WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Jan 7, 2025 – 12:21 PM JST

PDB ID	:	8JZP
EMDB ID	:	EMD-36750
Title	:	Structure of mouse C5a-human C5aR1-Go complex
Authors	:	Yadav, M.K.; Yadav, R.; Maharana, J.; Sarma, P.; Banerjee, R.; Shukla, A.K.; Gati, C.
Deposited on	:	2023-07-06
Resolution	:	3.45 Å(reported)
Based on initial model	:	8IA2

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 (i) 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 (i)) were used in the production of this report:
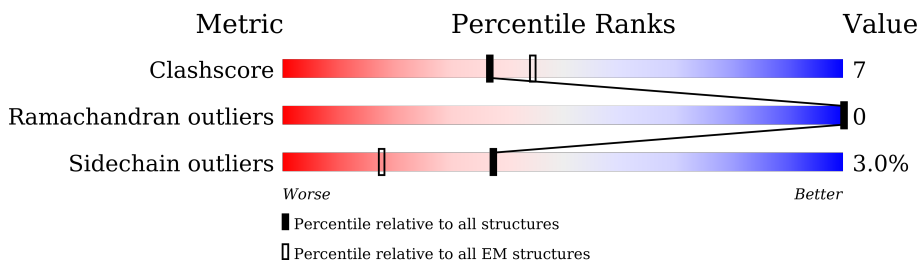
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.45 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		3.0%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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 <=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	406	60% 12% 28%
2	B	240	71% 15% 13%
3	C	350	80% 16% • •
4	F	109	50% 14% • 35%
5	G	71	62% 17% 21%
6	H	248	83% 10% 6%

2   Entry composition   ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8622 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 C5a anaphylatoxin chemotactic receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	294	2206	1473	355	366	12	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-55	MET	-	initiating methionine	UNP P21730
A	-54	GLY	-	expression tag	UNP P21730
A	-53	LYS	-	expression tag	UNP P21730
A	-52	THR	-	expression tag	UNP P21730
A	-51	ILE	-	expression tag	UNP P21730
A	-50	ILE	-	expression tag	UNP P21730
A	-49	ALA	-	expression tag	UNP P21730
A	-48	LEU	-	expression tag	UNP P21730
A	-47	SER	-	expression tag	UNP P21730
A	-46	TYR	-	expression tag	UNP P21730
A	-45	ILE	-	expression tag	UNP P21730
A	-44	PHE	-	expression tag	UNP P21730
A	-43	CYS	-	expression tag	UNP P21730
A	-42	LEU	-	expression tag	UNP P21730
A	-41	VAL	-	expression tag	UNP P21730
A	-40	PHE	-	expression tag	UNP P21730
A	-39	ALA	-	expression tag	UNP P21730
A	-38	ASP	-	expression tag	UNP P21730
A	-37	TYR	-	expression tag	UNP P21730
A	-36	LYS	-	expression tag	UNP P21730
A	-35	ASP	-	expression tag	UNP P21730
A	-34	ASP	-	expression tag	UNP P21730
A	-33	ASP	-	expression tag	UNP P21730
A	-32	ASP	-	expression tag	UNP P21730
A	-31	ALA	-	expression tag	UNP P21730
A	-30	ALA	-	expression tag	UNP P21730
A	-29	ASN	-	expression tag	UNP P21730
A	-28	PHE	-	expression tag	UNP P21730

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	THR	-	expression tag	UNP P21730
A	-26	PRO	-	expression tag	UNP P21730
A	-25	VAL	-	expression tag	UNP P21730
A	-24	ASN	-	expression tag	UNP P21730
A	-23	GLY	-	expression tag	UNP P21730
A	-22	SER	-	expression tag	UNP P21730
A	-21	SER	-	expression tag	UNP P21730
A	-20	GLY	-	expression tag	UNP P21730
A	-19	ASN	-	expression tag	UNP P21730
A	-18	GLN	-	expression tag	UNP P21730
A	-17	SER	-	expression tag	UNP P21730
A	-16	VAL	-	expression tag	UNP P21730
A	-15	ARG	-	expression tag	UNP P21730
A	-14	LEU	-	expression tag	UNP P21730
A	-13	VAL	-	expression tag	UNP P21730
A	-12	THR	-	expression tag	UNP P21730
A	-11	SER	-	expression tag	UNP P21730
A	-10	SER	-	expression tag	UNP P21730
A	-9	SER	-	expression tag	UNP P21730
A	-8	LEU	-	expression tag	UNP P21730
A	-7	GLU	-	expression tag	UNP P21730
A	-6	VAL	-	expression tag	UNP P21730
A	-5	LEU	-	expression tag	UNP P21730
A	-4	PHE	-	expression tag	UNP P21730
A	-3	GLN	-	expression tag	UNP P21730
A	-2	GLY	-	expression tag	UNP P21730
A	-1	PRO	-	expression tag	UNP P21730
A	0	GLY	-	expression tag	UNP P21730
A	1	SER	-	expression tag	UNP P21730

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(o) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	208	1509	969	259	274	7	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP P09471
B	-10	GLY	-	expression tag	UNP P09471
B	-9	HIS	-	expression tag	UNP P09471

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P09471
B	-7	HIS	-	expression tag	UNP P09471
B	-6	HIS	-	expression tag	UNP P09471
B	-5	HIS	-	expression tag	UNP P09471
B	-4	HIS	-	expression tag	UNP P09471
B	-3	GLU	-	expression tag	UNP P09471
B	-2	ASN	-	expression tag	UNP P09471
B	-1	LEU	-	expression tag	UNP P09471
B	0	TYR	-	expression tag	UNP P09471
B	1	PHE	-	expression tag	UNP P09471
B	2	GLN	-	expression tag	UNP P09471
B	3	GLY	-	expression tag	UNP P09471
B	42	ASP	GLY	engineered mutation	UNP P09471
B	43	ASN	GLU	engineered mutation	UNP P09471
B	174	GLY	-	linker	UNP P09471
B	175	GLY	-	linker	UNP P09471
B	176	SER	-	linker	UNP P09471
B	177	GLY	-	linker	UNP P09471
B	178	GLY	-	linker	UNP P09471
B	179	SER	-	linker	UNP P09471
B	180	GLY	-	linker	UNP P09471
B	181	GLY	-	linker	UNP P09471
B	227	ASP	ALA	engineered mutation	UNP P09471
B	230	ASP	GLY	engineered mutation	UNP P09471
B	?	-	ASP	deletion	UNP P09471
B	?	-	GLN	deletion	UNP P09471
B	?	-	VAL	deletion	UNP P09471
B	?	-	LEU	deletion	UNP P09471
B	?	-	HIS	deletion	UNP P09471
B	?	-	GLU	deletion	UNP P09471
B	?	-	ASP	deletion	UNP P09471
B	?	-	GLU	deletion	UNP P09471
B	?	-	THR	deletion	UNP P09471
B	?	-	THR	deletion	UNP P09471
B	332	ALA	ILE	engineered mutation	UNP P09471
B	335	ILE	VAL	engineered mutation	UNP P09471

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

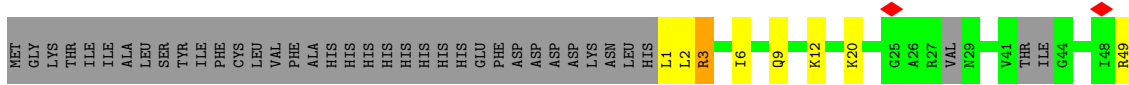| Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	338	2419	1501	438	463	17	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	MET	-	initiating methionine	UNP P62873
C	-8	HIS	-	expression tag	UNP P62873
C	-7	HIS	-	expression tag	UNP P62873
C	-6	HIS	-	expression tag	UNP P62873
C	-5	HIS	-	expression tag	UNP P62873
C	-4	HIS	-	expression tag	UNP P62873
C	-3	HIS	-	expression tag	UNP P62873
C	-2	GLY	-	expression tag	UNP P62873
C	-1	SER	-	expression tag	UNP P62873
C	0	SER	-	expression tag	UNP P62873
C	1	GLY	-	expression tag	UNP P62873

- Molecule 4 is a protein called C5a anaphylatoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	71	492	301	96	89	6	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-34	MET	-	initiating methionine	UNP P06684
F	-33	GLY	-	expression tag	UNP P06684
F	-32	LYS	-	expression tag	UNP P06684
F	-31	THR	-	expression tag	UNP P06684
F	-30	ILE	-	expression tag	UNP P06684
F	-29	ILE	-	expression tag	UNP P06684
F	-28	ALA	-	expression tag	UNP P06684
F	-27	LEU	-	expression tag	UNP P06684
F	-26	SER	-	expression tag	UNP P06684
F	-25	TYR	-	expression tag	UNP P06684
F	-24	ILE	-	expression tag	UNP P06684
F	-23	PHE	-	expression tag	UNP P06684
F	-22	CYS	-	expression tag	UNP P06684
F	-21	LEU	-	expression tag	UNP P06684
F	-20	VAL	-	expression tag	UNP P06684
F	-19	PHE	-	expression tag	UNP P06684
F	-18	ALA	-	expression tag	UNP P06684
F	-17	HIS	-	expression tag	UNP P06684
F	-16	HIS	-	expression tag	UNP P06684
F	-15	HIS	-	expression tag	UNP P06684

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	HIS	-	expression tag	UNP P06684
F	-13	HIS	-	expression tag	UNP P06684
F	-12	HIS	-	expression tag	UNP P06684
F	-11	HIS	-	expression tag	UNP P06684
F	-10	HIS	-	expression tag	UNP P06684
F	-9	GLU	-	expression tag	UNP P06684
F	-8	PHE	-	expression tag	UNP P06684
F	-7	ASP	-	expression tag	UNP P06684
F	-6	ASP	-	expression tag	UNP P06684
F	-5	ASP	-	expression tag	UNP P06684
F	-4	ASP	-	expression tag	UNP P06684
F	-3	LYS	-	expression tag	UNP P06684

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	56	381	237	68	74	2	0	0

- Molecule 6 is a protein called Antibody fragment ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	232	1615	1012	274	322	7	0	0

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: C5a anaphylatoxin chemotactic receptor 1

Chain A:
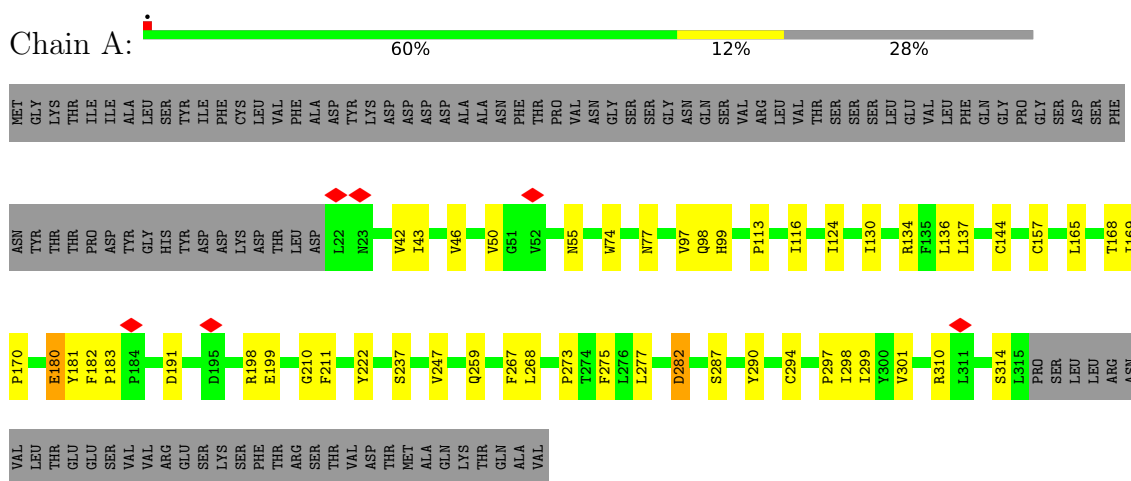
• Molecule 2: Guanine nucleotide-binding protein G(o) subunit alpha

Chain B:
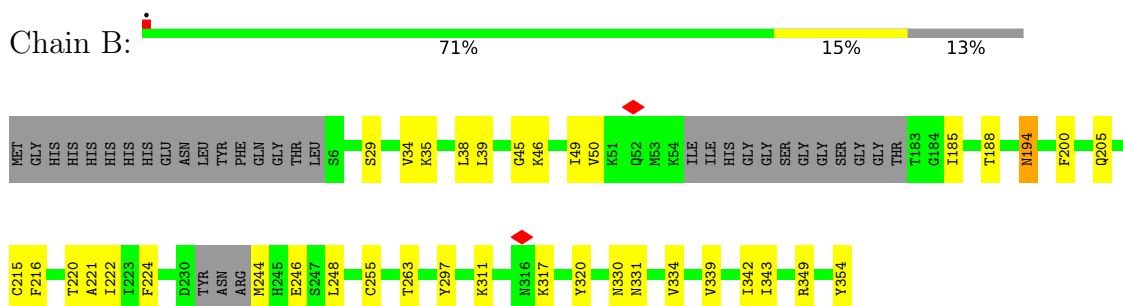
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain C:

W332 W339 N340
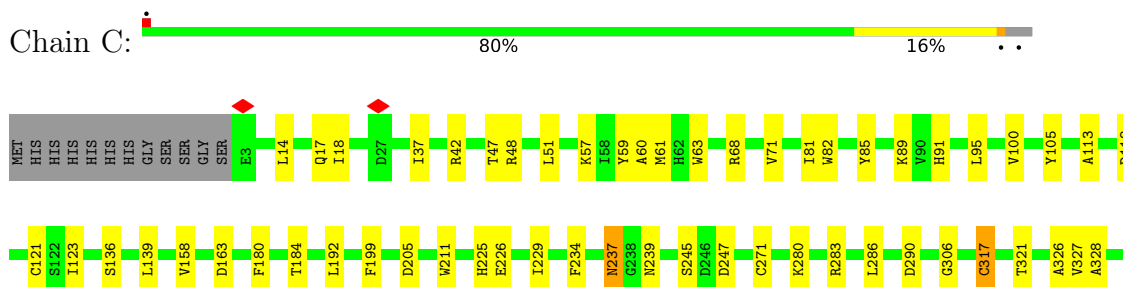
• Molecule 4: C5a anaphylatoxin

Chain F:

50% 14% . 35%

MET GLY LYS THR ILE ILE ALA LEU SER TYR ILE PHE CYS LEU VAL PHE ALA HIS HIS HIS HIS HIS HIS HIS GLU PHE ASP ASP ASP LYS ASN LEU HIS L1 L2 R3 I6 Q9 K12 K20 G25 A26 R27 VAL N29 V41 THR ILE G44 I48 R49

E53 N59 R62 K63 P66 Q71 L72 G73 R74

• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

62% 17% 21%

MET ALA SER ASN ASN THR A7 Q11 A12 L15 V16 E17 Q18 D26 R27 I28 K32 E42 P60 F61 R62 GLU LYS LYS PHE PHE CYS ALA ILE LEU
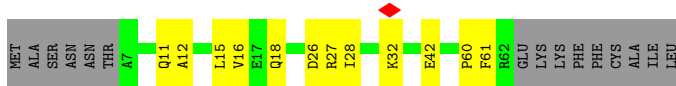
• Molecule 6: Antibody fragment ScFv16

Chain H:

83% 10% 6%

D1 F27 Q39 L45 Y50 R67 D90 T91 R98 Y103 D109 T118 V119 S120 S121 G122 GLY GLU GLY SER GLY GLY GLY SER GLY GLY GLY S136 L165 L174 L178 Q179 Q183 L188 R191 F212 D223 Y227

M230 Q231 H232 L233 E234 Y235 PRO LEU T238 F239 L247 LYS
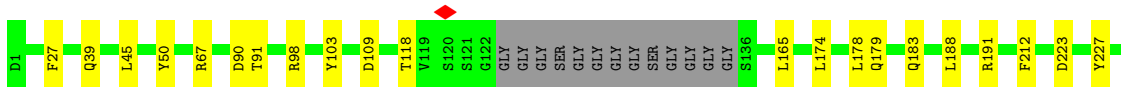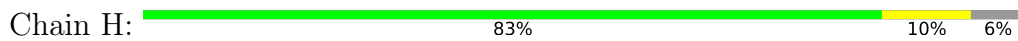
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	348496	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.412	Depositor
Minimum map value	-0.857	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	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	0.29	0/2265	0.53	0/3111
2	B	0.29	0/1535	0.48	0/2079
3	C	0.32	0/2464	0.56	0/3357
4	F	0.26	0/497	0.51	0/669
5	G	0.34	0/387	0.57	0/530
6	H	0.32	0/1651	0.53	0/2254
All	All	0.30	0/8799	0.53	0/12000

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2206	0	2210	32	0
2	B	1509	0	1405	20	0
3	C	2419	0	2188	40	0
4	F	492	0	441	14	0
5	G	381	0	339	7	0
6	H	1615	0	1397	18	0
All	All	8622	0	7980	123	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 7.

The worst 5 of 123 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)
6:H:174:LEU:HD13	6:H:212:PHE:HD1	1.43	0.84
3:C:81:ILE:HG12	3:C:91:HIS:HB2	1.67	0.76
2:B:194:ASN:O	2:B:194:ASN:ND2	2.18	0.74
1:A:182:PHE:HB2	1:A:183:PRO:HD3	1.70	0.73
1:A:181:TYR:OH	4:F:3:ARG:NH2	2.24	0.65

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	292/406 (72%)	259 (89%)	33 (11%)	0	100	100
2	B	202/240 (84%)	194 (96%)	8 (4%)	0	100	100
3	C	336/350 (96%)	315 (94%)	21 (6%)	0	100	100
4	F	65/109 (60%)	63 (97%)	2 (3%)	0	100	100
5	G	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
6	H	226/248 (91%)	218 (96%)	8 (4%)	0	100	100
All	All	1175/1424 (82%)	1102 (94%)	73 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	225/354 (64%)	219 (97%)	6 (3%)	40	67
2	B	141/206 (68%)	136 (96%)	5 (4%)	31	61
3	C	228/291 (78%)	224 (98%)	4 (2%)	54	75
4	F	44/97 (45%)	39 (89%)	5 (11%)	4	22
5	G	32/58 (55%)	30 (94%)	2 (6%)	15	43
6	H	151/201 (75%)	148 (98%)	3 (2%)	50	73
All	All	821/1207 (68%)	796 (97%)	25 (3%)	37	65

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	317	CYS
4	F	12	LYS
6	H	231	GLN
4	F	3	ARG
4	F	20	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
3	C	17	GLN
3	C	225	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-36750. 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
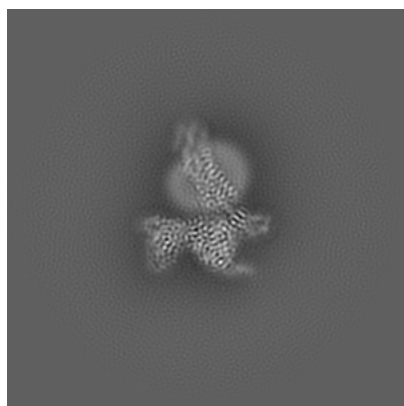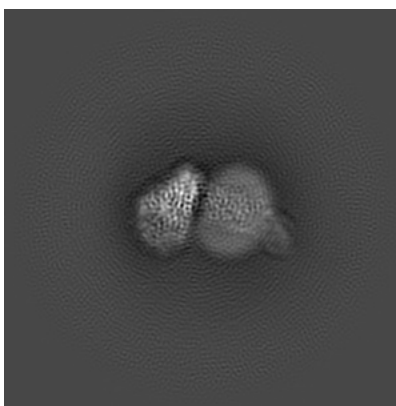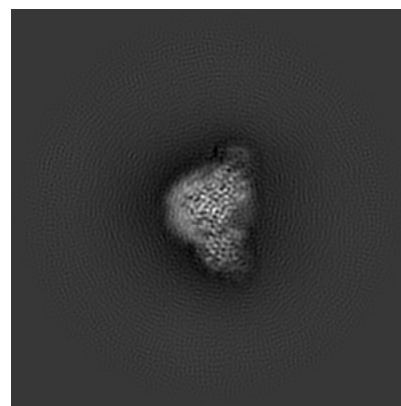
X   Y   Z

6.1.2   Raw map

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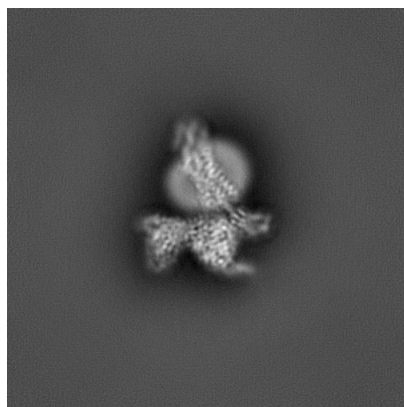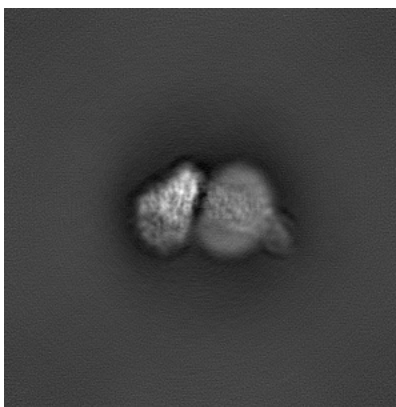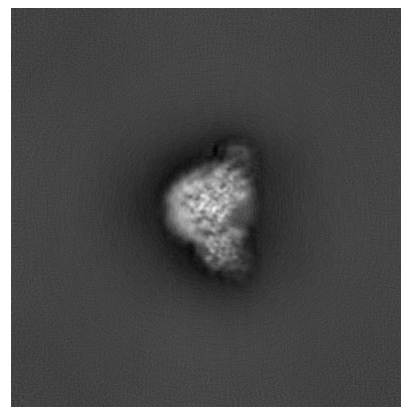
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
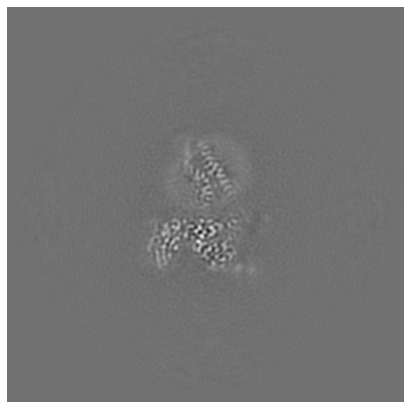
6.2.1 Primary map
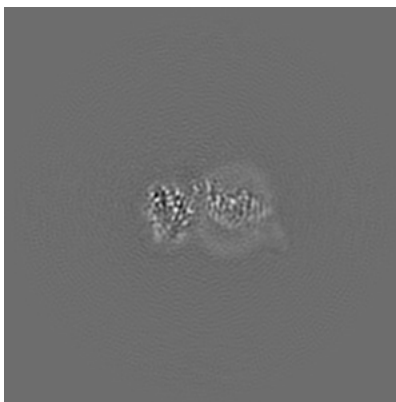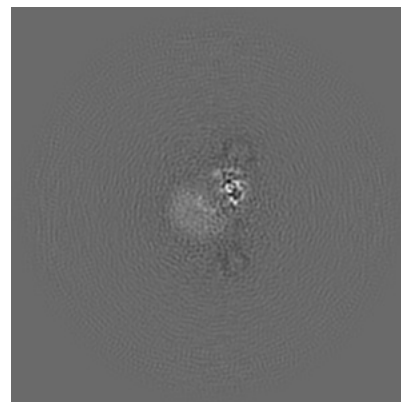
X Index: 180   Y Index: 180   Z Index: 180

6.2.2 Raw map
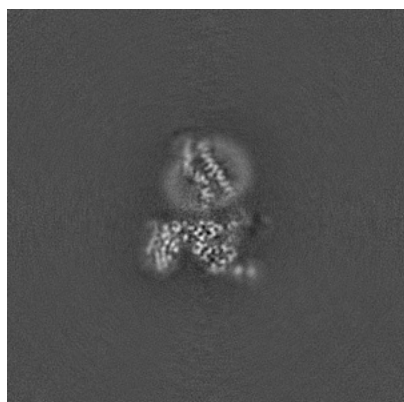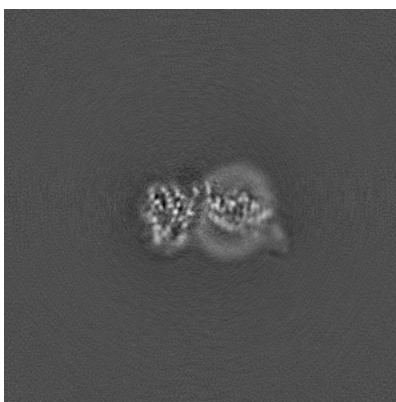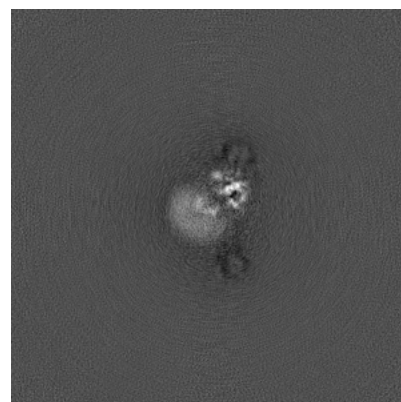
X Index: 180   Y Index: 180   Z Index: 180

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
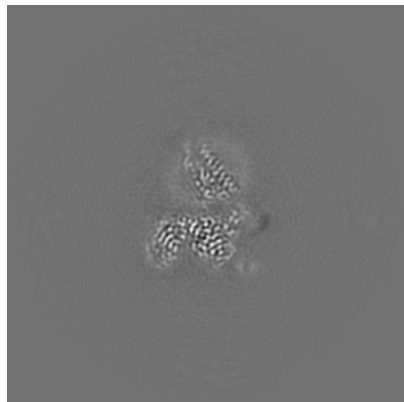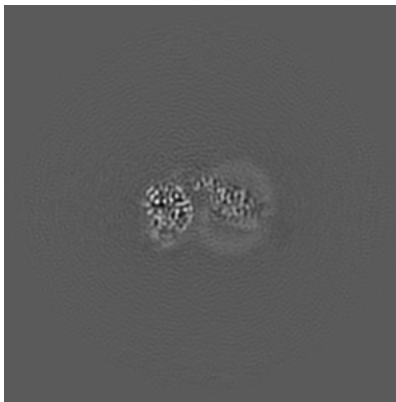
| X Index: 183 | Y Index: 185 | Z Index: 155 |
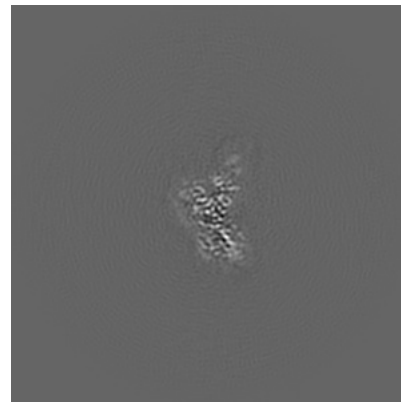
6.3.2 Raw map
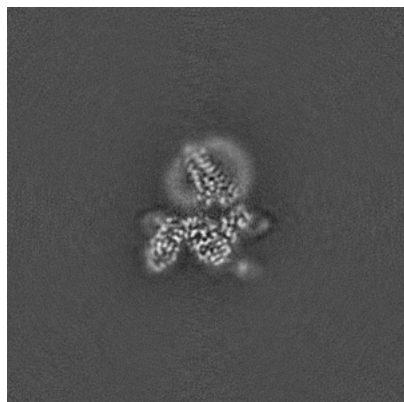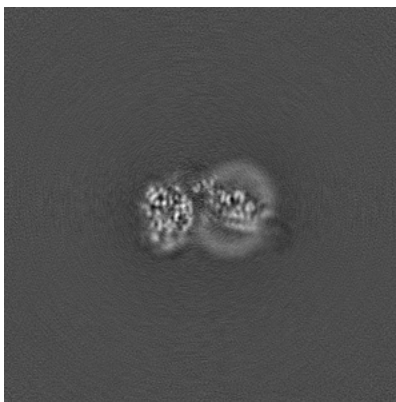
| X Index: 187 | Y Index: 184 | Z Index: 159 |
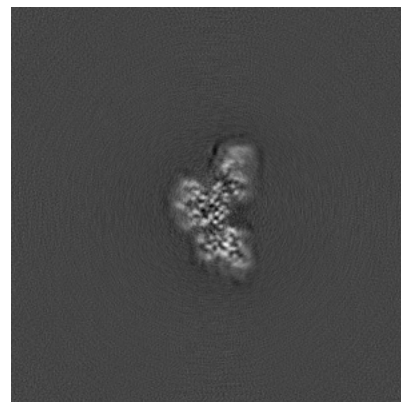
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
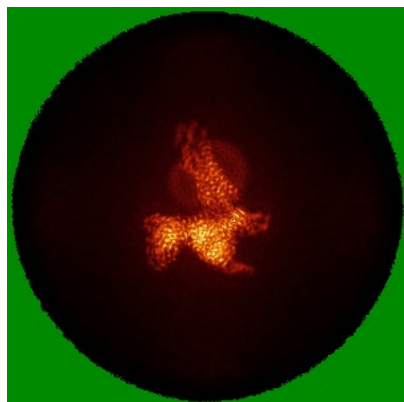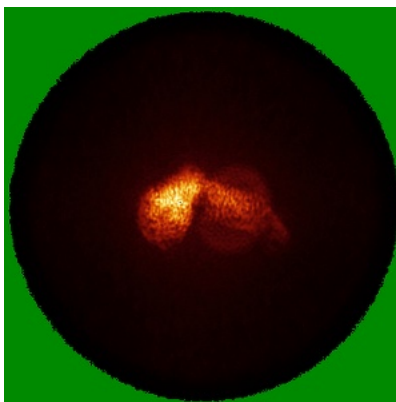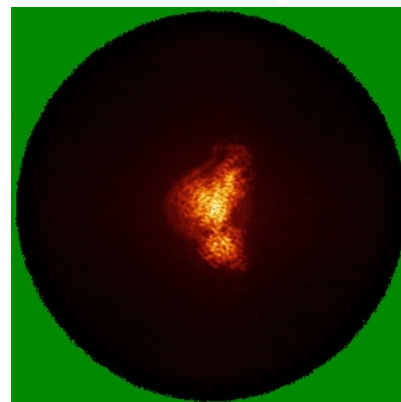
| X | Y | Z |

6.4.2 Raw map

| X | Y | Z |
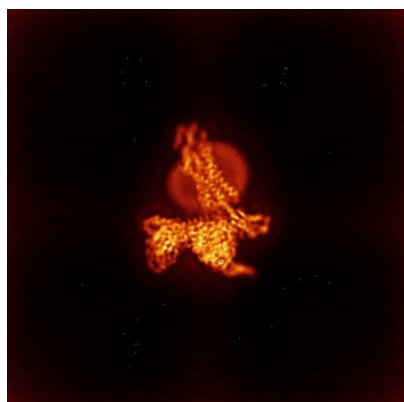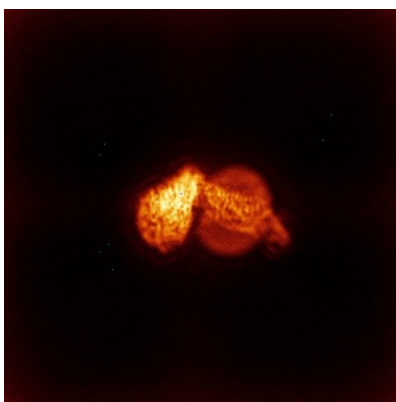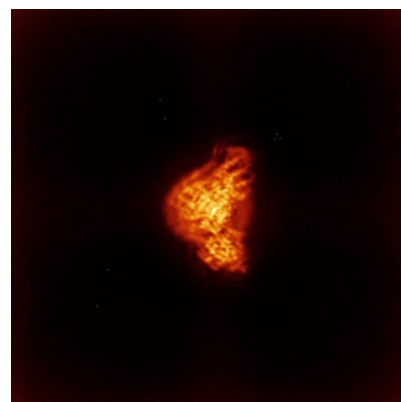
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
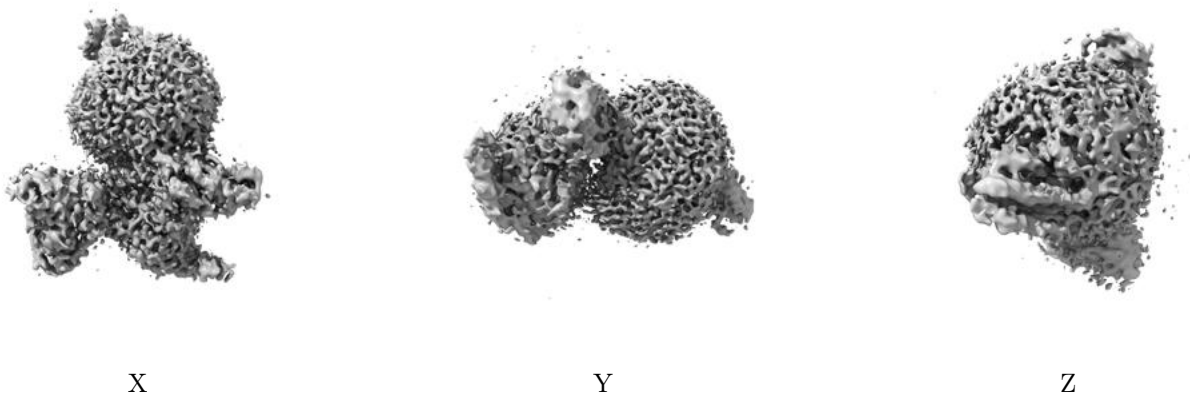
The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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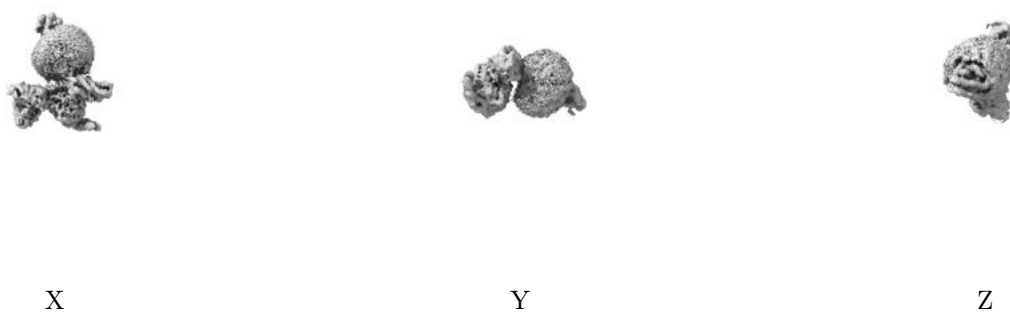
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
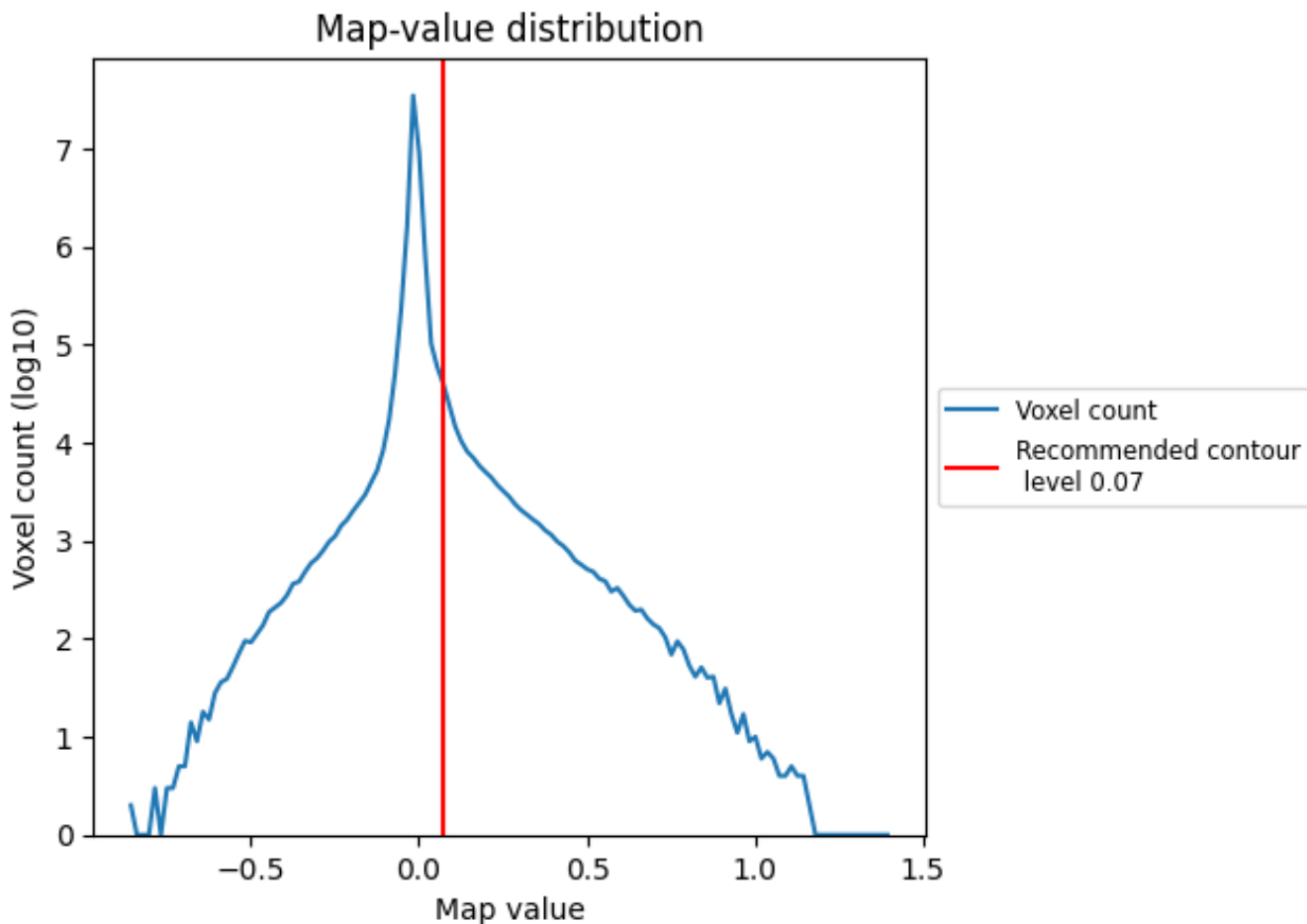
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
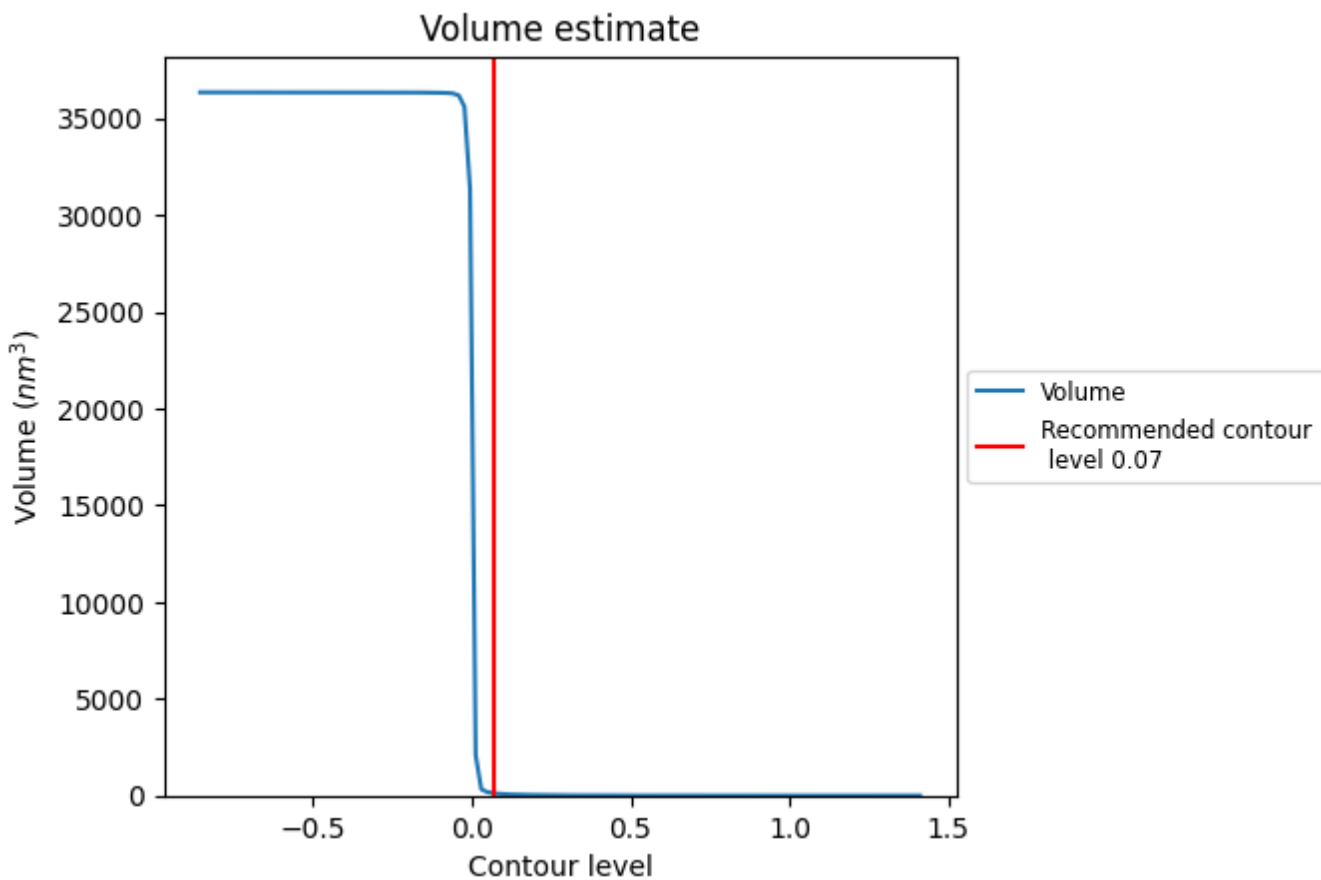
The volume at the recommended contour level is 123 nm^3; this corresponds to an approximate mass of 111 kDa.

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 ⓘ
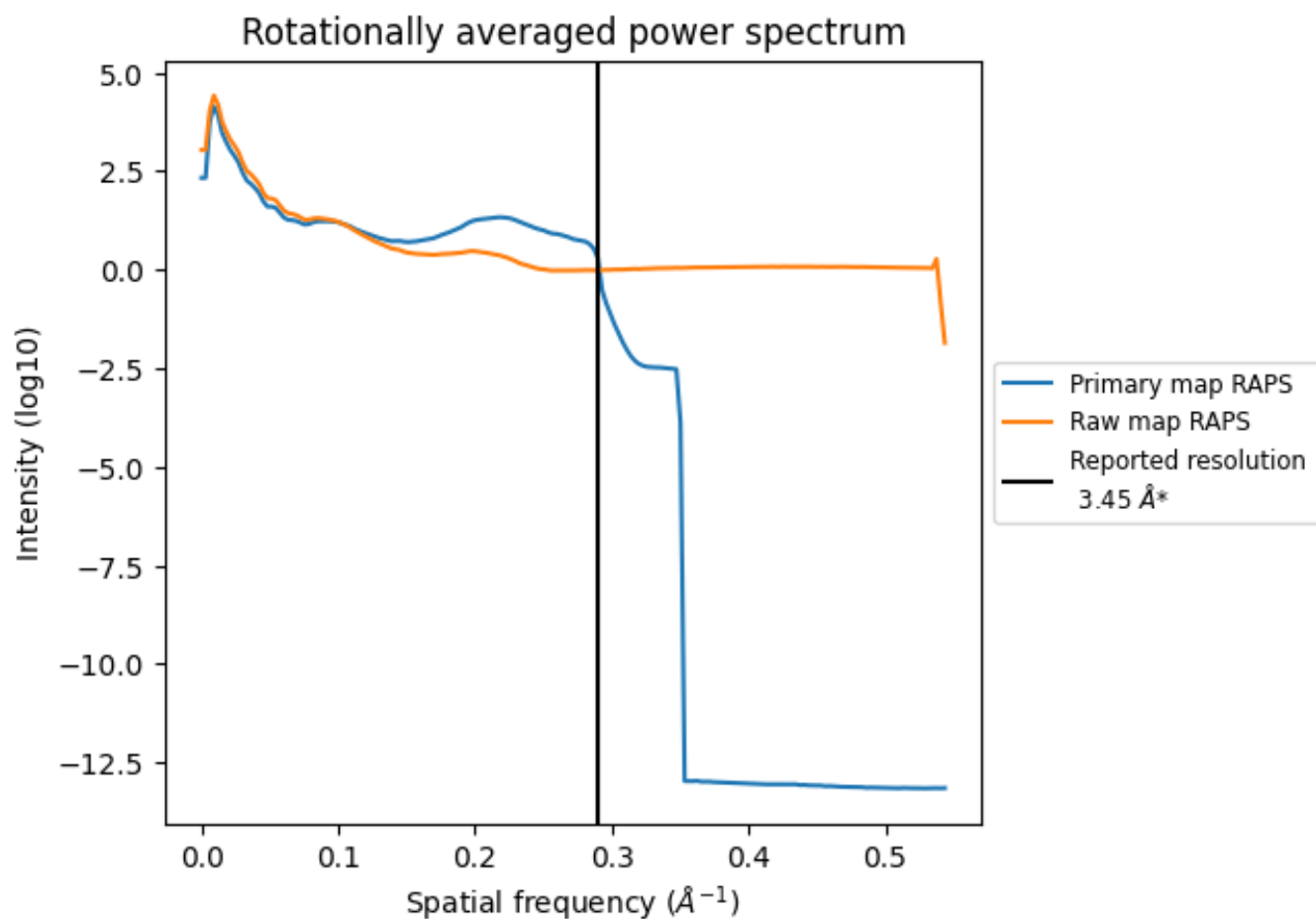
*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

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)
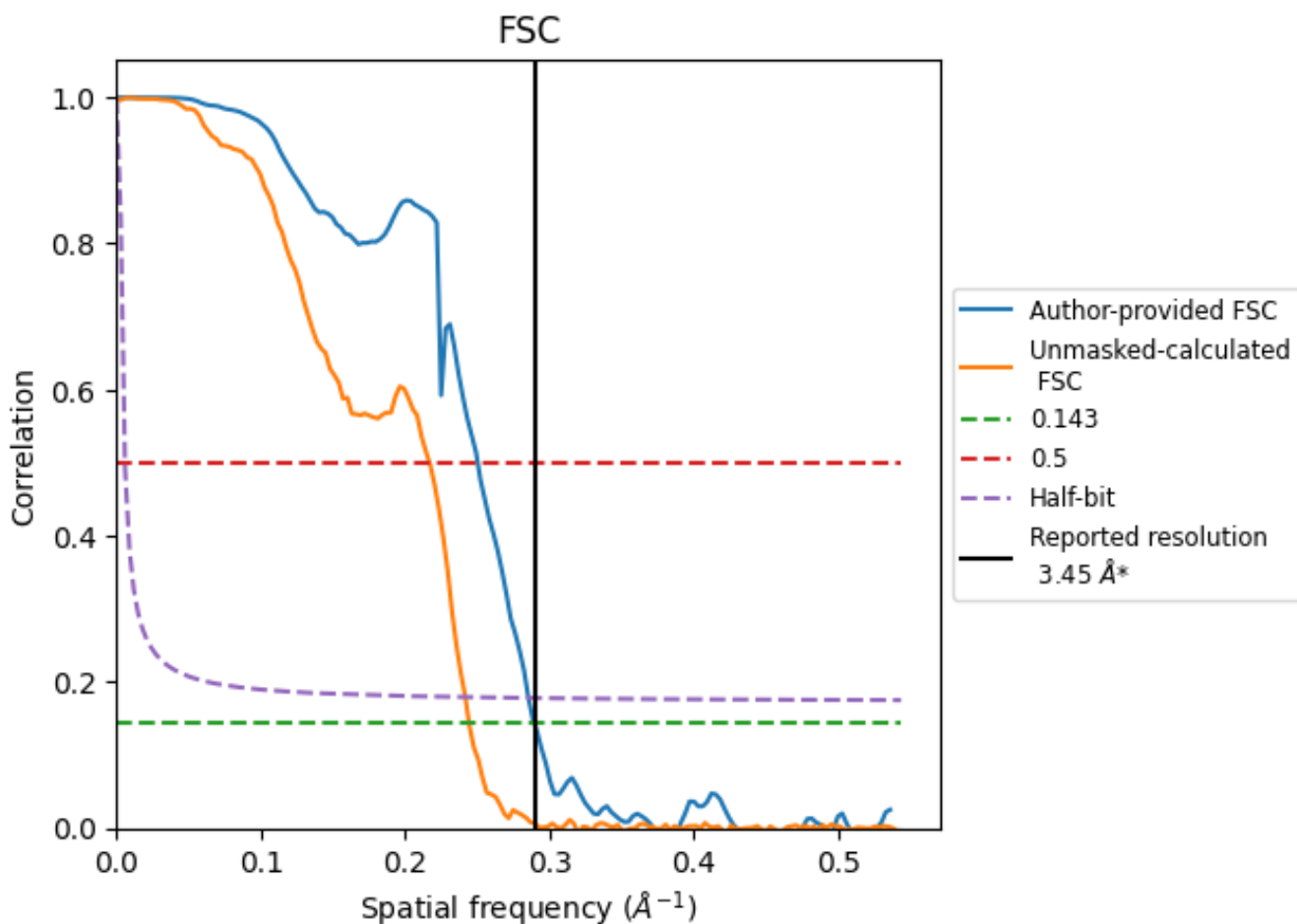
*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.45	4.00	3.50
Unmasked-calculated*	4.09	4.61	4.14

*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 4.09 differs from the reported value 3.45 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-36750 and PDB model 8JZP. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ

| X | Y | Z |
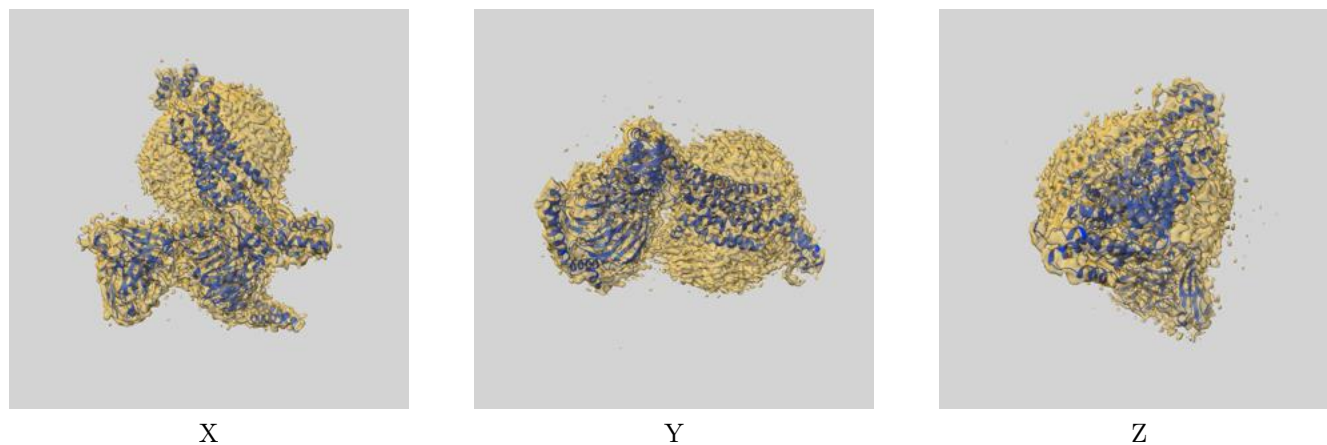
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model (i)
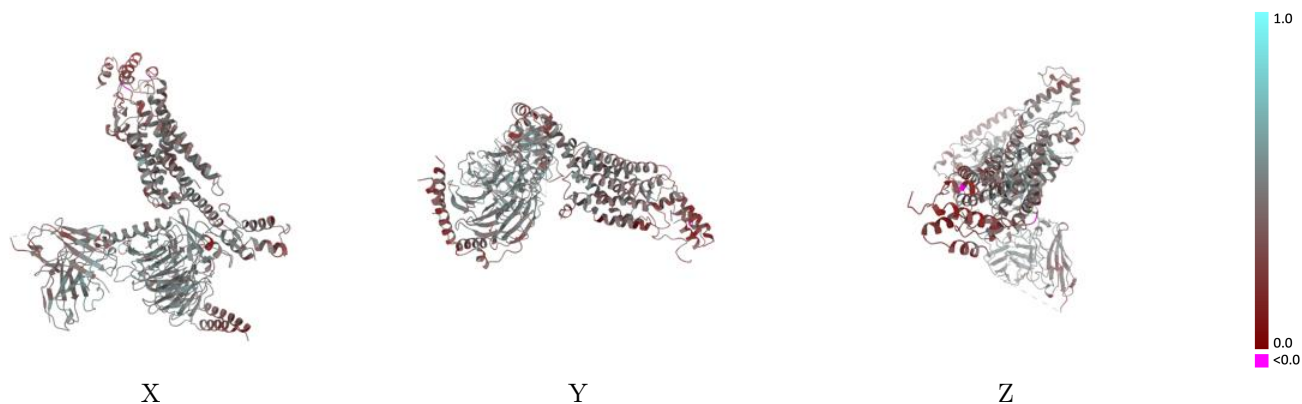
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)
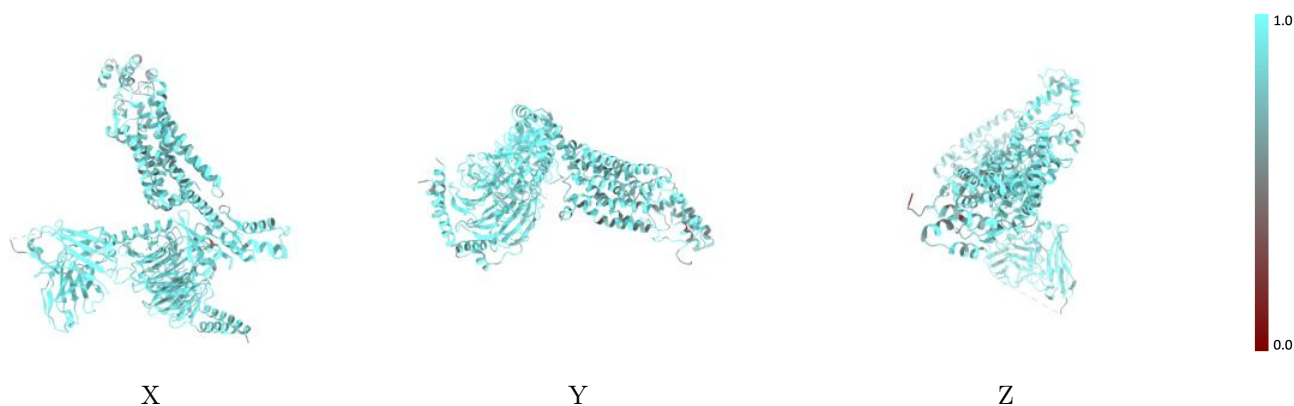
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4   Atom inclusion ⓘ
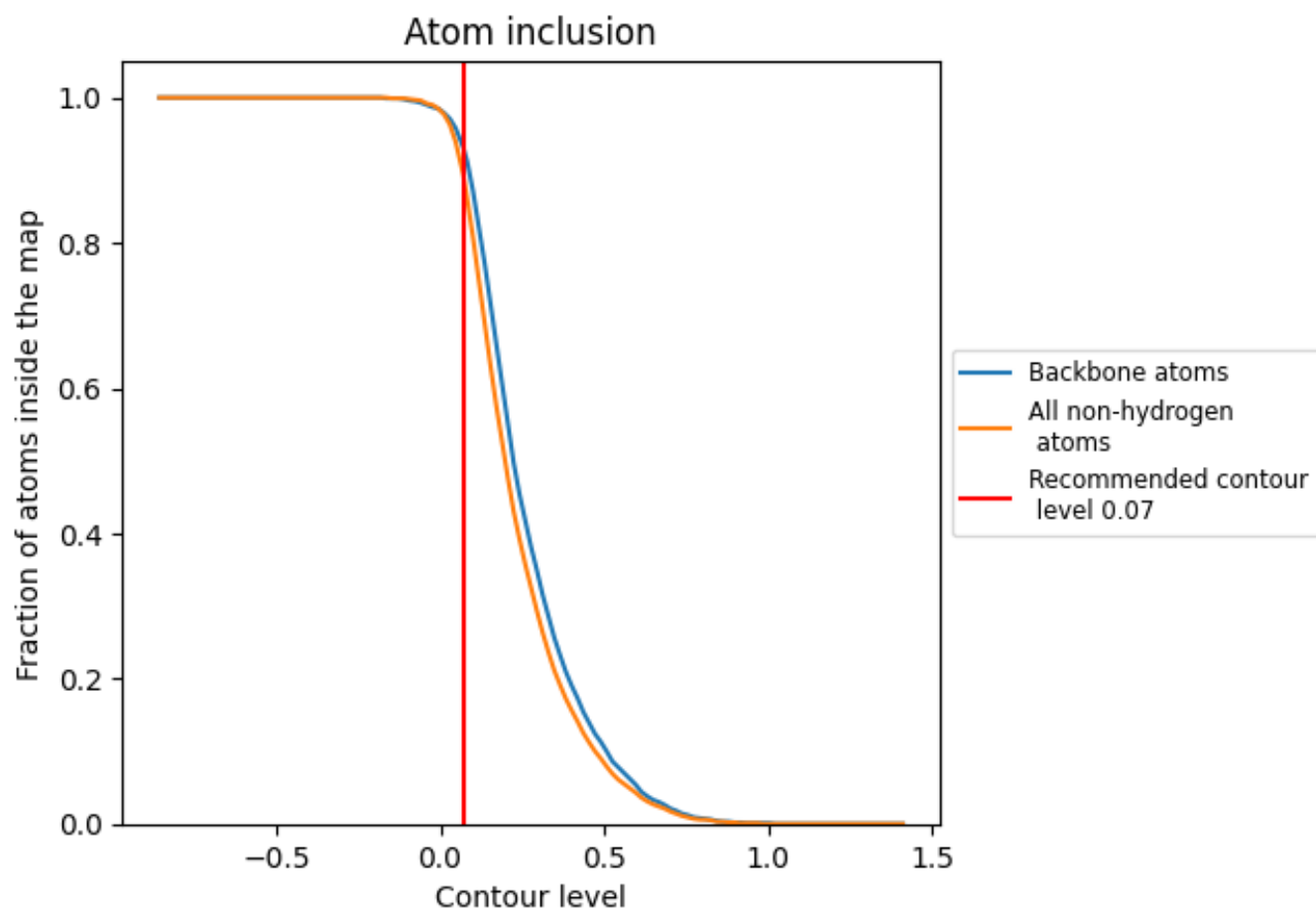
Atom inclusion

At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.4380
A	0.8550	0.4010
B	0.9180	0.4590
C	0.9230	0.4760
F	0.7700	0.2810
G	0.8700	0.3930
H	0.9310	0.4710

1.0

0.0
<0.0