



## wwPDB EM Validation Summary Report ⓘ

Jul 13, 2025 – 12:17 AM JST

PDB ID : 9J5M / pdb\_00009j5m  
EMDB ID : EMD-61146  
Title : Cryo-EM structure of the ectodomain of BTN2A1-BTN3A1-BTN3A2 in complex with gdTCR  
Authors : Zhu, Y.; Gao, W.; Huang, Z.  
Deposited on : 2024-08-12  
Resolution : 3.94 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>.

---

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

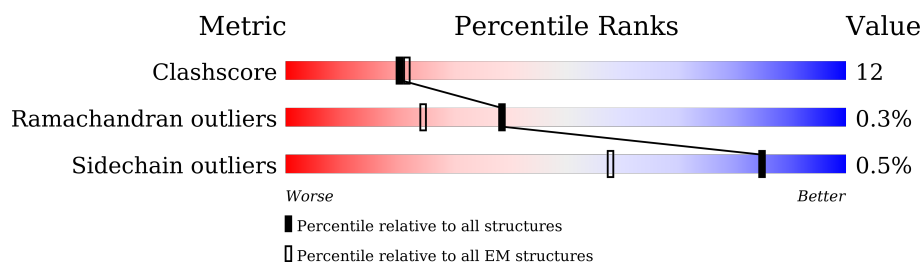
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.94 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	205	 8% 78% 22%
1	H	205	 67% 30% .
2	B	230	 5% 70% 29%
2	I	230	 80% 19%
3	C	305	 56% 14% 30%
4	D	484	 33% 12% 56%
5	E	499	 35% 8% 57%
5	G	499	 32% 10% 57%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12892 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 d subunit of gdTCR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	205	Total	C	N	O	S	0	0
			1399	878	244	271	6		
1	H	205	Total	C	N	O	S	0	0
			1585	1006	262	309	8		

- Molecule 2 is a protein called g subunit of gdTCR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	230	Total	C	N	O	S	0	0
			1732	1108	279	339	6		
2	I	229	Total	C	N	O	S	0	0
			1799	1146	301	346	6		

- Molecule 3 is a protein called Butyrophilin subfamily 3 member A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	215	Total	C	N	O	S	0	0
			1579	1000	269	303	7		

- Molecule 4 is a protein called Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1607	1010	274	315	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	427	THR	PRO	variant	UNP O00481

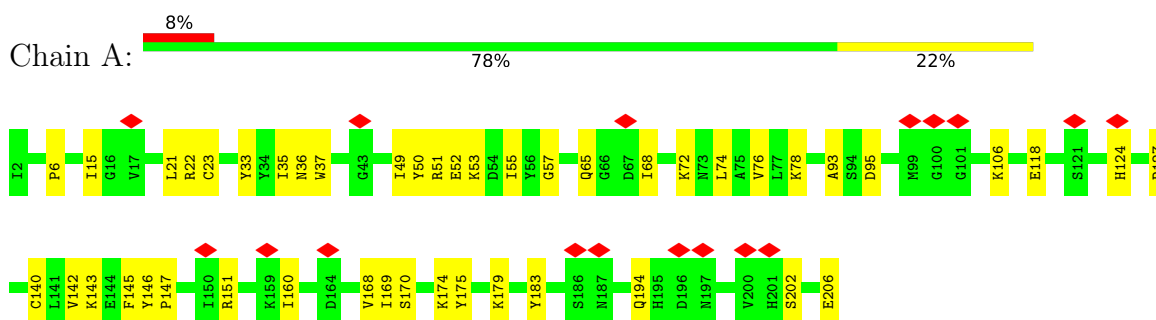
- Molecule 5 is a protein called Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1628	1031	284	302	11		
5	G	214	Total	C	N	O	S	0	0
			1563	989	271	293	10		

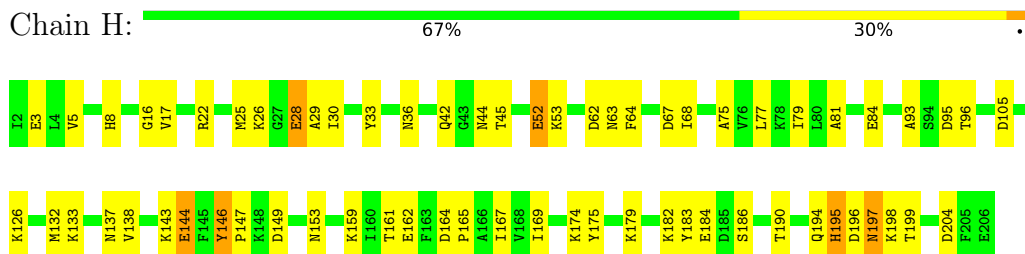
### 3 Residue-property plots

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.

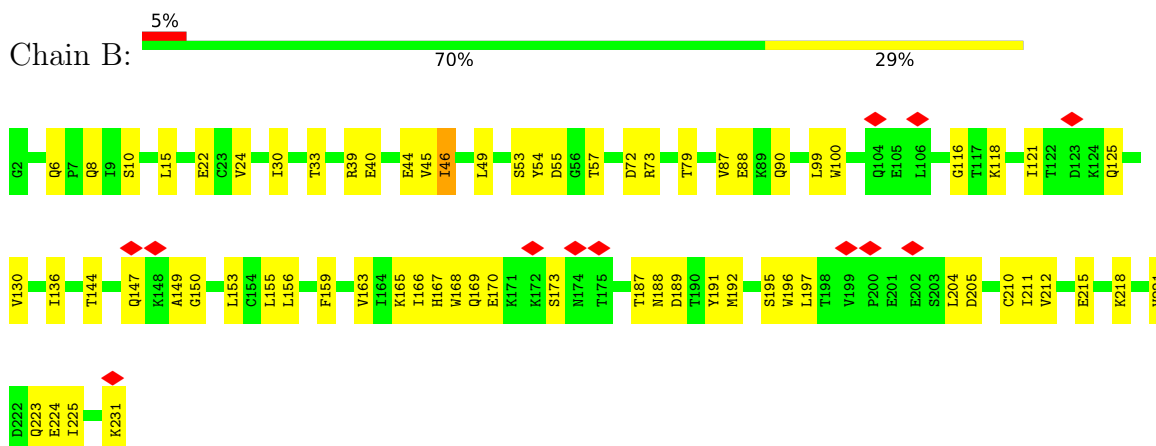
- Molecule 1: d subunit of gdTCR



- Molecule 1: d subunit of gdTCR

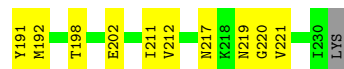


- Molecule 2: g subunit of gdTCR

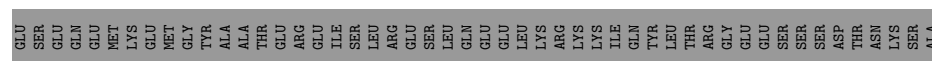
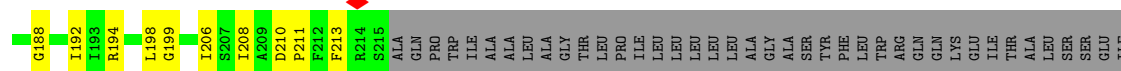


- Molecule 2: g subunit of gdTCR

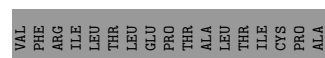
19%



- 30%



- 56%



- 57%

Q1	M189	ARG	VAL	LYS	SER
P7	Q200	ARG	ARG	GLY	HIS
T20	K201	ALA	CYS	ILE	THR
L21	K202	LEU	PRO	THR	THR
N30	I208	LEU	PRO	CYS	PRO
A31	P209	LEU	ARG	ARG	ARG
E35	F212	LEU	HIS	ILE	PRO
E82	M213	GLY	GLN	PRO	GLY
E63	P214	GLY	ASN	ASN	ASN
Y64	S215	GLY	THR	THR	THR
R65	VAL	LEU	PRO	VAL	VAL
F70	SER	GLU	ASP	GLU	GLU
I76	PRO	GLU	PRO	PRO	PRO
V80	ALA	GLU	ARG	GLU	GLU
A81	VAL	GLN	PHE	LEU	LEU
I82	LEU	LYS	ASP	LYS	LYS
I83	ILE	PRO	GLN	ALA	ALA
Q100	VAL	CYS	VAL	ASP	ASP
R103	VAL	LEU	LEU	PRO	PRO
L110	MET	ARG	GLY	ILE	ILE
G118	ILE	TRP	SER	CYS	PRO
M125	PRO	ARG	ALA	ALA	ALA
R126	VAL	THR	SER	THR	THR
G127	CYS	LEU	GLY	LYS	LYS
H128	ILE	LEU	LEU	GLY	GLY
G132	TRP	ALA	TYR	SER	SER
I133	ILE	VAL	TRP	CYS	CYS
R134	ASN	VAL	GLU	THR	THR
S139	LEU	VAL	VAL	PRO	PRO
W142	GLN	ASP	GLU	ASN	ASN
D152	LYS	PRO	ASP	VAL	VAL
G156	ILE	THR	THR	ILE	ILE
D170	SER	ASP	VAL	GLY	GLY
G171	GLY	LEU	VAL	VAL	VAL
L172	LYS	GLY	PHE	SER	SER
F173	LYS	LEU	CYS	THR	THR
M174	GLU	GLY	ASP	HIS	HIS
I181	PHE	ASP	GLN	TYR	TYR
V186	GLU	ASP	SER	ASN	ASN
	ARG	ARG	VAL	MET	MET
	THR	ARG	GLU	ARG	ARG
		THR	ASP	LEU	LEU
			ARG	ARG	ARG

● Molecule 5: Butyrophilin subfamily 2 member A1



GLN	F2	GLN	VAL	GLN	LEU
F2	I3	I3	F2	GLN	LEU
V4	V4	V4	I3	LYS	GLY
P7	P7	P7	V4	LYS	GLY
T8	T8	T8	P7	LYS	GLY
D9	D9	D9	T8	ILE	ILE
P10	P10	P10	D9	LEU	LEU
L25	L25	L25	P10	SER	SER
S26	S26	S26	L25	GLY	GLY
P27	P27	P27	S26	GLY	GLY
E35	E35	E35	P27	LYS	LYS
V36	V36	V36	E35	GLY	GLY
R37	R37	R37	V36	ARG	ARG
Q42	Q42	Q42	R37	GLU	GLU
F43	F43	F43	Q42	THR	THR
S44	S44	S44	F43	ARG	ARG
P45	P45	P45	S44	VAL	VAL
V49	V49	V49	P45	LYS	LYS
Y50	Y50	Y50	V49	ARG	ARG
K51	K51	K51	Y50	HIS	HIS
R54	R54	R54	K51	LEU	LEU
E55	E55	E55	R54	GLY	GLY
R56	R56	R56	E55	GLY	GLY
T57	T57	T57	R56	GLY	GLY
E58	E58	E58	T57	VAL	VAL
Q60	Q60	Q60	E58	PRO	PRO
M61	M61	M61	Q60	ASP	ASP
E62	E62	E62	M61	ASN	ASN
E63	E63	E63	E62	GLU	GLU
V71	V71	V71	E63	CYS	CYS
S72	S72	S72	V71	ALA	ALA
S76	S76	S76	S72	VAL	VAL
R77	R77	R77	S76	PRO	PRO
V83	V83	V83	R77	ILE	ILE
I84	I84	I84	V83	LEU	LEU
I87	I87	I87	I84	GLY	GLY
Q90	Q90	Q90	I87	ARG	ARG
Y98	Y98	Y98	Q90	THR	THR
F99	F99	F99	Y98	ARG	ARG
Q100	Q100	Q100	F99	ALA	ALA
E101	E101	E101	Q100	GLY	GLY
G102	G102	G102	E101	LYS	LYS
R103	R103	R103	G102	LEU	LEU
S104	S104	S104	R103	THR	THR
Y105	Y105	Y105	S104	VAL	VAL
D106	D106	D106	Y105	GLY	GLY
E107	E107	E107	D106	VAL	VAL
K120	K120	K120	E107	LEU	LEU
P121	P121	P121	K120	ASP	ASP
G127	G127	G127	P121	PRO	PRO
G131	G131	G131	G127	THR	THR
R134	R134	R134	G131	ALA	ALA
E136	E136	E136	R134	HIS	HIS
D152	D152	D152	E136	PRO	PRO
G156	G156	G156	D152	ASP	ASP
A160	A160	A160	G156	VAL	VAL
D170	D170	D170	A160	GLY	GLY
M174	M174	M174	D170	VAL	VAL
V179	V179	V179	M174	VAL	VAL
D183	D183	D183	V179	LEU	LEU
K184	K184	K184	D183	LEU	LEU
Q200	Q200	Q200	K184	GLY	GLY
P214	P214	P214	Q200	GLY	GLY
S215	S215	S215	P214	TRP	TRP
VAL	VAL	VAL	S215	THR	THR
SER	SER	SER	VAL	LEU	LEU
PRO	PRO	PRO	SER	LEU	LEU
CYS	CYS	CYS	PRO	GLY	GLY
ALA	ALA	ALA	CYS	ALA	ALA
VAL	VAL	VAL	ALA	VAL	VAL
LEU	LEU	LEU	VAL	LEU	LEU
GLN	GLN	GLN	LEU	GLY	GLY
VAL	VAL	VAL	GLN	ASP	ASP
LYS	LYS	LYS	VAL	THR	THR
ILE	ILE	ILE	LYS	GLN	GLN
THR	THR	THR	ILE	THR	THR
PRO	PRO	PRO	THR	LEU	LEU
ASP	ASP	ASP	PRO	GLY	GLY
ASN	ASN	ASN	ASP	VAL	VAL
GLU	GLU	GLU	ASN	GLY	GLY
LEU	LEU	LEU	GLU	THR	THR
THR	THR	THR	LEU	ASP	ASP
GLY	GLY	GLY	THR	VAL	VAL
VAL	VAL	VAL	GLY	GLY	GLY
PRO	PRO	PRO	VAL	VAL	VAL
GLU	GLU	GLU	PRO	VAL	VAL
LEU	LEU	LEU	GLU	THR	THR
GLY	GLY	GLY	LEU	ASP	ASP
THR	THR	THR	GLY	VAL	VAL
ALA	ALA	ALA	THR	GLY	GLY
GLY	GLY	GLY	ALA	THR	THR
HIS	HIS	HIS	GLY	ASP	ASP
LEU	LEU	LEU	HIS	VAL	VAL
SER	SER	SER	LEU	GLY	GLY
LEU	LEU	LEU	SER	THR	THR
LEU	LEU	LEU	LEU	ASP	ASP
LEU	LEU	LEU	LEU	VAL	VAL
LEU	LEU	LEU	LEU	GLY	GLY

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287533	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.395	Depositor
Minimum map value	-0.435	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.26	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.13	0/1424	0.37	0/1951
1	H	0.19	0/1620	0.59	1/2196 (0.0%)
2	B	0.14	0/1769	0.38	0/2415
2	I	0.14	0/1838	0.42	0/2494
3	C	0.14	0/1612	0.41	0/2194
4	D	0.13	0/1639	0.37	0/2225
5	E	0.13	0/1664	0.34	0/2261
5	G	0.17	0/1595	0.50	0/2173
All	All	0.15	0/13161	0.43	1/17909 (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
1	H	0	2
5	G	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	52	GLU	CA-CB-CG	5.04	124.17	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	26	SER	Peptide
5	G	44	SER	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	H	146	TYR	Peptide
1	H	28	GLU	Peptide

## 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	1399	0	1244	30	0
1	H	1585	0	1542	51	0
2	B	1732	0	1662	47	0
2	I	1799	0	1782	32	0
3	C	1579	0	1521	33	0
4	D	1607	0	1570	42	0
5	E	1628	0	1578	31	0
5	G	1563	0	1488	45	0
All	All	12892	0	12387	303	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 12.

The worst 5 of 303 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:G:51:LYS:HE3	5:G:56:ARG:HH22	1.44	0.81
1:A:22:ARG:HB3	1:A:74:LEU:HD11	1.64	0.79
2:I:139:PRO:HB3	2:I:151:THR:H	1.48	0.78
4:D:124:ASP:HB3	4:D:136:GLU:HB2	1.67	0.77
1:A:65:GLN:HB2	1:A:78:LYS:HB3	1.67	0.77

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	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
1	H	203/205 (99%)	161 (79%)	39 (19%)	3 (2%)	8	38
2	B	228/230 (99%)	216 (95%)	11 (5%)	1 (0%)	30	65
2	I	227/230 (99%)	205 (90%)	22 (10%)	0	100	100
3	C	213/305 (70%)	198 (93%)	15 (7%)	0	100	100
4	D	213/484 (44%)	202 (95%)	11 (5%)	0	100	100
5	E	213/499 (43%)	203 (95%)	10 (5%)	0	100	100
5	G	212/499 (42%)	176 (83%)	35 (16%)	1 (0%)	25	60
All	All	1712/2657 (64%)	1556 (91%)	151 (9%)	5 (0%)	38	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	144	GLU
1	H	197	ASN
2	B	188	ASN
5	G	35	GLU
1	H	79	ILE

### 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	128/180 (71%)	127 (99%)	1 (1%)	79	84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	175/180 (97%)	172 (98%)	3 (2%)	56	72
2	B	186/209 (89%)	184 (99%)	2 (1%)	70	79
2	I	201/209 (96%)	200 (100%)	1 (0%)	86	89
3	C	161/249 (65%)	161 (100%)	0	100	100
4	D	172/412 (42%)	172 (100%)	0	100	100
5	E	172/443 (39%)	172 (100%)	0	100	100
5	G	159/443 (36%)	159 (100%)	0	100	100
All	All	1354/2325 (58%)	1347 (100%)	7 (0%)	85	89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	8	HIS
1	H	190	THR
2	I	172	LYS
1	H	195	HIS
2	B	136	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
5	G	42	GLN
1	H	36	ASN
1	H	201	HIS
2	B	167	HIS
1	A	32	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

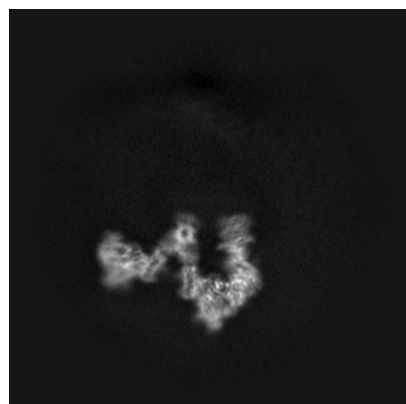
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61146. These allow visual inspection of the internal detail of the map and identification of artifacts.

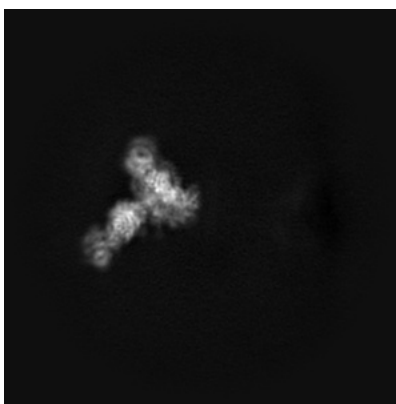
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

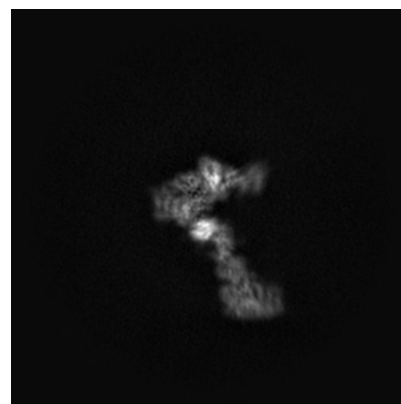
#### 6.1.1 Primary map



X

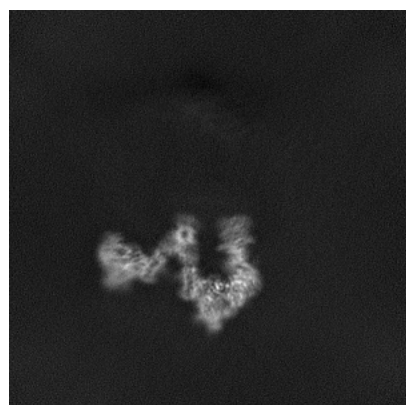


Y

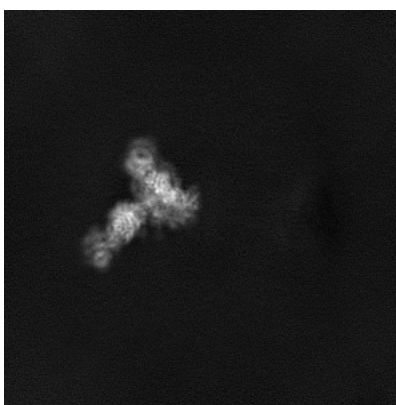


Z

#### 6.1.2 Raw map



X



Y

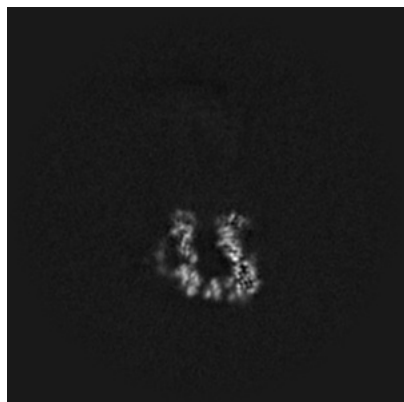


Z

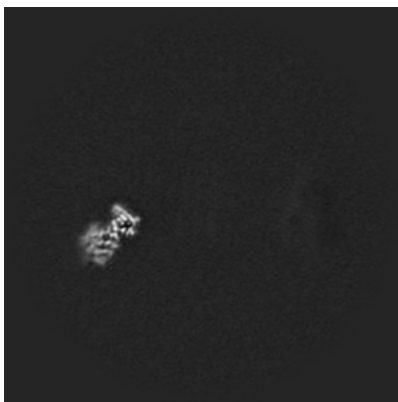
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

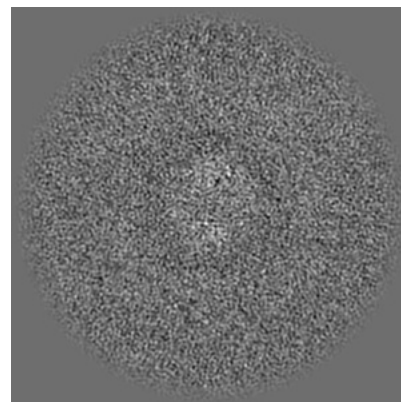
### 6.2.1 Primary map



X Index: 200

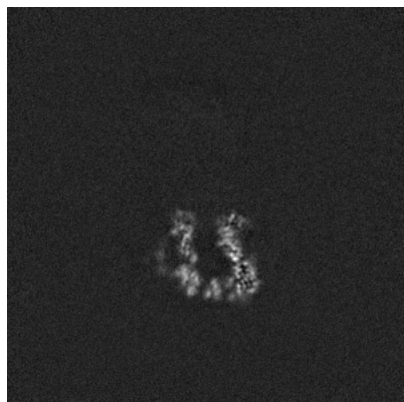


Y Index: 200



Z Index: 200

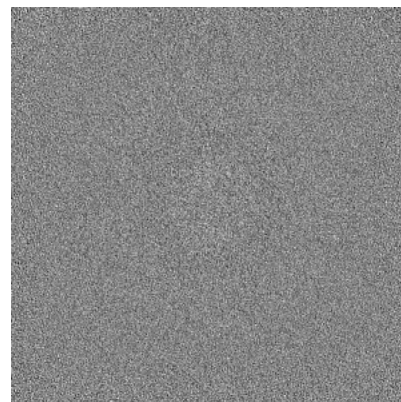
### 6.2.2 Raw map



X Index: 200



Y Index: 200



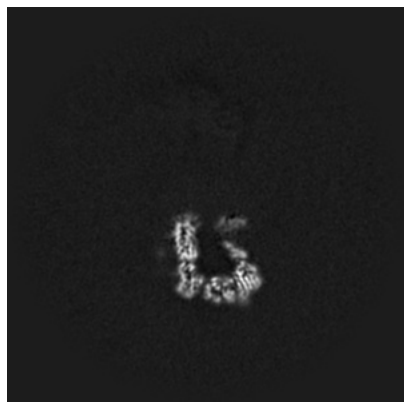
Z Index: 200

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

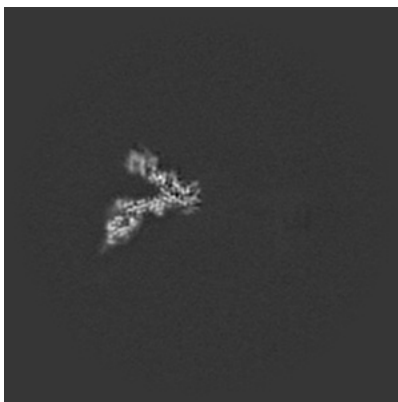


## 6.3 Largest variance slices [i](#)

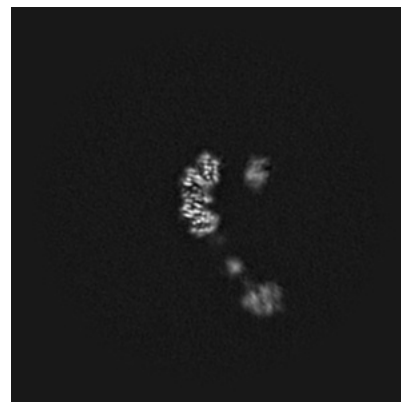
### 6.3.1 Primary map



X Index: 195

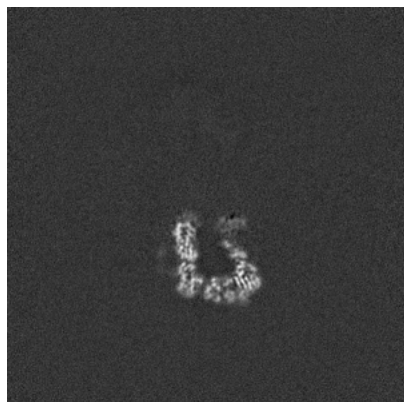


Y Index: 230

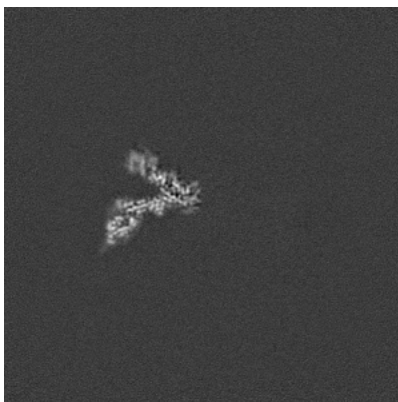


Z Index: 127

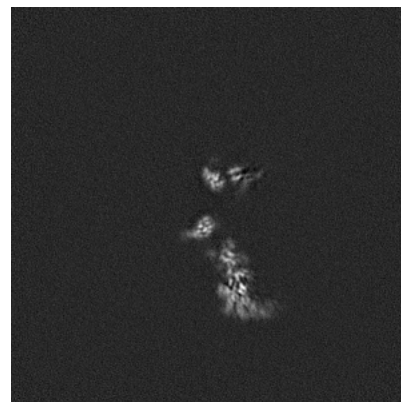
### 6.3.2 Raw map



X Index: 196



Y Index: 230



Z Index: 153

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

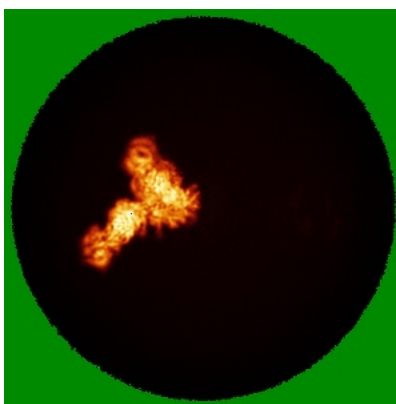


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X



Y

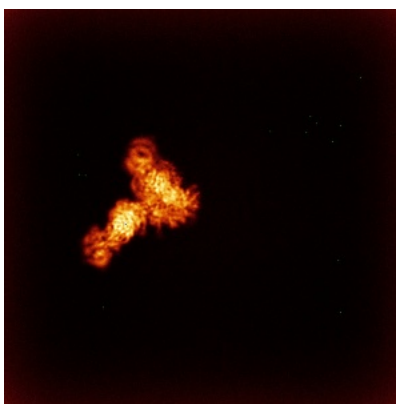


Z

### 6.4.2 Raw map



X



Y

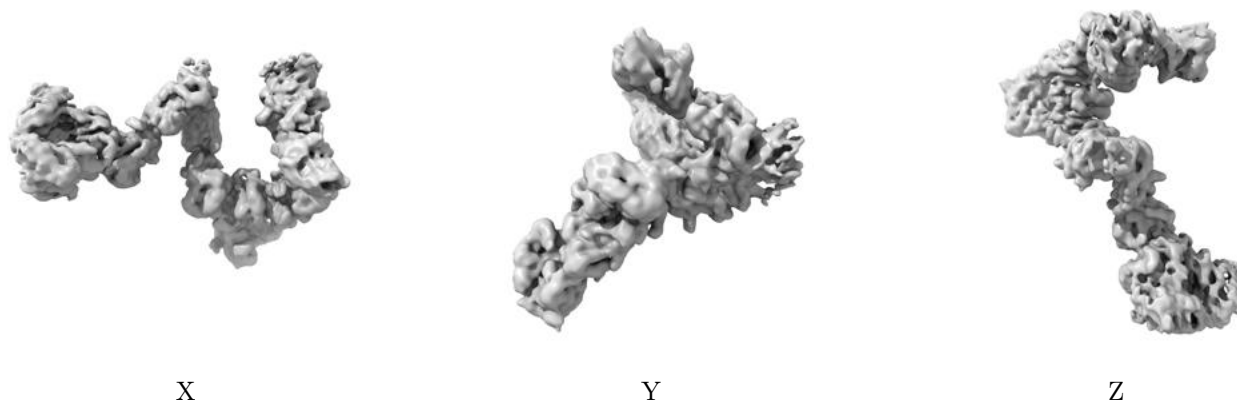


Z

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.

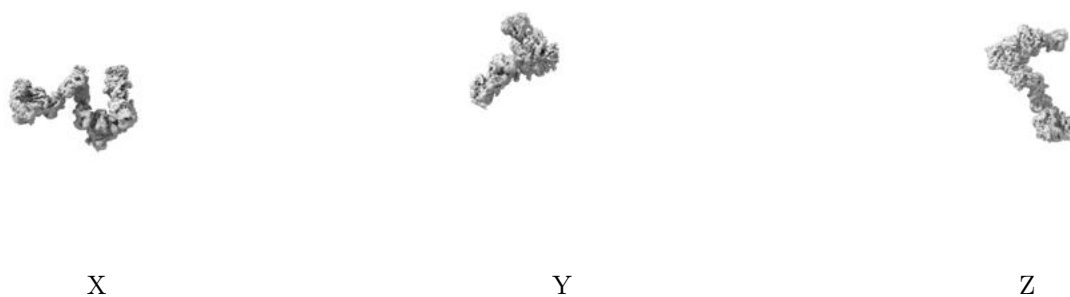
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

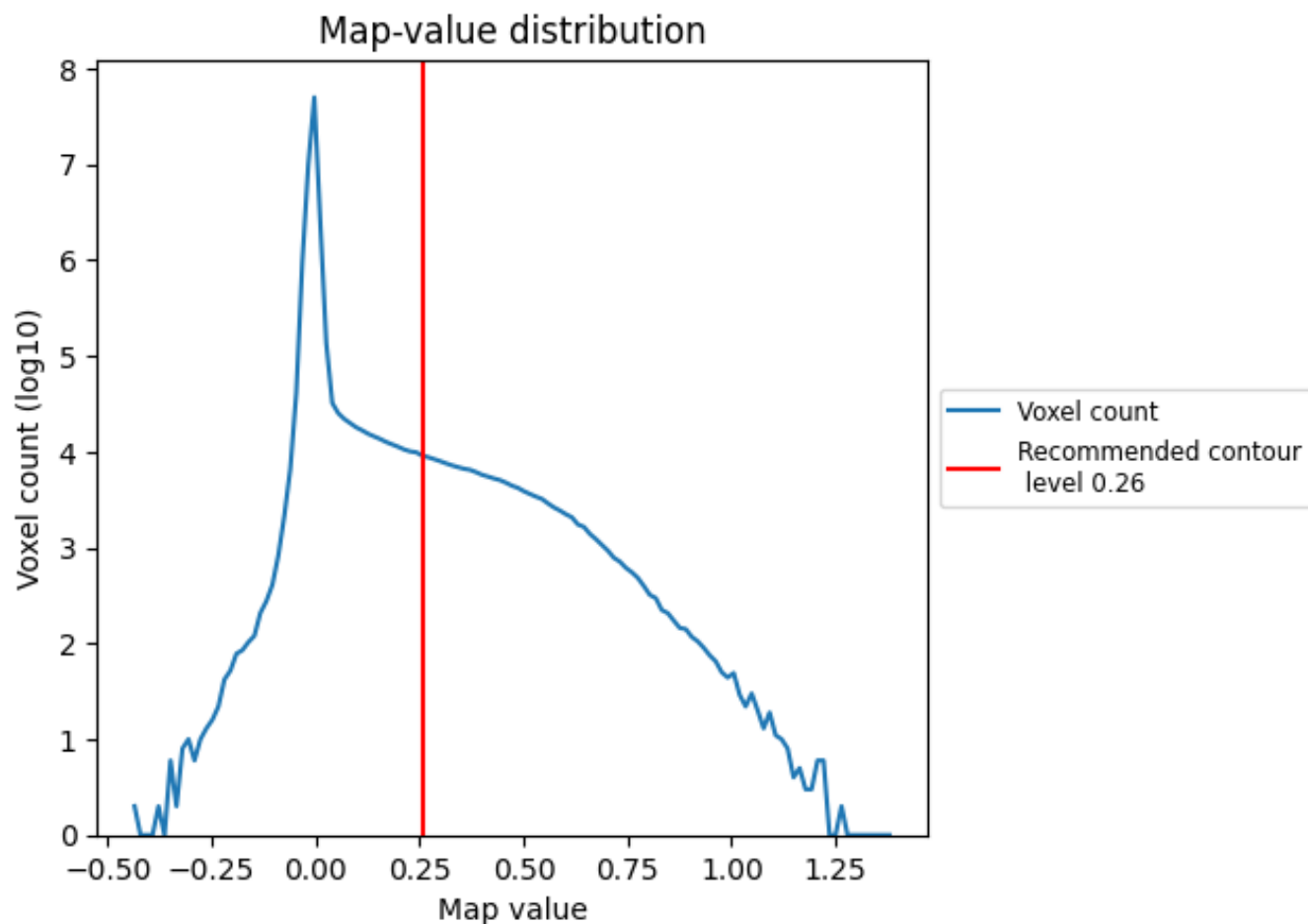
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

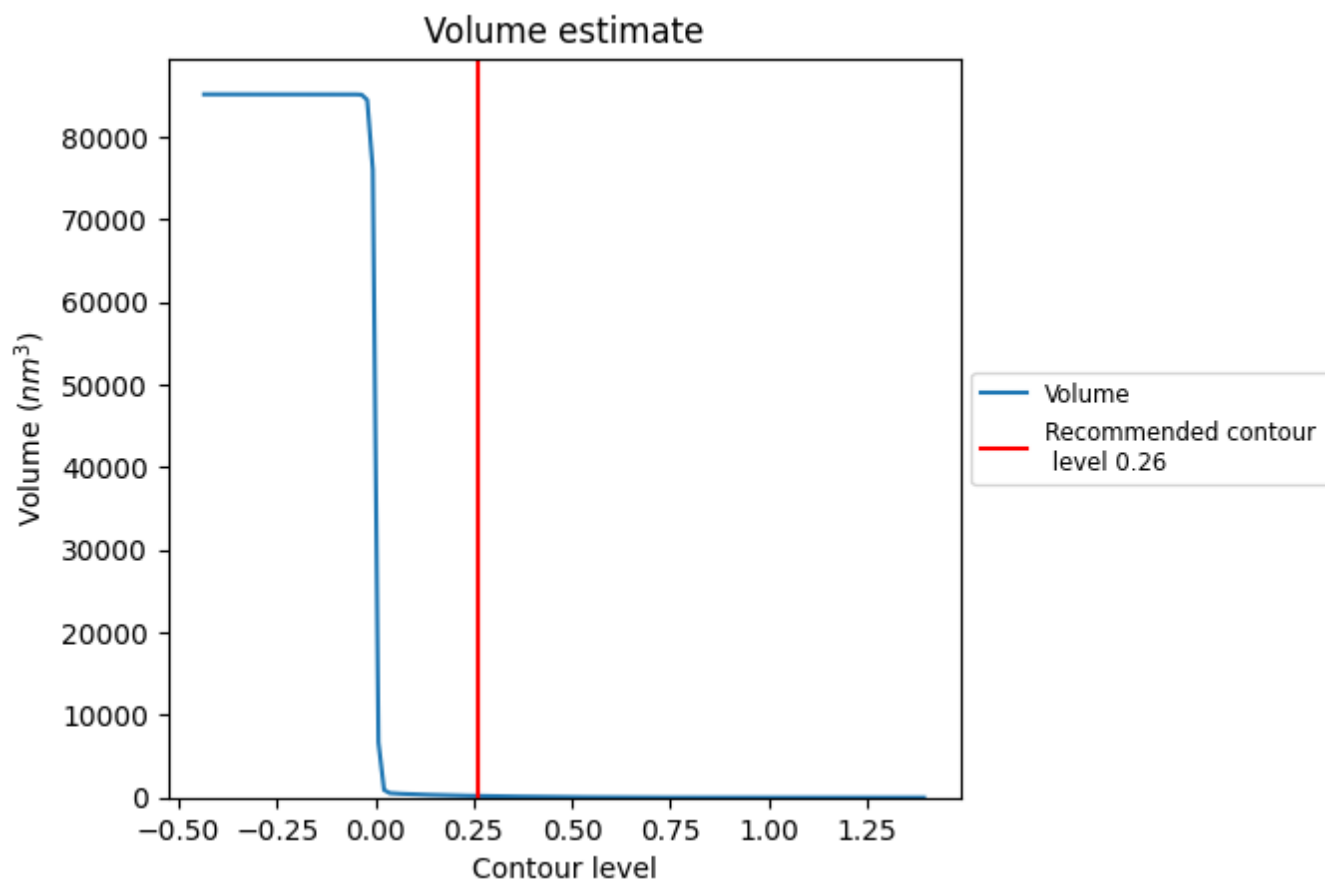
This section contains the results of statistical analysis of the map.

### 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.

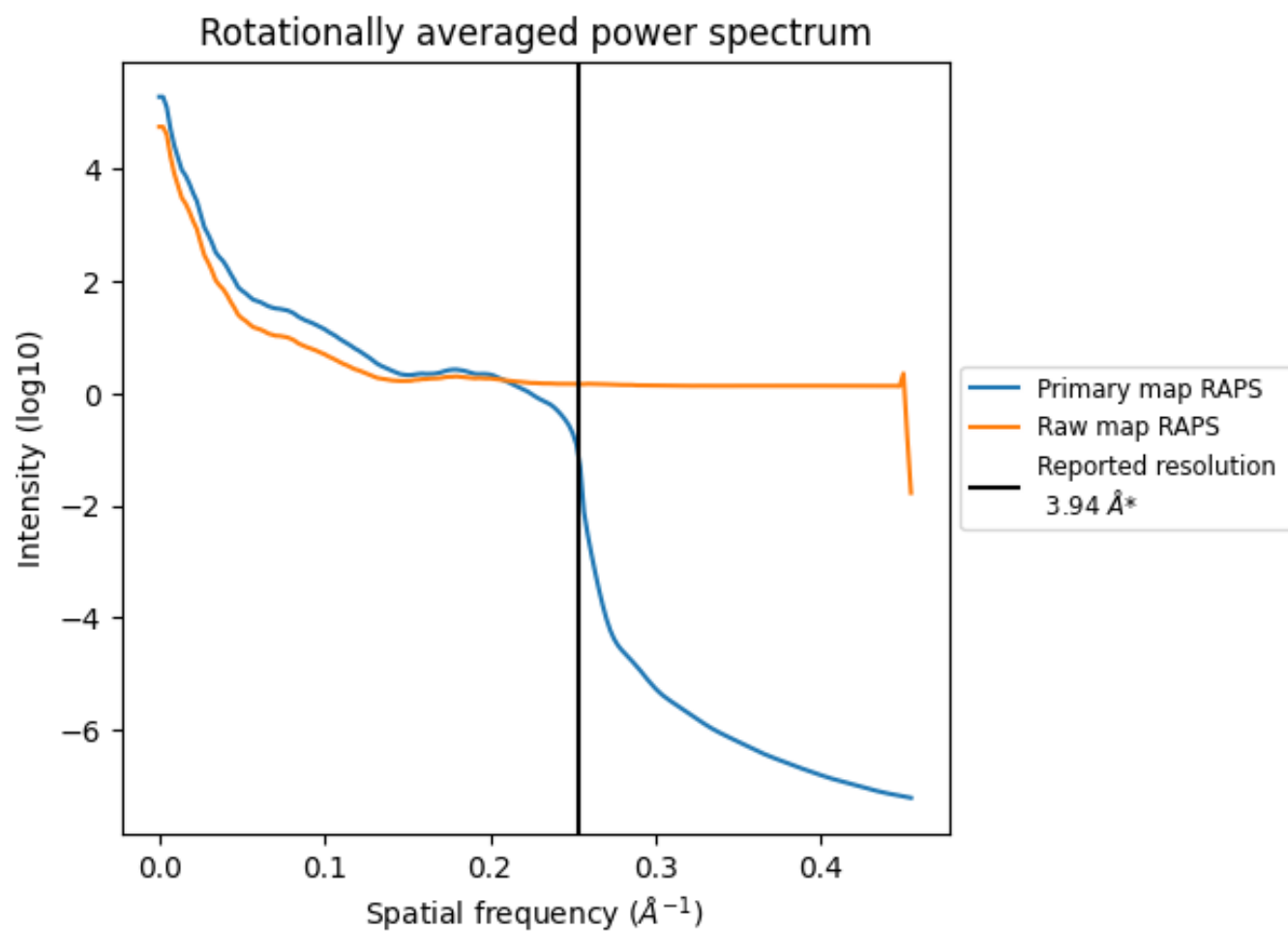
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm<sup>3</sup>; this corresponds to an approximate mass of 178 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 ⓘ

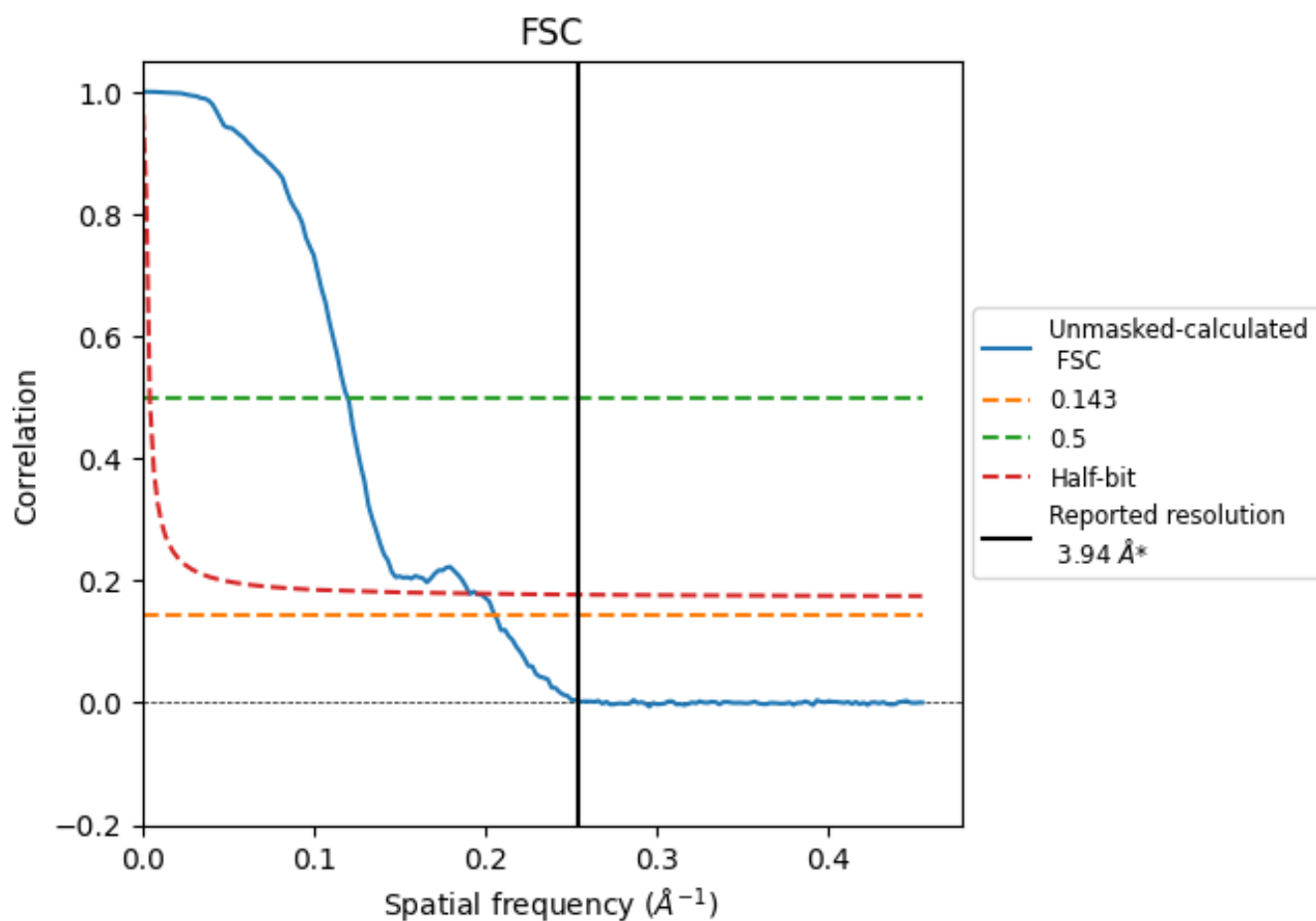


\*Reported resolution corresponds to spatial frequency of 0.254 Å<sup>-1</sup>

## 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  $0.254 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

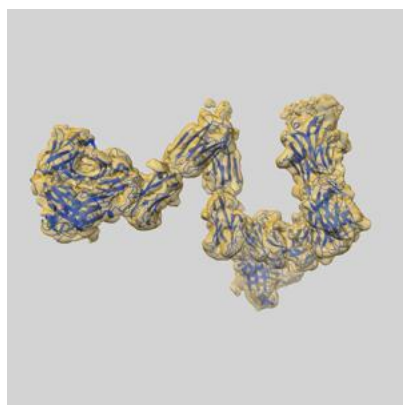
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.86	8.37	5.24

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.86 differs from the reported value 3.94 by more than 10 %

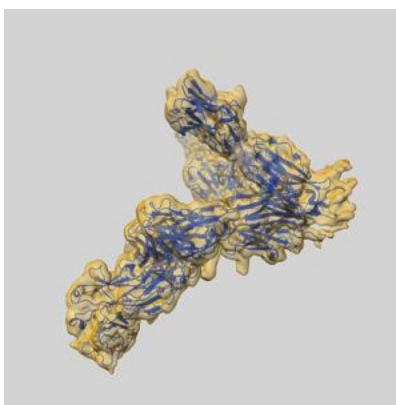
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61146 and PDB model 9J5M. Per-residue inclusion information can be found in section [3](#) on page [5](#).

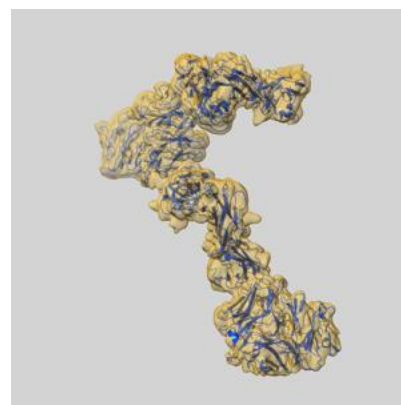
### 9.1 Map-model overlay [i](#)



X



Y

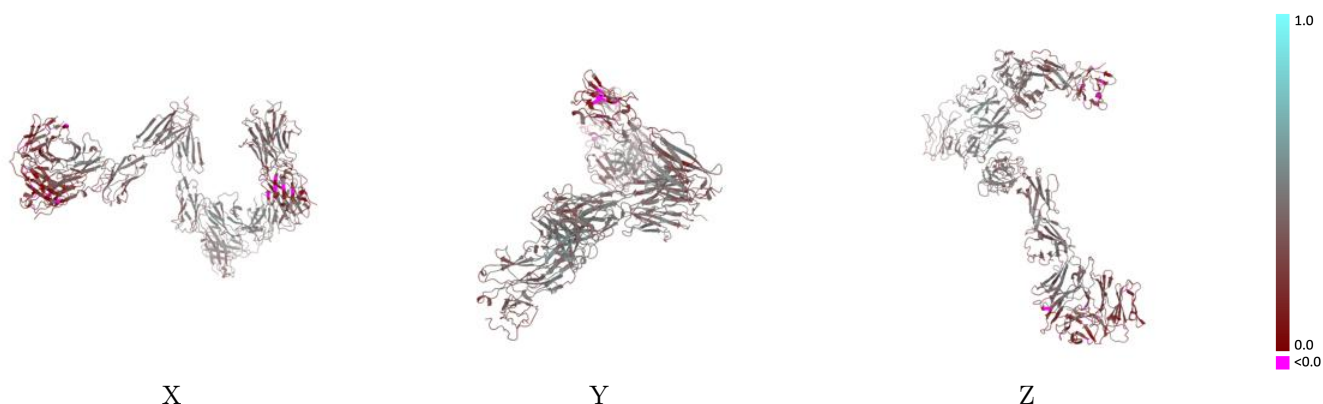


Z

The images above show the 3D surface view of the map at the recommended contour level 0.26 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](#)



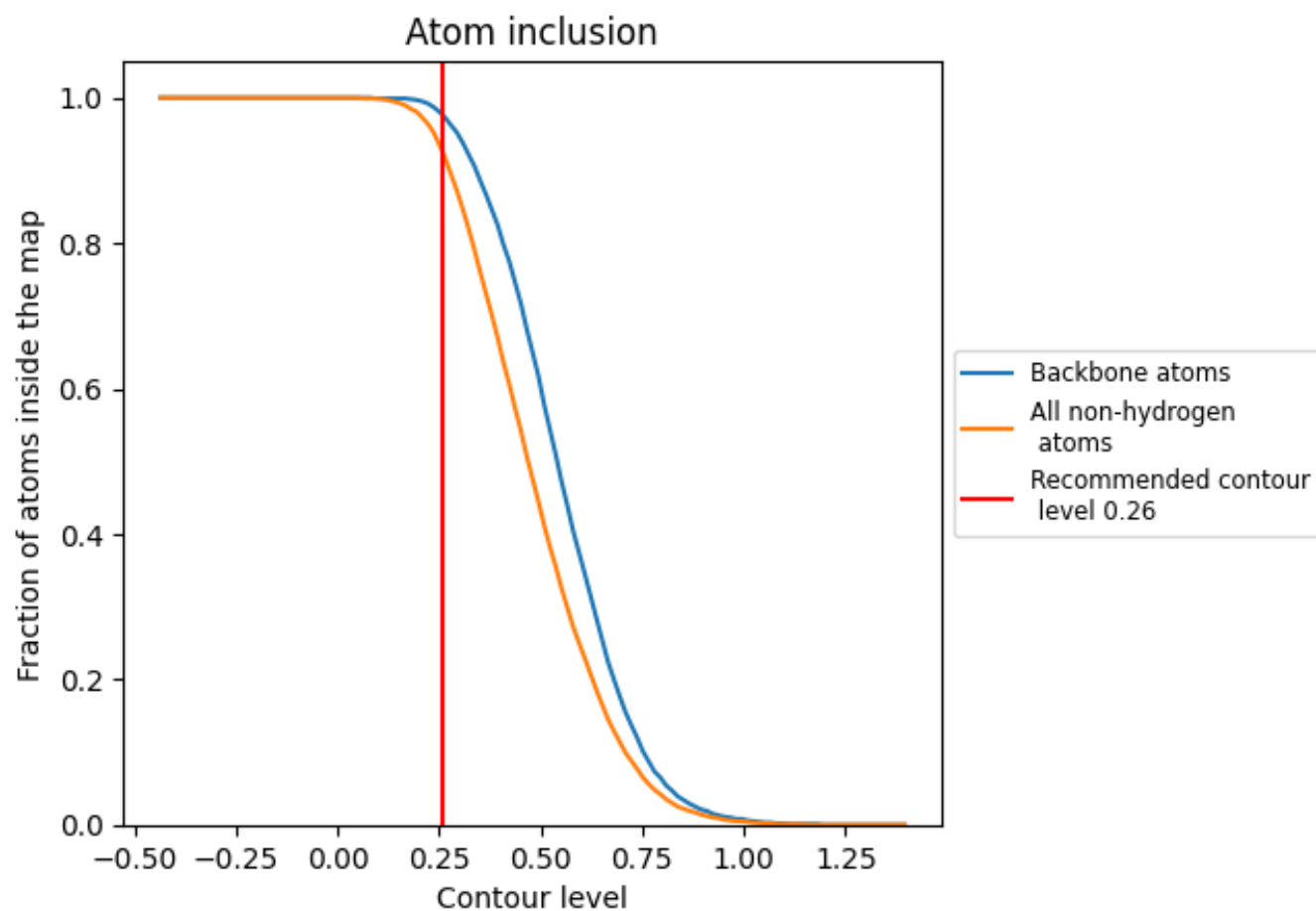
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.26).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9240	<div><div></div></div> 0.3650
A	<div><div></div></div> 0.8180	<div><div></div></div> 0.2450
B	<div><div></div></div> 0.8720	<div><div></div></div> 0.3320
C	<div><div></div></div> 0.9600	<div><div></div></div> 0.4060
D	<div><div></div></div> 0.8950	<div><div></div></div> 0.2950
E	<div><div></div></div> 0.9630	<div><div></div></div> 0.4100
G	<div><div></div></div> 0.9690	<div><div></div></div> 0.3850
H	<div><div></div></div> 0.9560	<div><div></div></div> 0.4010
I	<div><div></div></div> 0.9460	<div><div></div></div> 0.4280

1.0

0.0

<0.0