Preliminary Full wwPDB EM Validation Report ⓘ

Apr 11, 2022 – 04:43 PM PDT

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

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.

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

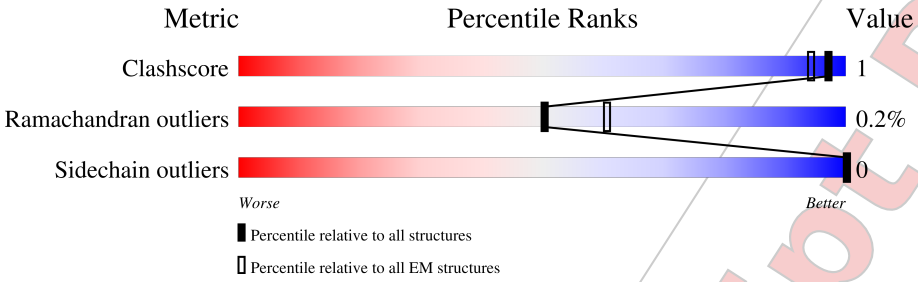
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 unknown.

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	525	12% 95%
1	B	525	11% 97%
1	C	525	11% 97%
1	D	525	13% 94% 6%
2	E	12	100%
2	F	12	8% 100%
2	G	12	8% 100%
2	H	12	100%

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2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33508 atoms, of which 16644 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	525	Total	C	H	N	O	S	0	0
			8213	2597	4085	727	787	17		
1	B	525	Total	C	H	N	O	S	0	0
			8213	2597	4085	727	787	17		
1	C	525	Total	C	H	N	O	S	0	0
			8213	2597	4085	727	787	17		
1	D	525	Total	C	H	N	O	S	0	0
			8213	2597	4085	727	787	17		

- Molecule 2 is a protein called PRO-GLN-PHE-GLY-VAL-GLY-GLN-GLY-SER-GLY-PHE-TYR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	12	Total	C	H	N	O	0	0
			164	58	76	14	16		
2	F	12	Total	C	H	N	O	0	0
			164	58	76	14	16		
2	G	12	Total	C	H	N	O	0	0
			164	58	76	14	16		
2	H	12	Total	C	H	N	O	0	0
			164	58	76	14	16		

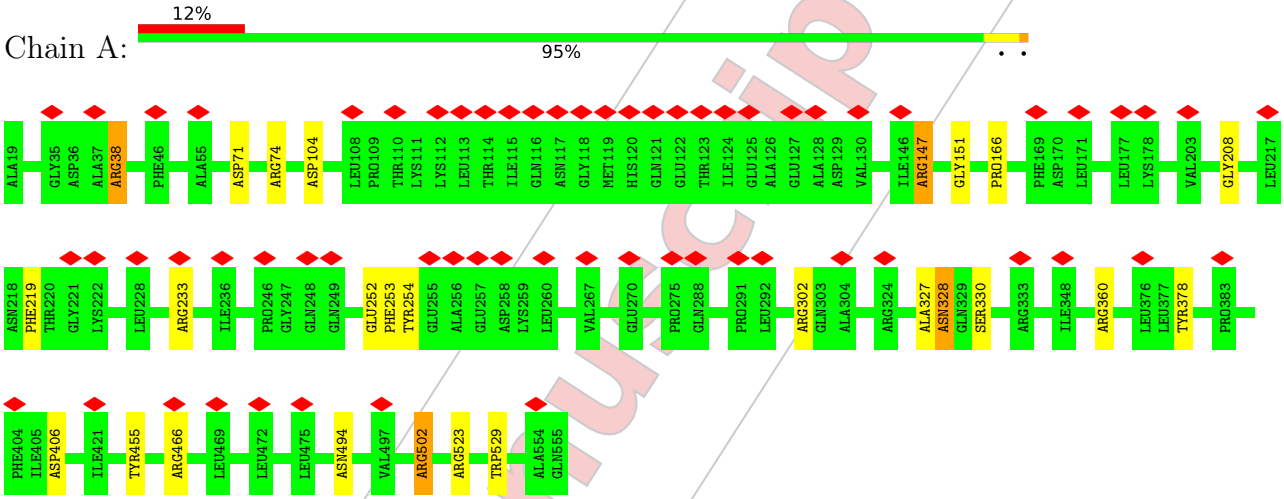
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3 Residue-property plots

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.

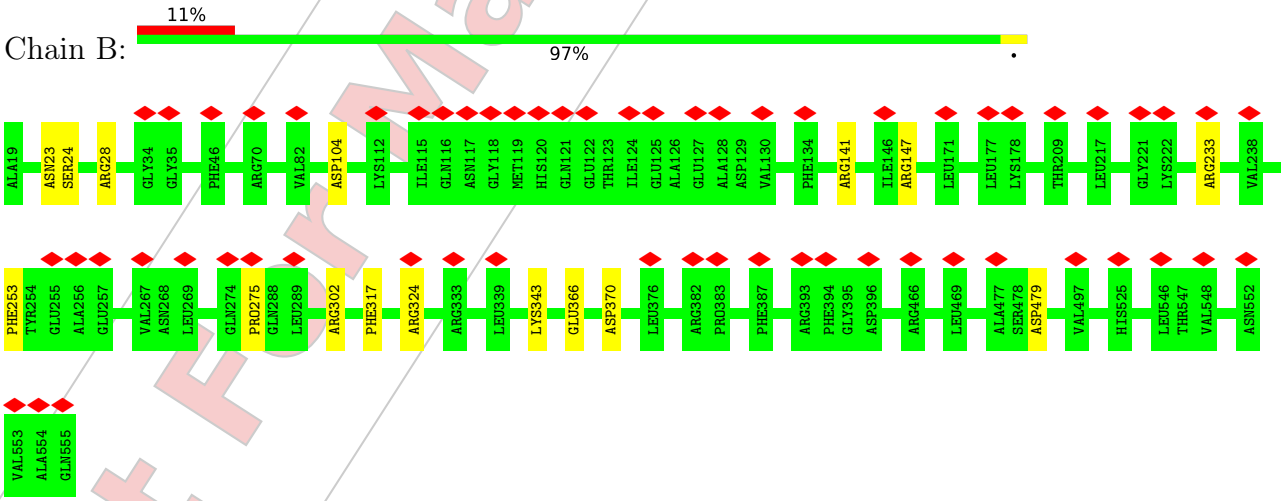
- Molecule 1:

Chain A:



- Molecule 1:

Chain B:

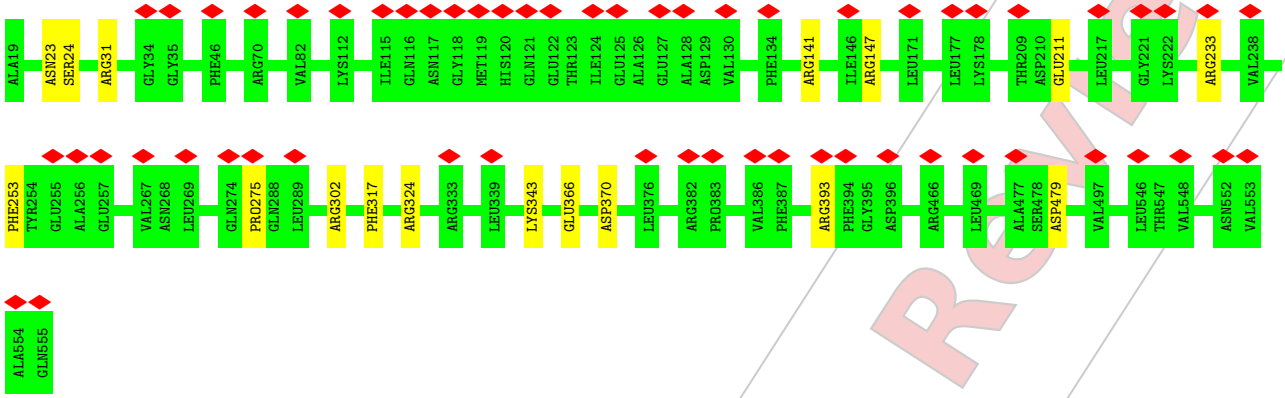


- Molecule 1:

Chain C:

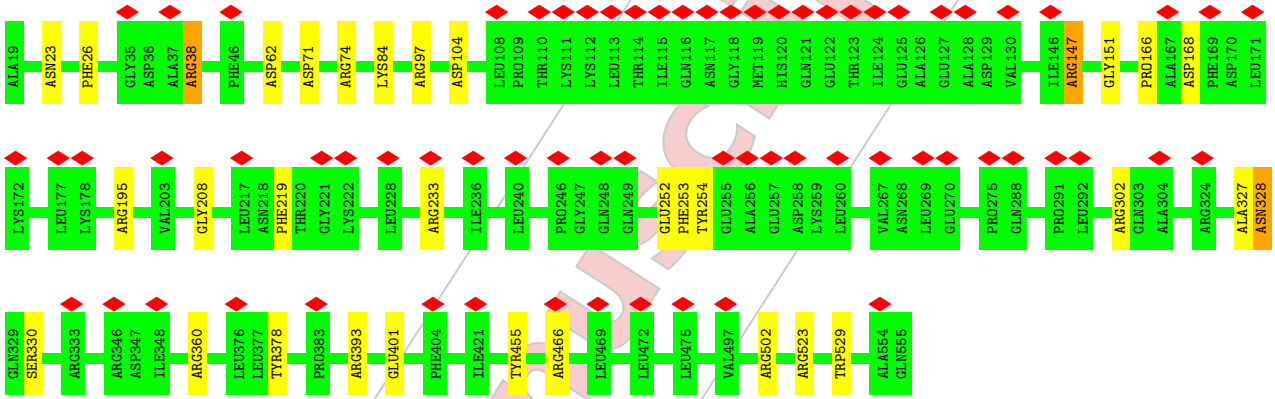


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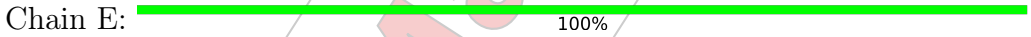


• Molecule 1:





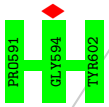
• Molecule 2: PRO-GLN-PHE-GLY-VAL-GLY-GLN-GLY-SER-GLY-PHE-TYR



There are no outlier residues recorded for this chain.

• Molecule 2: PRO-GLN-PHE-GLY-VAL-GLY-GLN-GLY-SER-GLY-PHE-TYR





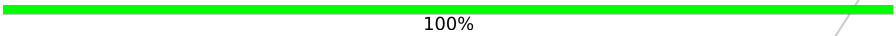
• Molecule 2: PRO-GLN-PHE-GLY-VAL-GLY-GLN-GLY-SER-GLY-PHE-TYR





• Molecule 2: PRO-GLN-PHE-GLY-VAL-GLY-GLN-GLY-SER-GLY-PHE-TYR

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Chain H: 

There are no outlier residues recorded for this chain.

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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	7.636	Depositor
Minimum map value	-4.272	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.216	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

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5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.07	7/4203 (0.2%)	1.02	16/5697 (0.3%)
1	B	1.01	4/4203 (0.1%)	0.94	8/5697 (0.1%)
1	C	1.02	5/4203 (0.1%)	0.93	9/5697 (0.2%)
1	D	1.04	8/4203 (0.2%)	1.03	19/5697 (0.3%)
2	E	1.23	0/91	0.95	0/120
2	F	0.97	0/91	0.89	0/120
2	G	0.97	0/91	0.89	0/120
2	H	0.80	0/91	0.87	0/120
All	All	1.03	24/17176 (0.1%)	0.98	52/23268 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	GLU	CG-CD	-5.87	1.43	1.51
1	D	252	GLU	CG-CD	-5.84	1.43	1.51
1	D	529	TRP	CB-CG	-5.52	1.40	1.50
1	C	211	GLU	CD-OE1	-5.49	1.19	1.25
1	A	529	TRP	CB-CG	-5.45	1.40	1.50
1	D	254	TYR	CB-CG	-5.45	1.43	1.51
1	A	254	TYR	CB-CG	-5.44	1.43	1.51
1	A	253	PHE	CB-CG	-5.40	1.42	1.51
1	B	253	PHE	CB-CG	-5.38	1.42	1.51
1	C	253	PHE	CB-CG	-5.36	1.42	1.51
1	D	253	PHE	CB-CG	-5.36	1.42	1.51
1	D	455	TYR	CB-CG	-5.27	1.43	1.51
1	A	455	TYR	CB-CG	-5.25	1.43	1.51
1	A	254	TYR	CG-CD2	-5.20	1.32	1.39
1	D	254	TYR	CG-CD2	-5.19	1.32	1.39
1	B	275	PRO	N-CD	5.12	1.55	1.47
1	A	219	PHE	CB-CG	-5.10	1.42	1.51
1	C	275	PRO	N-CD	5.09	1.54	1.47
1	B	366	GLU	CD-OE2	-5.09	1.20	1.25
1	D	219	PHE	CB-CG	-5.08	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	PHE	CB-CG	-5.05	1.42	1.51
1	C	317	PHE	CB-CG	-5.04	1.42	1.51
1	C	366	GLU	CD-OE2	-5.02	1.20	1.25
1	D	401	GLU	CD-OE1	-5.01	1.20	1.25

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ARG	NE-CZ-NH2	-14.88	112.86	120.30
1	D	74	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	C	141	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	D	147	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	B	141	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	D	466	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	466	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	233	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	D	302	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	A	302	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	233	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	C	324	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	74	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	D	74	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	C	302	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	B	302	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	324	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	147	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	393	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	28	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	D	466	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	466	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	523	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	233	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	D	523	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	233	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	406	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	378	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	D	378	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	D	302	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	147	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	C	147	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	302	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	502	ARG	NE-CZ-NH1	5.95	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	71	ASP	N-CA-C	-5.63	95.79	111.00
1	A	71	ASP	N-CA-C	-5.61	95.86	111.00
1	D	360	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	38	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	360	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	141	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	D	97	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	502	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	38	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	141	ARG	NH1-CZ-NH2	-5.34	113.52	119.40
1	D	147	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	393	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	208	GLY	N-CA-C	-5.11	100.32	113.10
1	B	233	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	195	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	208	GLY	N-CA-C	-5.09	100.39	113.10
1	C	233	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4128	4085	4083	5	0
1	B	4128	4085	4083	4	0
1	C	4128	4085	4083	3	0
1	D	4128	4085	4083	7	0
2	E	88	76	76	0	0
2	F	88	76	76	0	0
2	G	88	76	76	0	0
2	H	88	76	76	0	0
All	All	16864	16644	16636	19	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

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hydrogen atoms). The all-atom clashscore for this structure is 1.

All (19) 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:B:370:ASP:OD1	1:B:370:ASP:N	2.39	0.54
1:C:370:ASP:N	1:C:370:ASP:OD1	2.39	0.54
1:C:343:LYS:NZ	1:C:479:ASP:OD1	2.41	0.53
1:B:343:LYS:NZ	1:B:479:ASP:OD1	2.41	0.52
1:D:62:ASP:OD2	1:D:84:LYS:NZ	2.45	0.49
1:A:494:ASN:O	1:A:502:ARG:NH1	2.48	0.47
1:D:104:ASP:OD1	1:D:104:ASP:N	2.49	0.46
1:A:104:ASP:OD1	1:A:104:ASP:N	2.49	0.45
1:B:104:ASP:OD1	1:B:104:ASP:N	2.51	0.44
1:D:38:ARG:NH2	1:D:166:PRO:O	2.51	0.44
1:D:327:ALA:O	1:D:328:ASN:CB	2.66	0.44
1:A:38:ARG:NH2	1:A:166:PRO:O	2.51	0.43
1:B:23:ASN:O	1:B:24:SER:C	2.57	0.43
1:A:327:ALA:O	1:A:328:ASN:CB	2.66	0.43
1:C:23:ASN:O	1:C:24:SER:C	2.57	0.42
1:D:168:ASP:OD1	1:D:168:ASP:N	2.52	0.42
1:A:147:ARG:O	1:A:151:GLY:N	2.55	0.40
1:D:147:ARG:O	1:D:151:GLY:N	2.55	0.40
1:D:23:ASN:HA	1:D:26:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	521/525 (99%)	506 (97%)	13 (2%)	2 (0%)	34 34
1	B	521/525 (99%)	511 (98%)	10 (2%)	0	100 100
1	C	521/525 (99%)	511 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	521/525 (99%)	505 (97%)	14 (3%)	2 (0%)	34	34
2	E	10/12 (83%)	8 (80%)	2 (20%)	0	100	100
2	F	10/12 (83%)	10 (100%)	0	0	100	100
2	G	10/12 (83%)	10 (100%)	0	0	100	100
2	H	10/12 (83%)	8 (80%)	2 (20%)	0	100	100
All	All	2124/2148 (99%)	2069 (97%)	51 (2%)	4 (0%)	50	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	SER
1	D	330	SER
1	A	328	ASN
1	D	328	ASN

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	A	443/443 (100%)	443 (100%)	0	100	100
1	B	443/443 (100%)	443 (100%)	0	100	100
1	C	443/443 (100%)	443 (100%)	0	100	100
1	D	443/443 (100%)	443 (100%)	0	100	100
2	E	8/8 (100%)	8 (100%)	0	100	100
2	F	8/8 (100%)	8 (100%)	0	100	100
2	G	8/8 (100%)	8 (100%)	0	100	100
2	H	8/8 (100%)	8 (100%)	0	100	100
All	All	1804/1804 (100%)	1804 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

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no such sidechains identified.

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

There are no ligands in this entry.

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
1	B	1
1	C	1
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	275:PRO	C	288:GLN	N	9.99
1	C	275:PRO	C	288:GLN	N	9.99
1	A	275:PRO	C	288:GLN	N	9.30
1	D	275:PRO	C	288:GLN	N	9.30

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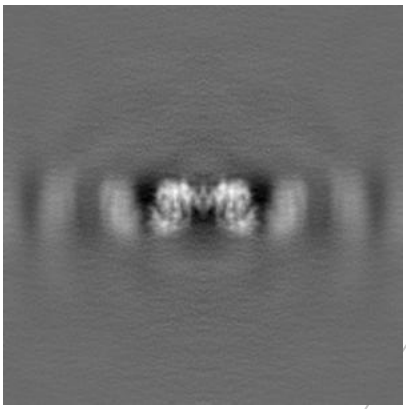
6 Map visualisation

This section contains visualisations of the EMDB entry D_9101001792. These allow visual inspection of the internal detail of the map and identification of artifacts.

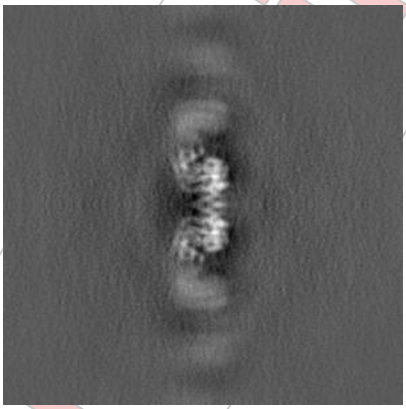
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

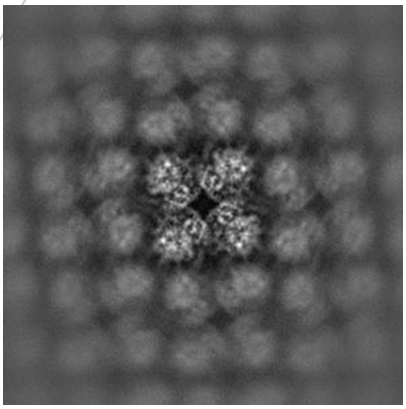
6.1.1 Primary map



X

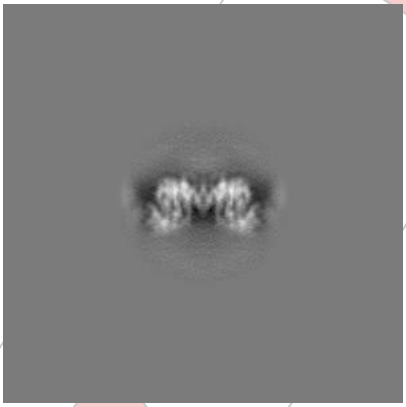


Y

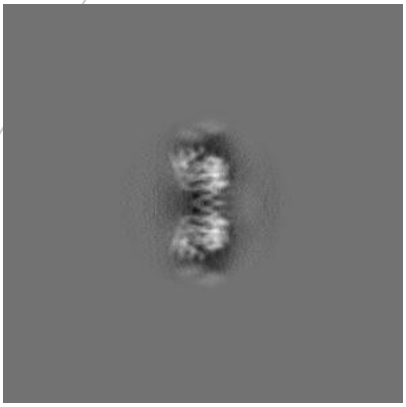


Z

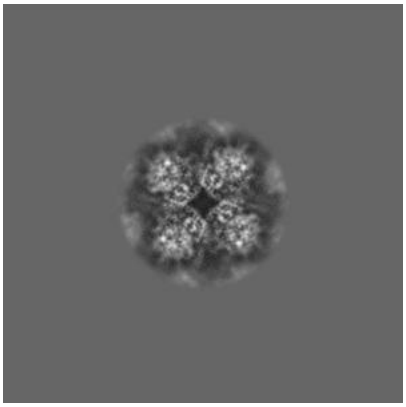
6.1.2 Raw map



X



Y



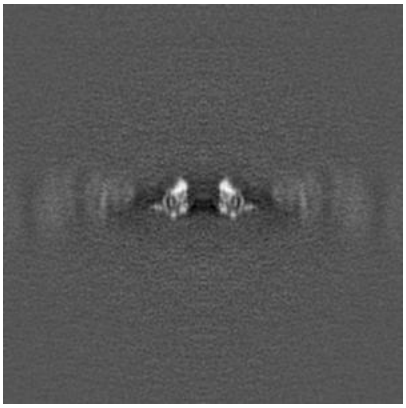
Z

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

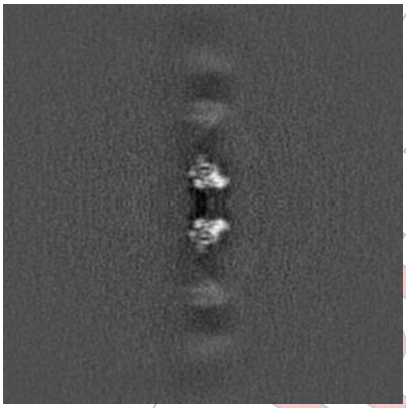
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6.2 Central slices (i)

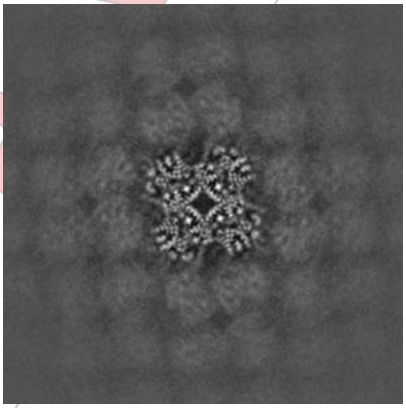
6.2.1 Primary map



X Index: 256

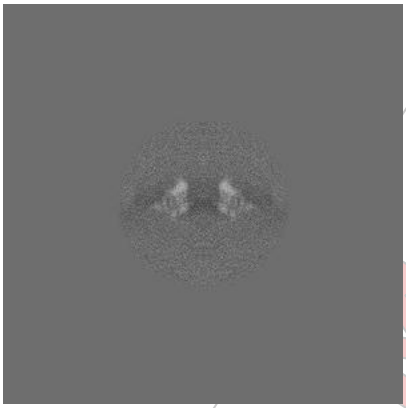


Y Index: 256

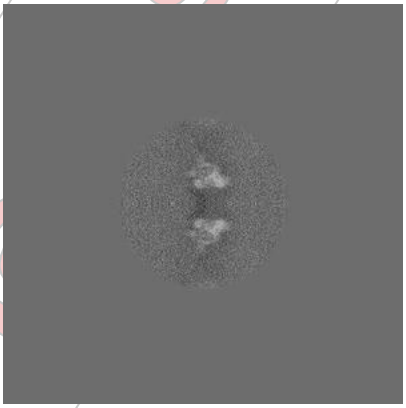


Z Index: 256

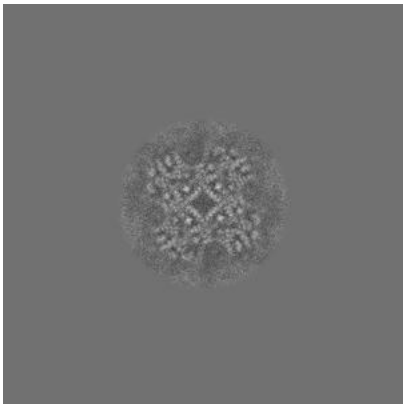
6.2.2 Raw map



X Index: 256



Y Index: 256



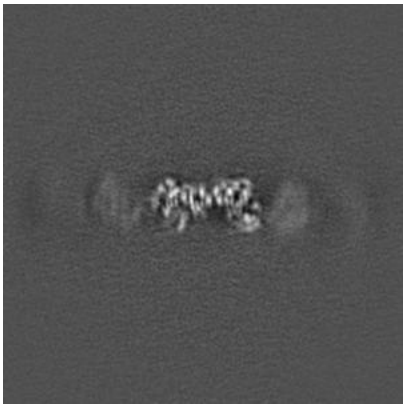
Z Index: 256

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

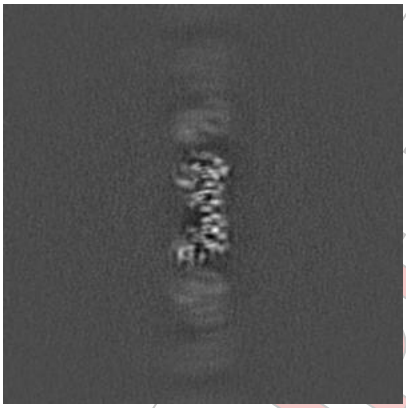
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6.3 Largest variance slices (i)

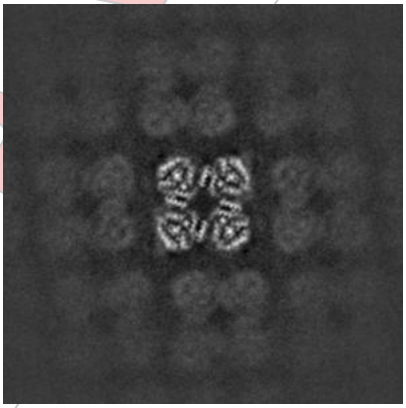
6.3.1 Primary map



X Index: 292

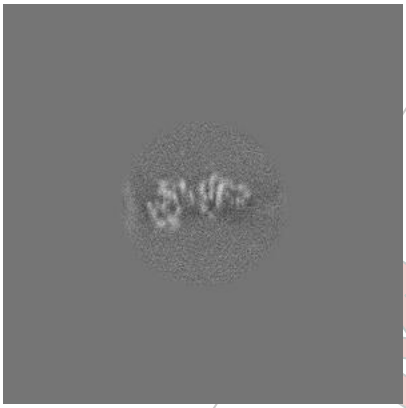


Y Index: 292

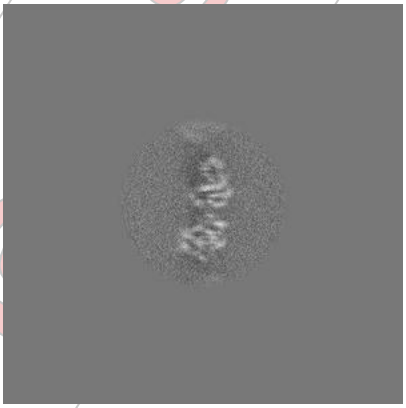


Z Index: 272

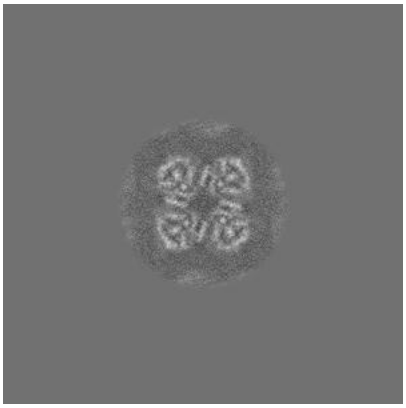
6.3.2 Raw map



X Index: 231



Y Index: 280



Z Index: 271

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

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6.4 Orthogonal surface views (i)

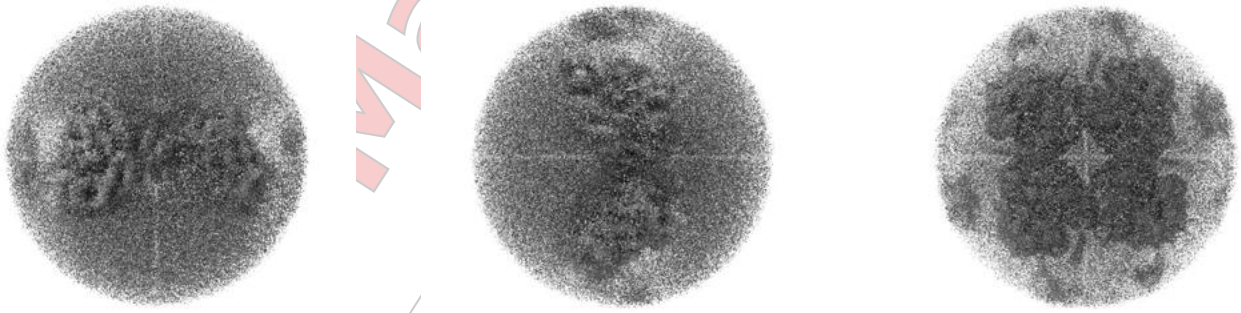
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

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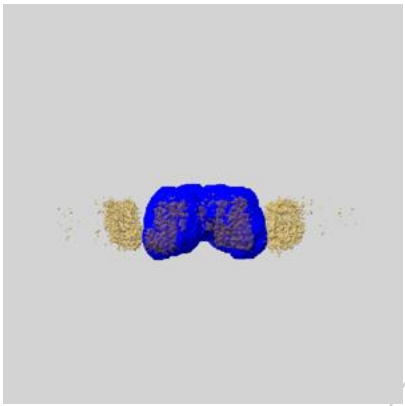
6.5 Mask visualisation

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

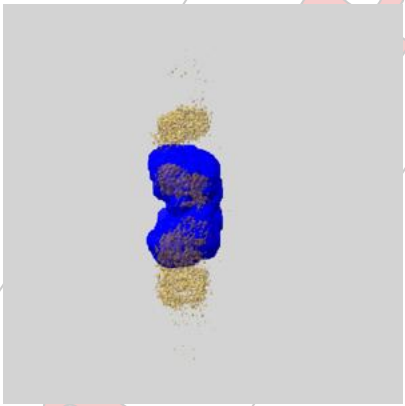
A mask typically either:

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

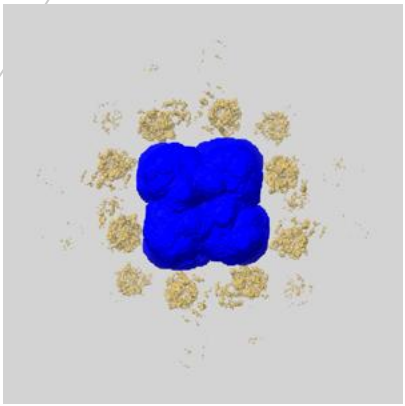
6.5.1 D_9101001792_em-mask-volume_P1.map.V14



X



Y



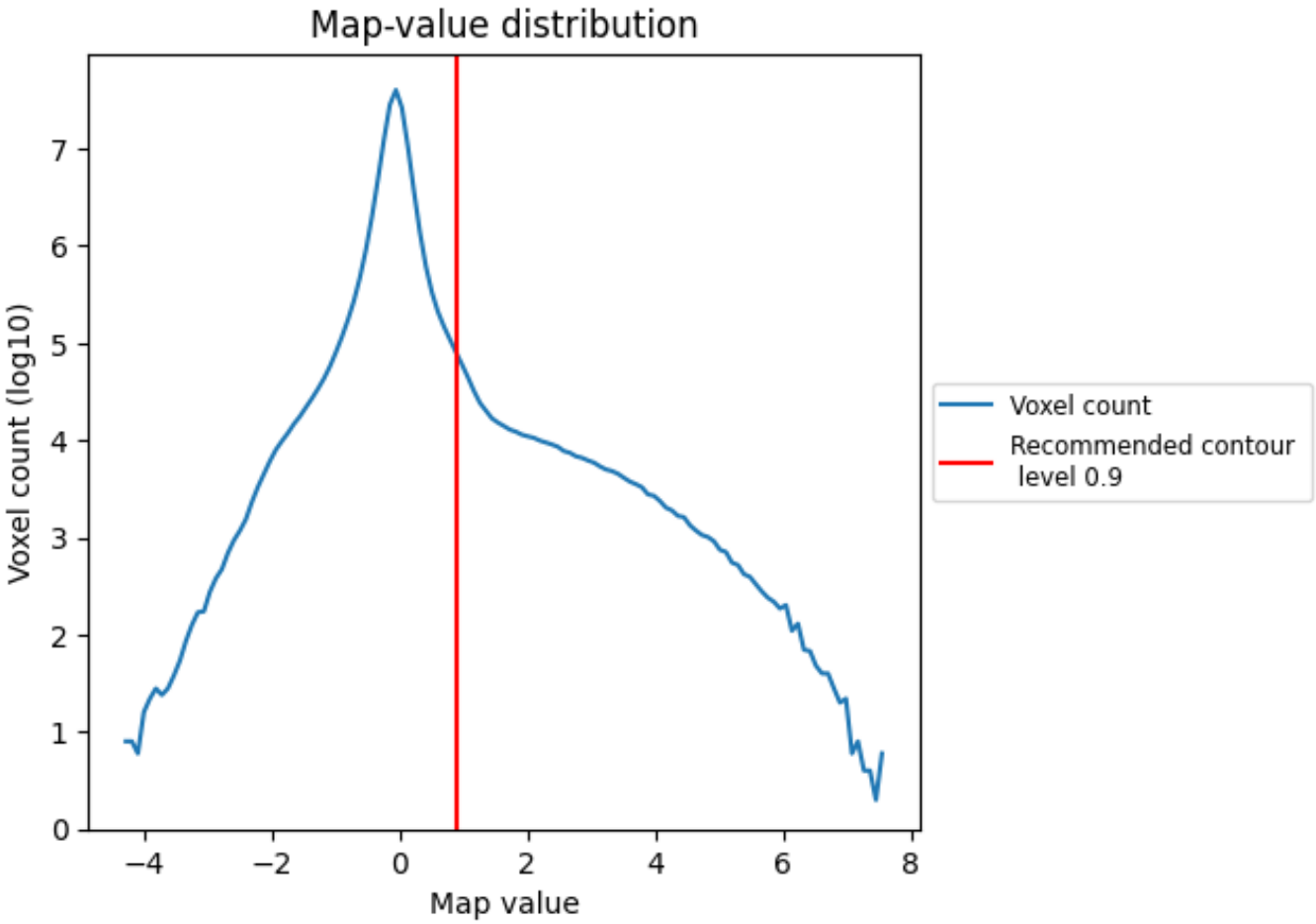
Z

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7 Map analysis

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

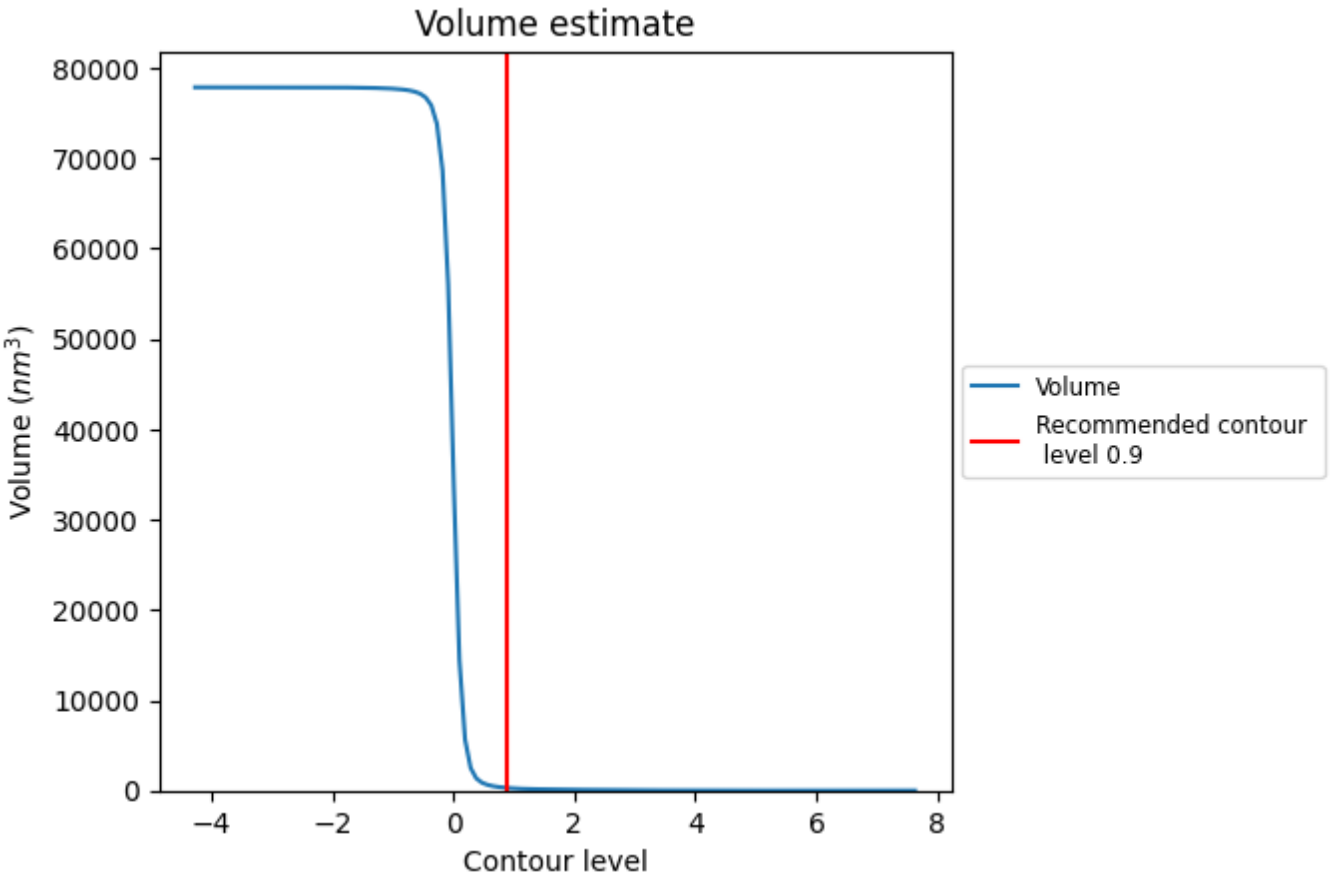
7.1 Map-value distribution



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.

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7.2 Volume estimate (i)

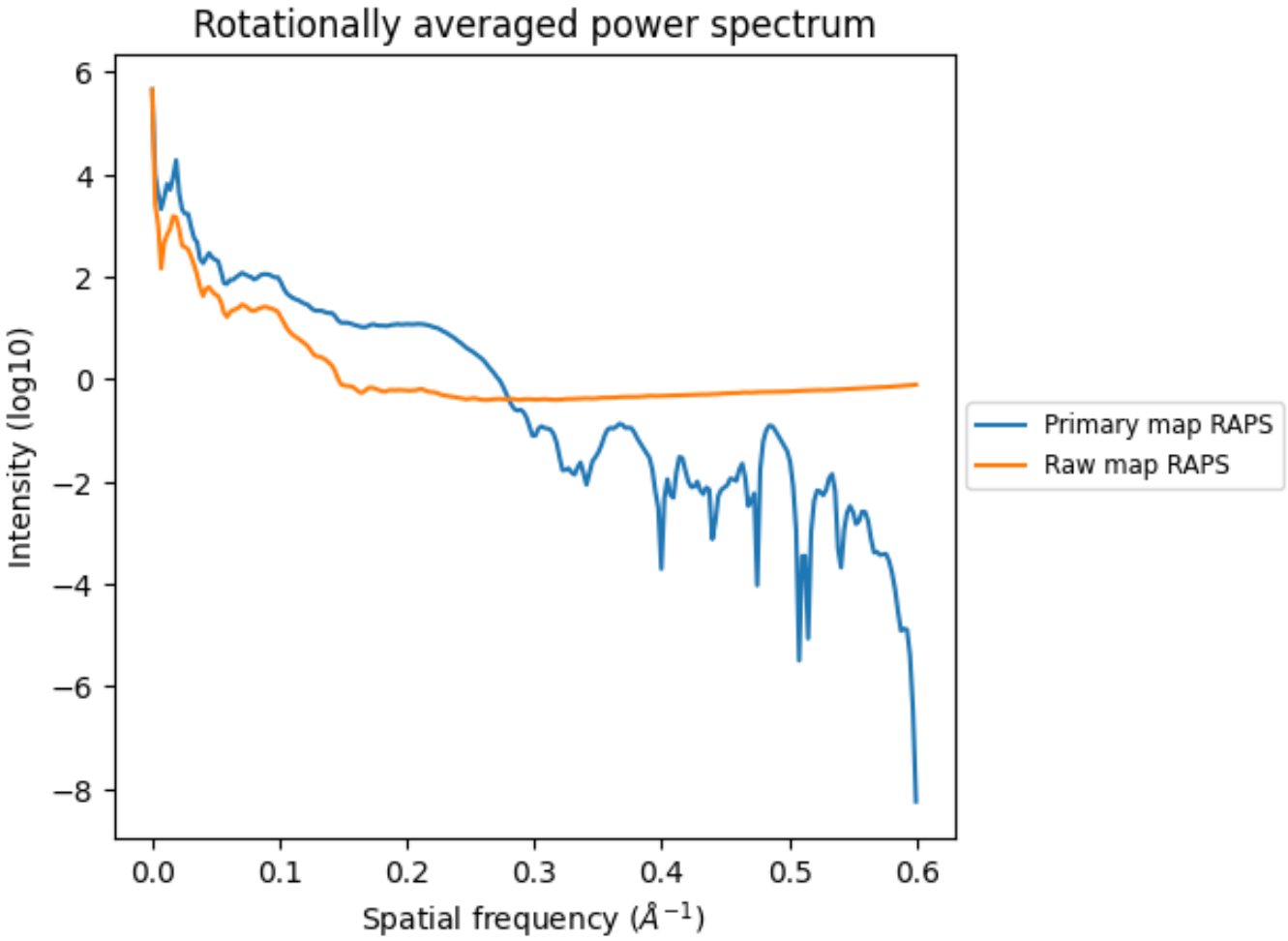


The volume at the recommended contour level is 287 nm^3; this corresponds to an approximate mass of 259 kDa.

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.

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7.3 Rotationally averaged power spectrum (i)

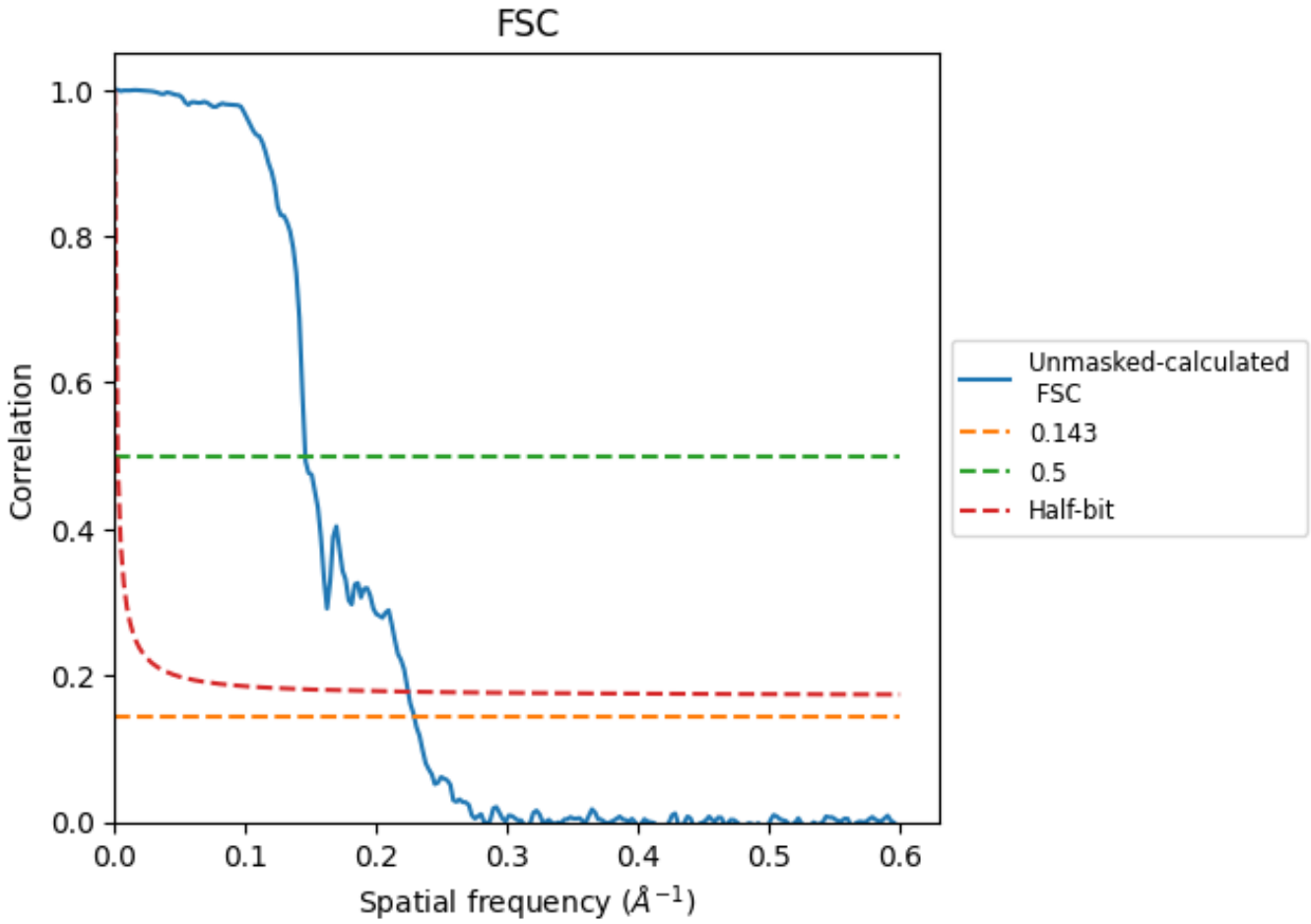


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8 Fourier-Shell correlation

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



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8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	6.87	4.46

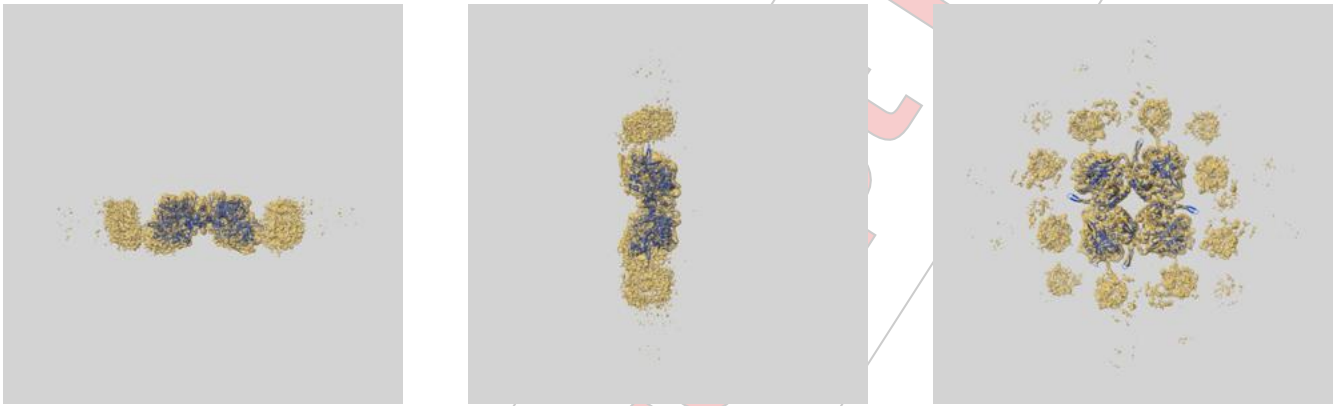
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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9 Map-model fit

This section contains information regarding the fit between EMDB map D_9101001792 and PDB model D_9101001792. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

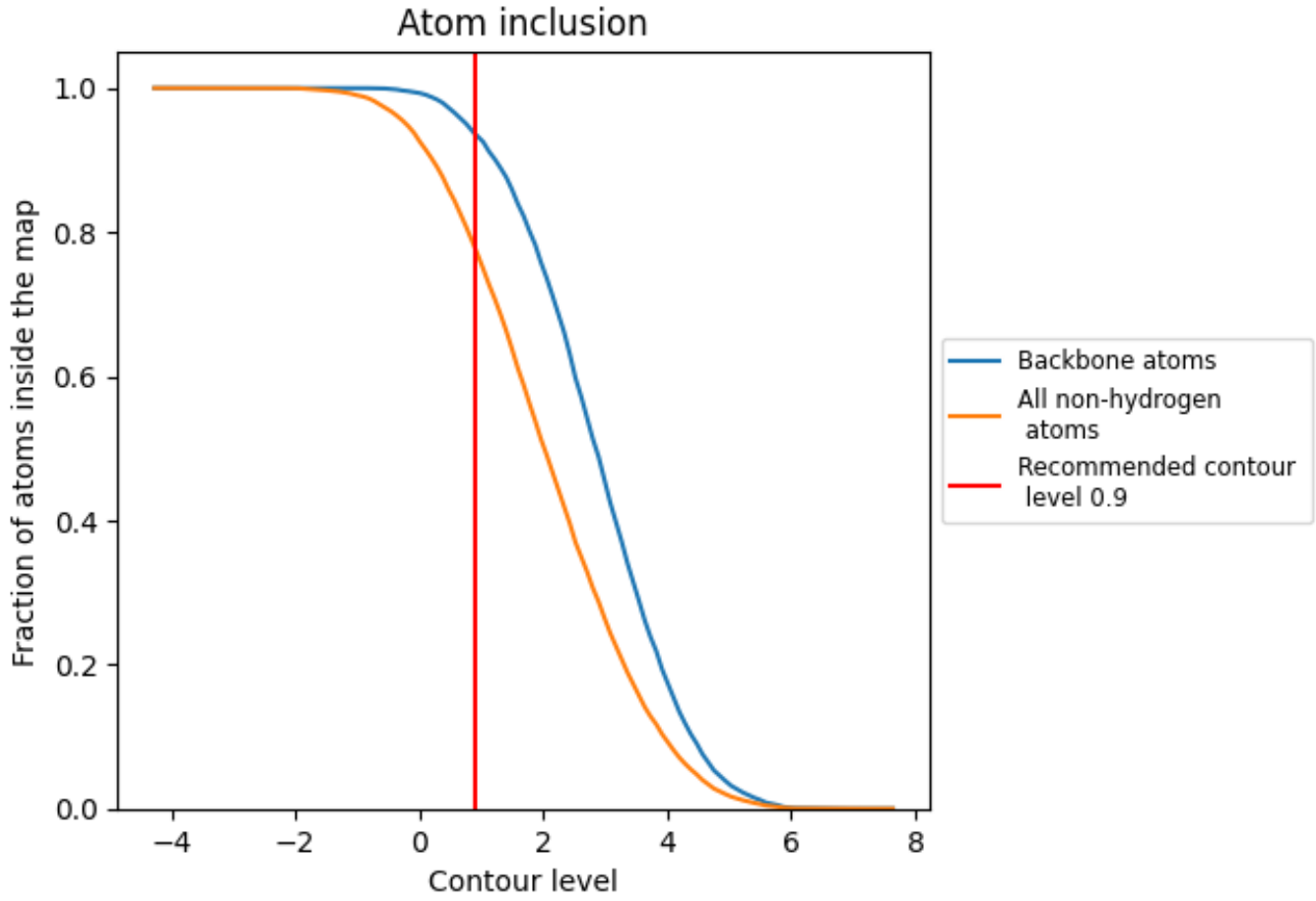


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

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9.2 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

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