



wwPDB EM Validation Summary Report ⓘ

Feb 12, 2024 – 08:40 PM EST

PDB ID : 3J2U
EMDB ID : EMD-5565
Title : Kinesin-13 KLP10A HD in complex with CS-tubulin and a microtubule
Authors : Asenjo, A.B.; Chatterjee, C.; Tan, D.; DePaoli, V.; Rice, W.J.; Diaz-Avalos, R.; Silvestry, M.; Sosa, H.
Deposited on : 2013-01-10
Resolution : 10.80 Å(reported)
Based on initial model : 1JFF

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.dev70
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) : 2.36

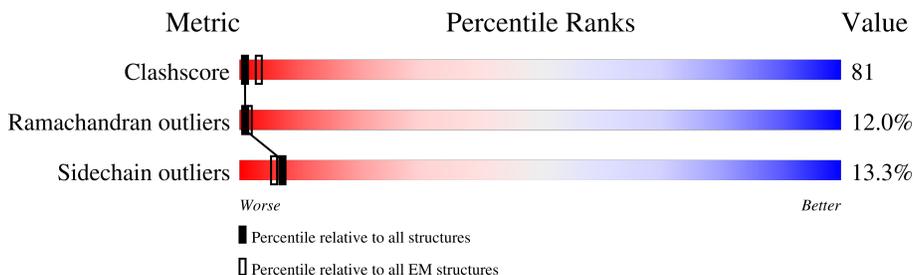
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.80 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 ≥ 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	K	374	
2	A	451	
2	C	451	
3	B	445	
3	D	445	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15575 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 Kinesin-like protein Klp10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	309	2419	1525	432	446	16	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	242	MET	-	expression tag	UNP Q960Z0
K	243	ARG	-	expression tag	UNP Q960Z0
K	244	GLY	-	expression tag	UNP Q960Z0
K	245	SER	-	expression tag	UNP Q960Z0
K	246	HIS	-	expression tag	UNP Q960Z0
K	247	HIS	-	expression tag	UNP Q960Z0
K	248	HIS	-	expression tag	UNP Q960Z0
K	249	HIS	-	expression tag	UNP Q960Z0
K	250	HIS	-	expression tag	UNP Q960Z0
K	251	HIS	-	expression tag	UNP Q960Z0
K	252	GLY	-	expression tag	UNP Q960Z0
K	253	MET	-	expression tag	UNP Q960Z0
K	254	ALA	-	expression tag	UNP Q960Z0
K	255	SER	-	expression tag	UNP Q960Z0
K	256	MET	-	expression tag	UNP Q960Z0
K	257	THR	-	expression tag	UNP Q960Z0
K	258	GLY	-	expression tag	UNP Q960Z0
K	259	GLY	-	expression tag	UNP Q960Z0
K	260	GLN	-	expression tag	UNP Q960Z0
K	261	GLN	-	expression tag	UNP Q960Z0
K	262	MET	-	expression tag	UNP Q960Z0
K	263	GLY	-	expression tag	UNP Q960Z0
K	264	ARG	-	expression tag	UNP Q960Z0
K	265	ASP	-	expression tag	UNP Q960Z0
K	266	LEU	-	expression tag	UNP Q960Z0
K	267	TYR	-	expression tag	UNP Q960Z0
K	268	ASP	-	expression tag	UNP Q960Z0
K	269	ASP	-	expression tag	UNP Q960Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	270	ASP	-	expression tag	UNP Q960Z0
K	271	ASP	-	expression tag	UNP Q960Z0
K	272	LYS	-	expression tag	UNP Q960Z0
K	273	ASP	-	expression tag	UNP Q960Z0
K	274	PRO	-	expression tag	UNP Q960Z0
K	275	SER	-	expression tag	UNP Q960Z0
K	276	SER	-	expression tag	UNP Q960Z0
K	277	ARG	-	expression tag	UNP Q960Z0
K	278	SER	-	expression tag	UNP Q960Z0

- Molecule 2 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	C	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There are 10 discrepancies between the modelled and reference sequences:

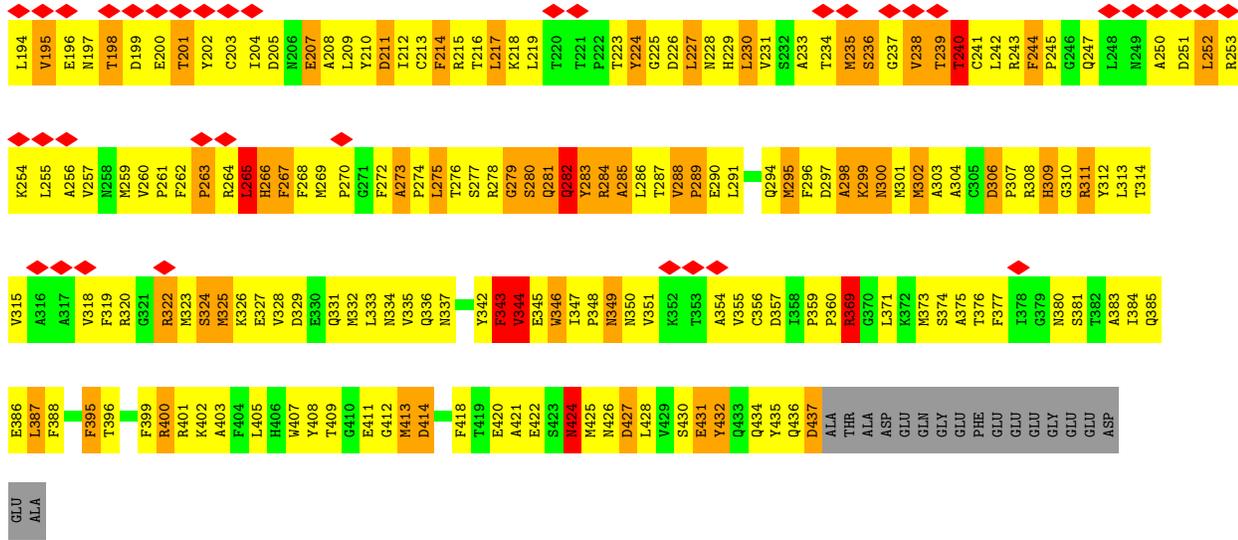
Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	conflict	UNP P81947
A	232	GLY	SER	conflict	UNP P81947
A	265	GLY	ILE	conflict	UNP P81947
A	340	THR	SER	conflict	UNP P81947
A	358	GLU	GLN	conflict	UNP P81947
C	136	SER	LEU	conflict	UNP P81947
C	232	GLY	SER	conflict	UNP P81947
C	265	GLY	ILE	conflict	UNP P81947
C	340	THR	SER	conflict	UNP P81947
C	358	GLU	GLN	conflict	UNP P81947

- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	D	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	ALA	THR	conflict	UNP Q6B856
B	172	VAL	MET	conflict	UNP Q6B856
B	298	ALA	SER	conflict	UNP Q6B856
B	318	VAL	ILE	conflict	UNP Q6B856
B	450	GLY	GLU	conflict	UNP Q6B856
B	451	GLU	GLY	conflict	UNP Q6B856
D	57	ALA	THR	conflict	UNP Q6B856
D	172	VAL	MET	conflict	UNP Q6B856
D	298	ALA	SER	conflict	UNP Q6B856
D	318	VAL	ILE	conflict	UNP Q6B856
D	450	GLY	GLU	conflict	UNP Q6B856
D	451	GLU	GLY	conflict	UNP Q6B856



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=168.087°, rise=5.553 Å, axial sym=C1	Depositor
Number of segments used	54584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each particle	Depositor
Microscope	JEOL 3200FSC, FEI TECNAI F20	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ($e^-/\text{Å}^2$)	Not provided	
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	Not provided	
Maximum map value	0.159	Depositor
Minimum map value	-0.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	580.0, 580.0, 160.0	wwPDB
Map dimensions	290, 290, 80	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2, 2, 2	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	K	0.93	0/2453	1.10	1/3290 (0.0%)
2	A	0.51	0/3300	0.73	0/4482
2	C	0.51	0/3300	0.73	0/4482
3	B	0.51	0/3426	0.76	2/4642 (0.0%)
3	D	0.51	0/3426	0.76	2/4642 (0.0%)
All	All	0.59	0/15905	0.81	5/21538 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	235	MET	CG-SD-CE	6.08	109.92	100.20
3	B	235	MET	CG-SD-CE	6.07	109.92	100.20
1	K	384	GLY	N-CA-C	-5.47	99.43	113.10
3	D	217	LEU	N-CA-C	-5.36	96.54	111.00
3	B	217	LEU	N-CA-C	-5.35	96.56	111.00

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	K	2419	0	2487	389	0
2	A	3227	0	3143	520	0
2	C	3227	0	3143	569	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3351	0	3229	563	0
3	D	3351	0	3229	568	0
All	All	15575	0	15231	2506	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 81.

The worst 5 of 2506 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:K:444:ASP:HA	3:B:419:THR:CG2	1.37	1.48
1:K:444:ASP:N	3:B:416:MET:HE1	1.26	1.43
1:K:444:ASP:N	3:B:416:MET:CE	1.87	1.37
1:K:444:ASP:CA	3:B:419:THR:CG2	2.01	1.35
2:C:407:TRP:CZ2	3:D:257:VAL:HA	1.60	1.34

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	K	303/374 (81%)	285 (94%)	12 (4%)	6 (2%)	7	38
2	A	408/451 (90%)	265 (65%)	84 (21%)	59 (14%)	0	4
2	C	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	4
3	B	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	5
3	D	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	5
All	All	1967/2166 (91%)	1364 (69%)	367 (19%)	236 (12%)	1	6

5 of 236 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	501	GLN
1	K	503	SER
1	K	506	ILE
2	A	96	LYS
2	A	97	GLU

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	K	269/323 (83%)	261 (97%)	8 (3%)	41	63
2	A	347/377 (92%)	298 (86%)	49 (14%)	3	16
2	C	347/377 (92%)	298 (86%)	49 (14%)	3	16
3	B	367/381 (96%)	308 (84%)	59 (16%)	2	13
3	D	367/381 (96%)	307 (84%)	60 (16%)	2	13
All	All	1697/1839 (92%)	1472 (87%)	225 (13%)	7	18

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	437	ASP
3	D	427	ASP
2	C	243	ARG
3	D	414	ASP
3	D	265	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	331	GLN
3	D	282	GLN
2	C	11	GLN
3	D	197	ASN
3	D	349	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

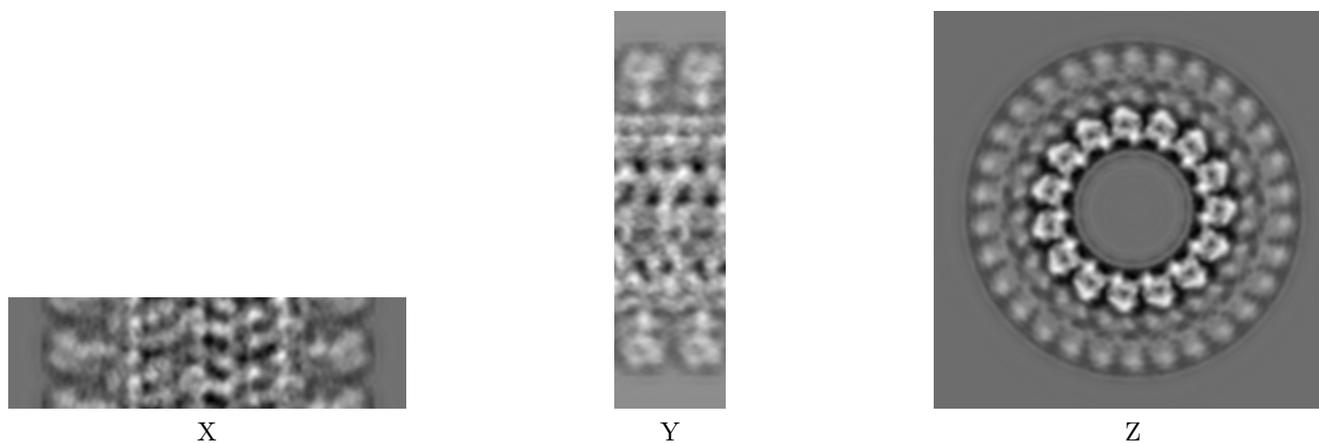
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5565. 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](#)

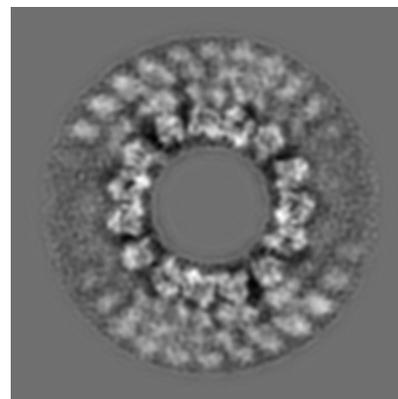
6.2.1 Primary map



X Index: 145



Y Index:
145



Z Index: 40

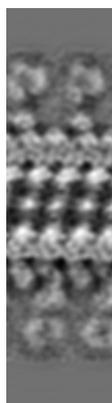
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

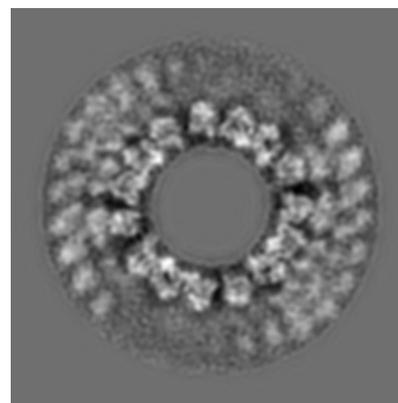
6.3.1 Primary map



X Index: 194



Y Index:
194

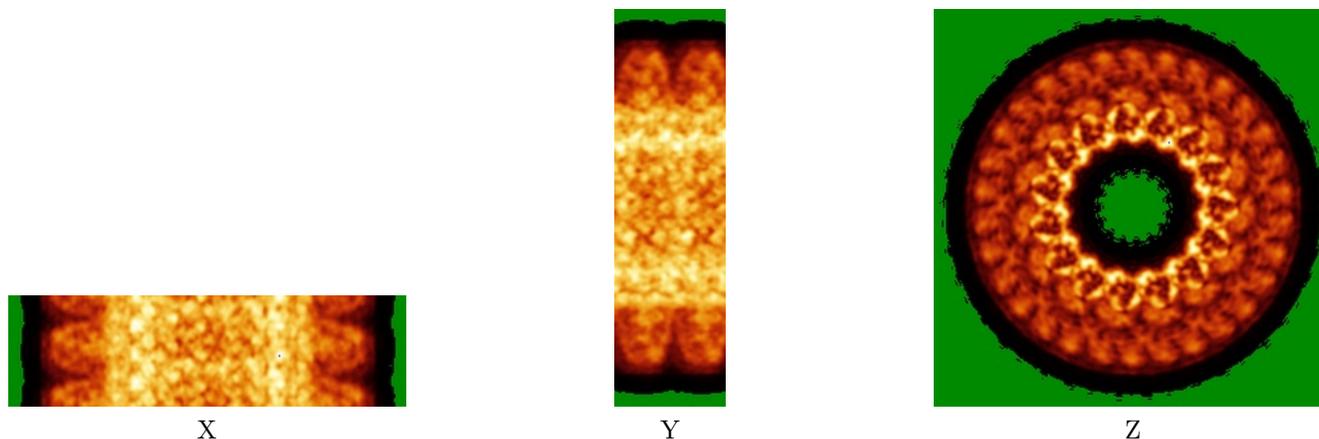


Z Index: 66

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

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

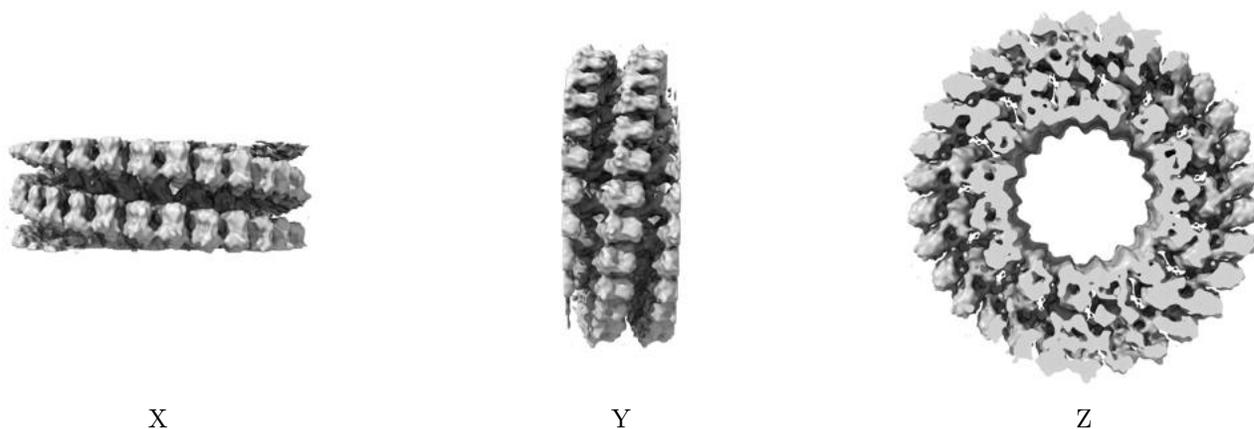
6.4.1 Primary map



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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

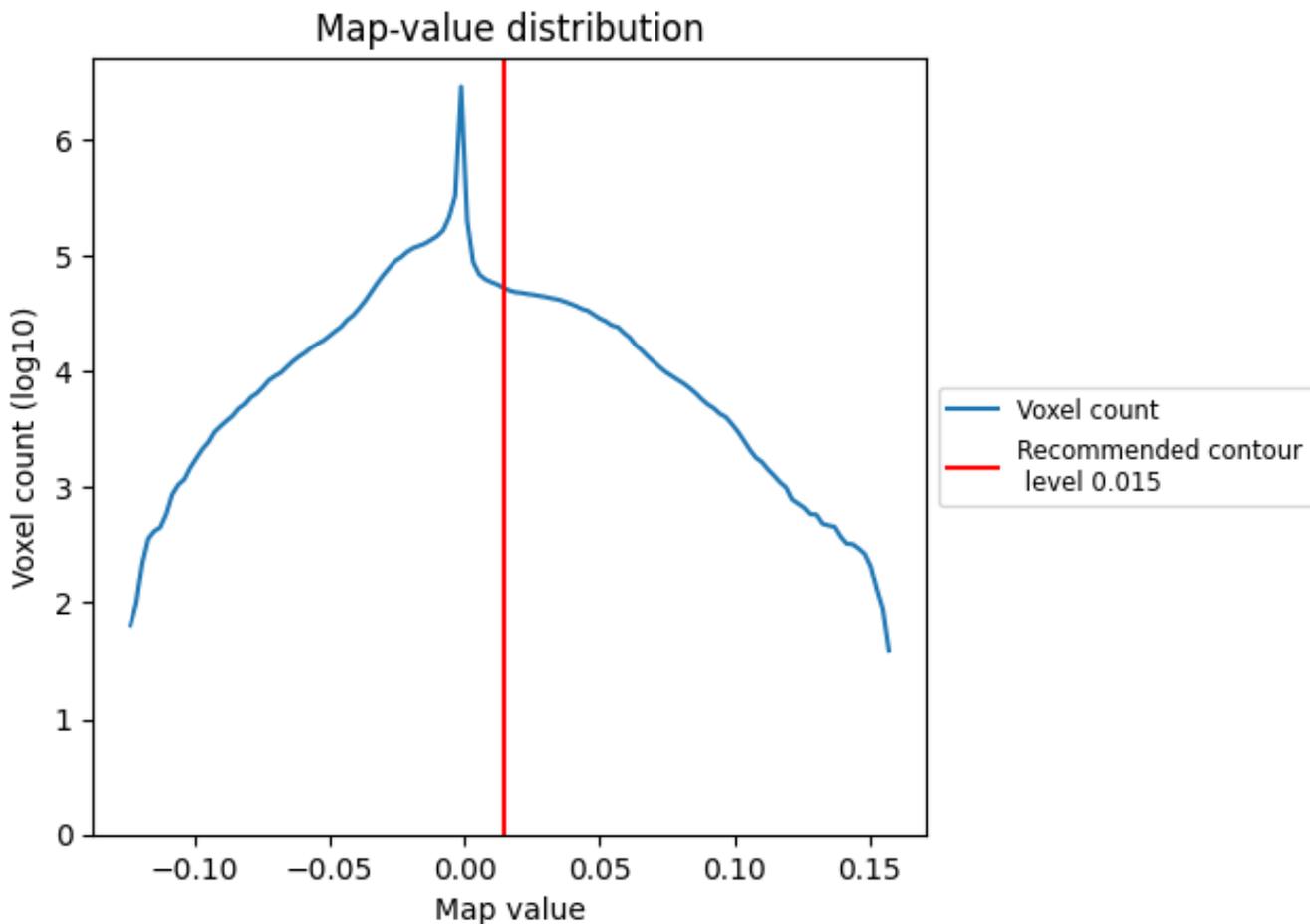
6.6 Mask visualisation

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

7 Map analysis [i](#)

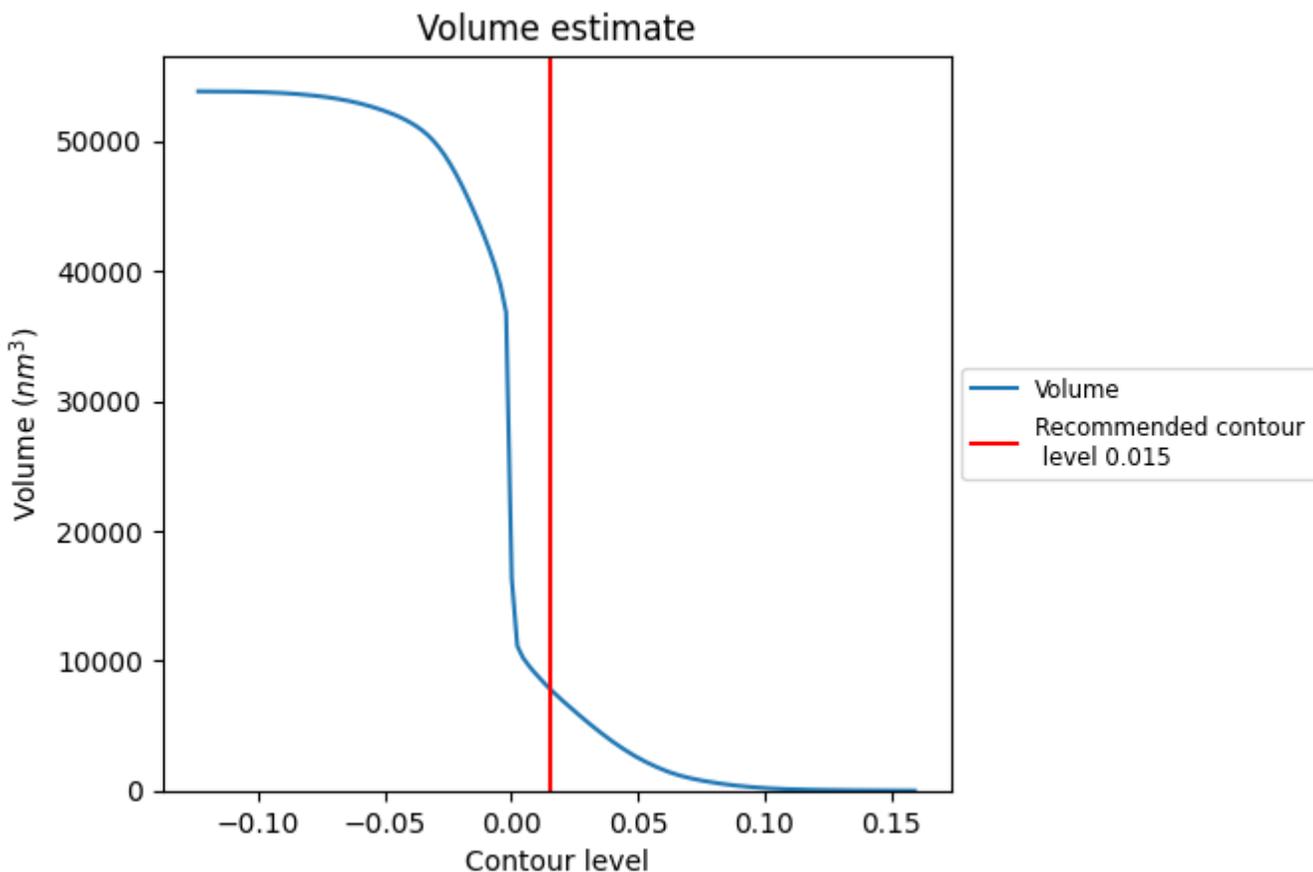
This section contains the results of statistical analysis of the map.

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 7876 nm³; this corresponds to an approximate mass of 7114 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](#)

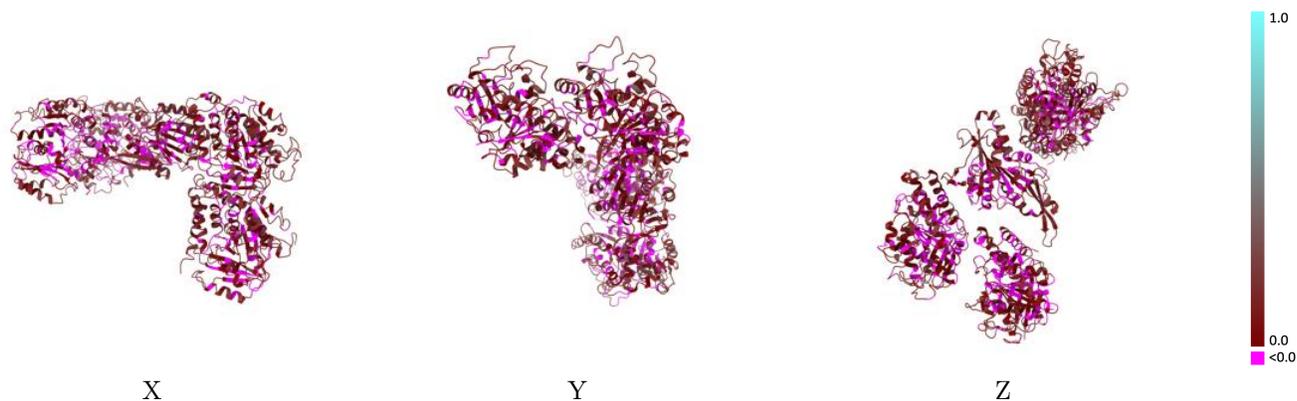
This section contains information regarding the fit between EMDB map EMD-5565 and PDB model 3J2U. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



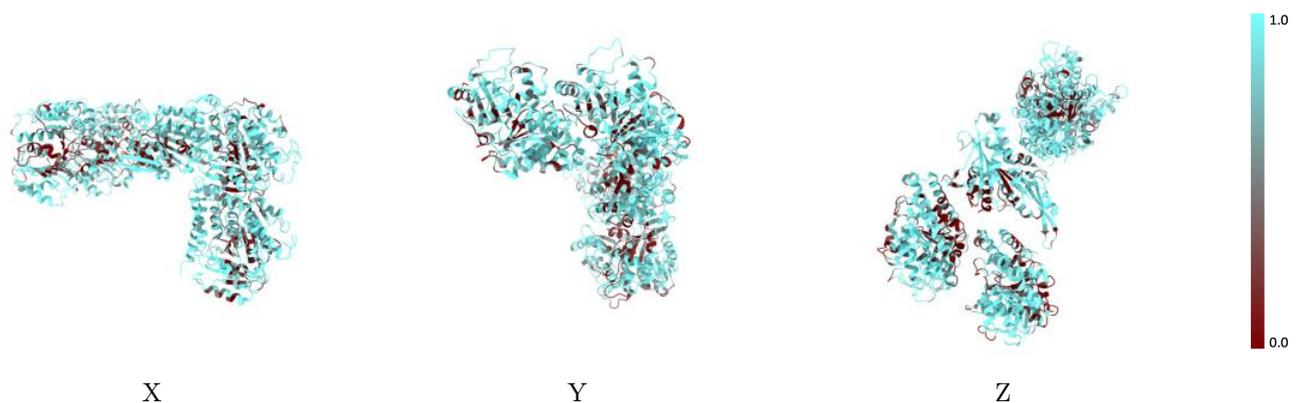
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



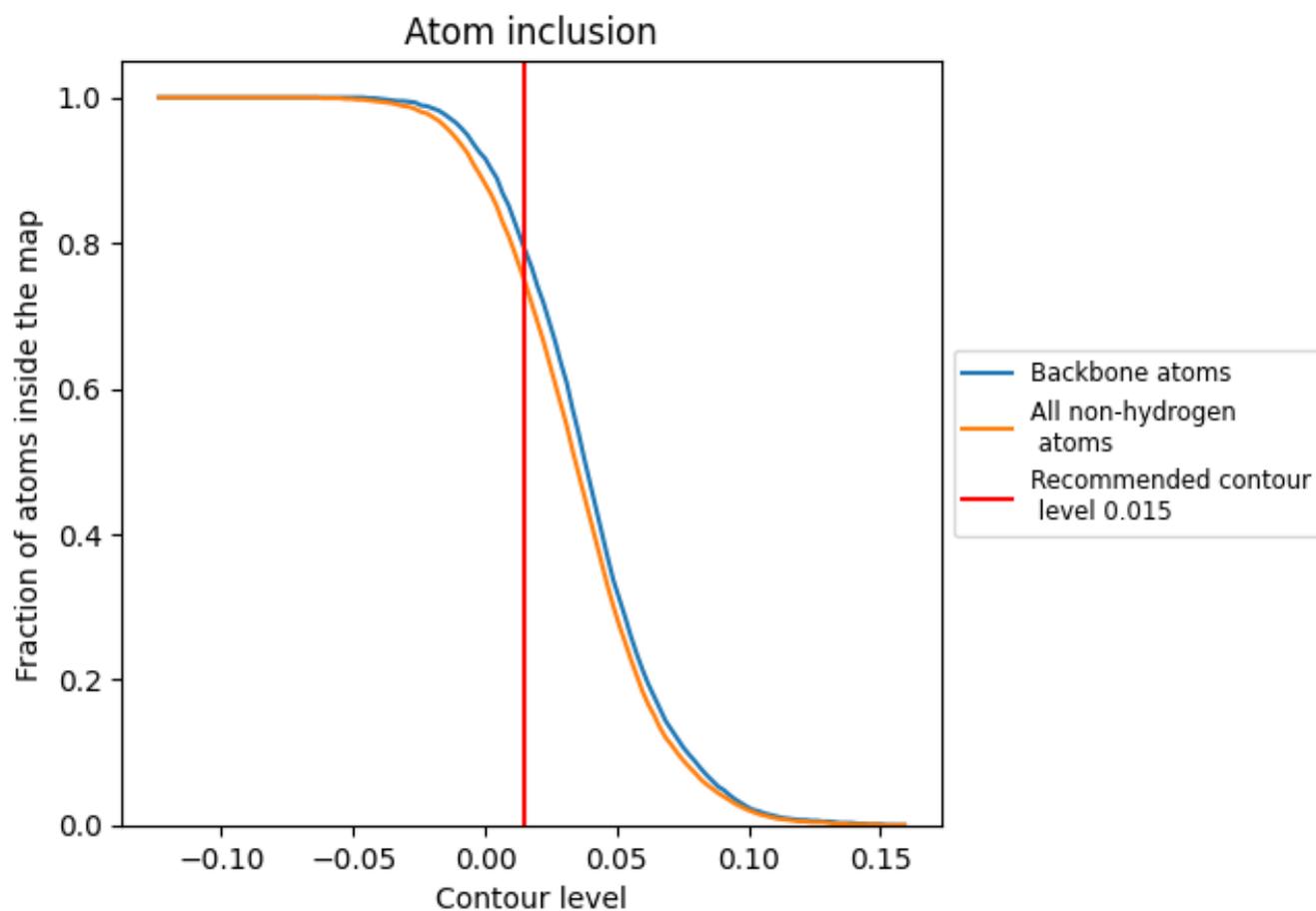
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.0710
A	 0.7060	 0.0520
B	 0.7260	 0.0560
C	 0.7840	 0.0810
D	 0.7840	 0.0910
K	 0.7340	 0.0780

