



## Full wwPDB EM Validation Report ⓘ

Jul 10, 2025 – 02:14 PM EDT

PDB ID : 7LZ6 / pdb\_00007lz6  
EMDB ID : EMD-23603  
Title : The Cryo-EM structure of a complex between GAD65 and b96.11 Fab  
Authors : Reboul, C.F.; Le, S.N.; Williams, D.E.; Buckle, A.M.  
Deposited on : 2021-03-09  
Resolution : 7.30 Å(reported)

This is a Full wwPDB EM Validation 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.dev118  
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) : 2.44

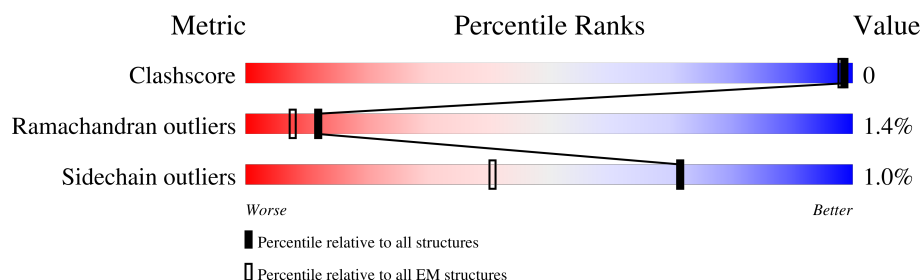
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.30 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	497	<div> <div>21%</div> <div>94%</div> <div>5%</div> </div>
1	B	497	<div> <div>22%</div> <div>94%</div> <div>6%</div> </div>
2	C	228	<div> <div>26%</div> <div>96%</div> <div>.</div> </div>
2	E	228	<div> <div>26%</div> <div>96%</div> <div>.</div> </div>
3	D	217	<div> <div>31%</div> <div>96%</div> <div>.</div> </div>
3	F	217	<div> <div>30%</div> <div>96%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14638 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 Glutamate decarboxylase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	497	Total	C	N	O	S	0	0
			3967	2546	669	719	33		
1	B	497	Total	C	N	O	S	0	0
			3967	2546	669	719	33		

- Molecule 2 is a protein called b96.11 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	228	Total	C	N	O	S	0	0
			1731	1097	290	338	6		
2	E	228	Total	C	N	O	S	0	0
			1731	1097	290	338	6		

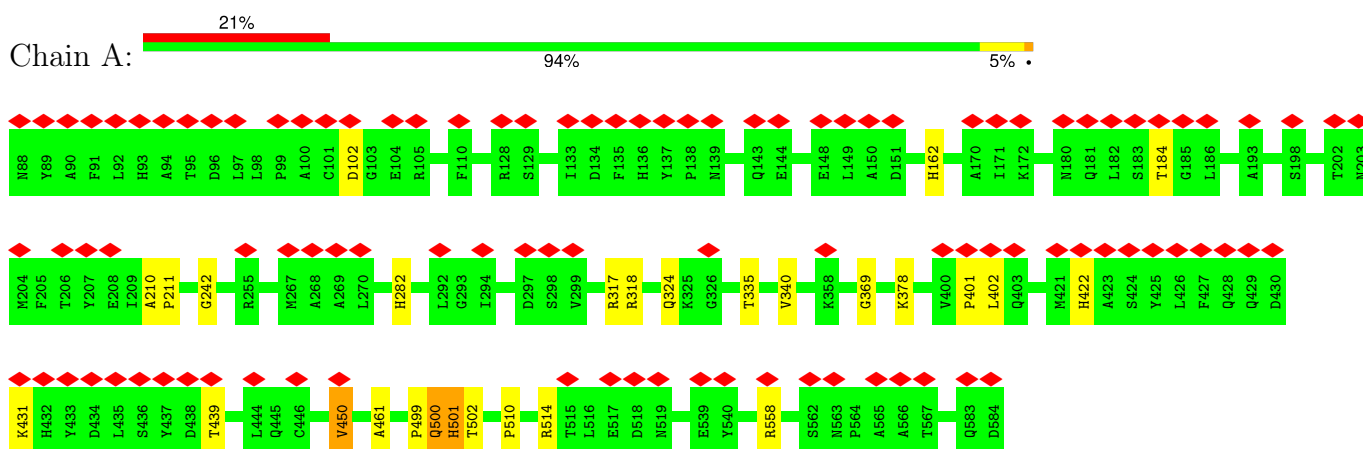
- Molecule 3 is a protein called b96.11 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	217	Total	C	N	O	S	0	0
			1621	1014	269	331	7		
3	F	217	Total	C	N	O	S	0	0
			1621	1014	269	331	7		

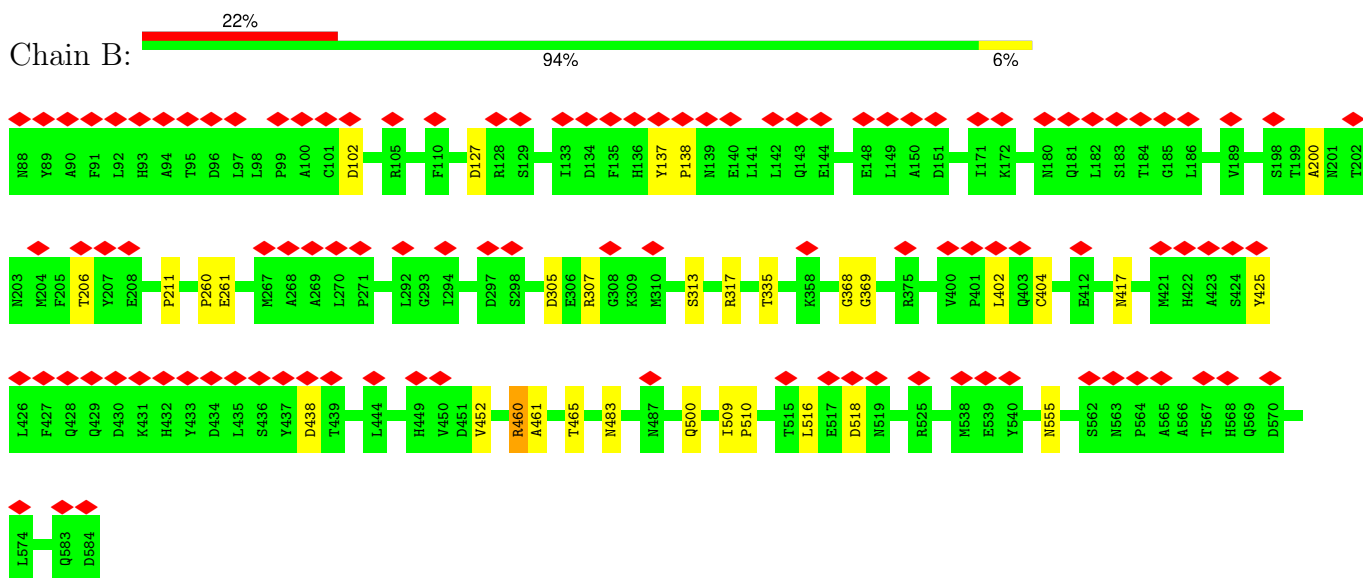
### 3 Residue-property plots

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: Glutamate decarboxylase 2

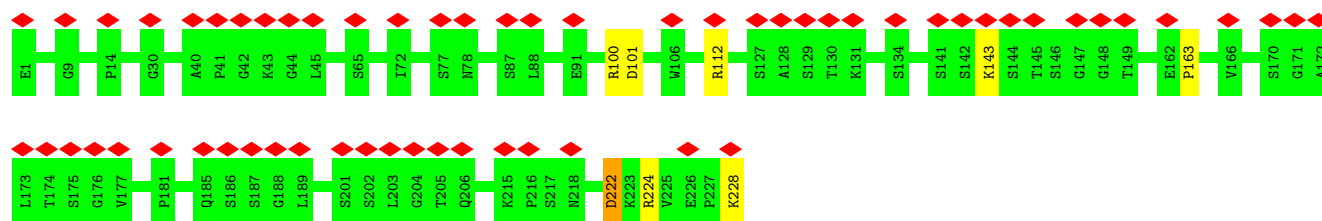


#### • Molecule 1: Glutamate decarboxylase 2

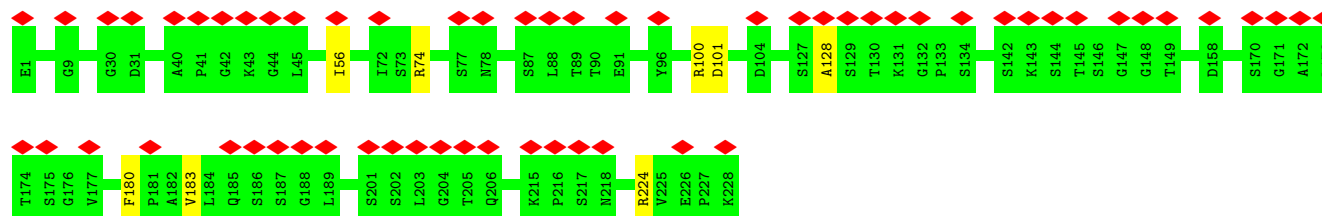


#### • Molecule 2: b96.11 Fab heavy chain

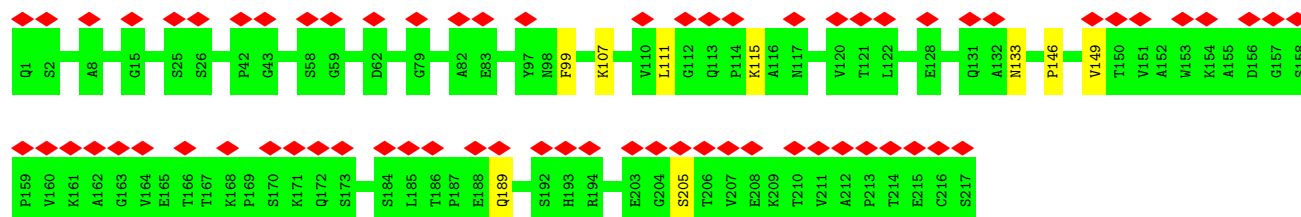




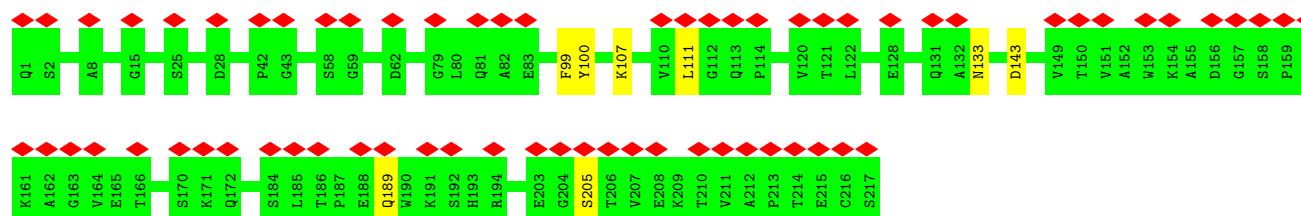
- Molecule 2: b96.11 Fab heavy chain



- Molecule 3: b96.11 Fab light chain



- Molecule 3: b96.11 Fab light chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	25700	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 ( $e^-/\text{\AA}^2$ )	63.63	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	0.032	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	305.27997, 305.27997, 305.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.90	0/4065	1.58	26/5497 (0.5%)
1	B	0.90	0/4065	1.57	33/5497 (0.6%)
2	C	0.86	0/1776	1.31	4/2416 (0.2%)
2	E	0.86	0/1776	1.33	3/2416 (0.1%)
3	D	0.85	0/1663	1.32	1/2264 (0.0%)
3	F	0.84	0/1663	1.31	0/2264
All	All	0.88	0/15008	1.46	67/20354 (0.3%)

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	2
1	B	0	2
2	E	0	2
All	All	0	6

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	500	GLN	N-CA-C	8.67	120.81	111.36
1	B	510	PRO	CA-C-O	-8.30	114.93	120.90
1	A	500	GLN	CA-C-N	8.11	136.30	121.70
1	A	500	GLN	C-N-CA	8.11	136.30	121.70
1	A	102	ASP	CA-C-N	7.73	128.56	119.98
1	A	102	ASP	C-N-CA	7.73	128.56	119.98
1	B	438	ASP	O-C-N	-7.45	116.02	123.62
1	B	500	GLN	CA-C-N	7.03	134.36	121.70
1	B	500	GLN	C-N-CA	7.03	134.36	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ARG	NE-CZ-NH1	6.55	128.05	121.50
2	E	180	PHE	CA-CB-CG	-6.38	107.42	113.80
1	B	368	GLY	CA-C-N	6.09	126.85	120.03
1	B	368	GLY	C-N-CA	6.09	126.85	120.03
1	B	438	ASP	CA-C-N	6.07	132.62	121.70
1	B	438	ASP	C-N-CA	6.07	132.62	121.70
1	A	317	ARG	NE-CZ-NH1	6.05	127.55	121.50
1	A	242	GLY	CA-C-N	6.01	126.65	119.98
1	A	242	GLY	C-N-CA	6.01	126.65	119.98
1	B	261	GLU	N-CA-C	5.93	119.34	111.75
2	C	101	ASP	CA-CB-CG	5.81	118.41	112.60
3	D	115	LYS	N-CA-C	5.81	117.62	111.28
1	A	318	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	A	402	LEU	N-CA-C	5.65	118.03	110.35
1	B	509	ILE	CA-C-N	5.65	123.78	119.66
1	B	509	ILE	C-N-CA	5.65	123.78	119.66
2	C	112	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	B	317	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	A	369	GLY	CA-C-N	5.56	126.26	120.03
1	A	369	GLY	C-N-CA	5.56	126.26	120.03
1	B	500	GLN	O-C-N	-5.53	115.85	122.15
1	B	260	PRO	CA-C-N	5.53	128.45	120.38
1	B	260	PRO	C-N-CA	5.53	128.45	120.38
1	A	450	VAL	CA-C-N	5.45	129.32	120.60
1	A	450	VAL	C-N-CA	5.45	129.32	120.60
1	B	137	TYR	CA-C-N	5.36	126.54	119.84
1	B	137	TYR	C-N-CA	5.36	126.54	119.84
1	A	378	LYS	CA-C-N	5.33	128.15	120.38
1	A	378	LYS	C-N-CA	5.33	128.15	120.38
1	A	422	HIS	CA-C-N	5.26	131.17	121.70
1	A	422	HIS	C-N-CA	5.26	131.17	121.70
1	B	402	LEU	N-CA-C	5.22	117.45	110.35
1	A	461	ALA	N-CA-C	5.21	117.04	111.36
1	A	431	LYS	N-CA-C	5.20	117.25	110.43
1	B	461	ALA	N-CA-C	5.20	117.03	111.36
1	B	516	LEU	CA-C-N	5.18	127.22	120.28
1	B	516	LEU	C-N-CA	5.18	127.22	120.28
2	C	143	LYS	N-CA-C	5.17	117.72	110.23
1	A	510	PRO	CA-C-N	5.16	126.29	119.84
1	A	510	PRO	C-N-CA	5.16	126.29	119.84
1	A	282	HIS	N-CA-C	5.16	117.36	110.35
2	E	101	ASP	CA-CB-CG	5.15	117.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	74	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	A	210	ALA	N-CA-C	5.12	116.93	109.30
1	B	425	TYR	CB-CA-C	5.12	119.82	110.10
1	A	340	VAL	N-CA-C	5.11	115.32	110.42
1	B	102	ASP	CA-C-N	5.09	125.60	120.00
1	B	102	ASP	C-N-CA	5.09	125.60	120.00
1	B	206	THR	CA-C-N	5.09	127.61	120.28
1	B	206	THR	C-N-CA	5.09	127.61	120.28
1	A	500	GLN	O-C-N	-5.08	115.84	122.59
1	B	369	GLY	CA-C-N	5.07	125.71	120.03
1	B	369	GLY	C-N-CA	5.07	125.71	120.03
1	B	417	ASN	CA-C-N	5.06	127.06	120.28
1	B	417	ASN	C-N-CA	5.06	127.06	120.28
1	B	452	VAL	N-CA-C	5.04	115.76	110.62
1	B	313	SER	N-CA-C	5.04	116.46	111.07
2	C	222	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	PRO	Peptide
1	A	558	ARG	Sidechain
1	B	200	ALA	Peptide
1	B	460	ARG	Sidechain
2	E	224	ARG	Sidechain
2	E	56	ILE	Peptide

## 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	3967	0	3936	2	0
1	B	3967	0	3936	1	0
2	C	1731	0	1678	1	0
2	E	1731	0	1678	0	0
3	D	1621	0	1557	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1621	0	1557	0	0
All	All	14638	0	14342	3	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (3) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:HIS:CE1	1:B:460:ARG:HH21	2.08	0.71
2:C:222:ASP:CG	2:C:224:ARG:HH12	2.21	0.49
1:A:501:HIS:CG	1:A:502:THR:H	2.39	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/497 (100%)	469 (95%)	20 (4%)	6 (1%)	11	44
1	B	495/497 (100%)	470 (95%)	19 (4%)	6 (1%)	11	44
2	C	226/228 (99%)	213 (94%)	12 (5%)	1 (0%)	30	68
2	E	226/228 (99%)	211 (93%)	14 (6%)	1 (0%)	30	68
3	D	215/217 (99%)	202 (94%)	7 (3%)	6 (3%)	4	24
3	F	215/217 (99%)	203 (94%)	6 (3%)	6 (3%)	4	24
All	All	1872/1884 (99%)	1768 (94%)	78 (4%)	26 (1%)	12	41

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	163	PRO
1	A	501	HIS
1	B	518	ASP
3	D	133	ASN
3	D	189	GLN
3	F	111	LEU
3	F	143	ASP
3	F	189	GLN
1	B	404	CYS
3	D	111	LEU
3	F	133	ASN
1	A	450	VAL
1	B	138	PRO
1	B	305	ASP
1	B	555	ASN
3	D	205	SER
3	F	99	PHE
3	F	205	SER
1	A	184	THR
3	D	99	PHE
2	E	128	ALA
1	A	211	PRO
1	A	499	PRO
1	A	500	GLN
1	B	211	PRO
3	D	146	PRO

### 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	425/425 (100%)	422 (99%)	3 (1%)	81	87
1	B	425/425 (100%)	420 (99%)	5 (1%)	67	78
2	C	192/192 (100%)	190 (99%)	2 (1%)	73	82
2	E	192/192 (100%)	190 (99%)	2 (1%)	73	82
3	D	181/181 (100%)	179 (99%)	2 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	181/181 (100%)	179 (99%)	2 (1%)	70	80
All	All	1596/1596 (100%)	1580 (99%)	16 (1%)	71	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	335	THR
1	A	439	THR
1	B	127	ASP
1	B	307	ARG
1	B	335	THR
1	B	465	THR
1	B	483	ASN
2	C	100	ARG
2	C	228	LYS
3	D	107	LYS
3	D	149	VAL
2	E	100	ARG
2	E	183	VAL
3	F	100	TYR
3	F	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	377	HIS
1	A	500	GLN
1	B	93	HIS
1	B	112	GLN
1	B	449	HIS
2	C	178	HIS
2	C	214	HIS
3	D	174	ASN
3	D	202	HIS
2	E	214	HIS
3	F	39	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 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 [i](#)

There are no chain breaks in this entry.

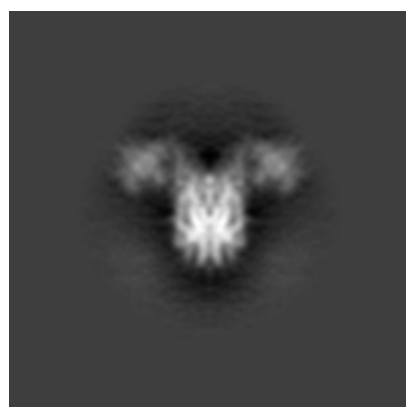
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23603. These allow visual inspection of the internal detail of the map and identification of artifacts.

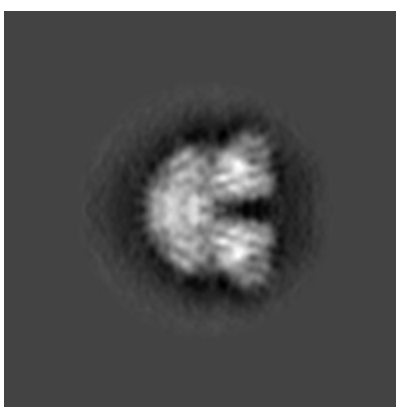
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

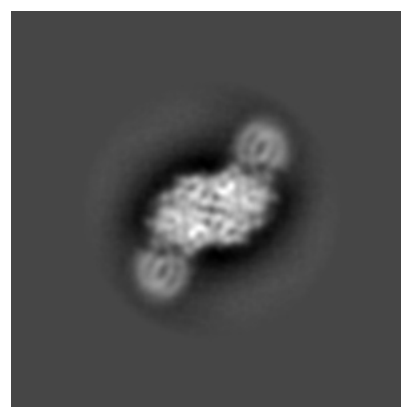
#### 6.1.1 Primary map



X



Y



Z

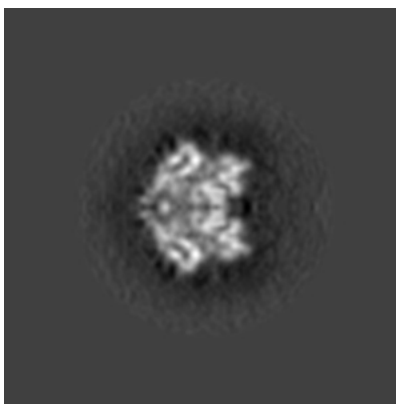
The images above show the map projected in three orthogonal directions.

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

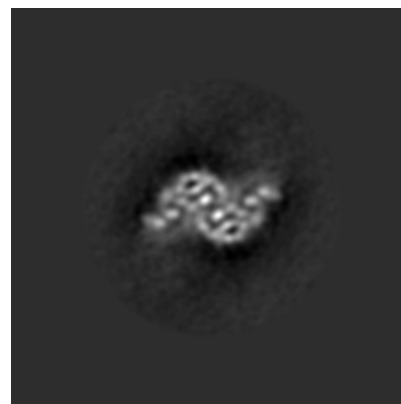
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

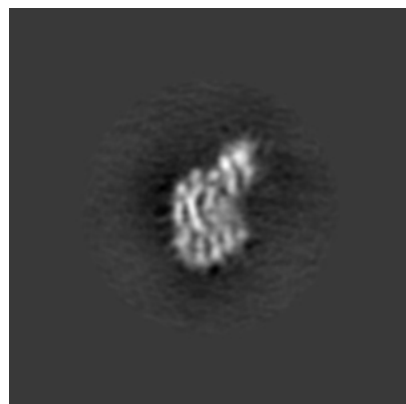


Z Index: 144

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

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

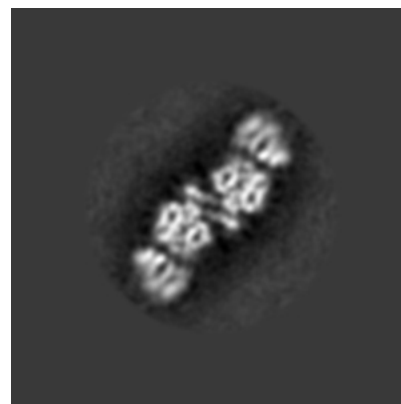
### 6.3.1 Primary map



X Index: 155



Y Index: 132

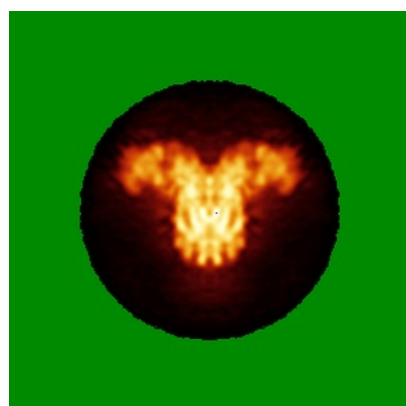


Z Index: 166

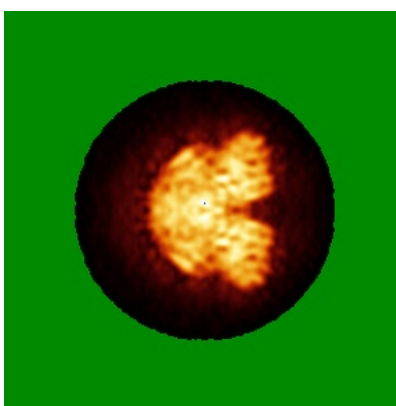
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y

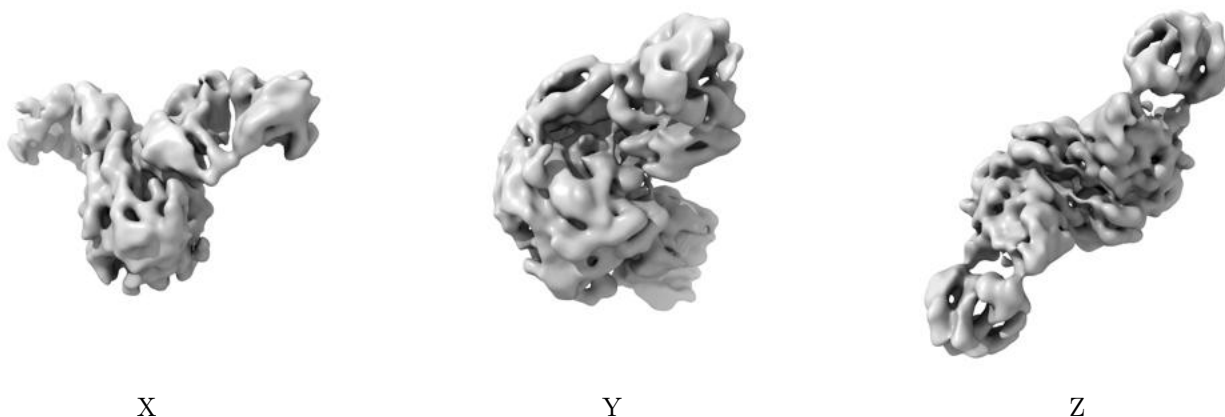


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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](#)

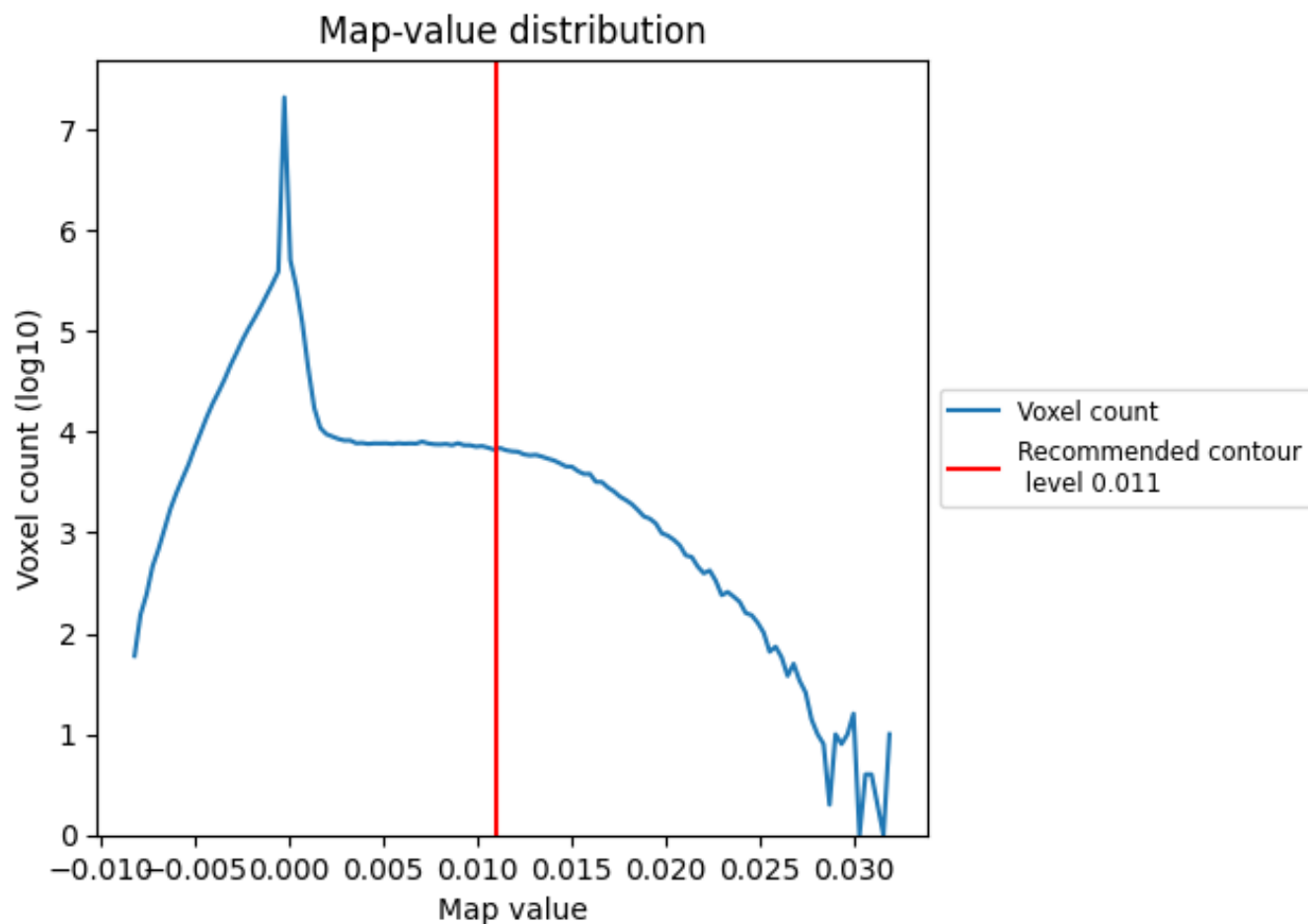
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

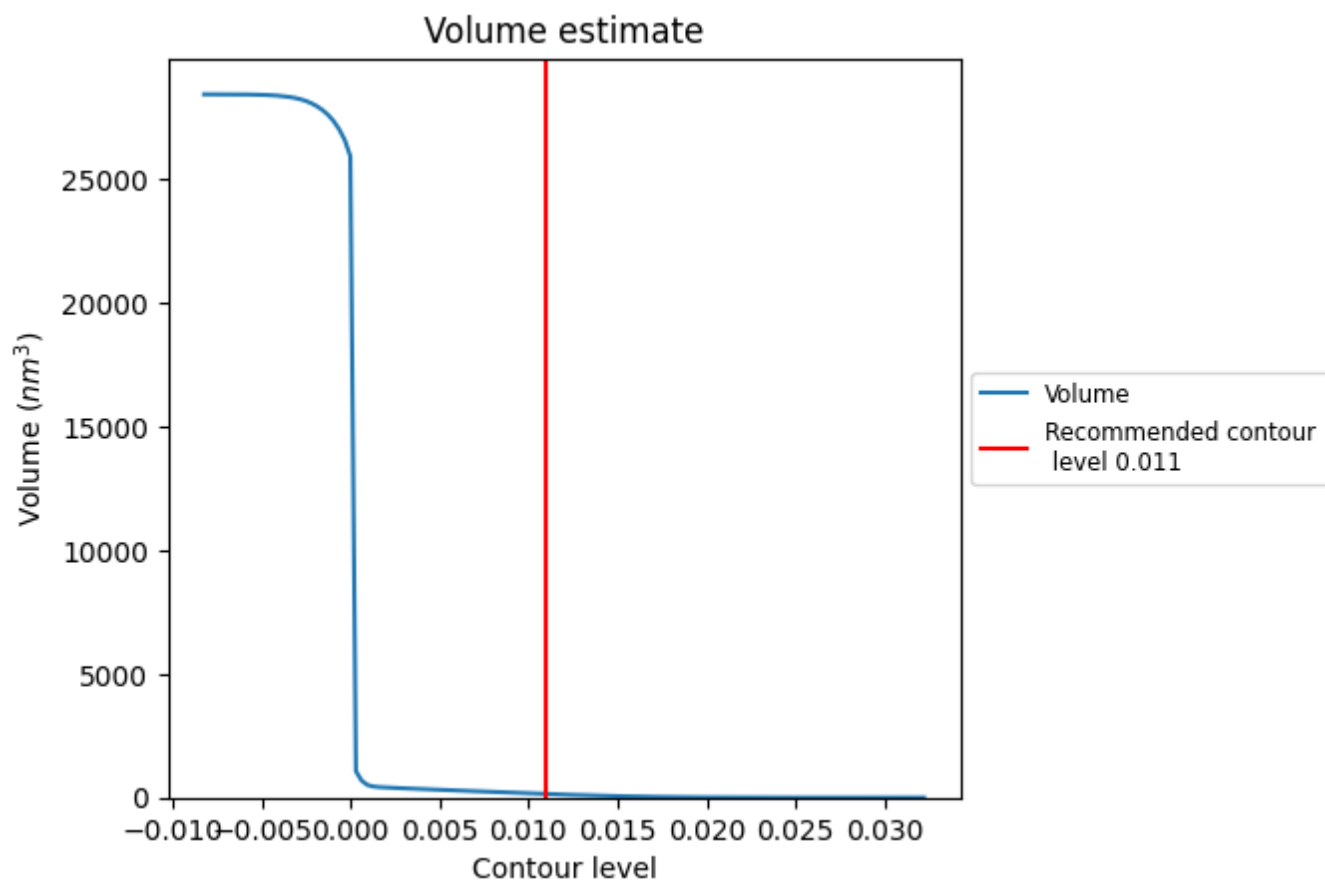
This section contains the results of statistical analysis of the map.

### 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.

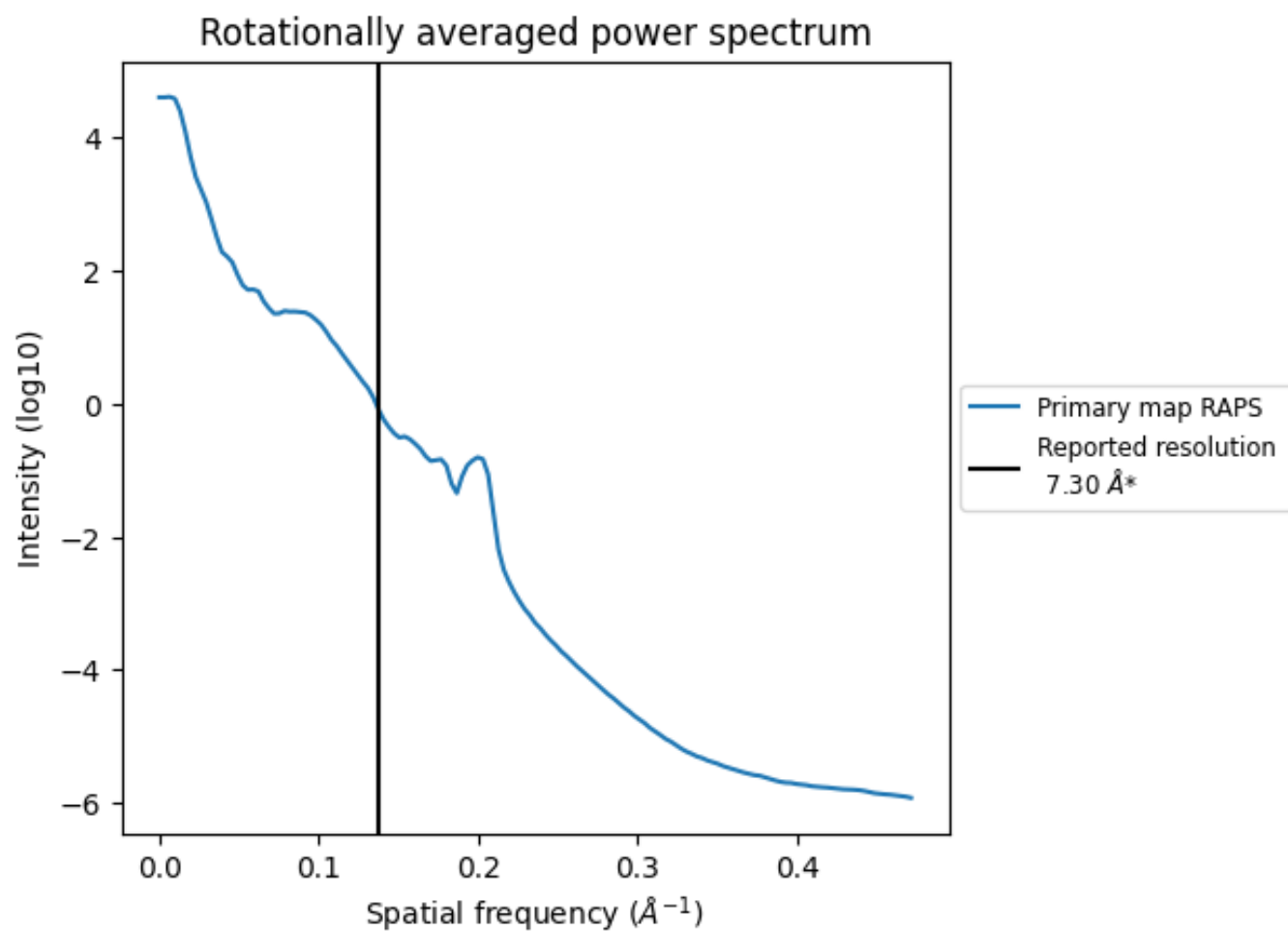
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm<sup>3</sup>; this corresponds to an approximate mass of 132 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 ⓘ

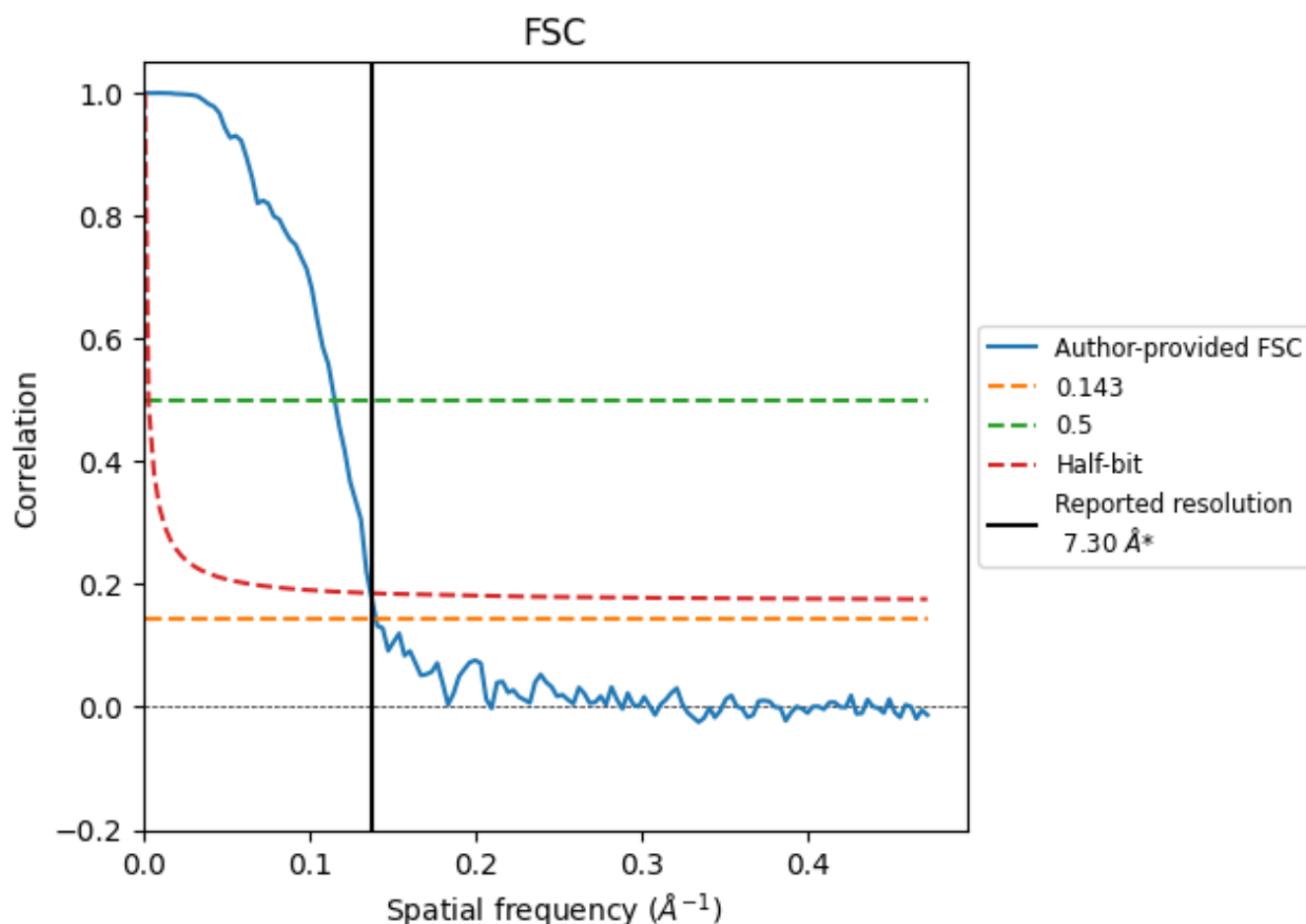


\*Reported resolution corresponds to spatial frequency of 0.137 Å<sup>-1</sup>

## 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 0.137 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

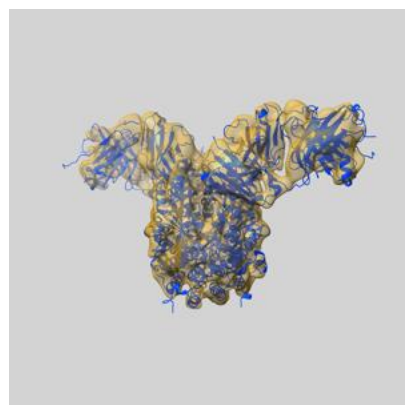
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	7.14	8.68	7.30
Unmasked-calculated*	-	-	-

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

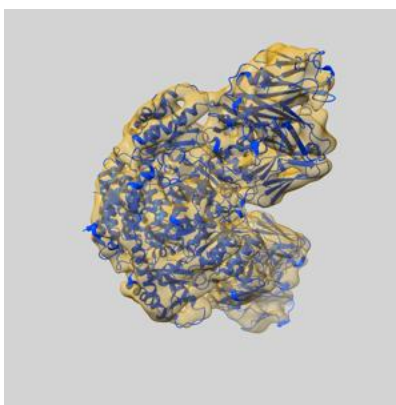
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23603 and PDB model 7LZ6. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

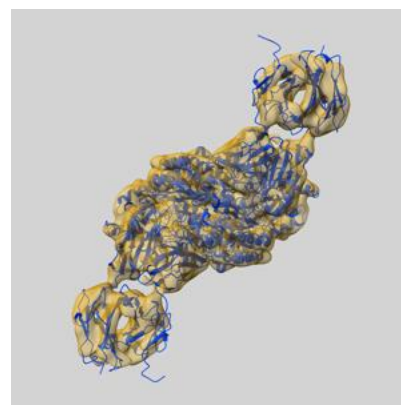
### 9.1 Map-model overlay [i](#)



X



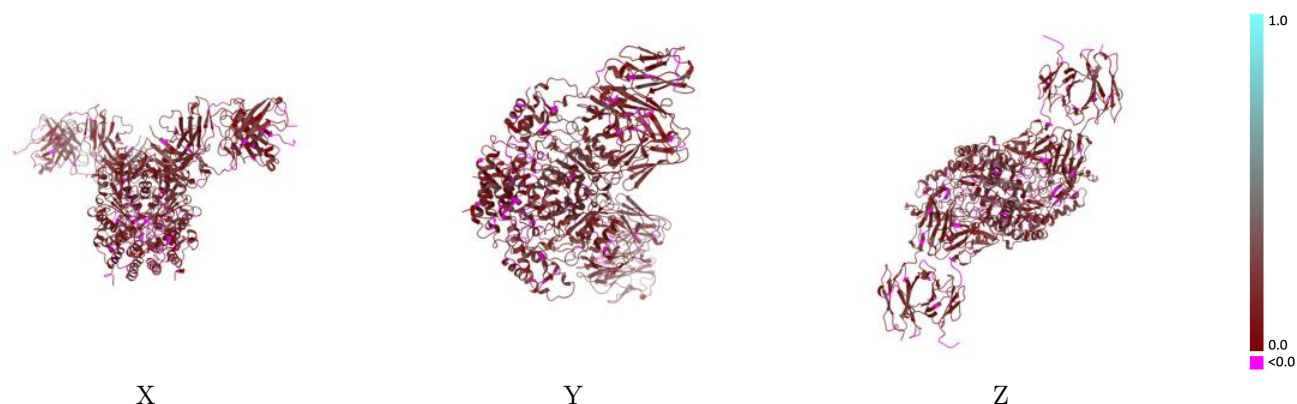
Y



Z

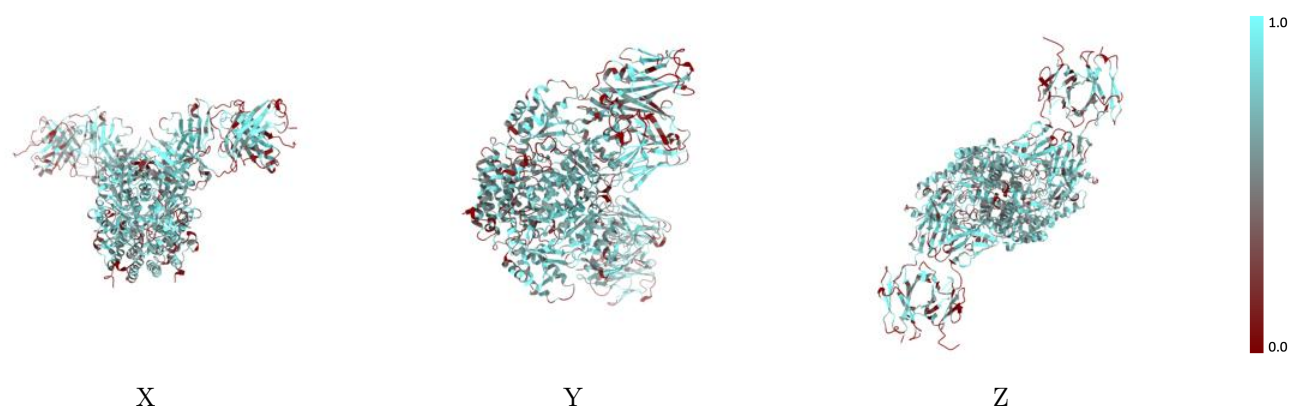
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



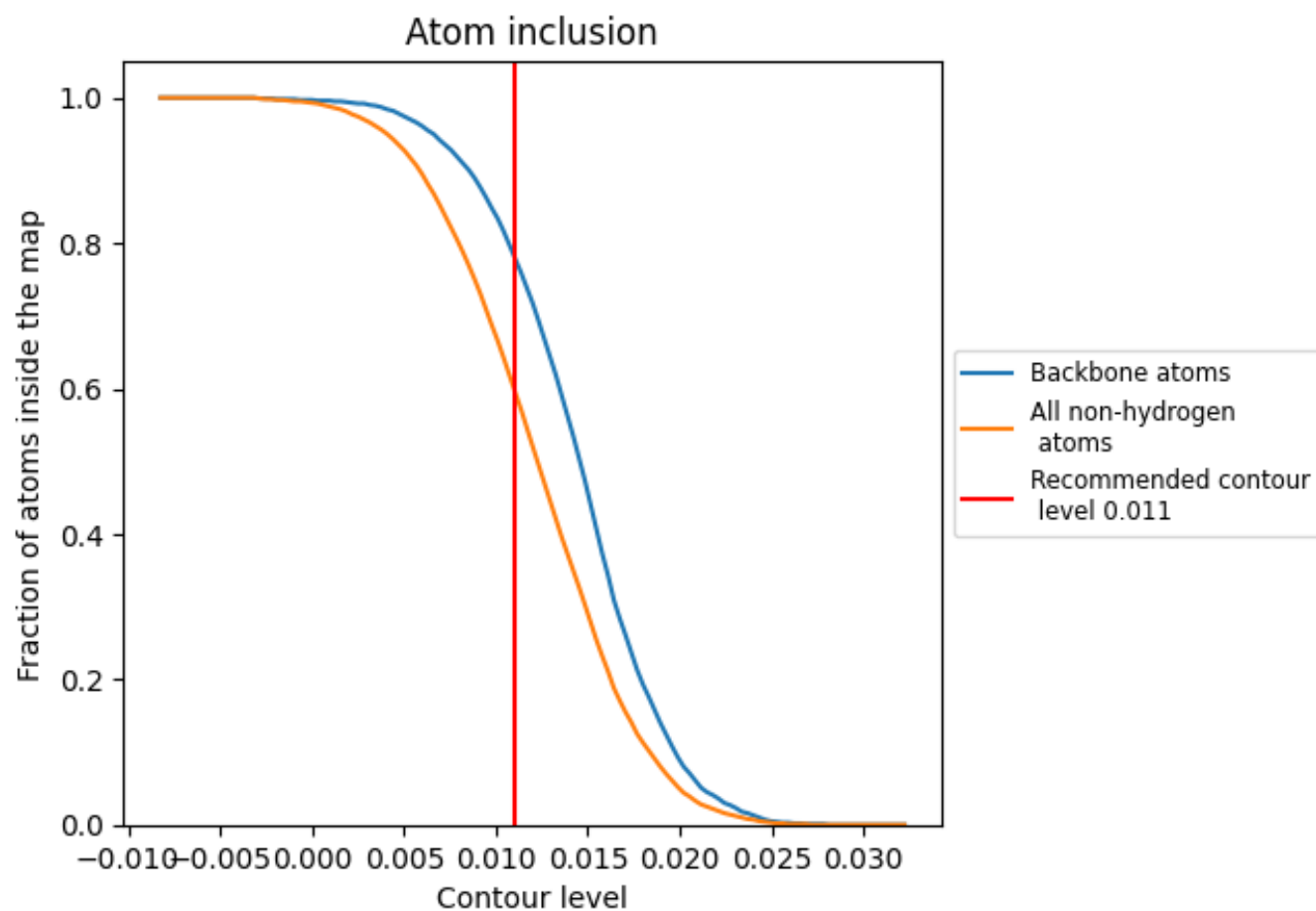
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 60% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5980	<div><div></div></div> 0.1390
A	<div><div></div></div> 0.6090	<div><div></div></div> 0.1330
B	<div><div></div></div> 0.6040	<div><div></div></div> 0.1320
C	<div><div></div></div> 0.5970	<div><div></div></div> 0.1510
D	<div><div></div></div> 0.5710	<div><div></div></div> 0.1420
E	<div><div></div></div> 0.6030	<div><div></div></div> 0.1500
F	<div><div></div></div> 0.5770	<div><div></div></div> 0.1430

1.0

0.0

<0.0