



## wwPDB EM Validation Summary Report ⓘ

Sep 1, 2025 – 01:57 pm BST

PDB ID : 9QCM / pdb\_00009qcm  
EMDB ID : EMD-53015  
Title : Botulinum neurotoxin type B1, 14-subunit, Large Progenitor Toxin Complex (L-PTC)  
Authors : Krc, A.; Persson Kosenina, S.; Masuyer, G.; Stenmark, P.  
Deposited on : 2025-03-04  
Resolution : 2.90 Å(reported)  
Based on initial model : .

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.dev126  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

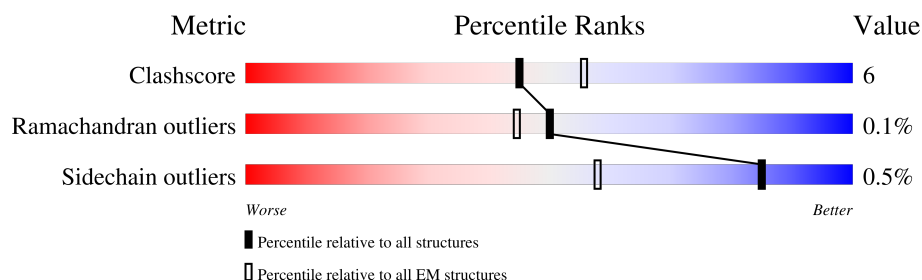
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1302	
2	B	1197	
3	C	626	
3	D	626	
3	E	626	
4	F	146	
4	G	146	
4	H	146	

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Mol	Chain	Length	Quality of chain
5	I	294	<div><div></div><div>7%</div><div>74%</div><div>19%</div><div>7%</div></div>
5	J	294	<div><div></div><div>78%</div><div>14%</div><div>7%</div></div>
5	K	294	<div><div></div><div>20%</div><div>83%</div><div>11%</div><div>7%</div></div>
5	L	294	<div><div></div><div>83%</div><div>9%</div><div>8%</div></div>
5	M	294	<div><div></div><div>36%</div><div>81%</div><div>13%</div><div>7%</div></div>
5	N	294	<div><div></div><div>80%</div><div>13%</div><div>7%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47012 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 Botulinum neurotoxin type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1250	Total	C	N	O	S	0	0
			9378	6124	1529	1695	30		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B1INP5
A	2	GLY	-	expression tag	UNP B1INP5
A	232	GLN	GLU	engineered mutation	UNP B1INP5
A	235	TYR	HIS	engineered mutation	UNP B1INP5
A	1293	HIS	-	expression tag	UNP B1INP5
A	1294	HIS	-	expression tag	UNP B1INP5
A	1295	HIS	-	expression tag	UNP B1INP5
A	1296	HIS	-	expression tag	UNP B1INP5
A	1297	HIS	-	expression tag	UNP B1INP5
A	1298	HIS	-	expression tag	UNP B1INP5
A	1299	HIS	-	expression tag	UNP B1INP5
A	1300	HIS	-	expression tag	UNP B1INP5
A	1301	HIS	-	expression tag	UNP B1INP5
A	1302	HIS	-	expression tag	UNP B1INP5

- Molecule 2 is a protein called Botulinum neurotoxin type B1, nontoxic-nonhemagglutinin component, NTNH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1187	Total	C	N	O	S	0	0
			8877	5797	1463	1592	25		

- Molecule 3 is a protein called Hemagglutinin component HA70.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	588	Total	C	N	O	S	0	0
			4694	2989	771	928	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	567	Total	C	N	O	S	0	0
			4384	2818	716	844	6		
3	E	566	Total	C	N	O	S	0	0
			4368	2809	718	835	6		

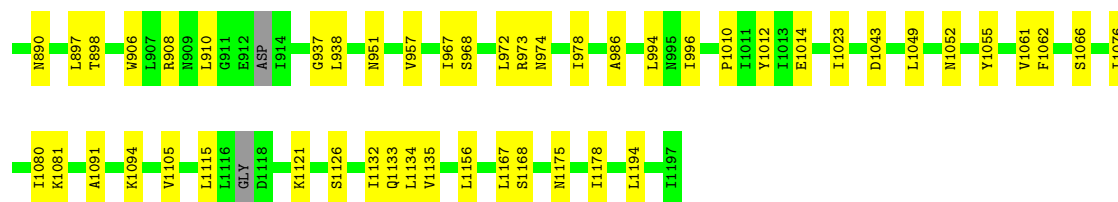
- Molecule 4 is a protein called Hemagglutinin component HA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	135	Total	C	N	O	S	0	0
			1024	669	161	192	2		
4	G	138	Total	C	N	O	S	0	0
			1062	696	168	196	2		
4	H	137	Total	C	N	O	S	0	0
			1050	686	166	195	3		

- Molecule 5 is a protein called Hemagglutinin component HA33.

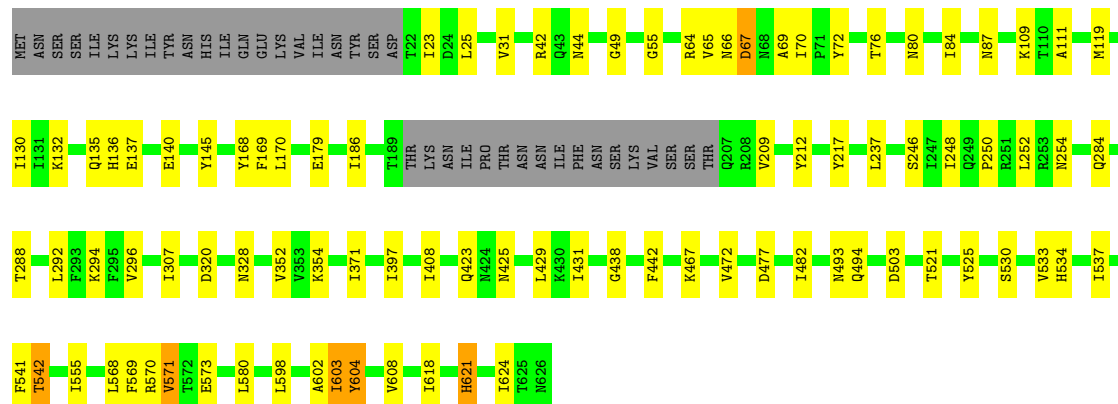
Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	273	Total	C	N	O	S	0	0
			2027	1305	343	376	3		
5	J	273	Total	C	N	O	S	0	0
			2027	1313	335	377	2		
5	K	274	Total	C	N	O	S	0	0
			2044	1319	343	378	4		
5	L	271	Total	C	N	O	S	0	0
			2025	1308	341	375	1		
5	M	274	Total	C	N	O	S	0	0
			2044	1319	343	378	4		
5	N	274	Total	C	N	O	S	0	0
			2008	1295	335	375	3		





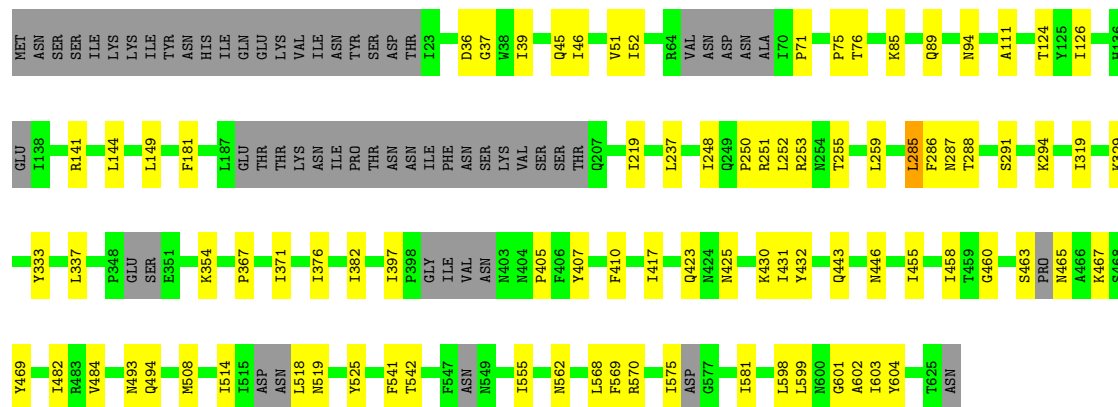
### • Molecule 3: Hemagglutinin component HA70

Chain C: 79% 14% 6%



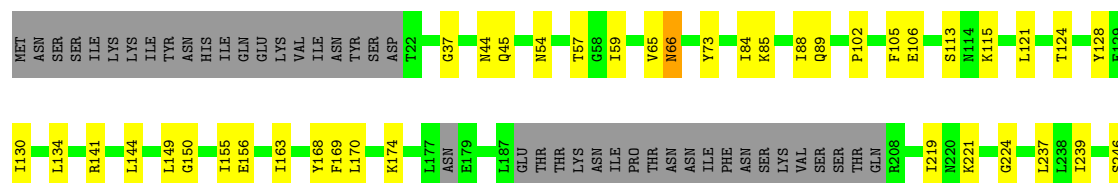
### • Molecule 3: Hemagglutinin component HA70

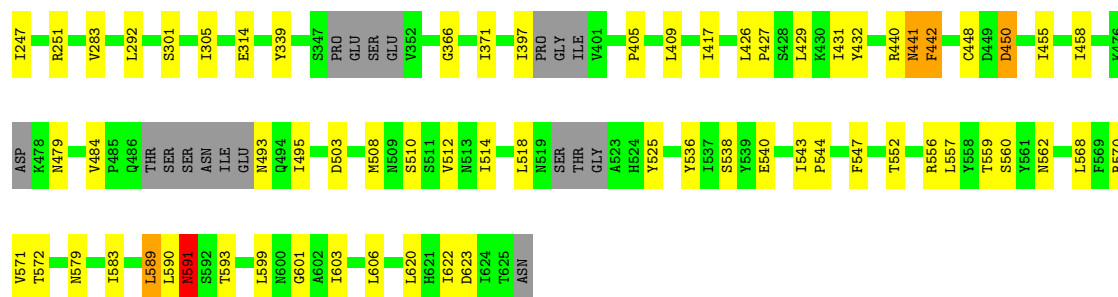
Chain D: 77% 14% 9%



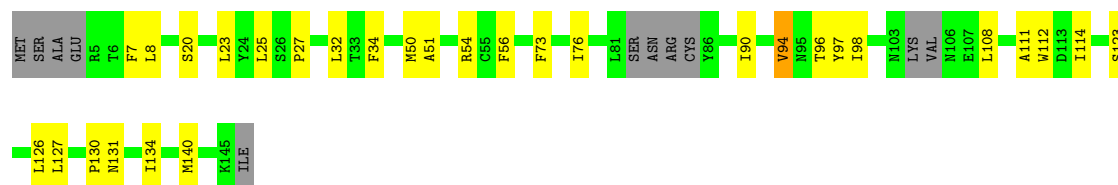
### • Molecule 3: Hemagglutinin component HA70

Chain E: 73% 16% 10%

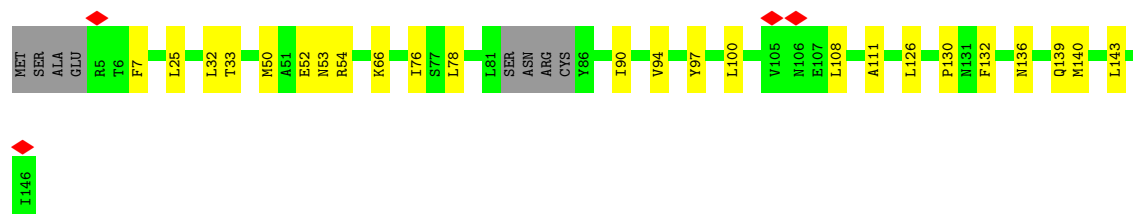
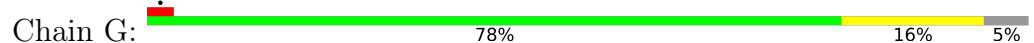




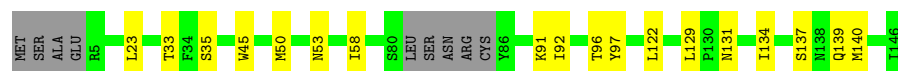
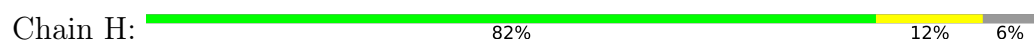
• Molecule 4: Hemagglutinin component HA17



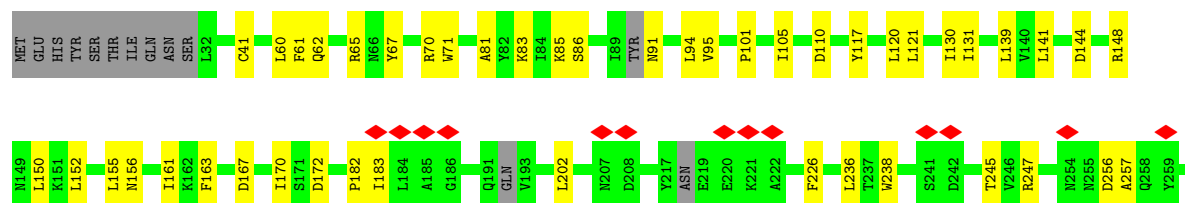
• Molecule 4: Hemagglutinin component HA17



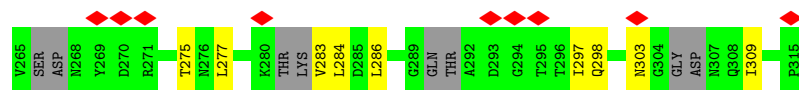
• Molecule 4: Hemagglutinin component HA17



• Molecule 5: Hemagglutinin component HA33

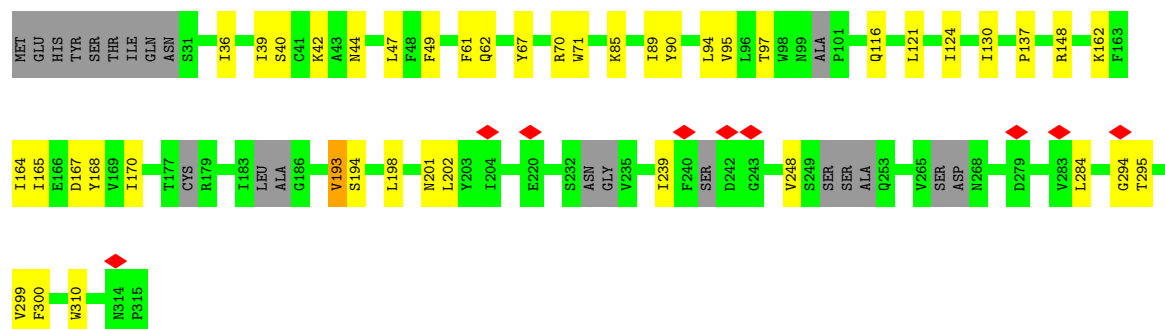






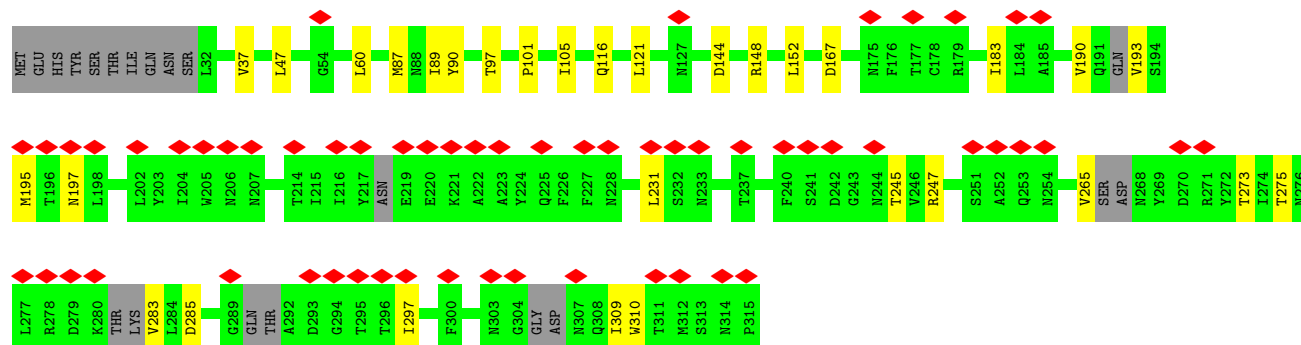
• Molecule 5: Hemagglutinin component HA33

Chain J: 78% 14% 7%



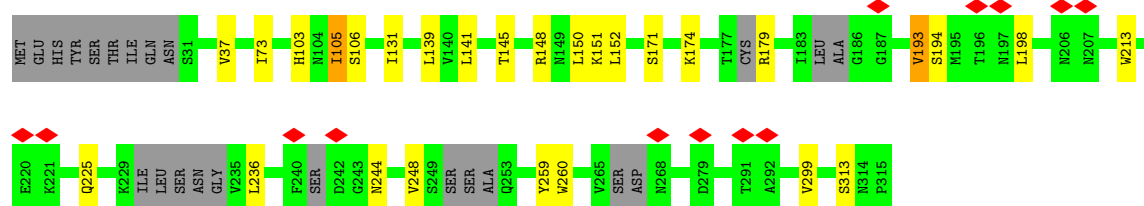
• Molecule 5: Hemagglutinin component HA33

Chain K: 20% 83% 11% 7%



• Molecule 5: Hemagglutinin component HA33

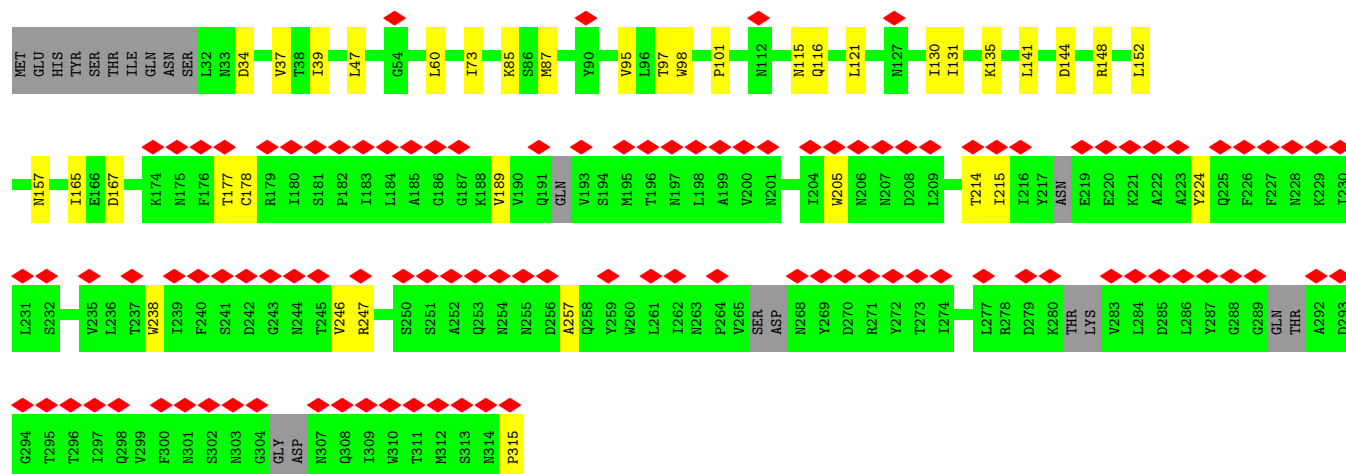
Chain L: 83% 9% 8%



• Molecule 5: Hemagglutinin component HA33

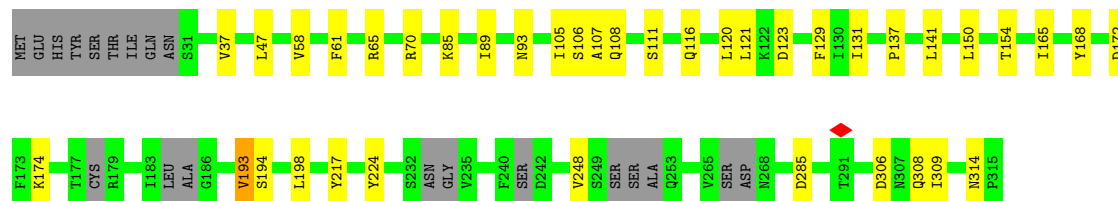
Chain M: 36% 81% 13% 7%





• Molecule 5: Hemagglutinin component HA33

Chain N: 80% 13% 7%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139594	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	74.186	Depositor
Minimum map value	-33.058	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	4	Depositor
Map size ( $\text{\AA}$ )	659.98804, 659.98804, 659.98804	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2222, 1.2222, 1.2222	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	0.15	0/9595	0.33	6/13091 (0.0%)
2	B	0.19	0/9079	0.36	6/12392 (0.0%)
3	C	0.22	0/4787	0.46	6/6509 (0.1%)
3	D	0.21	0/4468	0.47	5/6087 (0.1%)
3	E	0.21	0/4453	0.46	5/6069 (0.1%)
4	F	0.33	1/1051 (0.1%)	0.47	0/1439
4	G	0.09	0/1090	0.31	0/1487
4	H	0.09	0/1077	0.28	0/1470
5	I	0.11	0/2066	0.33	0/2827
5	J	0.11	0/2066	0.35	0/2829
5	K	0.10	0/2085	0.33	0/2852
5	L	0.17	1/2064 (0.0%)	0.36	1/2825 (0.0%)
5	M	0.09	0/2085	0.27	0/2852
5	N	0.16	1/2044 (0.0%)	0.30	0/2801
All	All	0.18	3/48010 (0.0%)	0.38	29/65530 (0.0%)

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
2	B	0	1
3	D	0	1
3	E	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	27	PRO	N-CD	-5.69	1.39	1.47
5	L	105	ILE	CA-C	5.69	1.59	1.52
5	N	107	ALA	C-N	-5.57	1.28	1.33

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	66	ASN	CB-CA-C	-11.57	94.61	112.31
3	D	286	PHE	N-CA-C	-9.23	101.28	112.54
3	D	75	PRO	N-CA-CB	-8.42	94.41	103.25
3	C	569	PHE	CA-CB-CG	7.34	121.14	113.80
3	E	442	PHE	CA-CB-CG	7.15	120.95	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	319	ARG	Sidechain
3	D	141	ARG	Sidechain
3	E	440	ARG	Sidechain

## 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	9378	0	8519	97	0
2	B	8877	0	8115	97	0
3	C	4694	0	4578	60	0
3	D	4384	0	4164	55	0
3	E	4368	0	4155	74	0
4	F	1024	0	915	22	0
4	G	1062	0	984	19	0
4	H	1050	0	971	13	0
5	I	2027	0	1831	36	0
5	J	2027	0	1835	26	0
5	K	2044	0	1859	22	0
5	L	2025	0	1855	21	0
5	M	2044	0	1859	22	0
5	N	2008	0	1809	24	0
All	All	47012	0	43449	553	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 6.

The worst 5 of 553 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:ILE:HD11	2:B:1167:LEU:HD13	1.24	1.16
2:B:1080:ILE:HD12	2:B:1175:ASN:HB2	1.29	1.08
2:B:1080:ILE:HD12	2:B:1175:ASN:CB	1.87	1.02
5:M:144:ASP:O	5:M:148:ARG:HA	1.64	0.96
1:A:69:ARG:NE	1:A:525:GLN:OE1	2.00	0.95

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	1234/1302 (95%)	1208 (98%)	25 (2%)	1 (0%)	48	77
2	B	1175/1197 (98%)	1125 (96%)	50 (4%)	0	100	100
3	C	584/626 (93%)	554 (95%)	28 (5%)	2 (0%)	37	66
3	D	547/626 (87%)	513 (94%)	34 (6%)	0	100	100
3	E	550/626 (88%)	528 (96%)	22 (4%)	0	100	100
4	F	129/146 (88%)	116 (90%)	13 (10%)	0	100	100
4	G	134/146 (92%)	132 (98%)	2 (2%)	0	100	100
4	H	133/146 (91%)	130 (98%)	3 (2%)	0	100	100
5	I	257/294 (87%)	240 (93%)	17 (7%)	0	100	100
5	J	257/294 (87%)	243 (95%)	12 (5%)	2 (1%)	16	45
5	K	260/294 (88%)	247 (95%)	13 (5%)	0	100	100
5	L	257/294 (87%)	234 (91%)	22 (9%)	1 (0%)	30	60
5	M	260/294 (88%)	244 (94%)	16 (6%)	0	100	100
5	N	260/294 (88%)	243 (94%)	15 (6%)	2 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6037/6579 (92%)	5757 (95%)	272 (4%)	8 (0%)	50 77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	675	ASN
5	J	193	VAL
5	L	193	VAL
5	N	193	VAL
3	C	67	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	880/1200 (73%)	877 (100%)	3 (0%)	91 97
2	B	836/1114 (75%)	833 (100%)	3 (0%)	89 97
3	C	525/570 (92%)	521 (99%)	4 (1%)	79 93
3	D	462/570 (81%)	461 (100%)	1 (0%)	92 98
3	E	458/570 (80%)	451 (98%)	7 (2%)	60 85
4	F	103/136 (76%)	101 (98%)	2 (2%)	52 81
4	G	109/136 (80%)	109 (100%)	0	100 100
4	H	108/136 (79%)	108 (100%)	0	100 100
5	I	193/266 (73%)	193 (100%)	0	100 100
5	J	193/266 (73%)	193 (100%)	0	100 100
5	K	196/266 (74%)	195 (100%)	1 (0%)	86 96
5	L	194/266 (73%)	194 (100%)	0	100 100
5	M	196/266 (74%)	196 (100%)	0	100 100
5	N	188/266 (71%)	188 (100%)	0	100 100
All	All	4641/6028 (77%)	4620 (100%)	21 (0%)	85 96

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	442	PHE
3	E	591	ASN
5	K	121	LEU
4	F	94	VAL
3	E	450	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	44	ASN
5	M	211	GLN
3	E	441	ASN
5	M	109	GLN
5	K	276	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

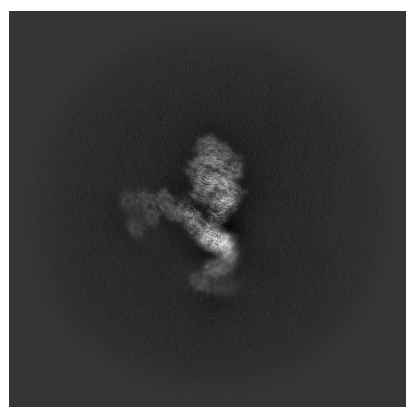
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53015. These allow visual inspection of the internal detail of the map and identification of artifacts.

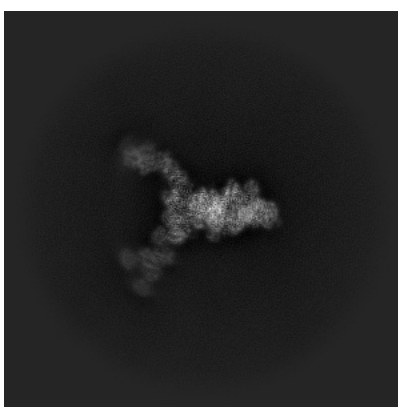
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

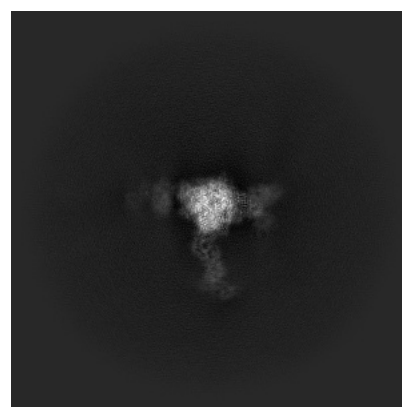
#### 6.1.1 Primary map



X



Y

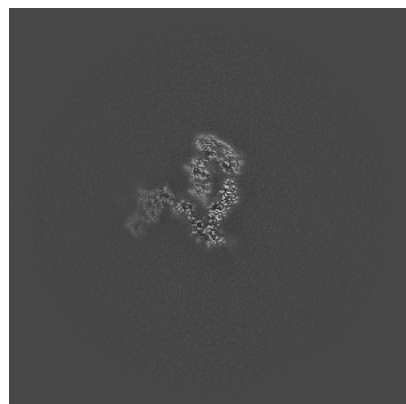


Z

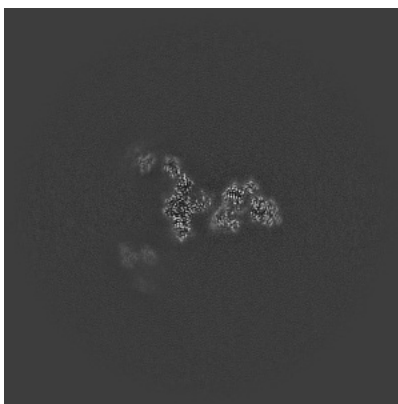
The images above show the map projected in three orthogonal directions.

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

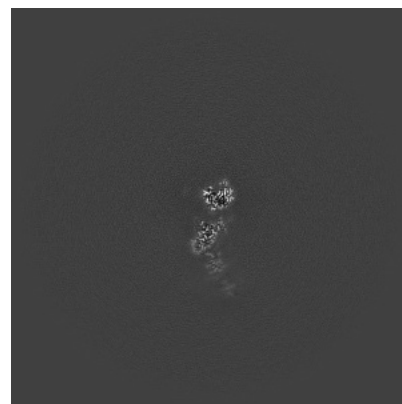
#### 6.2.1 Primary map



X Index: 270



Y Index: 270

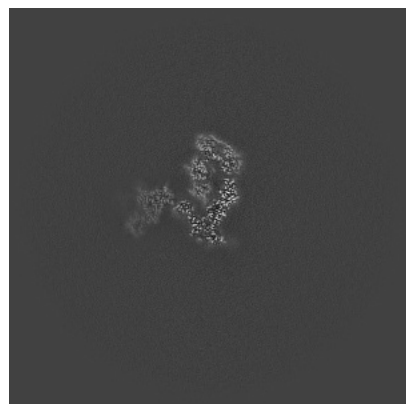


Z Index: 270

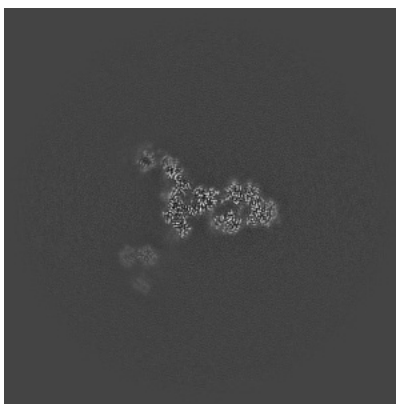
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 271



Y Index: 276



Z Index: 231

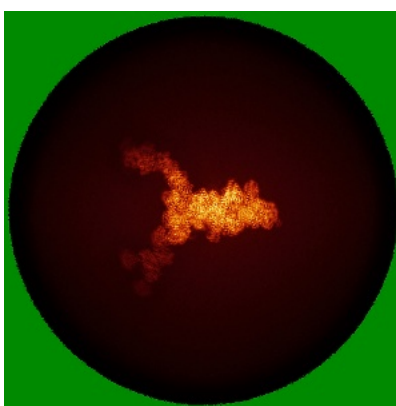
The images above show the largest variance slices of the map in three orthogonal directions.

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

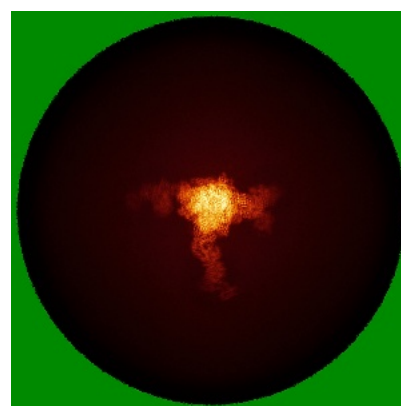
### 6.4.1 Primary map



X



Y



Z

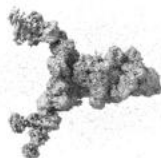
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

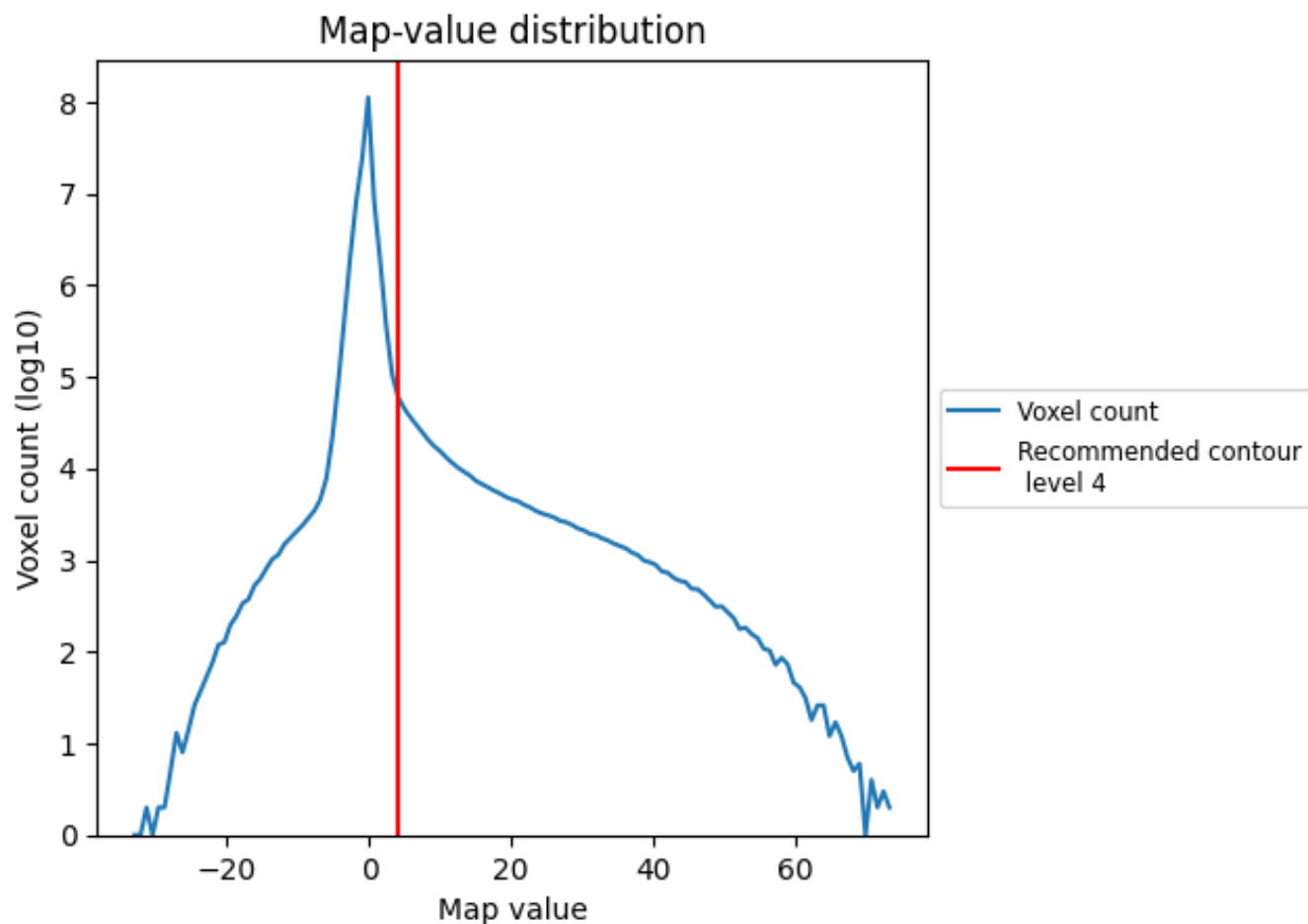
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

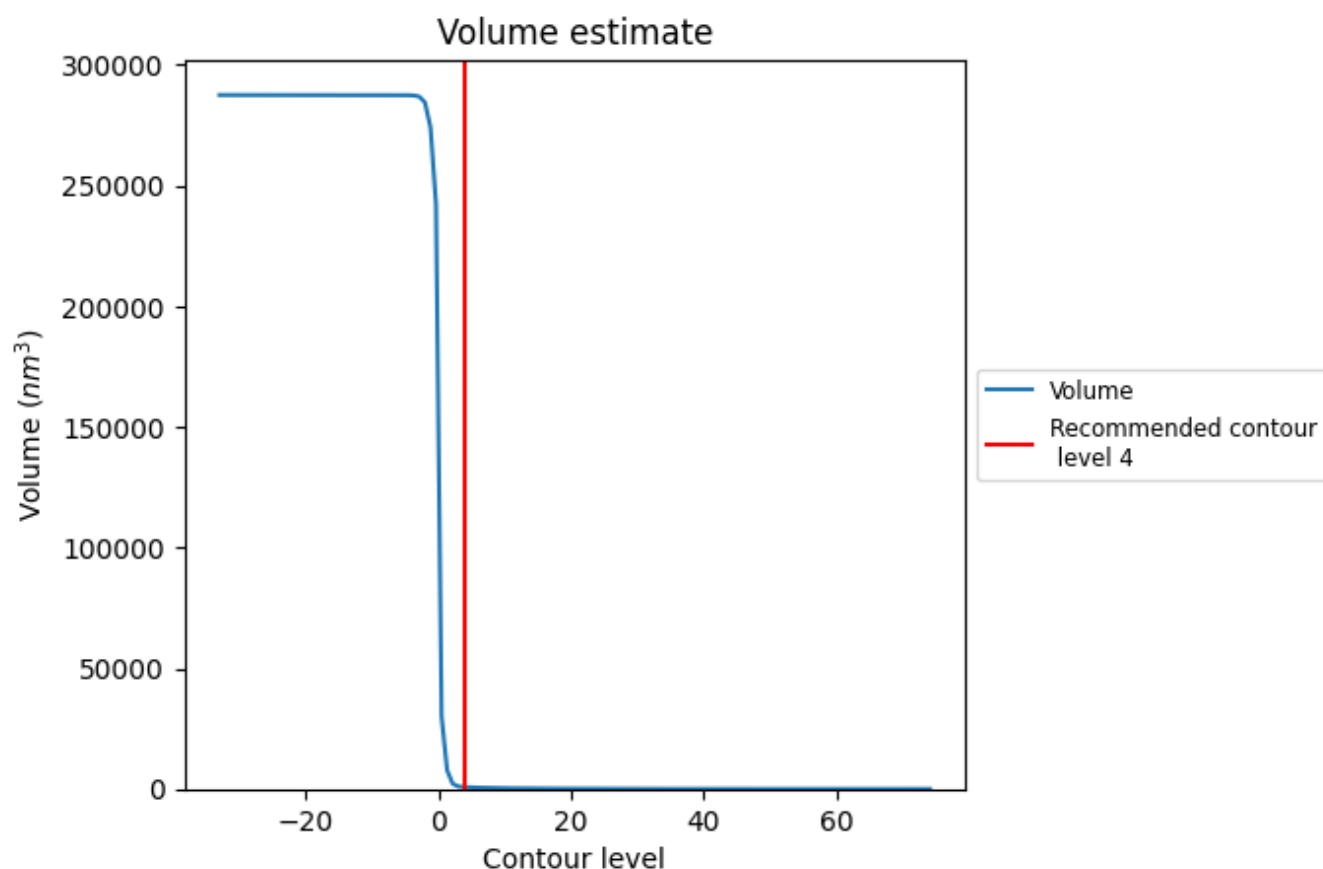
This section contains the results of statistical analysis of the map.

### 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.

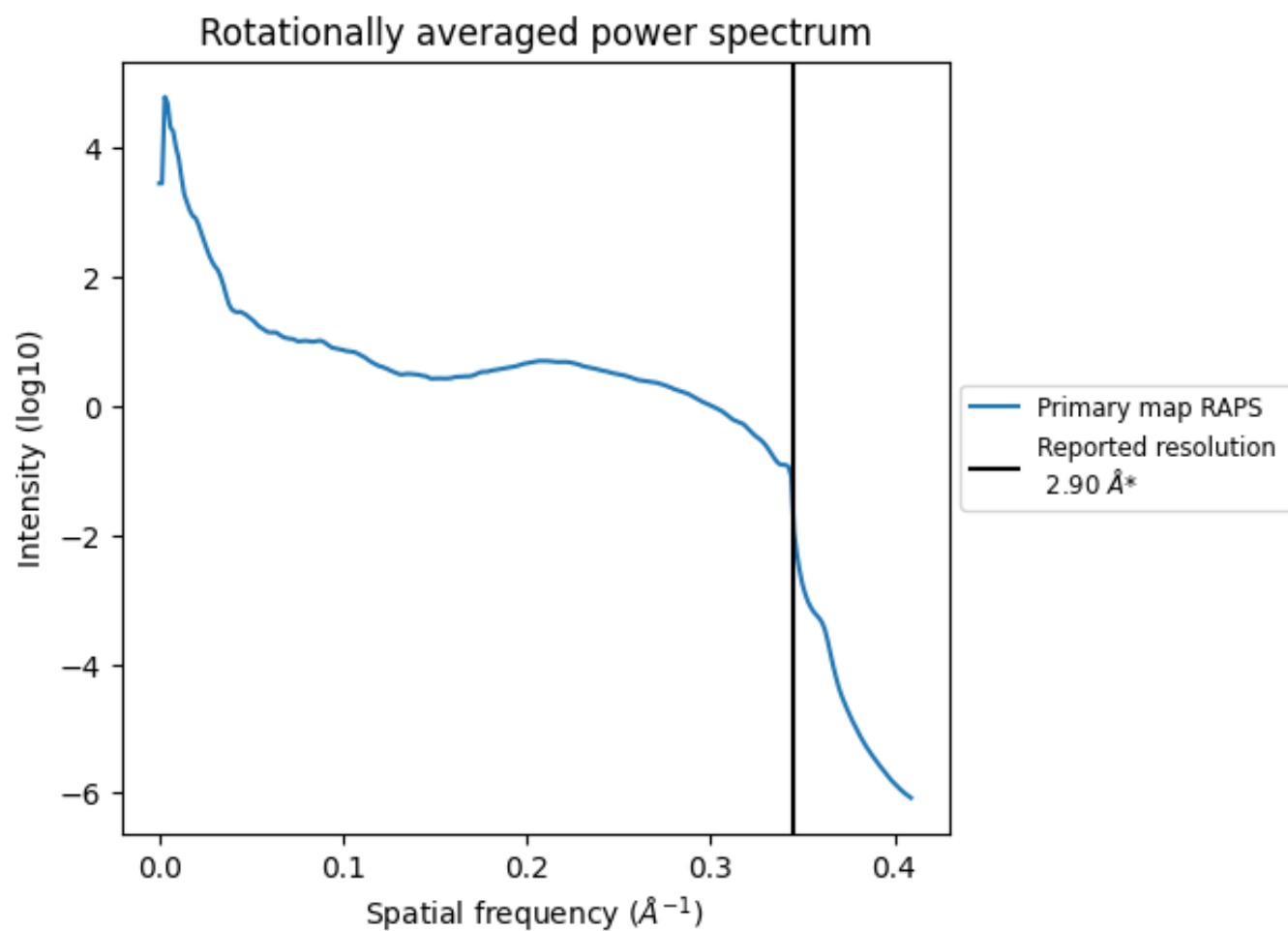
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 758  $\text{nm}^3$ ; this corresponds to an approximate mass of 685 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 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

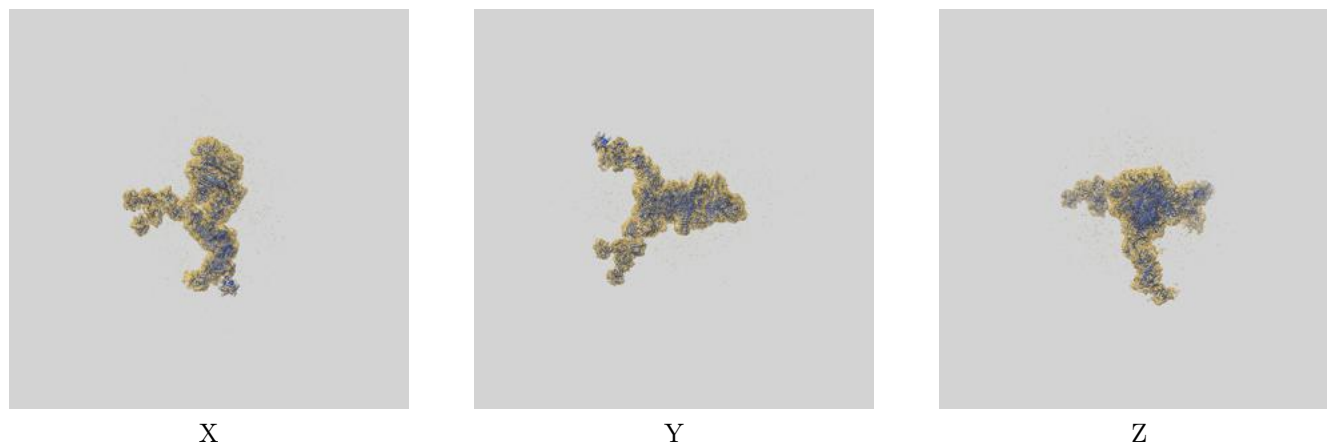
This section was not generated. No FSC curve or half-maps provided.



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

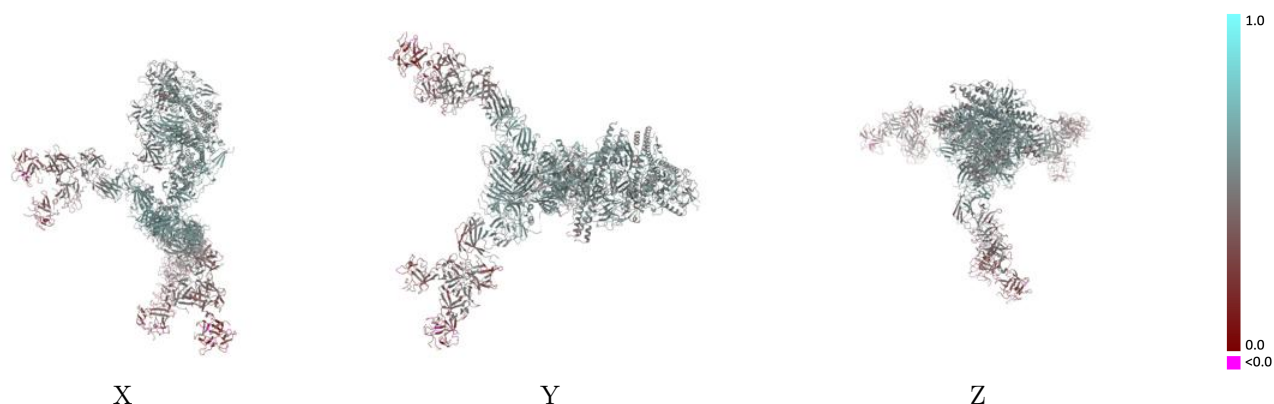
This section contains information regarding the fit between EMDB map EMD-53015 and PDB model 9QCM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



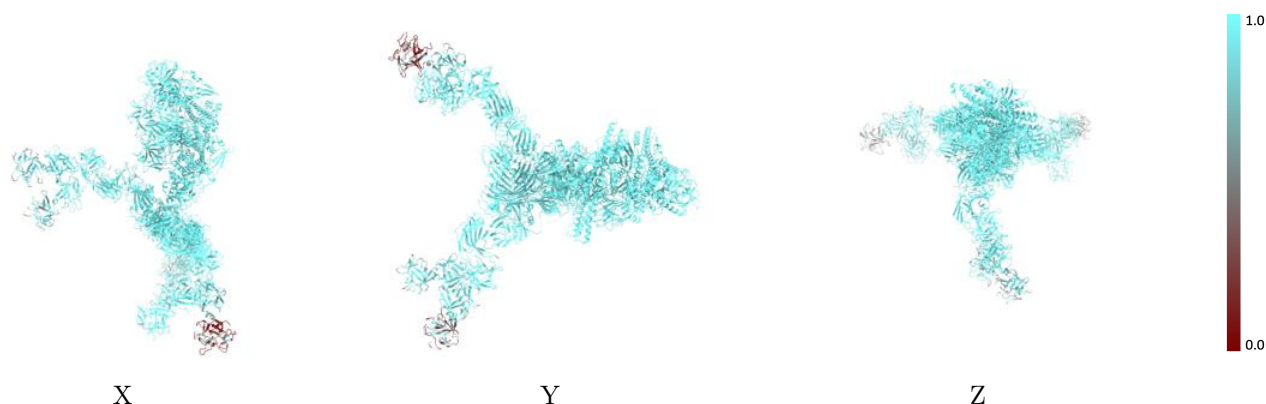
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



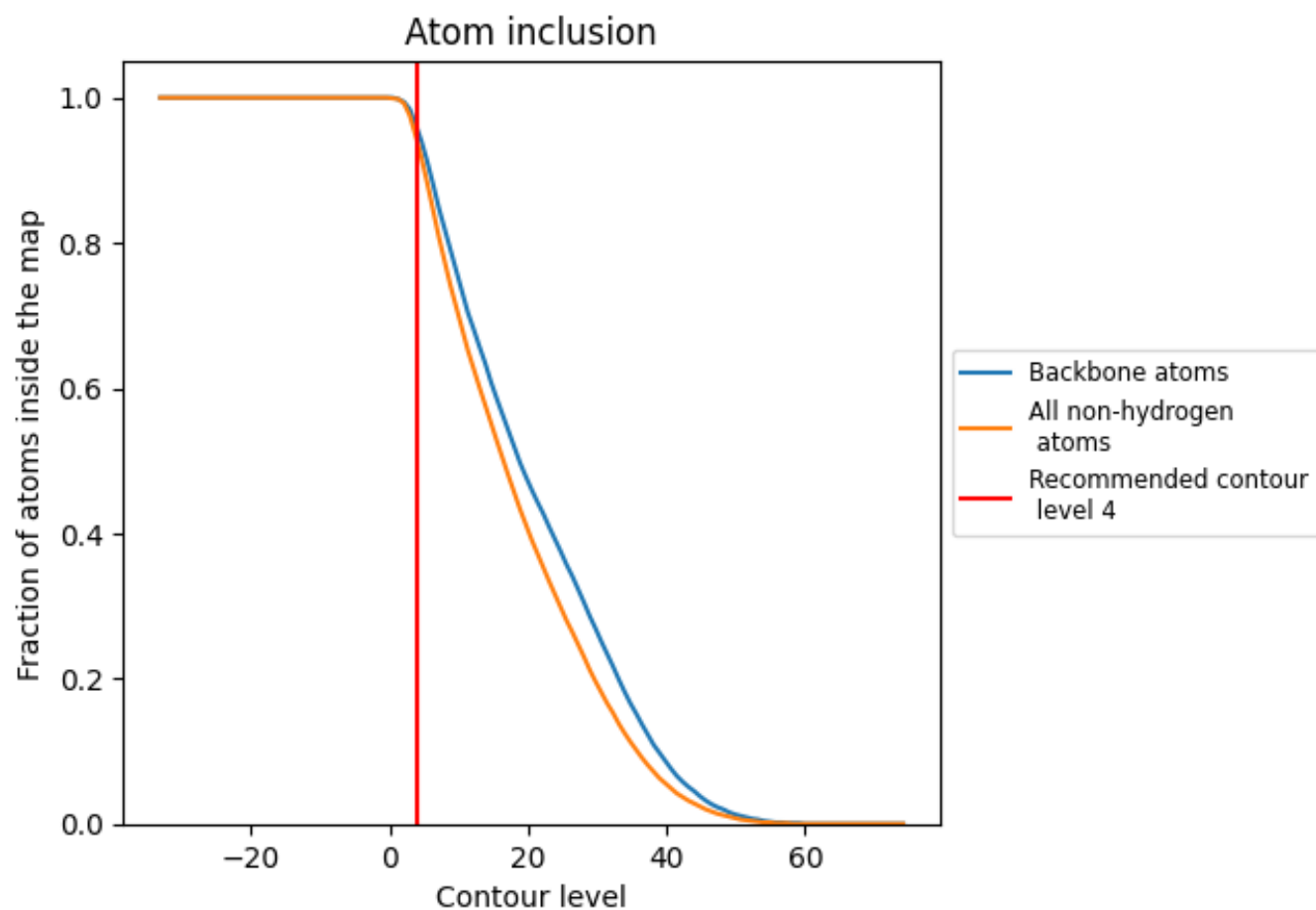
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9410	<div></div> 0.4800
A	<div></div> 0.9990	<div></div> 0.5200
B	<div></div> 0.9990	<div></div> 0.5530
C	<div></div> 0.9930	<div></div> 0.5460
D	<div></div> 0.9960	<div></div> 0.5230
E	<div></div> 0.9940	<div></div> 0.5600
F	<div></div> 0.9690	<div></div> 0.4230
G	<div></div> 0.9200	<div></div> 0.3790
H	<div></div> 0.9800	<div></div> 0.4200
I	<div></div> 0.8240	<div></div> 0.3480
J	<div></div> 0.8420	<div></div> 0.3510
K	<div></div> 0.6870	<div></div> 0.3410
L	<div></div> 0.8730	<div></div> 0.3670
M	<div></div> 0.5710	<div></div> 0.3150
N	<div></div> 0.9640	<div></div> 0.3590

1.0

0.0

<0.0