a protein called Fanconi anaemia protein FANCL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	Q	91	364	182	91	91	0	0
18	q	91	364	182	91	91	0	0

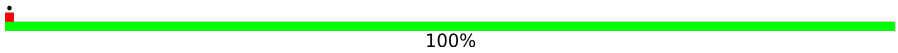
There are 2 discrepancies between the modelled and reference sequences:

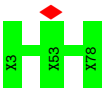
Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	ALA	-	expression tag	UNP Q3MUH5
q	96	ALA	-	expression tag	UNP Q3MUH5

3 Residue-property plots (i)

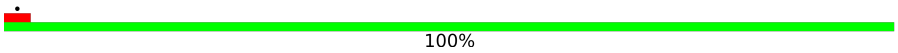
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

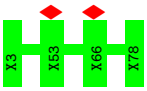
• Molecule 1: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain A: 

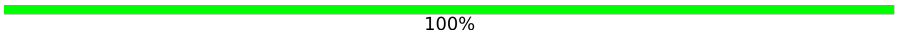


• Molecule 1: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain a: 

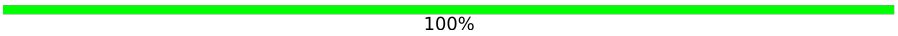


• Molecule 2: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain B: 

There are no outlier residues recorded for this chain.

• Molecule 2: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain b: 

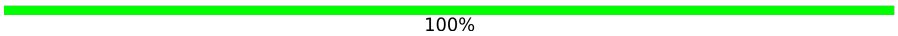
There are no outlier residues recorded for this chain.

• Molecule 3: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain C:

There are no outlier residues recorded for this chain.

• Molecule 3: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain c: 

There are no outlier residues recorded for this chain.

• Molecule 4: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain D: 100%

There are no outlier residues recorded for this chain.

• Molecule 4: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain d: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain E: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain e: 100%

There are no outlier residues recorded for this chain.

• Molecule 6: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain F: 100%

There are no outlier residues recorded for this chain.

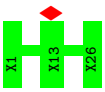
• Molecule 6: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain f: 100%

There are no outlier residues recorded for this chain.

• Molecule 7: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain G: 100%



• Molecule 7: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

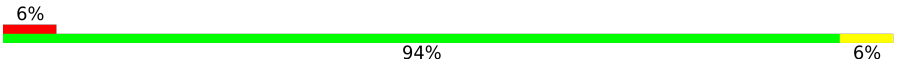
Chain g: 100%

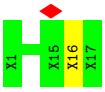
There are no outlier residues recorded for this chain.

• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

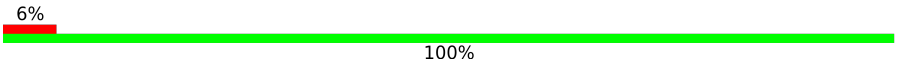
Chain H: 6% 100%

• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

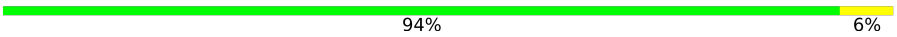
Chain J: 



• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain h: 

• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

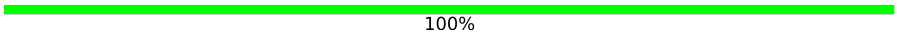
Chain j: 

• Molecule 9: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain I:

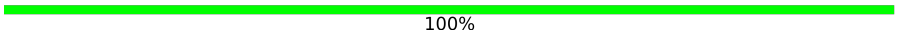
There are no outlier residues recorded for this chain.

• Molecule 9: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain i: 

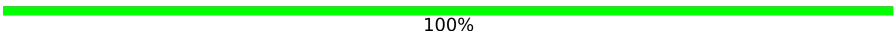
There are no outlier residues recorded for this chain.

• Molecule 10: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain K: 

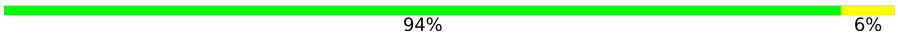
There are no outlier residues recorded for this chain.

• Molecule 10: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

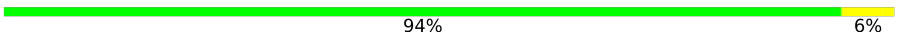
Chain k: 

There are no outlier residues recorded for this chain.

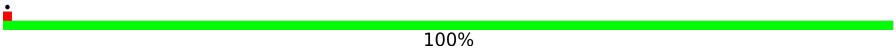
• Molecule 11: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

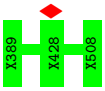
Chain L: 

• Molecule 11: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

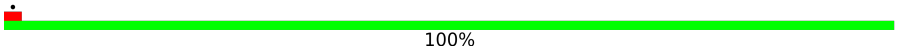
Chain l: 

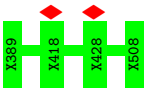
• Molecule 12: Unassigned secondary structure elements (proposed FANCB)

Chain M: 

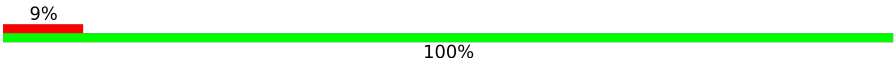


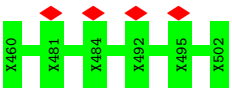
• Molecule 12: Unassigned secondary structure elements (proposed FANCB)

Chain m: 

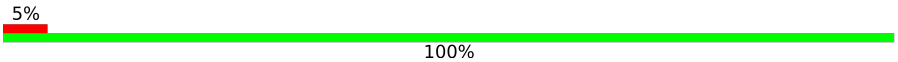


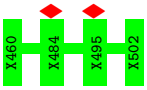
• Molecule 13: Unassigned secondary structure elements (proposed FAAP100)

Chain N: 

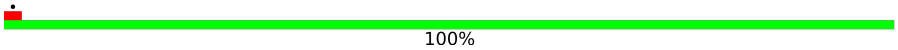


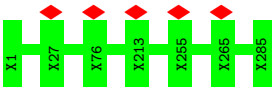
• Molecule 13: Unassigned secondary structure elements (proposed FAAP100)

Chain n: 



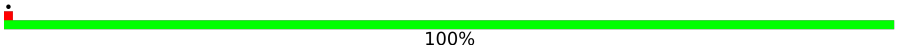
• Molecule 14: Unassigned secondary structure elements (proposed FANCB)

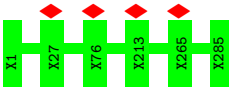
Chain O: 



• Molecule 14: Unassigned secondary structure elements (proposed FANCB)

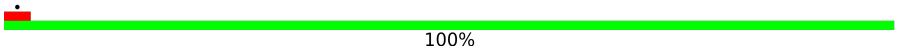
Chain o:

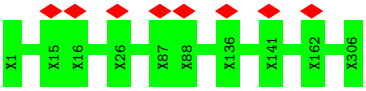




• Molecule 15: Unassigned secondary structure elements (proposed FAAP100)

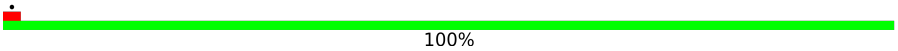
Chain P:

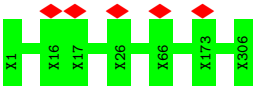




• Molecule 15: Unassigned secondary structure elements (proposed FAAP100)

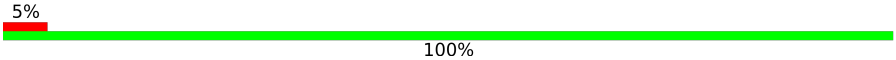
Chain p:

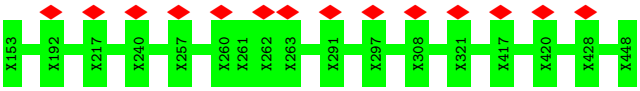




• Molecule 16: Unassigned secondary structure elements (proposed FANCG)

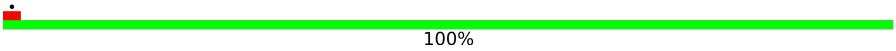
Chain R:

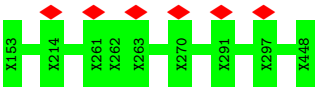




• Molecule 16: Unassigned secondary structure elements (proposed FANCG)

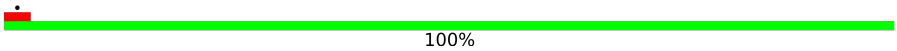
Chain r:

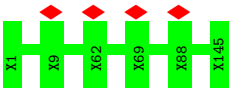




• Molecule 17: Unassigned secondary structure elements (proposed FANCG)

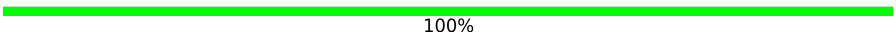
Chain S:





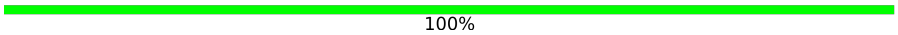
• Molecule 17: Unassigned secondary structure elements (proposed FANCG)

Chain s:



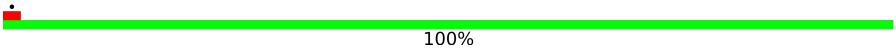
There are no outlier residues recorded for this chain.

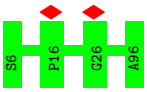
- Molecule 18: Fanconi anaemia protein FANCL

Chain Q: 

There are no outlier residues recorded for this chain.

- Molecule 18: Fanconi anaemia protein FANCL

Chain q: 



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49423	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 ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-4000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
18	Q	0.22	0/363	0.50	0/452
18	q	0.22	0/363	0.50	0/452
All	All	0.22	0/726	0.50	0/904

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
8	J	0	1
8	j	0	1
11	L	0	1
11	l	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	16	UNK	Mainchain
11	L	17	UNK	Mainchain
8	j	16	UNK	Mainchain
11	l	17	UNK	Mainchain

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	
18	Q	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
18	q	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
All	All	178/182 (98%)	176 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	P	10
15	p	10
14	O	10
14	o	10
1	A	3
1	a	3
7	G	2
7	g	2
17	S	1
17	s	1
16	R	1
16	r	1
4	D	1
4	d	1
12	M	1
12	m	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	228:UNK	C	232:UNK	N	12.83
1	p	228:UNK	C	232:UNK	N	12.83
1	S	123:UNK	C	124:UNK	N	11.74
1	s	123:UNK	C	124:UNK	N	11.74
1	O	128:UNK	C	129:UNK	N	11.32
1	o	128:UNK	C	129:UNK	N	11.32
1	P	240:UNK	C	244:UNK	N	10.60
1	p	240:UNK	C	244:UNK	N	10.60
1	O	146:UNK	C	150:UNK	N	10.44
1	o	146:UNK	C	150:UNK	N	10.44
1	P	108:UNK	C	118:UNK	N	8.98
1	p	108:UNK	C	118:UNK	N	8.98
1	A	65:UNK	C	66:UNK	N	8.86
1	a	65:UNK	C	66:UNK	N	8.85
1	O	115:UNK	C	118:UNK	N	8.75
1	o	115:UNK	C	118:UNK	N	8.75
1	O	98:UNK	C	100:UNK	N	8.42
1	o	98:UNK	C	100:UNK	N	8.42
1	P	126:UNK	C	128:UNK	N	8.35
1	p	126:UNK	C	128:UNK	N	8.35

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	18:UNK	C	19:UNK	N	7.93
1	g	18:UNK	C	19:UNK	N	7.93
1	P	136:UNK	C	138:UNK	N	7.73
1	p	136:UNK	C	138:UNK	N	7.73
1	R	381:UNK	C	393:UNK	N	7.27
1	r	381:UNK	C	393:UNK	N	7.27
1	P	66:UNK	C	68:UNK	N	6.98
1	p	66:UNK	C	68:UNK	N	6.97
1	O	60:UNK	C	61:UNK	N	6.67
1	o	60:UNK	C	61:UNK	N	6.67
1	o	95:UNK	C	96:UNK	N	6.60
1	O	95:UNK	C	96:UNK	N	6.59
1	G	16:UNK	C	17:UNK	N	6.48
1	g	16:UNK	C	17:UNK	N	6.48
1	P	27:UNK	C	30:UNK	N	6.48
1	p	27:UNK	C	30:UNK	N	6.48
1	P	96:UNK	C	100:UNK	N	6.41
1	p	96:UNK	C	100:UNK	N	6.41
1	P	281:UNK	C	288:UNK	N	5.92
1	p	281:UNK	C	288:UNK	N	5.92
1	A	61:UNK	C	62:UNK	N	5.82
1	a	61:UNK	C	62:UNK	N	5.82
1	A	43:UNK	C	44:UNK	N	5.29
1	a	43:UNK	C	44:UNK	N	5.29
1	P	74:UNK	C	76:UNK	N	5.16
1	p	74:UNK	C	76:UNK	N	5.16
1	D	43:UNK	C	44:UNK	N	5.02
1	d	43:UNK	C	44:UNK	N	5.02
1	O	39:UNK	C	40:UNK	N	4.73
1	o	39:UNK	C	40:UNK	N	4.73
1	O	188:UNK	C	189:UNK	N	4.58
1	o	188:UNK	C	189:UNK	N	4.58
1	O	80:UNK	C	81:UNK	N	3.77
1	o	80:UNK	C	81:UNK	N	3.77
1	o	51:UNK	C	52:UNK	N	3.58
1	M	430:UNK	C	431:UNK	N	3.57
1	O	51:UNK	C	52:UNK	N	3.57
1	m	430:UNK	C	431:UNK	N	3.57

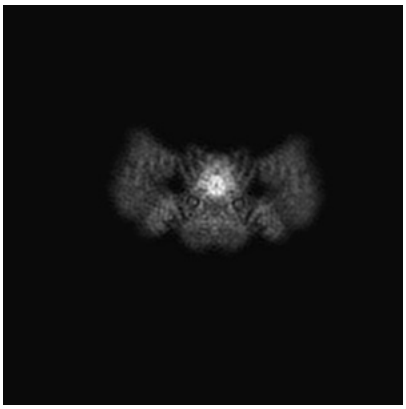
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10294. These allow visual inspection of the internal detail of the map and identification of artifacts.

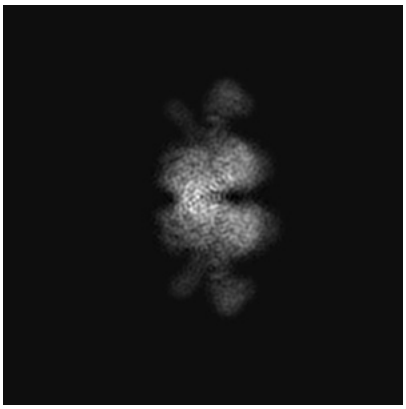
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

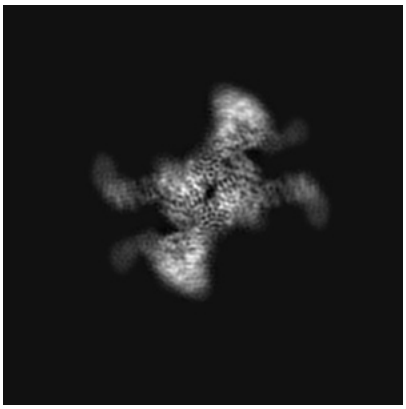
6.1.1 Primary map



X

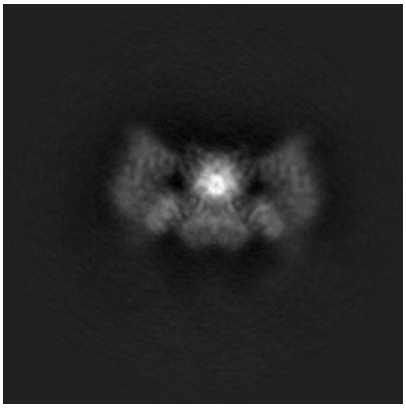


Y

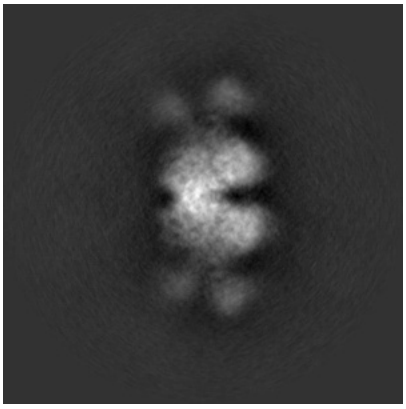


Z

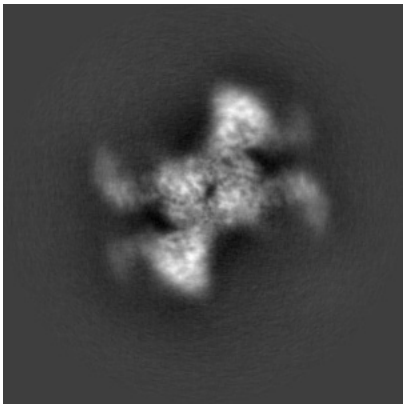
6.1.2 Raw map



X



Y

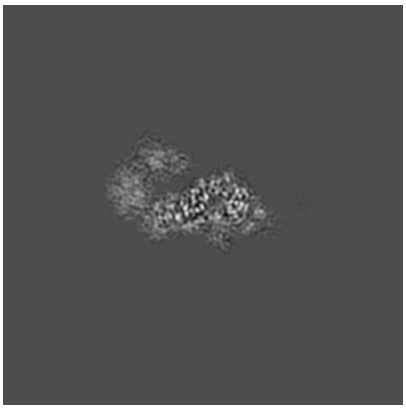


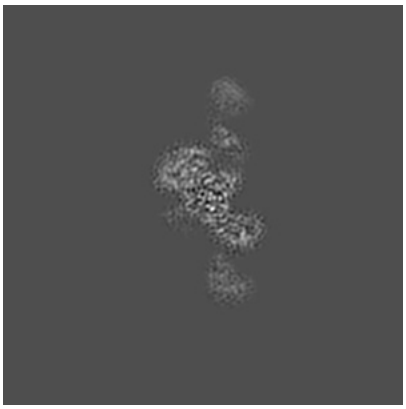
Z

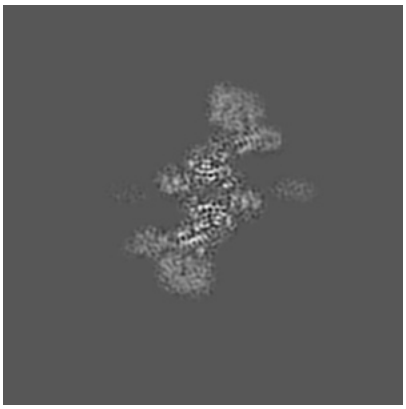
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

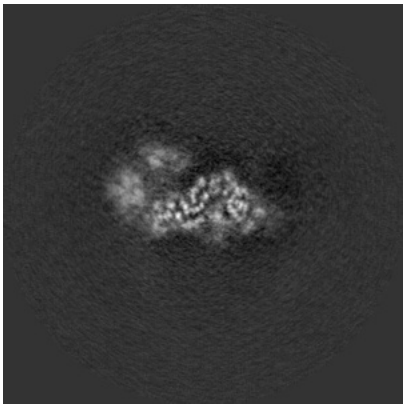
6.2.1 Primary map

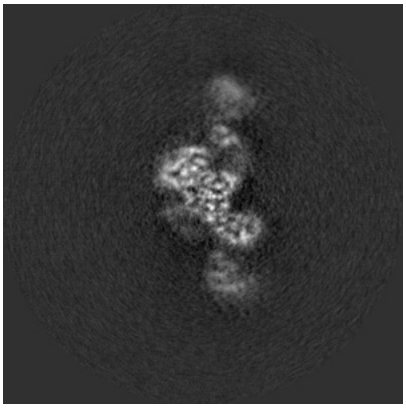

X Index: 190

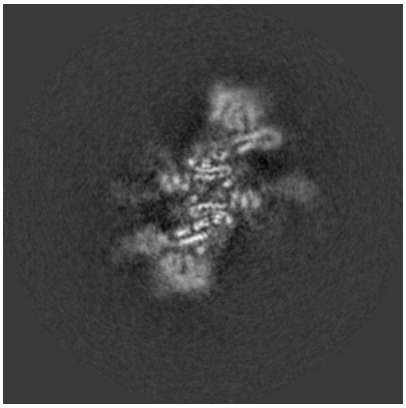

Y Index: 190


Z Index: 190

6.2.2 Raw map


X Index: 190

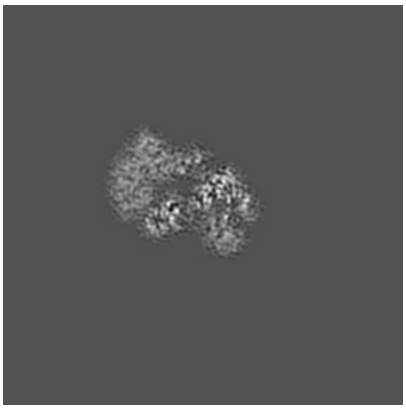

Y Index: 190

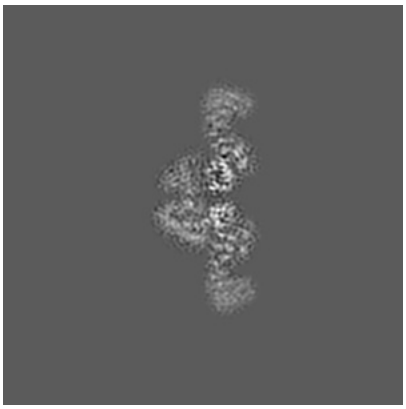

Z Index: 190

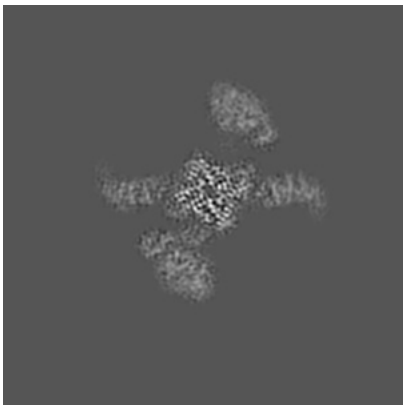
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

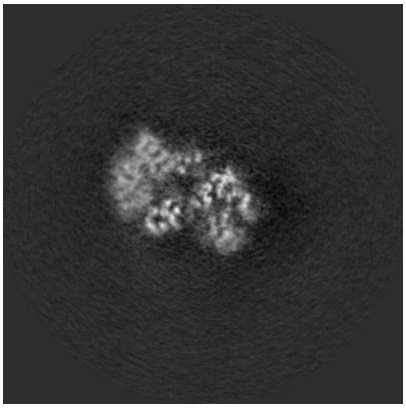
6.3.1 Primary map

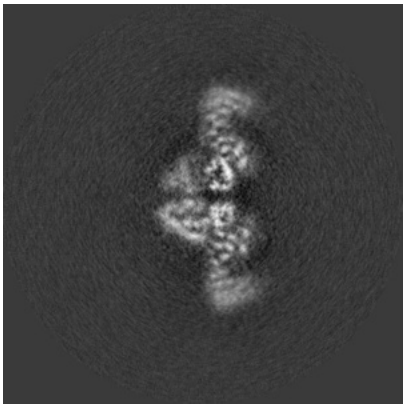

X Index: 180

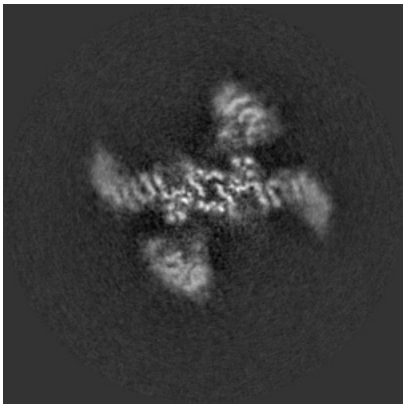

Y Index: 205


Z Index: 200

6.3.2 Raw map


X Index: 180


Y Index: 205


Z Index: 210

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

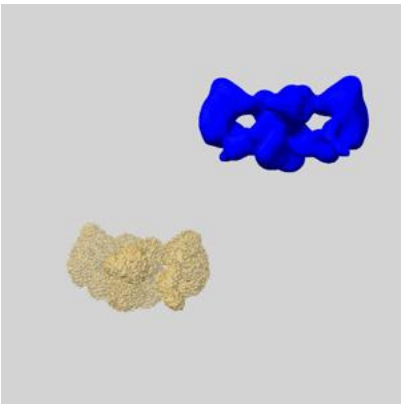
6.5 Mask visualisation (i)

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

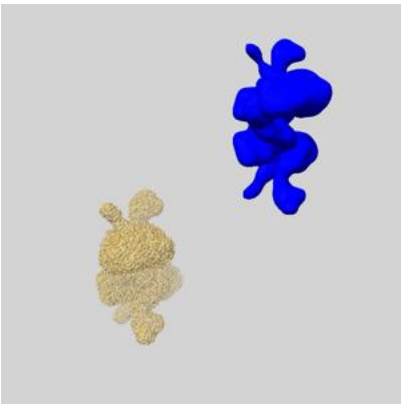
A mask typically either:

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

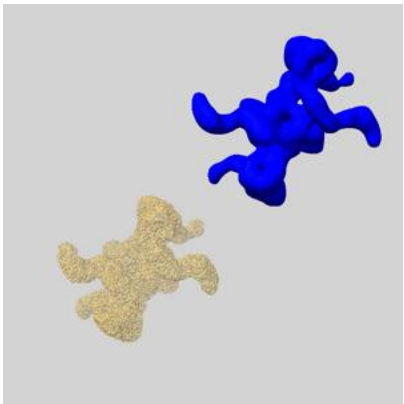
6.5.1 emd_10294_msk_3.map (i)



X

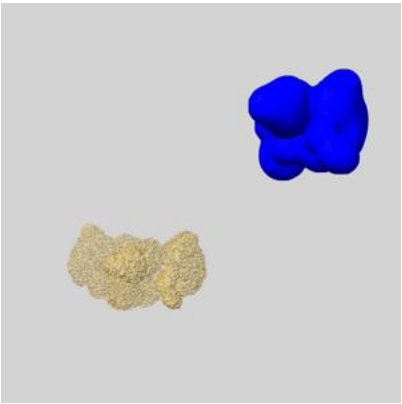


Y

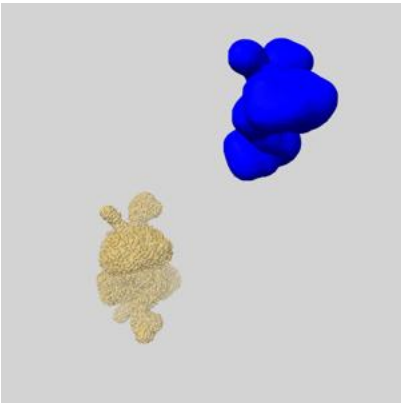


Z

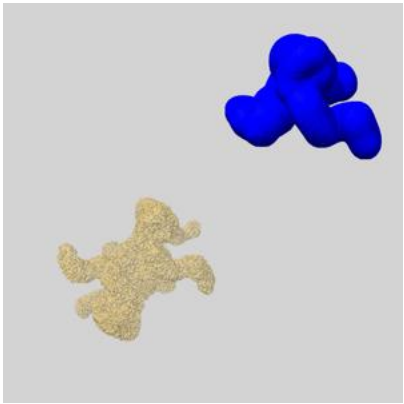
6.5.2 emd_10294_msk_2.map (i)



X

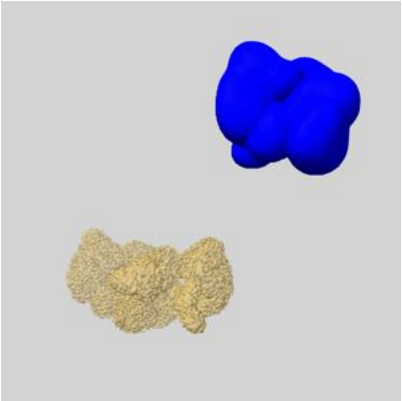


Y

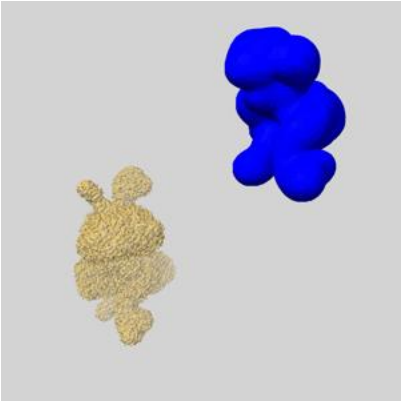


Z

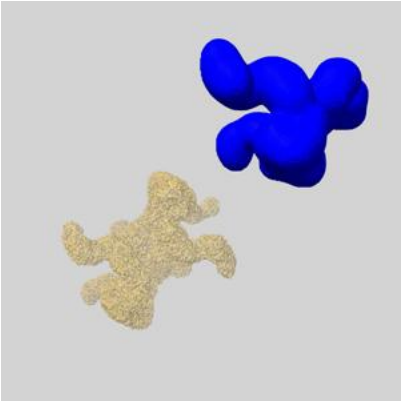
6.5.3 emd_10294_msk_1.map ⓘ



X



Y

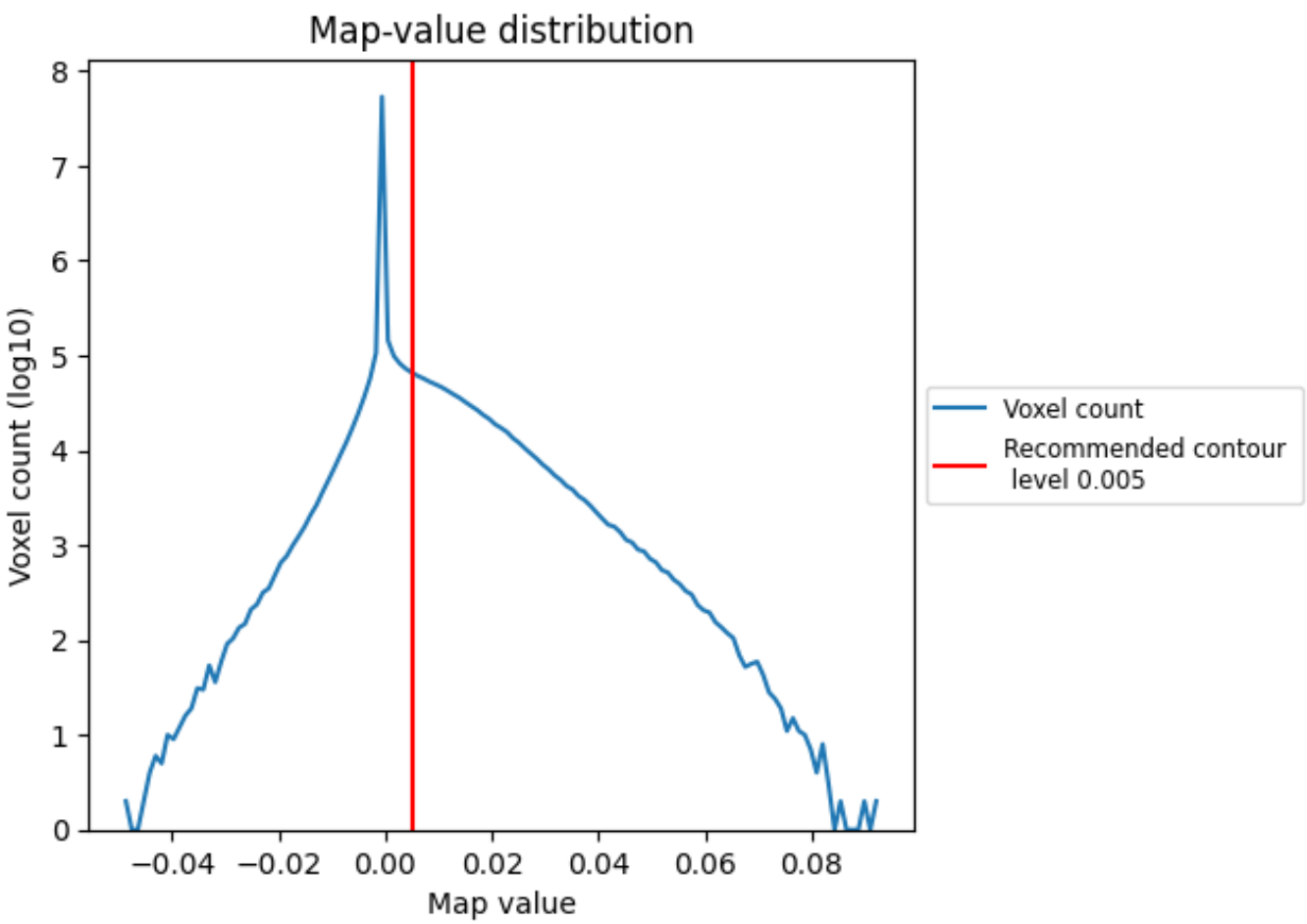


Z

7 Map analysis (i)

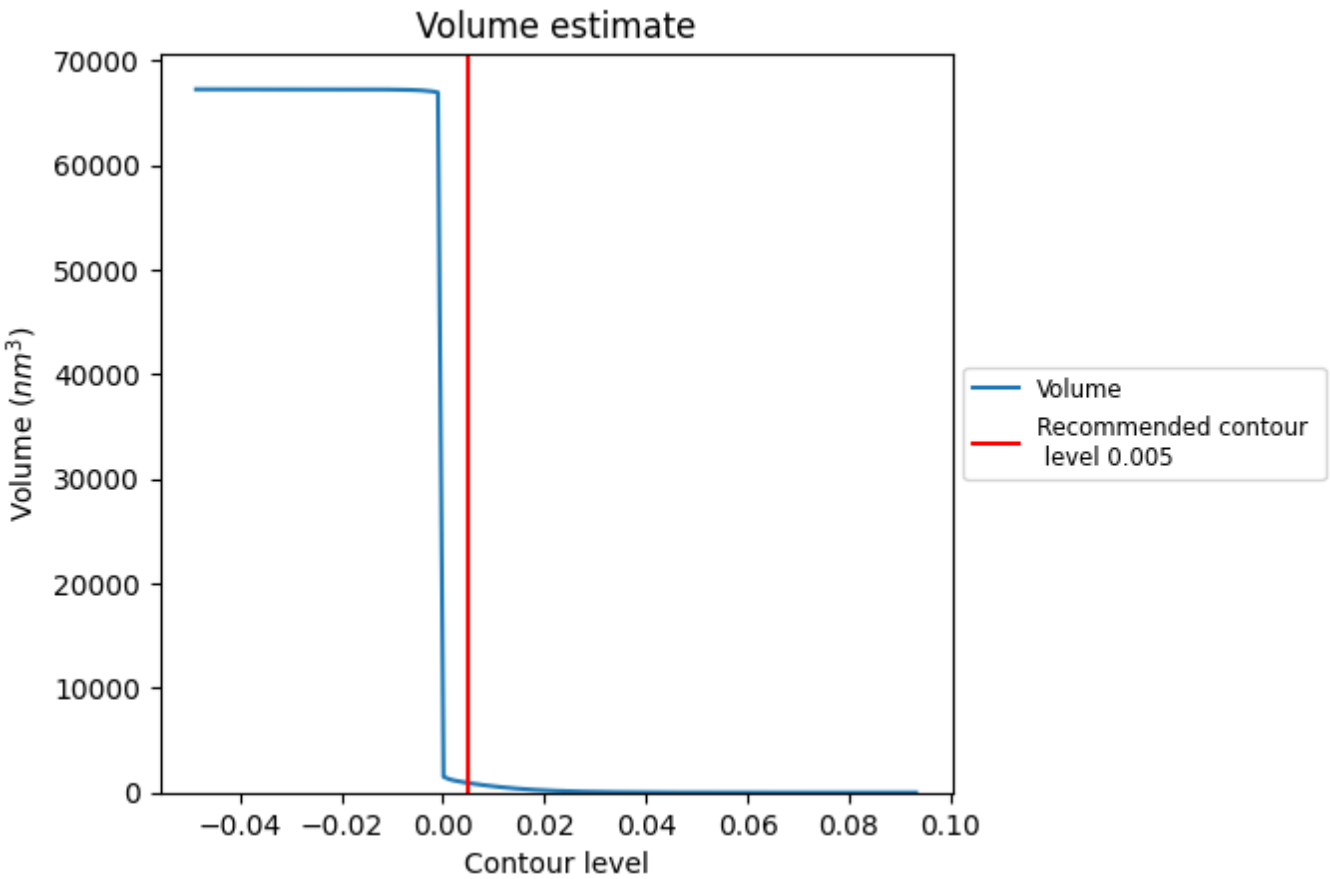
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

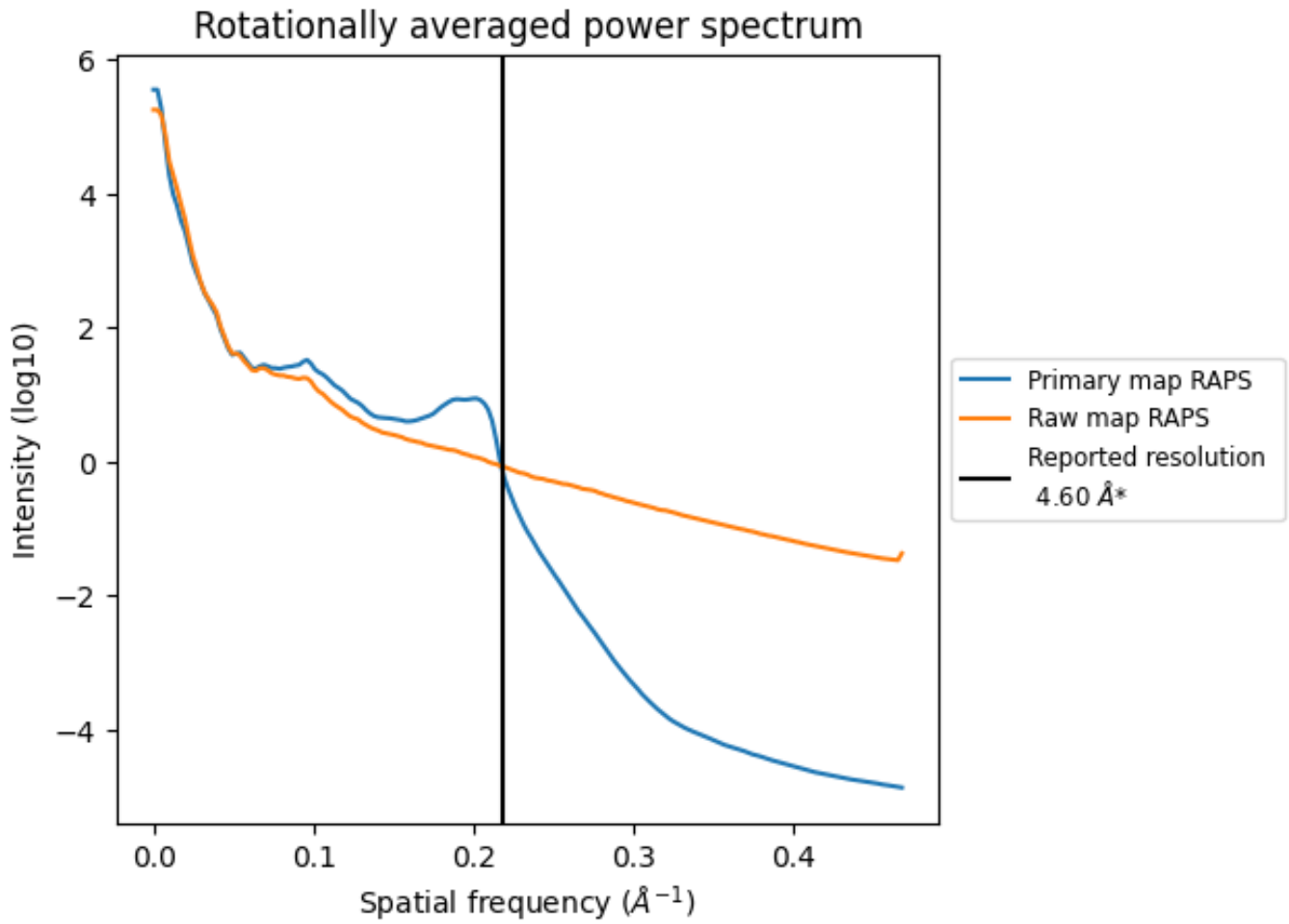
7.2 Volume estimate (i)



The volume at the recommended contour level is 914 nm^3; this corresponds to an approximate mass of 826 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)

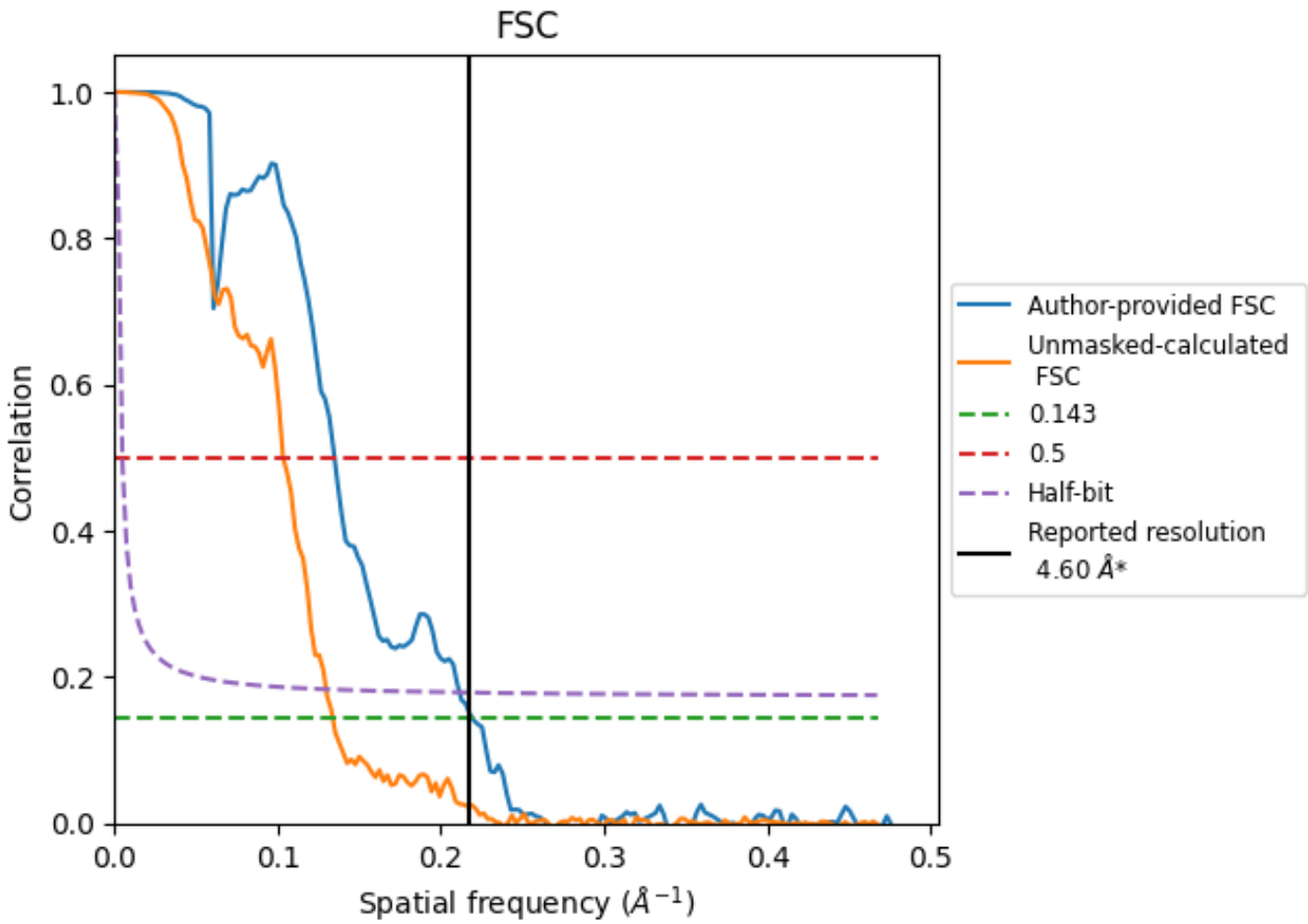


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

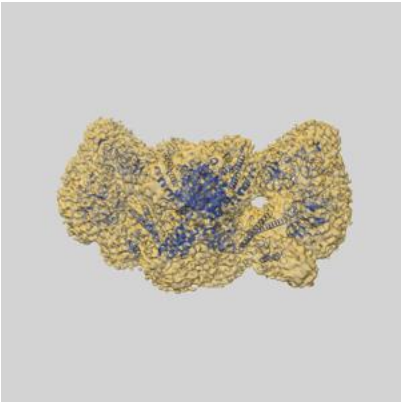
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.56	7.42	4.73
Unmasked-calculated*	7.48	9.68	7.71

*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 7.48 differs from the reported value 4.6 by more than 10 %

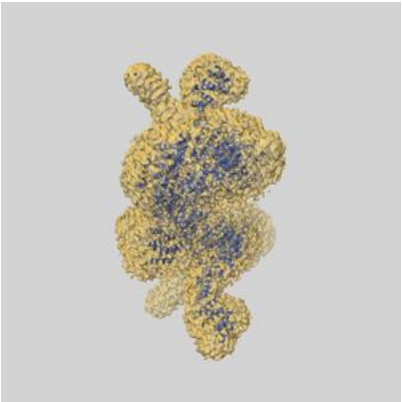
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10294 and PDB model 6SRS. Per-residue inclusion information can be found in section 3 on page 9.

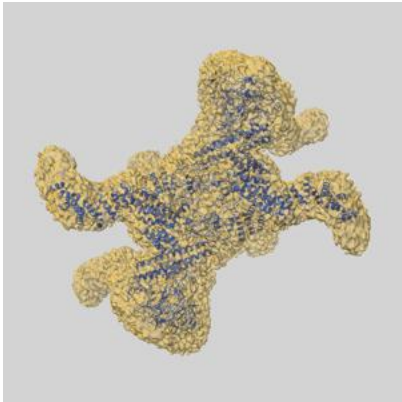
9.1 Map-model overlay (i)



X



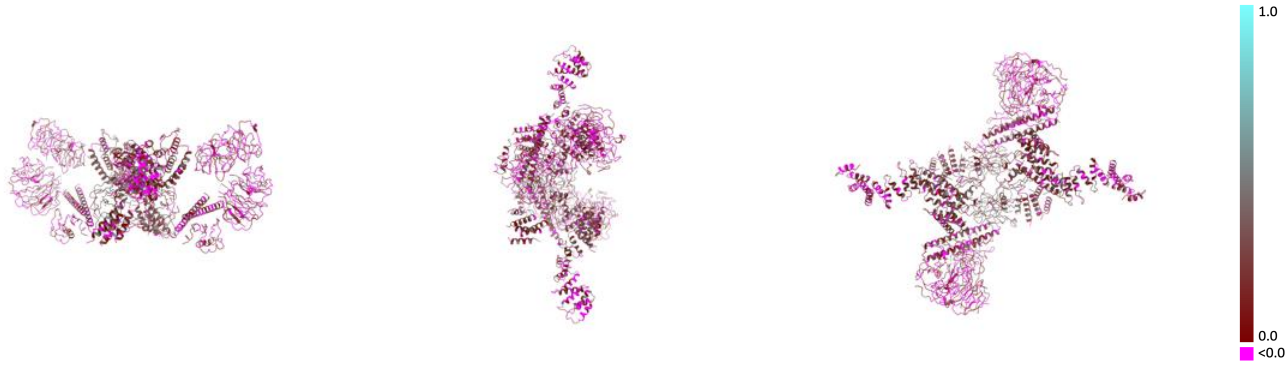
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

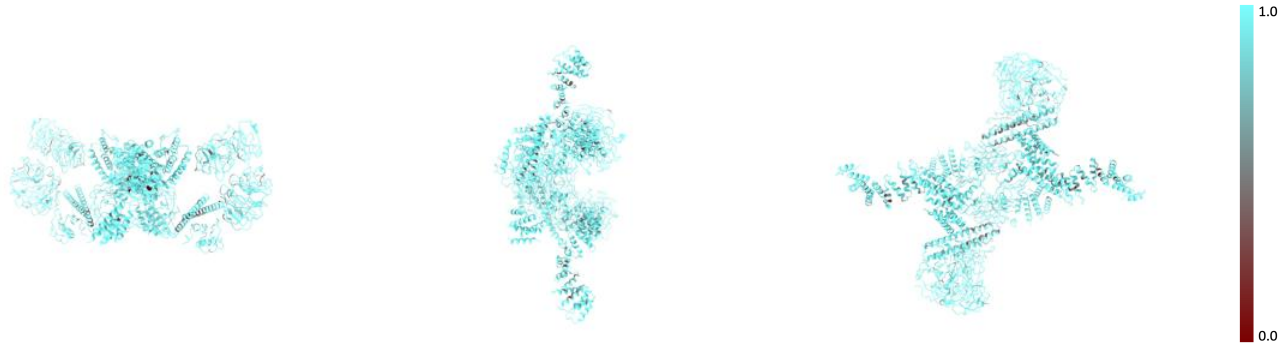
9.2 Q-score mapped to coordinate model (i)



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.

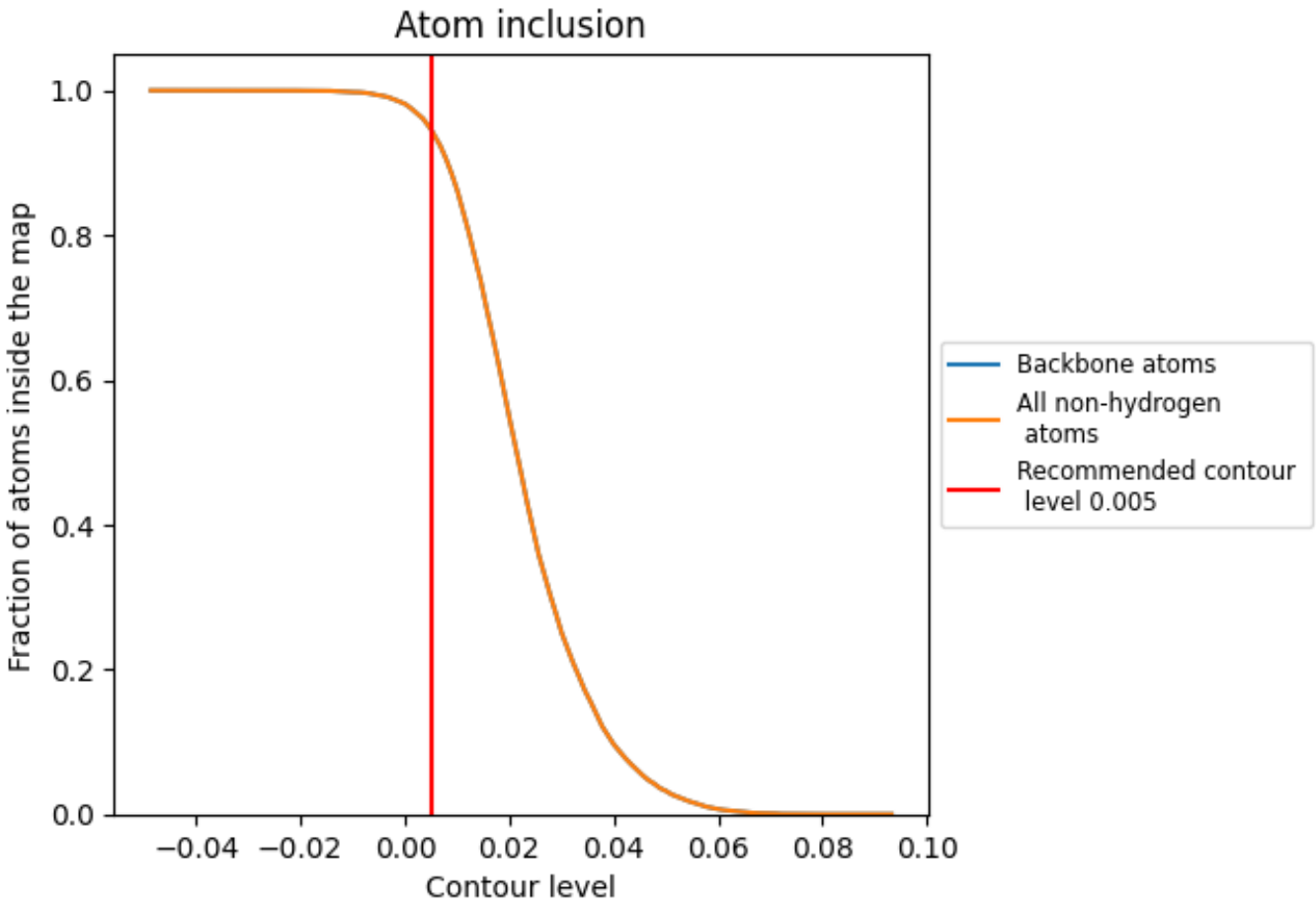
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9463	0.1350
A	0.9671	0.2920
B	0.9800	0.3820
C	0.9917	0.3800
D	1.0000	0.3570
E	1.0000	0.3920
F	1.0000	0.3630
G	0.9231	0.2900
H	0.9412	0.2400
I	1.0000	0.1760
J	0.9559	0.0970
K	0.9881	0.1830
L	1.0000	0.0990
M	0.9667	0.2610
N	0.8198	0.0840
O	0.9391	0.0440
P	0.9303	0.0300
Q	0.9368	0.0880
R	0.9202	0.1260
S	0.9379	0.1800
a	0.9309	0.2300
b	0.9800	0.1990
c	0.9667	0.2830
d	0.9891	0.1460
e	0.9722	0.2550
f	0.9833	0.1860
g	0.9712	0.1650
h	0.9265	0.2230
i	1.0000	0.2060
j	1.0000	0.1720
k	0.9881	0.2400
l	1.0000	0.1760
m	0.9646	0.2580
n	0.8779	0.1310
o	0.9561	0.0660

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Chain	Atom inclusion	Q-score
p	0.9420	0.0490
q	0.9341	0.0760
r	0.9386	0.1260
s	0.9741	0.2080