



# wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 09:13 am GMT

PDB ID : 5FJB  
EMDB ID : EMD-3076  
Title : Cyclophilin A Stabilize HIV-1 Capsid through a Novel Non- canonical Binding Site  
Authors : Liu, C.; Perilla, J.R.; Ning, J.; Lu, M.; Hou, G.; Ramalhu, R.; Bedwell, G.J.; Ahn, J.; Shi, J.; Gronenborn, A.M.; Prevelige Jr, P.E.; Rousso, I.; Aiken, C.; Polenova, T.; Schulten, K.; Zhang, P.  
Deposited on : 2015-10-07  
Resolution : 9.00 Å(reported)  
Based on initial model : 3J4F

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.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

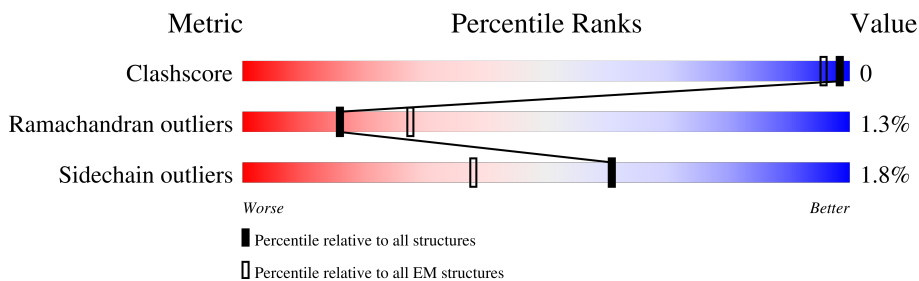
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	218	
1	B	218	
2	C	164	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4664 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GAG POLYPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	218	Total	C	N	O	S	0	0
			1703	1074	296	320	13		
1	B	218	Total	C	N	O	S	0	0
			1703	1074	296	320	13		

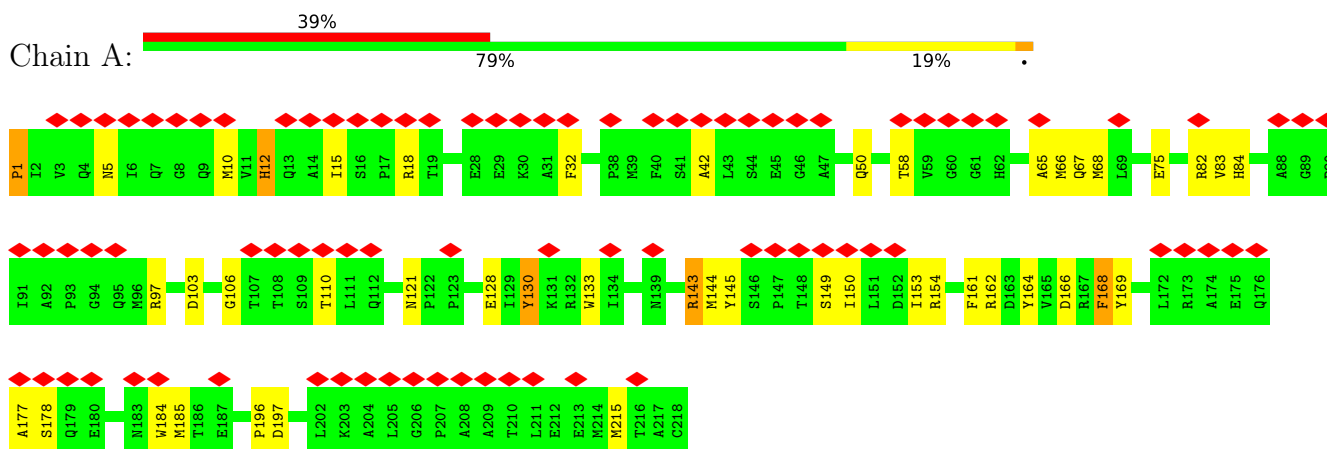
- Molecule 2 is a protein called PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	164	Total	C	N	O	S	0	0
			1258	797	217	236	8		

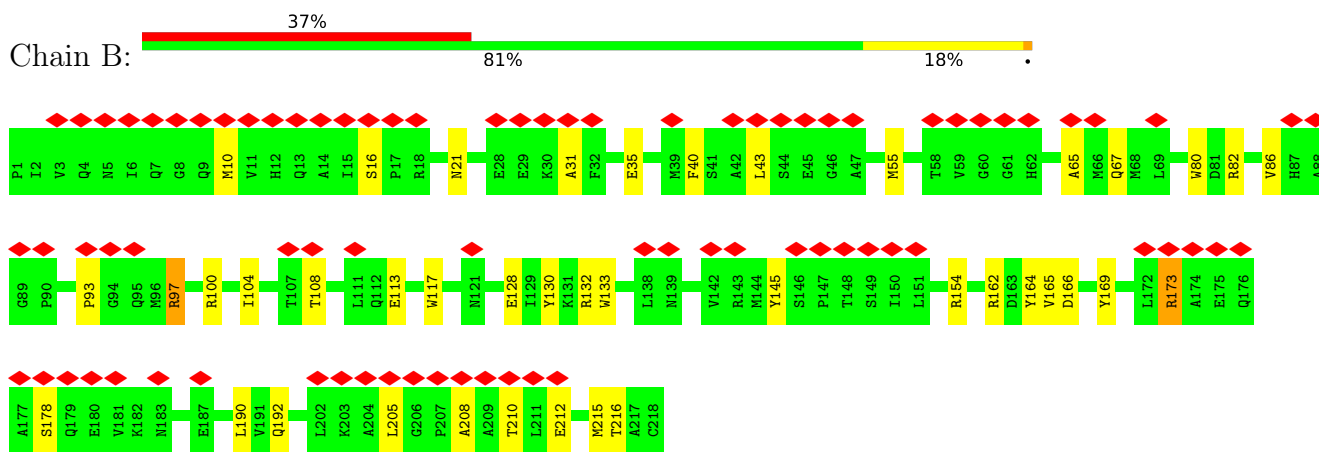
### 3 Residue-property plots

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.

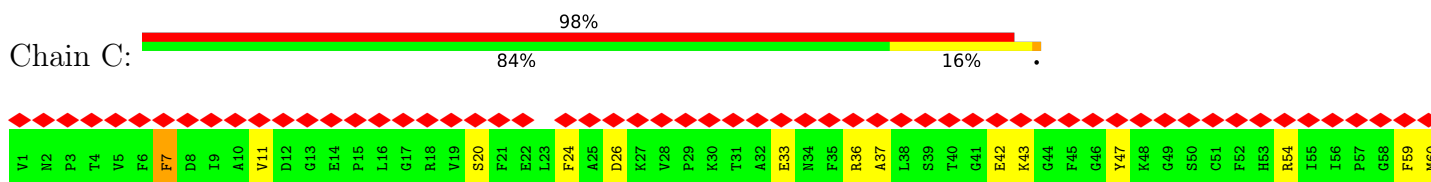
- Molecule 1: GAG POLYPROTEIN



- Molecule 1: GAG POLYPROTEIN



- Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



C61	Q62	G63	G64	D65	F66	T67	R68	H69	N70	G71	T72	G73	G74	K75	S76	I77	Y78	G79	E80	K81	F82	E83	D84	E85	N86	F87	I88	L89	K90	H91	T92	G93	P94	G95	I96	L97	S98	M99	A100	M101	A102	G103	P104	M105	T106	M107	G108	S109	Q110	F111	F112	I113	C114	T115	A116	K117	T118	E119	W120
L121	D122	G123	K124	H125	V126	V127	F128	G129	K130	V131	K132	E133	G134	M135	N136	I137	V138	E139	A140	M141	E142	R143	F144	G145	S146	R147	M148	G149	K150	T151	S152	K153	K154	I155	T156	I157	A158	D159	C160	G161	Q162	L163	E164																

## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	57.381	Depositor
Minimum map value	-44.915	Depositor
Average map value	0.244	Depositor
Map value standard deviation	11.385	Depositor
Recommended contour level	20.0	Depositor
Map size (Å)	462.15997, 462.15997, 275.59998	wwPDB
Map dimensions	436, 436, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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
1	A	1.66	10/1741 (0.6%)	1.99	32/2368 (1.4%)
1	B	1.59	9/1741 (0.5%)	1.95	35/2368 (1.5%)
2	C	1.67	8/1286 (0.6%)	1.86	22/1723 (1.3%)
All	All	1.64	27/4768 (0.6%)	1.94	89/6459 (1.4%)

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	7
1	B	0	2
2	C	0	2
All	All	0	11

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLY	CA-C	-7.34	1.40	1.51
1	B	16	SER	CA-CB	6.92	1.63	1.52
2	C	83	GLU	CD-OE1	6.88	1.33	1.25
1	B	65	ALA	N-CA	-6.44	1.33	1.46
1	A	145	TYR	CE1-CZ	6.38	1.46	1.38

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	NE-CZ-NH1	22.44	131.52	120.30
1	B	97	ARG	NE-CZ-NH2	-20.21	110.19	120.30
1	A	82	ARG	NE-CZ-NH1	18.10	129.35	120.30
1	B	132	ARG	NE-CZ-NH1	15.42	128.01	120.30
1	B	97	ARG	NE-CZ-NH1	15.29	127.95	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PRO	Peptide
1	A	121	ASN	Peptide
1	A	130	TYR	Sidechain
1	A	18	ARG	Sidechain
1	A	32	PHE	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	1703	0	1704	1	0
1	B	1703	0	1704	0	0
2	C	1258	0	1228	1	0
All	All	4664	0	4636	2	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 0.

All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HD12	1:A:153:ILE:HG13	1.82	0.61
2:C:11:VAL:HG22	2:C:155:ILE:HD12	2.03	0.41

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	216/218 (99%)	199 (92%)	12 (6%)	5 (2%)	6	34
1	B	216/218 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
2	C	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	66
All	All	594/600 (99%)	553 (93%)	33 (6%)	8 (1%)	16	48

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	149	SER
1	A	177	ALA
2	C	69	HIS
1	A	5	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	186/186 (100%)	181 (97%)	5 (3%)	44	65
1	B	186/186 (100%)	183 (98%)	3 (2%)	62	79
2	C	132/132 (100%)	131 (99%)	1 (1%)	81	89
All	All	504/504 (100%)	495 (98%)	9 (2%)	61	77

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	216	THR
2	C	60	MET
1	A	67	GLN
1	A	143	ARG
1	B	154	ARG

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

Mol	Chain	Res	Type
1	B	87	HIS

### 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](#)

There are no chain breaks in this entry.

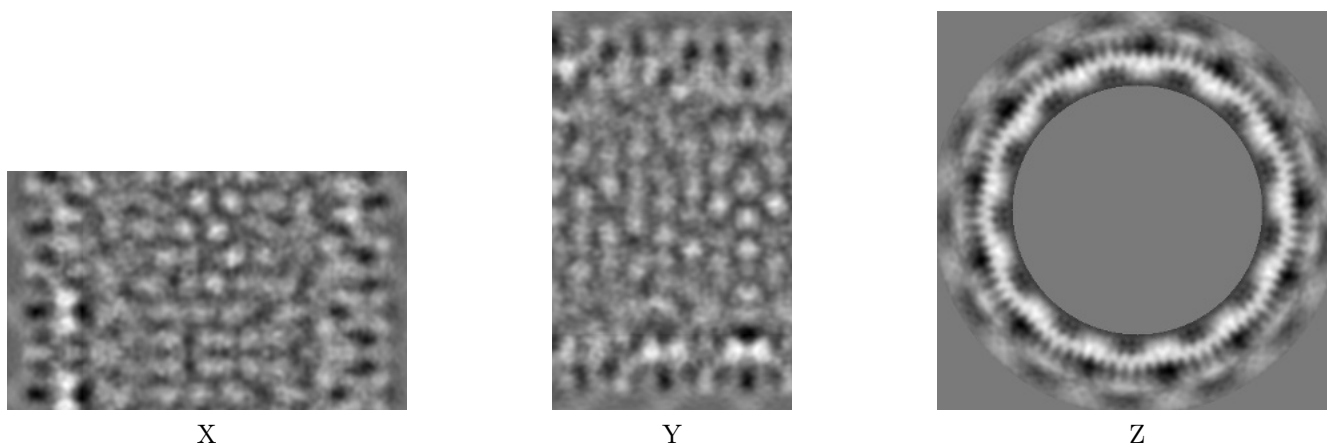
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3076. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

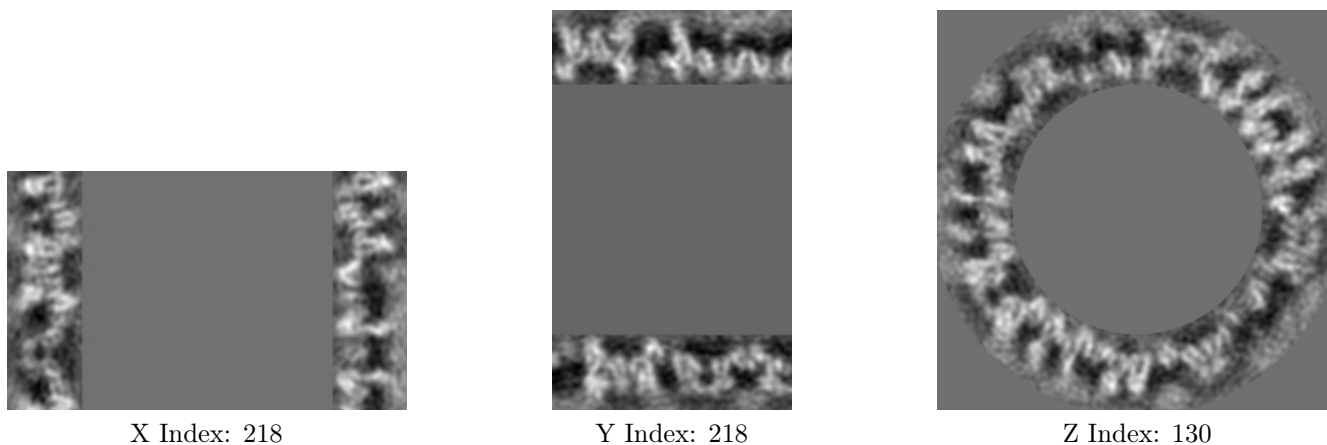
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

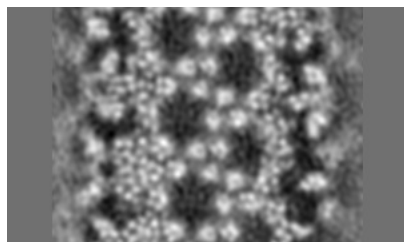
#### 6.2.1 Primary map



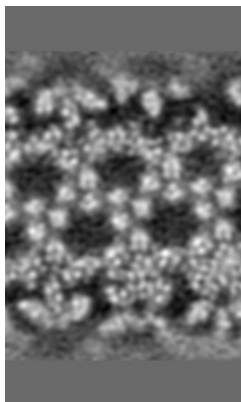
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

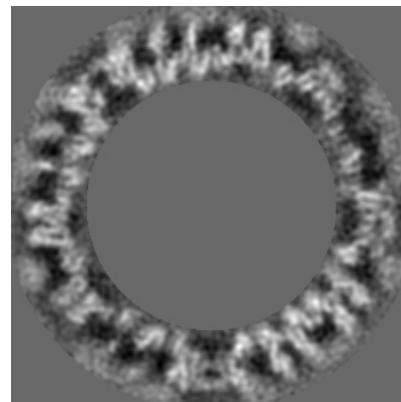
### 6.3.1 Primary map



X Index: 366



Y Index: 367

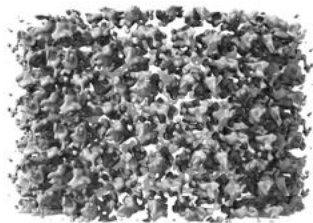


Z Index: 56

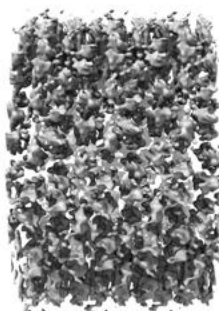
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

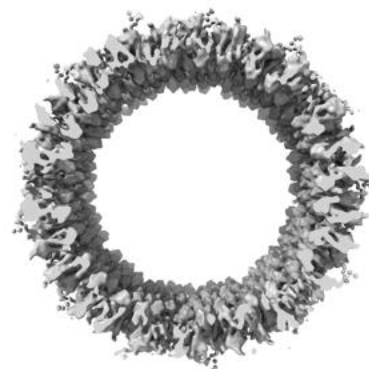
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 20.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

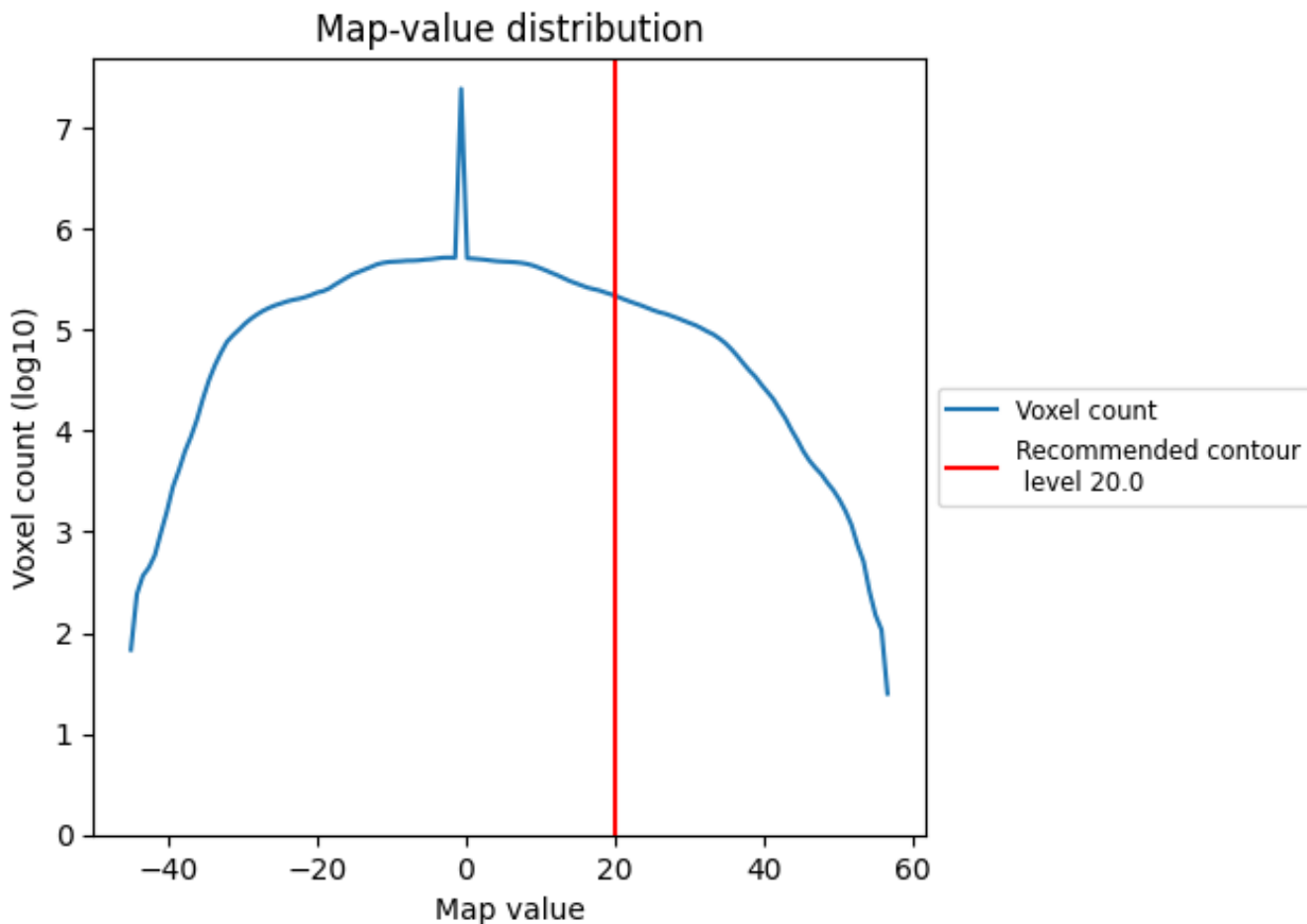
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

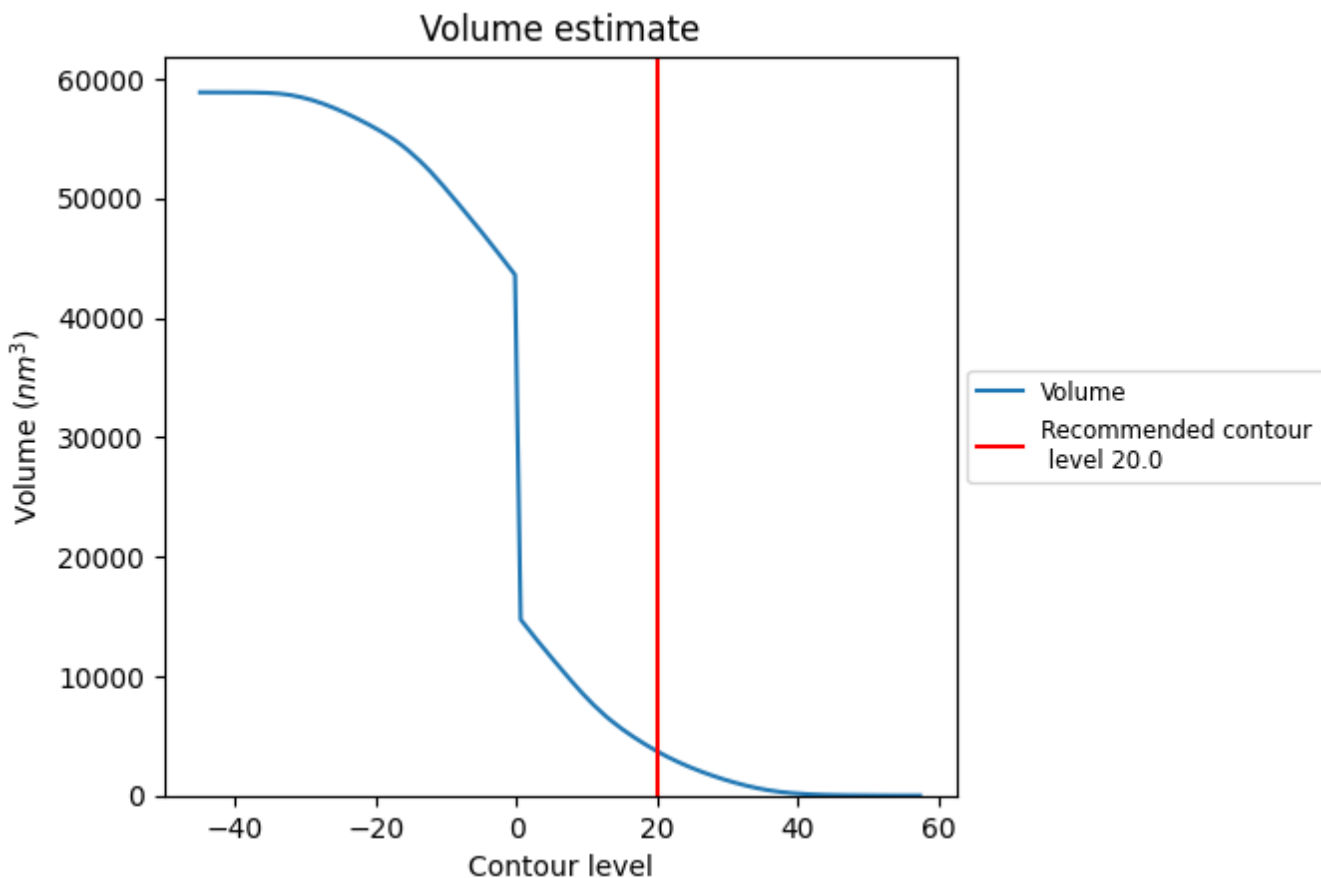
This section contains the results of statistical analysis of the map.

### 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 3713 nm<sup>3</sup>; this corresponds to an approximate mass of 3354 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

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

## 8 Fourier-Shell correlation

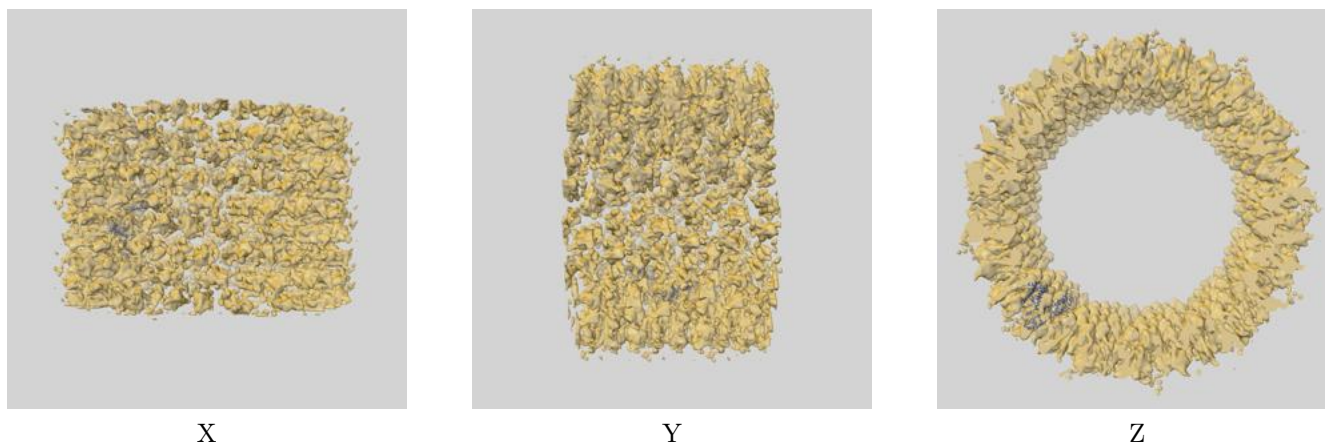
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

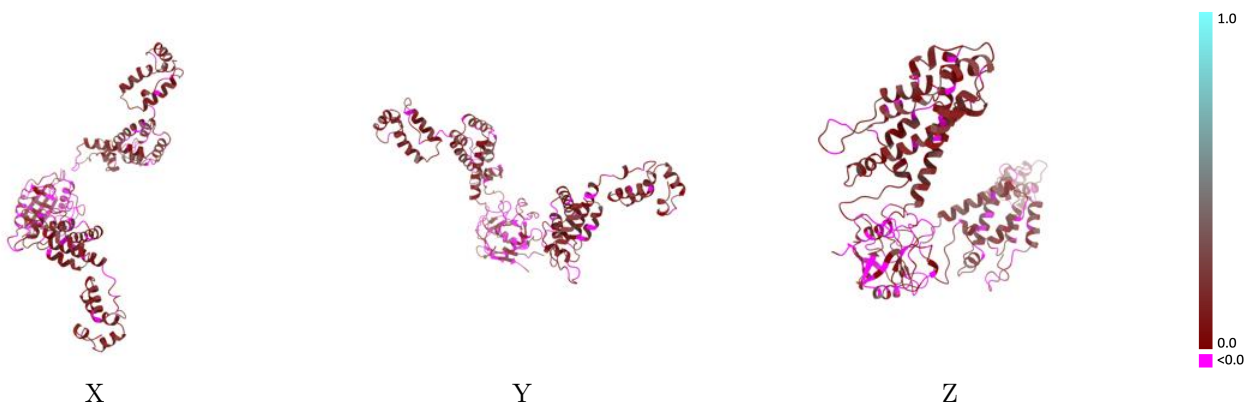
This section contains information regarding the fit between EMDB map EMD-3076 and PDB model 5FJB. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlay [i](#)



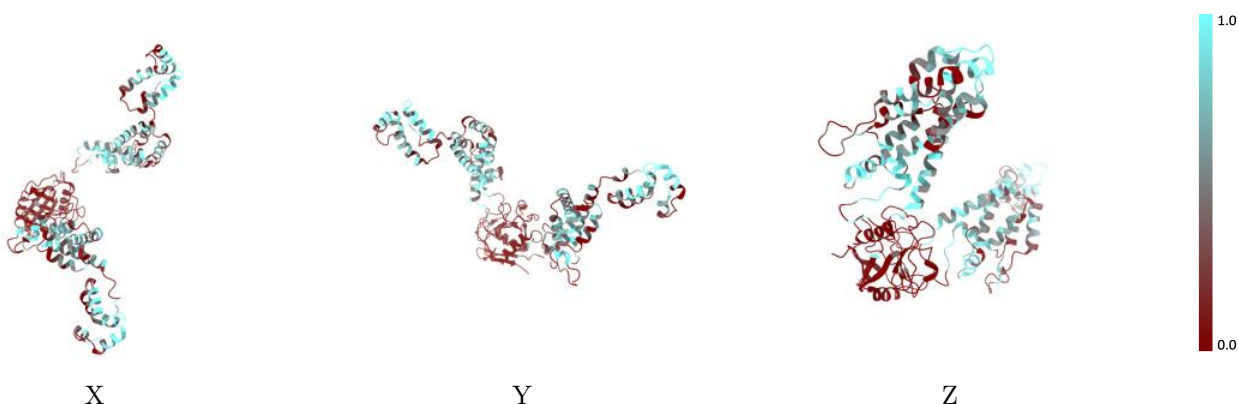
The images above show the 3D surface view of the map at the recommended contour level 20.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



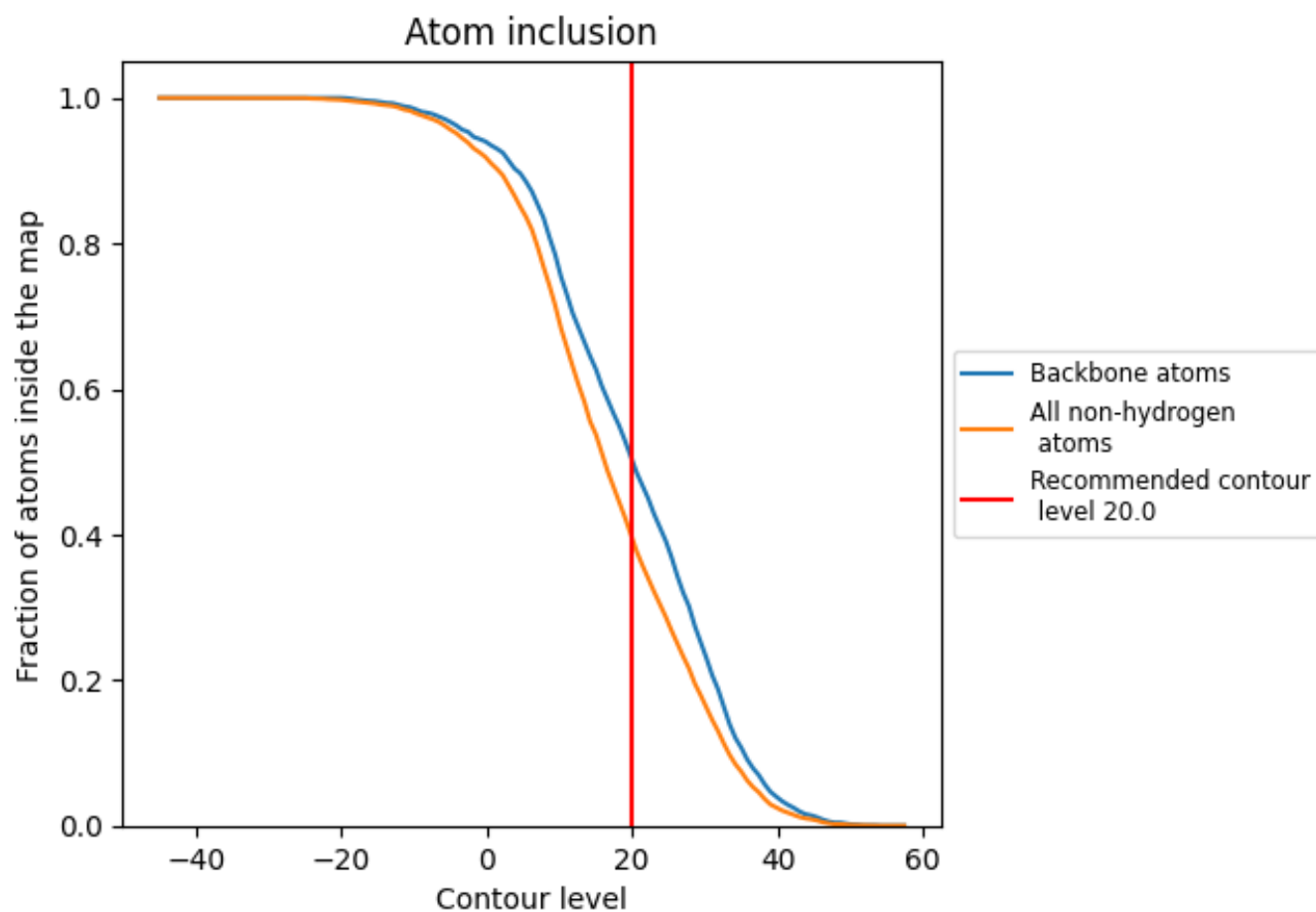
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (20.0).









## 9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 39% 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 (20.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3945	 0.1010
A	 0.5269	 0.1310
B	 0.5352	 0.1350
C	 0.0265	 0.0140

