



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 04:30 pm GMT

PDB ID : 5NVS
EMDB ID : EMD-3703
Title : Human cytoplasmic dynein-1 tail in the twisted N-terminus state
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on : 2017-05-04
Resolution : 8.40 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.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) : 2.31.2

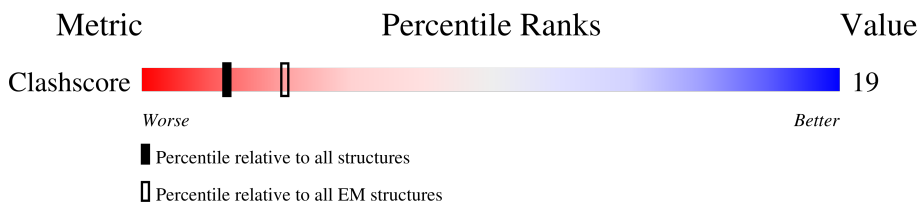
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


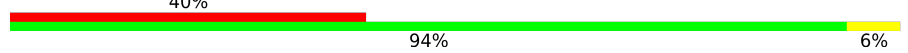
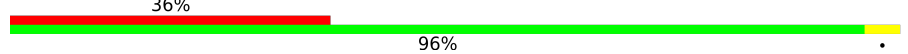

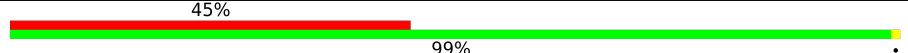



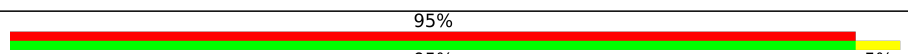
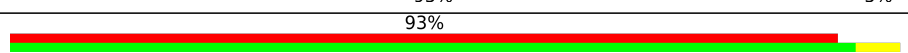
The reported resolution of this entry is 8.40 Å.

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

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	932	
2	C	350	
2	D	350	
3	B	893	
4	F	298	
5	E	295	
6	2	125	
7	1	124	
8	I	85	
8	J	85	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	K	103	100%
			92% 8%
10	L	104	99%
			91% 9%
11	M	27	100%
			100%
12	N	29	97%
			100%
13	R	120	52%
			100%
13	S	120	42%
			98%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 20072 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 dynein heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	932	4654	2790	932	932	0	0

- Molecule 2 is a protein called dynein intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	350	1723	1023	350	350	0	0
2	C	350	1723	1023	350	350	0	0

- Molecule 3 is a protein called dynein heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	B	893	4459	2673	893	893	0	0

- Molecule 4 is a protein called dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	298	1496	890	303	303	5	0

- Molecule 5 is a protein called dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	295	1459	869	295	295	0	0

- Molecule 6 is a protein called N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	2	125	Total	C	N	O	0	0
			625	375	125	125		

- Molecule 7 is a protein called N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	1	124	Total	C	N	O	0	0
			620	372	124	124		

- Molecule 8 is a protein called LC8.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	85	Total	C	N	O	0	0
			421	251	85	85		
8	J	85	Total	C	N	O	0	0
			421	251	85	85		

- Molecule 9 is a protein called Tctex.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	103	Total	C	N	O	0	0
			507	301	103	103		

- Molecule 10 is a protein called Tctex.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	104	Total	C	N	O	0	0
			513	305	104	104		

- Molecule 11 is a protein called intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	27	Total	C	N	O	0	0
			134	80	27	27		

- Molecule 12 is a protein called intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	N	29	Total	C	N	O	0	0
			143	85	29	29		

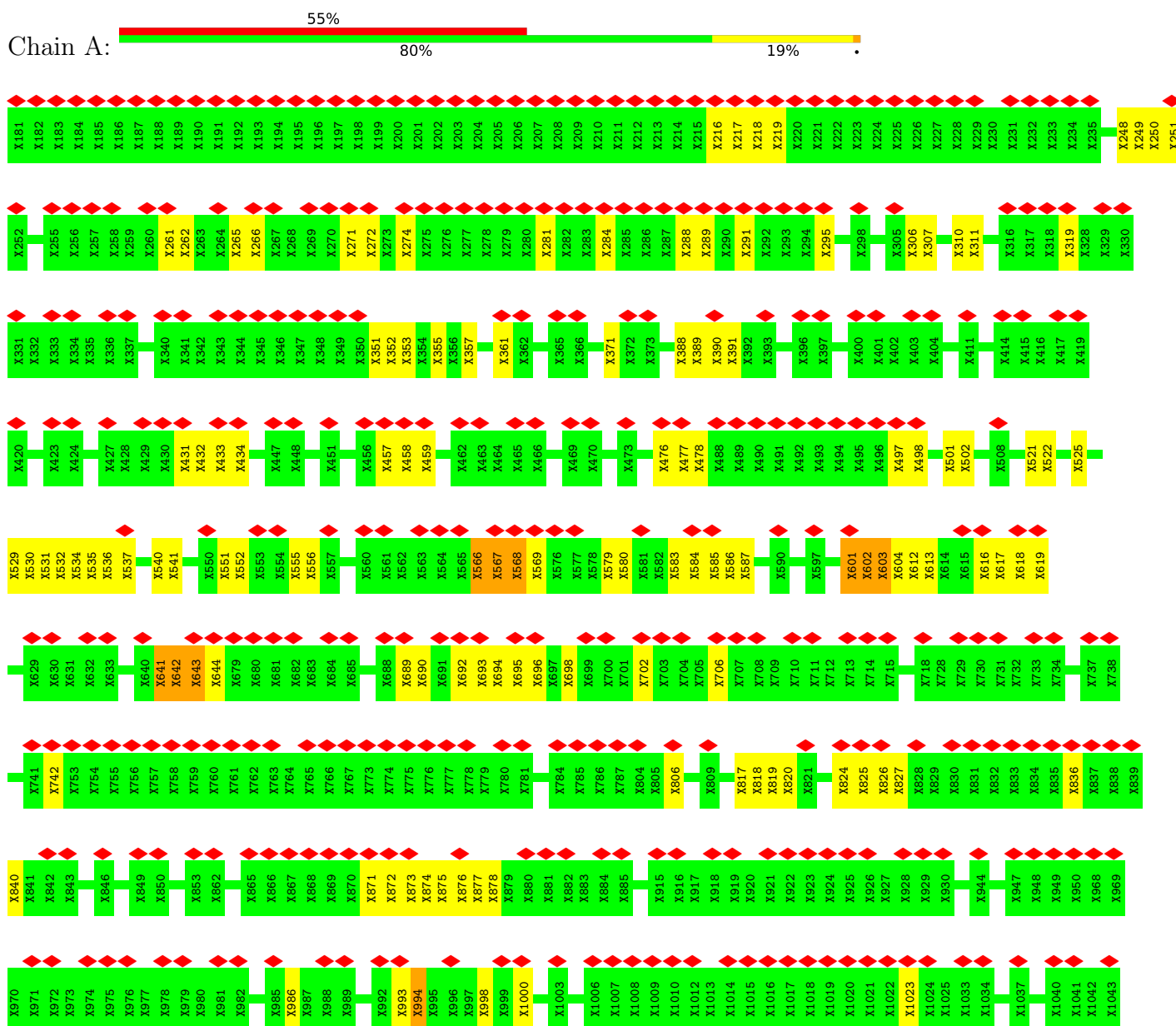
- Molecule 13 is a protein called Robl.

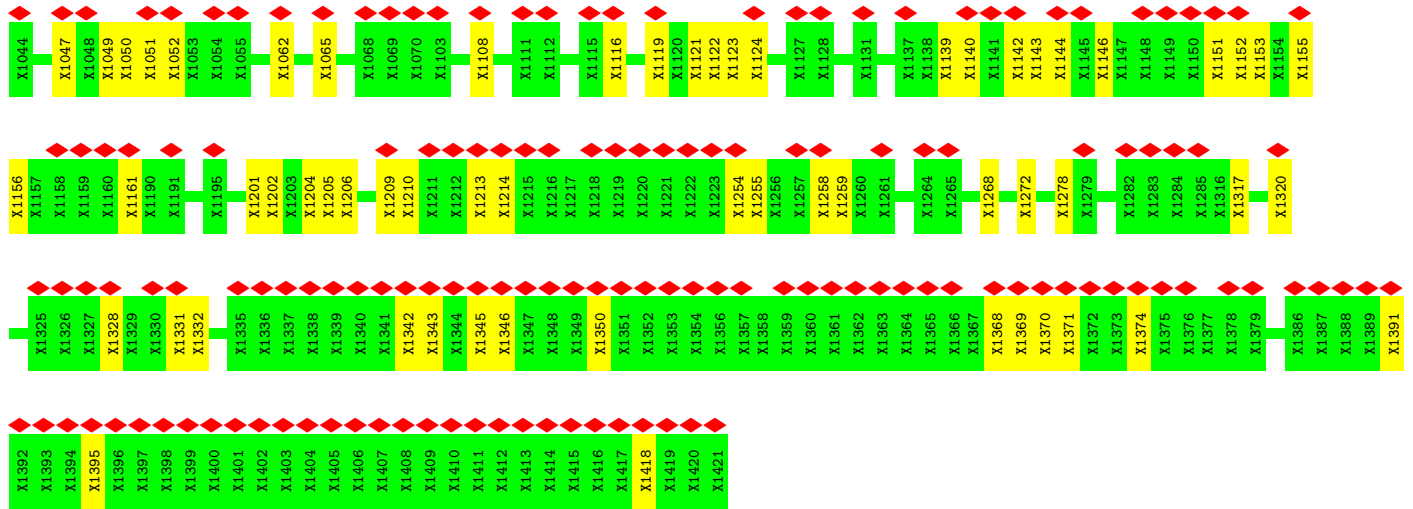
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	R	120	587	347	120	120	0	0
13	S	120	587	347	120	120	0	0

3 Residue-property plots

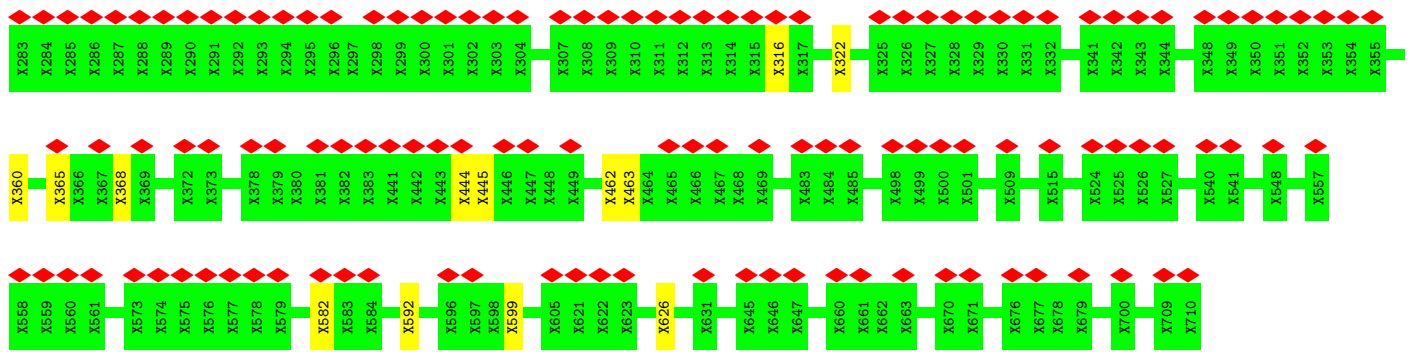
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

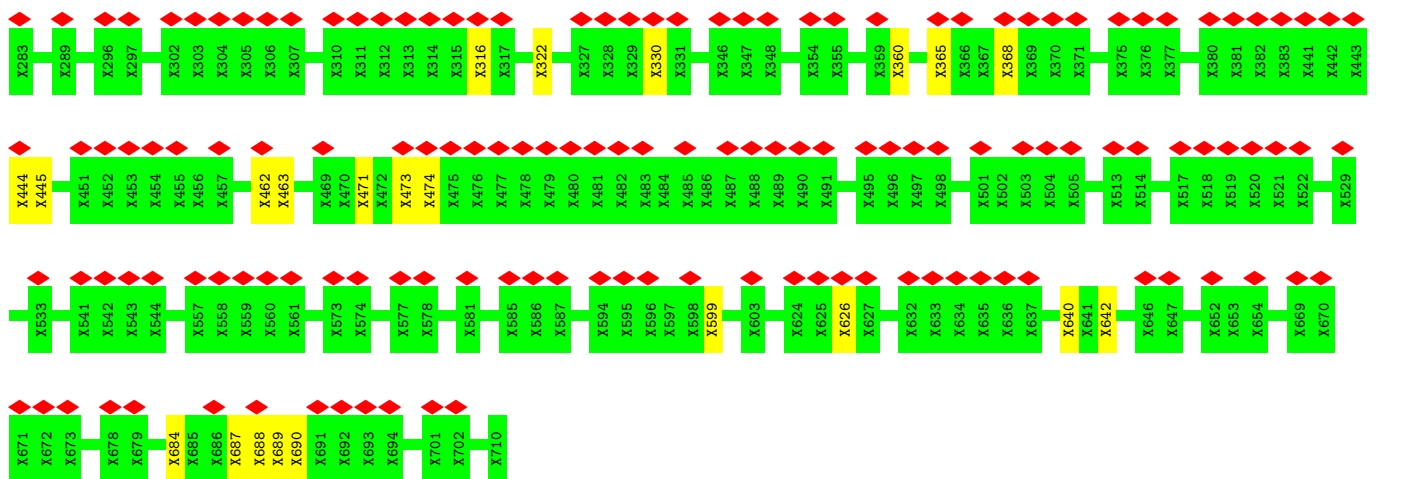
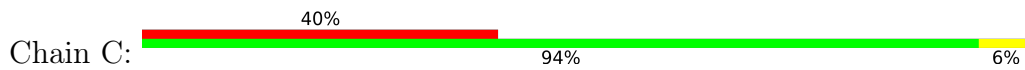




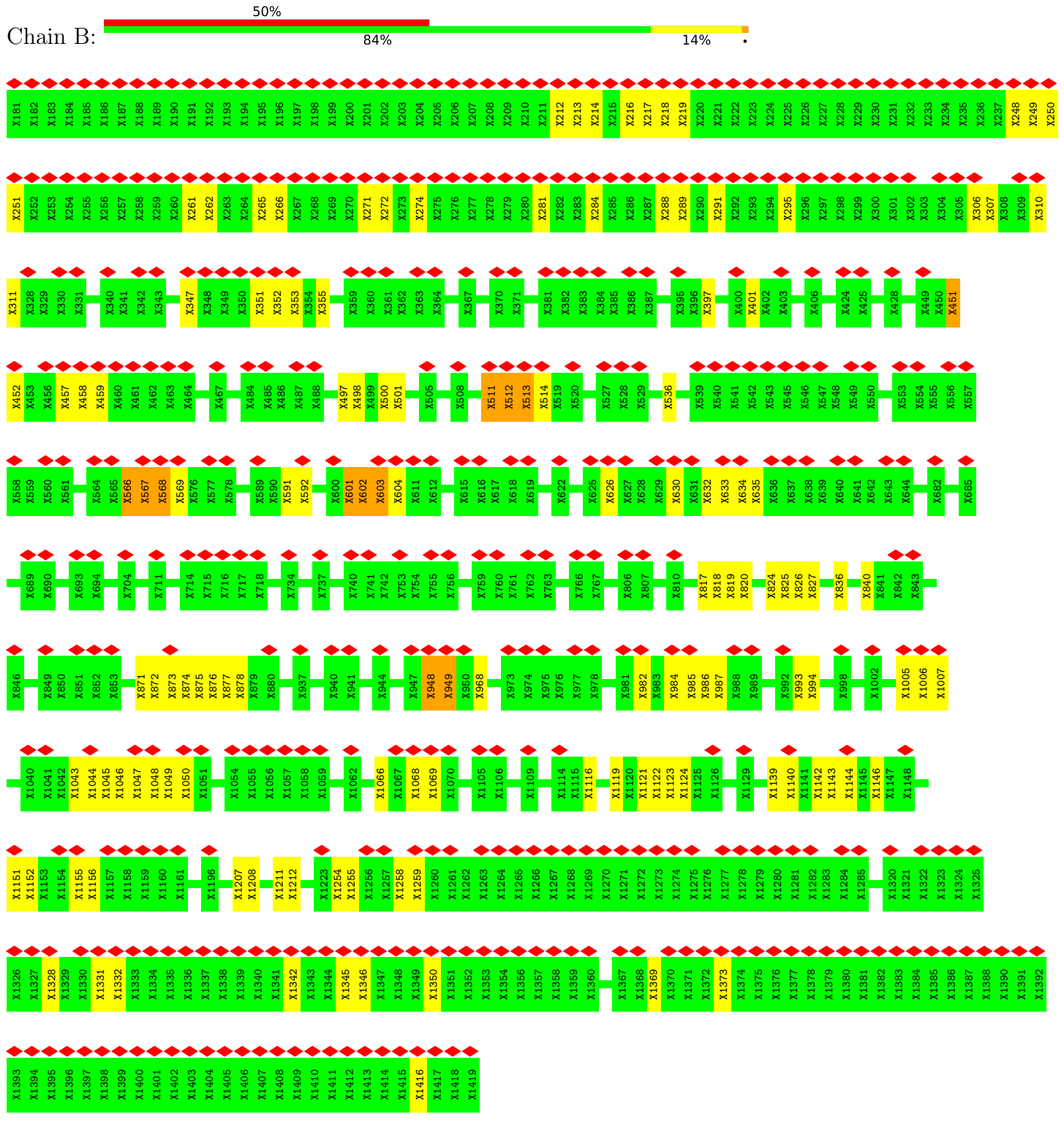
• Molecule 2: dynein intermediate chain



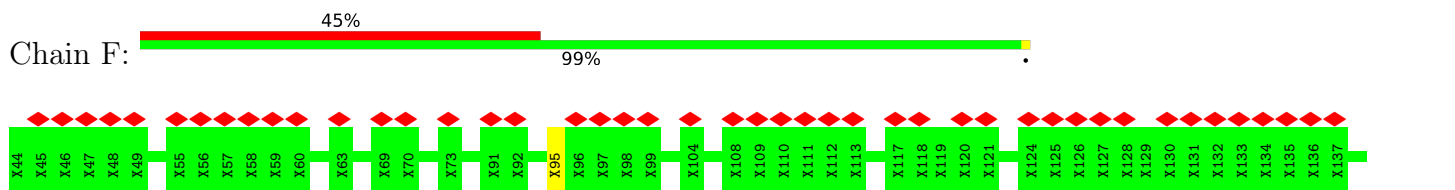
• Molecule 2: dynein intermediate chain

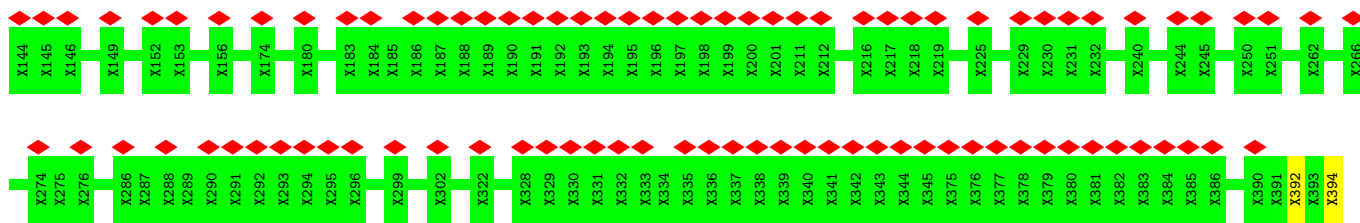


• Molecule 3: dynein heavy chain

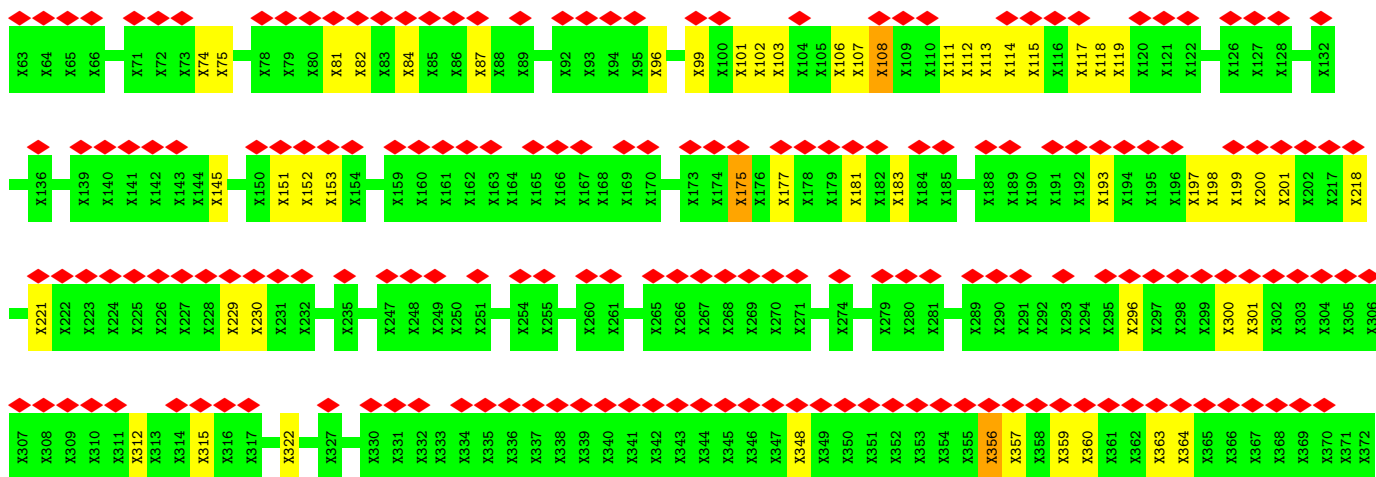
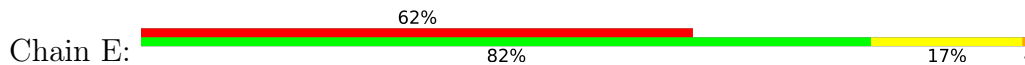


• Molecule 4: dynein light intermediate chain

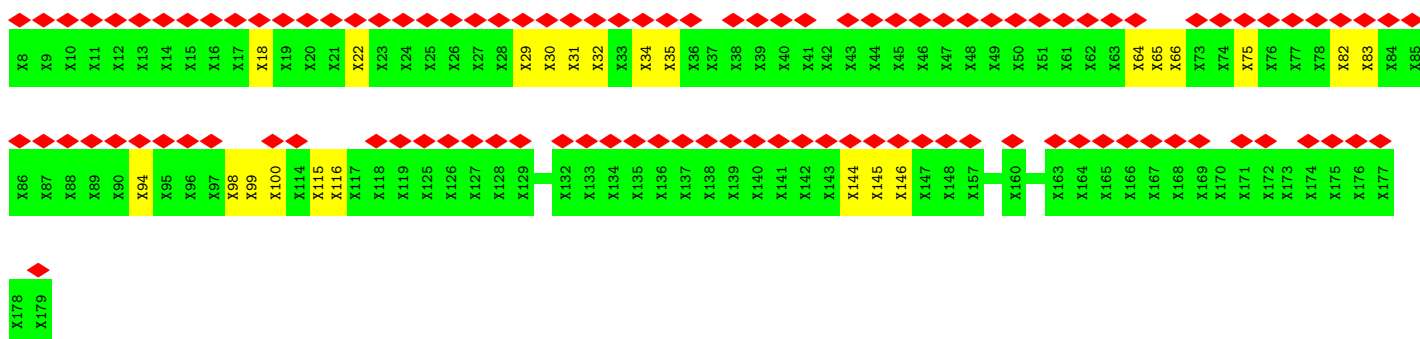
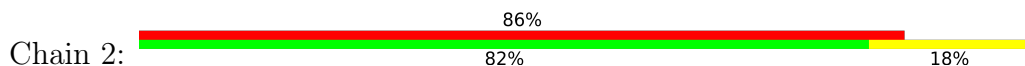




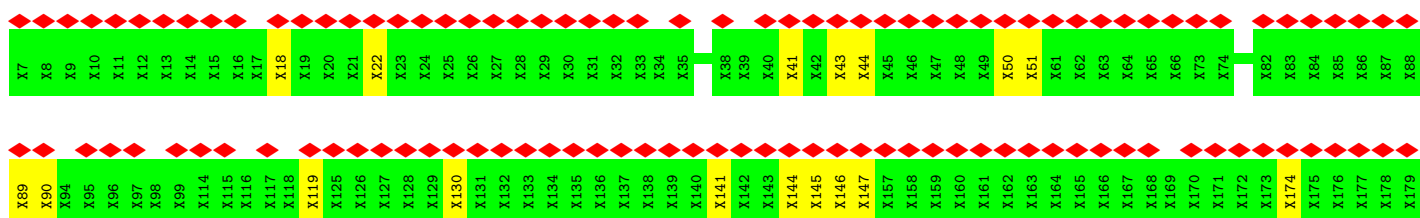
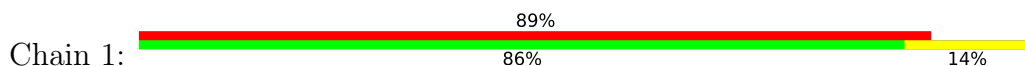
• Molecule 5: dynein light intermediate chain



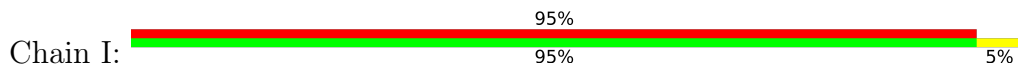
• Molecule 6: N-terminal dimerization domain



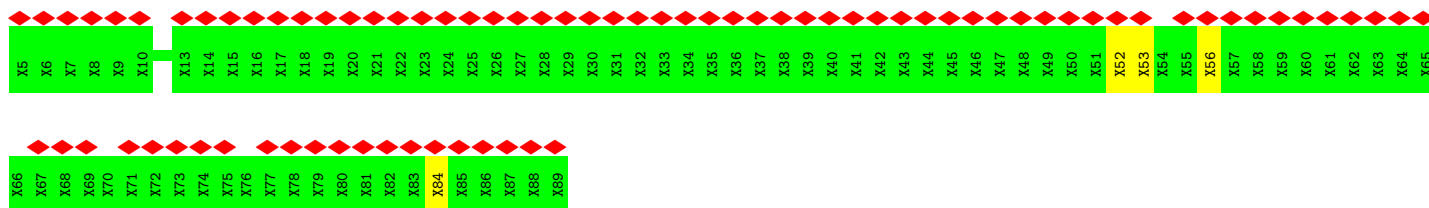
• Molecule 7: N-terminal dimerization domain



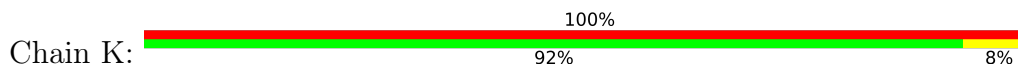
• Molecule 8: LC8



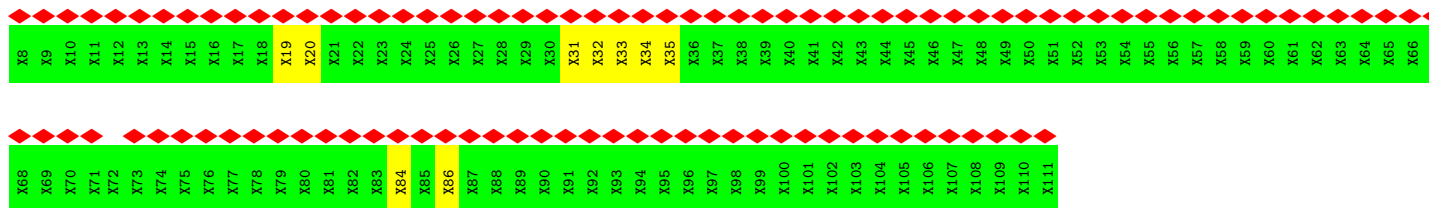
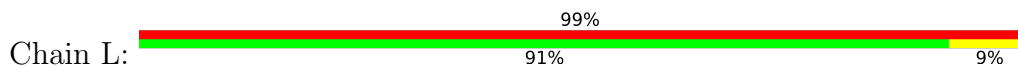
• Molecule 8: LC8



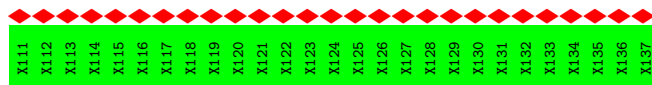
• Molecule 9: Tctex



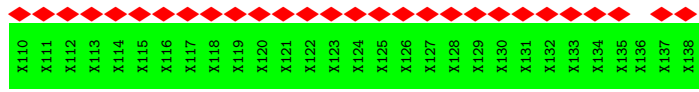
• Molecule 10: Tctex



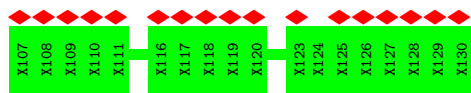
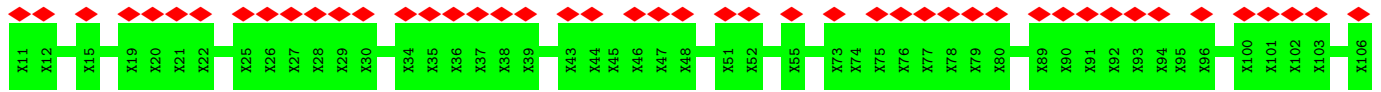
• Molecule 11: intermediate chain



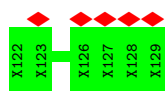
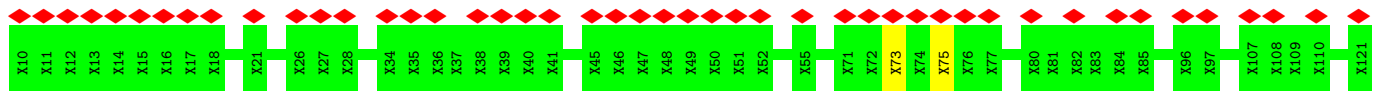
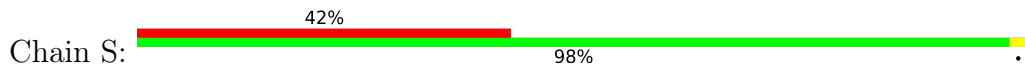
• Molecule 12: intermediate chain



• Molecule 13: Robl



• Molecule 13: Robl



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	187830	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 ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.241	Depositor
Minimum map value	-0.809	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.64, 2.64, 2.64	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	11
3	B	0	13
5	E	0	8
All	All	0	32

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	477	UNK	Mainchain
1	A	566	UNK	Mainchain
1	A	567	UNK	Mainchain
1	A	568	UNK	Mainchain
1	A	601	UNK	Mainchain

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	4654	0	984	213	0
2	C	1723	0	358	48	0
2	D	1723	0	360	9	0
3	B	4459	0	953	134	0
4	F	1496	0	300	2	0
5	E	1459	0	295	49	0
6	2	625	0	147	18	0
7	1	620	0	142	17	0
8	I	421	0	94	2	0
8	J	421	0	95	2	0
9	K	507	0	108	6	0
10	L	513	0	112	6	0
11	M	134	0	30	0	0
12	N	143	0	31	0	0
13	R	587	0	113	0	0
13	S	587	0	114	2	0
All	All	20072	0	4236	466	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 19.

The worst 5 of 466 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)
5:E:81:UNK:C	5:E:87:UNK:CB	1.85	1.54
1:A:497:UNK:O	1:A:501:UNK:CB	1.66	1.43
6:2:31:UNK:CB	6:2:34:UNK:CB	2.01	1.38
1:A:1161:UNK:O	1:A:1317:UNK:CA	1.72	1.35
3:B:817:UNK:O	3:B:819:UNK:N	1.58	1.33

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	28
1	A	27
6	2	7
7	1	7
4	F	3
2	D	3
2	C	3
5	E	3

The worst 5 of 81 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1161:UNK	C	1190:UNK	N	65.65
1	B	1161:UNK	C	1190:UNK	N	65.10
1	A	1354:UNK	C	1356:UNK	N	52.82
1	B	1354:UNK	C	1356:UNK	N	52.47

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1389:UNK	C	1391:UNK	N	50.96

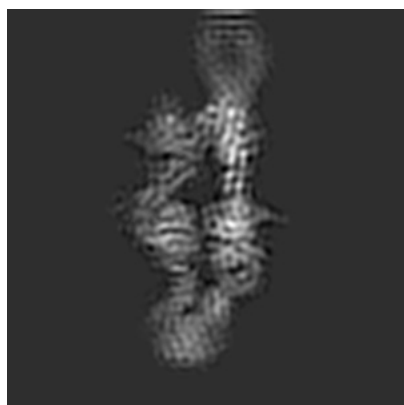
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3703. These allow visual inspection of the internal detail of the map and identification of artifacts.

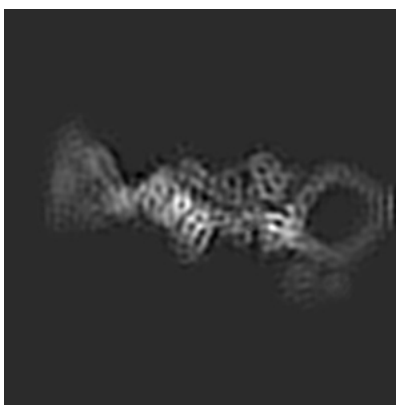
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

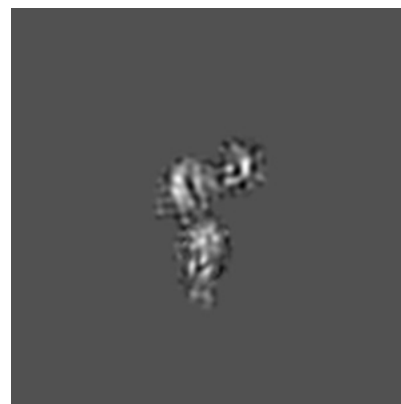
6.2.1 Primary map



X Index: 72



Y Index: 72

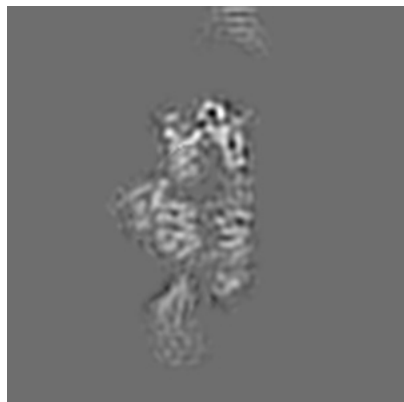


Z Index: 72

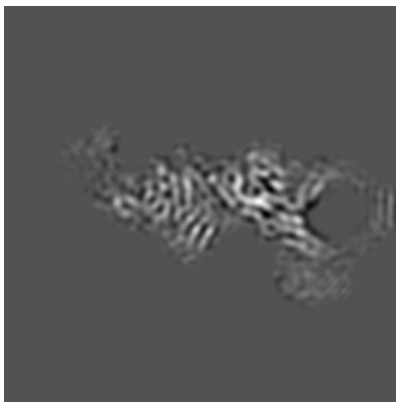
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 69



Y Index: 80



Z Index: 98

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

6.4 Orthogonal surface views [i](#)

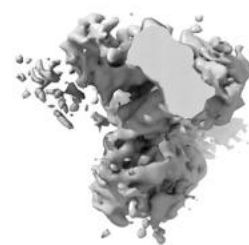
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

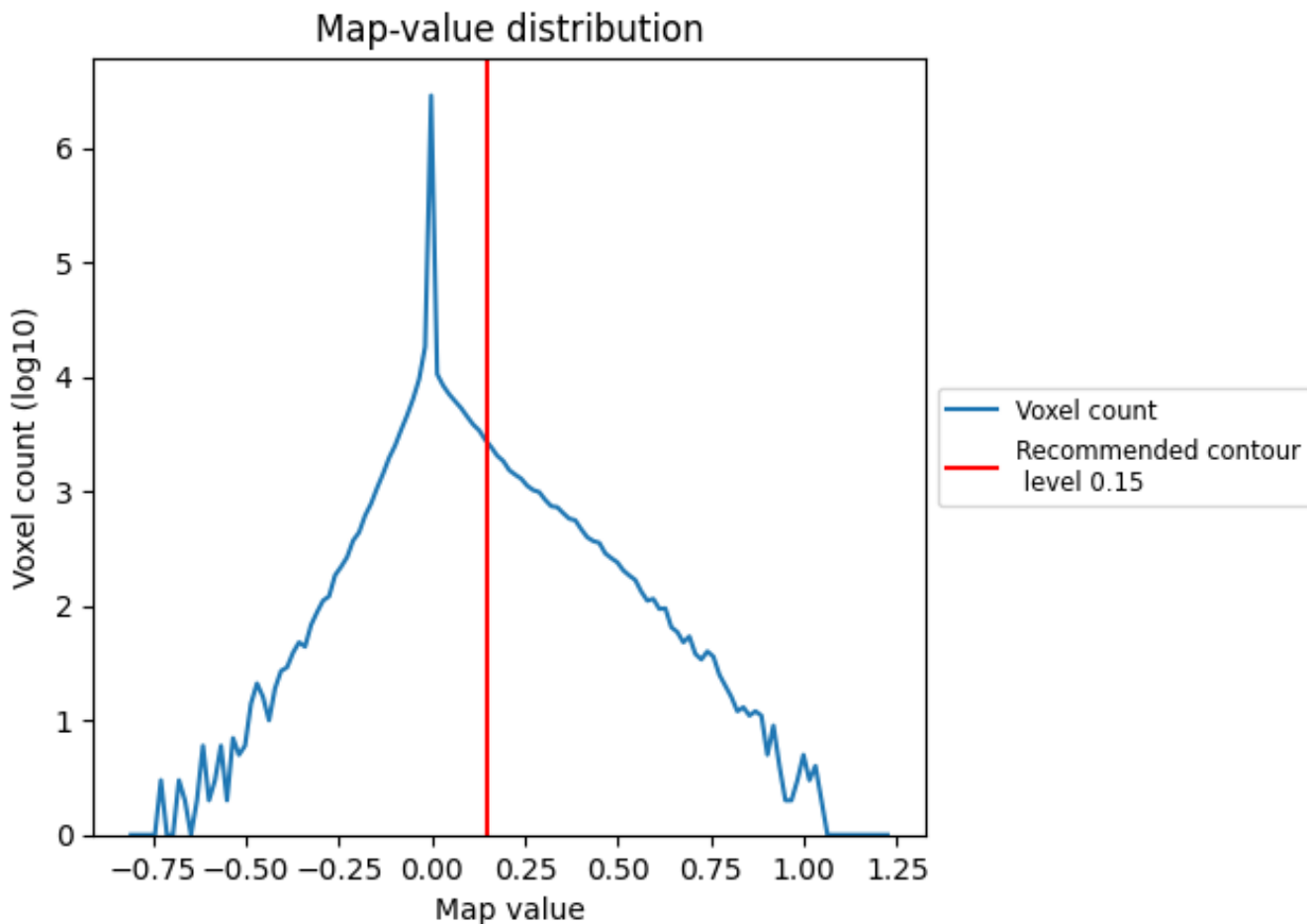
6.5 Mask visualisation

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

7 Map analysis [i](#)

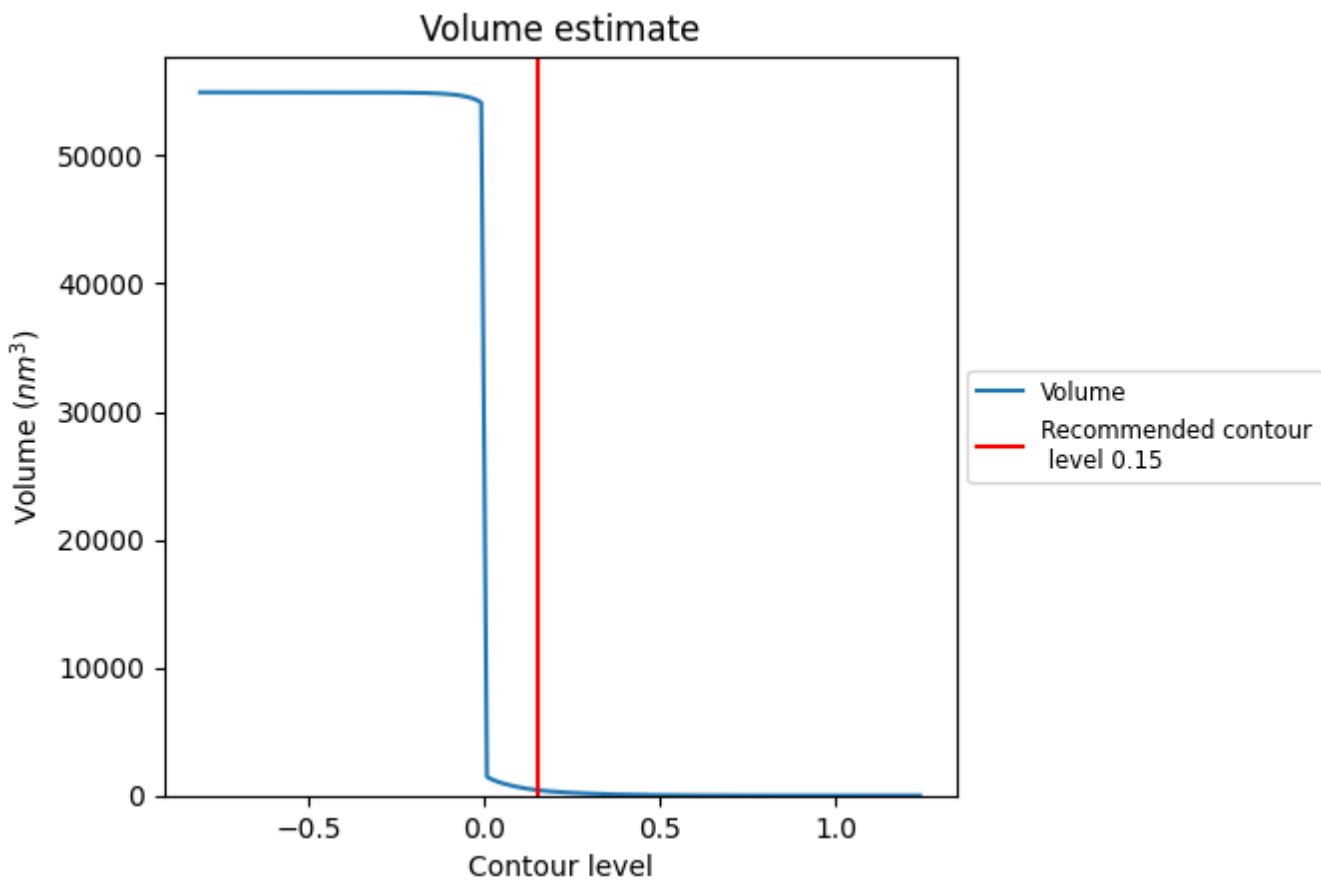
This section contains the results of statistical analysis of the map.

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.

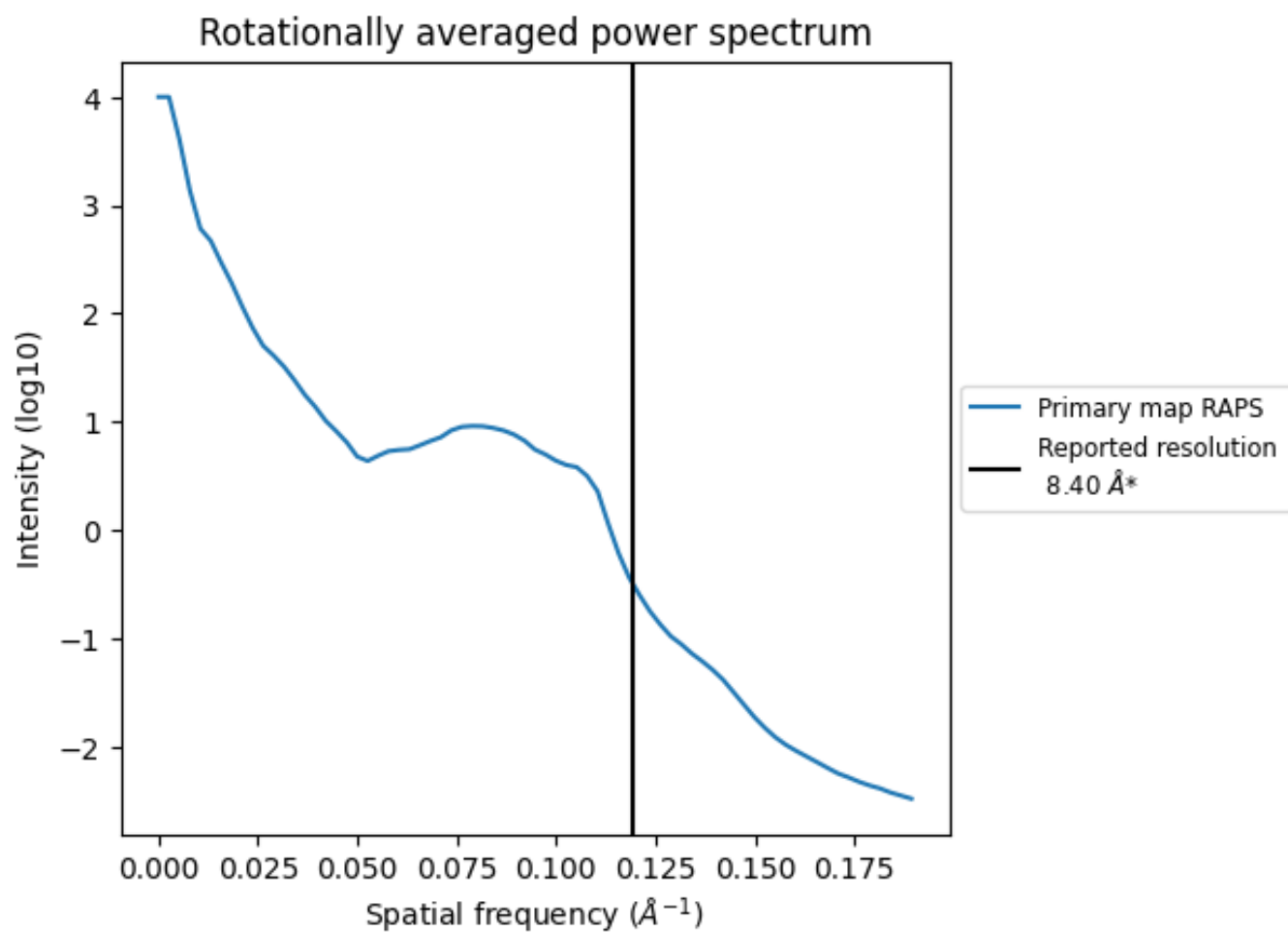
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431 nm³; this corresponds to an approximate mass of 389 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

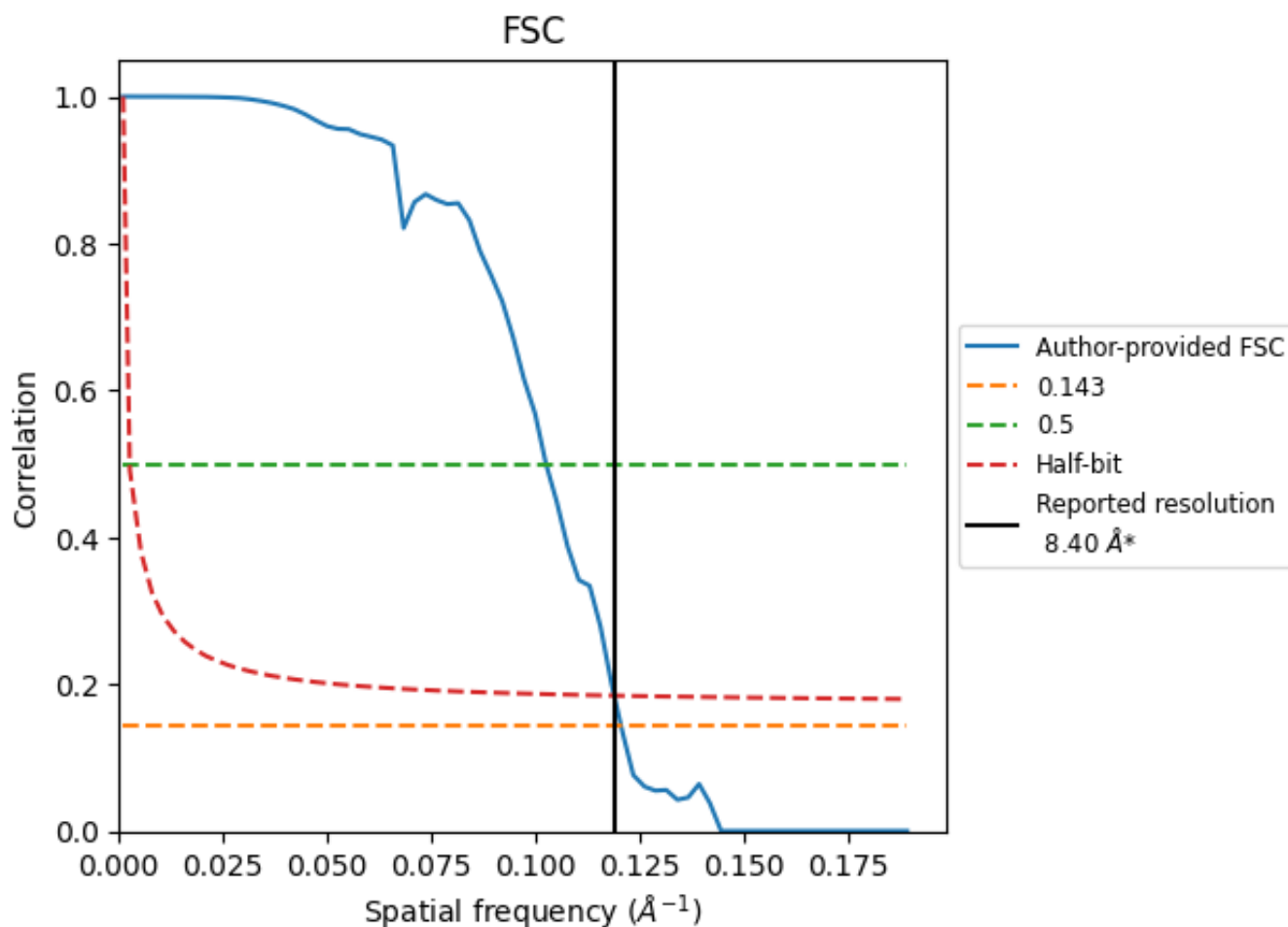


*Reported resolution corresponds to spatial frequency of 0.119 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.119 Å⁻¹

8.2 Resolution estimates [i](#)

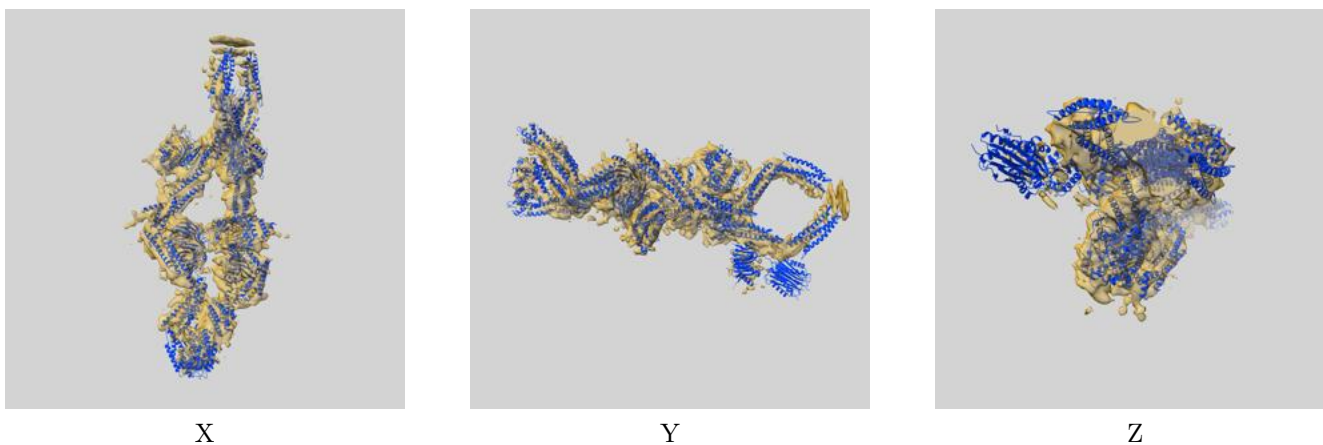
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.40	-	-
Author-provided FSC curve	8.29	9.75	8.40
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

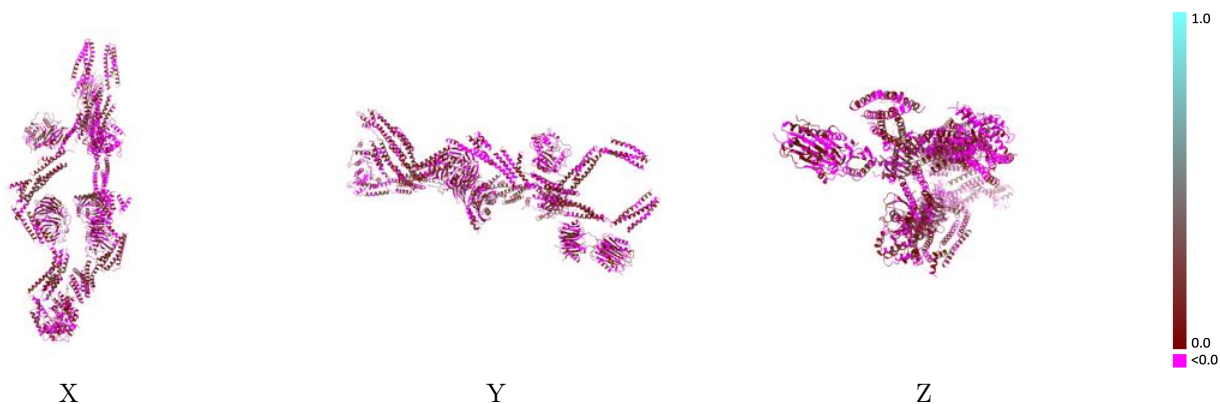
This section contains information regarding the fit between EMDB map EMD-3703 and PDB model 5NVS. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



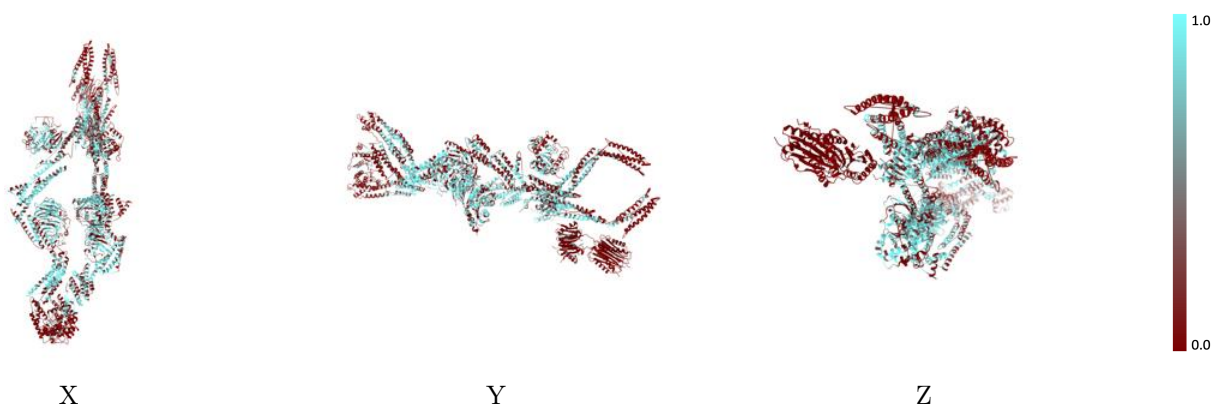
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



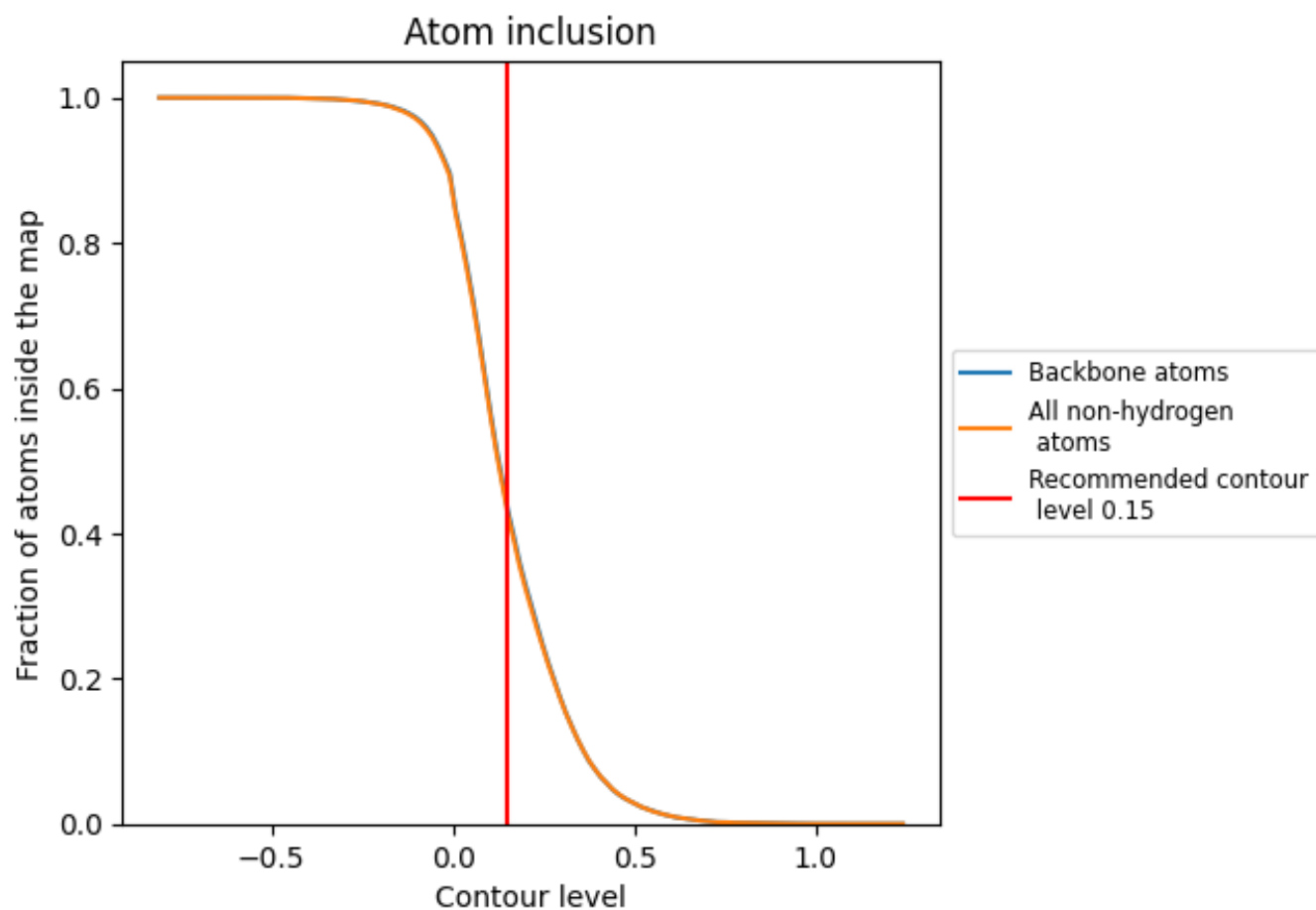
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 43% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4308	 0.0280
1	 0.1194	 0.0210
2	 0.1616	 -0.0390
A	 0.4557	 0.0290
B	 0.4925	 0.0560
C	 0.5920	 0.0050
D	 0.6193	 0.0440
E	 0.3838	 -0.0410
F	 0.5432	 0.0620
I	 0.0808	 -0.0010
J	 0.0974	 0.0210
K	 0.0000	 -0.0400
L	 0.0058	 0.0140
M	 0.0000	 0.0160
N	 0.0420	 -0.0100
R	 0.4770	 0.0180
S	 0.5690	 0.0900

