wwPDB EM Validation Summary Report (i)

Apr 14, 2025 – 04:10 pm BST

PDB ID	:	8QJ2 / pdb_00008qj2
EMDB ID	:	EMD-18442
Title	:	Structure of active state MC4R in complex with a potent ligand mimicking nanobody
Authors	:	Busch, A.; Jaakola, V.-P.; Masiulis, S.
Deposited on	:	2023-09-12
Resolution	:	3.40 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

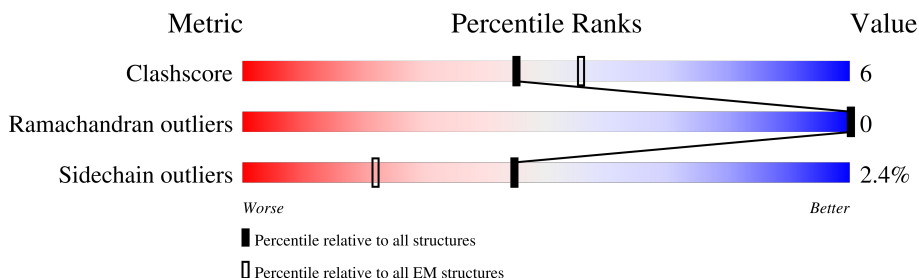|		
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.40 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		6
Ramachandran outliers		0
Sidechain outliers		2.4%

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	B	394	7% 48% 7% 44%
2	C	350	7% 77% 17% · 5%
3	G	71	14% 69% 7% 24%
4	N	138	8% 75% 15% · 9%
5	A	729	5% 28% 6% 66%
6	D	117	12% 62% 11% 27%

2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8108 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(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	219	Total 1781	C 1127	N 316	O 333	S 5	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	54	ASN	SER	engineered mutation	UNP P63092
B	226	ALA	GLY	engineered mutation	UNP P63092
B	268	ALA	GLU	engineered mutation	UNP P63092
B	271	LYS	ASN	engineered mutation	UNP P63092
B	274	ASP	LYS	engineered mutation	UNP P63092
B	280	LYS	ARG	engineered mutation	UNP P63092
B	284	ASP	THR	engineered mutation	UNP P63092
B	285	THR	ILE	engineered mutation	UNP P63092
B	366	SER	ALA	engineered mutation	UNP P63092

- 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	334	Total 2547	C 1575	N 452	O 499	S 21	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 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	G	54	Total 418	C 263	N 74	O 78	S 3	0	0

- Molecule 4 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	126	Total 922	C 578	N 160	O 178	S 6	0	0

- Molecule 5 is a protein called Soluble cytochrome b562,Melanocortin receptor 4,Red fluorescent protein drFP583.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	246	Total 1853	C 1234	N 284	O 312	S 23	0	0

There are 109 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-124	PHE	-	expression tag	UNP P0ABE7
A	-123	ALA	-	expression tag	UNP P0ABE7
A	-122	ASP	-	expression tag	UNP P0ABE7
A	-121	TYR	-	expression tag	UNP P0ABE7
A	-120	LYS	-	expression tag	UNP P0ABE7
A	-119	ASP	-	expression tag	UNP P0ABE7
A	-118	ASP	-	expression tag	UNP P0ABE7
A	-117	ASP	-	expression tag	UNP P0ABE7
A	-116	ASP	-	expression tag	UNP P0ABE7
A	-115	LYS	-	expression tag	UNP P0ABE7
A	-107	TRP	MET	engineered mutation	UNP P0ABE7
A	-12	ILE	HIS	engineered mutation	UNP P0ABE7
A	-8	LEU	-	linker	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	linker	UNP P0ABE7
A	-6	GLU	-	linker	UNP P0ABE7
A	-5	VAL	-	linker	UNP P0ABE7
A	-4	LEU	-	linker	UNP P0ABE7
A	-3	PHE	-	linker	UNP P0ABE7
A	-2	GLN	-	linker	UNP P0ABE7
A	-1	GLY	-	linker	UNP P0ABE7
A	0	PRO	-	linker	UNP P0ABE7
A	333	LEU	-	linker	UNP P32245
A	334	GLU	-	linker	UNP P32245
A	335	VAL	-	linker	UNP P32245
A	336	LEU	-	linker	UNP P32245
A	337	PHE	-	linker	UNP P32245
A	338	GLN	-	linker	UNP P32245
A	339	GLY	-	linker	UNP P32245
A	340	PRO	-	linker	UNP P32245
A	341	VAL	-	linker	UNP P32245
A	342	SER	-	linker	UNP P32245
A	343	LYS	-	linker	UNP P32245
A	344	GLY	-	linker	UNP P32245
A	345	GLU	-	linker	UNP P32245
A	346	GLU	-	linker	UNP P32245
A	347	ASP	-	linker	UNP P32245
A	348	ASN	-	linker	UNP P32245
A	349	MET	-	linker	UNP P32245
A	350	ALA	-	linker	UNP P32245
A	351	ILE	-	linker	UNP P32245
A	361	HIS	ARG	engineered mutation	UNP Q9U6Y8
A	365	SER	THR	engineered mutation	UNP Q9U6Y8
A	385	THR	HIS	engineered mutation	UNP Q9U6Y8
A	386	GLN	ASN	engineered mutation	UNP Q9U6Y8
A	388	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	410	MET	GLN	engineered mutation	UNP Q9U6Y8
A	415	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	427	LEU	LYS	engineered mutation	UNP Q9U6Y8
A	461	GLU	CYS	engineered mutation	UNP Q9U6Y8
A	468	LEU	PHE	engineered mutation	UNP Q9U6Y8
A	469	ARG	ILE	engineered mutation	UNP Q9U6Y8
A	471	THR	VAL	engineered mutation	UNP Q9U6Y8
A	491	SER	THR	engineered mutation	UNP Q9U6Y8
A	494	MET	LEU	engineered mutation	UNP Q9U6Y8
A	497	GLU	ARG	engineered mutation	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	500	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	506	LYS	HIS	engineered mutation	UNP Q9U6Y8
A	507	GLN	LYS	engineered mutation	UNP Q9U6Y8
A	508	ARG	ALA	engineered mutation	UNP Q9U6Y8
A	518	ASP	LEU	engineered mutation	UNP Q9U6Y8
A	519	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	521	VAL	PHE	engineered mutation	UNP Q9U6Y8
A	523	THR	SER	engineered mutation	UNP Q9U6Y8
A	524	THR	ILE	engineered mutation	UNP Q9U6Y8
A	526	LYS	MET	engineered mutation	UNP Q9U6Y8
A	536	ALA	TYR	engineered mutation	UNP Q9U6Y8
A	538	ASN	TYR	engineered mutation	UNP Q9U6Y8
A	540	ASN	ASP	engineered mutation	UNP Q9U6Y8
A	541	ILE	SER	engineered mutation	UNP Q9U6Y8
A	561	ALA	THR	engineered mutation	UNP Q9U6Y8
A	566	SER	-	expression tag	UNP Q9U6Y8
A	567	THR	-	expression tag	UNP Q9U6Y8
A	568	GLY	-	expression tag	UNP Q9U6Y8
A	569	GLY	-	expression tag	UNP Q9U6Y8
A	570	MET	-	expression tag	UNP Q9U6Y8
A	571	ASP	-	expression tag	UNP Q9U6Y8
A	572	GLU	-	expression tag	UNP Q9U6Y8
A	573	LEU	-	expression tag	UNP Q9U6Y8
A	574	TYR	-	expression tag	UNP Q9U6Y8
A	575	LYS	-	expression tag	UNP Q9U6Y8
A	576	HIS	-	expression tag	UNP Q9U6Y8
A	577	HIS	-	expression tag	UNP Q9U6Y8
A	578	HIS	-	expression tag	UNP Q9U6Y8
A	579	HIS	-	expression tag	UNP Q9U6Y8
A	580	HIS	-	expression tag	UNP Q9U6Y8
A	581	HIS	-	expression tag	UNP Q9U6Y8
A	582	HIS	-	expression tag	UNP Q9U6Y8
A	583	HIS	-	expression tag	UNP Q9U6Y8
A	584	HIS	-	expression tag	UNP Q9U6Y8
A	585	HIS	-	expression tag	UNP Q9U6Y8
A	586	GLY	-	expression tag	UNP Q9U6Y8
A	587	LEU	-	expression tag	UNP Q9U6Y8
A	588	ASN	-	expression tag	UNP Q9U6Y8
A	589	ASP	-	expression tag	UNP Q9U6Y8
A	590	ILE	-	expression tag	UNP Q9U6Y8
A	591	PHE	-	expression tag	UNP Q9U6Y8
A	592	GLU	-	expression tag	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	593	ALA	-	expression tag	UNP Q9U6Y8
A	594	GLN	-	expression tag	UNP Q9U6Y8
A	595	LYS	-	expression tag	UNP Q9U6Y8
A	596	ILE	-	expression tag	UNP Q9U6Y8
A	597	GLU	-	expression tag	UNP Q9U6Y8
A	598	TRP	-	expression tag	UNP Q9U6Y8
A	599	HIS	-	expression tag	UNP Q9U6Y8
A	600	GLU	-	expression tag	UNP Q9U6Y8
A	601	GLU	-	expression tag	UNP Q9U6Y8
A	602	PRO	-	expression tag	UNP Q9U6Y8
A	603	GLU	-	expression tag	UNP Q9U6Y8
A	604	ALA	-	expression tag	UNP Q9U6Y8

- Molecule 6 is a protein called pN162.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	85	587	369	109	106	3	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: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

14%

69% 7% 24%

MET ALA SER ASN THR ALA SER I9 A10 Q11 M21 D26 R27 D36 I37 M38 K46 L51 T52 A56 S57 E58 N59 P60 F61 R62 GLU LYS PHE CYS ALA ILE LEU

• Molecule 4: Nanobody-35

Chain N:

8%

75% 15% • 9%

Q1 V2 Q3 G9 G10 L11 V12 Q13 G16 S17 L18 C22 F27 T28 F29 M34 N35 W36 W47 D50 I51 S52 S57 Y60 V64 T69 I70 S71 R72 D73 L79 Y80 L81 N84 T91 Y94 R98 T113 T114 G121 V124

T125 V126 SER HIS HIS HIS HIS HIS GLU PRO GLU ALA

• Molecule 5: Soluble cytochrome b562,Melanocortin receptor 4,Red fluorescent protein drFP583

Chain A:

5%

28% 6% 66%

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

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

LEU PHE GLN GLY PRO MET VAL ASN SER THR HIS ARG GLY MET HIS THR SER LEU HIS LEU TRP ASN ARG SER SER TYR ARG LEU HIS SER ASN ALA SER GLU SER LEU GLY LYS GLY TYR SER ASP GLY G39 L44 E49 V50 F51 V52 T53 L54 G55 S58 L59 L60 E61 N62

I63 L64 V65 I66 V67 A68 I69 A70 K71 N72 LYS ASN L75 M79 Y80 F81 C84 V88 M91 S94 V95 S96 N97 G98 S99 I102 L106 LEU ASN SER THR ASP THR ALA GLN SER PHE THR VAL N120 I125 D126 S127 V128 I129 L133 L141 I160

M161 R165 I169 F184 I185 I186 Y187 S188 I198 M204 L207 Y212 A219 I223 I226 ALA VAL LEU PRO GLY THR GLY ALA ILE ARG GLN GLY ALA N240 G243 L247 V253 W258 L265 I266 C271 N274 P275 Y276 C277 V278 C279

S282 H283 L286 I289 I297 D298 A303 S306 Q307 E308 L309 R310 K311 T312 PHE LYS GLU ILE ILE CYS CYS TYR PRO LEU GLY GLY LEU CYS ASP LEU SER SER ARG TYR LEU GLU VAL LEU PHE GLN GLY VAL PRO VAL SER LYS GLY GLU GLU ASP ASN MET ALA ILE ILE LYS

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

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

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

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

GLN LYS ILE GLU TRP HIS GLU GLU PRO GLU ALA

• Molecule 6: pN162

Chain D:

12%

62%   11%   27%

GLN V2 Q3 S7 GLY GLY GLY LEU VAL GLN PRO GLY GLY SER LEU R19 A24 S25 G26 T40 P41 G42 R45 A46 D54 C55 N58 Y59 ALA ASP SER ALA LYS GLY ARG PHE T68 I69 S70 K75 N76 T77 V78 H79 L80 Q81 M82 ASP SER LEU LYS PRO GLU

D89 T90 Y93 V103 R104 P105 Q111 GLY THR GLN VAL THR VAL

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219891	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	30.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.837	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	256.5, 256.5, 256.5	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.425, 1.425, 1.425	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	B	0.25	0/1815	0.48	0/2447
2	C	0.25	0/2593	0.50	0/3518
3	G	0.25	0/424	0.45	0/572
4	N	0.27	0/942	0.51	0/1282
5	A	0.26	0/1888	0.42	0/2573
6	D	0.25	0/596	0.52	0/813
All	All	0.26	0/8258	0.48	0/11205

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	B	1781	0	1722	19	0
2	C	2547	0	2434	38	0
3	G	418	0	431	4	0
4	N	922	0	862	14	0
5	A	1853	0	1899	29	0
6	D	587	0	498	7	0
All	All	8108	0	7846	98	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 6.

The worst 5 of 98 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:C:201:SER:HG	2:C:211:TRP:HE1	1.29	0.80
6:D:24:ALA:HB3	6:D:76:ASN:HB3	1.66	0.78
1:B:232:ARG:NH1	2:C:204:CYS:SG	2.58	0.76
1:B:207:ILE:HD11	1:B:222:PHE:HB3	1.71	0.72
5:A:44:LEU:HD12	5:A:283:HIS:HD2	1.58	0.67

There are no symmetry-related clashes.

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	211/394 (54%)	194 (92%)	17 (8%)	0	100	100
2	C	330/350 (94%)	310 (94%)	20 (6%)	0	100	100
3	G	52/71 (73%)	48 (92%)	4 (8%)	0	100	100
4	N	124/138 (90%)	116 (94%)	8 (6%)	0	100	100
5	A	238/729 (33%)	227 (95%)	11 (5%)	0	100	100
6	D	77/117 (66%)	62 (80%)	15 (20%)	0	100	100
All	All	1032/1799 (57%)	957 (93%)	75 (7%)	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	189/350 (54%)	185 (98%)	4 (2%)	48	69
2	C	273/291 (94%)	263 (96%)	10 (4%)	29	54
3	G	44/58 (76%)	43 (98%)	1 (2%)	45	67
4	N	94/115 (82%)	93 (99%)	1 (1%)	70	81
5	A	205/629 (33%)	202 (98%)	3 (2%)	60	76
6	D	46/94 (49%)	45 (98%)	1 (2%)	47	68
All	All	851/1537 (55%)	831 (98%)	20 (2%)	45	66

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	59	ASN
5	A	265	LEU
6	D	40	THR
5	A	283	HIS
2	C	119	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	N	39	GLN
5	A	283	HIS
5	A	285	ASN
2	C	44	GLN
1	B	239	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-18442. 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 ⓘ
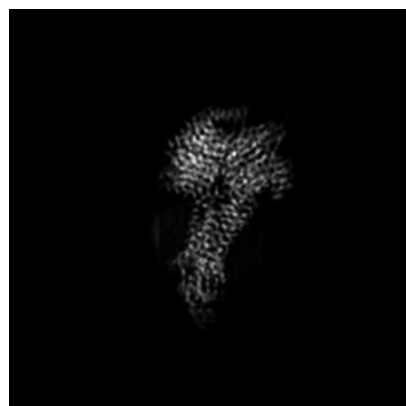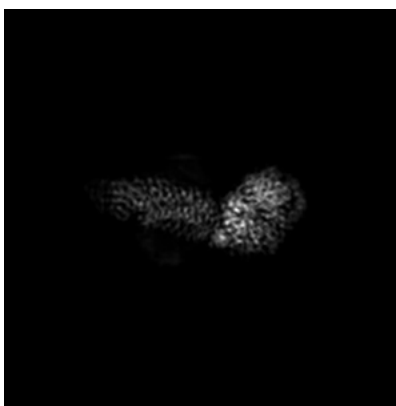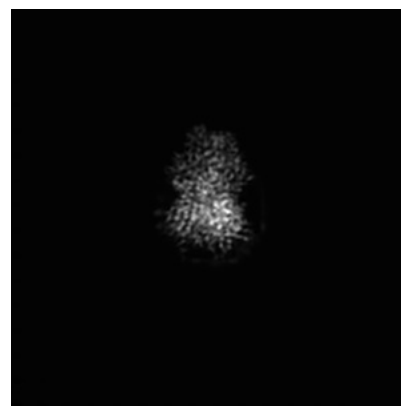
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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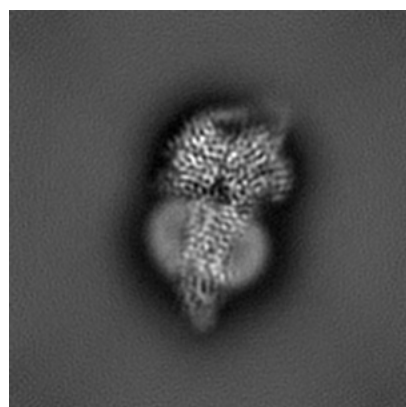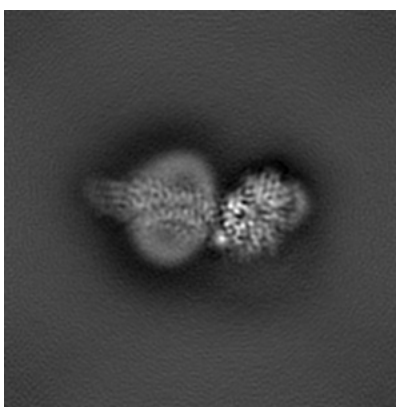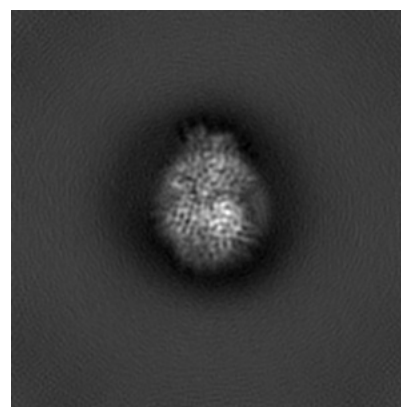
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ

6.2.1   Primary map

X Index: 90   Y Index: 90   Z Index: 90

6.2.2   Raw map
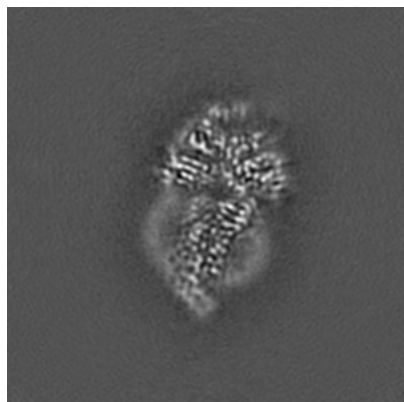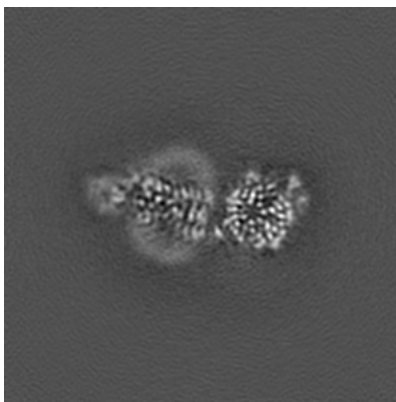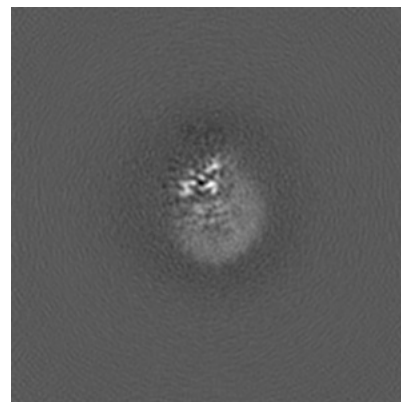
X Index: 90   Y Index: 90   Z Index: 90

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: 92   Y Index: 85   Z Index: 111

6.3.2 Raw map
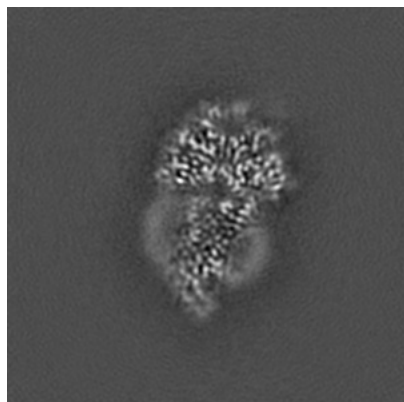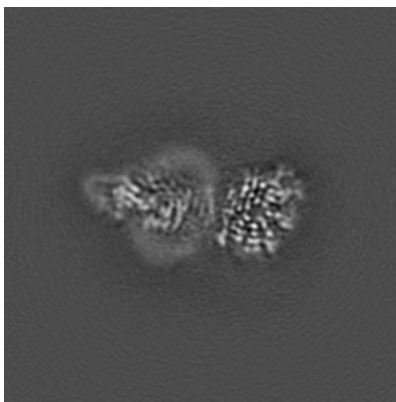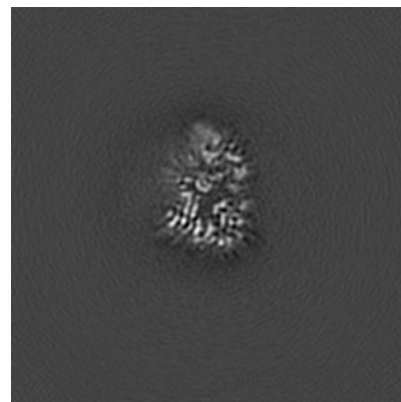
X Index: 91   Y Index: 85   Z Index: 111

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
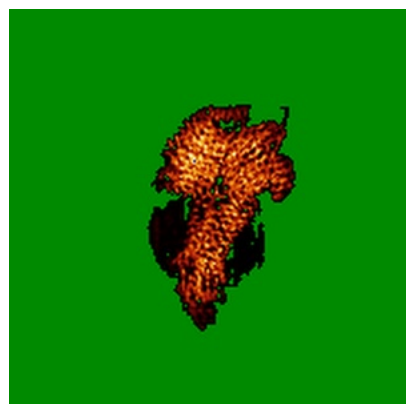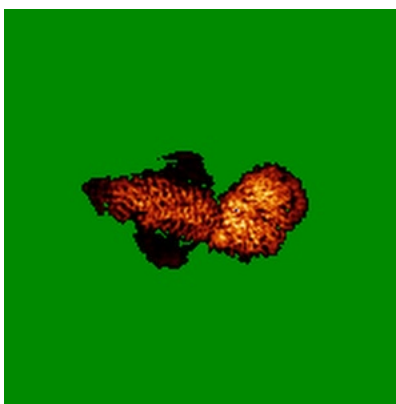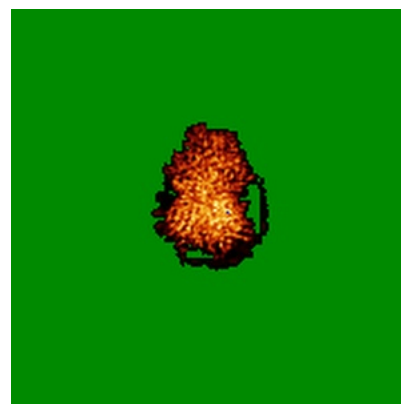
| X | Y | Z |

6.4.2 Raw map

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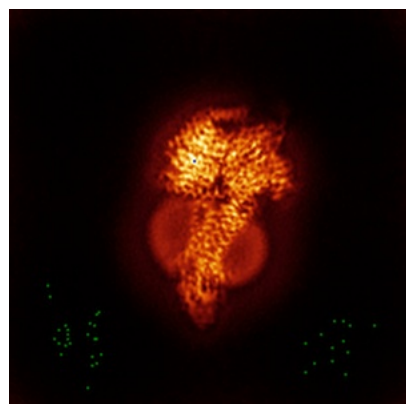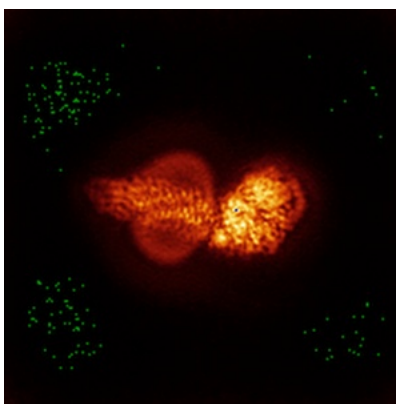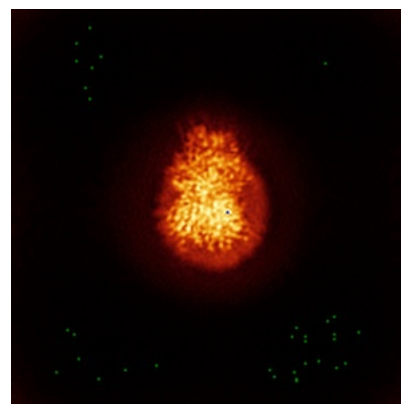
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views   ⓘ

6.5.1   Primary map

X   Y   Z
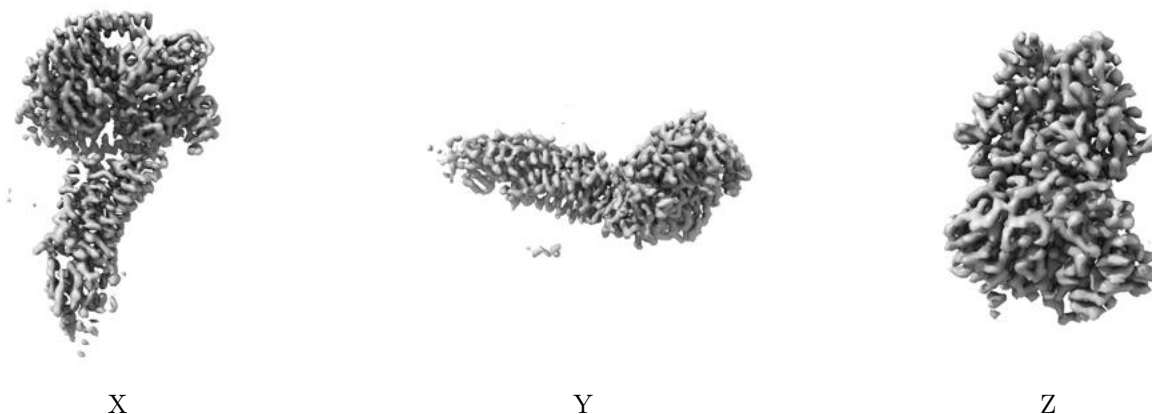
The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2   Raw map

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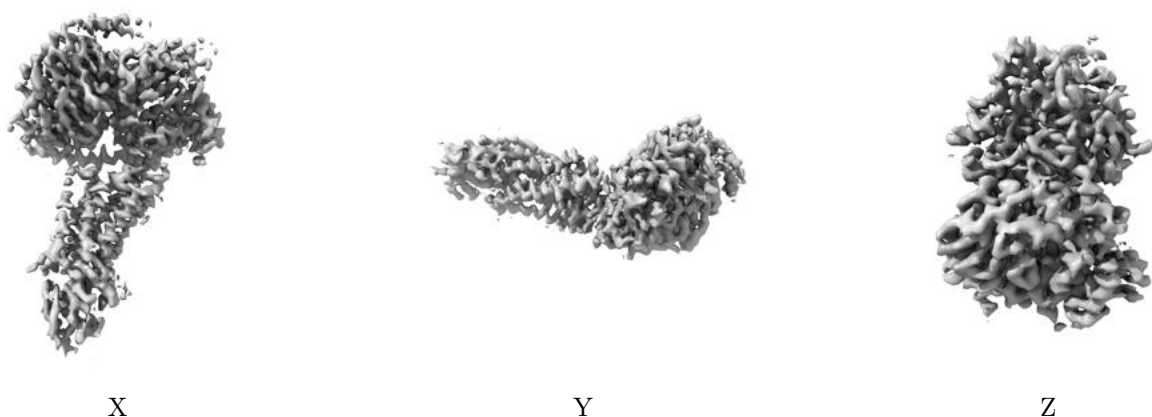
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6   Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1   emd_18442_msk_1.map ⓘ

X   Y   Z
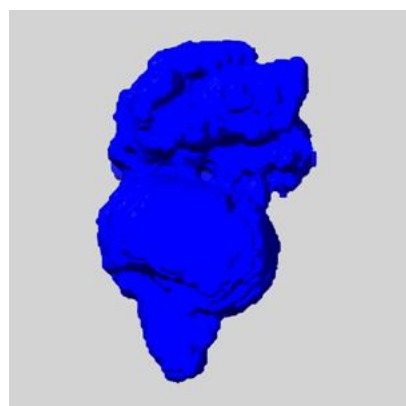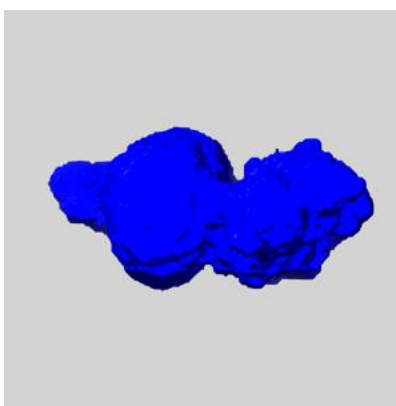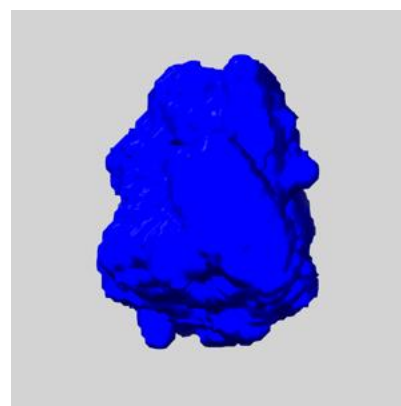
7 Map analysis ⓘ

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 ⓘ
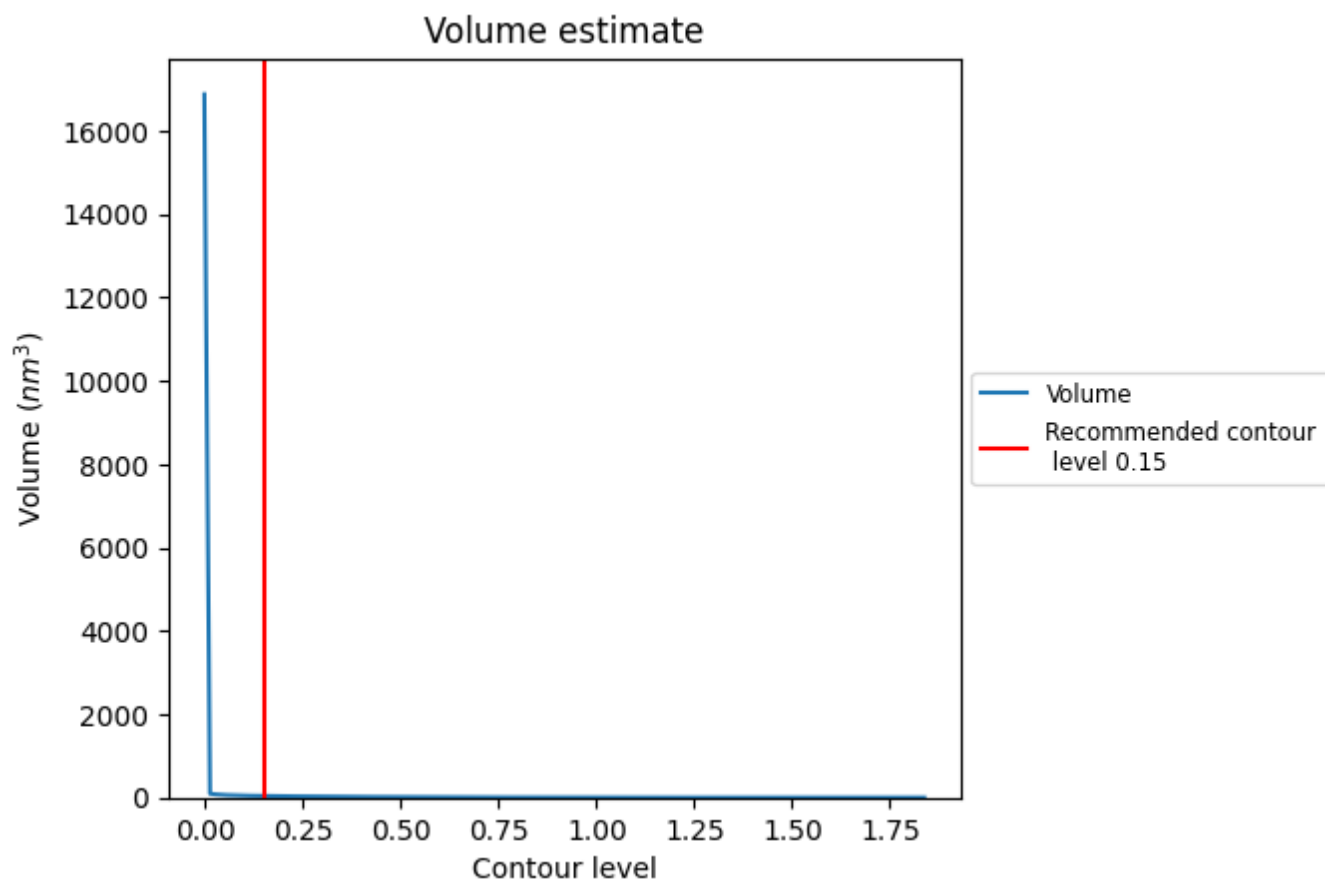
The volume at the recommended contour level is 38 nm^3; this corresponds to an approximate mass of 35 kDa.

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   ⓘ
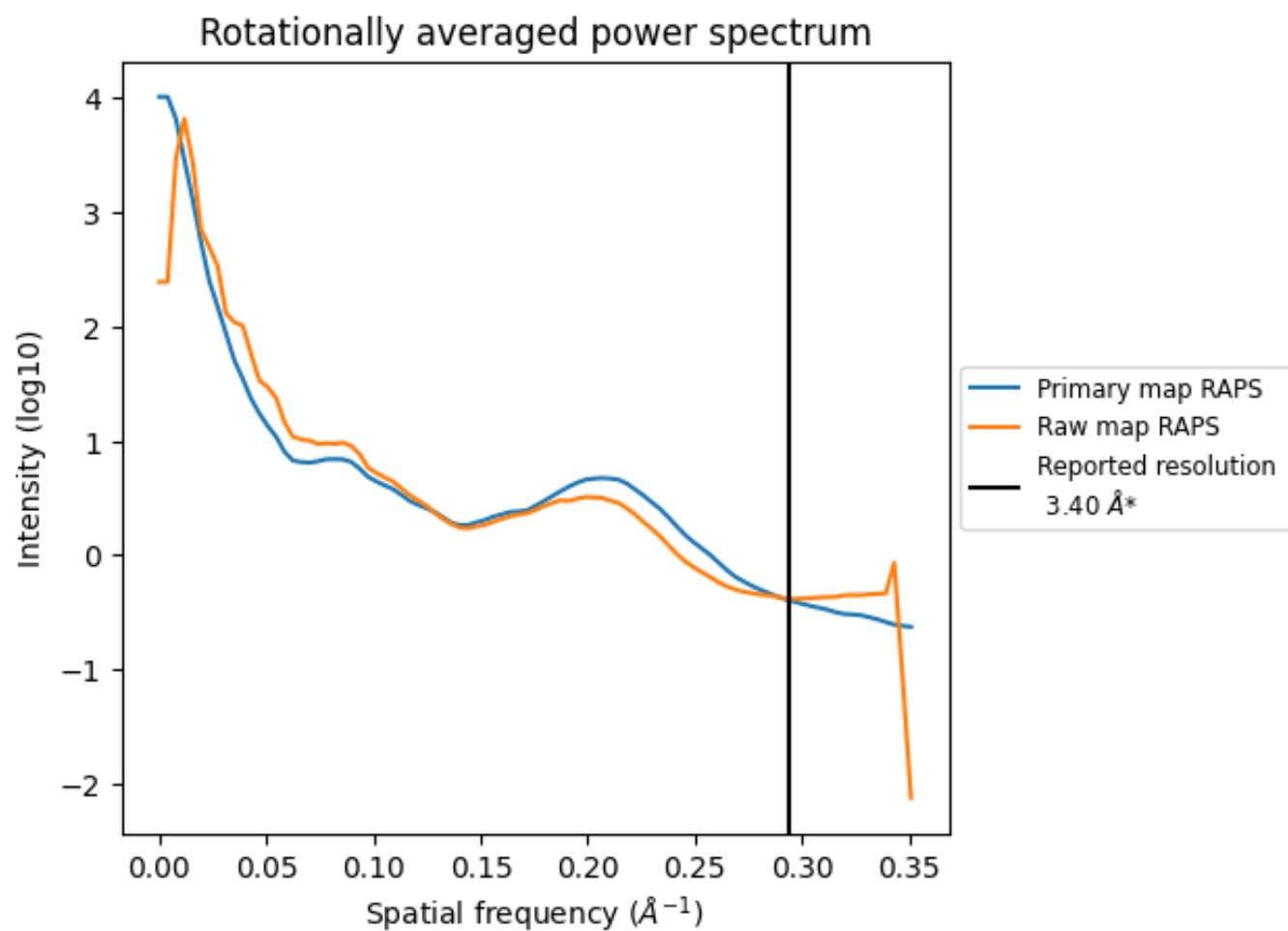
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
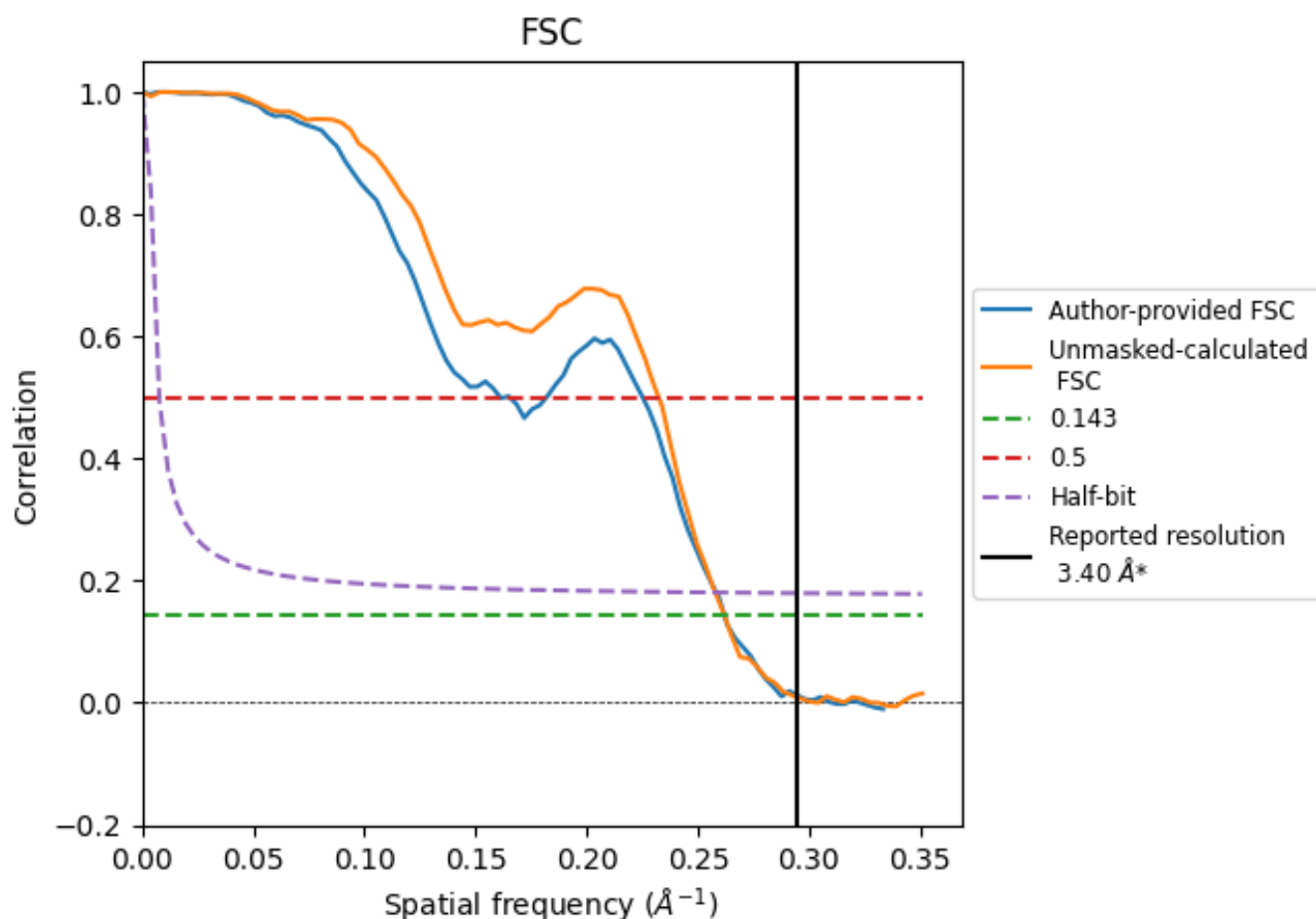
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.82	6.21	3.87
Unmasked-calculated*	3.82	4.30	3.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.4 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-18442 and PDB model 8QJ2. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ
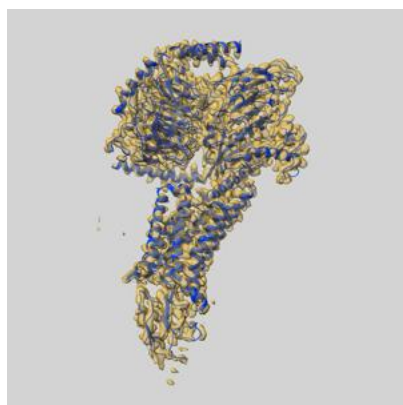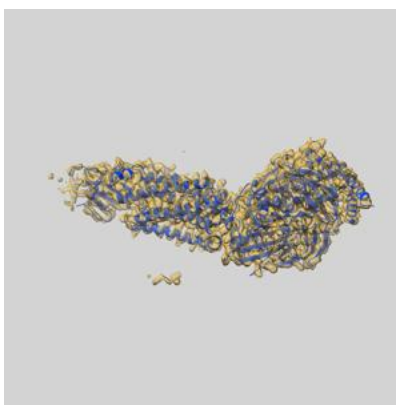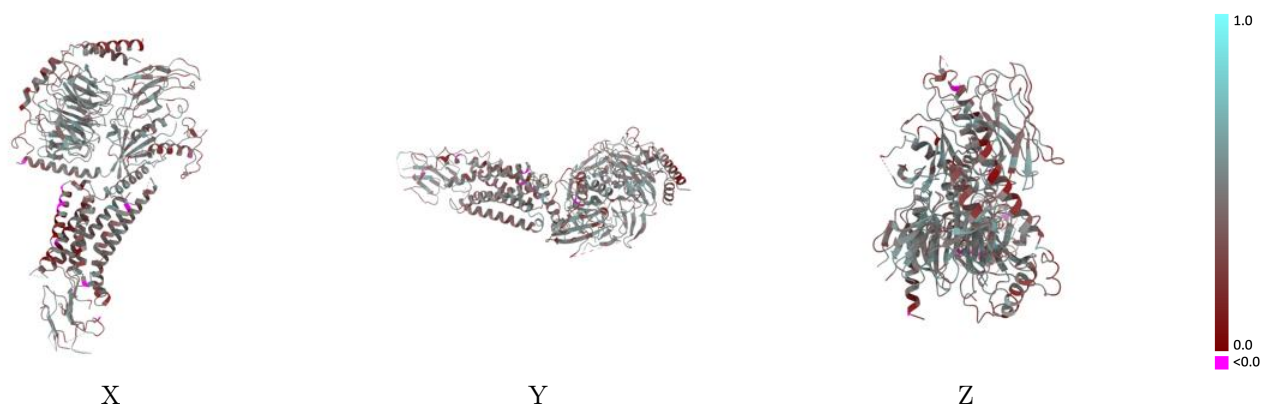

|		
X	Y	Z
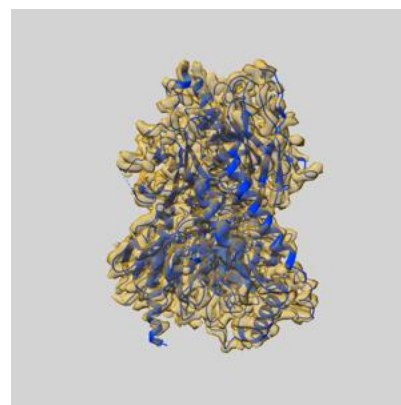
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model　ⓘ


X　　　　　　　　　　　Y　　　　　　　　　　　Z

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　ⓘ

X　　　　　　　　　　　Y　　　　　　　　　　　Z
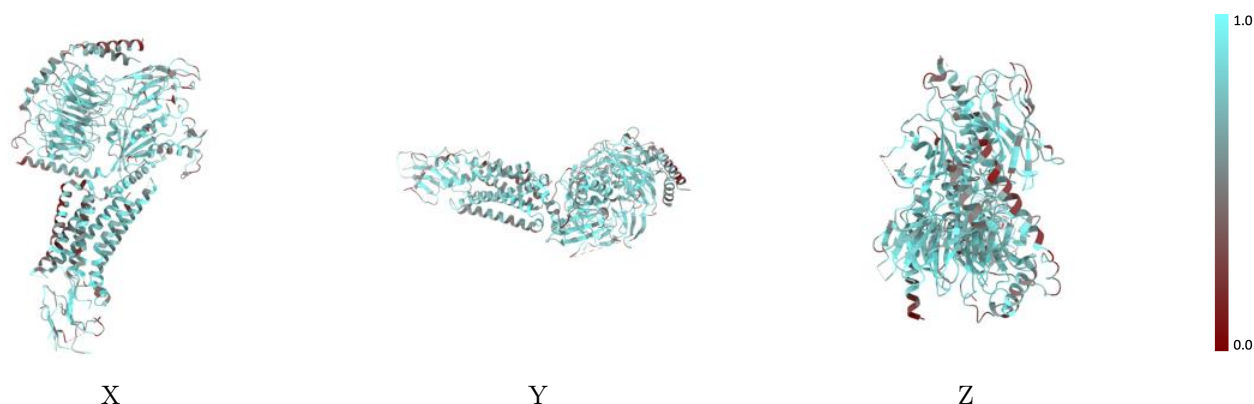
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4   Atom inclusion (i)
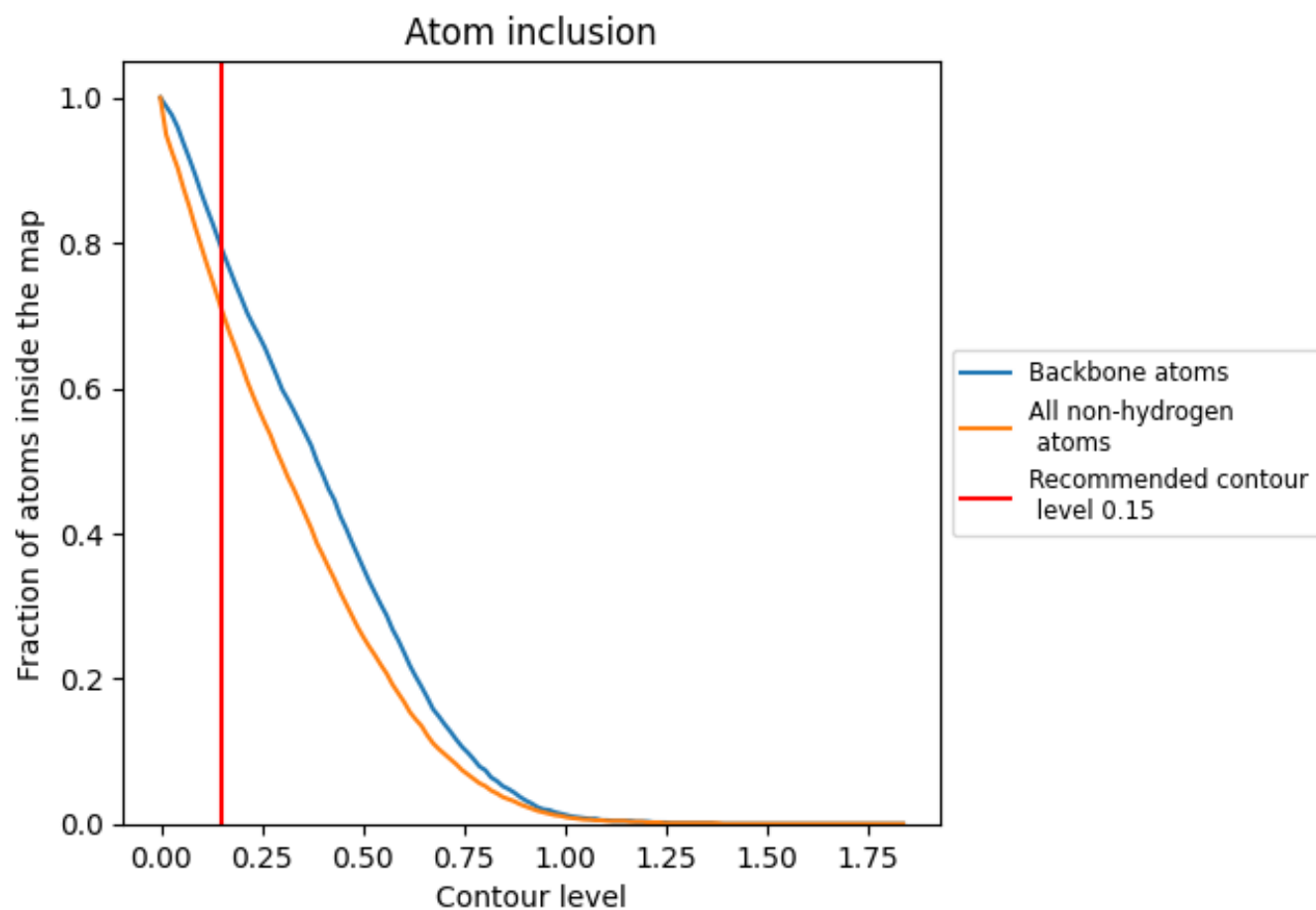
At the recommended contour level, 79% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.4310
A	0.6790	0.3790
B	0.7200	0.4370
C	0.7490	0.4690
D	0.6680	0.4340
G	0.5740	0.3650
N	0.7200	0.4440

1.0

0.0
<0.0