



Full wwPDB EM Validation Report ⓘ

Apr 27, 2026 – 04:15 PM JST

PDB ID : 22EM / pdb_000022em
EMDB ID : EMD-68208
Title : Gi bound kappa-opioid receptor in complex with beta01
Authors : Zhang, H.; Wang, R.; Shi, P.; He, X.; Zhu, Q.; Xu, Y.; Yuan, Q.; Hu, W.; Wu, K.; Zheng, Y.; Zhou, L.; Liang, J.; Lv, P.; Xu, Z.; Zhuang, Y.; Xu, H.; Wang, Y.; Tian, C.
Deposited on : 2026-01-08
Resolution : 2.86 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:

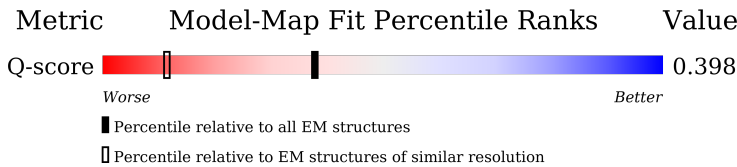
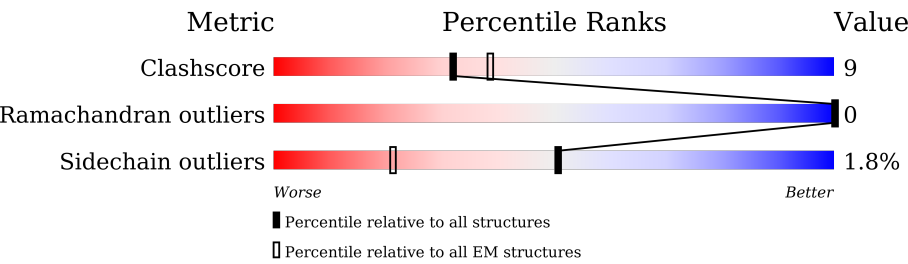
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12017 (2.36 - 3.36)

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	353	<div><div>9%</div><div>56%</div><div>8%</div><div>36%</div></div>
2	C	371	<div><div>13%</div><div>82%</div><div>8%</div><div>10%</div></div>
3	D	71	<div><div>59%</div><div>70%</div><div>7%</div><div>23%</div></div>
4	F	624	<div><div>6%</div><div>33%</div><div>11%</div><div>54%</div></div>

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Mol	Chain	Length	Quality of chain
5	A	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	A1E3Y	A	1	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7138 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	227	Total	C	N	O	S	0	0
			1826	1159	302	351	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	ALA	GLY	conflict	UNP P63096
B	326	SER	ALA	conflict	UNP P63096

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	335	Total	C	N	O	S	0	0
			2575	1589	464	501	21		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P62874
C	-3	HIS	-	expression tag	UNP P62874
C	-2	HIS	-	expression tag	UNP P62874
C	-1	HIS	-	expression tag	UNP P62874
C	0	HIS	-	expression tag	UNP P62874
C	1	HIS	-	expression tag	UNP P62874
C	2	GLY	-	expression tag	UNP P62874
C	3	SER	-	expression tag	UNP P62874
C	4	LEU	-	expression tag	UNP P62874
C	5	LEU	-	expression tag	UNP P62874
C	341	GLY	-	expression tag	UNP P62874
C	342	SER	-	expression tag	UNP P62874
C	343	SER	-	expression tag	UNP P62874
C	344	GLY	-	expression tag	UNP P62874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	345	GLY	-	expression tag	UNP P62874
C	346	GLY	-	expression tag	UNP P62874
C	347	GLY	-	expression tag	UNP P62874
C	348	SER	-	expression tag	UNP P62874
C	349	GLY	-	expression tag	UNP P62874
C	350	GLY	-	expression tag	UNP P62874
C	351	GLY	-	expression tag	UNP P62874
C	352	GLY	-	expression tag	UNP P62874
C	353	SER	-	expression tag	UNP P62874
C	354	SER	-	expression tag	UNP P62874
C	355	GLY	-	expression tag	UNP P62874
C	356	VAL	-	expression tag	UNP P62874
C	357	SER	-	expression tag	UNP P62874
C	358	GLY	-	expression tag	UNP P62874
C	359	TRP	-	expression tag	UNP P62874
C	360	ARG	-	expression tag	UNP P62874
C	361	LEU	-	expression tag	UNP P62874
C	362	PHE	-	expression tag	UNP P62874
C	363	LYS	-	expression tag	UNP P62874
C	364	LYS	-	expression tag	UNP P62874
C	365	ILE	-	expression tag	UNP P62874
C	366	SER	-	expression tag	UNP P62874

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	55	Total	C	N	O	S	0	0
			427	268	75	81	3		

- Molecule 4 is a protein called Soluble cytochrome b562,Kappa-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	284	Total	C	N	O	S	0	0
			2261	1499	357	387	18		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-107	MET	-	initiating methionine	UNP P0ABE7
F	-106	LYS	-	expression tag	UNP P0ABE7
F	-105	THR	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-104	ILE	-	expression tag	UNP P0ABE7
F	-103	ILE	-	expression tag	UNP P0ABE7
F	-102	ALA	-	expression tag	UNP P0ABE7
F	-101	LEU	-	expression tag	UNP P0ABE7
F	-100	SER	-	expression tag	UNP P0ABE7
F	-99	TYR	-	expression tag	UNP P0ABE7
F	-98	ILE	-	expression tag	UNP P0ABE7
F	-97	PHE	-	expression tag	UNP P0ABE7
F	-96	CYS	-	expression tag	UNP P0ABE7
F	-95	LEU	-	expression tag	UNP P0ABE7
F	-94	VAL	-	expression tag	UNP P0ABE7
F	-93	PHE	-	expression tag	UNP P0ABE7
F	-92	ALA	-	expression tag	UNP P0ABE7
F	-91	ASP	-	expression tag	UNP P0ABE7
F	-90	TYR	-	expression tag	UNP P0ABE7
F	-89	LYS	-	expression tag	UNP P0ABE7
F	-88	ASP	-	expression tag	UNP P0ABE7
F	-87	ASP	-	expression tag	UNP P0ABE7
F	-86	ASP	-	expression tag	UNP P0ABE7
F	-85	ASP	-	expression tag	UNP P0ABE7
F	-84	LYS	-	expression tag	UNP P0ABE7
F	-77	TRP	MET	conflict	UNP P0ABE7
F	18	ILE	HIS	conflict	UNP P0ABE7
F	22	LEU	-	linker	UNP P0ABE7
F	23	GLU	-	linker	UNP P0ABE7
F	24	ASN	-	linker	UNP P0ABE7
F	25	LEU	-	linker	UNP P0ABE7
F	26	TYR	-	linker	UNP P0ABE7
F	27	PHE	-	linker	UNP P0ABE7
F	28	GLN	-	linker	UNP P0ABE7
F	29	GLY	-	linker	UNP P0ABE7
F	30	MET	-	linker	UNP P0ABE7
F	31	GLY	-	linker	UNP P0ABE7
F	32	GLN	-	linker	UNP P0ABE7
F	33	PRO	-	linker	UNP P0ABE7
F	34	GLY	-	linker	UNP P0ABE7
F	35	ASN	-	linker	UNP P0ABE7
F	36	GLY	-	linker	UNP P0ABE7
F	37	SER	-	linker	UNP P0ABE7
F	38	ALA	-	linker	UNP P0ABE7
F	39	PHE	-	linker	UNP P0ABE7
F	40	LEU	-	linker	UNP P0ABE7

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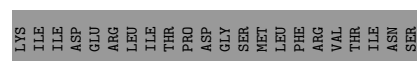
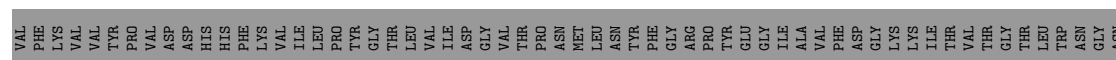
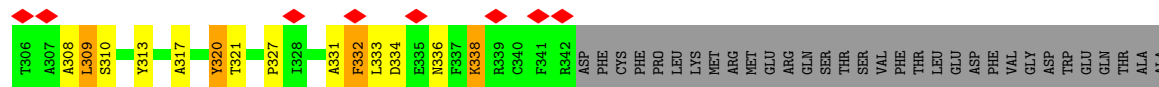
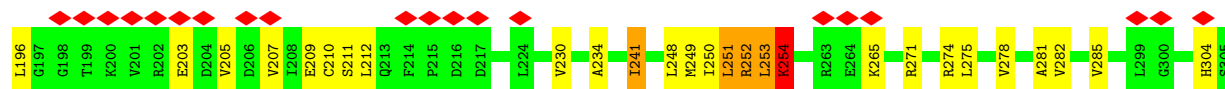
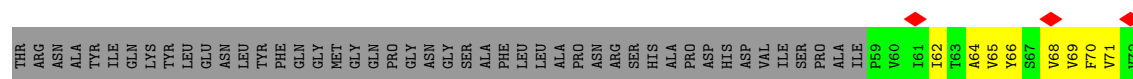
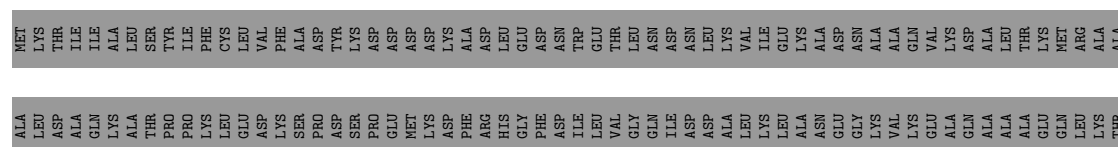
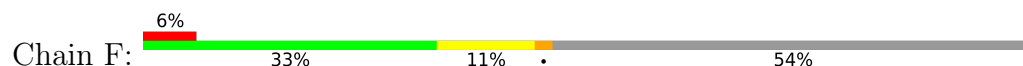
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Chain	Residue	Modelled	Actual	Comment	Reference
F	41	LEU	-	linker	UNP P0ABE7
F	42	ALA	-	linker	UNP P0ABE7
F	43	PRO	-	linker	UNP P0ABE7
F	44	ASN	-	linker	UNP P0ABE7
F	45	ARG	-	linker	UNP P0ABE7
F	46	SER	-	linker	UNP P0ABE7
F	47	HIS	-	linker	UNP P0ABE7
F	48	ALA	-	linker	UNP P0ABE7
F	49	PRO	-	linker	UNP P0ABE7
F	50	ASP	-	linker	UNP P0ABE7
F	51	HIS	-	linker	UNP P0ABE7
F	52	ASP	-	linker	UNP P0ABE7
F	53	VAL	-	linker	UNP P0ABE7

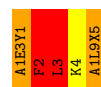
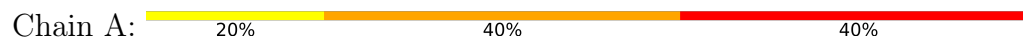
- Molecule 5 is a protein called A1E3Y-PHE-LEU-DLY-A1L9X.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	5	Total	C	N	O	0	0
			49	36	7	6		

- Molecule 4: Soluble cytochrome b562, Kappa-type opioid receptor



- Molecule 5: A1E3Y-PHE-LEU-DLY-A1L9X



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	431242	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)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.391	Depositor
Minimum map value	-2.076	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.227	Depositor
Map size (Å)	219.0, 219.0, 219.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DLY, A1E3Y, A1L9X

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	0.11	0/1856	0.25	0/2489
2	C	0.11	0/2622	0.27	0/3555
3	D	0.15	0/433	0.28	0/584
4	F	0.73	12/2314 (0.5%)	0.68	8/3153 (0.3%)
5	A	2.10	1/19 (5.3%)	1.61	1/24 (4.2%)
All	All	0.44	13/7244 (0.2%)	0.45	9/9805 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	252	ARG	CA-C	-9.44	1.40	1.52
5	A	2	PHE	C-N	8.18	1.44	1.33
4	F	241	ILE	C-O	-7.52	1.16	1.24
4	F	248	LEU	N-CA	-7.44	1.37	1.46
4	F	251	LEU	N-CA	-7.18	1.37	1.46
4	F	252	ARG	C-O	-6.16	1.16	1.24
4	F	241	ILE	CA-C	-6.15	1.44	1.52
4	F	151	MET	C-O	-6.03	1.16	1.24
4	F	254	LYS	N-CA	5.76	1.53	1.46
4	F	151	MET	CA-C	-5.58	1.45	1.52
4	F	248	LEU	CA-CB	-5.55	1.44	1.53
4	F	320	TYR	CA-C	-5.54	1.45	1.52
4	F	254	LYS	C-O	-5.11	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	254	LYS	N-CA-C	10.84	125.60	112.38
4	F	241	ILE	CB-CA-C	-8.83	101.26	110.88
4	F	310	SER	N-CA-C	-6.85	105.54	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	309	LEU	N-CA-C	-6.62	103.60	112.94
4	F	96	ILE	CA-C-N	6.38	129.15	120.54
4	F	96	ILE	C-N-CA	6.38	129.15	120.54
4	F	308	ALA	N-CA-C	-5.99	105.84	113.02
4	F	253	LEU	CB-CA-C	5.30	120.74	110.46
5	A	3	LEU	N-CA-C	-5.01	96.97	111.00

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	B	1826	0	1813	21	0
2	C	2575	0	2484	18	0
3	D	427	0	437	7	0
4	F	2261	0	2350	78	0
5	A	49	0	32	11	0
All	All	7138	0	7116	122	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 (122) 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)
4:F:115:GLN:NE2	5:A:1:A1E3Y:CA	2.22	1.02
4:F:115:GLN:HE21	5:A:1:A1E3Y:CA	1.74	1.00
4:F:90:MET:HB3	4:F:96:ILE:HD11	1.55	0.89
4:F:135:ILE:HD11	4:F:210:CYS:SG	2.15	0.85
4:F:81:MET:HE1	4:F:103:LEU:HD13	1.58	0.85
3:D:48:ASP:OD2	3:D:51:LEU:CD2	2.31	0.79
4:F:115:GLN:NE2	5:A:1:A1E3Y:C	2.46	0.79
4:F:70:PHE:HB2	4:F:112:MET:HE2	1.65	0.78
4:F:126:PHE:HB3	4:F:130:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:131:CYS:O	4:F:135:ILE:HD12	1.84	0.78
2:C:284:LEU:HD11	3:D:51:LEU:HB3	1.66	0.77
3:D:48:ASP:OD2	3:D:51:LEU:HD21	1.85	0.76
4:F:317:ALA:O	4:F:321:THR:HG23	1.88	0.74
4:F:81:MET:CE	4:F:103:LEU:HD13	2.17	0.74
4:F:70:PHE:CZ	4:F:74:LEU:HD12	2.25	0.72
4:F:95:ASN:HA	4:F:98:ILE:HG22	1.72	0.71
1:B:318:GLU:OE2	4:F:265:LYS:NZ	2.25	0.70
4:F:205:VAL:HG23	4:F:207:VAL:HG22	1.75	0.69
4:F:122:ASN:O	5:A:5:A1L9X:N	2.28	0.66
4:F:115:GLN:HE22	5:A:1:A1E3Y:C	2.07	0.65
1:B:254:CYS:O	1:B:317:LYS:NZ	2.32	0.62
4:F:70:PHE:HD2	4:F:109:THR:O	1.84	0.61
4:F:252:ARG:O	4:F:253:LEU:C	2.40	0.61
2:C:6:GLN:OE1	2:C:6:GLN:N	2.35	0.60
4:F:90:MET:HB3	4:F:96:ILE:CD1	2.29	0.60
1:B:251:ASP:HB2	1:B:310:LEU:HD21	1.81	0.60
4:F:62:ILE:O	4:F:65:VAL:HG12	2.02	0.59
4:F:70:PHE:CD2	4:F:113:PRO:HD3	2.37	0.59
4:F:70:PHE:CD2	4:F:109:THR:O	2.56	0.58
2:C:237:ASN:ND2	2:C:239:ASN:OD1	2.37	0.57
4:F:62:ILE:HG21	4:F:119:TYR:HE2	1.69	0.57
2:C:163:ASP:O	2:C:164:THR:OG1	2.19	0.57
1:B:298:GLU:N	1:B:298:GLU:OE1	2.36	0.57
3:D:48:ASP:OD1	3:D:50:LEU:CD2	2.52	0.57
4:F:211:SER:OG	5:A:4:DLY:NZ	2.39	0.56
3:D:48:ASP:OD1	3:D:50:LEU:HD23	2.06	0.55
2:C:83:ASP:OD2	2:C:86:THR:OG1	2.24	0.55
4:F:66:TYR:O	4:F:112:MET:HE1	2.06	0.55
2:C:303:ASP:OD1	2:C:304:ARG:N	2.39	0.55
4:F:70:PHE:HE2	4:F:110:THR:HA	1.72	0.54
4:F:241:ILE:O	4:F:241:ILE:CG2	2.54	0.54
3:D:12:ALA:O	3:D:16:VAL:HG23	2.07	0.54
4:F:76:GLY:O	4:F:80:VAL:HG23	2.08	0.54
4:F:241:ILE:O	4:F:241:ILE:HG22	2.06	0.54
4:F:66:TYR:C	4:F:112:MET:HE1	2.33	0.54
4:F:274:ARG:O	4:F:278:VAL:HG23	2.07	0.54
4:F:112:MET:HG2	4:F:320:TYR:CZ	2.42	0.54
4:F:191:ILE:O	4:F:195:VAL:HG22	2.08	0.53
4:F:64:ALA:O	4:F:68:VAL:HG23	2.08	0.53
4:F:114:PHE:O	4:F:118:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:GLU:OE2	2:C:263:THR:OG1	2.26	0.53
4:F:104:ALA:O	4:F:108:VAL:HG23	2.09	0.53
4:F:252:ARG:C	4:F:254:LYS:N	2.65	0.53
1:B:236:GLU:OE1	1:B:236:GLU:N	2.38	0.52
1:B:186:GLU:N	1:B:186:GLU:OE1	2.42	0.52
1:B:295:THR:N	1:B:298:GLU:OE2	2.40	0.52
4:F:135:ILE:HG12	5:A:3:LEU:HD12	1.92	0.52
1:B:18:MET:SD	1:B:21:ARG:NH2	2.83	0.52
4:F:195:VAL:HG23	4:F:196:LEU:HD12	1.90	0.51
2:C:254:ASP:OD2	2:C:257:ALA:N	2.42	0.51
1:B:9:ASP:O	1:B:13:VAL:HG23	2.10	0.51
4:F:119:TYR:HB2	4:F:313:TYR:CE1	2.46	0.51
2:C:87:THR:HG22	2:C:87:THR:O	2.11	0.51
4:F:252:ARG:O	4:F:254:LYS:N	2.44	0.51
4:F:69:VAL:HG11	4:F:321:THR:HG22	1.92	0.50
1:B:239:GLU:N	1:B:239:GLU:OE1	2.45	0.50
1:B:315:ASP:OD1	1:B:316:THR:N	2.44	0.50
4:F:95:ASN:HA	4:F:98:ILE:CG2	2.39	0.50
1:B:353:LEU:HD13	4:F:249:MET:HE1	1.93	0.50
2:C:30:LEU:O	2:C:30:LEU:HD23	2.11	0.49
4:F:119:TYR:CD1	4:F:313:TYR:CE2	3.00	0.49
3:D:48:ASP:CG	3:D:51:LEU:HG	2.38	0.49
4:F:185:LEU:O	4:F:185:LEU:HD23	2.12	0.48
4:F:62:ILE:HG21	4:F:119:TYR:CE2	2.47	0.48
4:F:332:PHE:O	4:F:338:LYS:HE2	2.14	0.48
4:F:304:HIS:CD2	4:F:309:LEU:HD11	2.49	0.48
4:F:278:VAL:O	4:F:282:VAL:HG23	2.13	0.48
4:F:334:ASP:OD1	4:F:336:ASN:ND2	2.46	0.48
2:C:331:SER:OG	2:C:333:ASP:OD1	2.27	0.48
4:F:275:LEU:HD13	4:F:333:LEU:HD12	1.94	0.48
4:F:112:MET:HG2	4:F:320:TYR:CE2	2.50	0.47
4:F:119:TYR:CD1	4:F:119:TYR:C	2.92	0.47
4:F:195:VAL:HG23	4:F:196:LEU:CD1	2.45	0.46
4:F:250:ILE:O	4:F:251:LEU:C	2.51	0.46
1:B:223:PHE:HE2	1:B:253:ILE:HD12	1.81	0.46
2:C:295:ASN:OD1	2:C:296:VAL:N	2.49	0.46
1:B:294:ASN:O	1:B:294:ASN:ND2	2.49	0.46
4:F:69:VAL:CG1	4:F:321:THR:HG22	2.46	0.46
1:B:247:MET:SD	1:B:310:LEU:HD22	2.56	0.45
4:F:70:PHE:CD1	4:F:71:VAL:N	2.84	0.45
4:F:332:PHE:O	4:F:338:LYS:NZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LEU:HD13	1:B:253:ILE:HD13	1.99	0.45
1:B:230:TYR:OH	1:B:283:LEU:O	2.28	0.44
1:B:233:VAL:HG12	1:B:234:LEU:HD23	2.00	0.44
4:F:139:TYR:CE1	5:A:2:PHE:CG	3.06	0.44
2:C:149:CYS:O	2:C:150:ARG:NH1	2.51	0.43
4:F:70:PHE:HB2	4:F:112:MET:CE	2.44	0.43
4:F:62:ILE:CG2	4:F:119:TYR:HE2	2.30	0.43
5:A:1:A1E3Y:O	5:A:3:LEU:HG	2.18	0.43
4:F:191:ILE:O	4:F:195:VAL:HG13	2.18	0.43
4:F:320:TYR:OH	5:A:1:A1E3Y:N	2.52	0.43
4:F:87:TYR:O	4:F:88:THR:C	2.62	0.42
4:F:281:ALA:O	4:F:285:VAL:HG22	2.20	0.42
4:F:230:VAL:O	4:F:234:ALA:HB3	2.19	0.42
4:F:327:PRO:O	4:F:331:ALA:HB3	2.19	0.42
2:C:171:ILE:N	2:C:171:ILE:HD12	2.34	0.42
4:F:118:VAL:HG11	5:A:3:LEU:O	2.20	0.42
1:B:201:VAL:HG21	1:B:211:TRP:CZ3	2.55	0.42
2:C:269:ILE:HD11	2:C:271:CYS:SG	2.60	0.41
4:F:70:PHE:CE2	4:F:110:THR:HA	2.54	0.41
4:F:332:PHE:HD1	4:F:332:PHE:HA	1.75	0.41
2:C:108:SER:OG	2:C:154:ASP:OD1	2.33	0.41
4:F:271:ARG:O	4:F:275:LEU:HG	2.20	0.41
1:B:247:MET:HE3	1:B:310:LEU:HD13	2.02	0.41
4:F:332:PHE:O	4:F:338:LYS:CE	2.68	0.41
1:B:230:TYR:O	1:B:241:ASN:ND2	2.49	0.41
2:C:30:LEU:HD22	2:C:262:MET:HE1	2.03	0.41
4:F:62:ILE:O	4:F:65:VAL:CG1	2.69	0.41
4:F:70:PHE:CD1	4:F:70:PHE:C	2.99	0.41
4:F:203:GLU:OE1	4:F:203:GLU:N	2.55	0.40
2:C:90:VAL:HG12	2:C:91:HIS:CE1	2.57	0.40
4:F:69:VAL:HG11	4:F:321:THR:CG2	2.52	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	223/353 (63%)	219 (98%)	4 (2%)	0	100	100
2	C	333/371 (90%)	330 (99%)	3 (1%)	0	100	100
3	D	53/71 (75%)	49 (92%)	4 (8%)	0	100	100
4	F	282/624 (45%)	272 (96%)	10 (4%)	0	100	100
5	A	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	893/1424 (63%)	871 (98%)	22 (2%)	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	B	202/305 (66%)	202 (100%)	0	100	100
2	C	278/302 (92%)	277 (100%)	1 (0%)	84	92
3	D	45/58 (78%)	45 (100%)	0	100	100
4	F	258/549 (47%)	247 (96%)	11 (4%)	26	50
5	A	2/2 (100%)	0	2 (100%)	0	0
All	All	785/1216 (65%)	771 (98%)	14 (2%)	51	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	234	PHE
4	F	96	ILE
4	F	112	MET
4	F	119	TYR
4	F	122	ASN
4	F	131	CYS
4	F	168	ASP

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Mol	Chain	Res	Type
4	F	209	GLU
4	F	212	LEU
4	F	254	LYS
4	F	332	PHE
4	F	338	LYS
5	A	2	PHE
5	A	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	306	GLN
1	B	322	HIS
2	C	6	GLN
2	C	183	HIS
2	C	220	GLN
2	C	259	GLN
4	F	77	ASN
4	F	95	ASN
4	F	115	GLN
4	F	322	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	A1L9X	A	5	5	8,10,10	2.92	2 (25%)	9,14,14	1.91	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1E3Y	A	1	5	11,11,12	0.83	0	10,13,15	1.55	3 (30%)
5	DLY	A	4	5	7,8,9	0.64	0	3,8,10	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1L9X	A	5	5	-	1/5/16/16	0/1/1/1
5	A1E3Y	A	1	5	-	3/7/7/8	0/1/1/1
5	DLY	A	4	5	-	2/6/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5	A1L9X	CB-CA	-6.71	1.47	1.54
5	A	5	A1L9X	CZ-CA	-3.86	1.50	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5	A1L9X	CG-CB-CA	-3.24	110.00	112.97
5	A	1	A1E3Y	O-C-CA	-2.60	117.86	125.43
5	A	5	A1L9X	CZ-CA-CB	2.56	112.47	108.40
5	A	1	A1E3Y	CD1-CG-CD2	2.33	121.20	118.29
5	A	1	A1E3Y	CB-CA-C	-2.30	104.57	114.50
5	A	5	A1L9X	OXT-C-CA	2.27	119.79	113.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	A1E3Y	O-C-CA-CB
5	A	1	A1E3Y	C-CA-CB-CG
5	A	5	A1L9X	OXT-C-CA-N
5	A	4	DLY	CE-CD-CG-CB
5	A	1	A1E3Y	C-CA-CB-N
5	A	4	DLY	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5	A1L9X	1	0
5	A	1	A1E3Y	6	0
5	A	4	DLY	1	0

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.

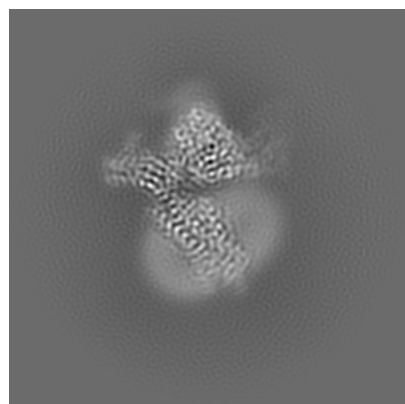
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68208. These allow visual inspection of the internal detail of the map and identification of artifacts.

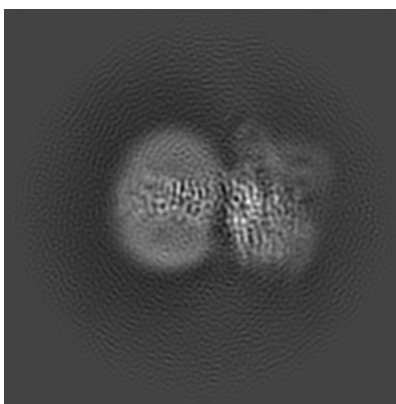
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

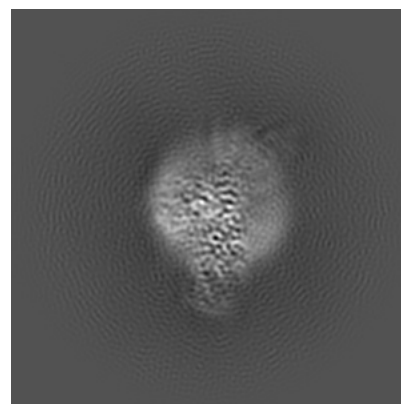
6.1.1 Primary map



X

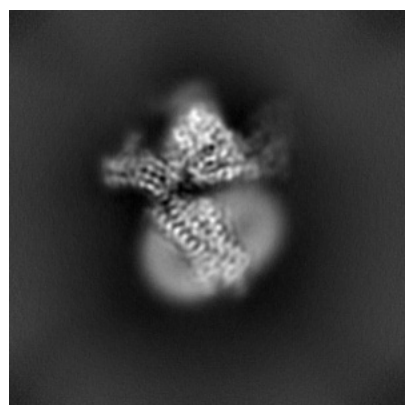


Y

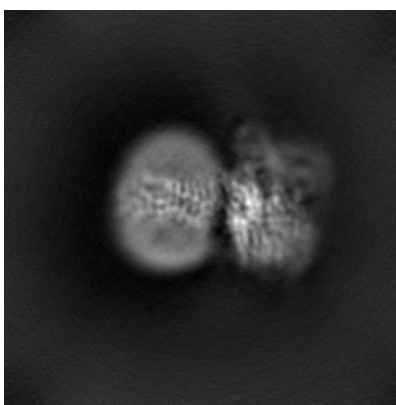


Z

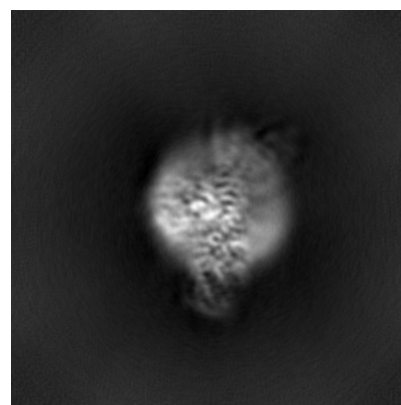
6.1.2 Raw map



X



Y

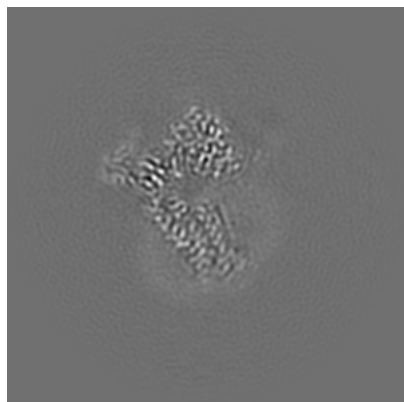


Z

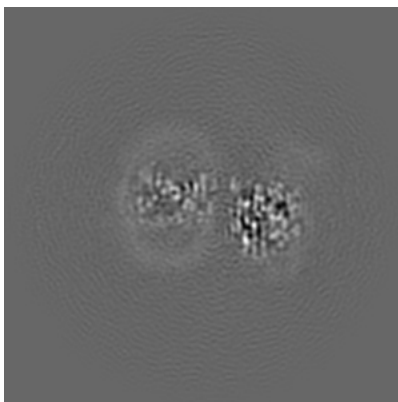
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

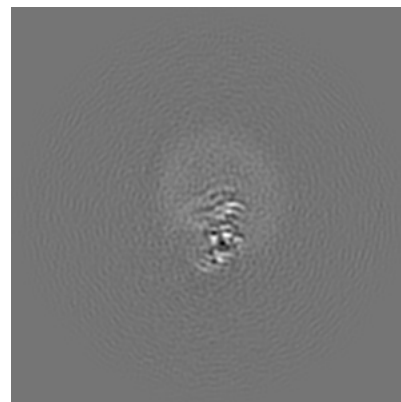
6.2.1 Primary map



X Index: 150

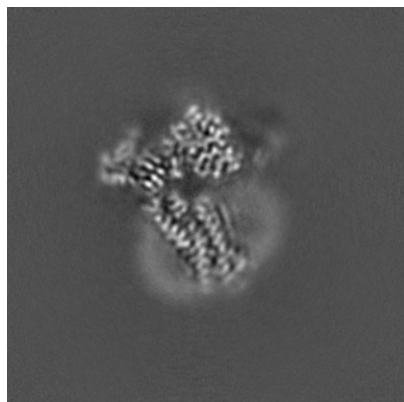


Y Index: 150

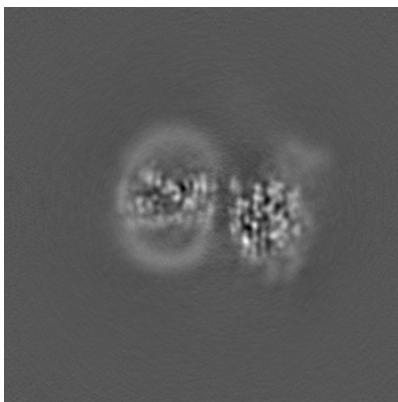


Z Index: 150

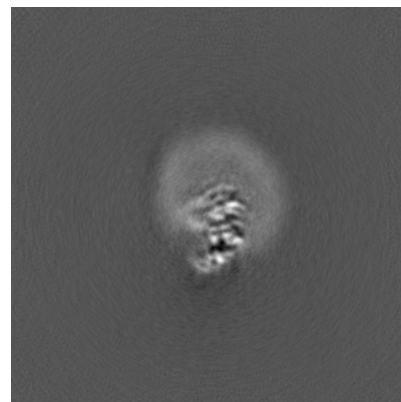
6.2.2 Raw map



X Index: 150



Y Index: 150

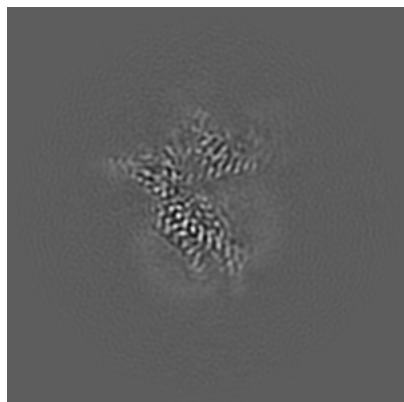


Z Index: 150

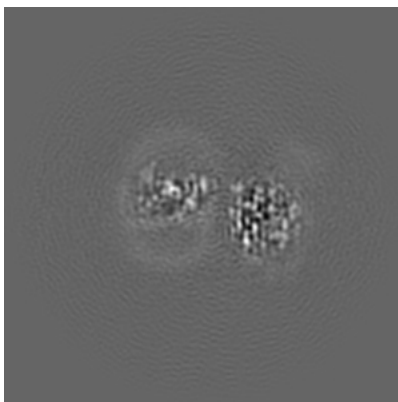
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

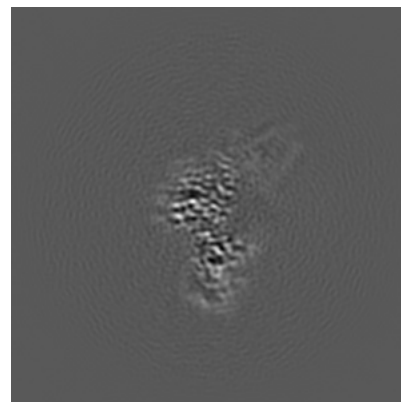
6.3.1 Primary map



X Index: 162

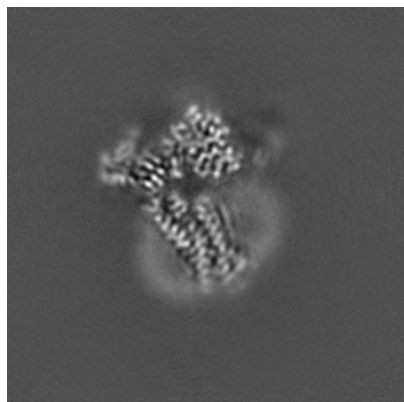


Y Index: 151

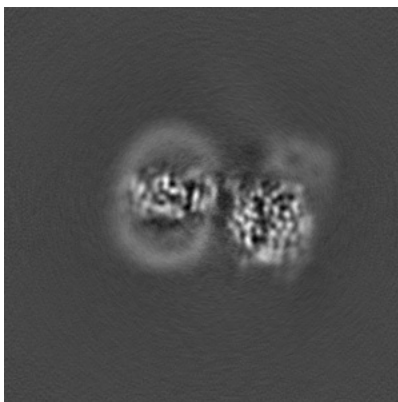


Z Index: 182

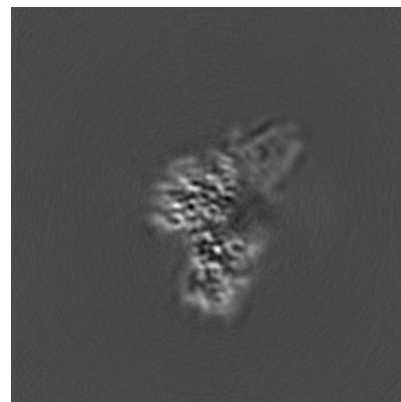
6.3.2 Raw map



X Index: 150



Y Index: 144

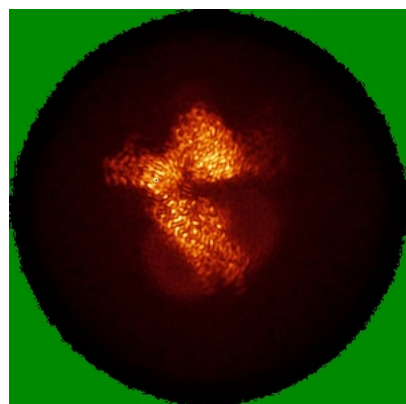


Z Index: 181

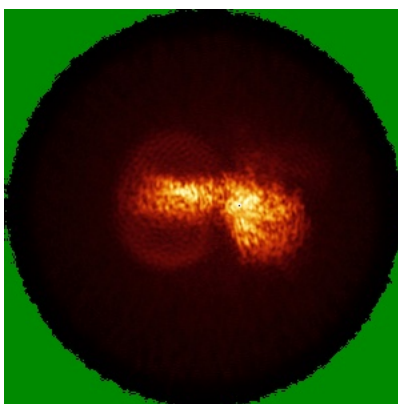
The images above show the largest variance slices of the map in three orthogonal directions.

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

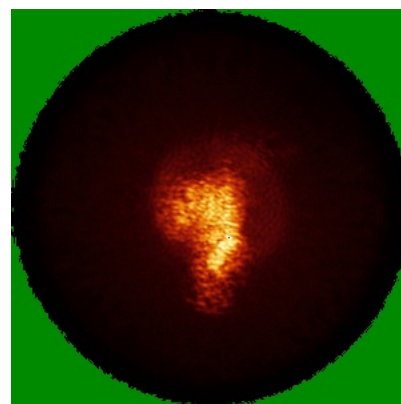
6.4.1 Primary map



X

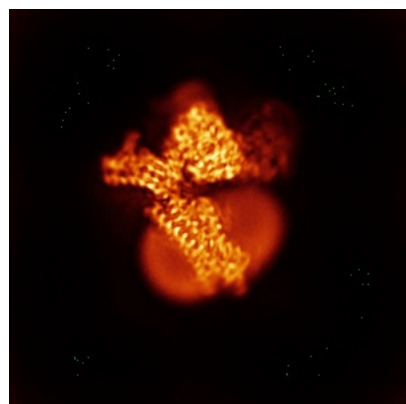


Y

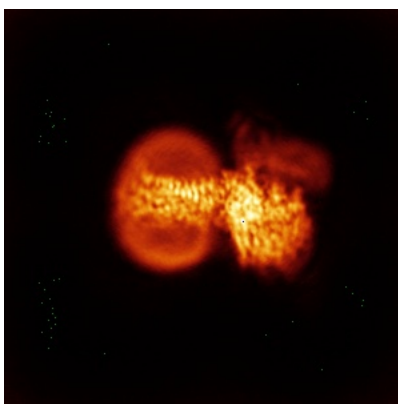


Z

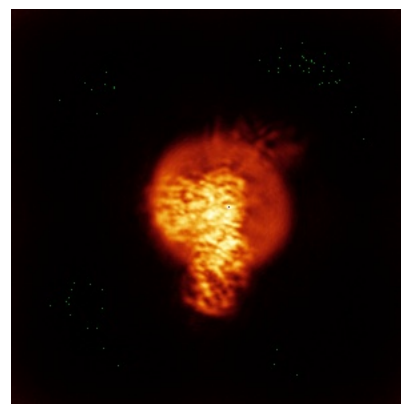
6.4.2 Raw map



X



Y

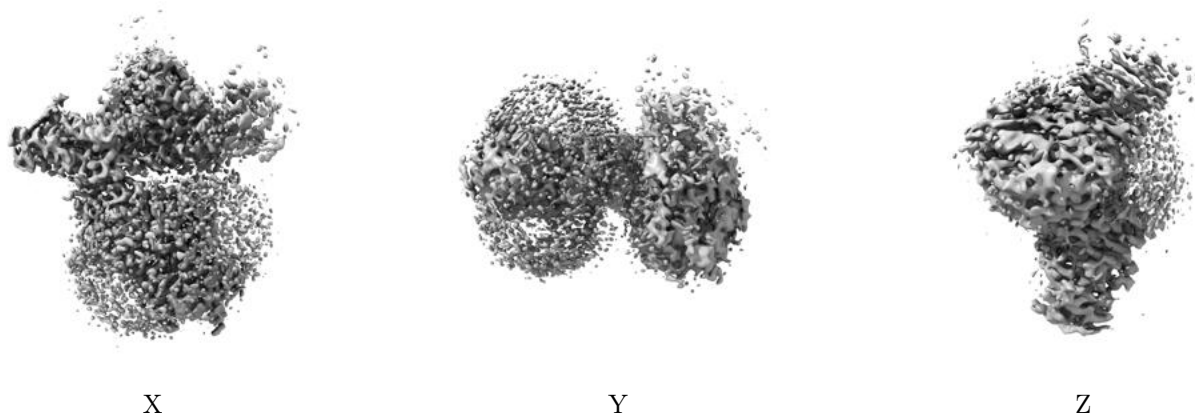


Z

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 0.227. 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.

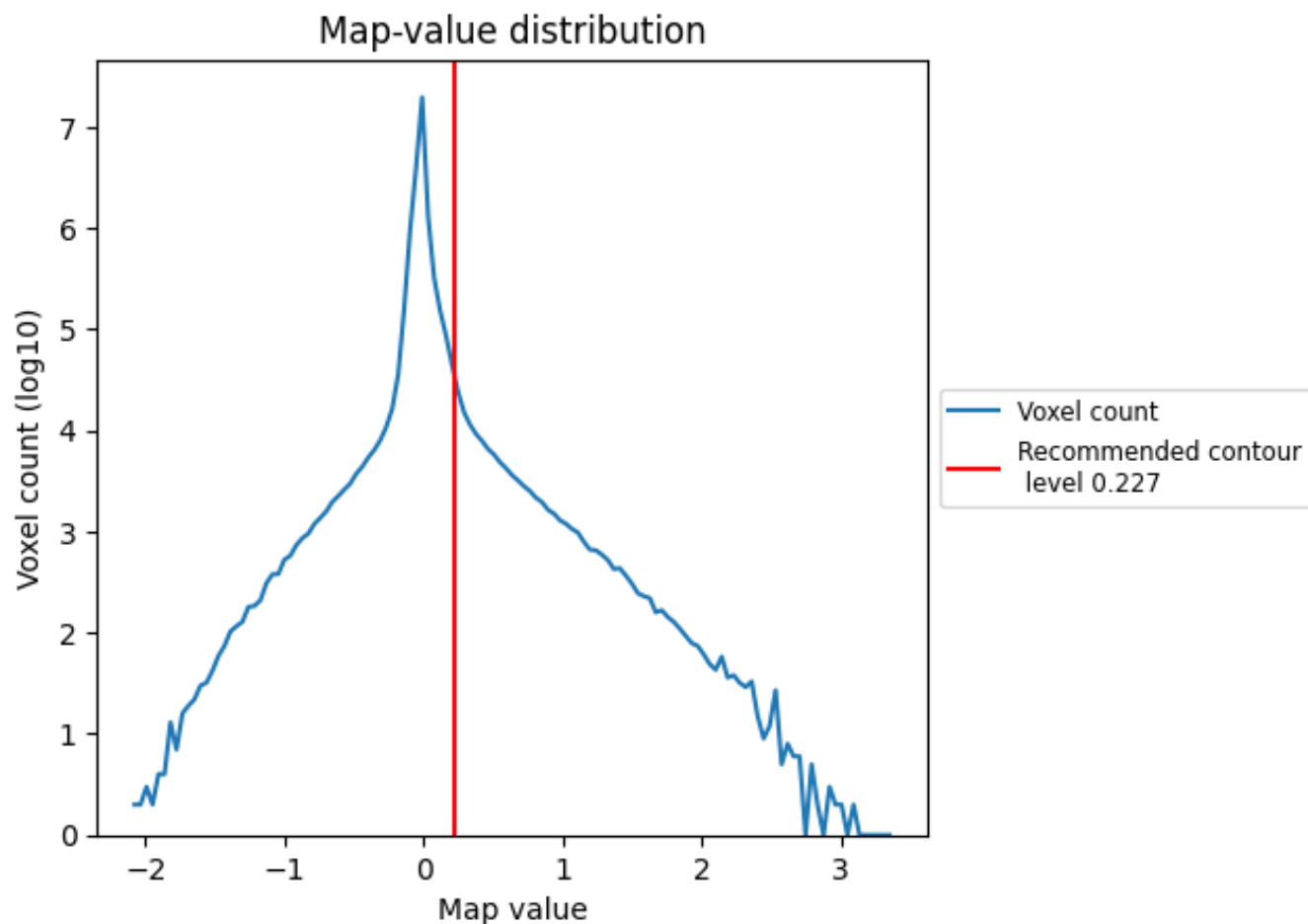
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

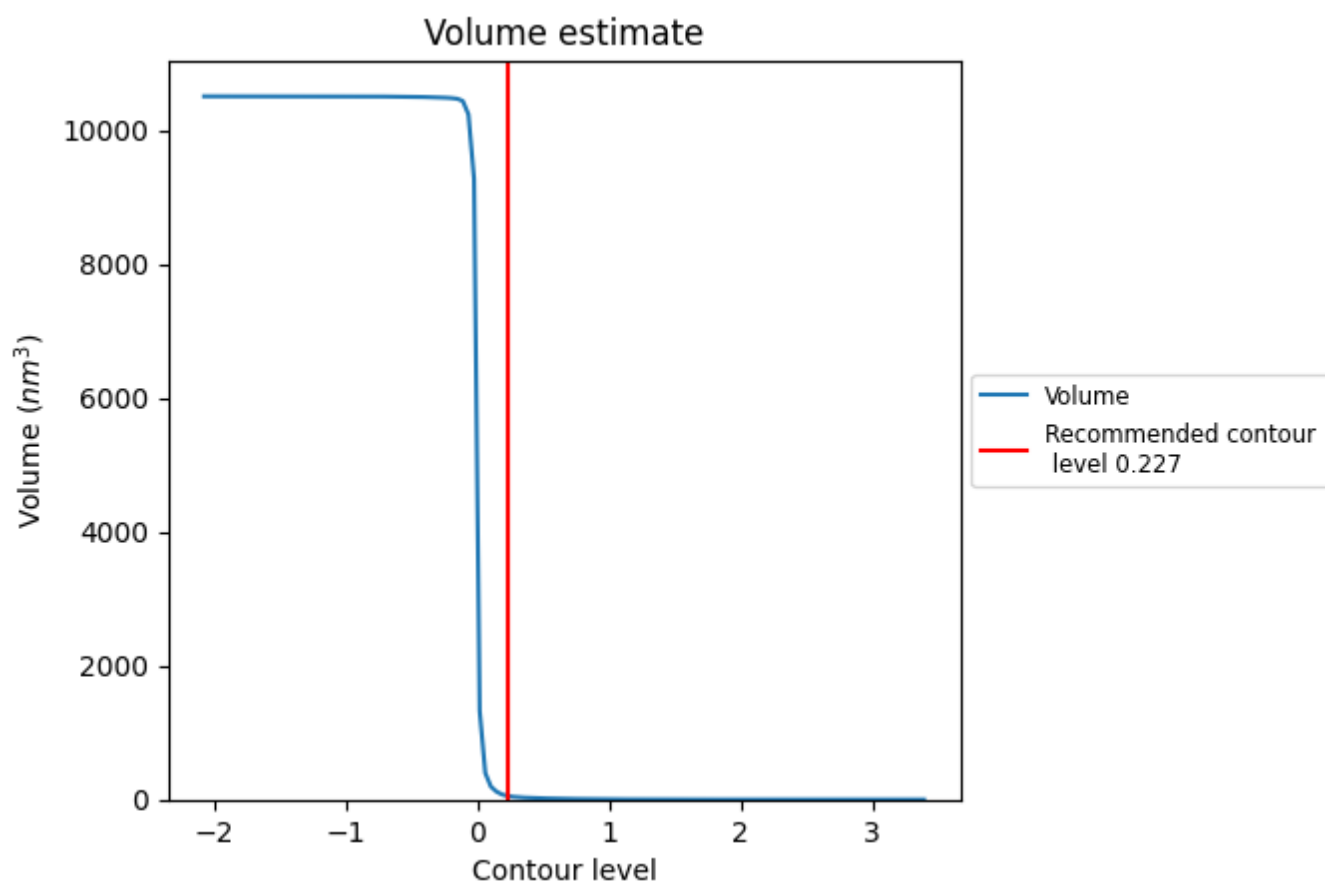
This section contains the results of statistical analysis of the map.

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.

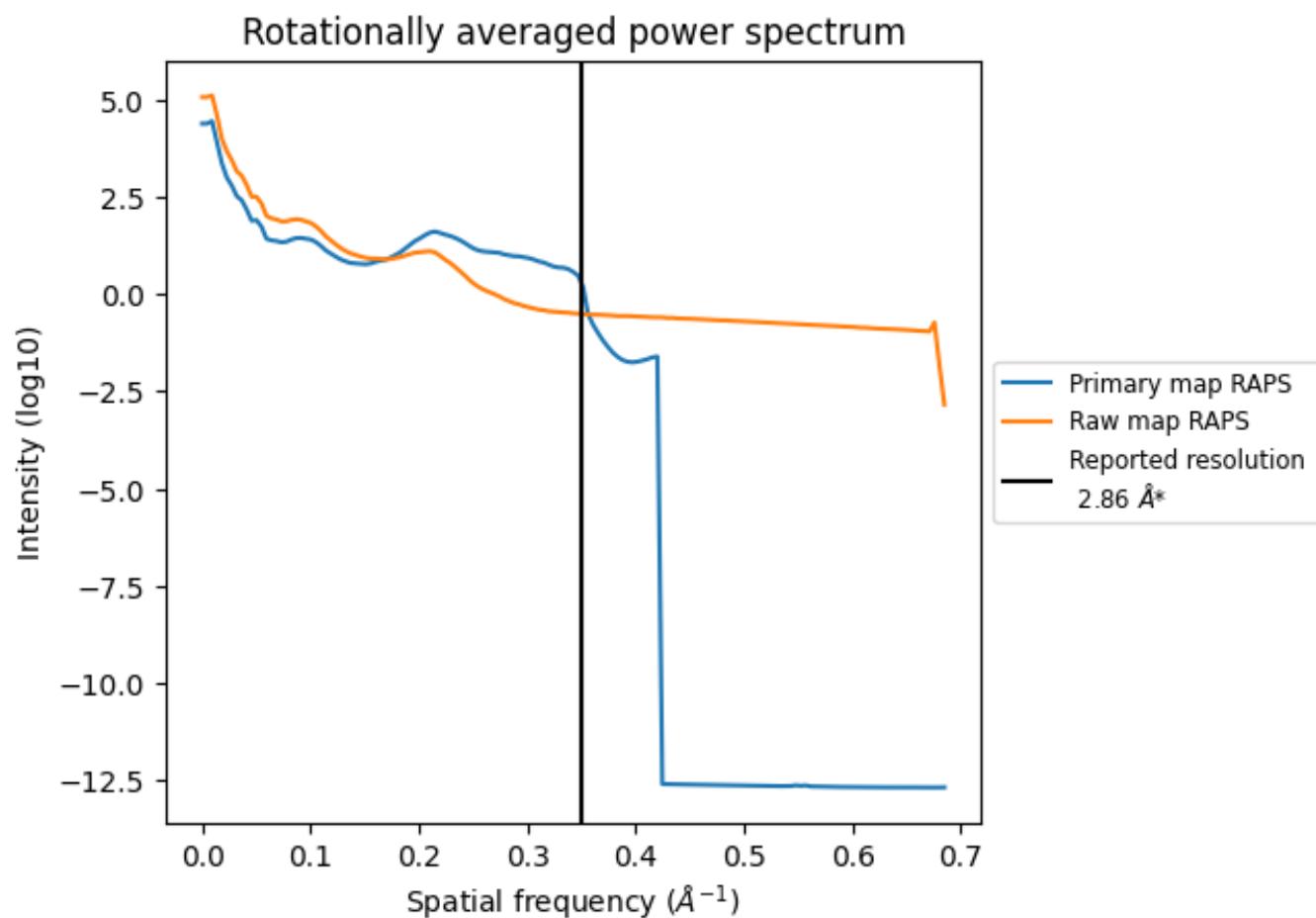
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm³; this corresponds to an approximate mass of 49 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 ⓘ

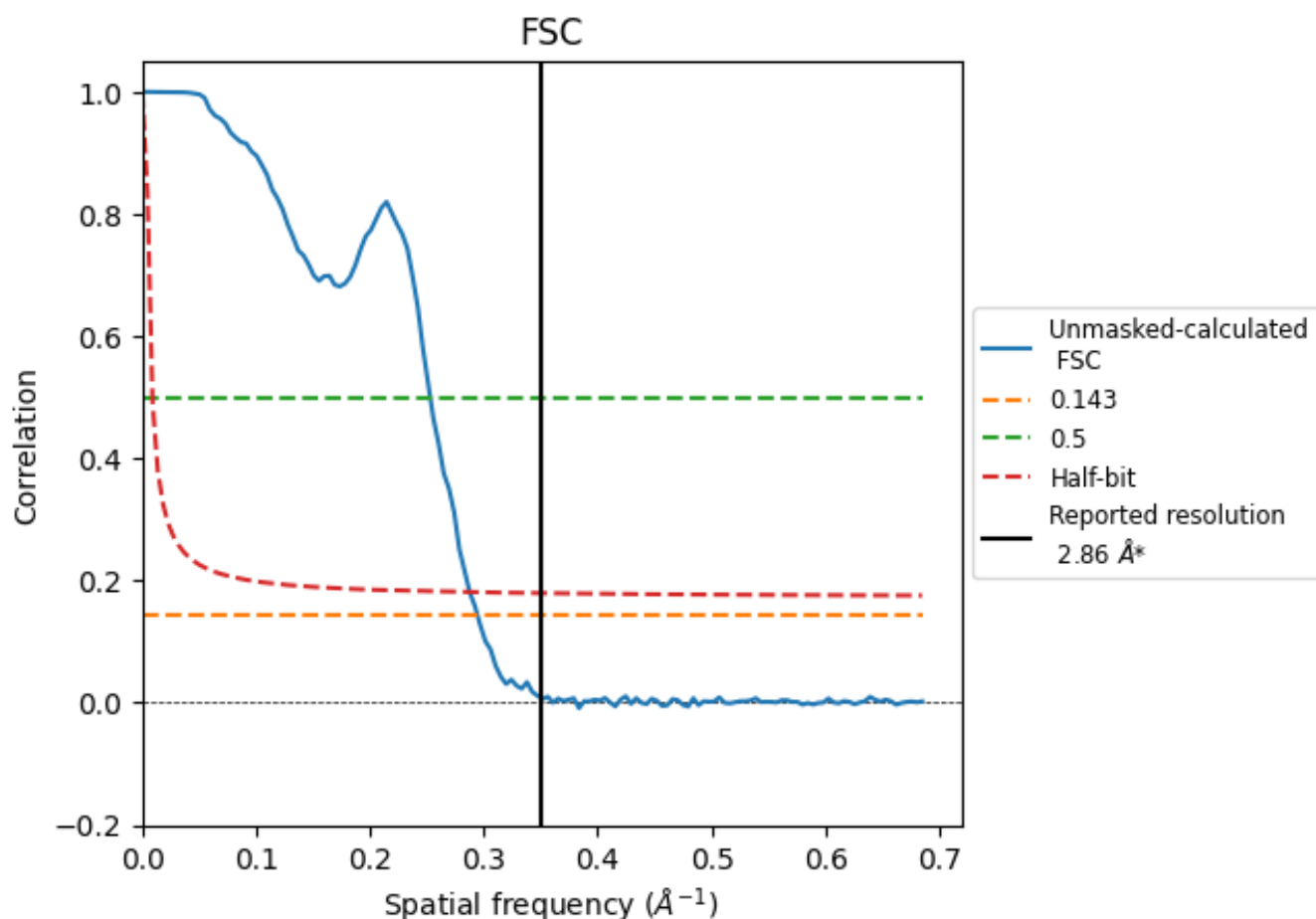


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 \AA^{-1}

8.2 Resolution estimates [i](#)

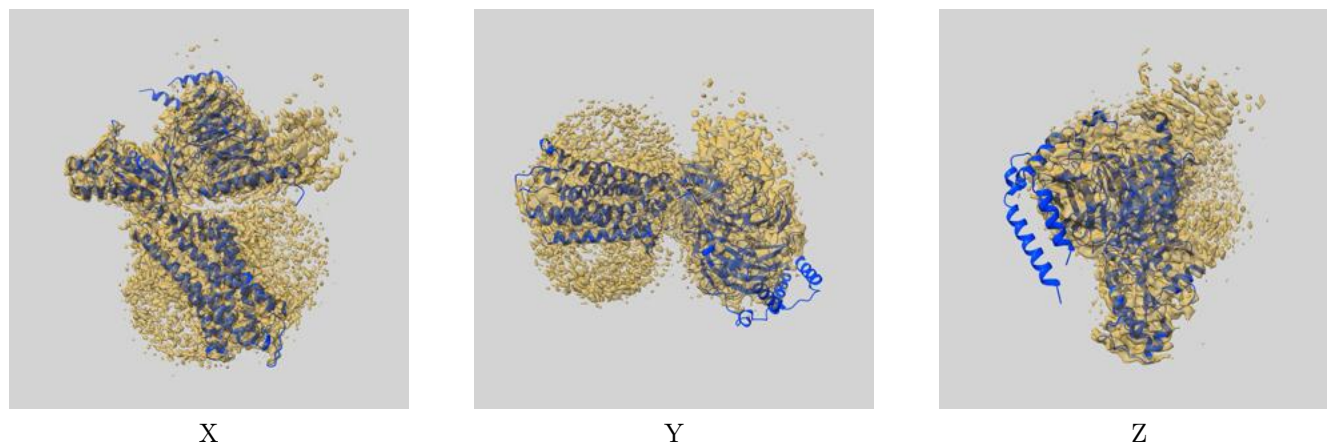
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	3.95	3.48

*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 3.40 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

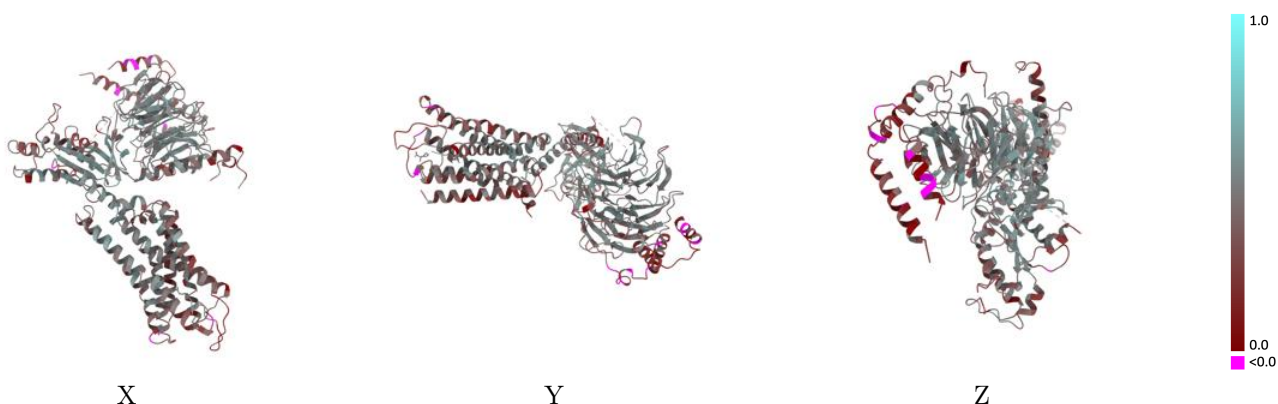
This section contains information regarding the fit between EMDB map EMD-68208 and PDB model 22EM. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.227 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](#)



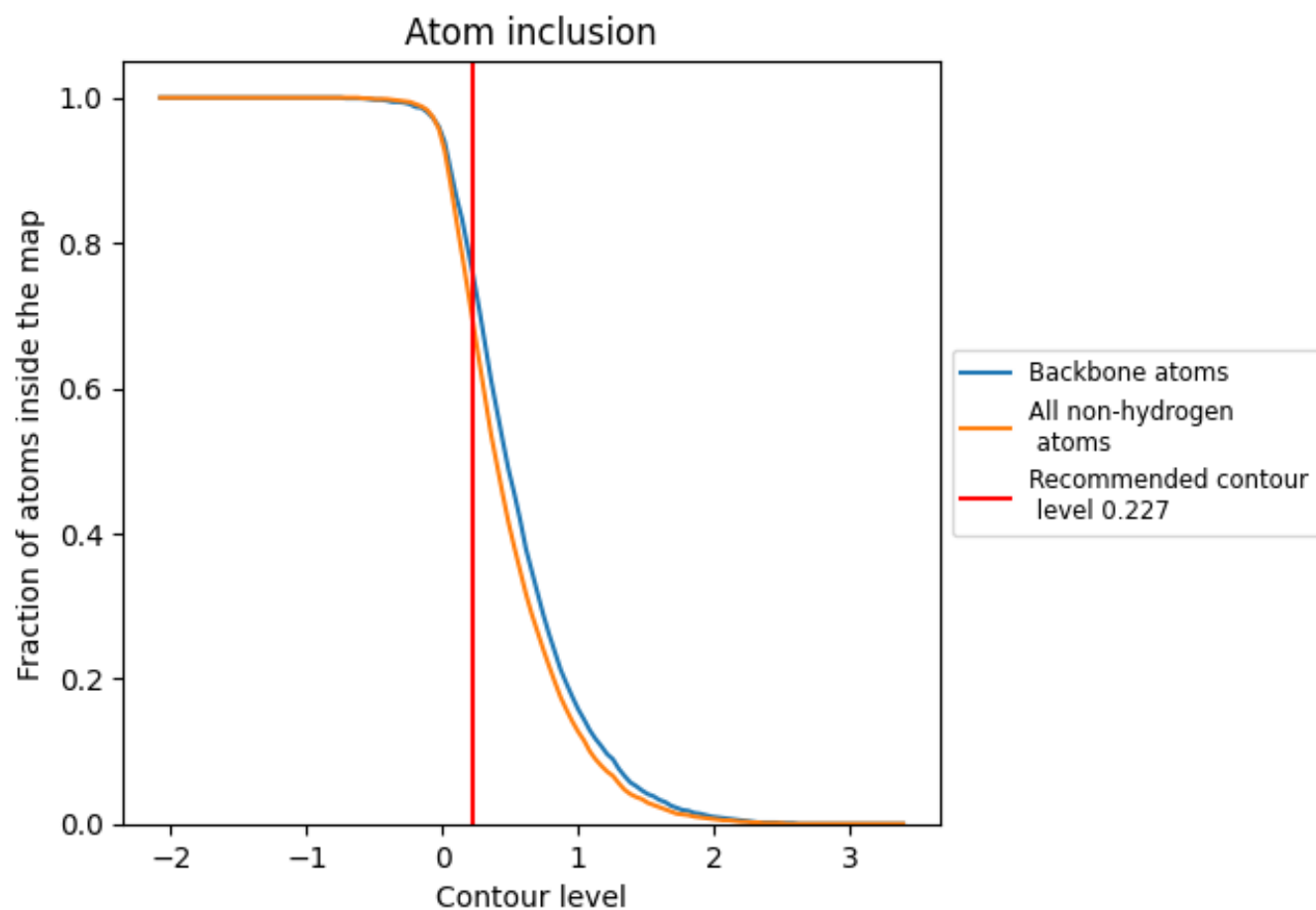
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.227).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 69% 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 (0.227) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6880	<div></div> 0.3980
A	<div></div> 0.9390	<div></div> 0.5390
B	<div></div> 0.7110	<div></div> 0.4170
C	<div></div> 0.7380	<div></div> 0.4300
D	<div></div> 0.2240	<div></div> 0.2200
F	<div></div> 0.6940	<div></div> 0.3780

