



Full wwPDB EM Validation 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 Full wwPDB EM Validation 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

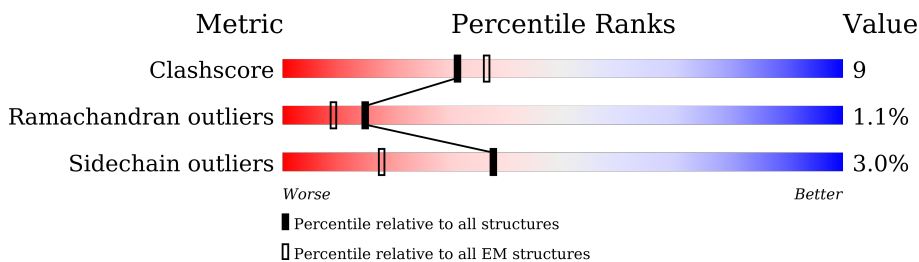
1 Overall quality at a glance

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

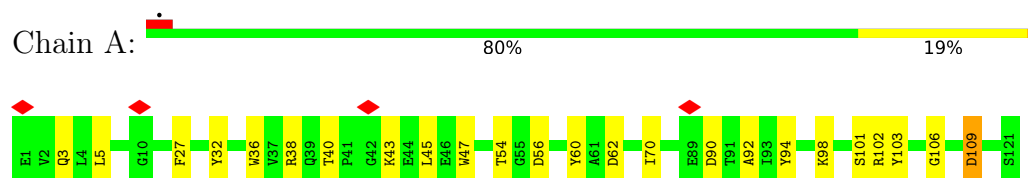
- Molecule 1: Spike glycoprotein

Chain C: 13% .. 84%

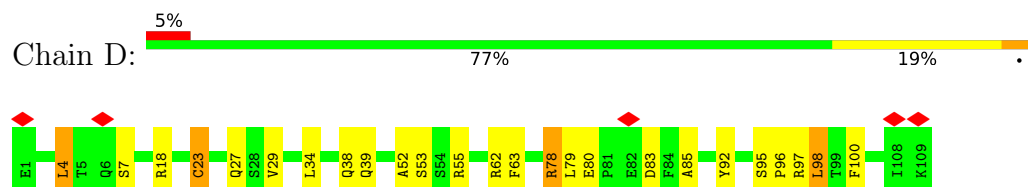
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- Molecule 2: P3E6 heavy chain



- 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(°)	Ideal(°)
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.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	109	ASP	Sidechain

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Mol	Chain	Res	Type	Group
2	A	32	TYR	Sidechain
2	A	38	ARG	Mainchain
2	A	60	TYR	Sidechain
2	A	62	ASP	Sidechain
2	A	90	ASP	Sidechain
2	A	92	ALA	Peptide
2	A	94	TYR	Sidechain
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
1	C	498	ARG	Sidechain
3	D	7	SER	Peptide
3	D	95	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:CYS:HB3	1:C:382:VAL:HG23	1.56	0.87
1:C:378:LYS:HD3	1:C:380:TYR:OH	1.79	0.82
2:A:101:SER:OG	2:A:103:TYR:O	2.03	0.76
1:B:372:ALA:H	1:B:373:PRO:HD2	1.50	0.74
3:D:96:PRO:C	3:D:98:LEU:H	1.96	0.69
1:C:373:PRO:CD	1:C:374:PHE:CD1	2.67	0.69
1:C:373:PRO:HD2	1:C:374:PHE:N	2.10	0.67
2:A:47:TRP:CD1	3:D:98:LEU:HD23	2.30	0.66
1:C:378:LYS:HD3	1:C:380:TYR:CZ	2.31	0.66
3:D:96:PRO:O	3:D:98:LEU:N	2.29	0.65
2:A:40:THR:HG23	2:A:43:LYS:HE2	1.79	0.65
1:C:445:VAL:HG11	3:D:96:PRO:HD3	1.80	0.64
1:C:379:CYS:HB3	1:C:382:VAL:CG2	2.28	0.63
1:B:374:PHE:HB2	1:B:434:ILE:HD11	1.79	0.63
1:B:375:PHE:HD2	1:B:436:TRP:HA	1.63	0.62
1:C:495:TYR:O	1:C:496:SER:CB	2.48	0.61
1:C:350:VAL:HG21	1:C:418:ILE:HD11	1.82	0.60
1:C:383:SER:HB2	1:C:386:LYS:HG3	1.82	0.60
3:D:55:ARG:NH1	3:D:63:PHE:O	2.36	0.59
1:B:447:GLY:HA3	1:B:449:TYR:CZ	2.39	0.58
3:D:39:GLN:O	3:D:85:ALA:HB1	2.03	0.57
1:B:454:ARG:HH11	1:B:457:ARG:HD2	1.68	0.57
1:C:406:GLU:HB3	1:C:418:ILE:HG21	1.87	0.57
1:C:444:LYS:HG2	2:A:103:TYR:CD1	2.41	0.56
2:A:36:TRP:CD1	2:A:70:ILE:HD11	2.44	0.53
1:B:457:ARG:HH22	1:B:461:LEU:HA	1.74	0.52
3:D:96:PRO:C	3:D:98:LEU:N	2.63	0.52
3:D:78:ARG:NH2	3:D:80:GLU:OE2	2.43	0.52
2:A:45:LEU:H	2:A:45:LEU:HD12	1.75	0.52
1:C:373:PRO:CD	1:C:374:PHE:N	2.73	0.51
1:B:476:GLY:H	1:B:487:ASN:HB3	1.76	0.51
1:B:476:GLY:N	1:B:487:ASN:HB3	2.26	0.51
1:C:445:VAL:CG1	3:D:96:PRO:HD3	2.42	0.50
3:D:27:GLN:HE22	3:D:29:VAL:HG12	1.77	0.50
3:D:34:LEU:HB3	3:D:52:ALA:HB2	1.94	0.49
1:C:496:SER:O	1:C:501:TYR:HE2	1.95	0.49
1:C:395:VAL:HG23	1:C:524:VAL:HG21	1.95	0.49
2:A:54:THR:OG1	2:A:56:ASP:OD1	2.28	0.49
1:B:355:ARG:HB2	1:B:466:ARG:HH12	1.79	0.48
1:B:454:ARG:NH1	1:B:457:ARG:HD2	2.29	0.48
1:B:375:PHE:CD2	1:B:436:TRP:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ILE:HD11	1:B:495:TYR:OH	2.13	0.48
1:C:418:ILE:HD12	1:C:422:ASN:HD22	1.79	0.47
1:C:422:ASN:OD1	1:C:454:ARG:HB3	2.14	0.47
2:A:27:PHE:CE1	2:A:98:LYS:HD3	2.49	0.47
1:B:448:ASN:O	1:B:497:PHE:HB2	2.14	0.47
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.80	0.46
1:C:386:LYS:HE2	1:C:386:LYS:HB2	1.62	0.46
3:D:79:LEU:HD23	3:D:80:GLU:O	2.15	0.46
1:B:338:PHE:CZ	1:B:363:ALA:HB1	2.51	0.46
2:A:3:GLN:OE1	2:A:5:LEU:HD23	2.15	0.46
1:C:378:LYS:HG2	1:C:380:TYR:CE2	2.52	0.45
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.99	0.45
3:D:38:GLN:HG3	3:D:85:ALA:HB3	1.99	0.45
1:C:393:THR:HG23	1:C:517:LEU:O	2.16	0.45
1:B:420:ASP:OD2	3:D:18:ARG:NH2	2.48	0.45
1:B:355:ARG:HH12	1:B:464:PHE:HB3	1.82	0.44
1:C:336:CYS:HB2	1:C:337:PRO:HD2	2.00	0.44
1:C:416:GLY:N	1:C:420:ASP:OD1	2.45	0.44
3:D:62:ARG:NH1	3:D:83:ASP:OD2	2.51	0.44
3:D:34:LEU:HD12	3:D:34:LEU:HA	1.83	0.44
1:B:453:TYR:HB3	1:B:495:TYR:CE2	2.52	0.43
1:B:447:GLY:HA3	1:B:449:TYR:OH	2.18	0.43
1:C:441:LEU:HD23	2:A:102:ARG:HB2	2.00	0.43
1:B:423:TYR:HD1	1:B:424:LYS:N	2.17	0.42
1:B:474:GLN:HG2	1:B:476:GLY:O	2.20	0.42
2:A:45:LEU:HD13	3:D:100:PHE:CD2	2.54	0.42
1:C:373:PRO:HD2	1:C:374:PHE:H	1.82	0.41
3:D:4:LEU:HD22	3:D:23:CYS:SG	2.59	0.41
1:B:353:TRP:O	1:B:466:ARG:NH1	2.54	0.41
1:B:418:ILE:HA	1:B:418:ILE:HD13	1.94	0.41
2:A:106:GLY:HA2	3:D:92:TYR:CD2	2.56	0.40
1:B:353:TRP:CD2	1:B:466:ARG:HD3	2.57	0.40
1:B:375:PHE:HE2	1:B:437:ASN:H	1.65	0.40
1:C:342:PHE:CZ	1:C:511:VAL:HG11	2.57	0.40
1:C:444:LYS:HE3	1:C:444:LYS:HB3	1.82	0.40

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

All (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
1	C	496	SER
1	C	517	LEU

5.3.2 Protein sidechains [i](#)

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

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Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	88/90 (98%)	85 (97%)	3 (3%)	32	60
All	All	503/2297 (22%)	488 (97%)	15 (3%)	37	63

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	369	TYR
1	B	423	TYR
1	B	493	ARG
1	C	377	PHE
1	C	386	LYS
1	C	403	ARG
1	C	422	ASN
1	C	498	ARG
1	C	501	TYR
1	C	515	PHE
1	C	518	LEU
2	A	109	ASP
3	D	23	CYS
3	D	78	ARG
3	D	98	LEU

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 ⓘ

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.

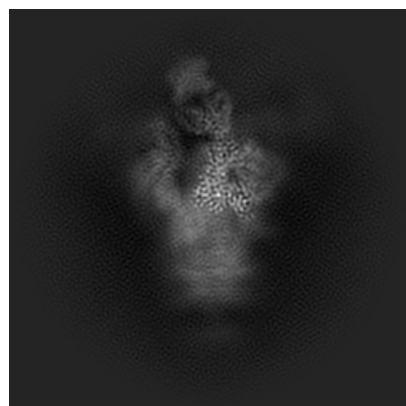
6 Map visualisation [i](#)

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

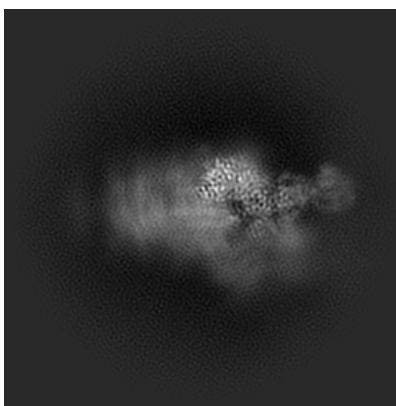
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

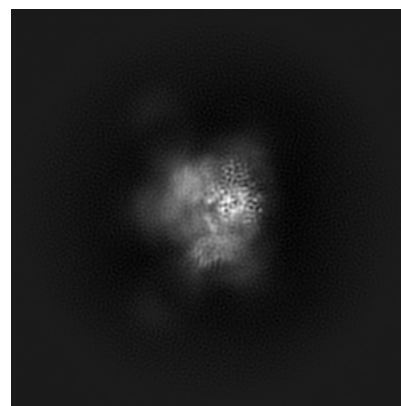
6.1.1 Primary map



X

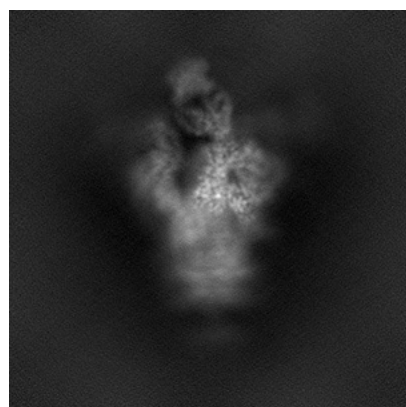


Y

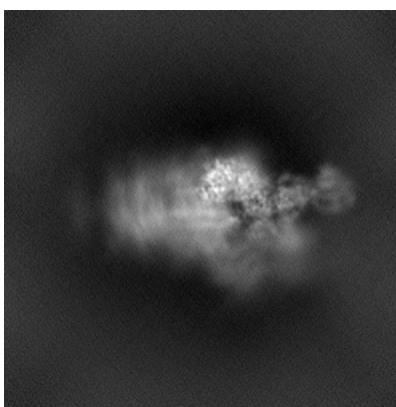


Z

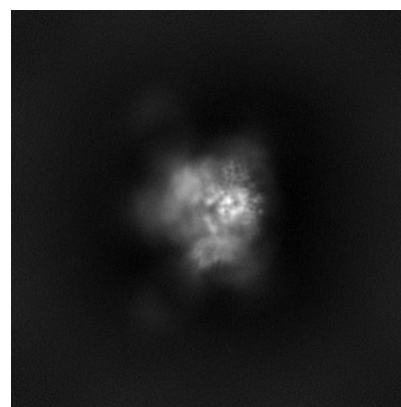
6.1.2 Raw map



X



Y

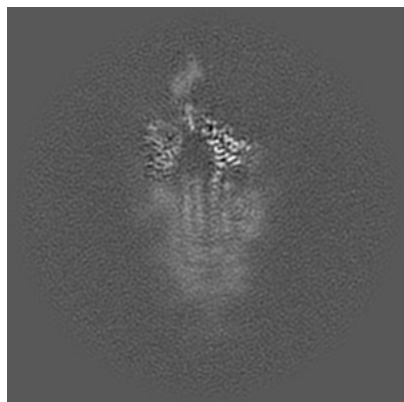


Z

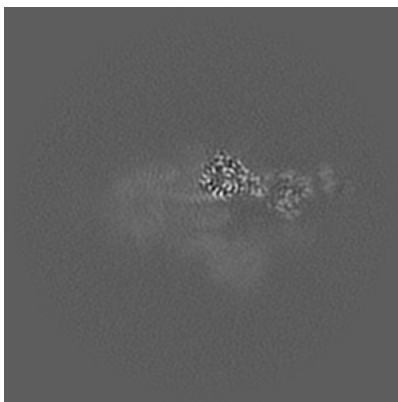
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

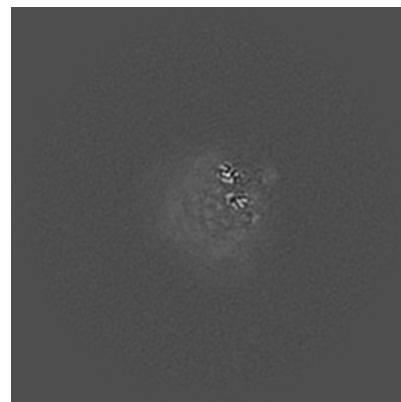
6.2.1 Primary map



X Index: 160

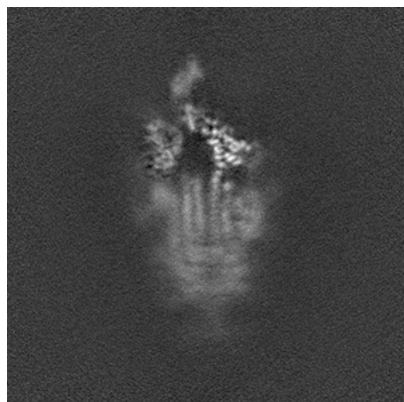


Y Index: 160

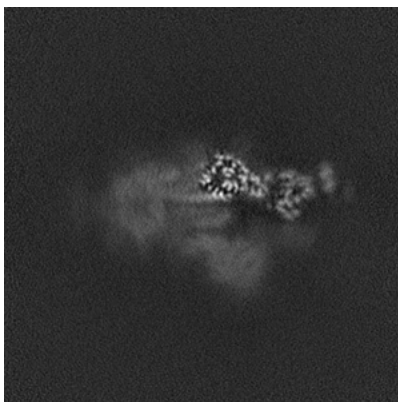


Z Index: 160

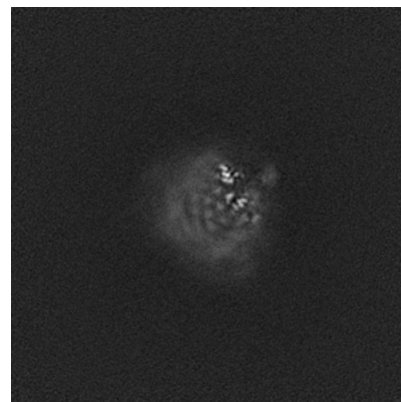
6.2.2 Raw map



X Index: 160



Y Index: 160

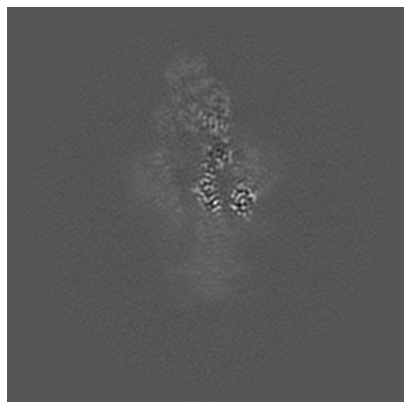


Z Index: 160

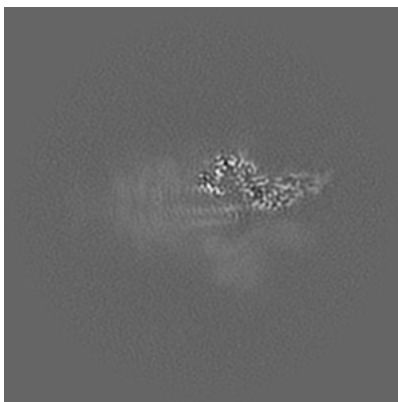
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

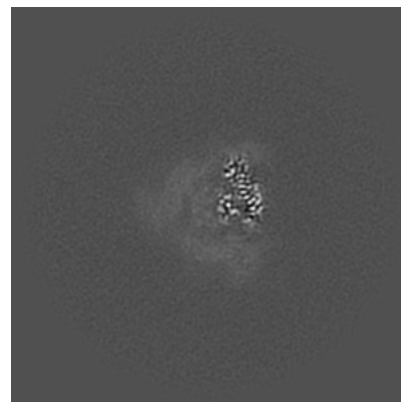
6.3.1 Primary map



X Index: 176

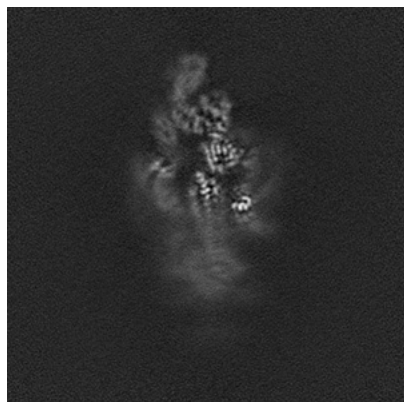


Y Index: 167

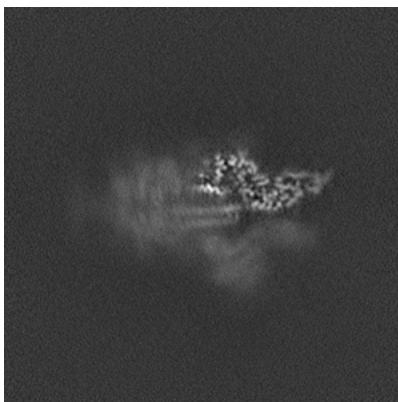


Z Index: 170

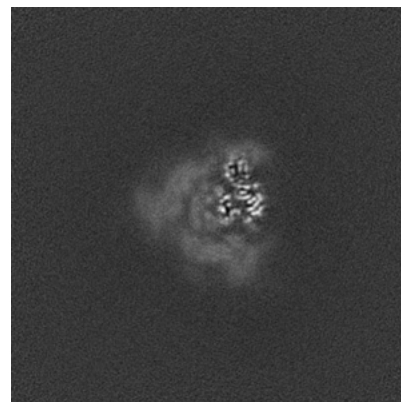
6.3.2 Raw map



X Index: 170



Y Index: 167

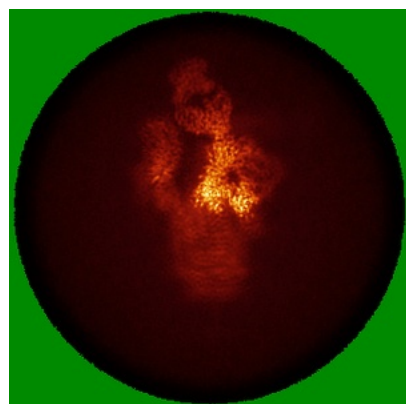


Z Index: 171

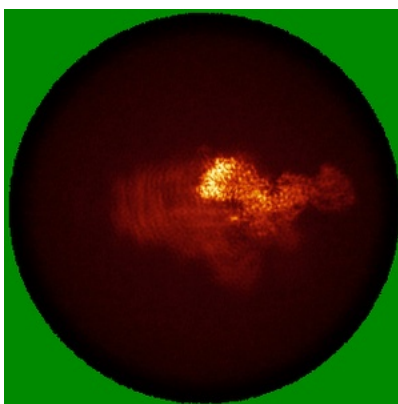
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

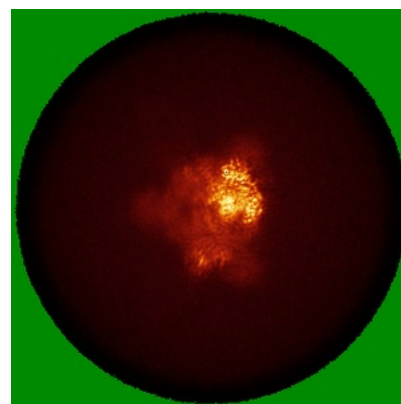
6.4.1 Primary map



X

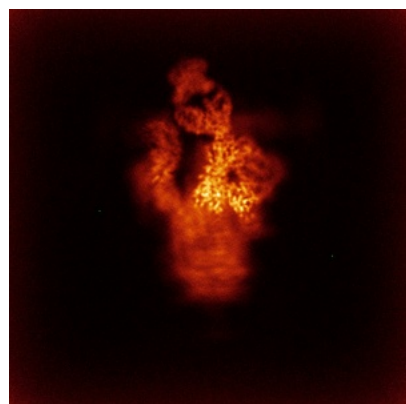


Y

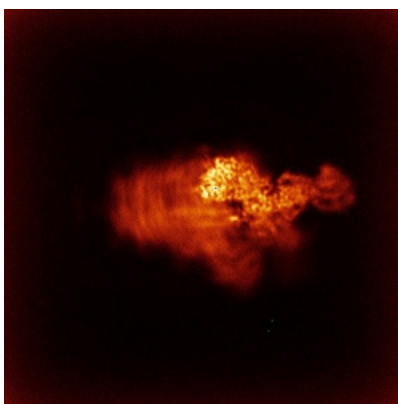


Z

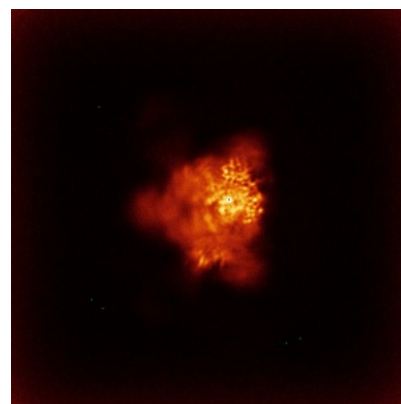
6.4.2 Raw map



X



Y

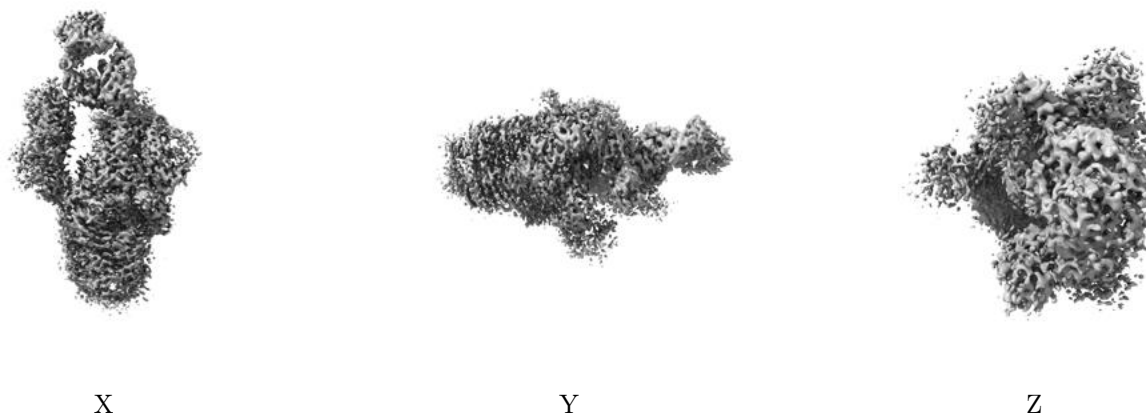


Z

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.

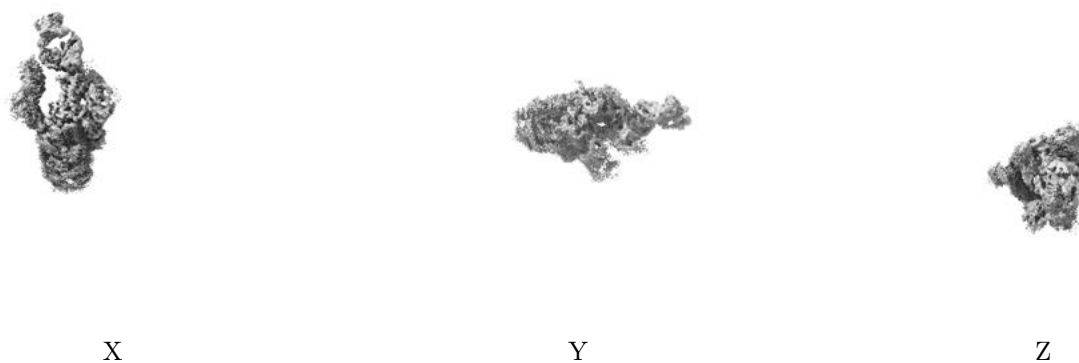
6.5 Orthogonal surface views [i](#)

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.

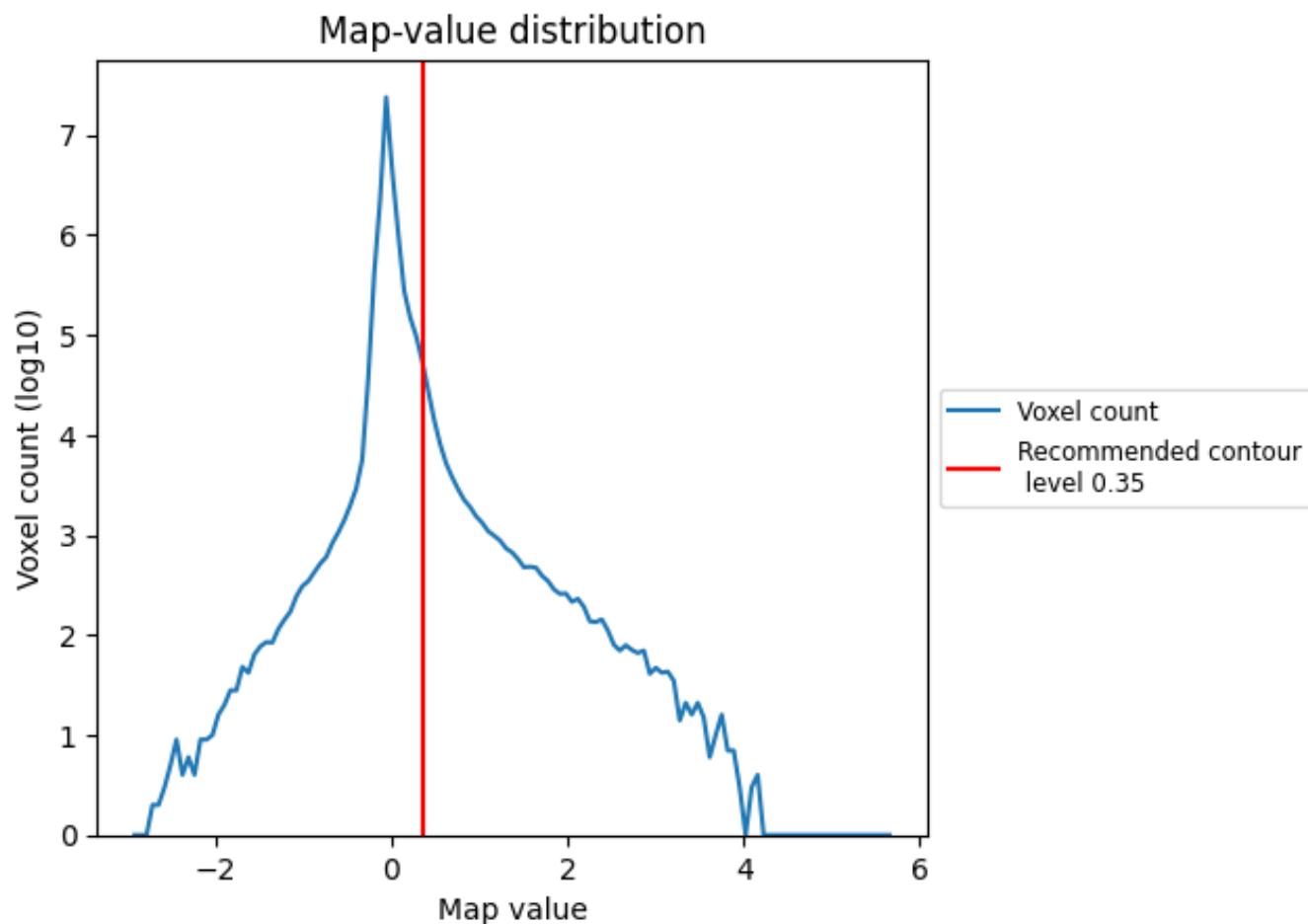
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

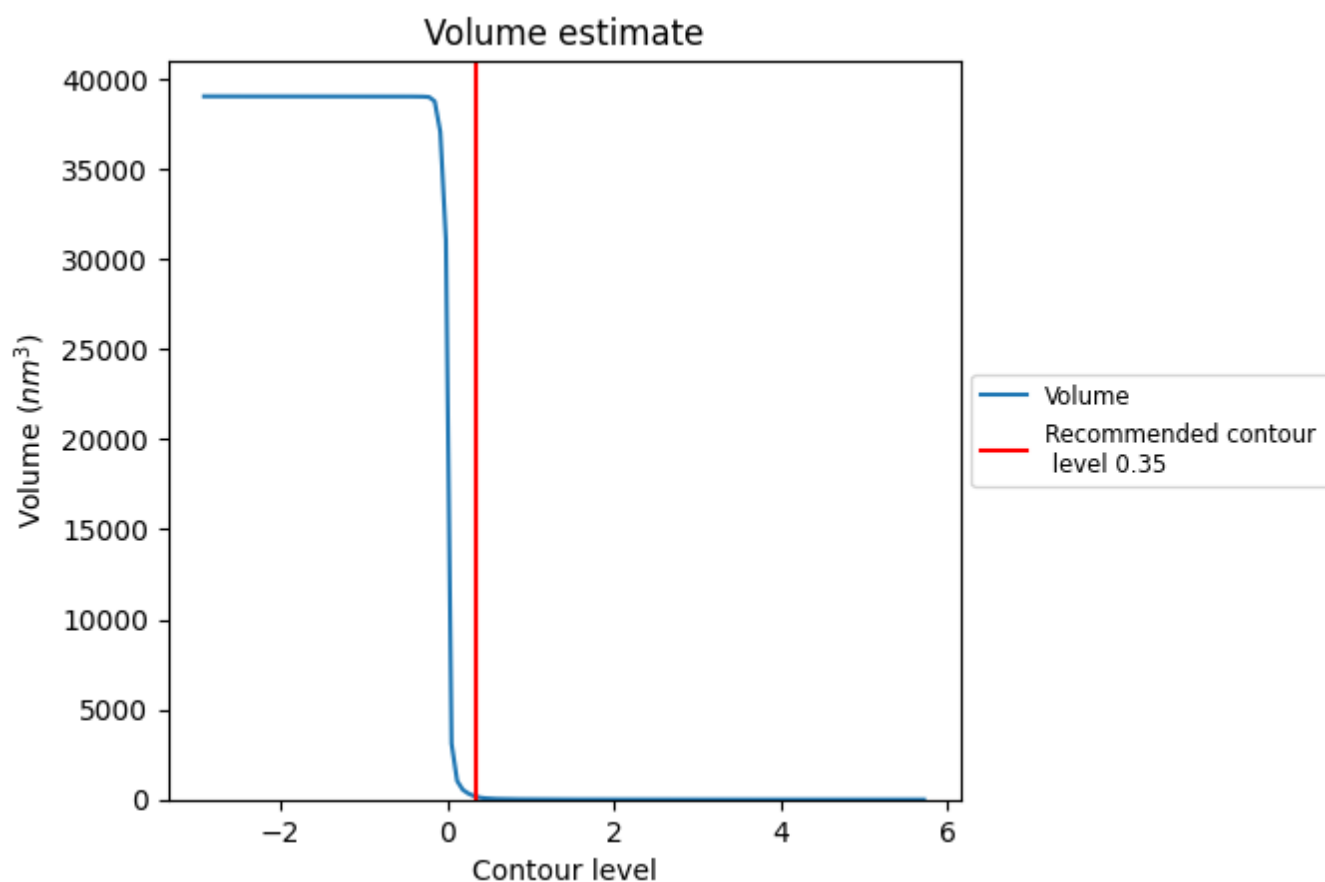
This section contains the results of statistical analysis of the map.

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.

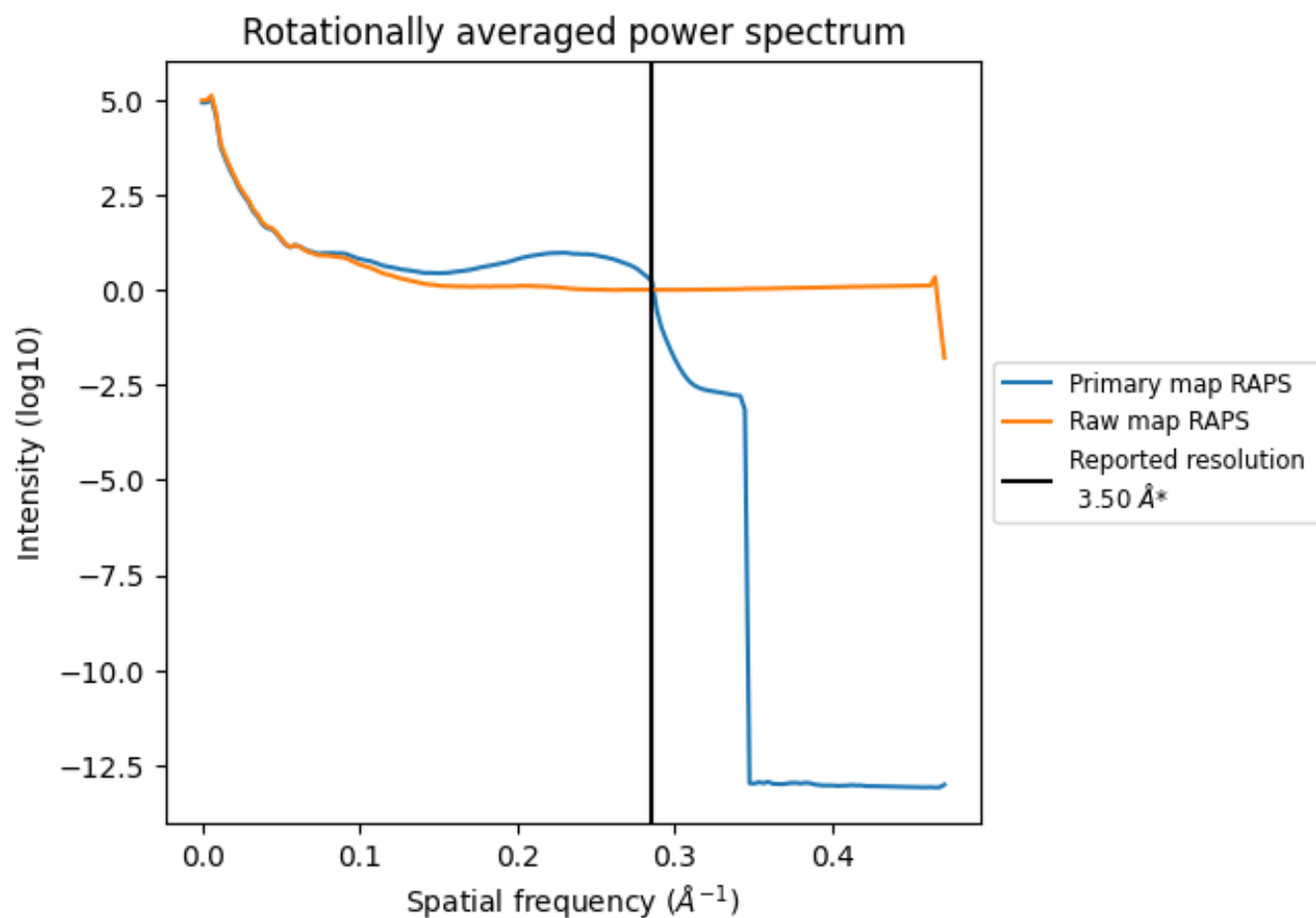
7.2 Volume estimate [i](#)



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 ⓘ

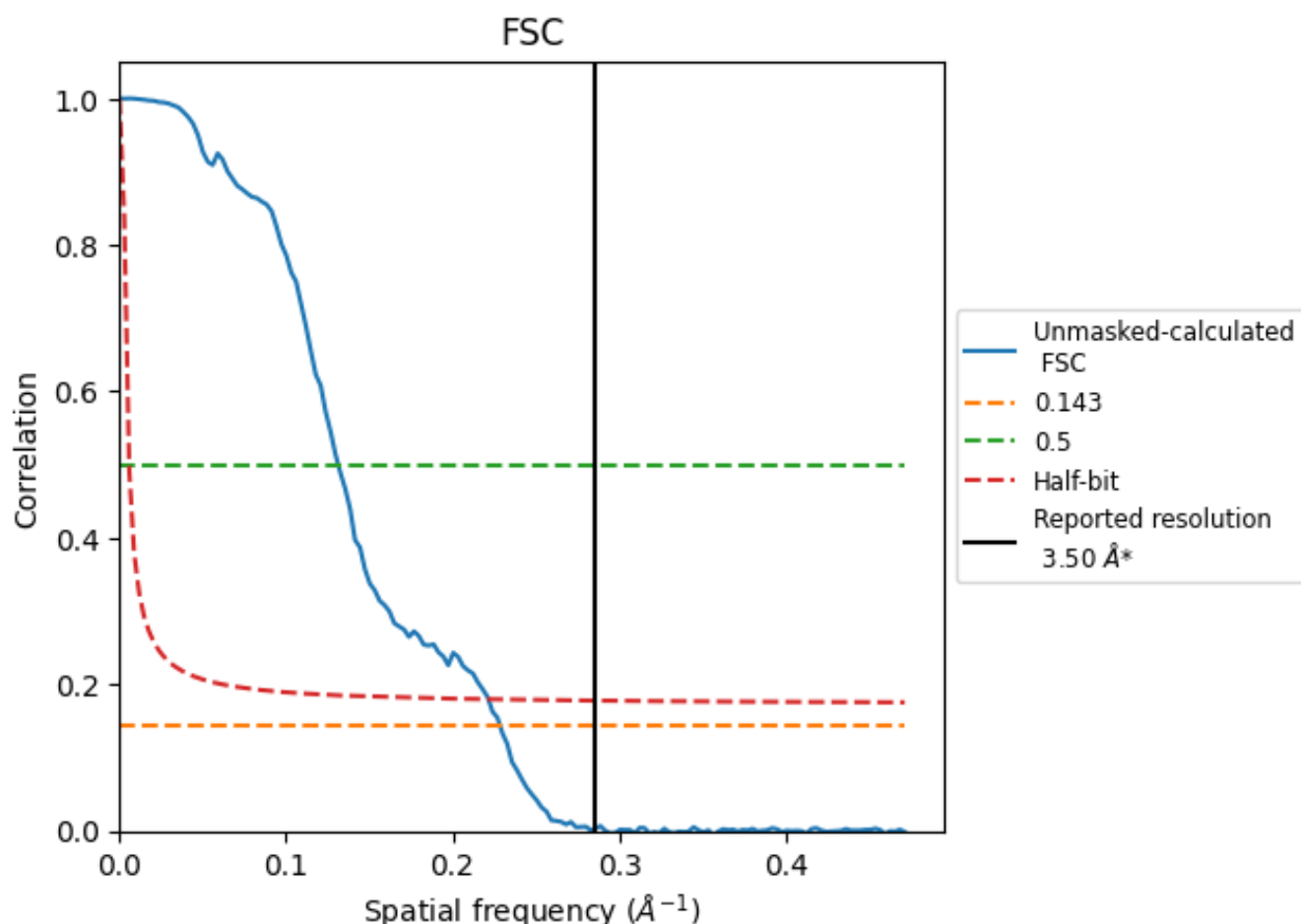


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

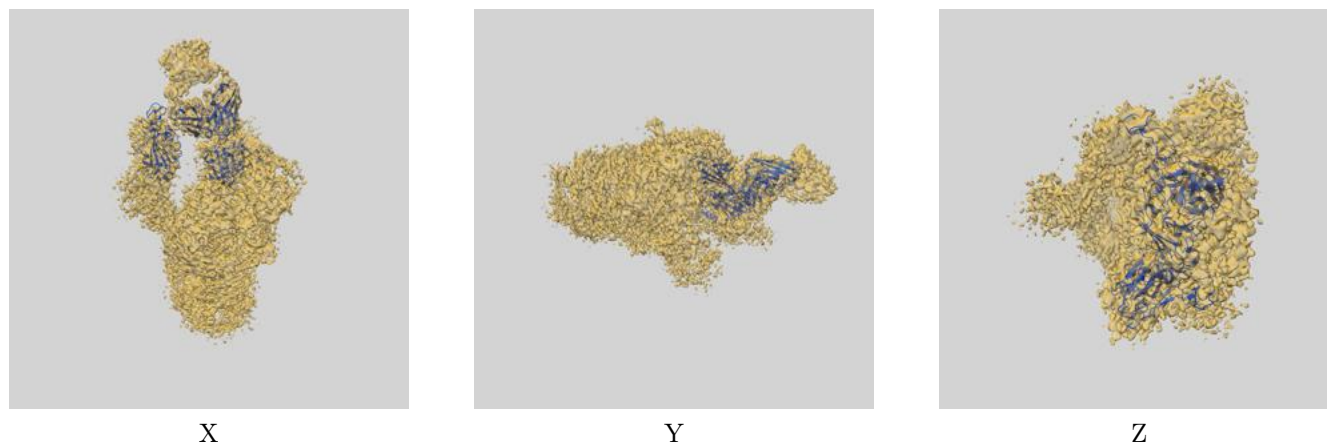
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	7.61	4.51

*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](#)

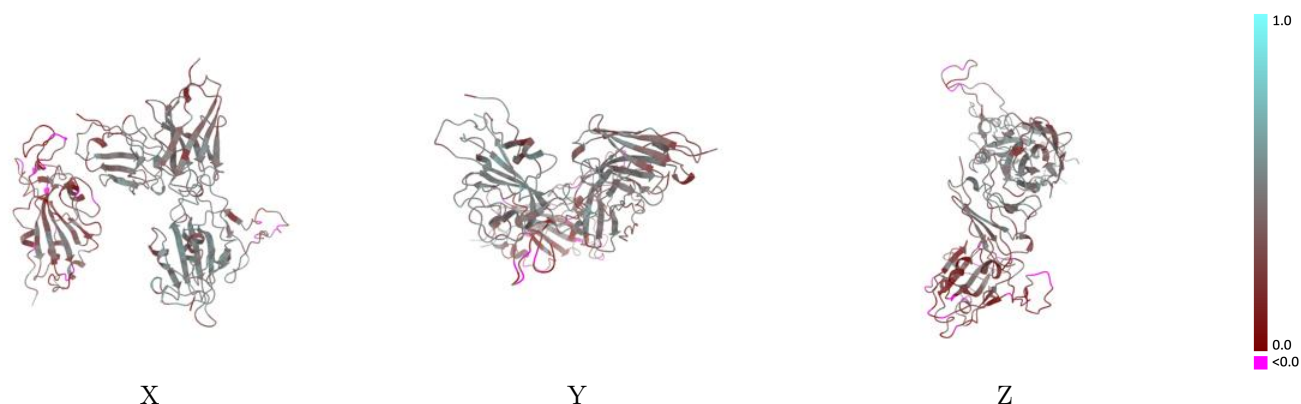
This section contains information regarding the fit between EMDB map EMD-33892 and PDB model 7YKJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



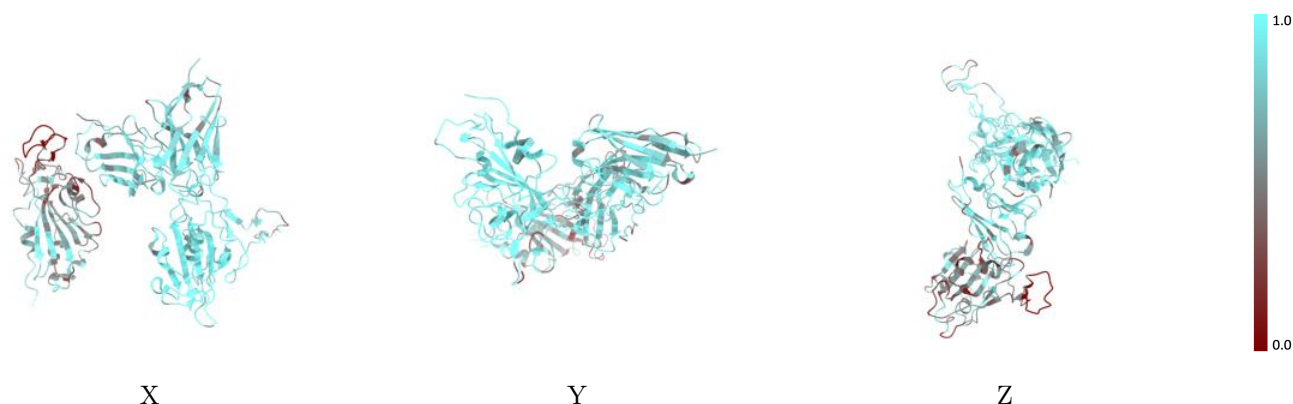
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



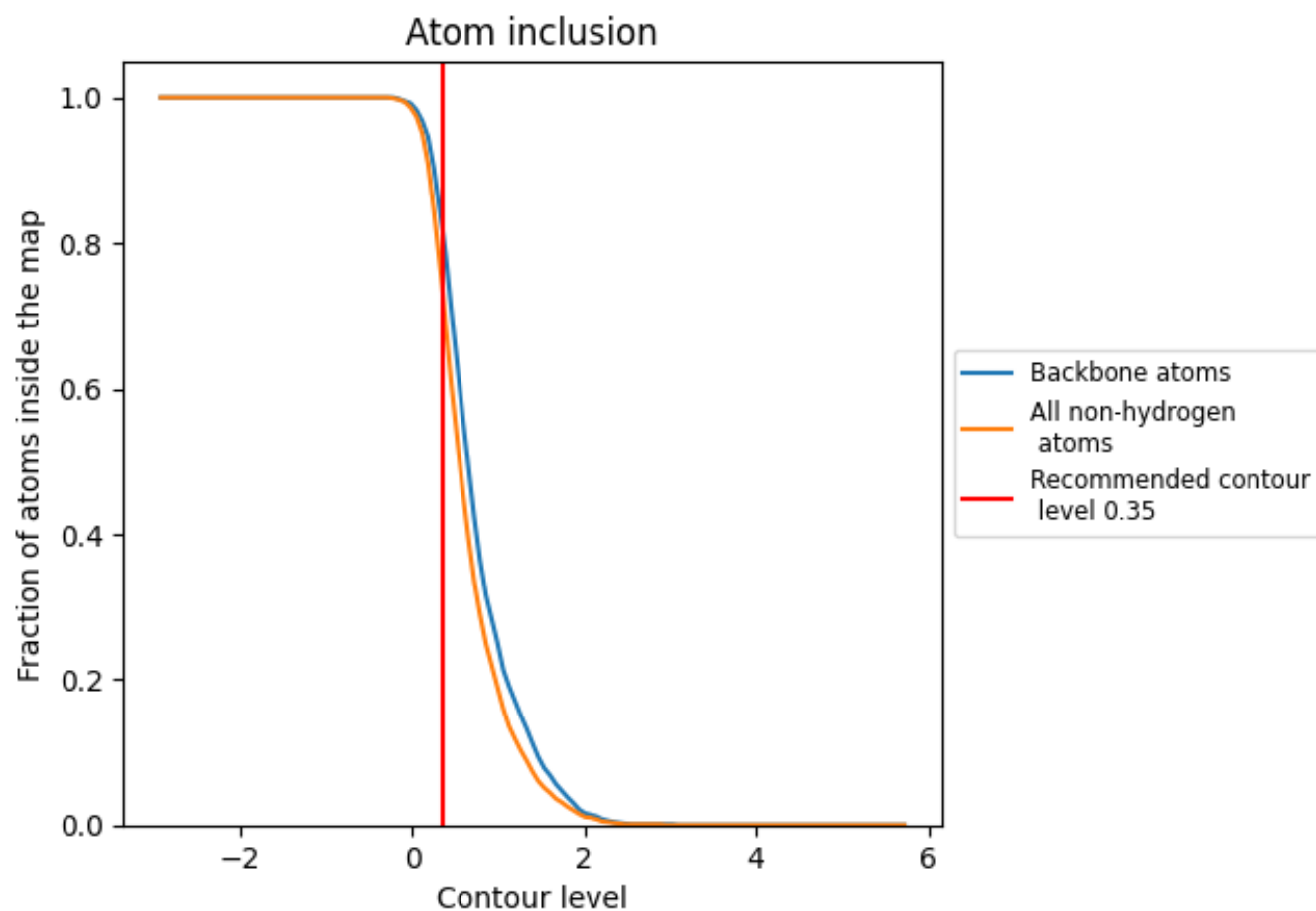
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

