



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 01:36 PM JST

PDB ID : 7YKJ
EMDB ID : EMD-33892
Title : Omicron RBDs bound with P3E6 Fab (one up and one down)
Authors : Tang, B.; Dang, S.
Deposited on : 2022-07-22
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
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) : 2.39

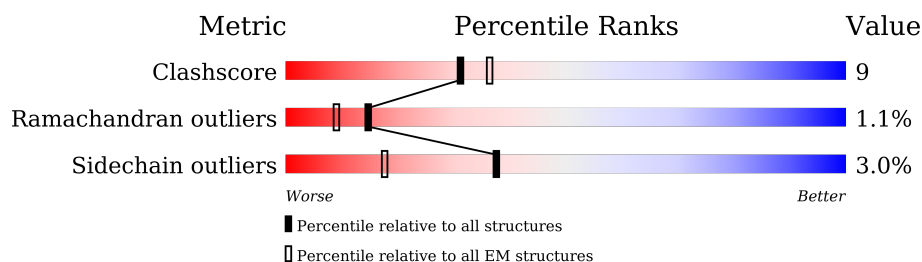
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 ≥ 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	B	1205	<div> <div>5%</div> <div>14%</div> <div>84%</div> </div>
1	C	1205	<div> <div>13%</div> <div>84%</div> </div>
2	A	121	<div> <div>80%</div> <div>19%</div> </div>
3	D	109	<div> <div>5%</div> <div>77%</div> <div>19%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4811 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	198	Total	C	N	O	S	0	0
			1529	984	257	280	8		
1	C	198	Total	C	N	O	S	0	0
			1556	1003	263	282	8		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	70	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	96	ILE	THR	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	variant	UNP P0DTC2
B	212	GLU	-	insertion	UNP P0DTC2
B	213	PRO	-	insertion	UNP P0DTC2
B	214	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	70	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	96	ILE	THR	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	209	ILE	LEU	variant	UNP P0DTC2
C	212	GLU	-	insertion	UNP P0DTC2
C	213	PRO	-	insertion	UNP P0DTC2
C	214	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called P3E6 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	121	Total	C	N	O	S	0	0
			906	570	151	180	5		

- Molecule 3 is a protein called P3E6 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	109	Total	C	N	O	S	0	0
			820	515	139	164	2		

ASP	GLY	VAL	TLE	GLN	PRO
LYS	VAL	LEU	SER	GLN	ILE
THR	PHE	GLY	SER	VAL	ASN
PHE	VAL	GLN	VAL	LYS	PHE
LYS	SER	SER	LEU	TVR	GLY
ASN	ASN	LYS	ASN	GLU	LEU
HIS	GLY	ARG	ASP	ASN	GLY
THR	VAL	VAL	ILE	GLN	PHE
SER	HIS	ASP	PHE	LYS	ASN
PRO	TRP	PHE	SER	LEU	PRO
ASP	PHE	CYS	ARG	ILE	SER
VAL	VAL	GLY	LEU	ALA	GLN
ASP	THR	LYS	ASP	ASN	ILE
LEU	GLN	GLY	PRO	GLN	LEU
GLY	ARG	TVR	PRO	PHE	THR
ASN	GLN	HIS	GLU	ASP	ASP
ILE	PHE	LEU	ALA	SER	GLU
ASP	TVR	MET	GLU	ILE	PRO
GLY	PRO	SER	VAL	ILE	LYS
ILE	GLU	PHE	GLN	GLY	PRO
ASN	GLN	GLN	ILE	LYS	THR
ALA	ILE	GLN	ASP	ILE	LYS
SER	ILE	PRO	ARG	GLN	SER
VAL	THR	ALA	LEU	ASP	ARG
VAL	THR	PRO	ILE	ASP	SER
ASN	ASP	HIS	THR	LEU	PHE
ILE	ASN	GLY	GLY	LEU	ILE
GLN	THR	VAL	ARG	SER	GLY
LYS	PHE	VAL	LEU	THR	ASP
GLU	VAL	PHE	LEU	THR	LEU
ILE	SER	LEU	GLN	ALA	LEU
ASP	GLY	HTS	LEU	SER	PHE
ARG	CYS	VAL	GLN	ALA	LYS
LEU	CYS	THR	THR	GLY	VAL
ASN	ASP	TVR	TVR	LYS	THR
GLU	VAL	PRO	VAL	LEU	LEU
VAL	VAL	PRO	THR	GLN	ALA
ALA	ILE	ALA	GLN	VAL	ASP
LYS	GLY	GLN	GLN	VAL	ALA
ASN	ILE	GLU	LEU	VAL	GLY
LEU	VAL	LYS	ILE	ASN	PHE
ASN	ASN	ASN	ARG	HIS	ILE
GLU	ASN	PHE	ALA	ASN	LYS
SER	THR	THR	ALA	ALA	GLN
LEU	VAL	THR	GLU	GLN	TVR
ILE	TVR	ALA	ILE	ALA	GLY
ASP	ASP	PRO	ARG	LEU	ASP
LEU	PRO	ALA	ALA	ASN	CYS
GLN	LEU	ILE	SER	THR	LEU
GLU	GLN	CYS	ALA	LEU	GLY
LEU	PRO	HIS	ASN	VAL	ASP
GLY	GLY	LEU	LYS	TVR	ILE
LYS	LEU	GLY	ALA	GLN	ALA
THR	ASP	LYS	ALA	LEU	PHE
GLN	SER	VAL	THR	SER	ASN
GLU	PHE	HIS	LYS	SER	ARG
GLN	LYS	PHE	MET	LYS	THR
ILE	GLU	PRO	SER	PHE	ILE
GLY	GLU	ARG	GLY	GLY	GLY
VAL	TVR	GLU	CYS	ALA	CYS
THR	GLN	ALA	GLY	THR	ALA

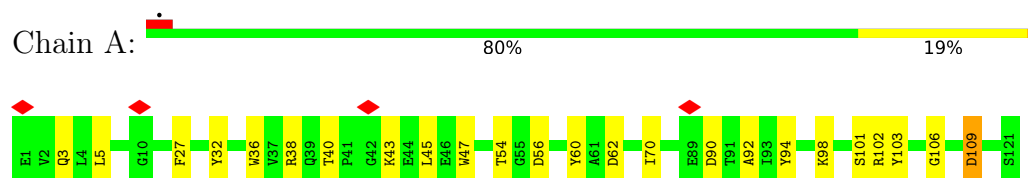
- Molecule 1: Spike glycoprotein

Chain C:  13% .. 84%

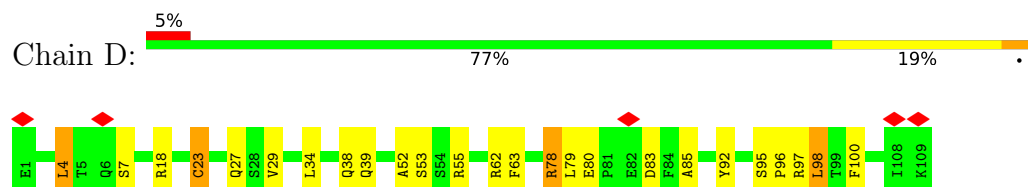
LEU	PRO	ALA	GLY	GLN	LYS	LEU	GLY	LYS	LEU	PHE	ALA	ASN	MET
VAL	GLY	VAL	GLY	VAL	N417	HIS	THR	SER	ARG	THR	THR	VAL	PHE
ILE	ILE	VAL	GLY	VAL	I418	SER	ALA	PHE	SER	ASN	ASN	THR	THR
MET	CYS	VAL	VAL	VAL	A419	THR	THR	THR	TYR	ARG	VAL	TRP	PHE
THR	ALA	TYR	LEU	VAL	Y421	LEU	GLY	VAL	LEU	GLU	ILE	HIS	VAL
LYS	SER	GLN	THR	THR	N422	THR	LYS	LYS	THR	PHE	LYS	VAL	LEU
THR	TYR	GLY	THR	GLU	L441	PRO	VAL	GLY	PRO	VAL	VAL	ILE	LEU
GLN	VAL	VAL	SER	SER	K444	GLY	ILE	ILE	GLY	PHE	CYS	GLY	LEU
VAL	THR	THR	ASN	ASN	V445	ASP	ASN	TYR	ASP	LYS	GLU	GLY	PRO
ASP	GLN	CYS	LYS	LYS	Y451	SER	GLN	THR	SER	ASN	PHE	THR	VAL
THR	CYS	THR	PHE	PHE	K458	SER	VAL	ARG	SER	ASP	THR	GLY	SER
MET	LYS	VAL	LEU	LEU	Y451	GLY	GLN	ASN	GLY	GLY	CYS	THR	GLN
THR	HIS	VAL	PRO	PRO	R454	THR	THR	PHE	TRP	TYR	ASN	LYS	CYS
TYR	GLY	VAL	PHE	PHE	K458	ALA	ALA	VAL	ALA	PHE	ASP	LYS	ASN
VAL	SER	VAL	GLN	GLN	K458	GLY	VAL	VAL	GLY	LYS	PRO	PHE	VAL
GLY	ALA	ILE	PHE	PHE	A475	THR	PRO	GLN	ALA	TYR	LEU	ASP	LEU
ASP	SER	HIS	GLY	GLY	K478	ALA	THR	THR	ALA	SER	ASP	PRO	THR
SER	SER	ALA	ARG	ARG	K478	GLY	GLU	GLY	ALA	LYS	HIS	VAL	THR
THR	VAL	ASP	ASN	ASN	K478	THR	THR	THR	ALA	THR	LYS	VAL	ARG
GLU	ALA	LEU	ASN	ASN	N481	THR	ILE	ILE	THR	HIS	ASN	LEU	THR
CYS	SER	GLN	ALA	ALA	G482	VAL	VAL	VAL	VAL	PRO	ASN	PHE	THR
SER	GLN	THR	THR	THR	G482	ARG	ARG	ARG	GLY	ILE	LYS	ASP	LEU
ASN	SER	THR	THR	THR	G482	PHE	PHE	PHE	THR	ILE	THR	ASP	PRO
LEU	ILE	THR	THR	THR	Y495	THR	PRO	PRO	LEU	VAL	TRP	GLY	ALA
LEU	ALA	ARG	ASP	ASP	S496	GLN	N331	N331	GLN	ARG	MET	VAL	THR
GLN	TYR	VAL	ALA	ALA	F497	PRO	C336	C336	GLU	GLU	GLY	VAL	THR
GLY	THR	THR	VAL	VAL	R498	ARG	PRO	PRO	THR	GLU	GLU	PHE	ASN
THR	MET	SER	GLY	GLY	R498	THR	THR	THR	THR	ASP	ALA	ASN	SER
SER	SER	THR	THR	THR	Y501	GLY	PHE	PHE	THR	THR	THR	THR	THR
THR	LEU	GLY	GLY	GLY	Y501	LEU	LEU	LEU	ARG	ILE	THR	THR	THR
CYS	GLY	ASN	SER	SER	V511	LEU	LYS	LYS	VAL	GLU	VAL	GLY	ARG
THR	ALA	VAL	GLU	GLU	F515	THR	GLY	GLY	PRO	THR	THR	LYS	VAL
GLN	GLU	ASN	PHE	PHE	E516	TYR	GLN	PHE	GLN	GLY	THR	ILE	ARG
LEU	LEU	SER	GLN	GLN	L517	ASN	ASN	ASN	GLU	THR	THR	GLY	THR
ARG	VAL	VAL	THR	THR	L518	ASN	ASN	ALA	GLY	THR	THR	THR	VAL
ALA	ALA	ALA	ARG	ARG	L518	THR	ASN	ALA	GLY	THR	THR	THR	VAL
LEU	TYR	ALA	ALA	ALA	V524	THR	THR	GLY	THR	THR	THR	THR	LEU
THR	SER	SER	GLY	GLY	K528	ILE	THR	F377	ILE	PRO	CYS	GLY	LYS
GLY	ASN	ASN	ASN	ASN	LYS	THR	THR	K378	THR	THR	PHE	TRP	VAL
ILE	ASN	ASN	ASN	ASN	LYS	THR	THR	C379	ASP	VAL	THR	TRP	VAL
ALA	SER	ILE	ILE	ILE	LYS	THR	THR	Y380	ALA	VAL	THR	PHE	ARG
VAL	VAL	THR	PHE	PHE	THR	THR	THR	G381	ALA	ASP	TYR	GLY	SER
GLU	ALA	ALA	ALA	ALA	ASN	ASN	ASN	V382	VAL	VAL	VAL	THR	SER
GLN	ILE	ILE	GLY	GLY	VAL	LEU	LEU	S383	CYS	ILE	GLN	LEU	LEU
ASP	PRO	VAL	VAL	VAL	VAL	VAL	VAL	K386	ALA	GLY	PRO	ASP	HIS
THR	ASN	THR	SER	SER	VAL	VAL	VAL	LYS	ILE	THR	PHE	THR	THR
ASN	ASN	VAL	VAL	VAL	ASN	VAL	VAL	ASN	ASN	ILE	THR	LYS	SER
THR	PHE	THR	ASN	ASN	LYS	THR	THR	T393	PRO	ILE	THR	THR	THR
GLN	THR	THR	SER	SER	CYS	THR	THR	N394	LEU	THR	ASP	GLN	ASP
GLU	ILE	THR	THR	THR	VAL	VAL	VAL	V395	SER	ARG	THR	SER	LEU
VAL	SER	THR	GLY	GLY	ASN	THR	THR	R403	GLU	PHE	GLY	LEU	PHE
PHE	VAL	VAL	THR	THR	PHE	THR	THR	N406	LYS	GLN	GLY	LEU	LEU
THR	THR	THR	ASN	ASN	ASN	THR	THR	E406	CYS	THR	GLY	VAL	PHE
GLU	THR	THR	THR	THR	ASN	THR	THR	ASN	THR	THR	GLY	ASN	THR
ILE	ILE	ILE	ILE	ILE	GLY	ASN	ASN	G416	LEU	ALA	ASN	ASN	SER

[illegible]

- Molecule 2: P3E6 heavy chain



- Molecule 3: P3E6 light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107197	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.723	Depositor
Minimum map value	-2.915	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.67	0/1574	0.92	0/2151
1	C	0.74	0/1602	1.01	4/2184 (0.2%)
2	A	0.72	0/927	1.07	0/1262
3	D	0.57	0/838	0.85	0/1137
All	All	0.69	0/4941	0.97	4/6734 (0.1%)

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	B	0	3
1	C	0	3
2	A	0	8
3	D	0	2
All	All	0	16

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	373	PRO	CA-N-CD	-9.19	98.63	111.50
1	C	451	TYR	CB-CG-CD2	-8.27	116.04	121.00
1	C	451	TYR	CB-CG-CD1	6.33	124.80	121.00
1	C	357	ARG	NE-CZ-NH1	6.07	123.33	120.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	357	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	466	ARG	Sidechain
1	B	493	ARG	Sidechain
1	C	454	ARG	Sidechain
1	C	458	LYS	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1529	0	1403	26	0
1	C	1556	0	1465	31	0
2	A	906	0	845	12	0
3	D	820	0	798	19	0
All	All	4811	0	4511	80	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 9.

The worst 5 of 80 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:C:373:PRO:HD2	1:C:374:PHE:HD1	1.08	1.12
1:C:495:TYR:O	1:C:496:SER:OG	1.76	1.04
1:C:373:PRO:HD2	1:C:374:PHE:CD1	1.97	0.99
1:C:373:PRO:CD	1:C:374:PHE:HD1	1.76	0.97
1:C:379:CYS:HB3	1:C:382:VAL:HG23	1.56	0.87

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	B	196/1205 (16%)	191 (97%)	4 (2%)	1 (0%)	25	59
1	C	196/1205 (16%)	172 (88%)	21 (11%)	3 (2%)	8	39
2	A	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
3	D	107/109 (98%)	92 (86%)	12 (11%)	3 (3%)	4	27
All	All	618/2640 (23%)	570 (92%)	41 (7%)	7 (1%)	15	45

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	373	PRO
3	D	53	SER
3	D	97	ARG
3	D	4	LEU
1	B	372	ALA

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	B	156/1053 (15%)	153 (98%)	3 (2%)	52	73
1	C	164/1053 (16%)	156 (95%)	8 (5%)	21	50
2	A	95/101 (94%)	94 (99%)	1 (1%)	70	83
3	D	88/90 (98%)	85 (97%)	3 (3%)	32	60
All	All	503/2297 (22%)	488 (97%)	15 (3%)	37	63

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	498	ARG
3	D	78	ARG
1	C	501	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	98	LEU
2	A	109	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	448	ASN
1	B	505	HIS
1	C	422	ASN
2	A	3	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.

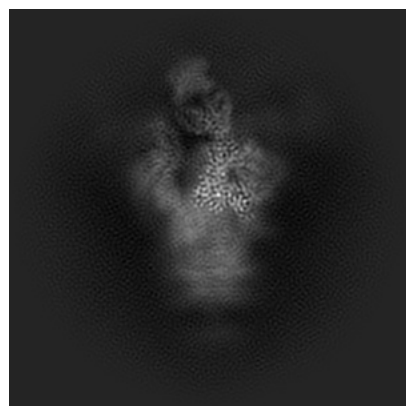
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33892. These allow visual inspection of the internal detail of the map and identification of artifacts.

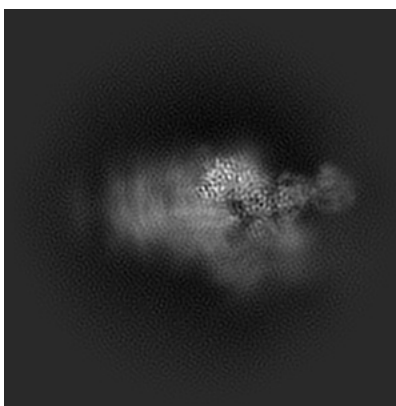
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

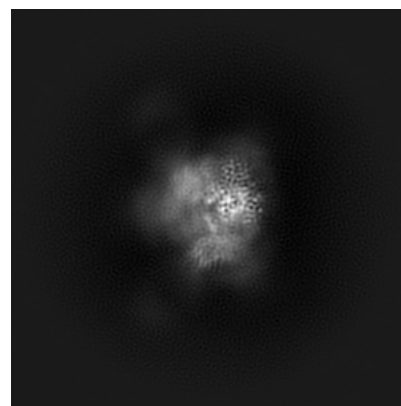
6.1.1 Primary map



X

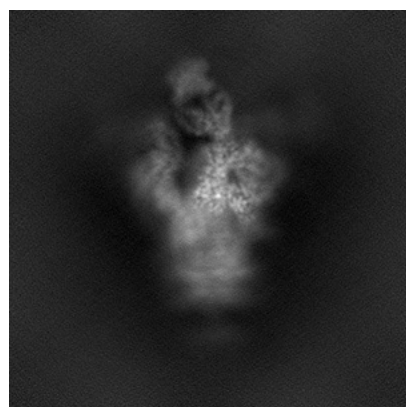


Y

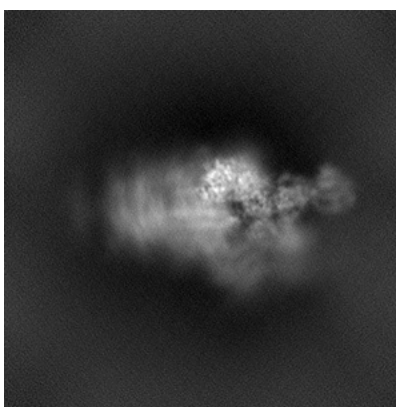


Z

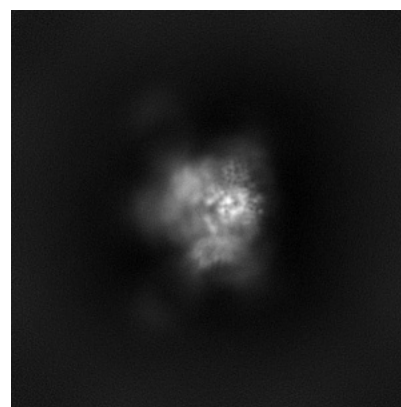
6.1.2 Raw map



X



Y

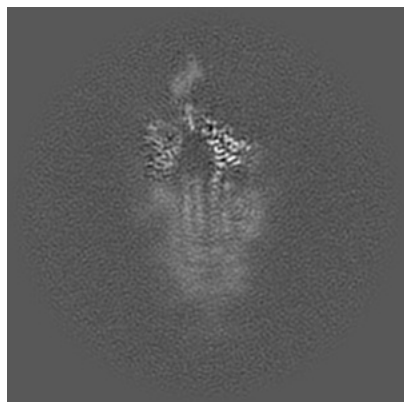


Z

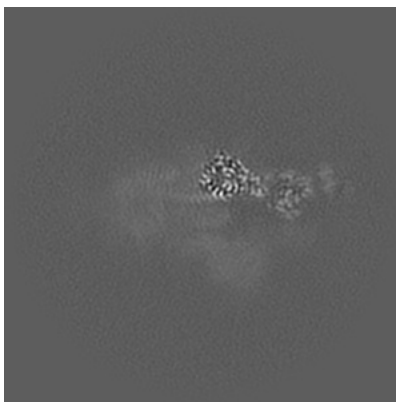
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

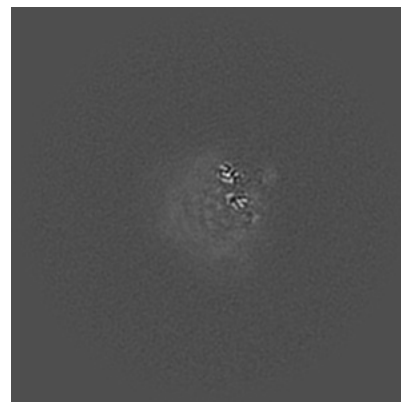
6.2.1 Primary map



X Index: 160

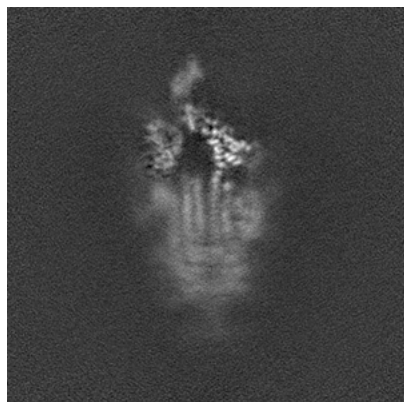


Y Index: 160

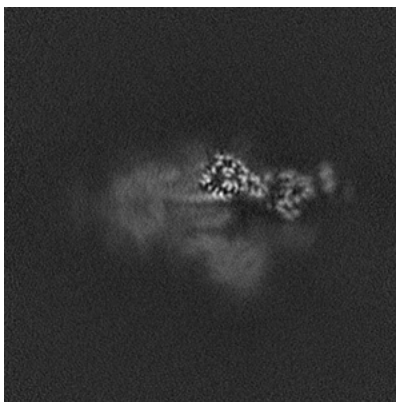


Z Index: 160

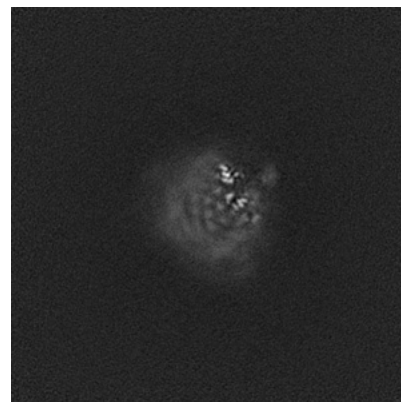
6.2.2 Raw map



X Index: 160



Y Index: 160

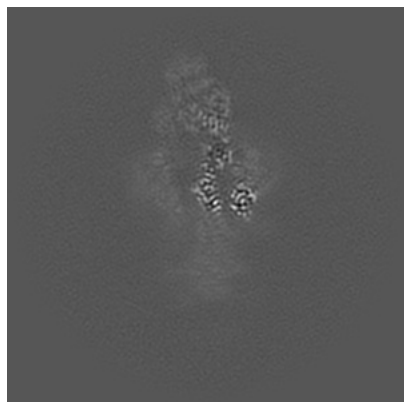


Z Index: 160

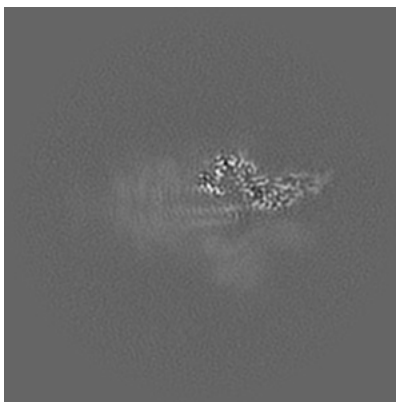
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

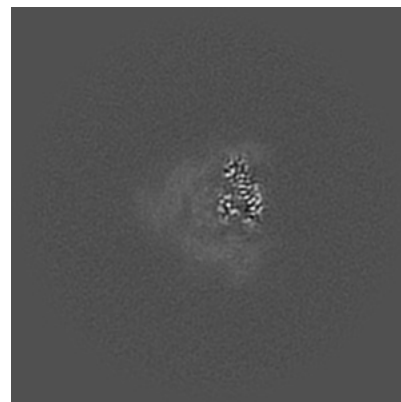
6.3.1 Primary map



X Index: 176



Y Index: 167

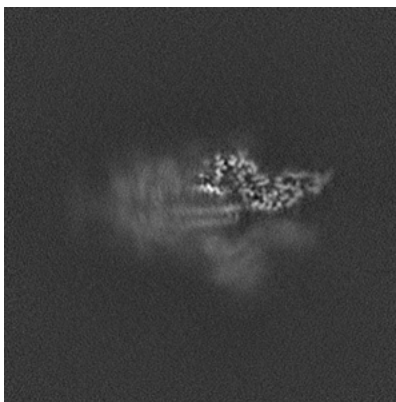


Z Index: 170

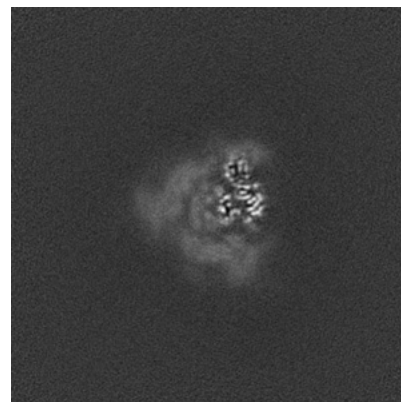
6.3.2 Raw map



X Index: 170



Y Index: 167

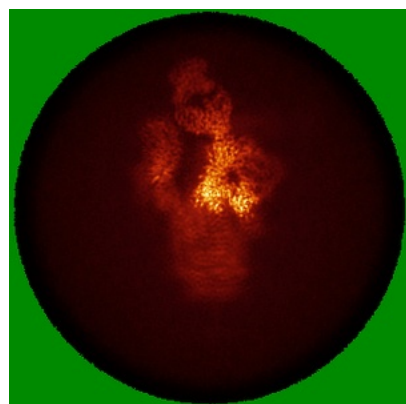


Z Index: 171

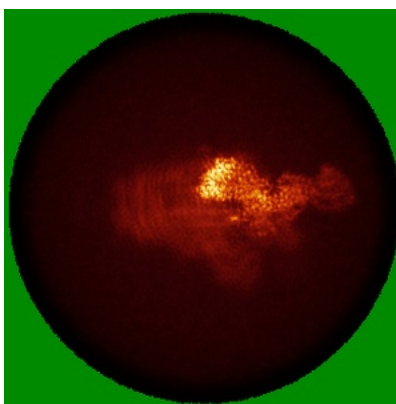
The images above show the largest variance slices of the map in three orthogonal directions.

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

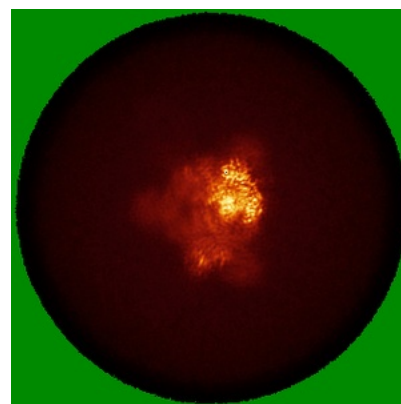
6.4.1 Primary map



X

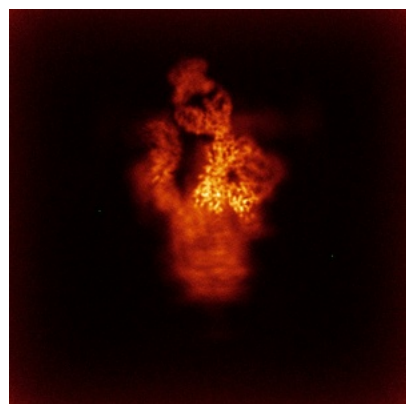


Y

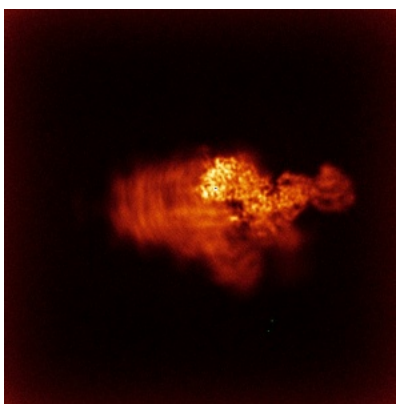


Z

6.4.2 Raw map



X



Y

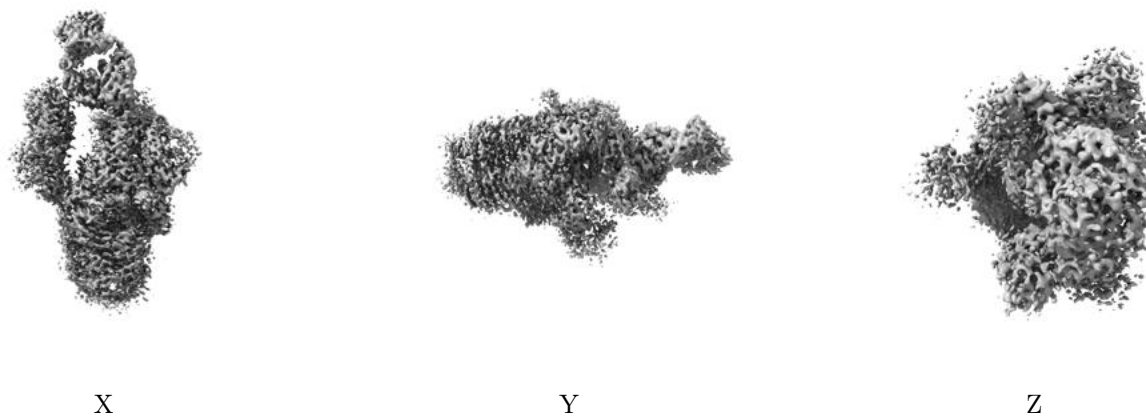


Z

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.

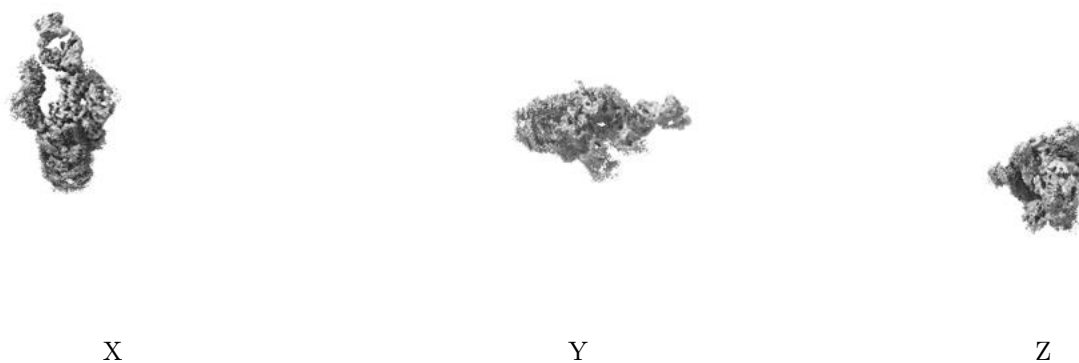
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

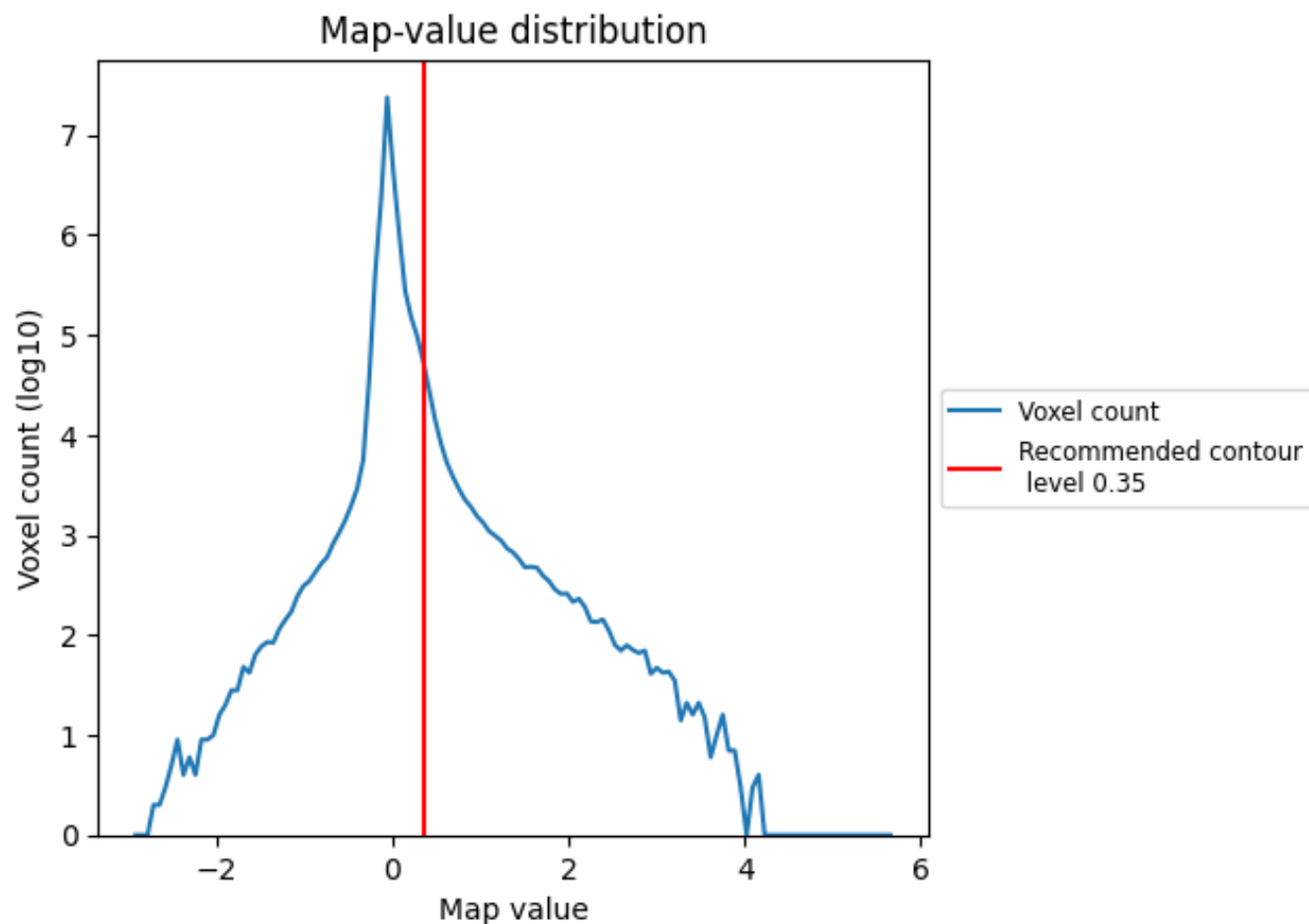
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

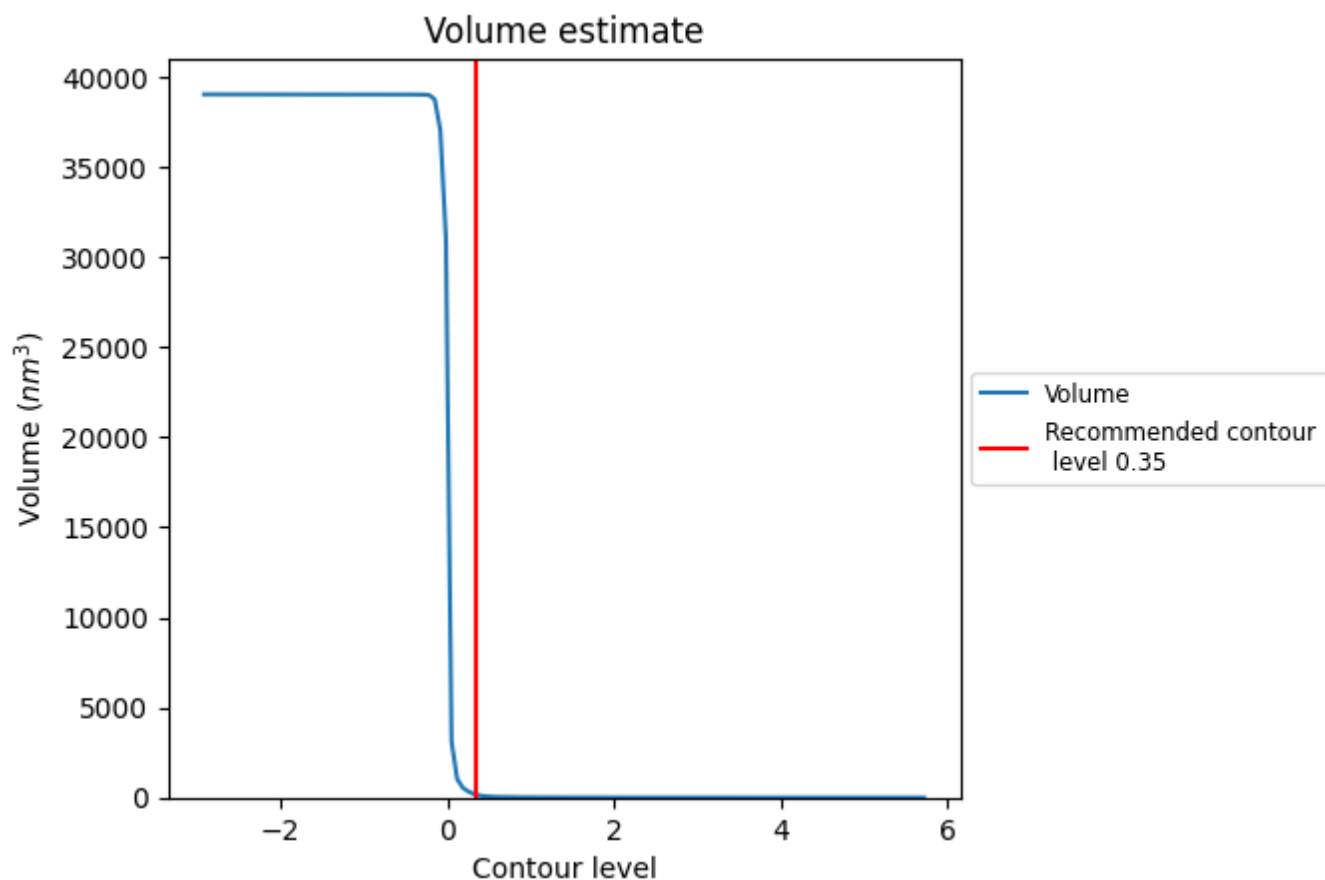
This section contains the results of statistical analysis of the map.

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.

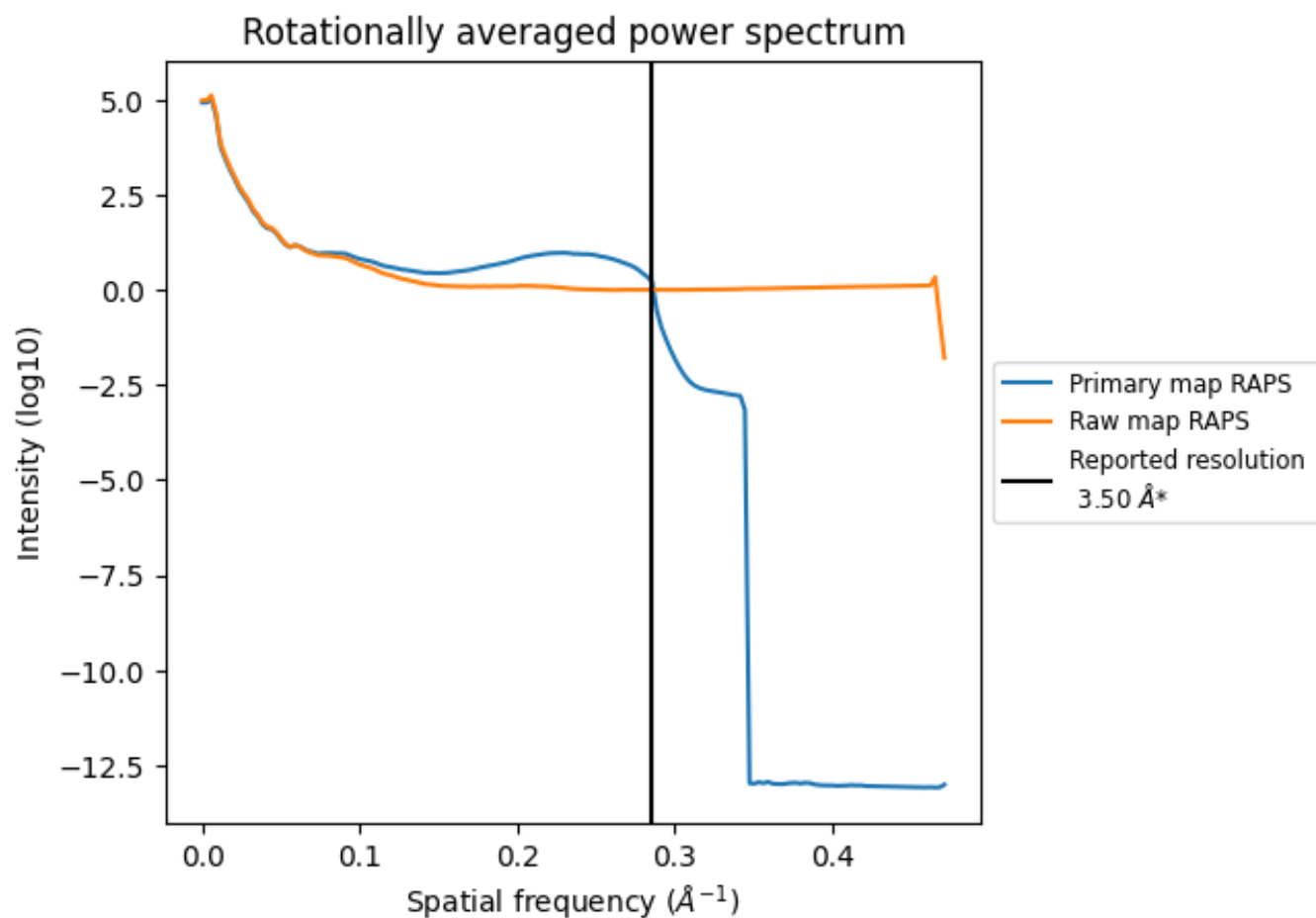
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 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 ⓘ

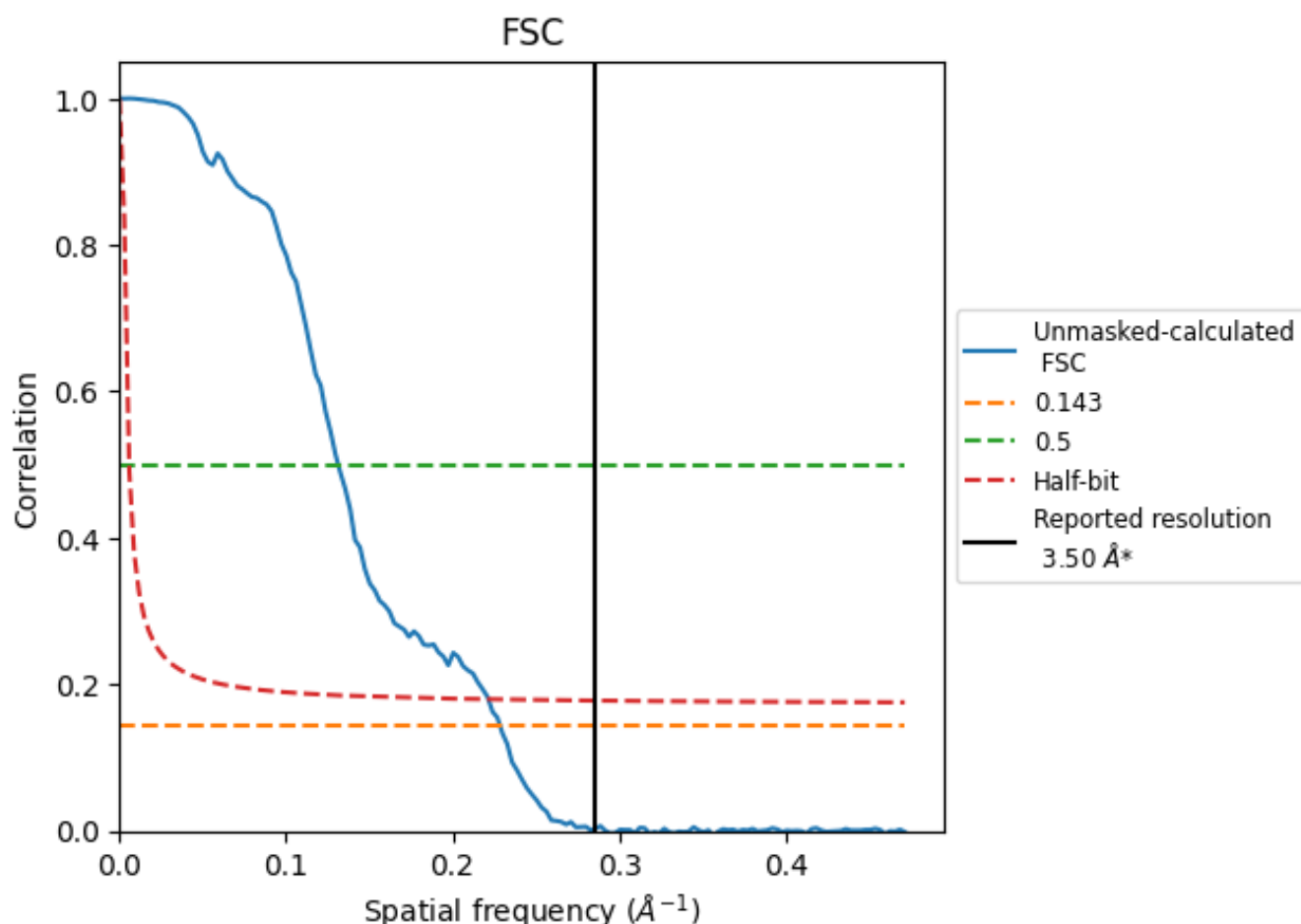


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

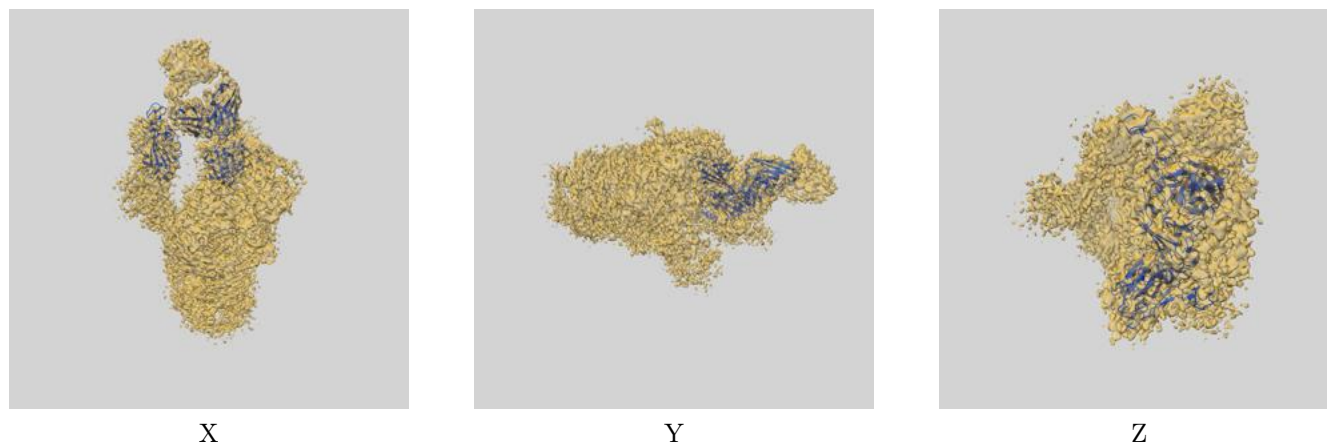
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	7.61	4.51

*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 4.37 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

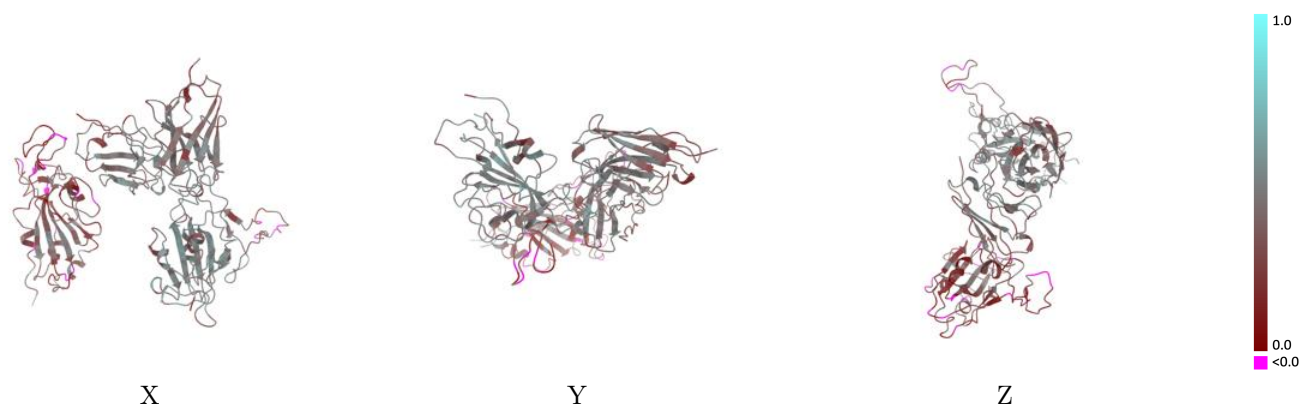
This section contains information regarding the fit between EMDB map EMD-33892 and PDB model 7YKJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



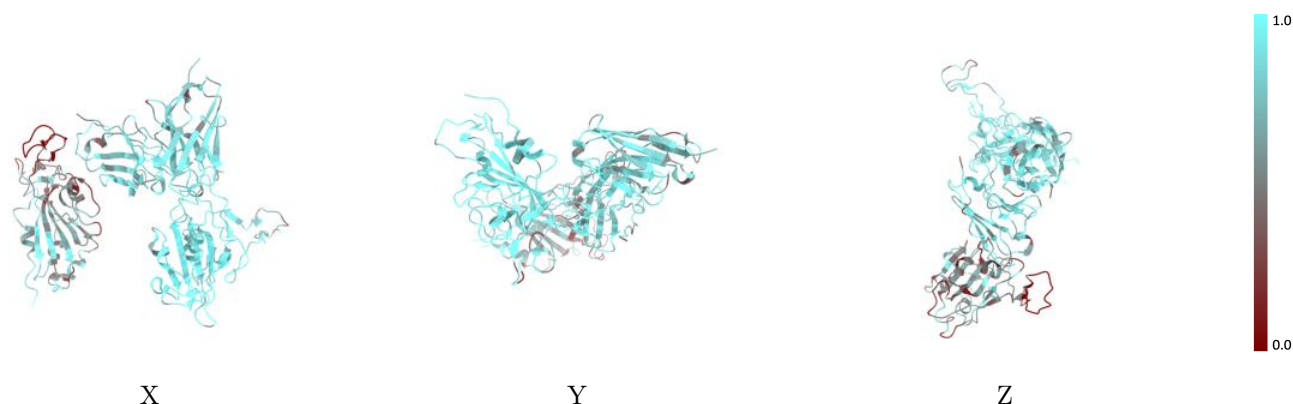
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



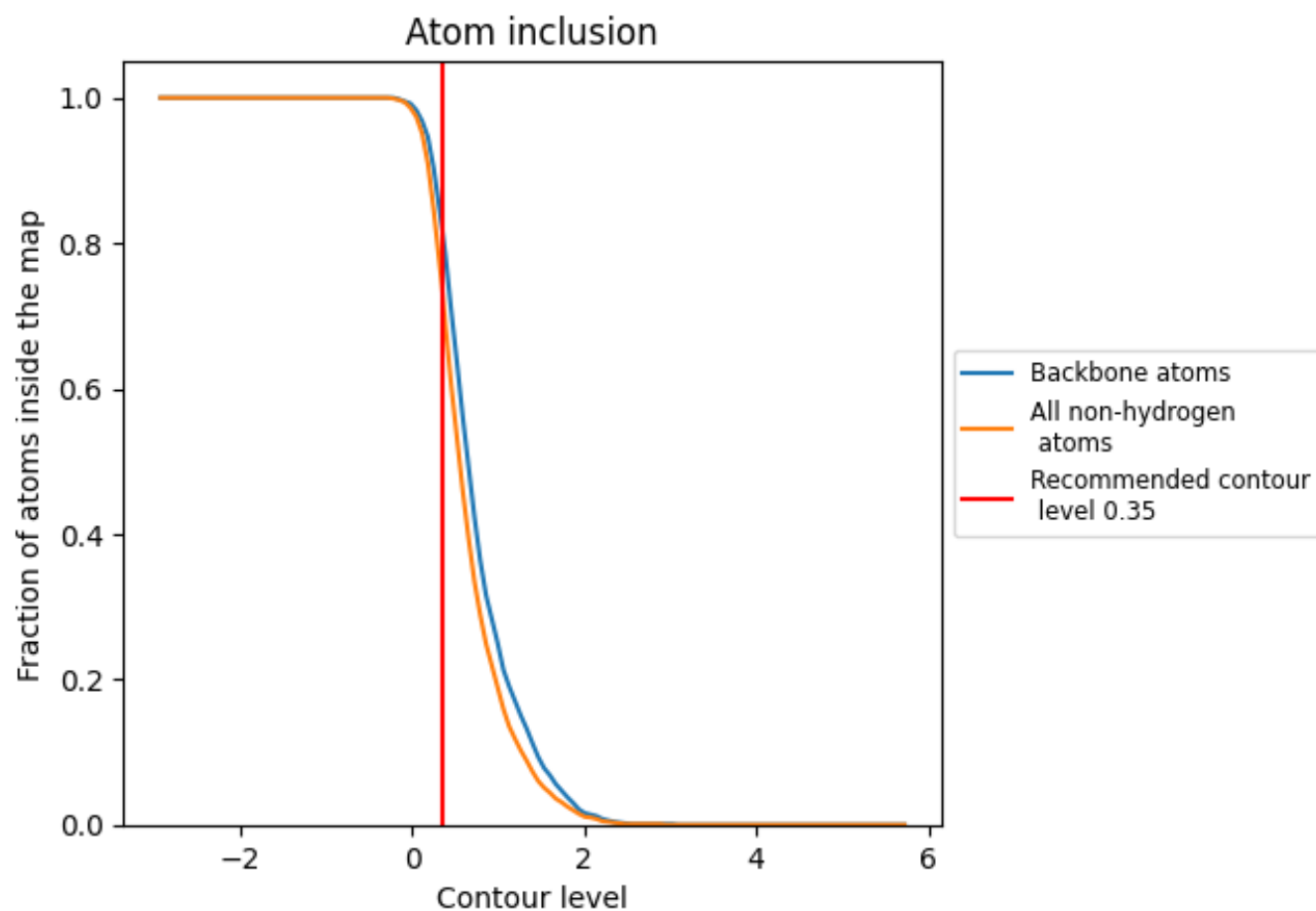
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7430	<div></div> 0.3690
A	<div></div> 0.8080	<div></div> 0.4250
B	<div></div> 0.5270	<div></div> 0.2410
C	<div></div> 0.8880	<div></div> 0.4420
D	<div></div> 0.7960	<div></div> 0.4070

