



## wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 07:34 AM EST

PDB ID : 7KZN  
EMDB ID : EMD-23083  
Title : Outer dynein arm core subcomplex from *C. reinhardtii*  
Authors : Walton, T.; Wu, H.; Brown, A.B.  
Deposited on : 2020-12-10  
Resolution : 4.00 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](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) : 2.31.2

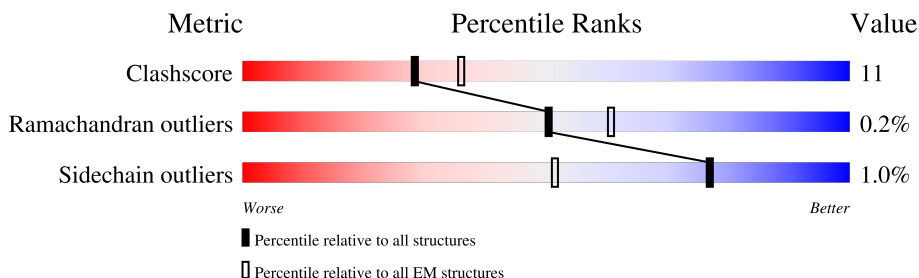
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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.




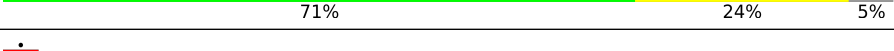
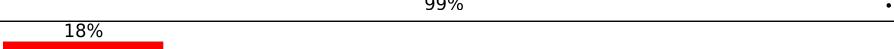
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4503	
2	B	4568	
3	C	4485	
4	D	683	
5	E	567	
6	F	136	
7	G	159	
8	H	120	

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Mol	Chain	Length	Quality of chain
9	I	105	 70%26%...
10	J	100	 78%16%6%
11	K	91	 63%27%10%
11	L	91	 65%25%10%
11	M	91	 60%30%10%
11	N	91	 8%80%10%10%
12	O	117	 12%81%17%
13	P	103	 71%24%5%
14	X	121	 100%
15	Y	168	 99%
16	Z	184	 18%64%21%15%

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 31205 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 Heavy chain alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	315	Total	C	N	O	0	0
			1544	914	315	315		

- Molecule 2 is a protein called Flagellar outer dynein arm heavy chain beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	683	Total	C	N	O	S	0	0
			5028	3180	878	946	24		

- Molecule 3 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	965	Total	C	N	O	S	0	0
			7293	4574	1296	1386	37		

- Molecule 4 is a protein called Dynein, 78 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	456	Total	C	N	O	S	0	0
			3609	2297	610	678	24		

- Molecule 5 is a protein called Dynein, 70 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	474	Total	C	N	O	S	0	0
			3697	2332	623	725	17		

- Molecule 6 is a protein called Flagellar outer dynein arm light chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	100	Total	C	N	O	0	0
			495	295	100	100		

- Molecule 7 is a protein called Dynein 18 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		

- Molecule 8 is a protein called Dynein 11 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	91	Total	C	N	O	0	0
			451	269	91	91		

- Molecule 9 is a protein called Dynein light chain roadblock LC7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	103	Total	C	N	O	S	0	0
			827	525	148	153	1		

- Molecule 10 is a protein called Dynein light chain roadblock LC7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	94	Total	C	N	O	S	0	0
			741	466	133	140	2		

- Molecule 11 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
11	L	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
11	M	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
11	N	82	Total	C	N	O		0	0
			407	243	82	82			

- Molecule 12 is a protein called Dynein light chain 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	97	Total	C	N	O	0	0
			481	286	97	98		

- Molecule 13 is a protein called Dynein light chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	98	Total	C	N	O	S	0	0
			805	523	128	146	8		

- Molecule 14 is a protein called DC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	121	Total	C	N	O	0	0
			605	363	121	121		

- Molecule 15 is a protein called DC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Y	168	Total	C	N	O	0	0
			840	504	168	168		

- Molecule 16 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	157	Total	C	N	O	S	0	0
			1280	798	221	252	9		























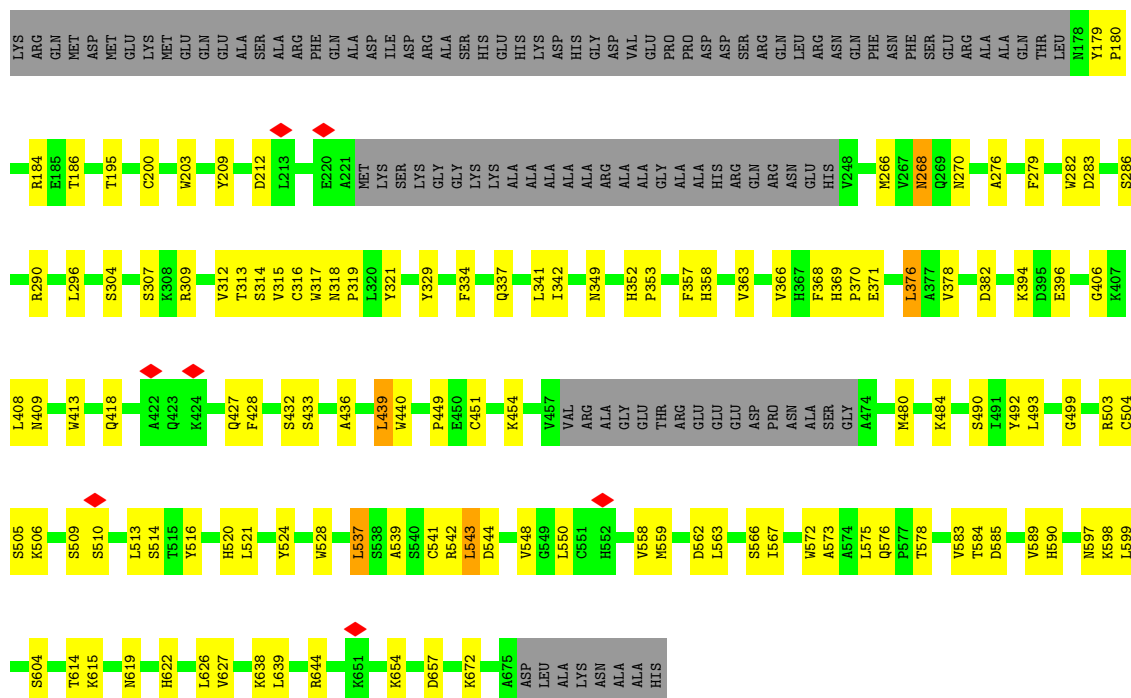




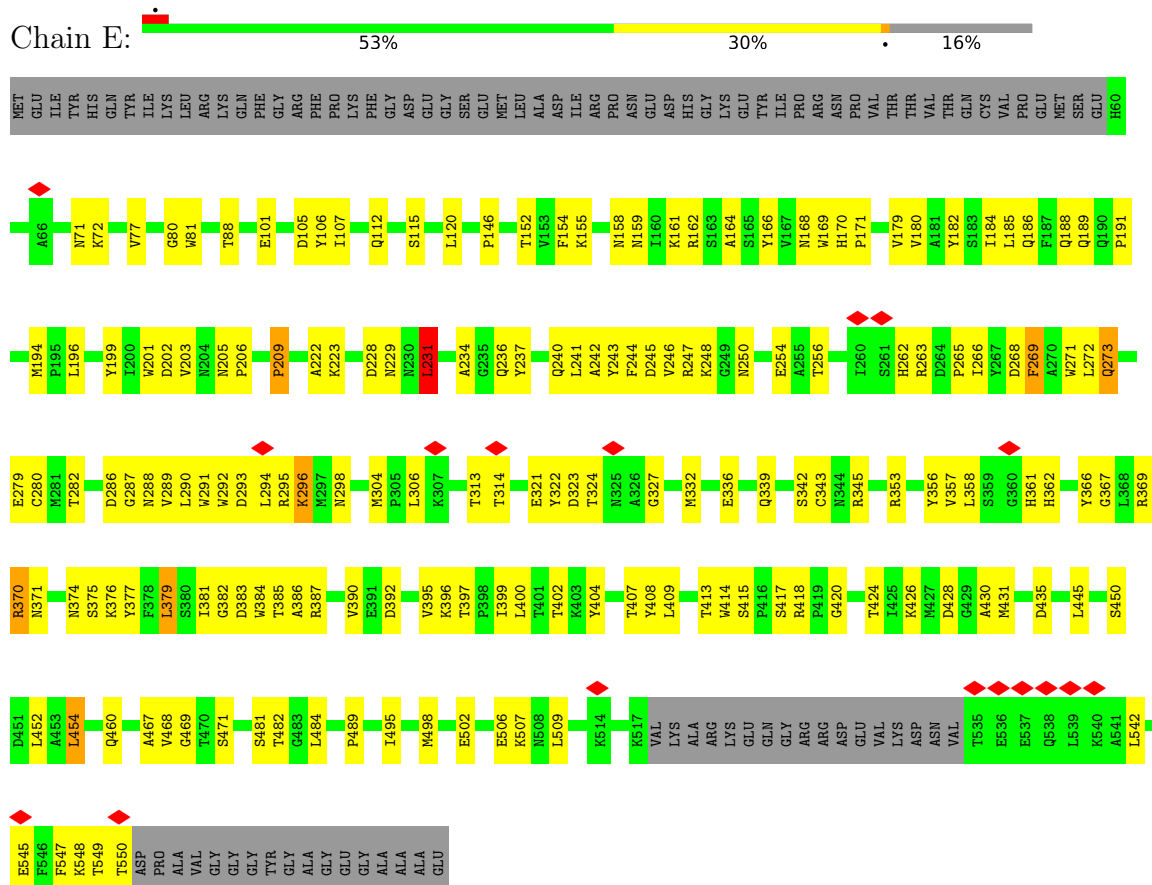
- Molecule 4: Dynein, 78 kDa intermediate chain, flagellar outer arm

Chain D:

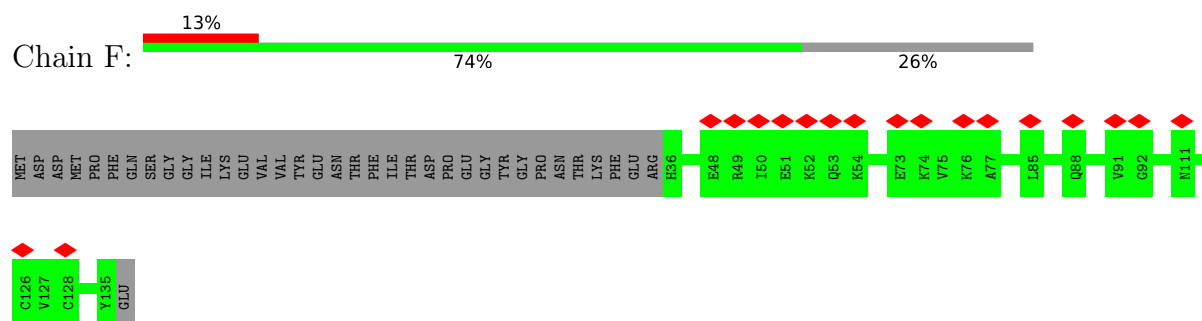
[illegible]



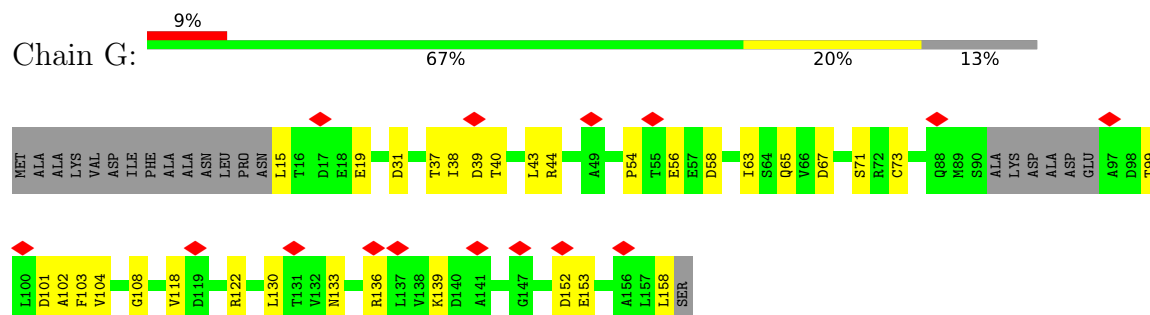
- Molecule 5: Dynein, 70 kDa intermediate chain, flagellar outer arm



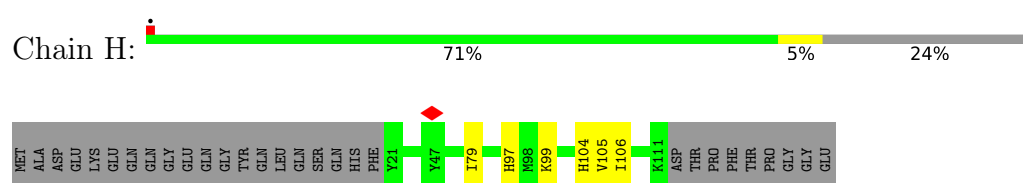
- Molecule 6: Flagellar outer dynein arm light chain 2



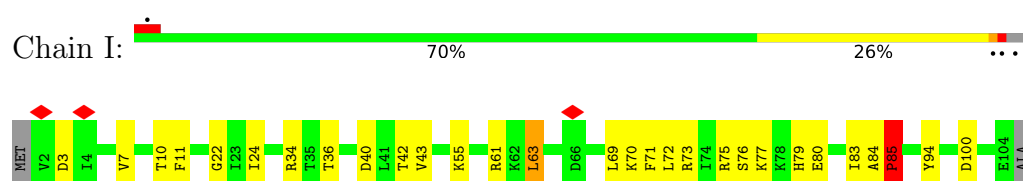
- Molecule 7: Dynein 18 kDa light chain, flagellar outer arm



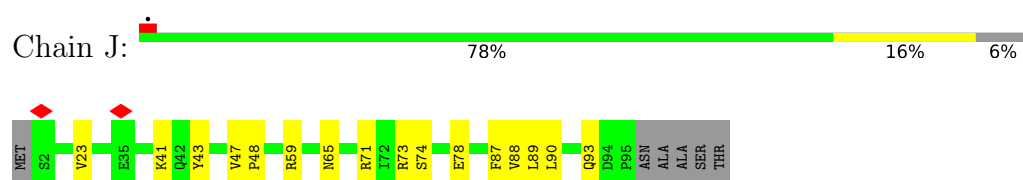
- Molecule 8: Dynein 11 kDa light chain, flagellar outer arm



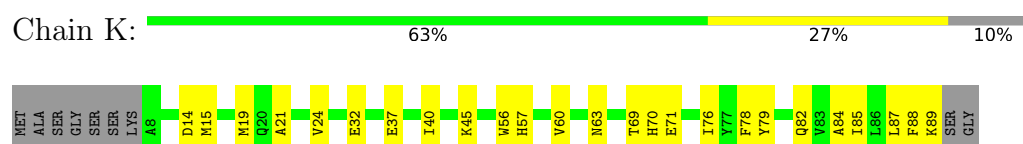
- Molecule 9: Dynein light chain roadblock LC7a



- Molecule 10: Dynein light chain roadblock LC7b



- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm



- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm

Chain L: 




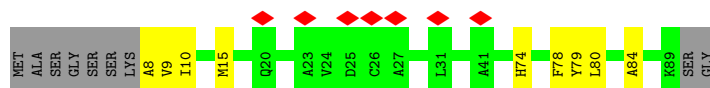
- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm

Chain M: 




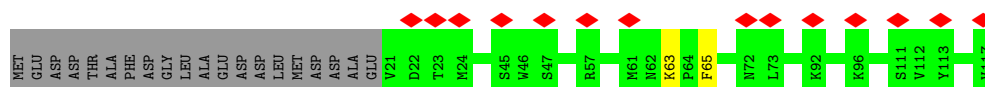
- Molecule 11: Dynein 8 kDa light chain, flagellar outer arm

Chain N: 



- Molecule 12: Dynein light chain 9

Chain O: 



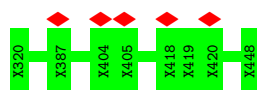
- Molecule 13: Dynein light chain 10

Chain P: 



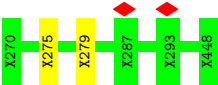
- Molecule 14: DC1

Chain X: 

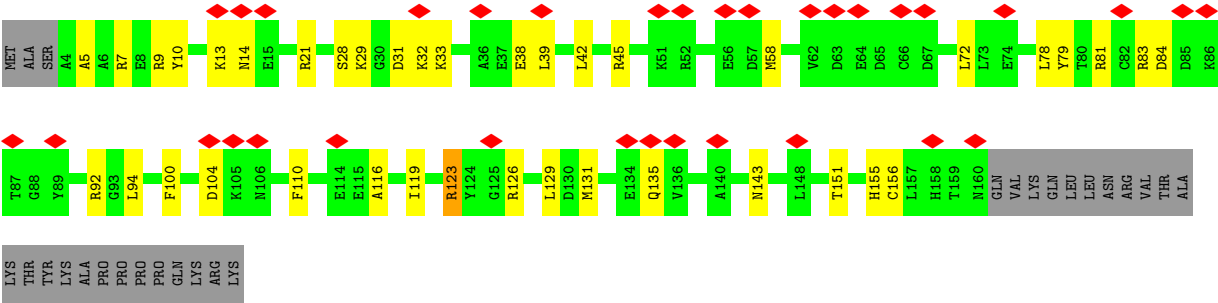


- Molecule 15: DC2

Chain Y: 



• Molecule 16: Outer dynein arm-docking complex protein DC3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=82 Å, axial sym=C1	Depositor
Number of segments used	485694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	61.48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	353.6, 353.6, 353.6	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.26	0/1543	0.50	0/2140
2	B	0.43	0/5090	0.72	5/6881 (0.1%)
3	C	0.46	0/7381	0.71	8/9958 (0.1%)
4	D	0.70	2/3699 (0.1%)	0.88	6/5023 (0.1%)
5	E	0.71	1/3784 (0.0%)	0.90	7/5152 (0.1%)
6	F	0.24	0/494	0.52	0/687
7	G	0.34	0/1098	0.63	0/1471
8	H	0.26	0/450	0.46	0/626
9	I	0.57	0/840	0.85	3/1133 (0.3%)
10	J	0.55	0/752	0.78	0/1019
11	K	0.53	0/687	0.70	0/926
11	L	0.56	0/687	0.74	0/926
11	M	0.43	0/687	0.73	0/926
11	N	0.25	0/406	0.49	0/565
12	O	0.26	0/480	0.56	0/666
13	P	0.58	0/823	0.87	1/1108 (0.1%)
16	Z	0.32	0/1299	0.57	0/1745
All	All	0.52	3/30200 (0.0%)	0.74	30/40952 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	314	SER	CA-CB	-5.72	1.44	1.52
5	E	336	GLU	CA-C	-5.47	1.38	1.52
4	D	378	VAL	CB-CG2	-5.17	1.42	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	376	LEU	CB-CG-CD1	8.76	125.89	111.00
3	C	129	PRO	CA-N-CD	-7.70	100.72	111.50
5	E	370	ARG	C-N-CA	-7.35	103.32	121.70
3	C	455	MET	CB-CG-SD	-6.89	91.72	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	552	LEU	CA-CB-CG	6.71	130.74	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1544	0	701	10	0
2	B	5028	0	4588	121	0
3	C	7293	0	6812	143	0
4	D	3609	0	3534	91	0
5	E	3697	0	3534	133	0
6	F	495	0	221	0	0
7	G	1089	0	1072	22	0
8	H	451	0	204	3	0
9	I	827	0	841	21	0
10	J	741	0	750	13	0
11	K	671	0	654	20	0
11	L	671	0	654	18	0
11	M	671	0	654	23	0
11	N	407	0	192	5	0
12	O	481	0	230	1	0
13	P	805	0	801	20	0
14	X	605	0	129	0	0
15	Y	840	0	181	1	0
16	Z	1280	0	1239	23	0
All	All	31205	0	26991	613	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 11.

The worst 5 of 613 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)
8:H:79:ILE:O	8:H:105:VAL:HA	1.63	0.99
2:B:382:MET:O	2:B:386:VAL:HG23	1.69	0.92
2:B:503:GLU:HG2	4:D:510:SER:HB2	1.56	0.88
4:D:200:CYS:HG	13:P:89:TYR:HH	1.23	0.84
2:B:627:LEU:HG	2:B:631:MET:HE2	1.58	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	313/4503 (7%)	279 (89%)	34 (11%)	0	100	100
2	B	647/4568 (14%)	615 (95%)	31 (5%)	1 (0%)	47	79
3	C	925/4485 (21%)	858 (93%)	65 (7%)	2 (0%)	47	79
4	D	450/683 (66%)	387 (86%)	63 (14%)	0	100	100
5	E	470/567 (83%)	371 (79%)	94 (20%)	5 (1%)	14	51
6	F	98/136 (72%)	94 (96%)	4 (4%)	0	100	100
7	G	134/159 (84%)	125 (93%)	9 (7%)	0	100	100
8	H	89/120 (74%)	77 (86%)	12 (14%)	0	100	100
9	I	101/105 (96%)	89 (88%)	11 (11%)	1 (1%)	15	53
10	J	92/100 (92%)	81 (88%)	11 (12%)	0	100	100
11	K	80/91 (88%)	73 (91%)	7 (9%)	0	100	100
11	L	80/91 (88%)	72 (90%)	8 (10%)	0	100	100
11	M	80/91 (88%)	73 (91%)	7 (9%)	0	100	100
11	N	80/91 (88%)	68 (85%)	12 (15%)	0	100	100
12	O	95/117 (81%)	92 (97%)	3 (3%)	0	100	100
13	P	96/103 (93%)	89 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Z	155/184 (84%)	136 (88%)	19 (12%)	0	100	100
All	All	3985/16194 (25%)	3579 (90%)	397 (10%)	9 (0%)	50	79

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	625	ASP
5	E	298	ASN
9	I	85	PRO
5	E	295	ARG
3	C	114	TRP

### 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	
2	B	463/3998 (12%)	455 (98%)	8 (2%)	60	78
3	C	701/3945 (18%)	695 (99%)	6 (1%)	78	88
4	D	401/584 (69%)	396 (99%)	5 (1%)	71	84
5	E	400/489 (82%)	396 (99%)	4 (1%)	76	86
7	G	121/136 (89%)	121 (100%)	0	100	100
9	I	90/91 (99%)	89 (99%)	1 (1%)	73	85
10	J	83/87 (95%)	83 (100%)	0	100	100
11	K	70/76 (92%)	70 (100%)	0	100	100
11	L	70/76 (92%)	69 (99%)	1 (1%)	67	81
11	M	70/76 (92%)	70 (100%)	0	100	100
13	P	86/90 (96%)	86 (100%)	0	100	100
16	Z	138/162 (85%)	136 (99%)	2 (1%)	67	81
All	All	2693/9810 (28%)	2666 (99%)	27 (1%)	77	86

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	268	ASN
4	D	312	VAL
11	L	45	LYS
4	D	309	ARG
4	D	672	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	65	GLN
5	E	374	ASN
5	E	205	ASN
5	E	158	ASN
5	E	273	GLN

### 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
15	Y	3
14	X	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	396:UNK	C	403:UNK	N	28.65
1	Y	387:UNK	C	394:UNK	N	22.26
1	Y	420:UNK	C	424:UNK	N	12.82
1	X	345:UNK	C	348:UNK	N	10.08
1	Y	281:UNK	C	284:UNK	N	6.72

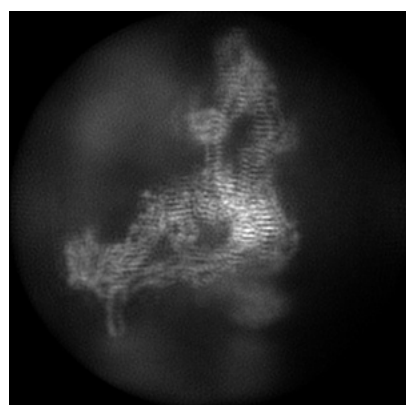
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23083. These allow visual inspection of the internal detail of the map and identification of artifacts.

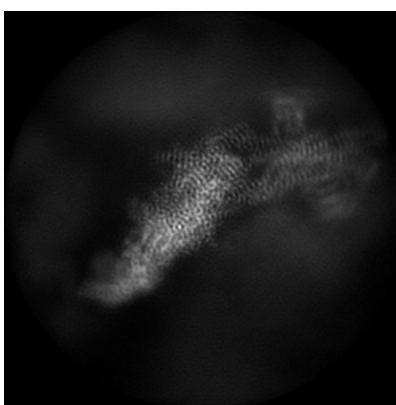
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

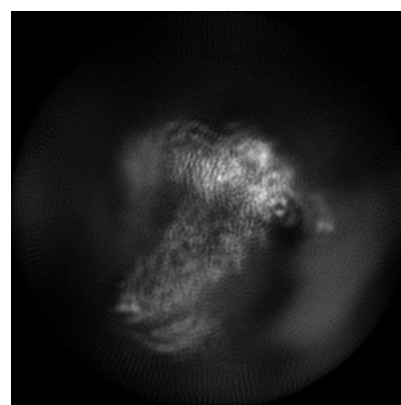
#### 6.1.1 Primary map



X



Y

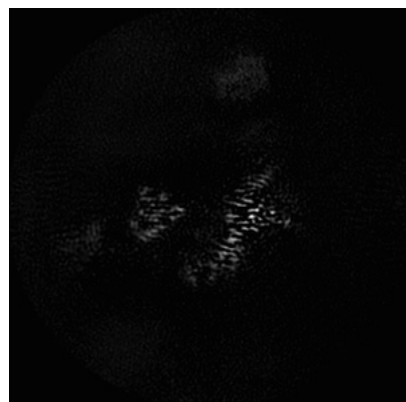


Z

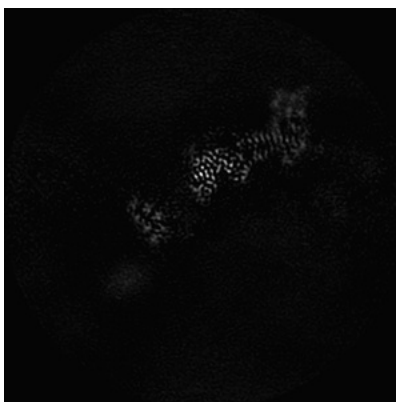
The images above show the map projected in three orthogonal directions.

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

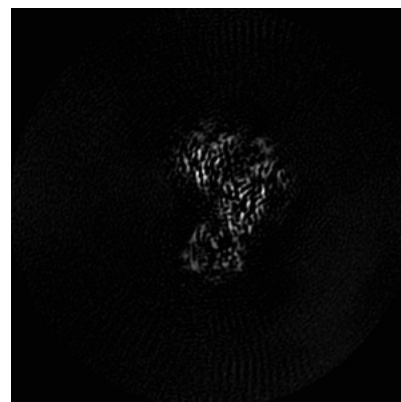
#### 6.2.1 Primary map



X Index: 130



Y Index: 130

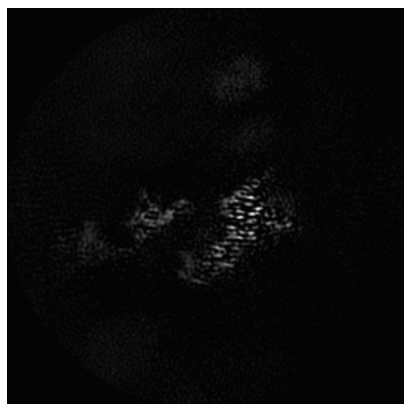


Z Index: 130

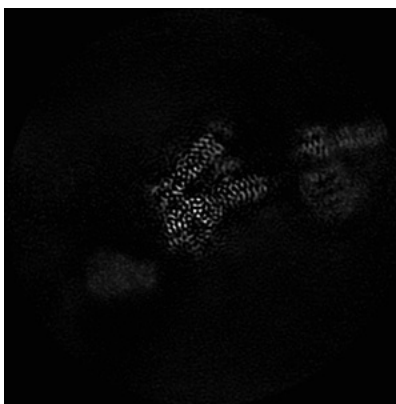
The images above show central slices of the map in three orthogonal directions.

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

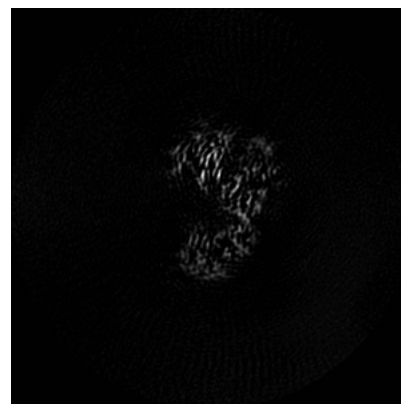
### 6.3.1 Primary map



X Index: 127



Y Index: 152



Z Index: 126

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 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

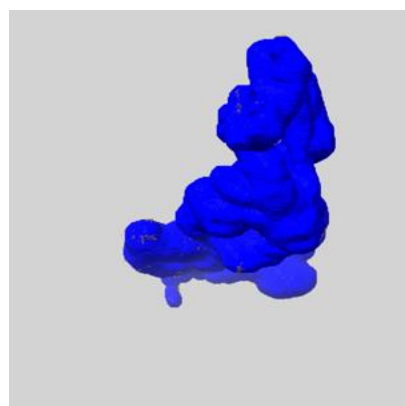
## 6.5 Mask visualisation [i](#)

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

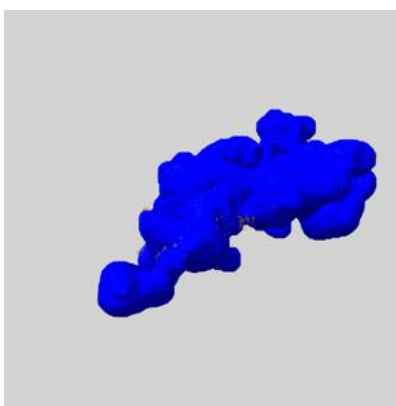
A mask typically either:

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

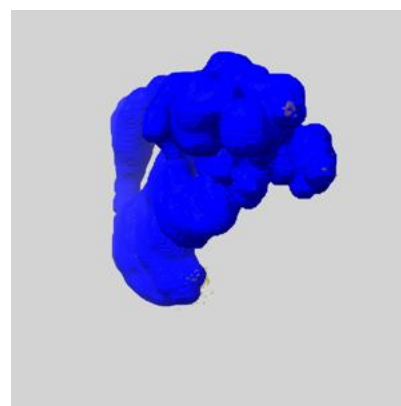
### 6.5.1 emd\_23083\_msk\_1.map [i](#)



X



Y



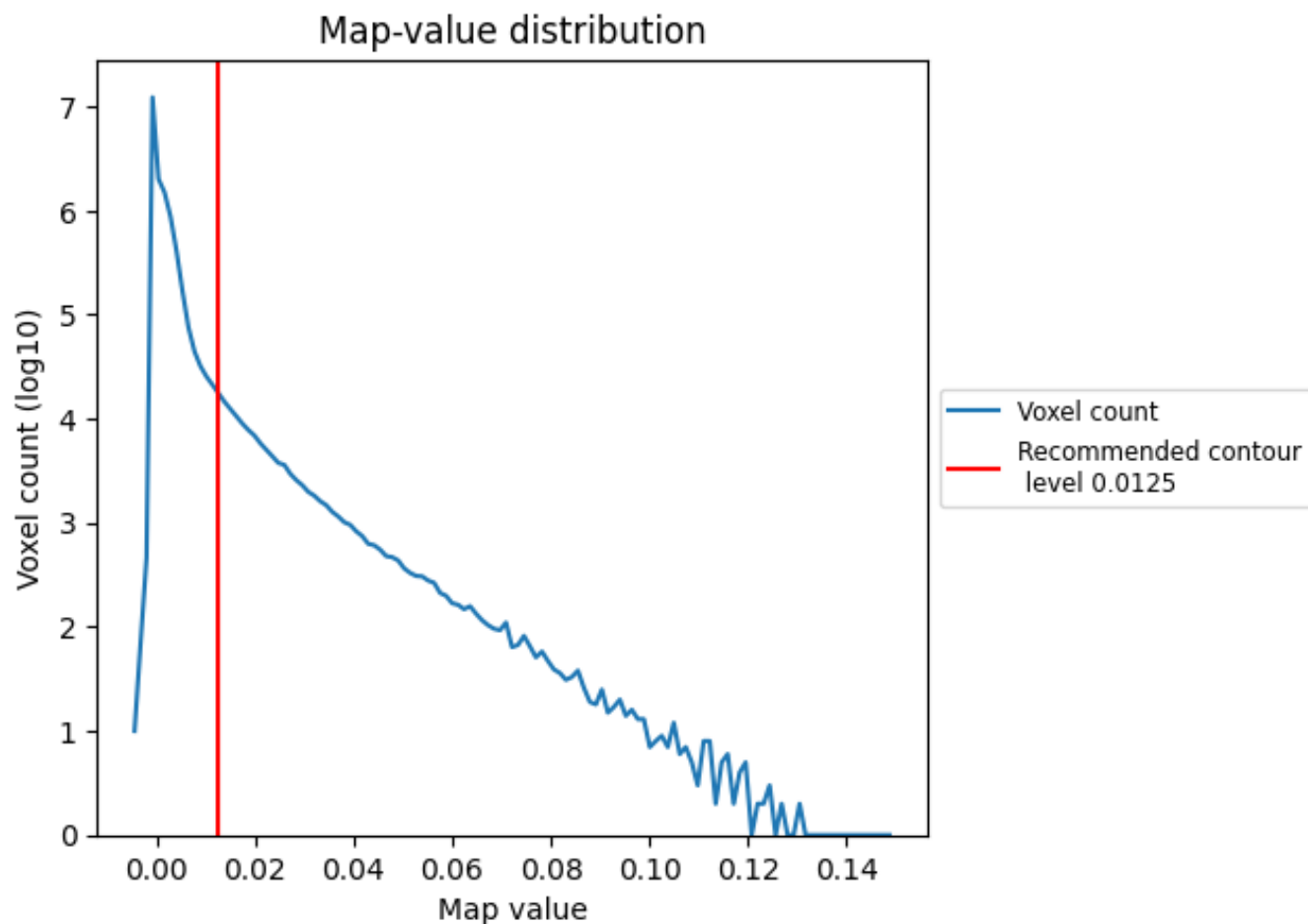
Z



## 7 Map analysis [i](#)

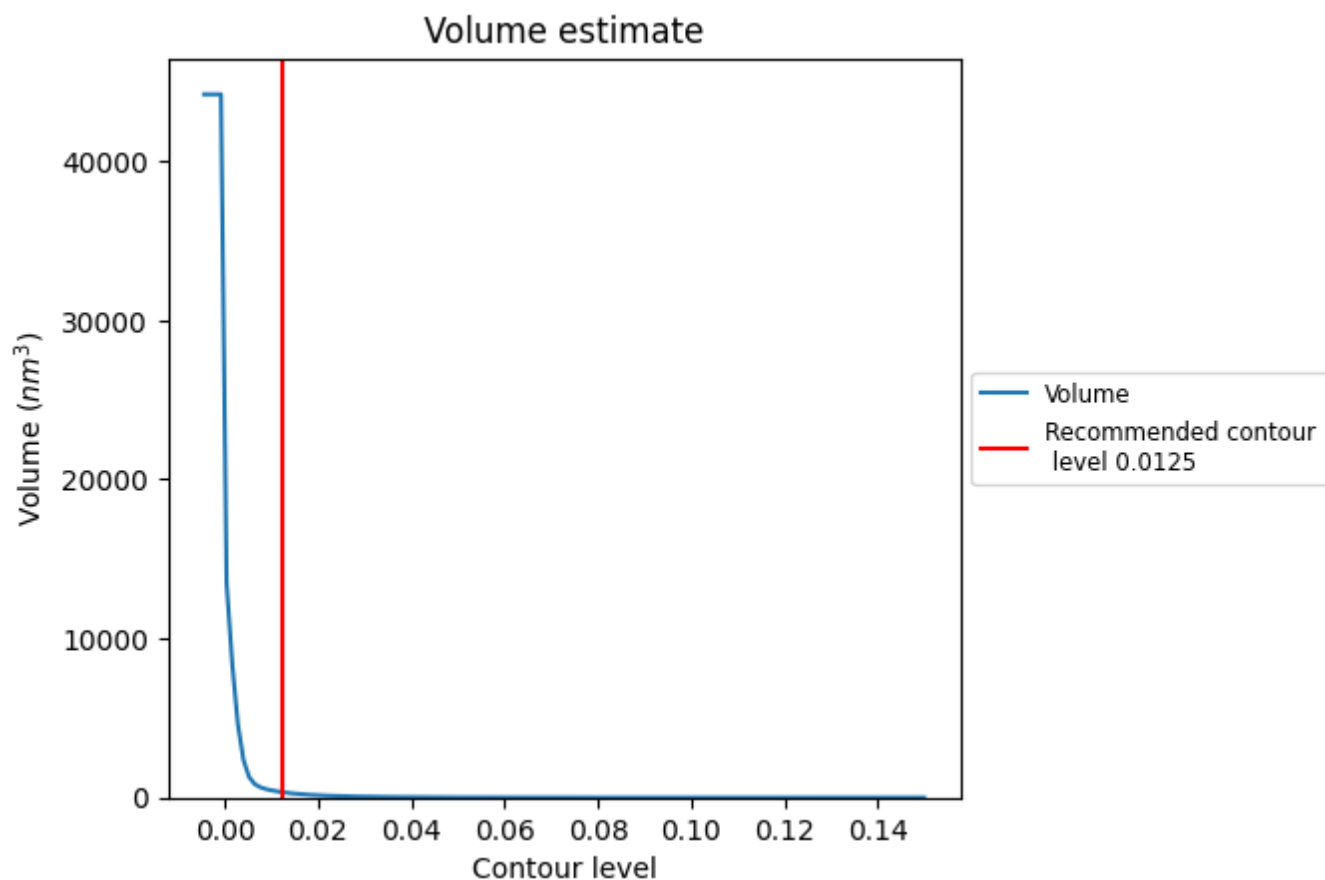
This section contains the results of statistical analysis of the map.

### 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.

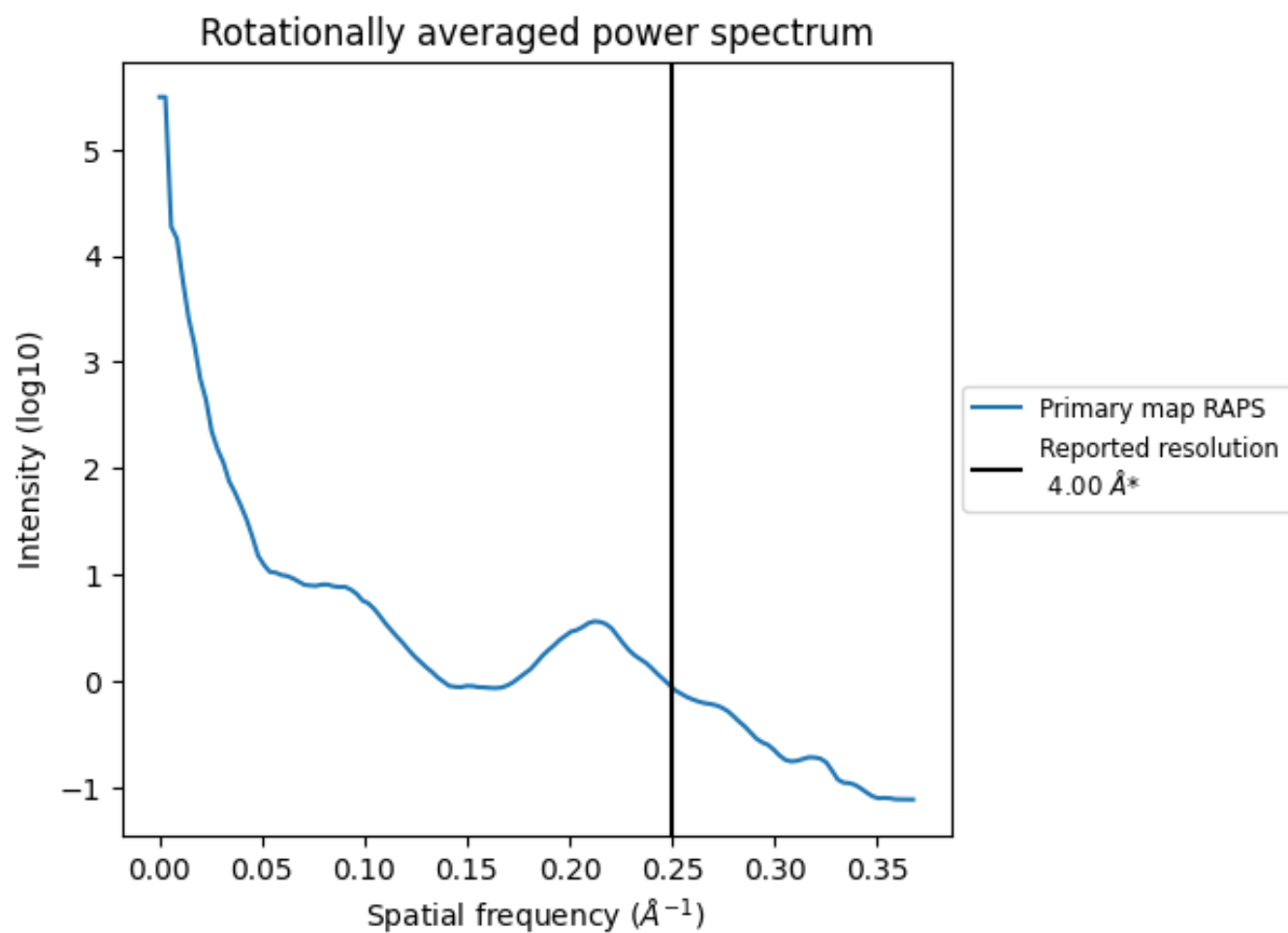
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm<sup>3</sup>; this corresponds to an approximate mass of 298 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 0.250 Å<sup>-1</sup>

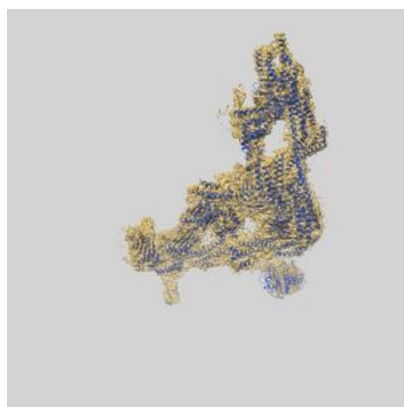
## 8 Fourier-Shell correlation

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

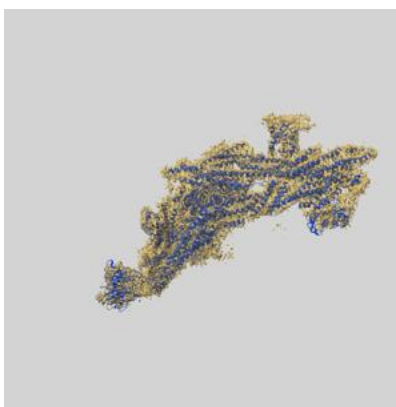
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23083 and PDB model 7KZN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

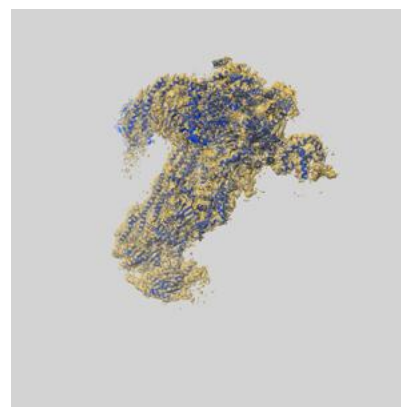
### 9.1 Map-model overlay [i](#)



X



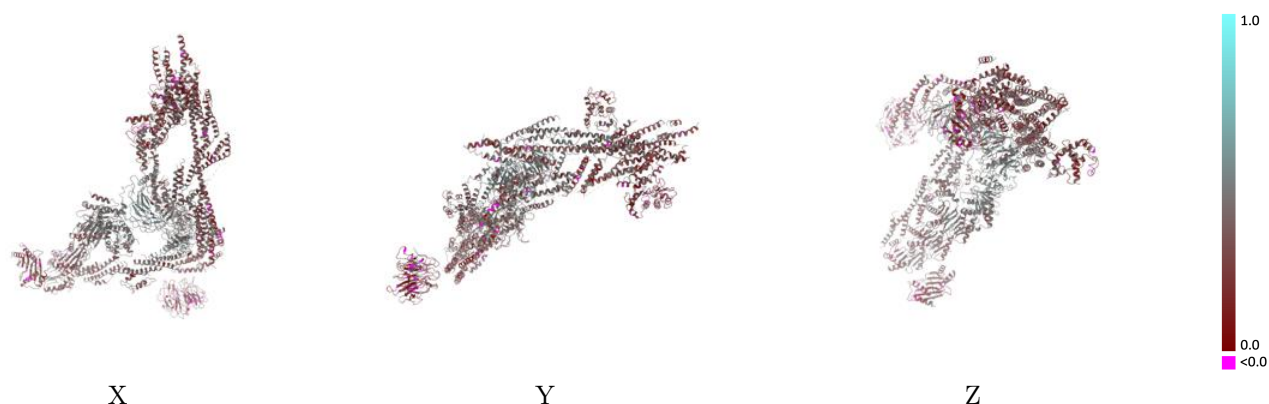
Y



Z

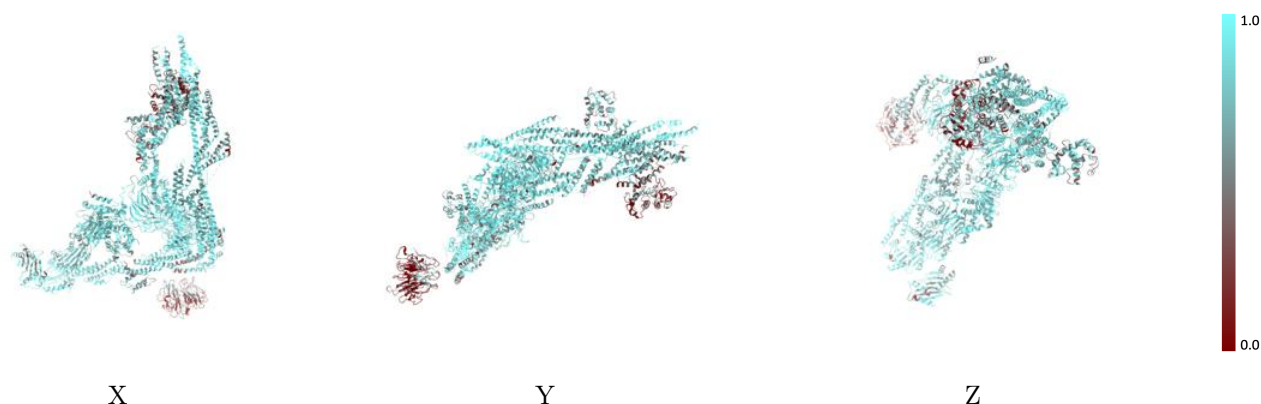
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



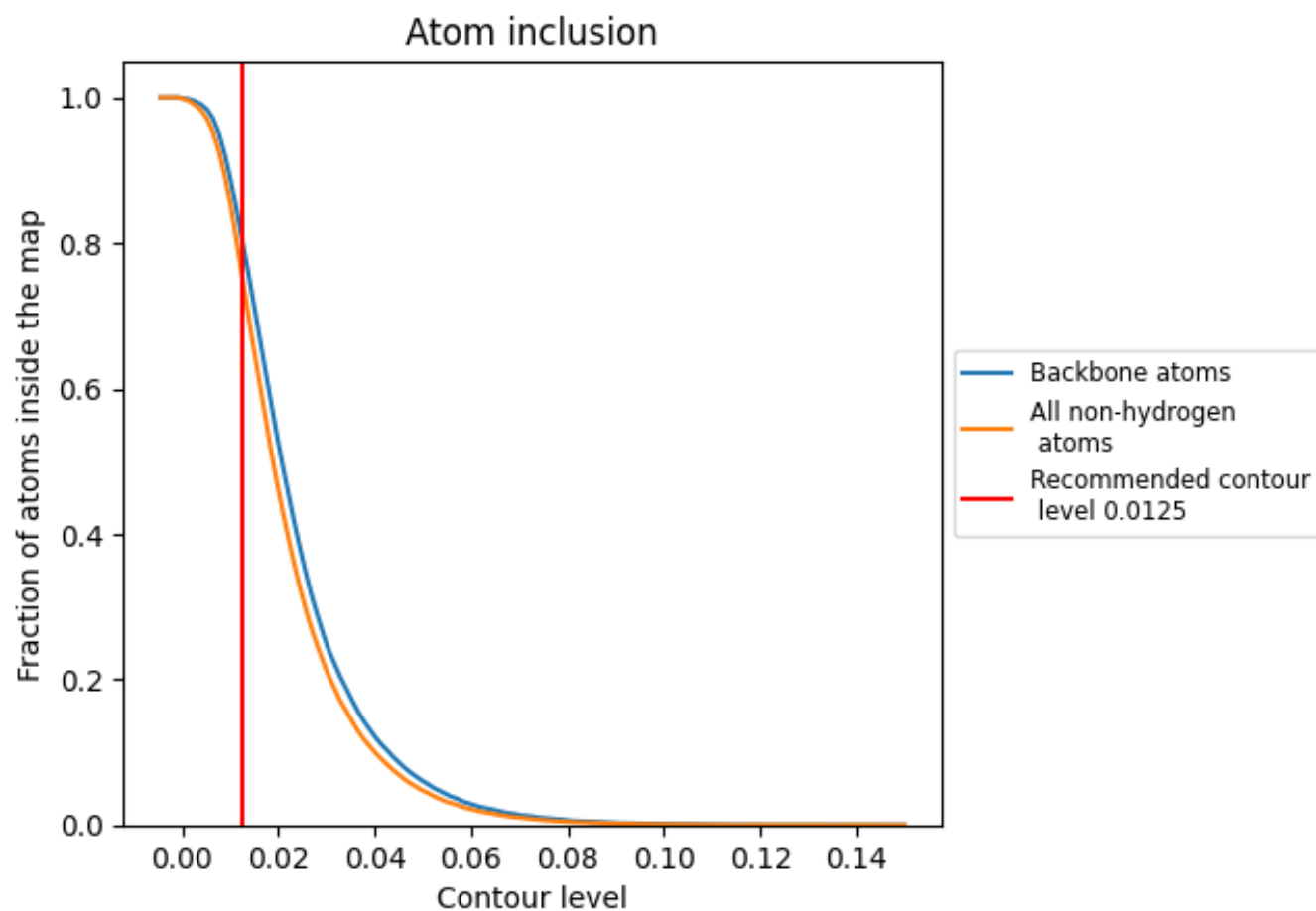
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7545	 0.3760
A	 0.2163	 0.2390
B	 0.6776	 0.3280
C	 0.7654	 0.3780
D	 0.8843	 0.4800
E	 0.8438	 0.4280
F	 0.7313	 0.2340
G	 0.7037	 0.3780
H	 0.9202	 0.3880
I	 0.8292	 0.4610
J	 0.8887	 0.4840
K	 0.8306	 0.4030
L	 0.7852	 0.3470
M	 0.8427	 0.3440
N	 0.8624	 0.3230
O	 0.7796	 0.2730
P	 0.7851	 0.4020
X	 0.8347	 0.3370
Y	 0.8845	 0.3590
Z	 0.6070	 0.2890

