



wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 12:45 AM EDT

PDB ID : 8DP5
EMDB ID : EMD-27630
Title : Structure of the PEAK3/14-3-3 complex
Authors : Torosyan, H.; Paul, M.; Jura, N.; Verba, K.A.
Deposited on : 2022-07-14
Resolution : 3.10 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
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) : 2.39

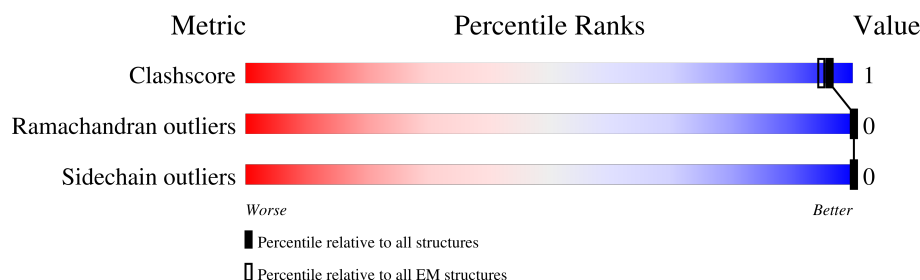
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	66% 32% 7%
1	B	491	65% 32% 7%
2	C	246	91% 7%
3	D	255	88% 9%
4	E	491	98%
4	P	491	99%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17780 atoms, of which 8916 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 Protein PEAK3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0
			5051	1606	2544	453	438	10		
1	B	335	Total	C	H	N	O	S	0	0
			5084	1618	2563	456	437	10		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	LEU	-	expression tag	UNP Q6ZS72
A	475	GLU	-	expression tag	UNP Q6ZS72
A	476	GLY	-	expression tag	UNP Q6ZS72
A	477	GLY	-	expression tag	UNP Q6ZS72
A	478	GLY	-	expression tag	UNP Q6ZS72
A	479	GLY	-	expression tag	UNP Q6ZS72
A	480	ALA	-	expression tag	UNP Q6ZS72
A	481	ASP	-	expression tag	UNP Q6ZS72
A	482	TYR	-	expression tag	UNP Q6ZS72
A	483	LYS	-	expression tag	UNP Q6ZS72
A	484	ASP	-	expression tag	UNP Q6ZS72
A	485	ASP	-	expression tag	UNP Q6ZS72
A	486	ASP	-	expression tag	UNP Q6ZS72
A	487	ASP	-	expression tag	UNP Q6ZS72
A	488	LYS	-	expression tag	UNP Q6ZS72
A	489	GLY	-	expression tag	UNP Q6ZS72
A	490	PRO	-	expression tag	UNP Q6ZS72
A	491	VAL	-	expression tag	UNP Q6ZS72
B	474	LEU	-	expression tag	UNP Q6ZS72
B	475	GLU	-	expression tag	UNP Q6ZS72
B	476	GLY	-	expression tag	UNP Q6ZS72
B	477	GLY	-	expression tag	UNP Q6ZS72
B	478	GLY	-	expression tag	UNP Q6ZS72
B	479	GLY	-	expression tag	UNP Q6ZS72
B	480	ALA	-	expression tag	UNP Q6ZS72
B	481	ASP	-	expression tag	UNP Q6ZS72

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Chain	Residue	Modelled	Actual	Comment	Reference
B	482	TYR	-	expression tag	UNP Q6ZS72
B	483	LYS	-	expression tag	UNP Q6ZS72
B	484	ASP	-	expression tag	UNP Q6ZS72
B	485	ASP	-	expression tag	UNP Q6ZS72
B	486	ASP	-	expression tag	UNP Q6ZS72
B	487	ASP	-	expression tag	UNP Q6ZS72
B	488	LYS	-	expression tag	UNP Q6ZS72
B	489	GLY	-	expression tag	UNP Q6ZS72
B	490	PRO	-	expression tag	UNP Q6ZS72
B	491	VAL	-	expression tag	UNP Q6ZS72

- Molecule 2 is a protein called 14-3-3 protein beta/alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	230	Total	C	H	N	O	S	0	0
			3691	1161	1836	312	373	9		

- Molecule 3 is a protein called 14-3-3 protein epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	231	Total	C	H	N	O	S	0	0
			3698	1166	1846	312	363	11		

- Molecule 4 is a protein called Protein PEAK3 fragment.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	8	Total	C	H	N	O	P	0	0
			140	39	70	15	15	1		
4	P	7	Total	C	H	N	O	P	0	0
			116	33	57	11	14	1		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	474	LEU	-	expression tag	UNP Q6ZS72
E	475	GLU	-	expression tag	UNP Q6ZS72
E	476	GLY	-	expression tag	UNP Q6ZS72
E	477	GLY	-	expression tag	UNP Q6ZS72
E	478	GLY	-	expression tag	UNP Q6ZS72
E	479	GLY	-	expression tag	UNP Q6ZS72
E	480	ALA	-	expression tag	UNP Q6ZS72
E	481	ASP	-	expression tag	UNP Q6ZS72

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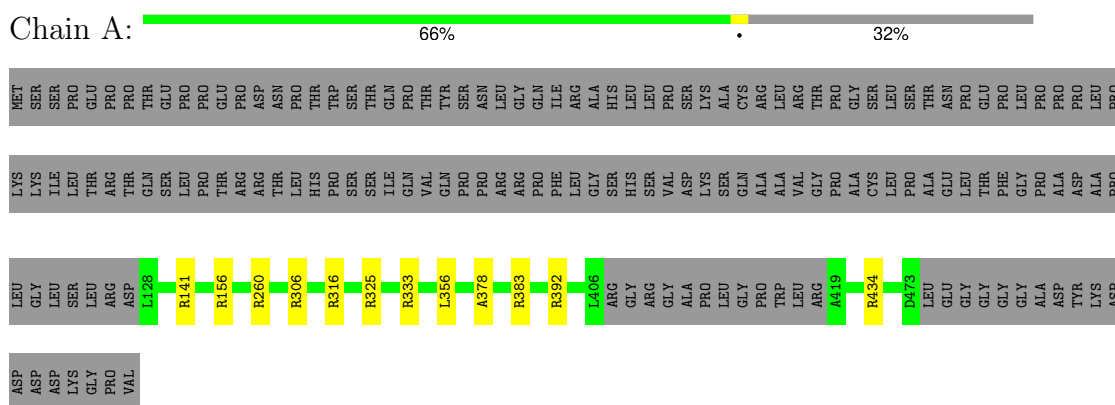
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Chain	Residue	Modelled	Actual	Comment	Reference
E	482	TYR	-	expression tag	UNP Q6ZS72
E	483	LYS	-	expression tag	UNP Q6ZS72
E	484	ASP	-	expression tag	UNP Q6ZS72
E	485	ASP	-	expression tag	UNP Q6ZS72
E	486	ASP	-	expression tag	UNP Q6ZS72
E	487	ASP	-	expression tag	UNP Q6ZS72
E	488	LYS	-	expression tag	UNP Q6ZS72
E	489	GLY	-	expression tag	UNP Q6ZS72
E	490	PRO	-	expression tag	UNP Q6ZS72
E	491	VAL	-	expression tag	UNP Q6ZS72
P	474	LEU	-	expression tag	UNP Q6ZS72
P	475	GLU	-	expression tag	UNP Q6ZS72
P	476	GLY	-	expression tag	UNP Q6ZS72
P	477	GLY	-	expression tag	UNP Q6ZS72
P	478	GLY	-	expression tag	UNP Q6ZS72
P	479	GLY	-	expression tag	UNP Q6ZS72
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P	484	ASP	-	expression tag	UNP Q6ZS72
P	485	ASP	-	expression tag	UNP Q6ZS72
P	486	ASP	-	expression tag	UNP Q6ZS72
P	487	ASP	-	expression tag	UNP Q6ZS72
P	488	LYS	-	expression tag	UNP Q6ZS72
P	489	GLY	-	expression tag	UNP Q6ZS72
P	490	PRO	-	expression tag	UNP Q6ZS72
P	491	VAL	-	expression tag	UNP Q6ZS72

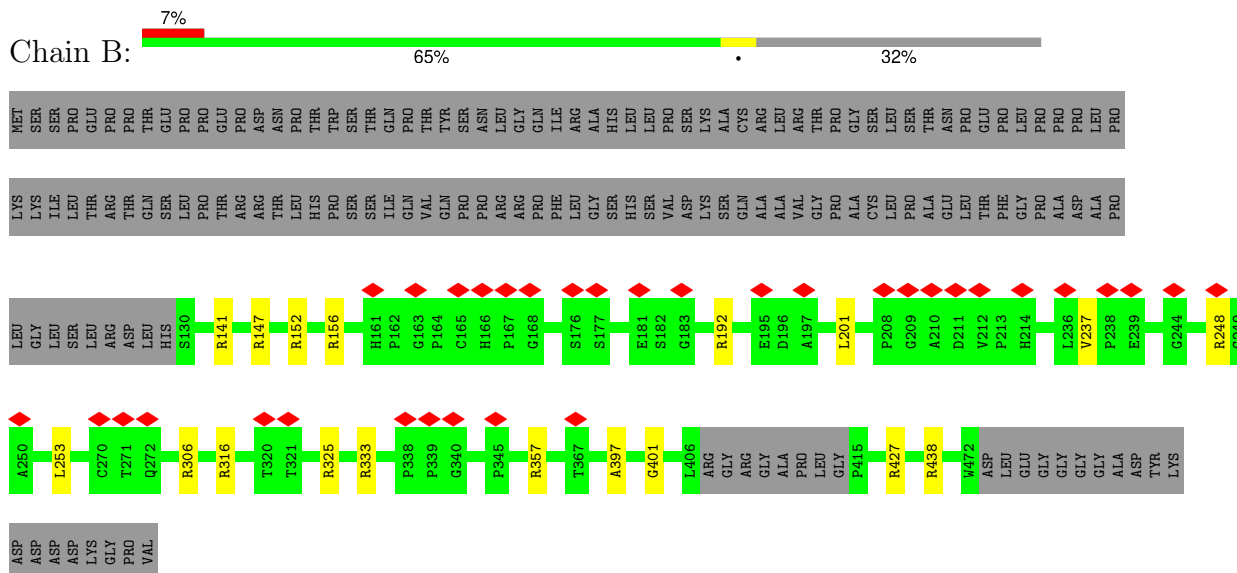
3 Residue-property plots

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: Protein PEAK3



• Molecule 1: Protein PEAK3



• Molecule 2: 14-3-3 protein beta/alpha



Lys ASP ASP ASP ASP Lys GLY GLY VAL	TRP	ALA	VAL	PRO	GLY	ASP
	LEU	ALA	GLU	GLY	PRO	GLY
	ARG	PRO	LEU	ALA	PRO	LEU
	VAL	SER	ARG	ARG	TRP	TYR
	ARG	THR	GLU	ARG	TYR	TYR
	GLY	PRO	ASN	GLY	GLY	ARG
	LEU	LEU	LEU	VAL	VAL	VAL
	LEU	ALA	LEU	ALA	ARG	VAL
	LEU	GLY	VAL	LEU	ALA	ALA
	ARG	LEU	ALA	ALA	ALA	HIS
ASP ASP ASP ASP Lys GLY GLY VAL	ARG	LEU	PRO	PRO	GLU	GLU
	ALA	LEU	ARG	GLU	ASP	ASP
	ALA	LEU	GLY	VAL	ALA	ASP
	GLU	GLU	CYS	PRO	TRP	TRP
	ARG	ALA	ALA	GLU	HIS	HIS
	ALA	ALA	THR	ARG	ILE	ILE
	ALA	GLN	THR	ARG	LEU	LEU
	GLY	THR	GLY	VAL	VAL	VAL
	GLU	ARG	PRO	ALA	ALA	ALA
	GLU	LEU	PRO	GLN	LYS	LYS
TRP	PRO	ARG	ARG	TRP	VAL	VAL
	SER	PRO	LEU	LEU	PRO	PRO
	LEU	SER	LEU	ALA	LYS	LYS
	GLU	ALA	LEU	GLU	GLY	GLY
	ASP	SER	THR	ALA	ALA	ALA
	TRP	THR	PHE	CYS	ASP	ASP
	LEU	THR	PHE	THR	ASP	ASP
	CYS	ARG	GLY	GLN	VAL	VAL
	GLY	GLY	ARG	PRO	PRO	PRO
	CYS	ALA	VAL	PRO	HIS	HIS
GLY GLY VAL	TYR	LEU	CYS	GLU	PRO	PRO
	LEU	GLN	LEU	GLU	TRP	TRP
	ALA	ALA	GLN	PHE	GLY	GLY
	GLU	LEU	PRO	VAL	LEU	LEU
	ALA	LEU	GLY	ALA	ALA	ALA
	SER	PRO	PRO	ALA	SER	SER
	MET	GLY	SER	LEU	LEU	LEU
	GLY	GLU	PRO	LEU	GLY	GLY
	ALA	LEU	PRO	GLN	HIS	PHE
	ALA	ARG	HIS	LEU	ASN	ASN
GLY GLY VAL	LEU	GLY	LEU	ALA	LEU	LEU
	LEU	PRO	GLY	GLN	GLY	GLN
	TRP	PRO	LEU	LEU	LEU	GLY
	ASP	LEU	GLY	LYS	GLY	GLY
	LEU	GLY	SER	PHE	CYS	CYS
	GLU	PRO	LEU	LEU	GLY	GLY
	GLY	TRP	LEU	GLU	LEU	LEU
	GLY	LEU	ARG	ALA	VAL	VAL
	GLY	ARG	ALA	TRP	GLY	GLY
	ASP	GLY	LEU	ALA	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.383	Depositor
Minimum map value	-1.276	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.268	Depositor
Map size (Å)	267.19998, 267.19998, 267.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8349999, 0.8349999, 0.8349999	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	0/2578	1.02	9/3533 (0.3%)
1	B	0.68	0/2594	1.01	13/3555 (0.4%)
2	C	0.64	0/1882	0.92	3/2533 (0.1%)
3	D	0.64	0/1880	0.99	8/2534 (0.3%)
4	E	0.83	0/59	1.34	1/77 (1.3%)
4	P	0.81	0/48	1.21	0/63
All	All	0.66	0/9041	0.99	34/12295 (0.3%)

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	A	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ARG	NE-CZ-NH1	8.93	124.76	120.30
3	D	42	ARG	NE-CZ-NH1	8.26	124.43	120.30
3	D	86	ARG	NE-CZ-NH1	7.94	124.27	120.30
3	D	130	ARG	NE-CZ-NH1	7.51	124.06	120.30
3	D	57	ARG	NE-CZ-NH1	7.38	123.99	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	ARG	Sidechain
2	C	127	TYR	Sidechain

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	2507	2544	2542	1	0
1	B	2521	2563	2562	7	0
2	C	1855	1836	1835	6	0
3	D	1852	1846	1845	0	0
4	E	70	70	68	0	0
4	P	59	57	55	0	0
All	All	8864	8916	8907	14	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 14 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)
2:C:205:LEU:HD11	2:C:213:TYR:CD1	1.88	1.06
1:B:201:LEU:HD22	1:B:253:LEU:HD13	1.56	0.88
2:C:205:LEU:HD21	2:C:213:TYR:CE1	2.13	0.83
1:B:201:LEU:HD22	1:B:253:LEU:CD1	2.08	0.81
2:C:205:LEU:HD11	2:C:213:TYR:HD1	1.41	0.81

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	330/491 (67%)	330 (100%)	0	0	100	100
1	B	331/491 (67%)	325 (98%)	6 (2%)	0	100	100
2	C	228/246 (93%)	225 (99%)	3 (1%)	0	100	100
3	D	229/255 (90%)	226 (99%)	3 (1%)	0	100	100
4	E	5/491 (1%)	5 (100%)	0	0	100	100
4	P	4/491 (1%)	4 (100%)	0	0	100	100
All	All	1127/2465 (46%)	1115 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/387 (66%)	254 (100%)	0	100	100
1	B	255/387 (66%)	255 (100%)	0	100	100
2	C	204/215 (95%)	204 (100%)	0	100	100
3	D	199/220 (90%)	199 (100%)	0	100	100
4	E	7/386 (2%)	7 (100%)	0	100	100
4	P	6/386 (2%)	6 (100%)	0	100	100
All	All	925/1981 (47%)	925 (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 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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	SEP	P	69	4	8,9,10	1.08	0	7,12,14	2.99	1 (14%)
4	SEP	E	69	4	8,9,10	1.14	0	7,12,14	2.17	1 (14%)

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
4	SEP	P	69	4	-	4/6/8/10	-
4	SEP	E	69	4	-	1/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	P	69	SEP	OG-CB-CA	7.48	115.42	108.14
4	E	69	SEP	OG-CB-CA	5.34	113.34	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	69	SEP	C-CA-CB-OG
4	P	69	SEP	CB-OG-P-O2P
4	P	69	SEP	CB-OG-P-O3P
4	P	69	SEP	CB-OG-P-O1P
4	P	69	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

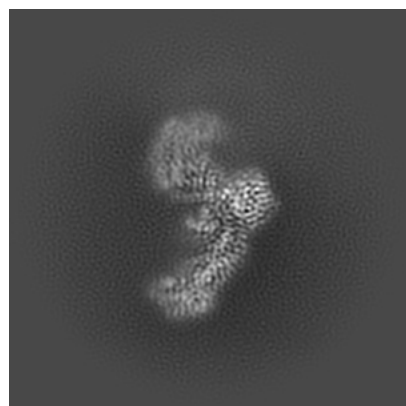
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27630. These allow visual inspection of the internal detail of the map and identification of artifacts.

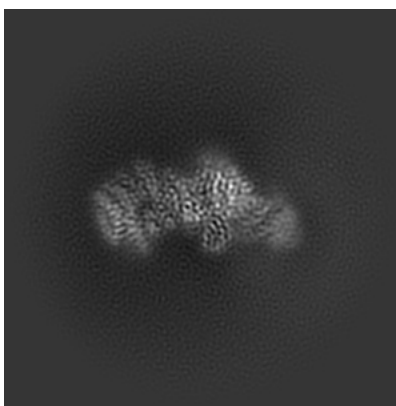
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

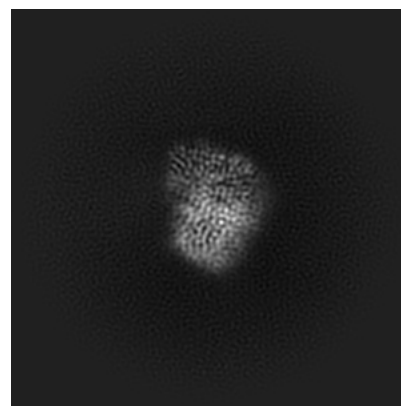
6.1.1 Primary map



X

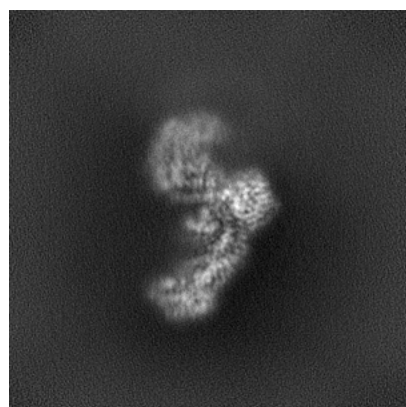


Y

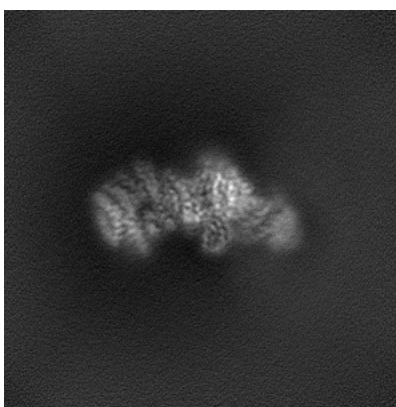


Z

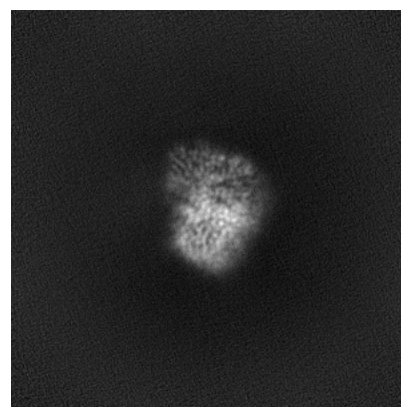
6.1.2 Raw map



X



Y

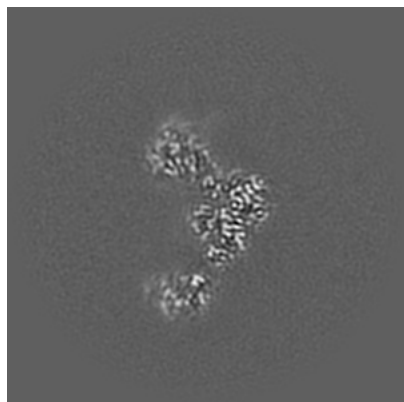


Z

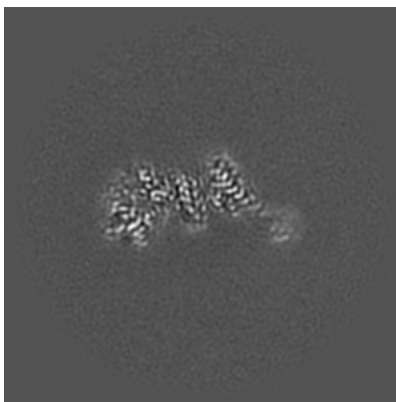
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

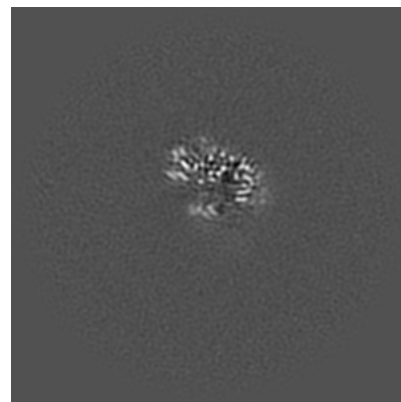
6.2.1 Primary map



X Index: 160

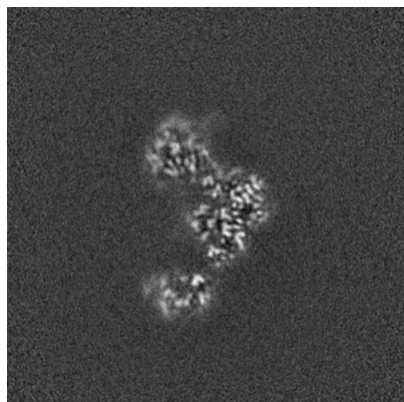


Y Index: 160

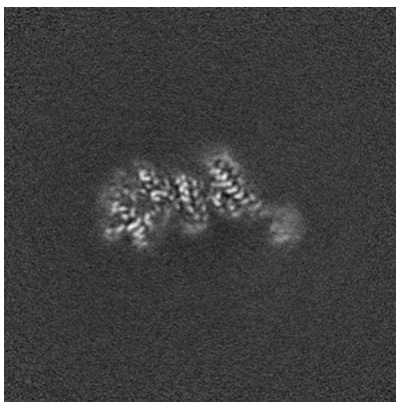


Z Index: 160

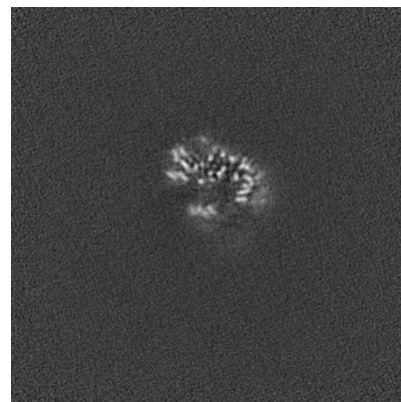
6.2.2 Raw map



X Index: 160



Y Index: 160

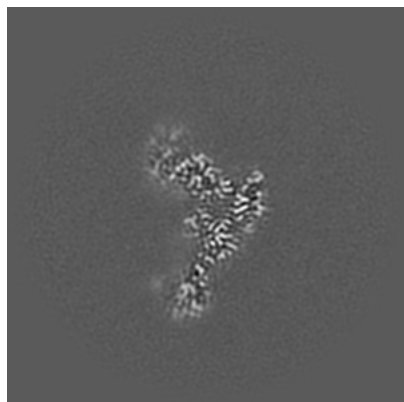


Z Index: 160

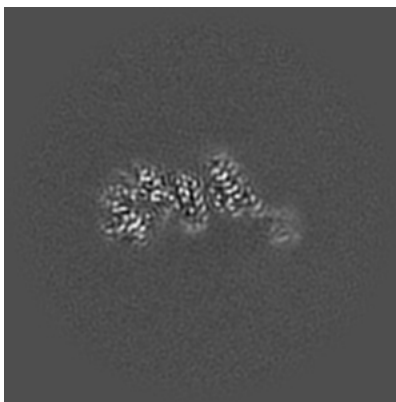
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

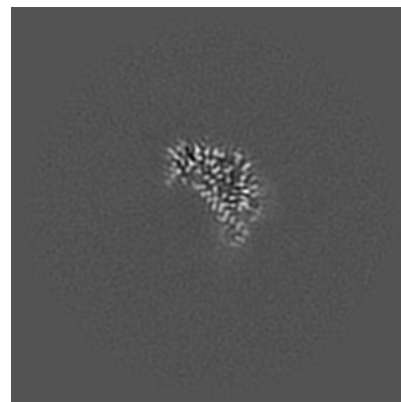
6.3.1 Primary map



X Index: 169

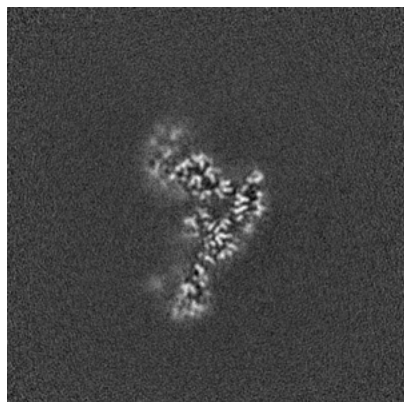


Y Index: 159

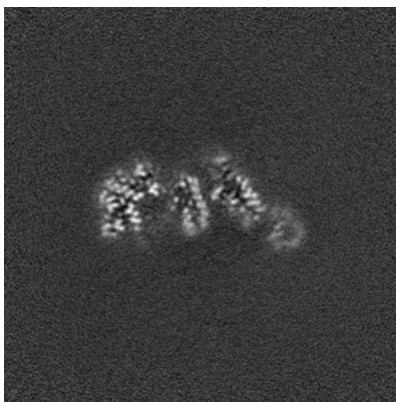


Z Index: 171

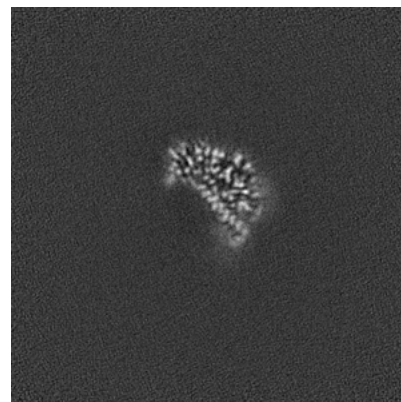
6.3.2 Raw map



X Index: 169



Y Index: 155

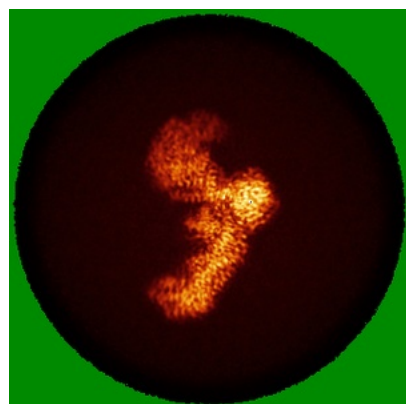


Z Index: 170

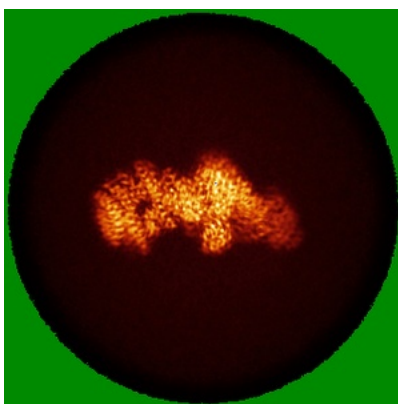
The images above show the largest variance slices of the map in three orthogonal directions.

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

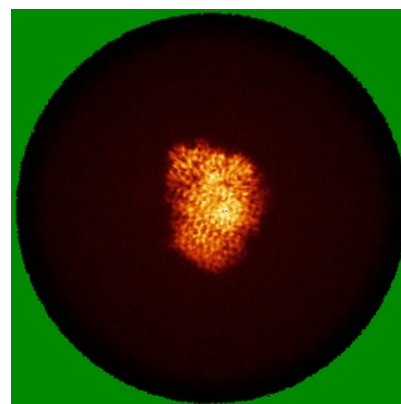
6.4.1 Primary map



X

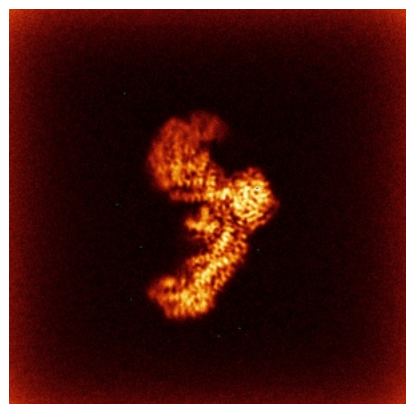


Y

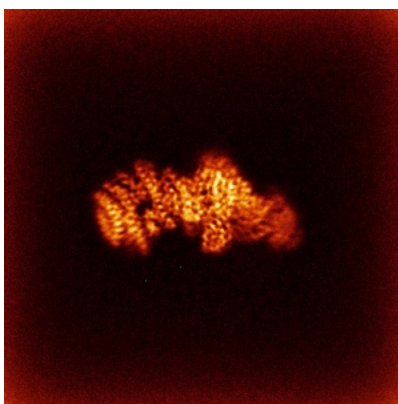


Z

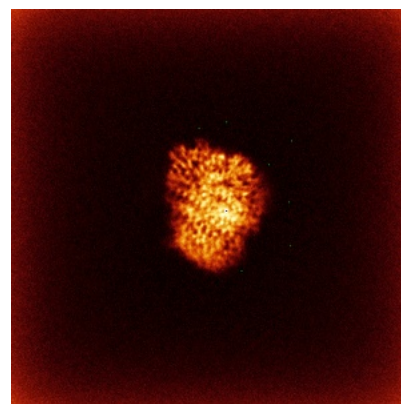
6.4.2 Raw map



X



Y

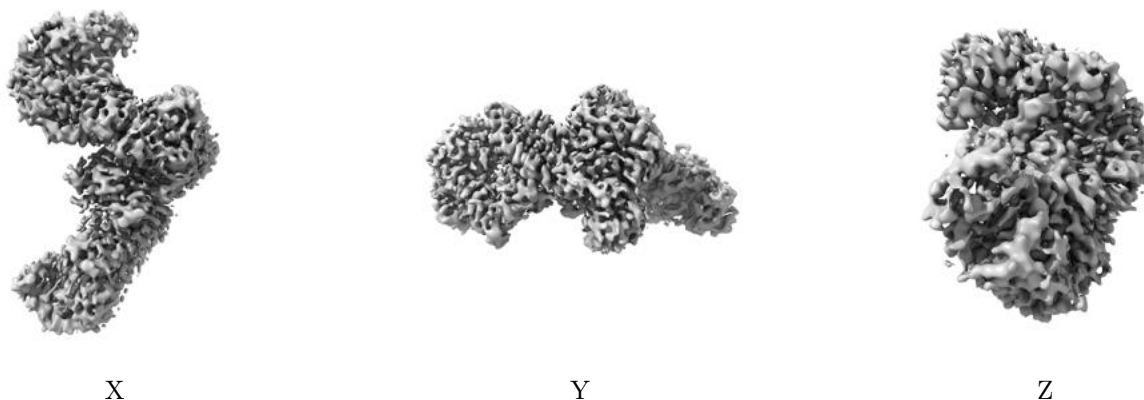


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

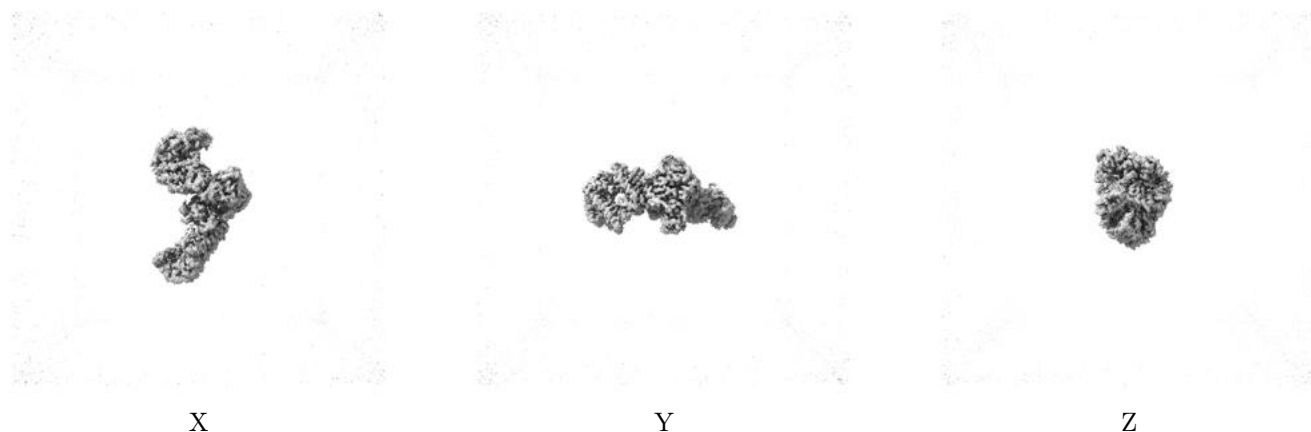
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.268. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

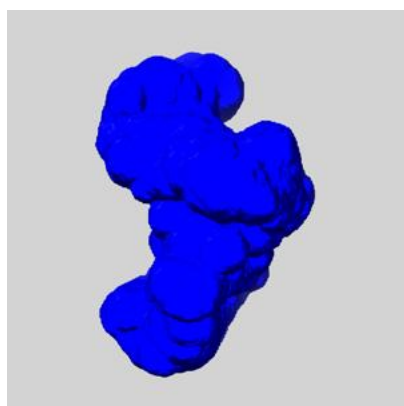
6.6 Mask visualisation [i](#)

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

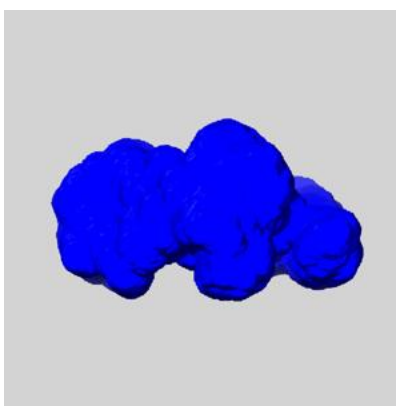
A mask typically either:

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

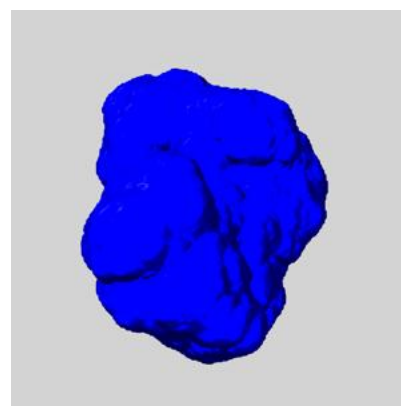
6.6.1 emd_27630_msk_1.map [i](#)



X



Y

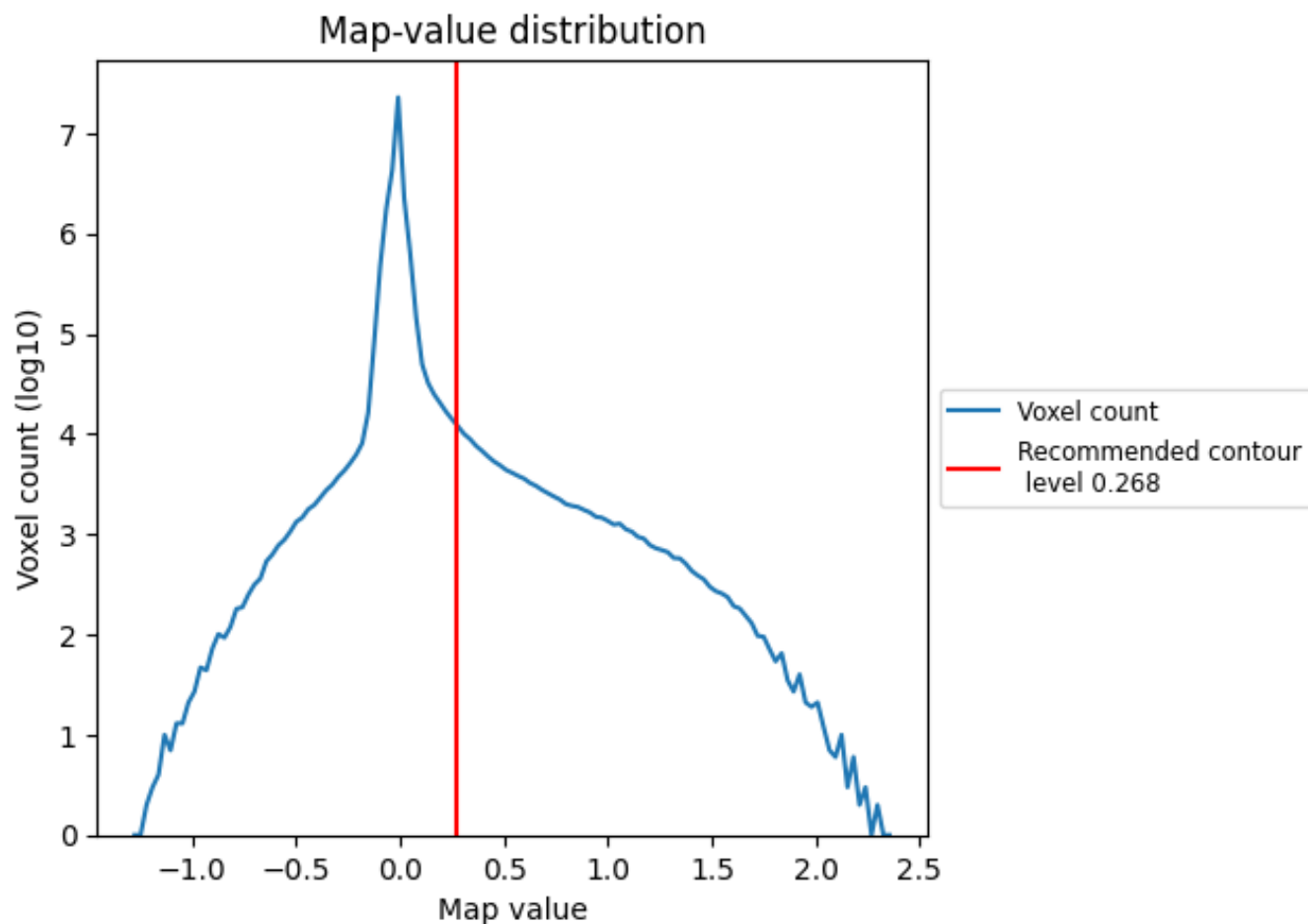


Z

7 Map analysis [i](#)

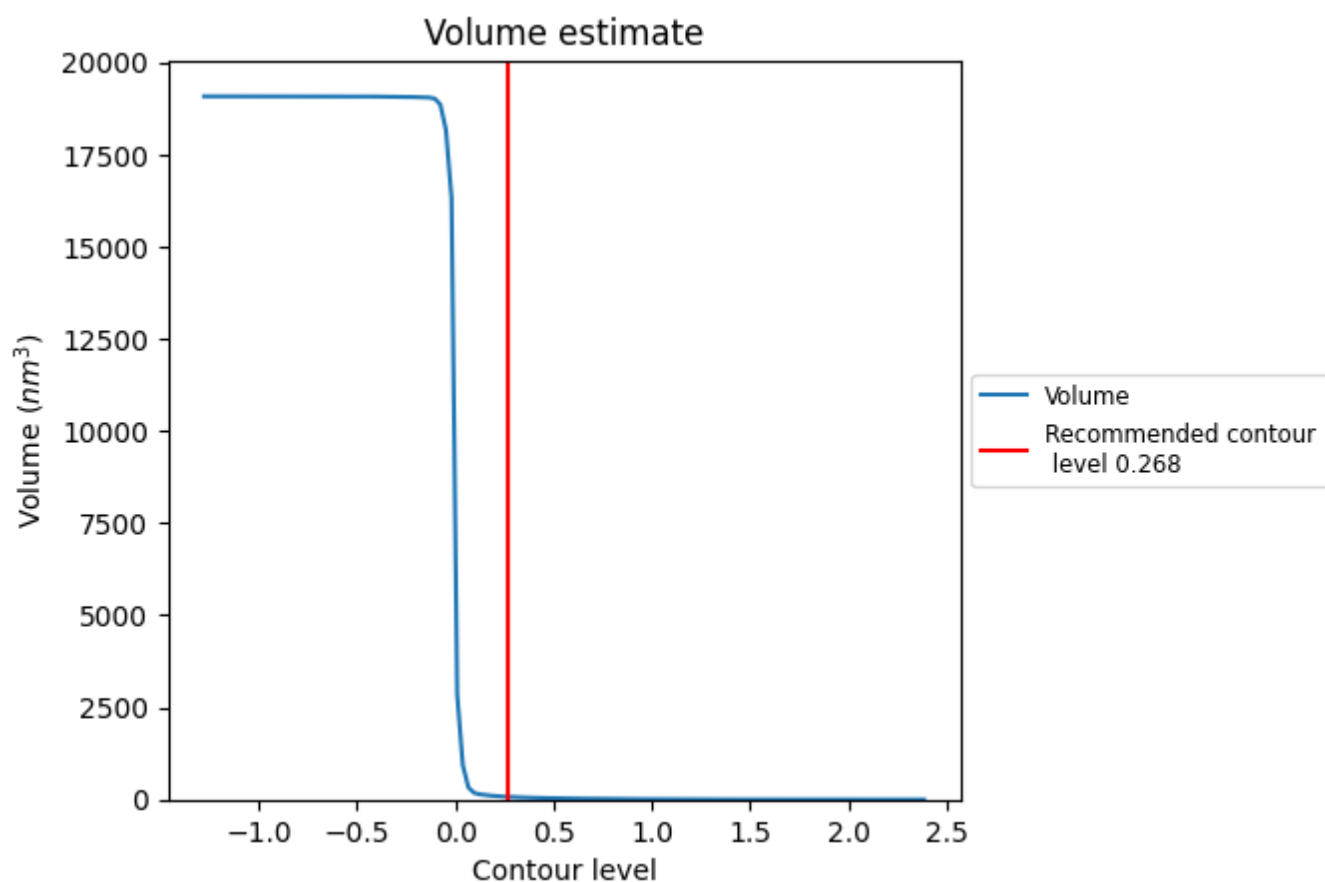
This section contains the results of statistical analysis of the map.

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.

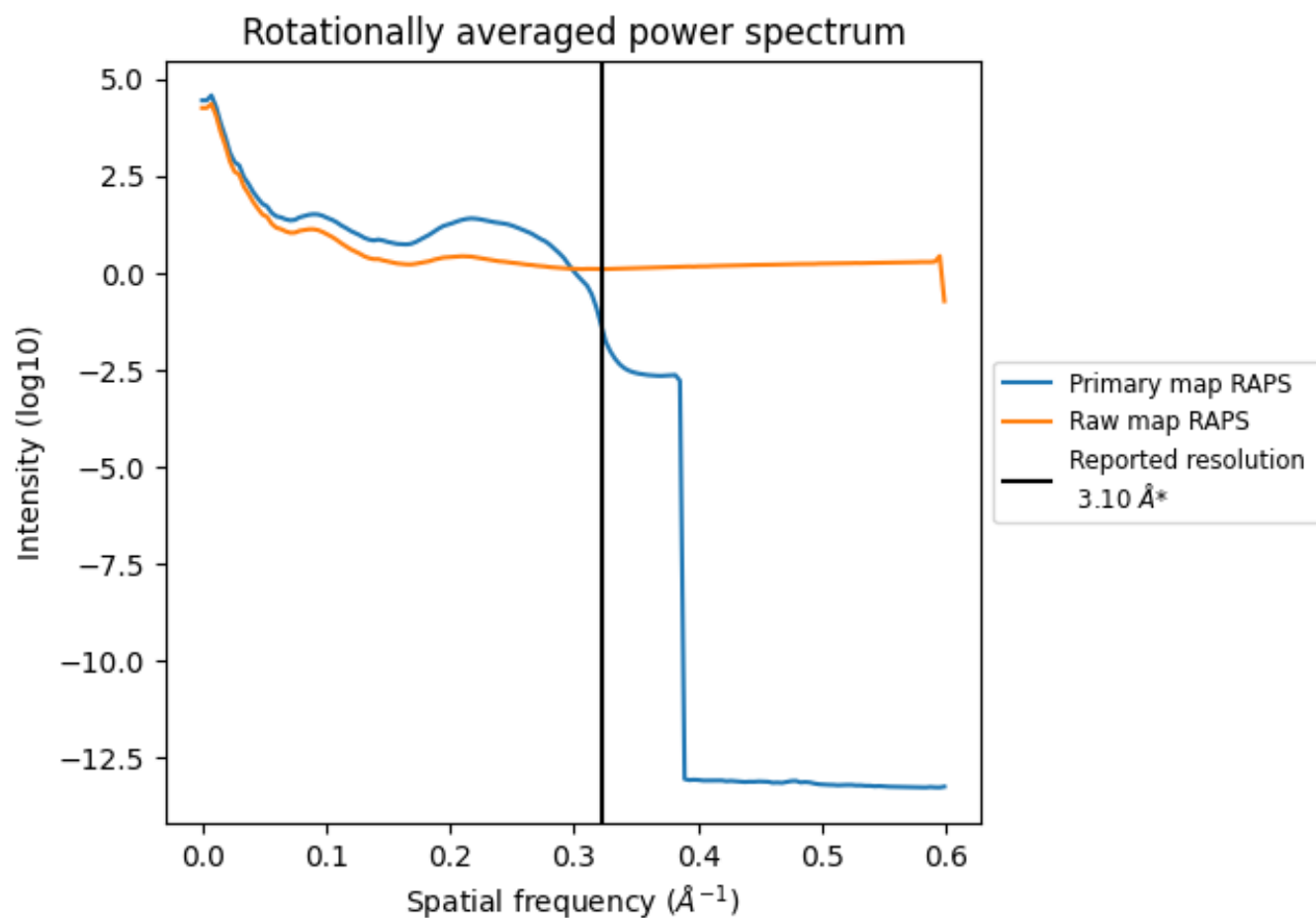
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

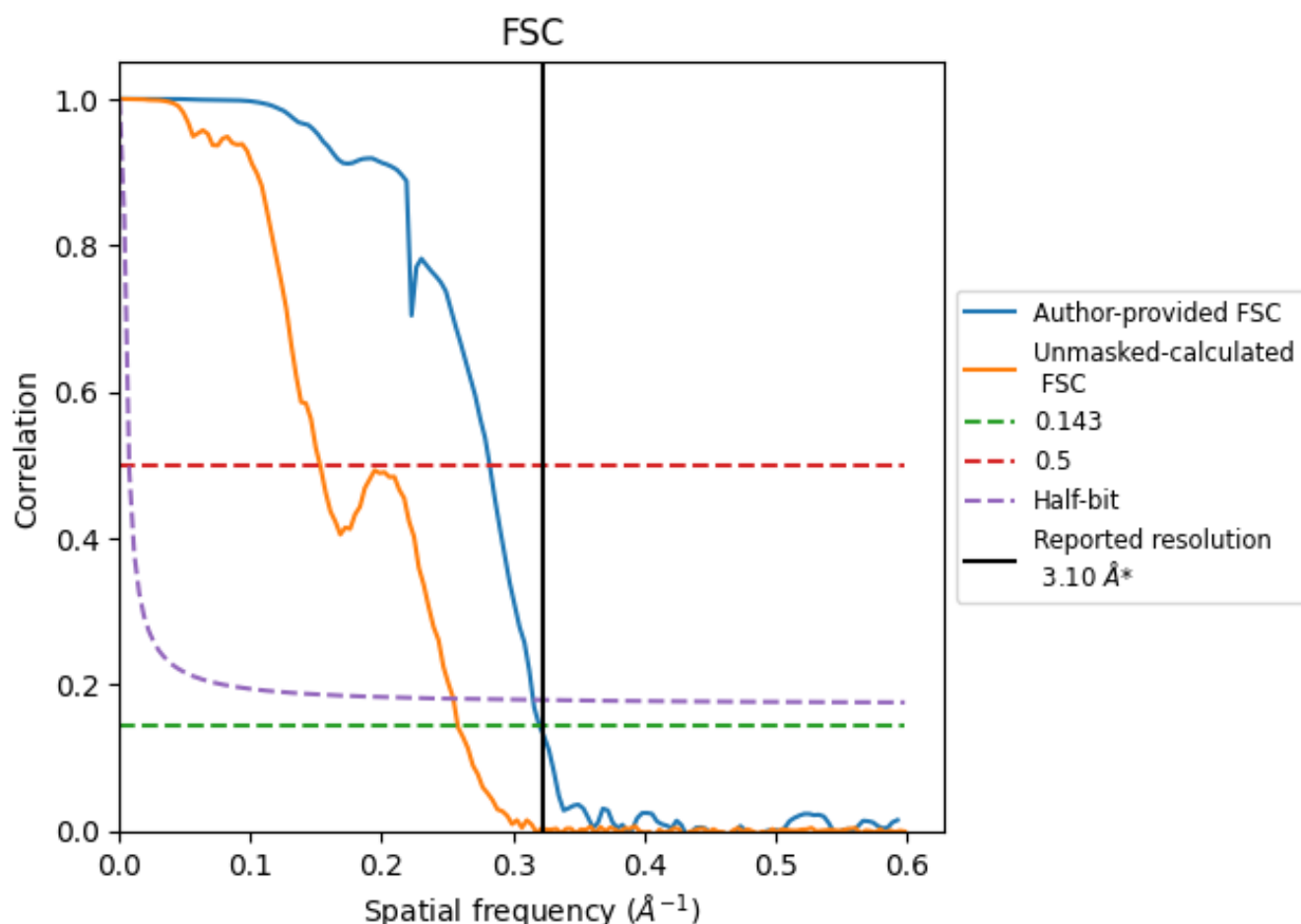


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

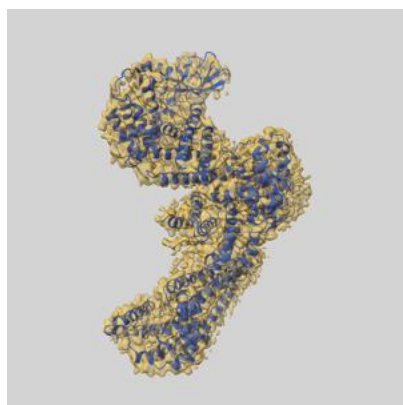
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.54	3.17
Unmasked-calculated*	3.88	6.54	3.93

*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 3.88 differs from the reported value 3.1 by more than 10 %

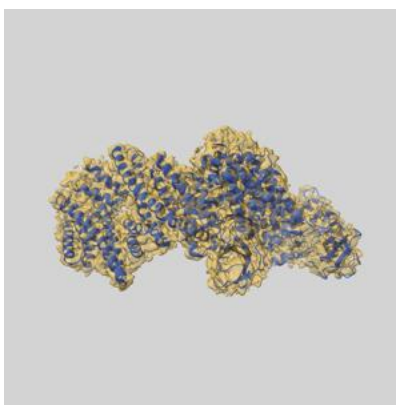
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27630 and PDB model 8DP5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

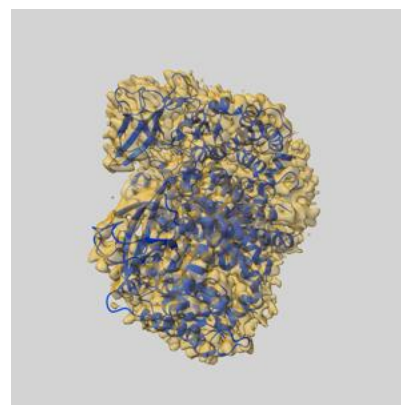
9.1 Map-model overlay [i](#)



X



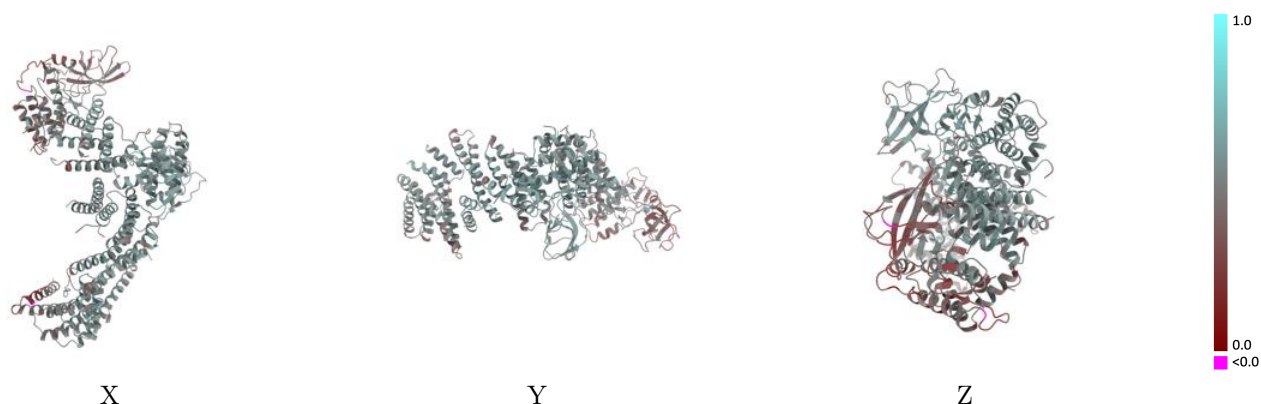
Y



Z

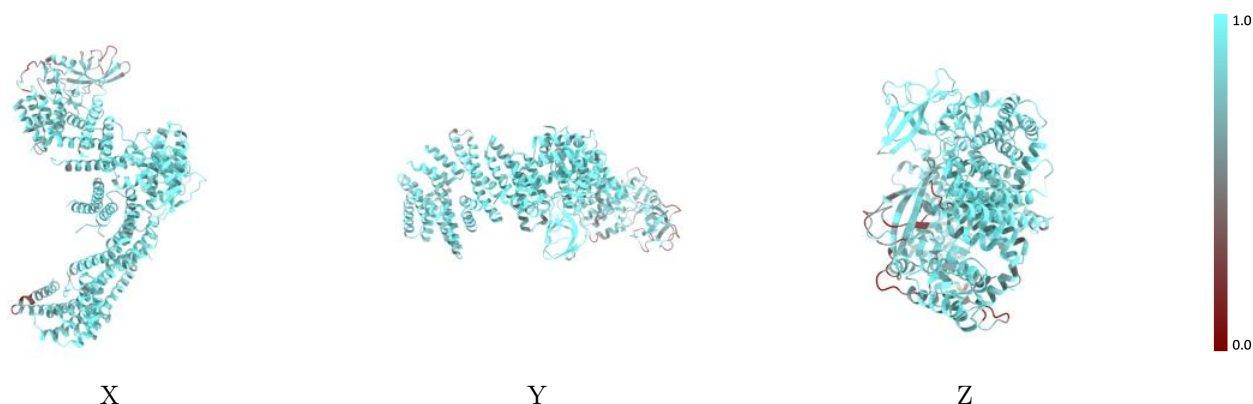
The images above show the 3D surface view of the map at the recommended contour level 0.268 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



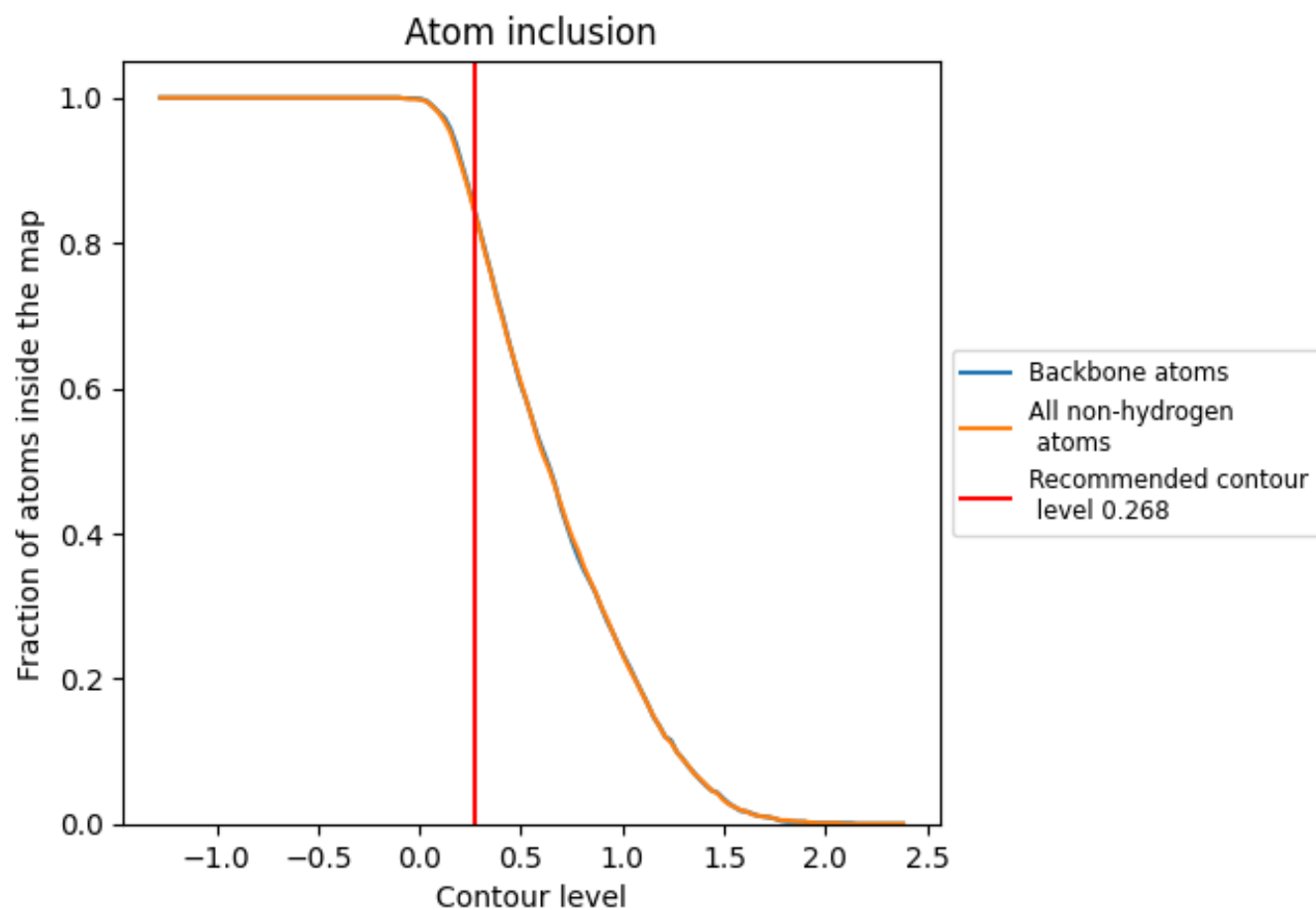
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.268).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.268) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8470	<div><div></div></div> 0.4930
A	<div><div></div></div> 0.9200	<div><div></div></div> 0.5420
B	<div><div></div></div> 0.7690	<div><div></div></div> 0.4180
C	<div><div></div></div> 0.8660	<div><div></div></div> 0.4840
D	<div><div></div></div> 0.8980	<div><div></div></div> 0.5390
E	<div><div></div></div> 0.8790	<div><div></div></div> 0.5000
P	<div><div></div></div> 0.8600	<div><div></div></div> 0.4730

1.0

0.0

<0.0