



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 07:19 AM UTC

PDB ID : 7YKJ / pdb_00007ykj
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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

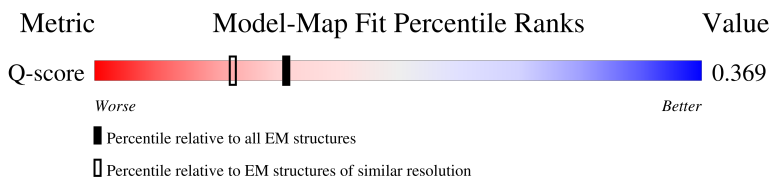
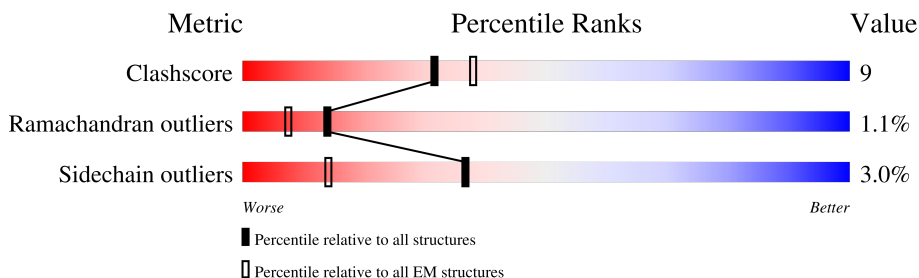
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	
1	C	1205	
2	A	121	
3	D	109	

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
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C	214	GLU	-	insertion	UNP P0DTC2
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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	ARG
VAL	THR	ALA	LEU	ASP	SER
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	ASN
LEU	CYS	THR	THR	GLY	LYS
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	PHE
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	GLY	ILE
LYS	LEU	GLY	ALA	GLN	ALA
THR	ASP	LYS	ALA	LEU	ALA
GLN	SER	VAL	THR	SER	ARG
GLU	PHE	HIS	LYS	SER	ASN
GLN	LYS	PHE	MET	LYS	THR
ILE	GLU	PRO	SER	PHE	ALA
GLY	GLU	ARG	GLU	GLY	THR
VAL	LEU	GLN	CYS	ALA	VAL

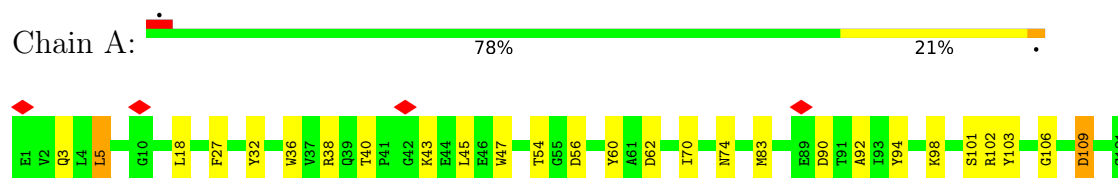
- Molecule 1: Spike glycoprotein

Chain C: 13% 2% 84%

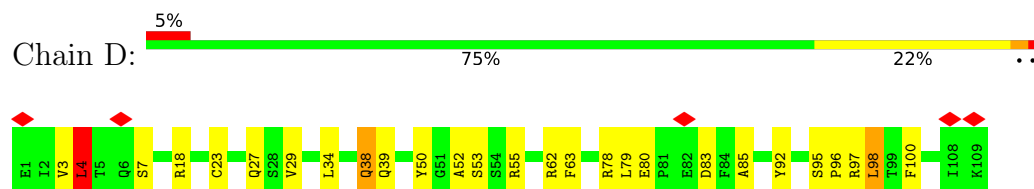
GLU	ILE	LEU	LEU	PRO	SER	GLY	Q409	LYS	LEU	PHE	LYS	THR	ALA	ASN	MET	
ILE	LEU	LEU	GLY	GLY	ASN	LEU	Q409	SER	HIS	ASN	SER	THR	THR	VAL	PHE	
PRO	PRO	ALA	GLY	VAL	GLN	GLY	T415	PHE	ARG	THR	PHE	THR	VAL	THR	ASN	ASN
VAL	VAL	VAL	THR	ALA	ALA	THR	N417	VAL	TYR	VAL	VAL	VAL	VAL	VAL	ARG	VAL
ILE	ILE	VAL	GLY	VAL	VAL	GLY	I418	GLU	LEU	GLU	GLU	ILE	ILE	ILE	GLU	ILE
CYS	MET	THR	VAL	CYS	LEU	VAL	A419	LYS	THR	PHE	THR	LYS	LYS	LYS	PHE	VAL
THR	THR	ALA	THR	SER	TYR	LEU	D420	GLY	PRO	PHE	GLY	VAL	VAL	VAL	CYS	LEU
LYS	LYS	SER	SER	SER	GLN	THR	Y421	ILE	GLY	THR	TYR	CYS	CYS	CYS	PHE	LEU
THR	THR	THR	THR	THR	GLY	GLU	N422	TYR	ASP	ASP	GLN	GLY	GLU	GLY	GLY	LEU
SER	SER	VAL	SER	GLN	VAL	SER		GLN	SER	THR	ASN	PHE	THR	THR	ASN	SER
VAL	ASP	THR	VAL	THR	ASN	ASN	N439	THR	SER	ASN	THR	ILE	GLN	GLN	ASN	SER
ASP	ASP	LYS	LYS	GLN	CYS	LYS	K440	SER	SER	SER	SER	ASP	PHE	PHE	GLY	SER
CYS	THR	THR	THR	THR	THR	THR	L441	ASN	GLY	THR	ASN	CYS	THR	THR	GLN	CYS
THR	THR	PHE	PHE	GLY	GLU	PHE		PHE	TRP	GLY	THR	GLY	VAL	VAL	LYS	ASN
MET	MET	THR	VAL	VAL	VAL	LEU	K444	ARG	THR	PHE	ARG	PHE	PRO	VAL	ARG	VAL
TYR	TYR	GLY	VAL	HIS	PRO	PHE	V444	VAL	ALA	LYS	VAL	THR	ALA	ALA	THR	ASN
ILE	ILE	CYS	SER	SER	ALA	GLN	R454	PRO	GLY	ILE	GLN	PHE	THR	PHE	ASP	LEU
CYS	GLY	GLY	ALA	ILE	ILE	GLN		THR	ALA	SER	THR	ASP	ASP	ASP	ASN	THR
GLY	GLY	ASP	SER	SER	HIS	PHE	K458	GLY	ALA	ARG	GLY	SER	HIS	VAL	VAL	THR
SER	SER	SER	SER	SER	ALA	GLY		SER	TYR	THR	THR	ASN	ASN	LEU	THR	THR
THR	THR	VAL	VAL	VAL	ASP	ARG	A475	ILE	TYR	THR	ILE	THR	ASN	PRO	GLN	THR
ALA	ALA	SER	GLN	GLN	GLN	ASP		VAL	VAL	GLN	THR	ASN	ASN	PHE	LEU	LEU
SER	CYS	SER	THR	GLN	THR	ALA	K478	ARG	GLY	ILE	ARG	LYS	LYS	ASN	ASN	PRO
GLY	GLY	THR	THR	THR	THR	THR		VAL	VAL	ILE	THR	GLY	GLY	THR	THR	LEU
CYS	CYS	ASN	ASN	ILE	THR	ASP	N481	PRO	GLN	THR	PRO	THR	TRP	GLY	ALA	ALA
ASN	LEU	LEU	LEU	ILE	THR	THR	G482	THR	ARG	THR	THR	GLY	GLY	VAL	THR	TYR
LEU	LEU	LEU	THR	ALA	THR	ASP		THR	PRO	THR	THR	THR	GLY	THR	THR	ASN
GLN	THR	THR	VAL	THR	VAL	VAL	Y495	THR	ARG	ASP	C336	SER	SER	PHE	ASN	ASN
THR	THR	THR	VAL	THR	VAL	VAL		THR	THR	THR	P337	GLU	GLU	ALA	ALA	SER
GLY	GLY	GLY	THR	MET	THR	ARG	S496	THR	PHE	THR	ASN	PHE	THR	THR	THR	SER
SER	SER	SER	THR	SER	THR	ASP	F497	THR	LEU	THR	V341	ARG	ILE	GLU	GLY	THR
LEU	PHE	LEU	GLY	GLY	GLY	PRO	R498	THR	LYS	GLN	V342	VAL	VAL	GLU	VAL	ARG
CYS	CYS	THR	THR	GLY	SER	GLN	Y501	THR	TYR	GLY	V350	THR	THR	SER	GLY	GLY
THR	THR	THR	ALA	ALA	ASN	THR		THR	ASN	PHE	THR	SER	SER	ASN	VAL	THR
GLN	GLN	LEU	LEU	ASN	PHE	GLU	V511	THR	GLU	SER	V362	ALA	ASN	ILE	THR	TYR
LYS	LYS	SER	GLN	VAL	GLN	ILE	L517	GLY	THR	ALA	ASN	ILE	ASN	ILE	THR	PRO
ARG	ALA	ALA	THR	VAL	THR	ASP	L518	THR	ILE	GLY	F373	ARG	ASN	ARG	LYS	ASN
ALA	ALA	THR	ARG	ALA	ARG	ASP		THR	ILE	PRO	F374	CYS	CYS	GLY	LYS	VAL
LEU	LEU	THR	ALA	THR	ALA	ILE	V524	THR	THR	THR	K378	THR	PHE	THR	VAL	VAL
THR	THR	GLY	GLY	CYS	GLY	THR		ASN	ASP	VAL	C379	VAL	VAL	PHE	ARG	PHE
ILE	ILE	ASN	LEU	ASN	LEU	CYS	K528	LYS	ALA	ALA	V380	VAL	THR	GLY	GLY	SER
ALA	ALA	SER	ILE	SER	ILE	SER		SER	ASP	ASP	G381	LEU	VAL	THR	SER	SER
VAL	VAL	VAL	THR	ILE	GLY	PHE	K528	THR	CYS	THR	V382	GLY	GLN	THR	THR	VAL
GLU	GLU	GLN	GLN	ILE	ALA	GLY		ASN	ALA	GLY	V383	ALA	GLN	LEU	LEU	LEU
ASP	ASP	GLN	GLN	ILE	GLU	GLY	T385	THR	LEU	ILE	P384	GLY	PRO	ASP	THR	HIS
LYS	LYS	ASN	THR	THR	VAL	SER		VAL	ASP	ASN	K386	PHE	THR	LYS	THR	THR
ASN	ASN	ASN	VAL	ASN	VAL	VAL	T393	LYS	LEU	ILE	THR	THR	ASN	GLN	ASP	ASN
THR	THR	PHE	THR	PHE	ASN	ILE		ASN	SER	ARG	N394	LEU	LEU	SER	LEU	LEU
GLN	GLN	THR	THR	THR	SER	THR	V395	CYS	GLU	PHE	V395	GLY	GLY	THR	PHE	PHE
VAL	VAL	VAL	ILE	ILE	TYR	PRO		VAL	THR	GLN	R403	THR	LYS	ILE	VAL	PRO
PHE	PHE	VAL	GLY	GLY	GLU	GLY		ASN	CYS	THR	R403	THR	LYS	LYS	PHE	THR
THR	THR	THR	THR	THR	ASP	THR	PHE	PHE	THR	THR	E406	THR	GLN	VAL	ASN	SER
ALA	ALA	THR	THR	THR	THR	THR	ASN	ASN	LEU	ALA	E406	THR	GLY	ASN	ASN	THR

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

- 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	0.82	0/1574	1.22	0/2151
1	C	0.82	0/1602	1.30	5/2184 (0.2%)
2	A	0.78	0/927	1.33	1/1262 (0.1%)
3	D	0.64	0/838	1.03	1/1137 (0.1%)
All	All	0.78	0/4941	1.24	7/6734 (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.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	373	PRO	CA-N-CD	-9.55	98.63	112.00
2	A	74	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	C	409	GLN	OE1-CD-NE2	-5.20	117.41	122.60
1	C	439	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	C	394	ASN	OD1-CG-ND2	-5.11	117.49	122.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	357	ARG	Sidechain
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 ⓘ

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	13	0
3	D	820	0	798	19	0
All	All	4811	0	4511	81	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 81 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 ⓘ

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	B	196/1205 (16%)	191 (97%)	4 (2%)	1 (0%)	24	57
1	C	196/1205 (16%)	172 (88%)	21 (11%)	3 (2%)	8	37
2	A	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
3	D	107/109 (98%)	92 (86%)	12 (11%)	3 (3%)	4	26
All	All	618/2640 (23%)	570 (92%)	41 (7%)	7 (1%)	14	43

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%)	155 (99%)	1 (1%)	78	79
1	C	164/1053 (16%)	155 (94%)	9 (6%)	19	46
2	A	95/101 (94%)	93 (98%)	2 (2%)	47	66
3	D	88/90 (98%)	85 (97%)	3 (3%)	32	57
All	All	503/2297 (22%)	488 (97%)	15 (3%)	37	60

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

Mol	Chain	Res	Type
1	C	498	ARG
3	D	4	LEU
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. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	84	ASN
3	D	38	GLN
3	D	91	GLN
1	C	487	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.

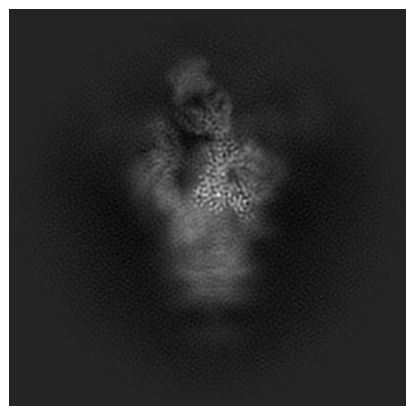
6 Map visualisation [i](#)

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.

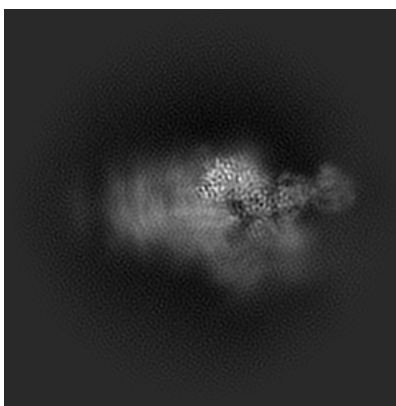
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

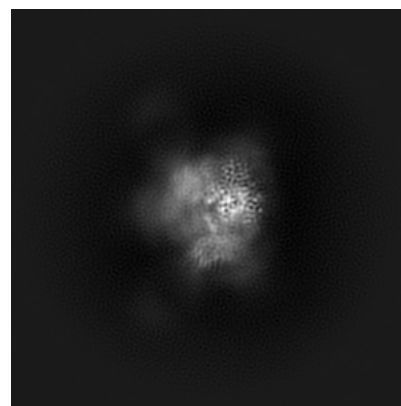
6.1.1 Primary map



X

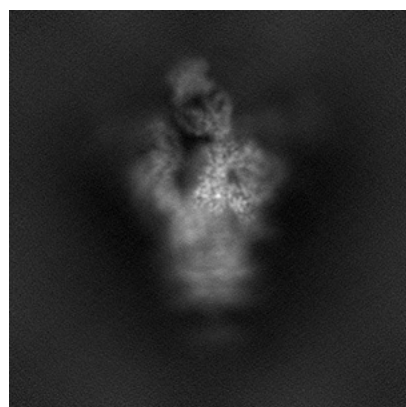


Y

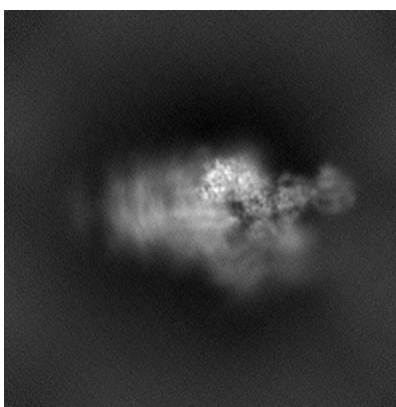


Z

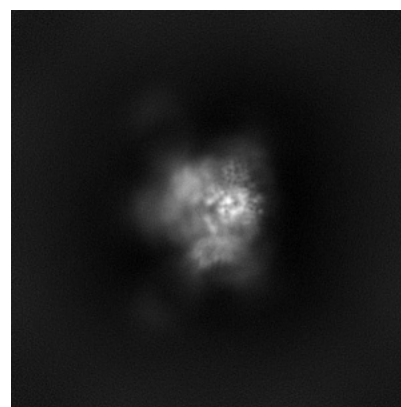
6.1.2 Raw map



X



Y

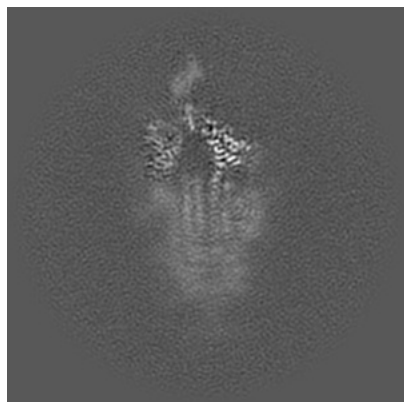


Z

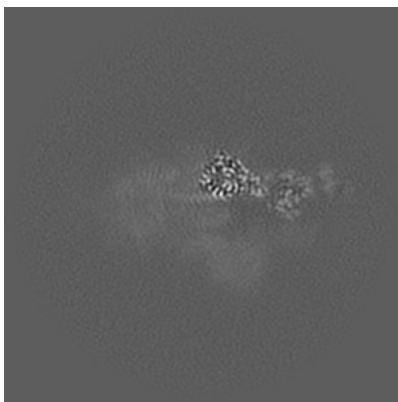
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

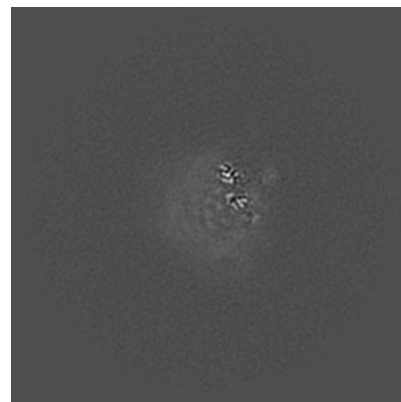
6.2.1 Primary map



X Index: 160

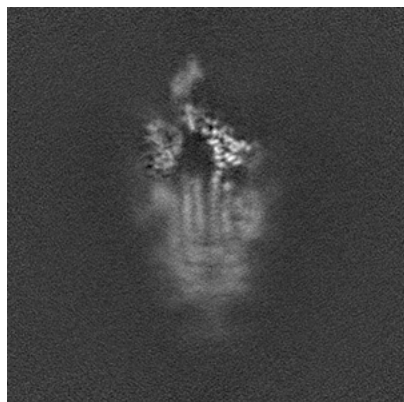


Y Index: 160

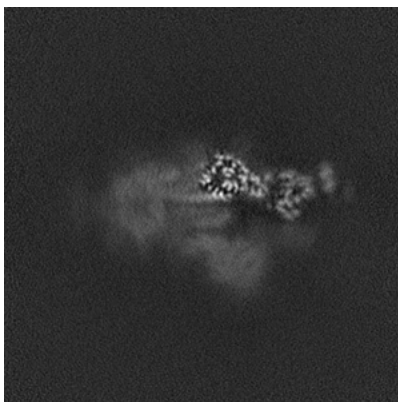


Z Index: 160

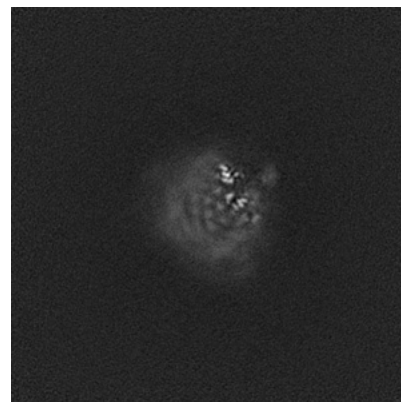
6.2.2 Raw map



X Index: 160



Y Index: 160

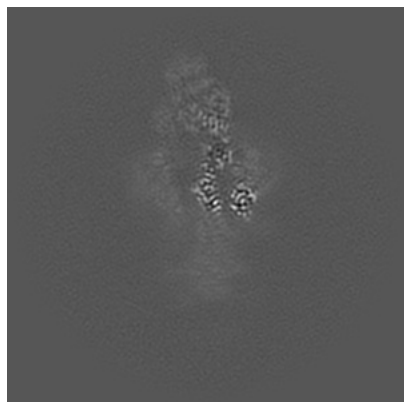


Z Index: 160

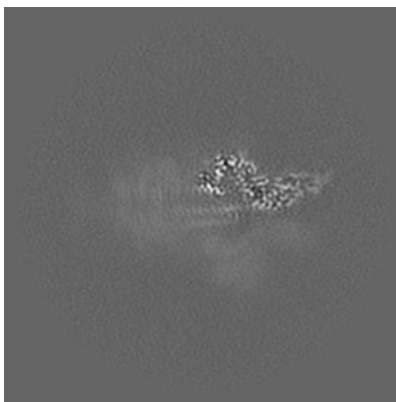
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

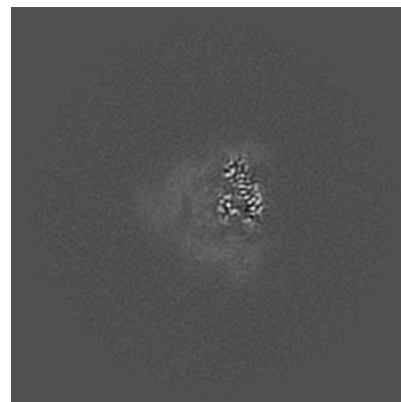
6.3.1 Primary map



X Index: 176

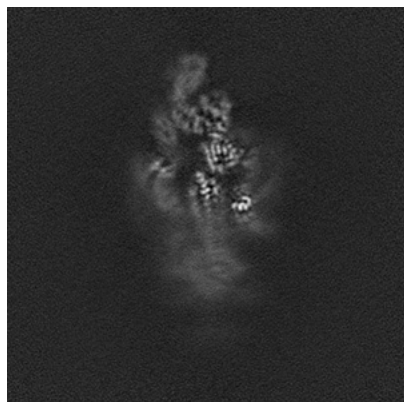


Y Index: 167

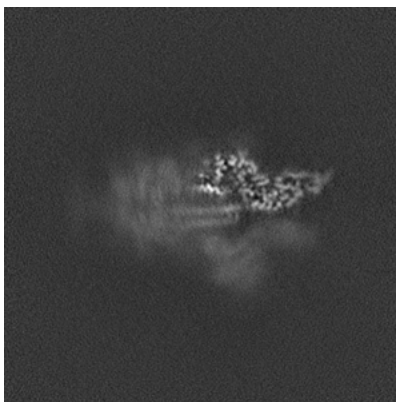


Z Index: 170

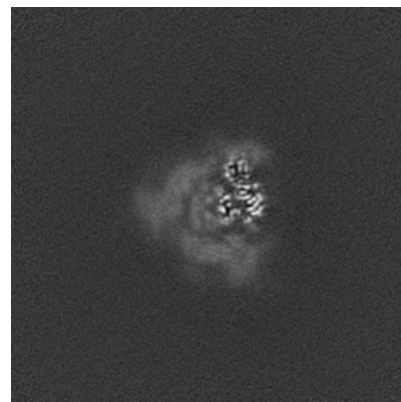
6.3.2 Raw map



X Index: 170



Y Index: 167

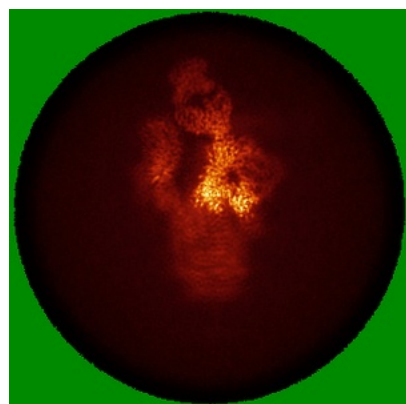


Z Index: 171

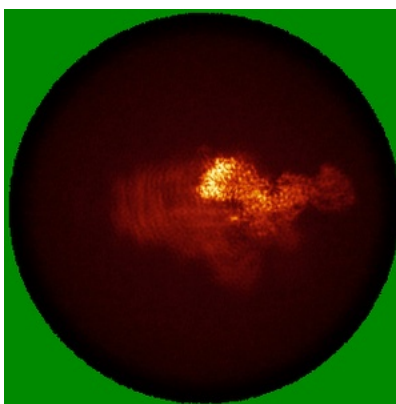
The images above show the largest variance slices of the map in three orthogonal directions.

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

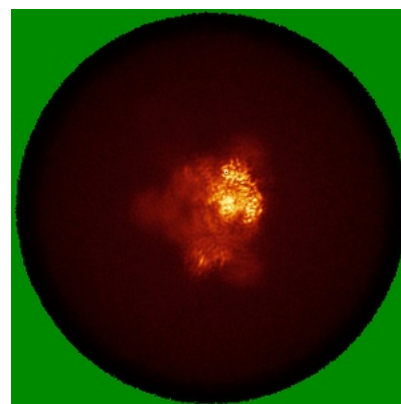
6.4.1 Primary map



X

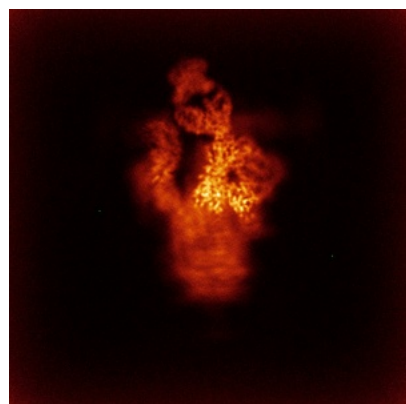


Y

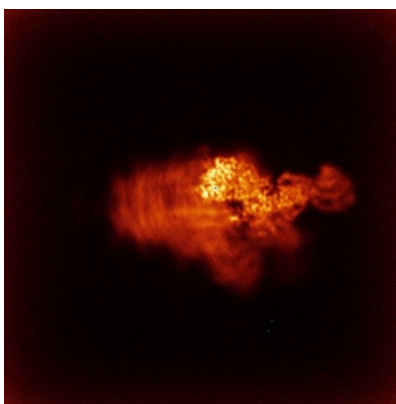


Z

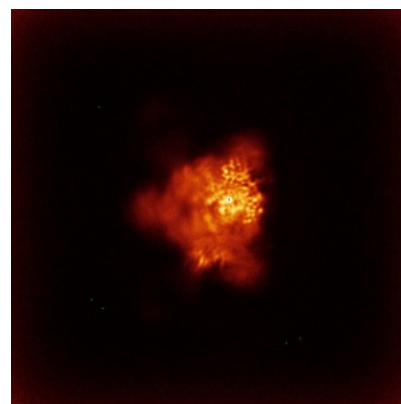
6.4.2 Raw map



X



Y

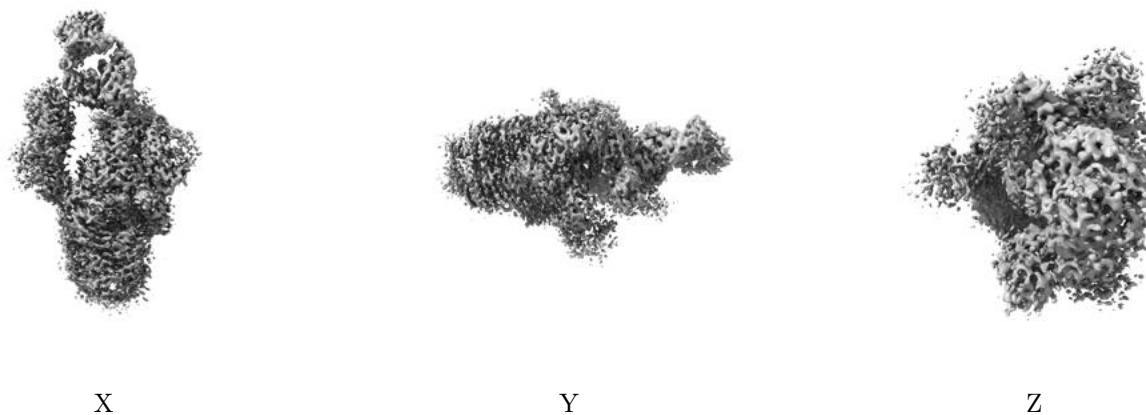


Z

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.

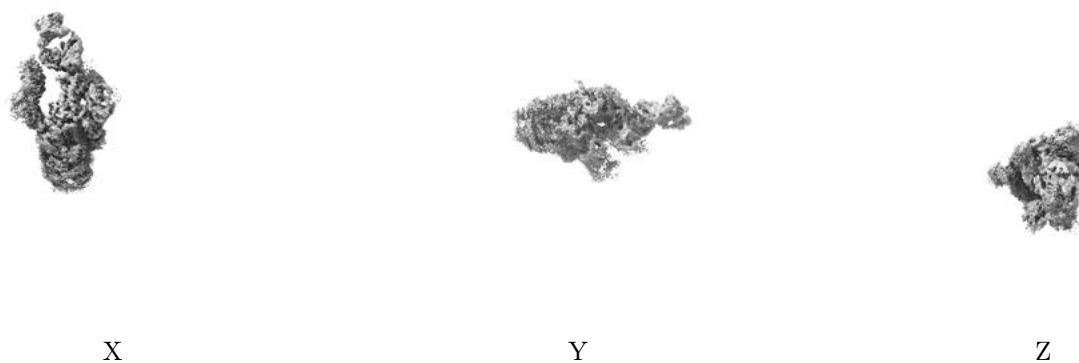
6.5 Orthogonal surface views [i](#)

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.

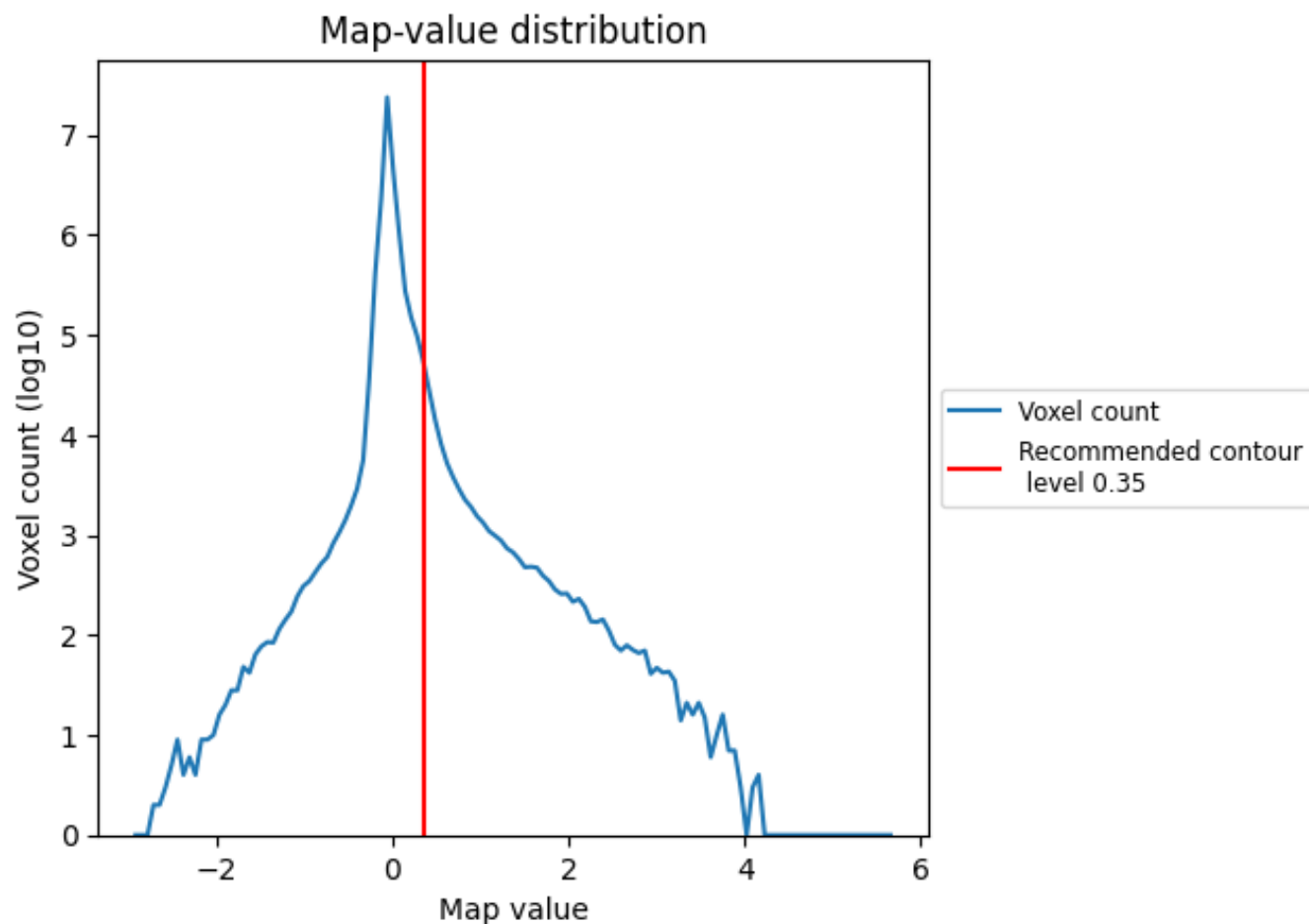
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

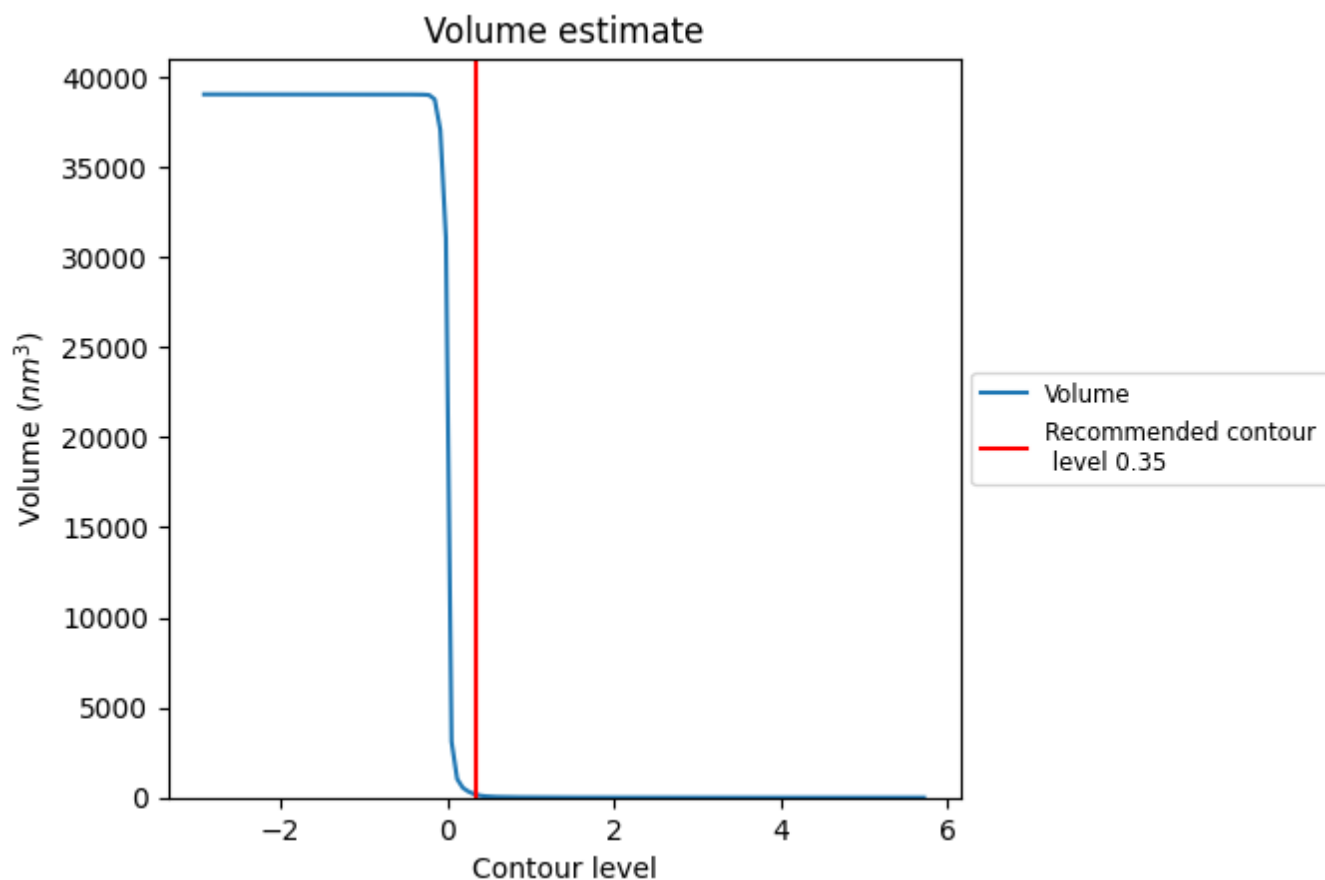
This section contains the results of statistical analysis of the map.

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.

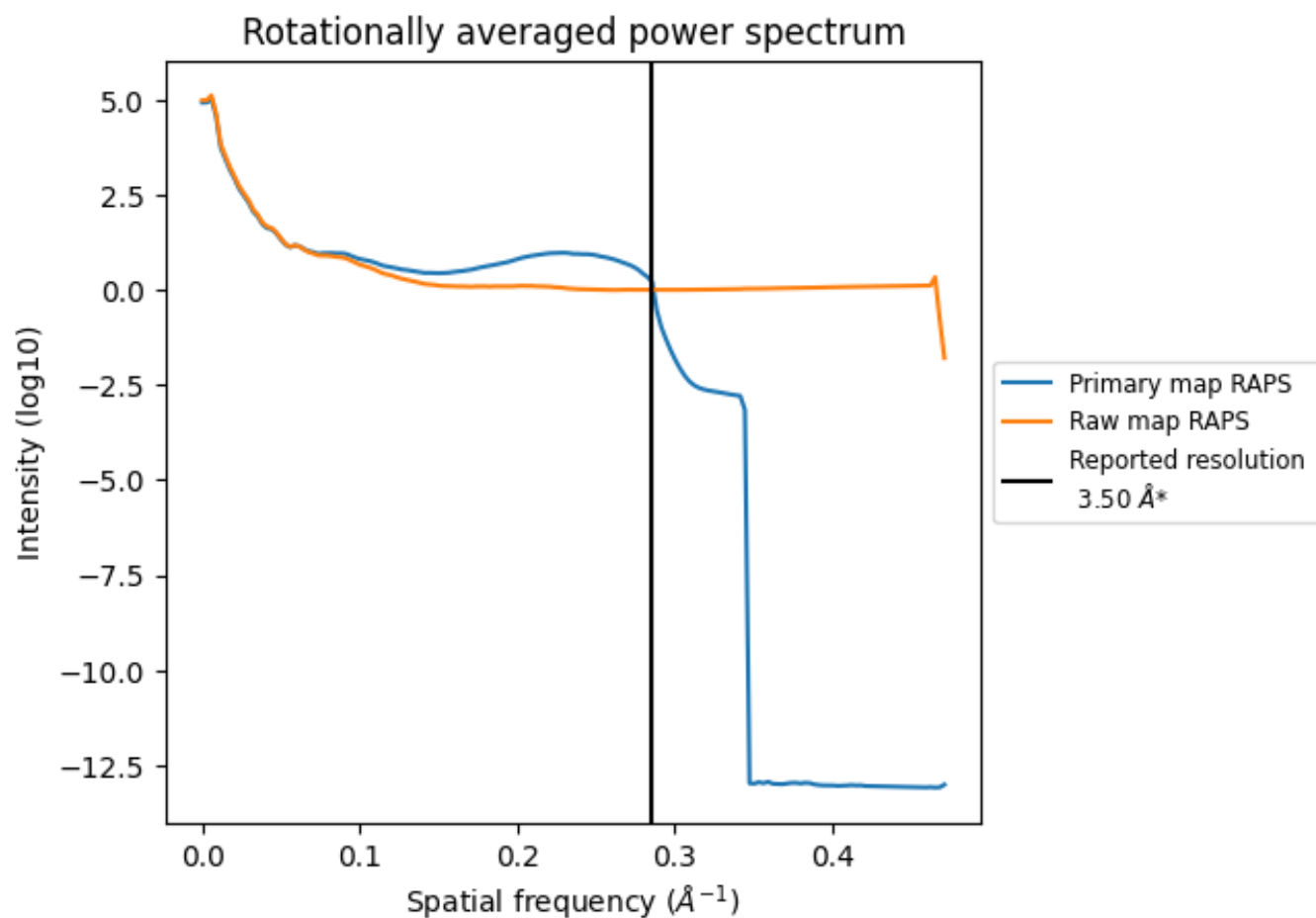
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm^3 ; 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 ⓘ

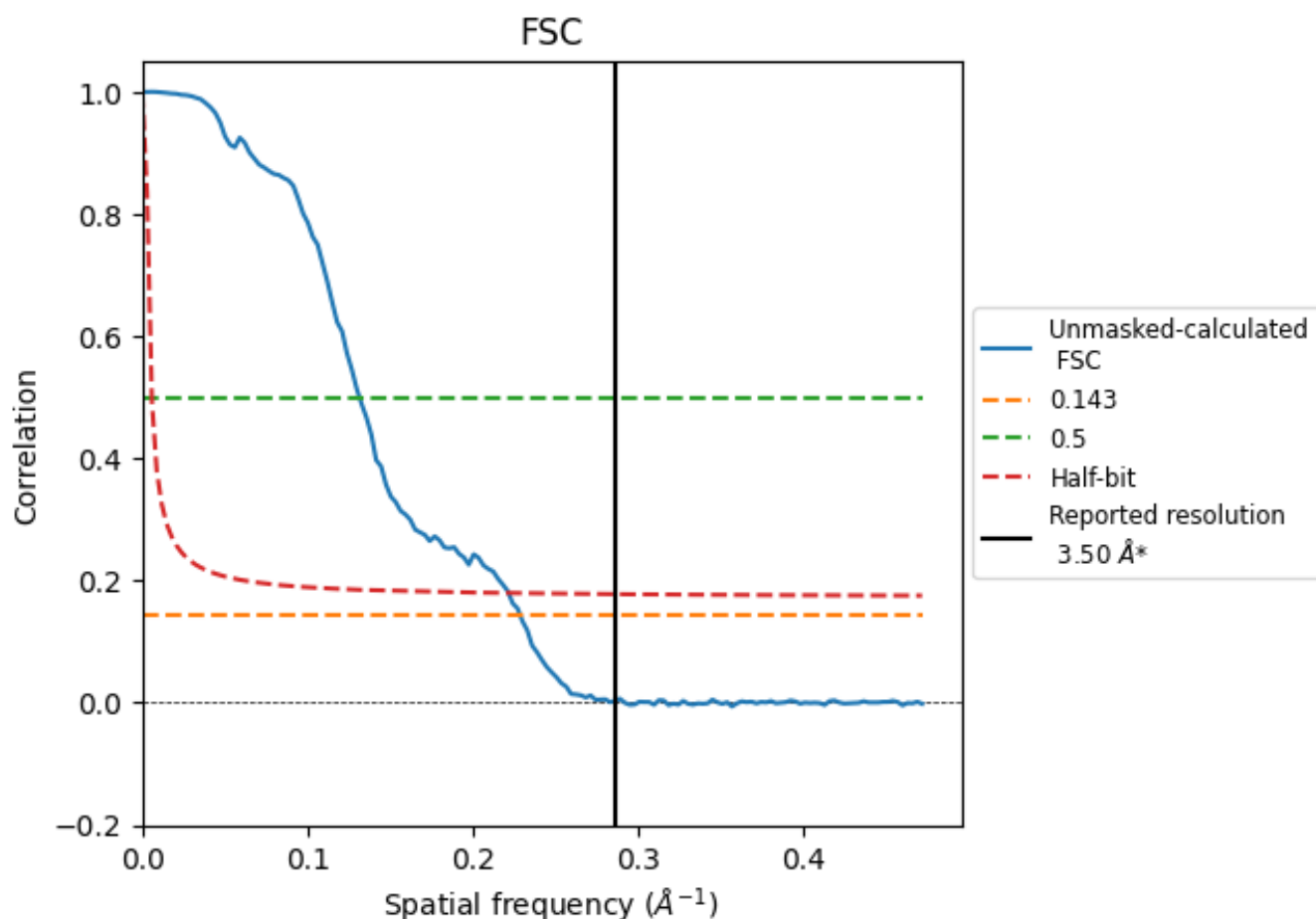


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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

8.2 Resolution estimates [i](#)

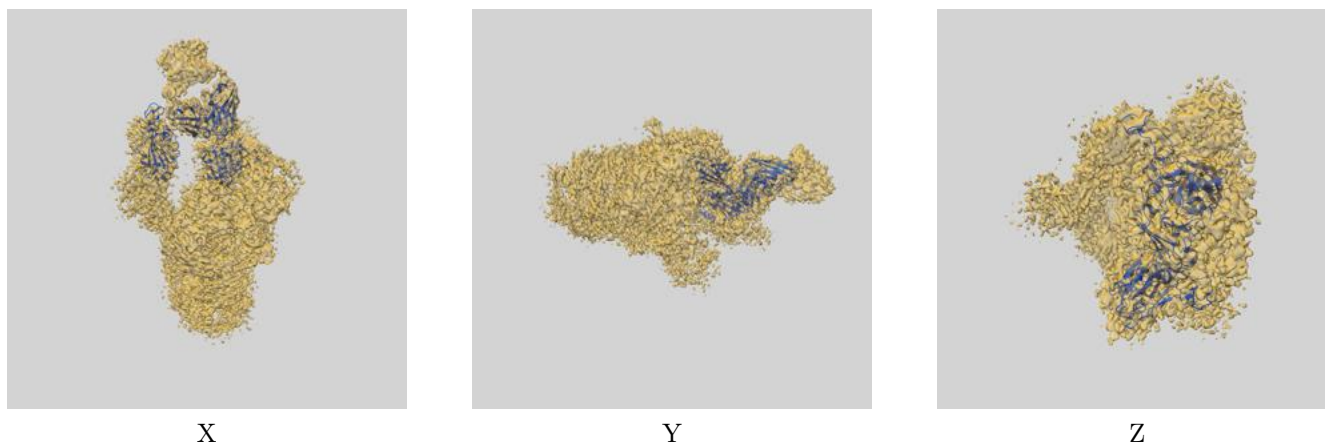
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	7.61	4.51

*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](#)

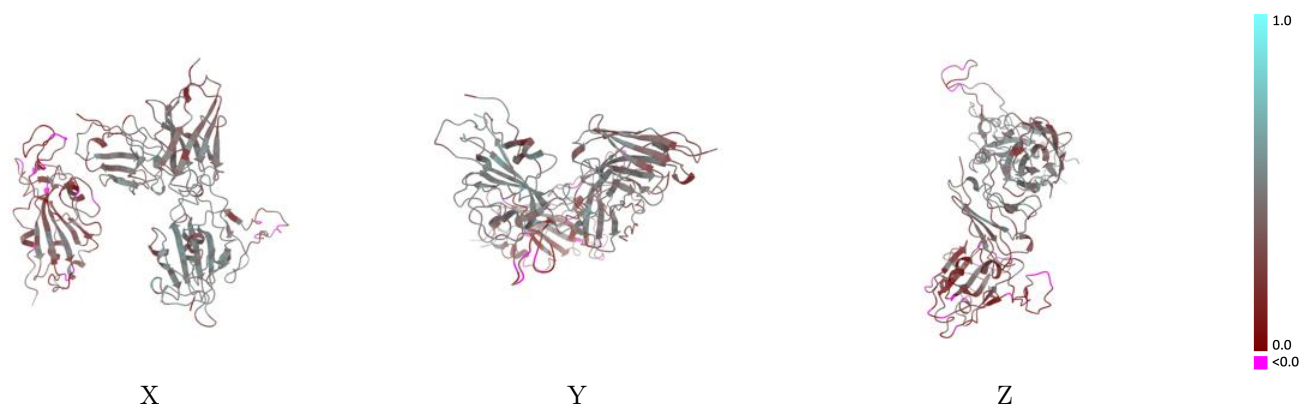
This section contains information regarding the fit between EMDB map EMD-33892 and PDB model 7YKJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



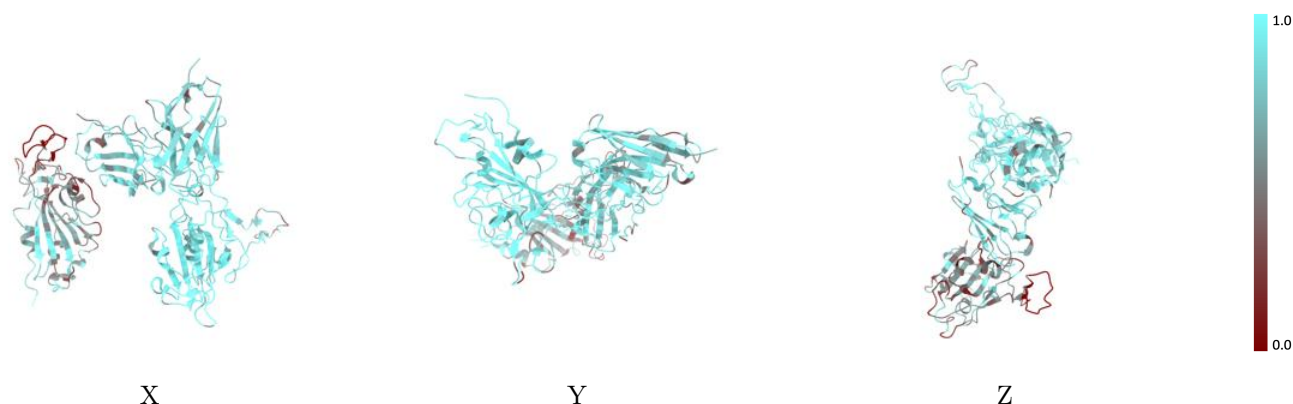
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



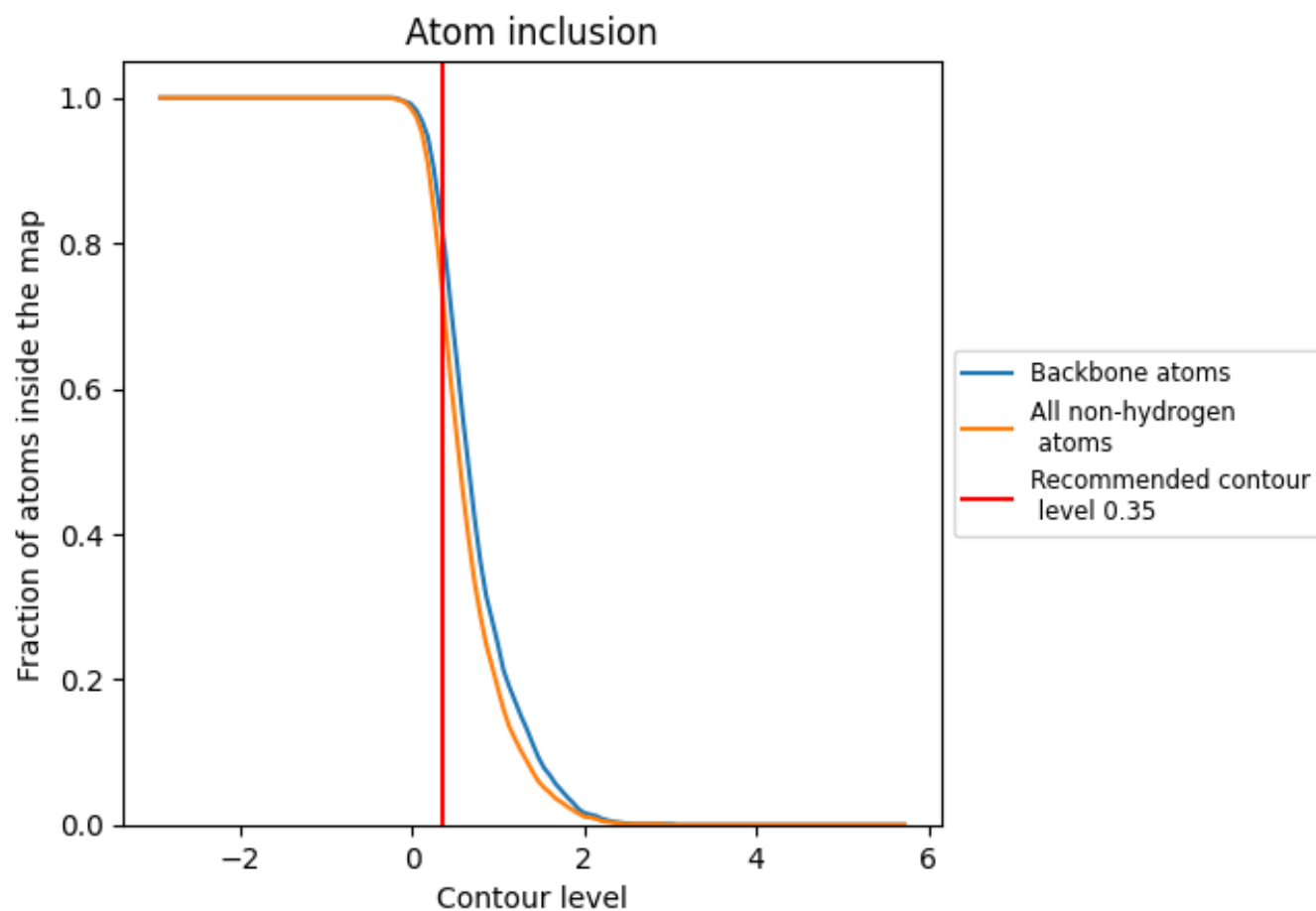
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.7430	0.3690
A	0.8080	0.4250
B	0.5270	0.2410
C	0.8880	0.4420
D	0.7960	0.4070

