



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2024 – 03:34 AM JST

PDB ID : 8WTJ
EMDB ID : EMD-37835
Title : XBB.1.5.70 spike protein in complex with ACE2
Authors : Feng, L.L.; Feng, L.L.
Deposited on : 2023-10-18
Resolution : 4.64 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

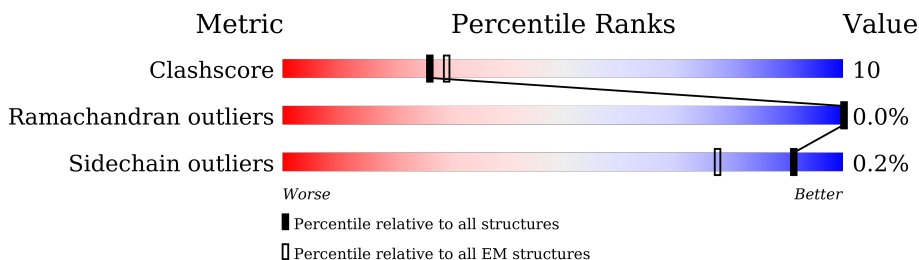
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.64 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	A	1317	 6% 61% 20% 19%
1	B	1317	 6% 60% 21% 19%
1	C	1317	 14% 61% 19% 19%
2	E	594	 65% 76% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29931 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	A	1066	Total	C	N	O	S	0	0
			8360	5346	1396	1579	39		
1	B	1066	Total	C	N	O	S	0	0
			8359	5344	1396	1580	39		
1	C	1067	Total	C	N	O	S	0	0
			8367	5350	1397	1581	39		

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	variant	UNP P0DTC2
A	80	ALA	VAL	variant	UNP P0DTC2
A	139	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	GLN	HIS	variant	UNP P0DTC2
A	179	GLU	GLN	variant	UNP P0DTC2
A	209	GLU	VAL	variant	UNP P0DTC2
A	248	VAL	GLY	variant	UNP P0DTC2
A	335	HIS	GLY	variant	UNP P0DTC2
A	342	THR	ARG	variant	UNP P0DTC2
A	364	ILE	LEU	variant	UNP P0DTC2
A	367	PHE	SER	variant	UNP P0DTC2
A	369	PRO	SER	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	372	ALA	THR	variant	UNP P0DTC2
A	401	ASN	ASP	variant	UNP P0DTC2
A	404	SER	ARG	variant	UNP P0DTC2
A	413	ASN	LYS	variant	UNP P0DTC2
A	436	LYS	ASN	variant	UNP P0DTC2
A	441	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	442	SER	GLY	variant	UNP P0DTC2
A	451	PHE	LEU	conflict	UNP P0DTC2
A	452	LEU	PHE	variant	UNP P0DTC2
A	456	LYS	ASN	variant	UNP P0DTC2
A	473	ASN	SER	variant	UNP P0DTC2
A	474	LYS	THR	variant	UNP P0DTC2
A	480	ALA	GLU	variant	UNP P0DTC2
A	482	PRO	PHE	variant	UNP P0DTC2
A	486	SER	PHE	variant	UNP P0DTC2
A	494	ARG	GLN	variant	UNP P0DTC2
A	497	TYR	ASN	variant	UNP P0DTC2
A	501	HIS	TYR	variant	UNP P0DTC2
A	610	GLY	ASP	variant	UNP P0DTC2
A	651	TYR	HIS	variant	UNP P0DTC2
A	675	LYS	ASN	variant	UNP P0DTC2
A	677	HIS	PRO	variant	UNP P0DTC2
A	678	GLY	ARG	conflict	UNP P0DTC2
A	679	SER	ARG	conflict	UNP P0DTC2
A	681	SER	ARG	conflict	UNP P0DTC2
A	760	LYS	ASN	variant	UNP P0DTC2
A	792	TYR	ASP	variant	UNP P0DTC2
A	813	PRO	PHE	conflict	UNP P0DTC2
A	825	THR	ALA	conflict	UNP P0DTC2
A	832	LYS	GLN	conflict	UNP P0DTC2
A	888	PRO	ALA	conflict	UNP P0DTC2
A	895	PRO	ALA	conflict	UNP P0DTC2
A	938	PRO	ALA	conflict	UNP P0DTC2
A	950	HIS	GLN	variant	UNP P0DTC2
A	965	LYS	ASN	variant	UNP P0DTC2
A	982	PRO	LYS	engineered mutation	UNP P0DTC2
A	983	PRO	VAL	engineered mutation	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	24	SER	ALA	variant	UNP P0DTC2
B	80	ALA	VAL	variant	UNP P0DTC2
B	139	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	GLN	HIS	variant	UNP P0DTC2
B	179	GLU	GLN	variant	UNP P0DTC2
B	209	GLU	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	248	VAL	GLY	variant	UNP P0DTC2
B	335	HIS	GLY	variant	UNP P0DTC2
B	342	THR	ARG	variant	UNP P0DTC2
B	364	ILE	LEU	variant	UNP P0DTC2
B	367	PHE	SER	variant	UNP P0DTC2
B	369	PRO	SER	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	372	ALA	THR	variant	UNP P0DTC2
B	401	ASN	ASP	variant	UNP P0DTC2
B	404	SER	ARG	variant	UNP P0DTC2
B	413	ASN	LYS	variant	UNP P0DTC2
B	436	LYS	ASN	variant	UNP P0DTC2
B	441	PRO	VAL	variant	UNP P0DTC2
B	442	SER	GLY	variant	UNP P0DTC2
B	451	PHE	LEU	conflict	UNP P0DTC2
B	452	LEU	PHE	variant	UNP P0DTC2
B	456	LYS	ASN	variant	UNP P0DTC2
B	473	ASN	SER	variant	UNP P0DTC2
B	474	LYS	THR	variant	UNP P0DTC2
B	480	ALA	GLU	variant	UNP P0DTC2
B	482	PRO	PHE	variant	UNP P0DTC2
B	486	SER	PHE	variant	UNP P0DTC2
B	494	ARG	GLN	variant	UNP P0DTC2
B	497	TYR	ASN	variant	UNP P0DTC2
B	501	HIS	TYR	variant	UNP P0DTC2
B	610	GLY	ASP	variant	UNP P0DTC2
B	651	TYR	HIS	variant	UNP P0DTC2
B	675	LYS	ASN	variant	UNP P0DTC2
B	677	HIS	PRO	variant	UNP P0DTC2
B	678	GLY	ARG	conflict	UNP P0DTC2
B	679	SER	ARG	conflict	UNP P0DTC2
B	681	SER	ARG	conflict	UNP P0DTC2
B	760	LYS	ASN	variant	UNP P0DTC2
B	792	TYR	ASP	variant	UNP P0DTC2
B	813	PRO	PHE	conflict	UNP P0DTC2
B	825	THR	ALA	conflict	UNP P0DTC2
B	832	LYS	GLN	conflict	UNP P0DTC2
B	888	PRO	ALA	conflict	UNP P0DTC2
B	895	PRO	ALA	conflict	UNP P0DTC2
B	938	PRO	ALA	conflict	UNP P0DTC2
B	950	HIS	GLN	variant	UNP P0DTC2
B	965	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	982	PRO	LYS	engineered mutation	UNP P0DTC2
B	983	PRO	VAL	engineered mutation	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	24	SER	ALA	variant	UNP P0DTC2
C	80	ALA	VAL	variant	UNP P0DTC2
C	139	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	GLN	HIS	variant	UNP P0DTC2
C	179	GLU	GLN	variant	UNP P0DTC2
C	209	GLU	VAL	variant	UNP P0DTC2
C	248	VAL	GLY	variant	UNP P0DTC2
C	335	HIS	GLY	variant	UNP P0DTC2
C	342	THR	ARG	variant	UNP P0DTC2
C	364	ILE	LEU	variant	UNP P0DTC2
C	367	PHE	SER	variant	UNP P0DTC2
C	369	PRO	SER	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	372	ALA	THR	variant	UNP P0DTC2
C	401	ASN	ASP	variant	UNP P0DTC2
C	404	SER	ARG	variant	UNP P0DTC2
C	413	ASN	LYS	variant	UNP P0DTC2
C	436	LYS	ASN	variant	UNP P0DTC2
C	441	PRO	VAL	variant	UNP P0DTC2
C	442	SER	GLY	variant	UNP P0DTC2
C	451	PHE	LEU	conflict	UNP P0DTC2
C	452	LEU	PHE	variant	UNP P0DTC2
C	456	LYS	ASN	variant	UNP P0DTC2
C	473	ASN	SER	variant	UNP P0DTC2
C	474	LYS	THR	variant	UNP P0DTC2
C	480	ALA	GLU	variant	UNP P0DTC2
C	482	PRO	PHE	variant	UNP P0DTC2
C	486	SER	PHE	variant	UNP P0DTC2
C	494	ARG	GLN	variant	UNP P0DTC2
C	497	TYR	ASN	variant	UNP P0DTC2
C	501	HIS	TYR	variant	UNP P0DTC2
C	610	GLY	ASP	variant	UNP P0DTC2
C	651	TYR	HIS	variant	UNP P0DTC2
C	675	LYS	ASN	variant	UNP P0DTC2
C	677	HIS	PRO	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	678	GLY	ARG	conflict	UNP P0DTC2
C	679	SER	ARG	conflict	UNP P0DTC2
C	681	SER	ARG	conflict	UNP P0DTC2
C	760	LYS	ASN	variant	UNP P0DTC2
C	792	TYR	ASP	variant	UNP P0DTC2
C	813	PRO	PHE	conflict	UNP P0DTC2
C	825	THR	ALA	conflict	UNP P0DTC2
C	832	LYS	GLN	conflict	UNP P0DTC2
C	888	PRO	ALA	conflict	UNP P0DTC2
C	895	PRO	ALA	conflict	UNP P0DTC2
C	938	PRO	ALA	conflict	UNP P0DTC2
C	950	HIS	GLN	variant	UNP P0DTC2
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C	982	PRO	LYS	engineered mutation	UNP P0DTC2
C	983	PRO	VAL	engineered mutation	UNP P0DTC2

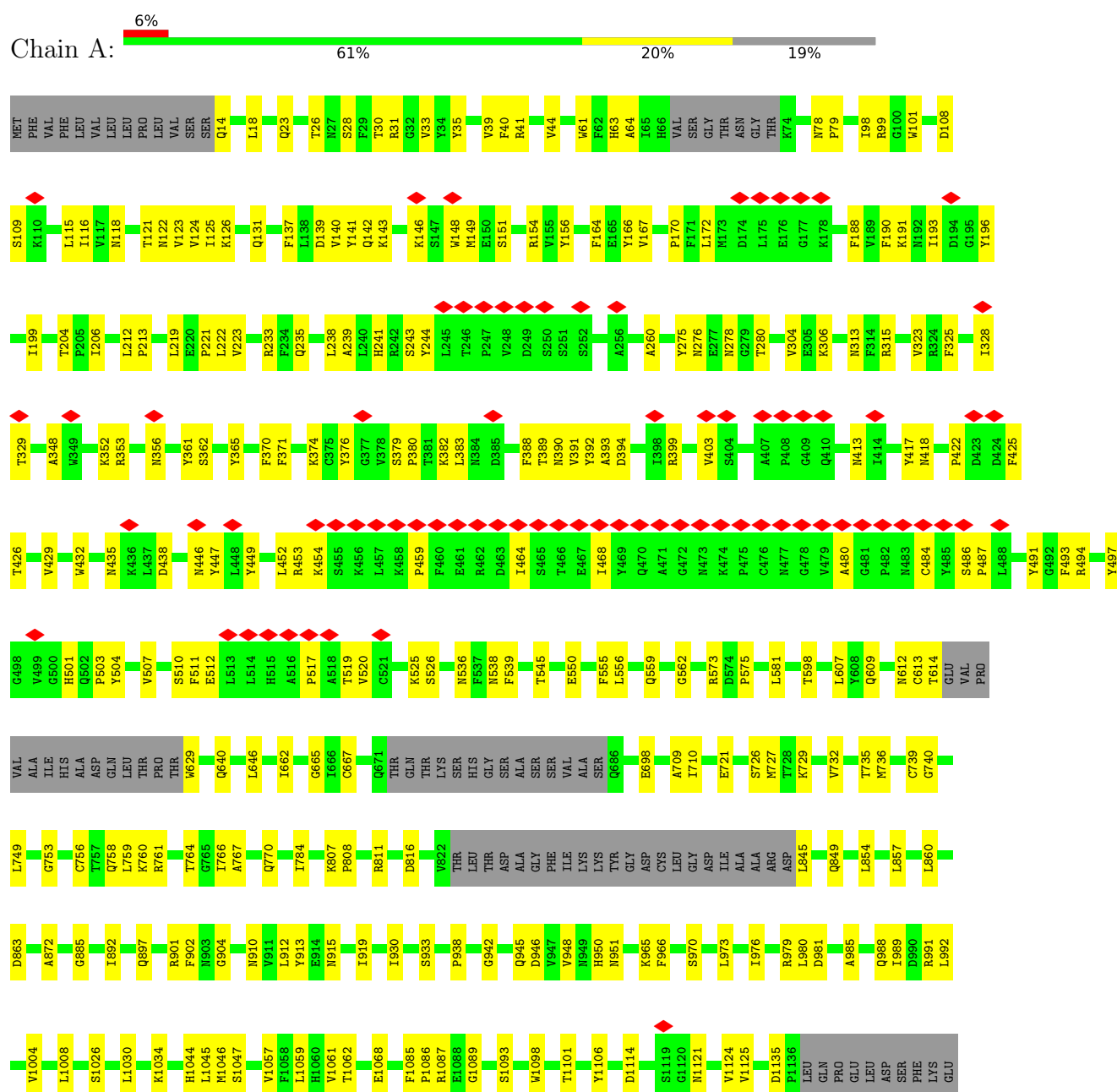
- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	594	Total	C	N	O	S	0	0
			4845	3099	803	914	29		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein



PHE LEU LEU ARG SER SER GLU VAL LEU LEU PHE PHE GLN GLN PRO PRO GLY TRP SER SER HIS PRO PRO GLN PHE PHE GLU GLY LYS GLY GLY GLY SER SER GLY GLY GLY SER SER SER SER ALA TRP TRP SER HIS PRO GLN PHE PHE GLU GLU LYS HIS HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Spike glycoprotein

Chain B:



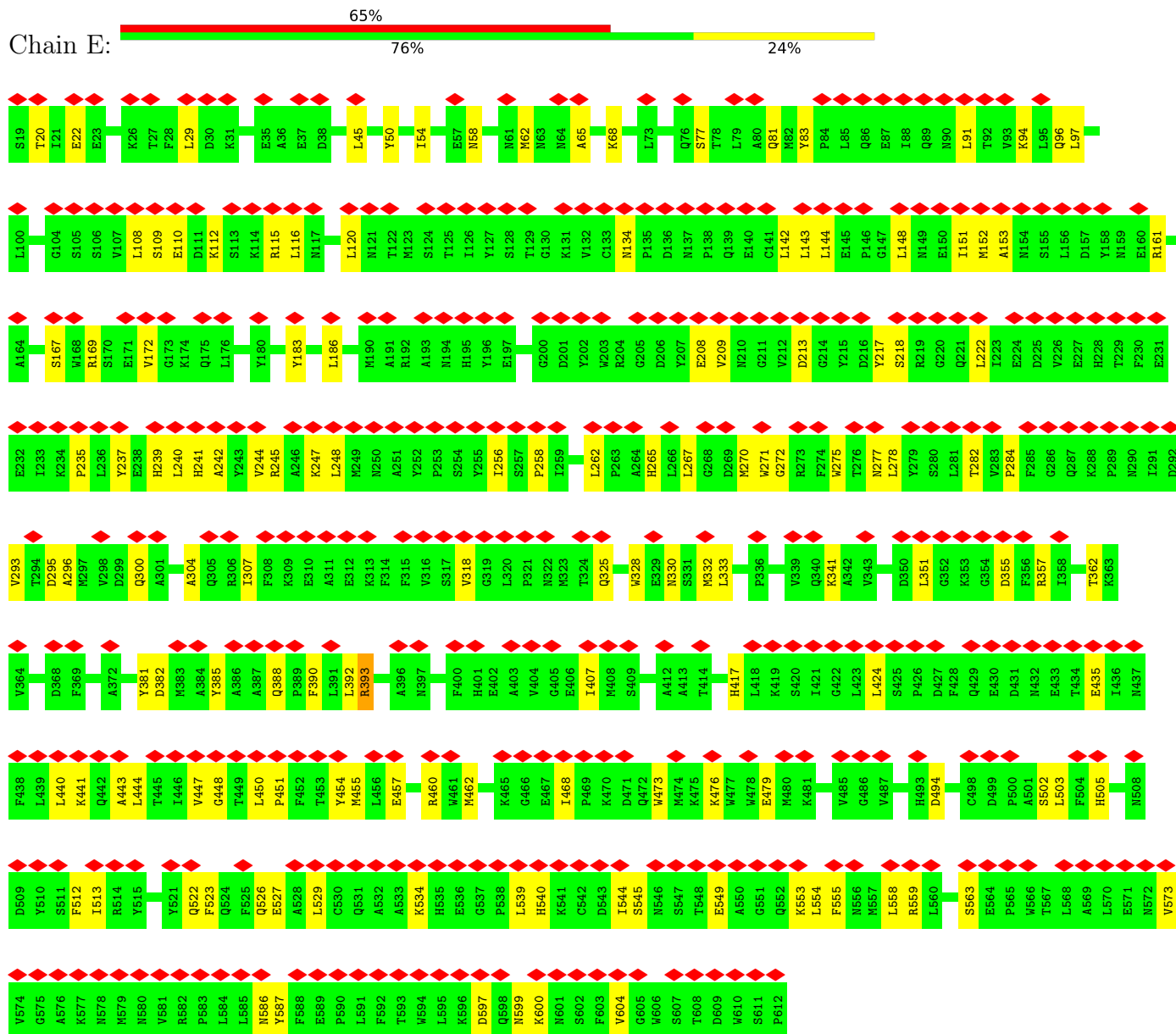
ASN	L860	E721	G613	H501	N433	N327	S201	S95	ASN	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
HIS	Y1061	I722	T614	Q502	S434	I328	K202	N96	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
THR	I866	I722	T614	P503	N435	I328	K202	N96	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
SER	A1066	K729	VAL	P503	N435	L331	G215	N97	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
PRO	Q1067	K729	VAL	P504	N436	L331	G215	N97	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
ASP	A872	D733	VAL	R505	L437	F343	L219	R99	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
ASP	L800	D733	VAL	R508	S439	F343	L219	R99	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
ASP	I905	K736	ILE	L513	K440	Y347	L225	I102	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
GLY	T1071	I737	HIS	L513	K440	Y347	L225	I102	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
GLY	T1072	I738	ALA	A516	K444	W349	L227	K110	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
ASP	T1073	Y752	ASP	A516	K444	W349	L227	K110	THR	VAL	LEU	LEU	PRO	VAL	SER	SER	Q14	L18	S24	Y25	T26	R21	S28	F29	T30	R31	F40	D50	L51	P54	F55	F56	S57	W61	H66	VAL	SER	GLY	THR	R75	F76	D77	N78	P79	A80	L81	P82	F89	Y99	Z00																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
ILE	Y913	Y		F517	N446		R233																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

Chain C: 



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

● Molecule 2: Processed angiotensin-converting enzyme 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64562	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.962	Depositor
Minimum map value	-0.234	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/8563	0.57	1/11654 (0.0%)
1	B	0.28	0/8562	0.55	1/11653 (0.0%)
1	C	0.27	0/8570	0.58	4/11664 (0.0%)
2	E	0.28	0/4981	0.57	2/6767 (0.0%)
All	All	0.28	0/30676	0.57	8/41738 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	MET	CA-CB-CG	6.28	123.97	113.30
1	C	289	LEU	CA-CB-CG	6.17	129.49	115.30
1	C	138	LEU	CA-CB-CG	6.07	129.25	115.30
2	E	455	MET	CB-CG-SD	6.03	130.48	112.40
1	C	578	LEU	CA-CB-CG	5.57	128.11	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	242	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8360	0	8174	179	0
1	B	8359	0	8170	181	0
1	C	8367	0	8183	164	0
2	E	4845	0	4625	91	0
All	All	29931	0	29152	583	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 10.

The worst 5 of 583 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)
2:E:296:ALA:O	2:E:300:GLN:HB2	1.73	0.89
1:B:1089:GLY:HA3	1:B:1101:THR:O	1.77	0.83
1:A:1089:GLY:HA3	1:A:1101:THR:O	1.86	0.75
1:A:352:LYS:HB2	1:A:393:ALA:HB3	1.69	0.74
1:C:427:GLY:HA3	1:C:509:LEU:O	1.88	0.73

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1056/1317 (80%)	955 (90%)	101 (10%)	0	100	100
1	B	1056/1317 (80%)	960 (91%)	96 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1057/1317 (80%)	953 (90%)	103 (10%)	1 (0%)	48	83
2	E	592/594 (100%)	567 (96%)	25 (4%)	0	100	100
All	All	3761/4545 (83%)	3435 (91%)	325 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	23	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	934/1139 (82%)	933 (100%)	1 (0%)	92	95
1	B	934/1139 (82%)	932 (100%)	2 (0%)	92	93
1	C	935/1139 (82%)	932 (100%)	3 (0%)	91	91
2	E	525/525 (100%)	523 (100%)	2 (0%)	89	90
All	All	3328/3942 (84%)	3320 (100%)	8 (0%)	91	93

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	559	ARG
2	E	393	ARG
1	C	390	ASN
1	C	186	ARG
1	C	1015	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	640	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	820	ASN
1	C	134	ASN
1	C	783	GLN
2	E	134	ASN

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.

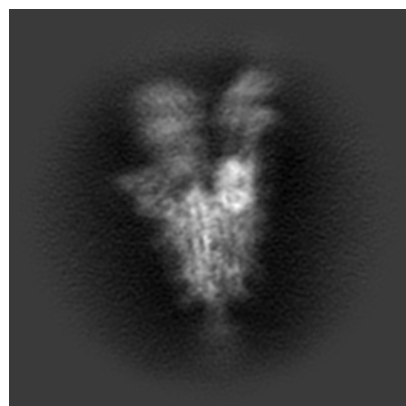
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37835. These allow visual inspection of the internal detail of the map and identification of artifacts.

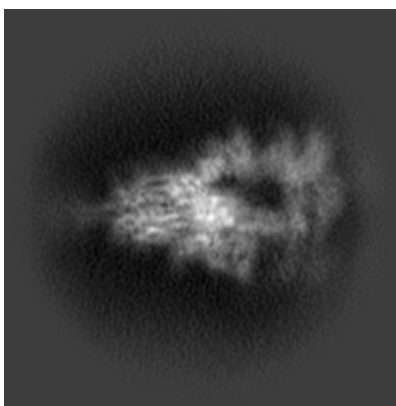
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

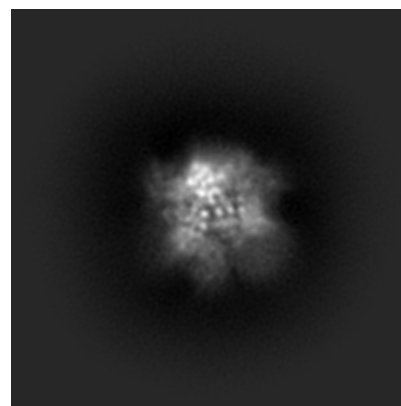
6.1.1 Primary map



X

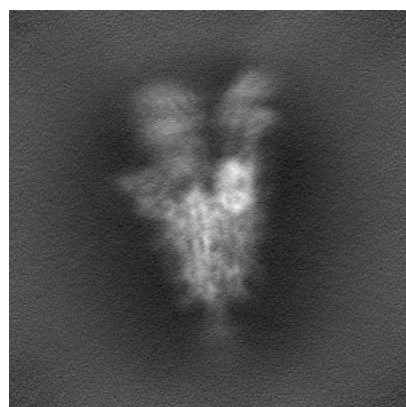


Y

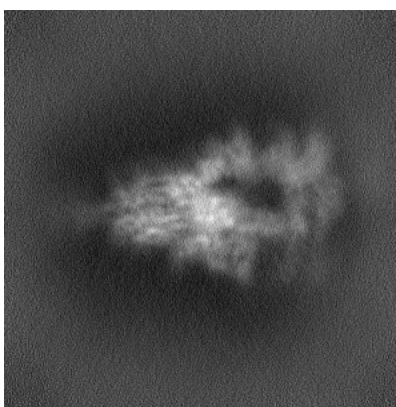


Z

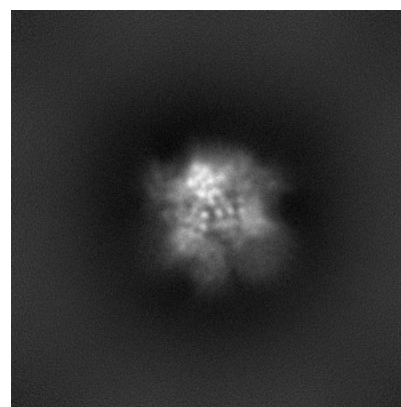
6.1.2 Raw map



X



Y

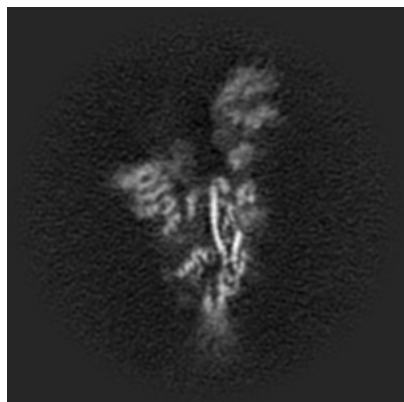


Z

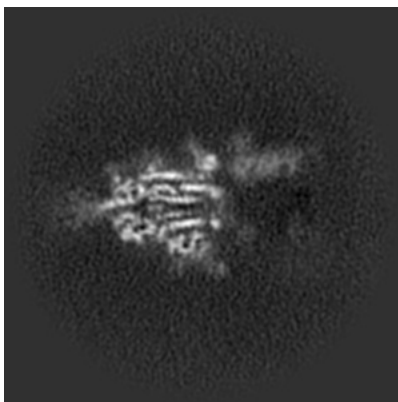
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

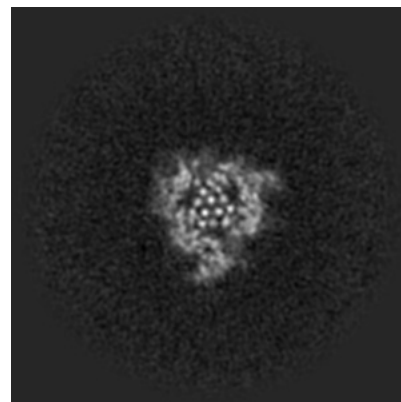
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

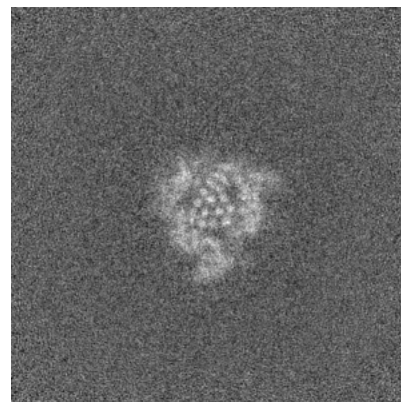
6.2.2 Raw map



X Index: 180



Y Index: 180

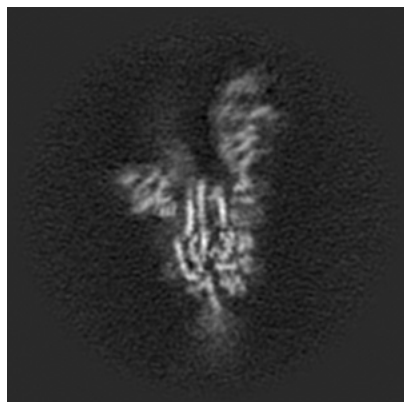


Z Index: 180

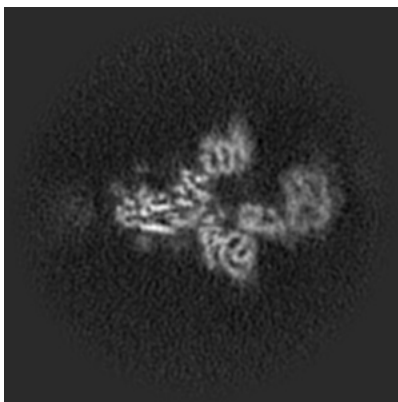
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

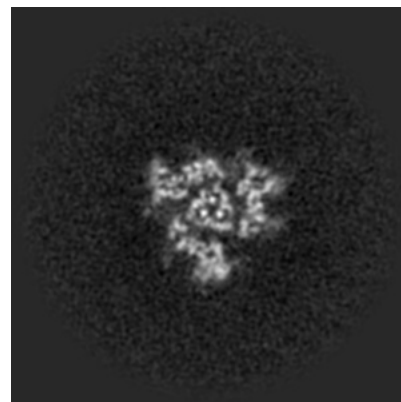
6.3.1 Primary map



X Index: 172

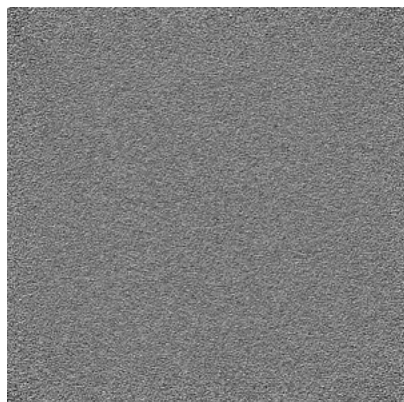


Y Index: 204

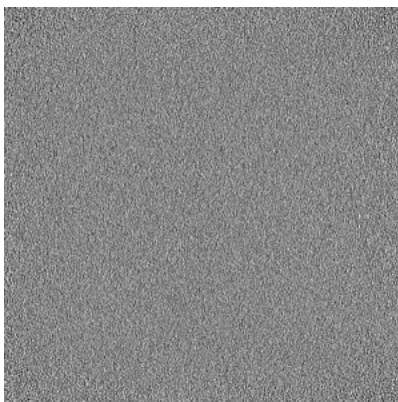


Z Index: 188

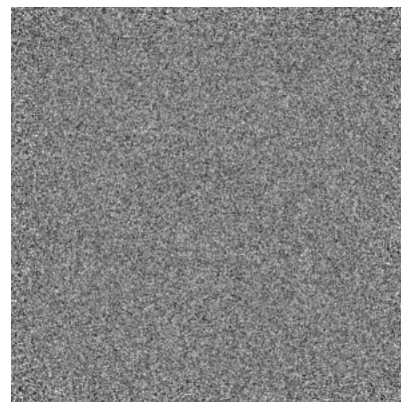
6.3.2 Raw map



X Index: 0



Y Index: 0

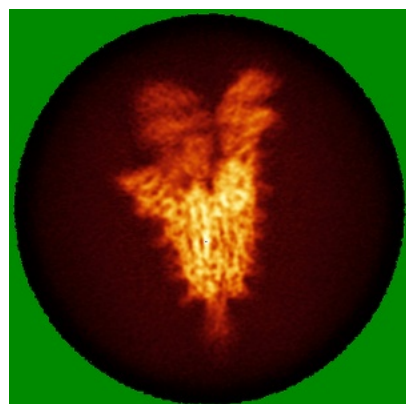


Z Index: 359

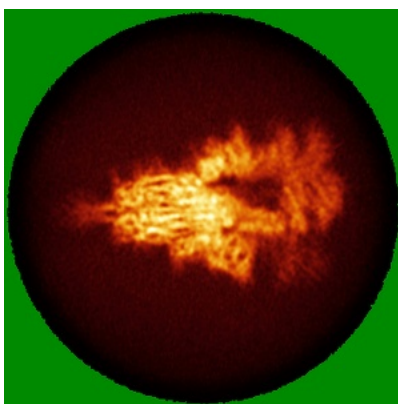
The images above show the largest variance slices of the map in three orthogonal directions.

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

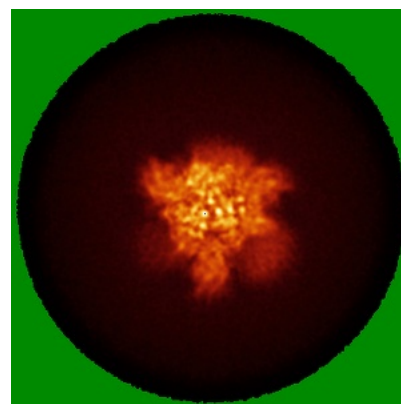
6.4.1 Primary map



X

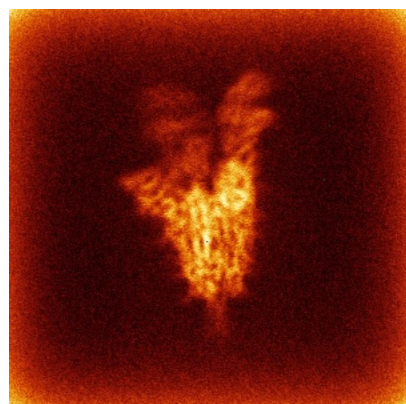


Y

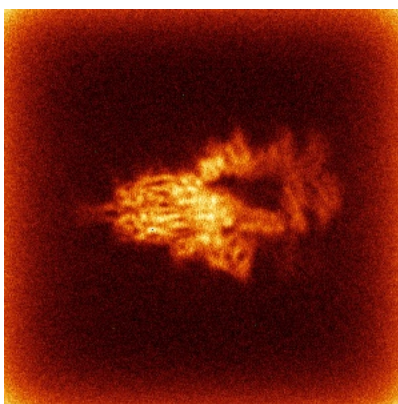


Z

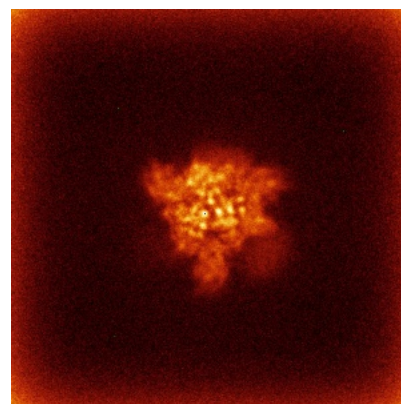
6.4.2 Raw map



X



Y

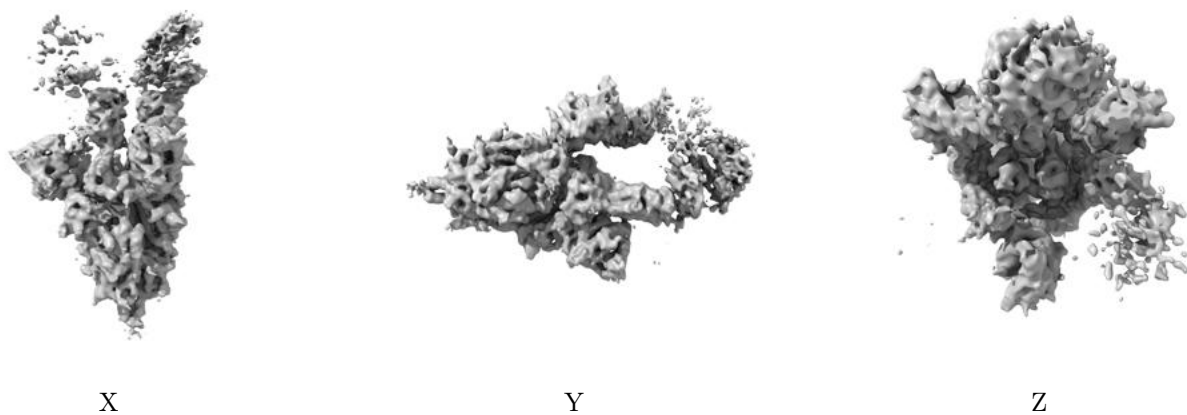


Z

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.

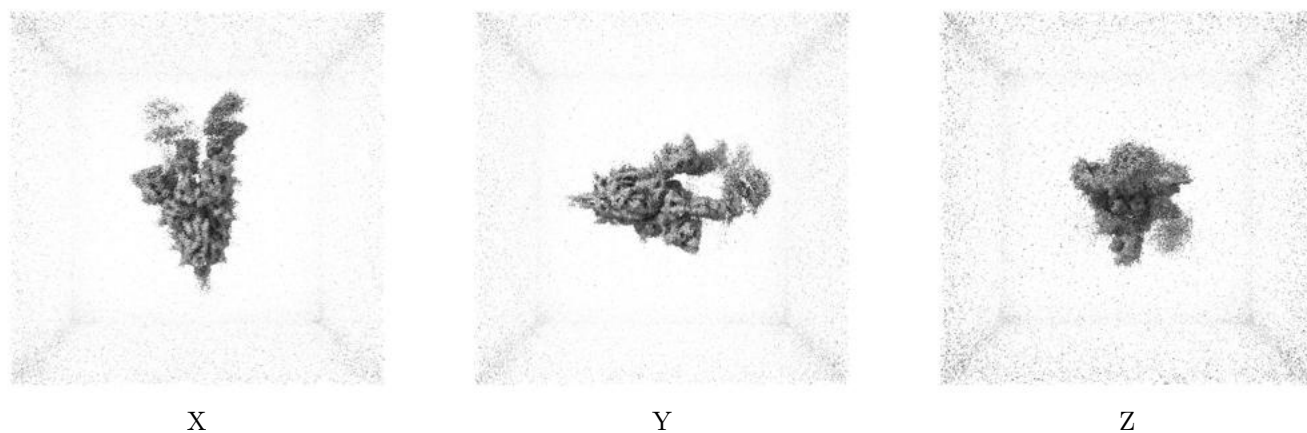
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

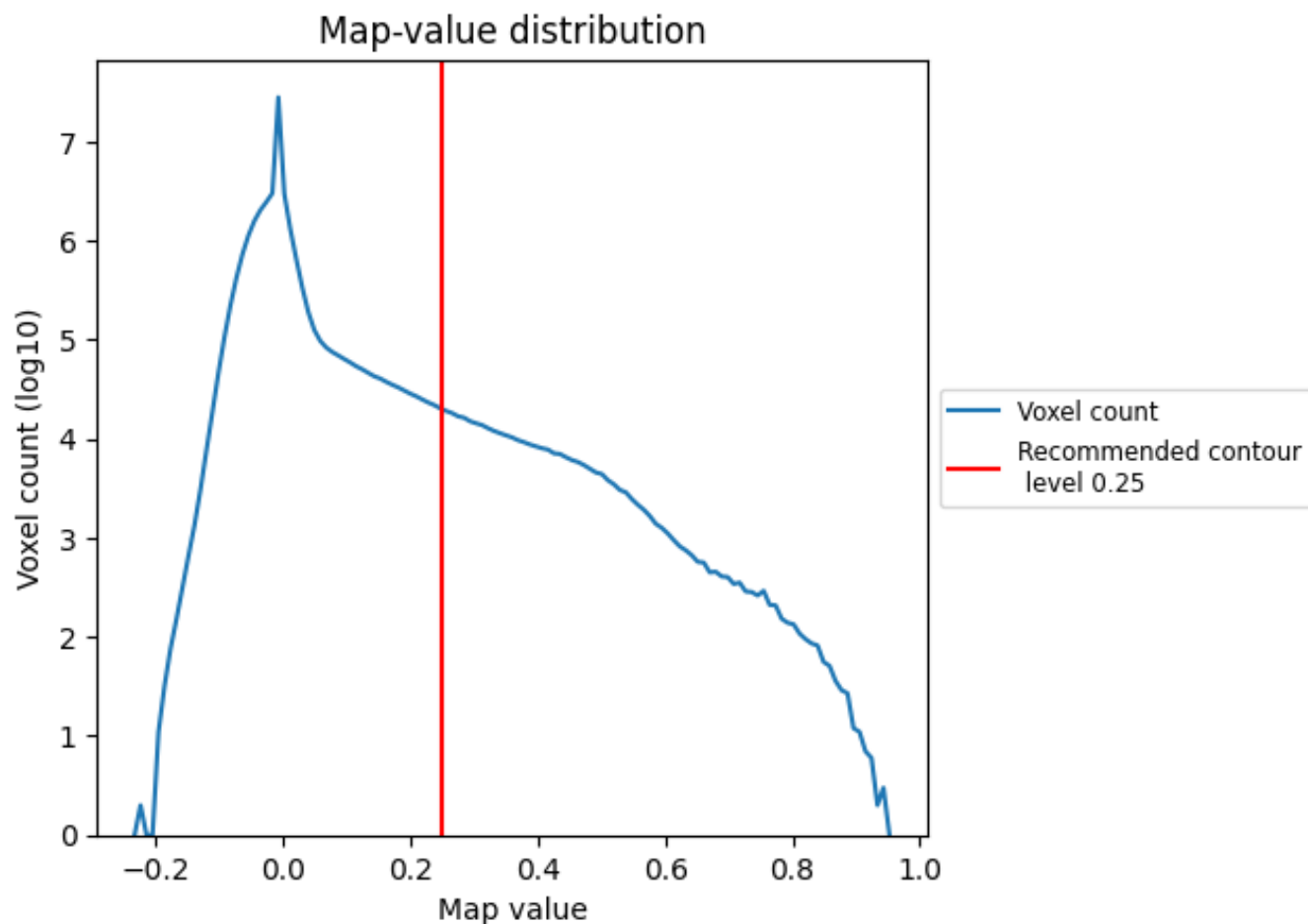
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

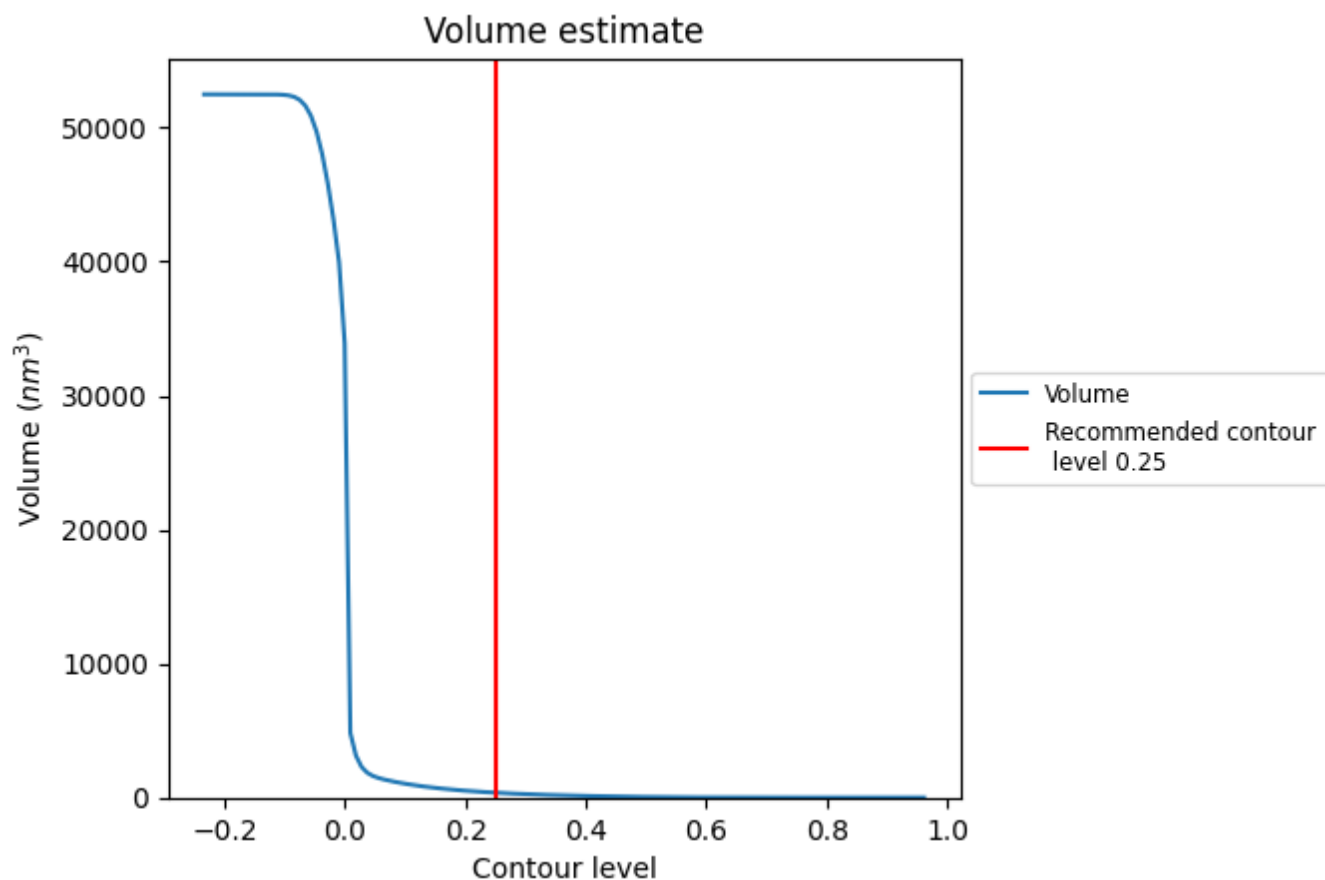
This section contains the results of statistical analysis of the map.

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.

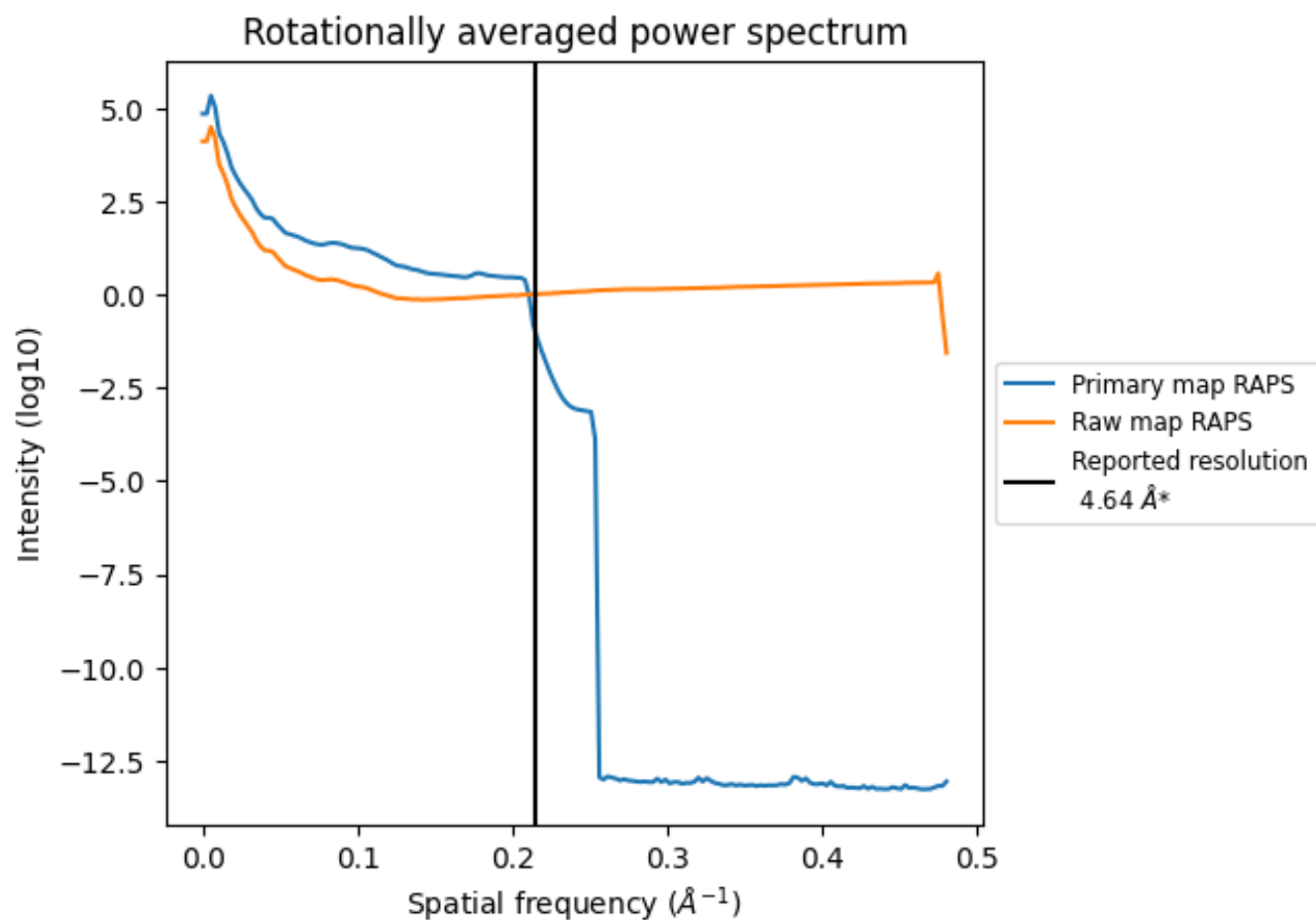
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm³; this corresponds to an approximate mass of 327 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 ⓘ

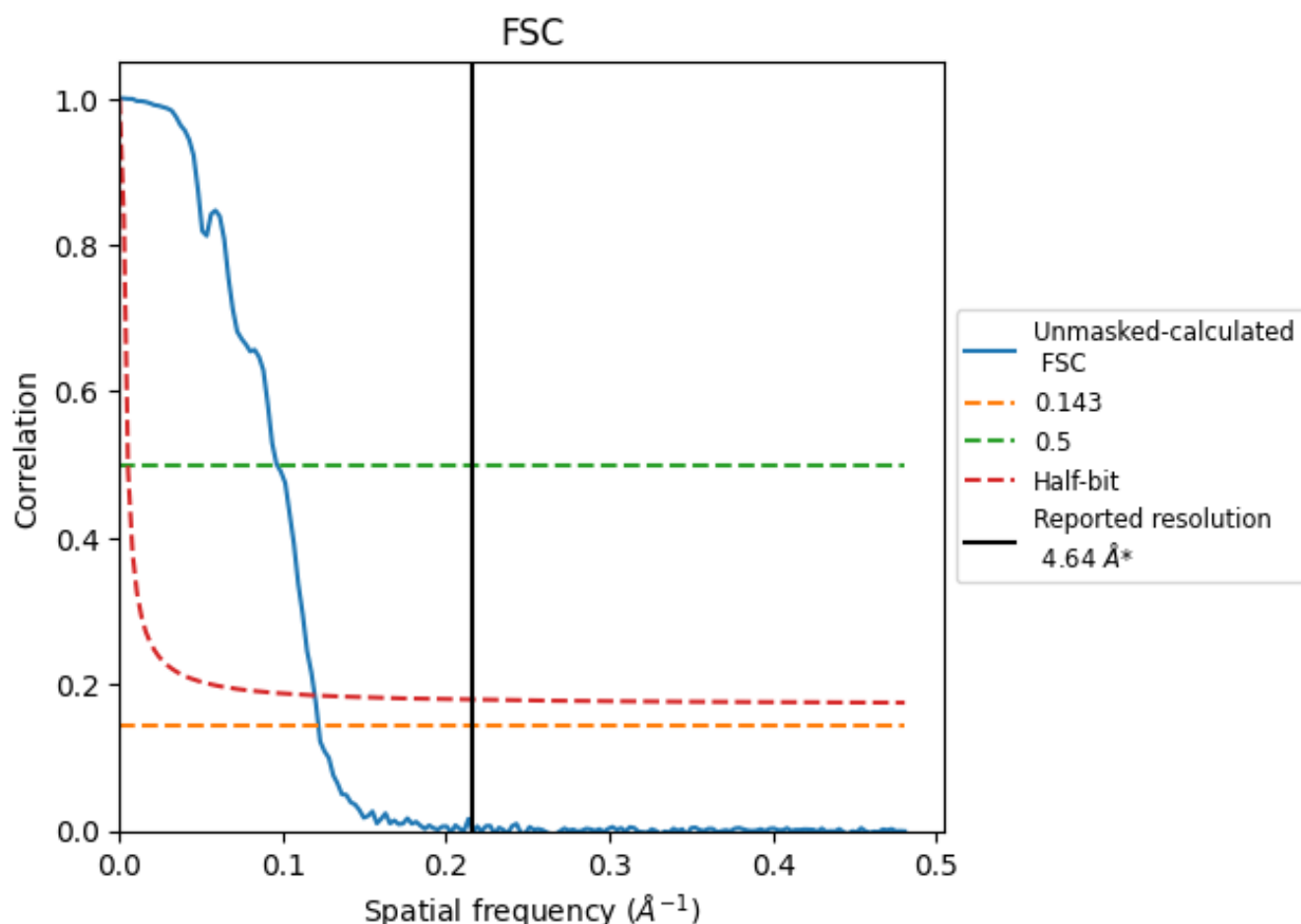


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

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 0.216 Å⁻¹

8.2 Resolution estimates [i](#)

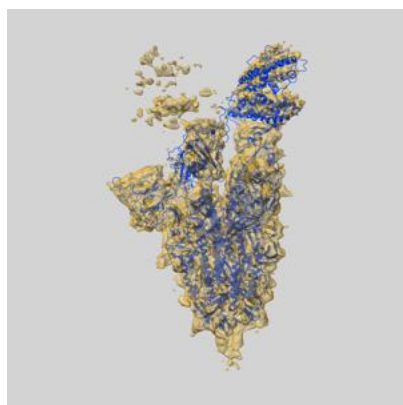
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.21	10.40	8.36

*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 8.21 differs from the reported value 4.64 by more than 10 %

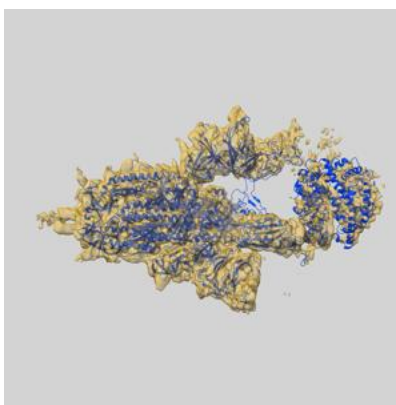
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37835 and PDB model 8WTJ. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

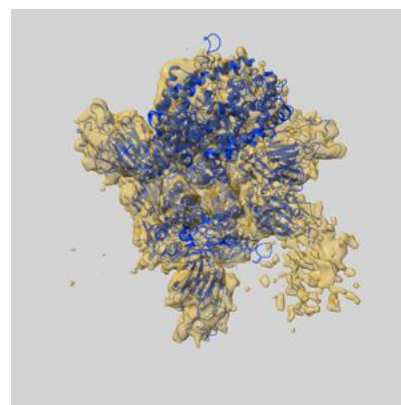
9.1 Map-model overlay [i](#)



X



Y



Z

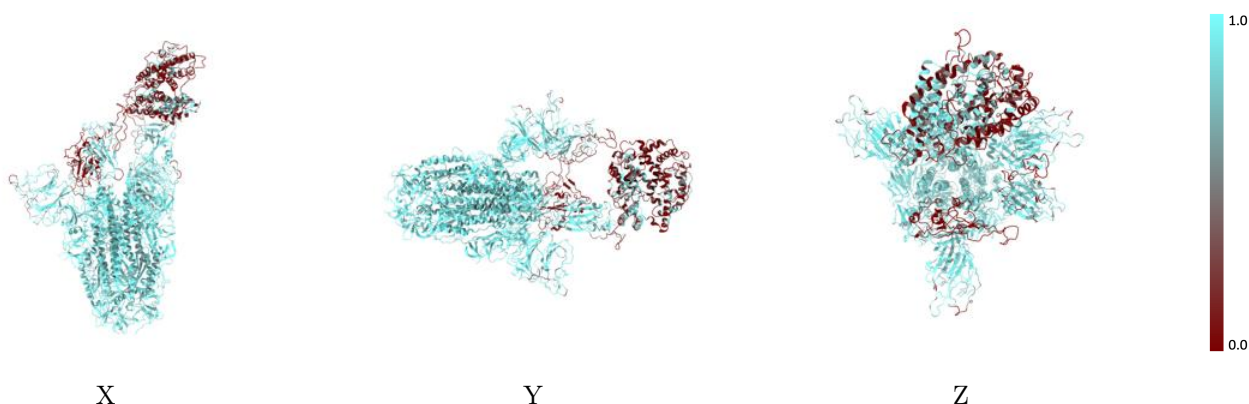
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



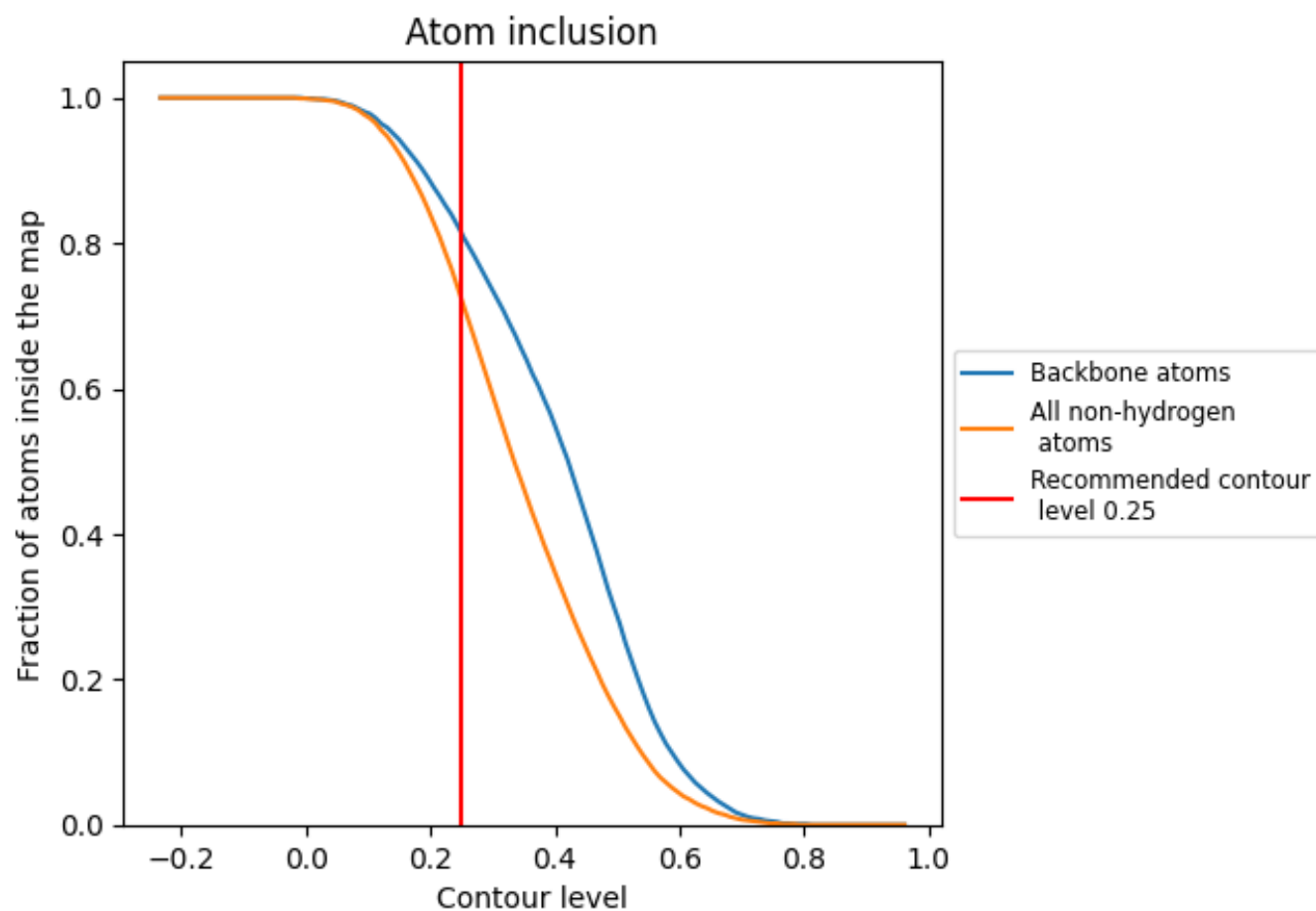
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7230	<div></div> 0.2020
A	<div></div> 0.8170	<div></div> 0.2210
B	<div></div> 0.8510	<div></div> 0.2300
C	<div></div> 0.7350	<div></div> 0.2210
E	<div></div> 0.3220	<div></div> 0.0900

