Full wwPDB EM Validation Report ⓘ

Apr 14, 2025 – 04:11 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)

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:

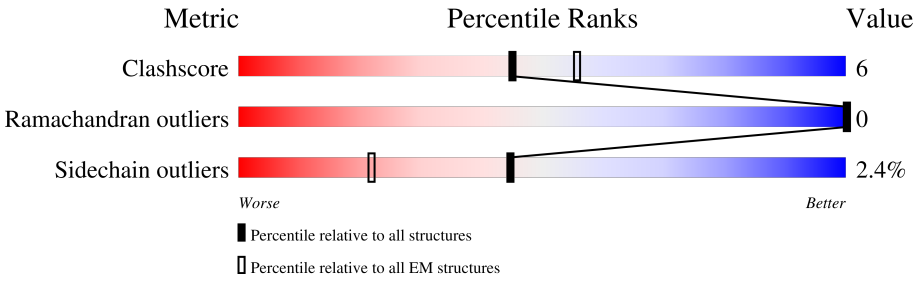
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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	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 (i)

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
			Total	C	N	O	S		
1	B	219	1781	1127	316	333	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
			Total	C	N	O	S		
2	C	334	2547	1575	452	499	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	C	N	O	S	0	0
			418	263	74	78	3		

- Molecule 4 is a protein called Nanobody-35.

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

- 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	C	N	O	S	0	0
			1853	1234	284	312	23		

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.

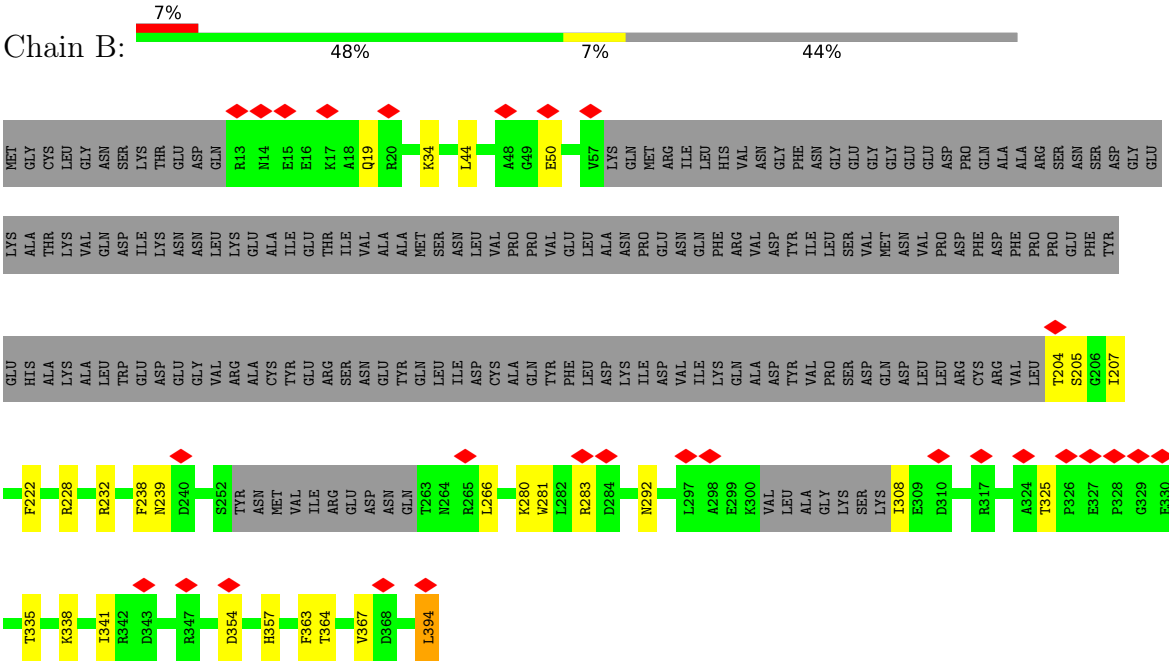
Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	85	Total	C	N	O	S	0	0
			587	369	109	106	3		

3 Residue-property plots (i)

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.

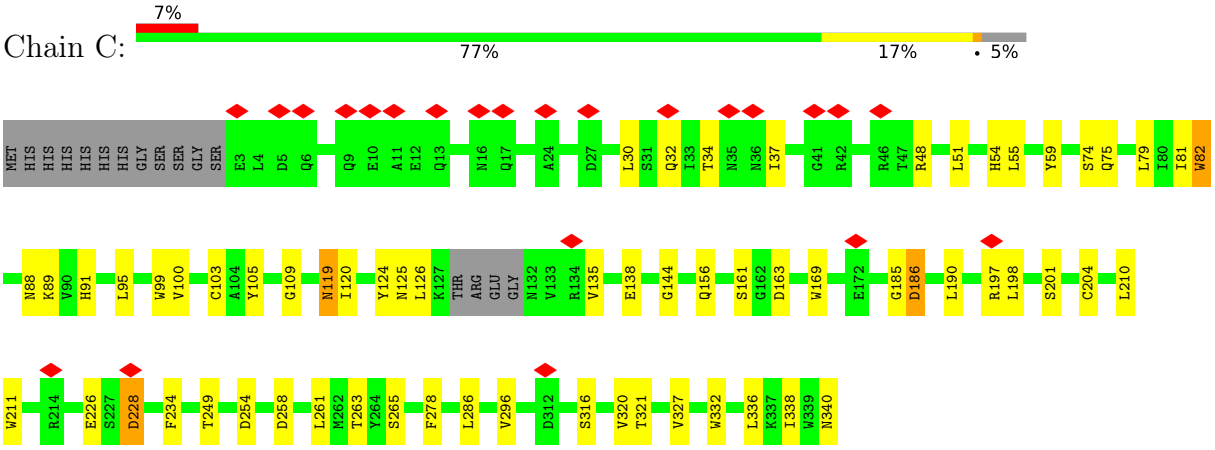
• Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain B:



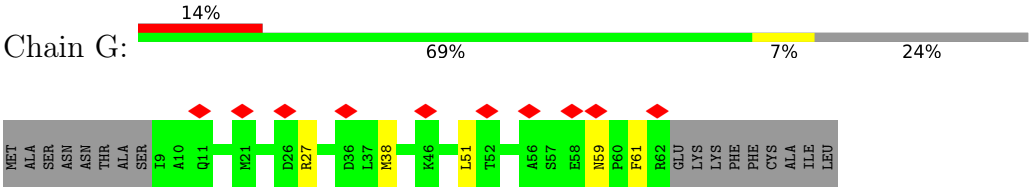
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain C:



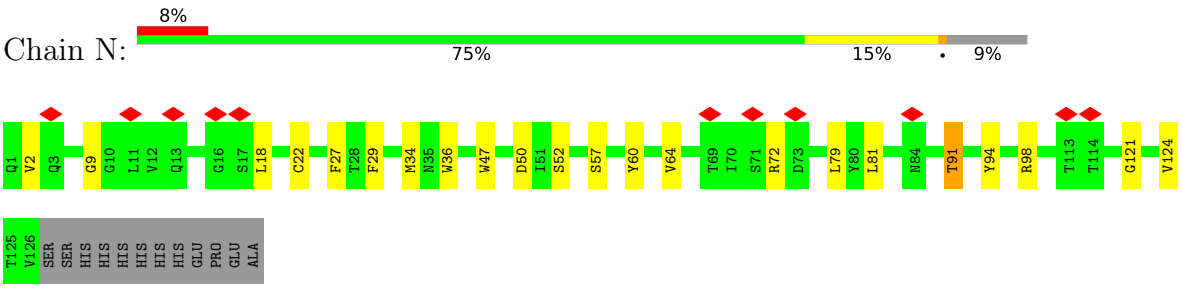
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



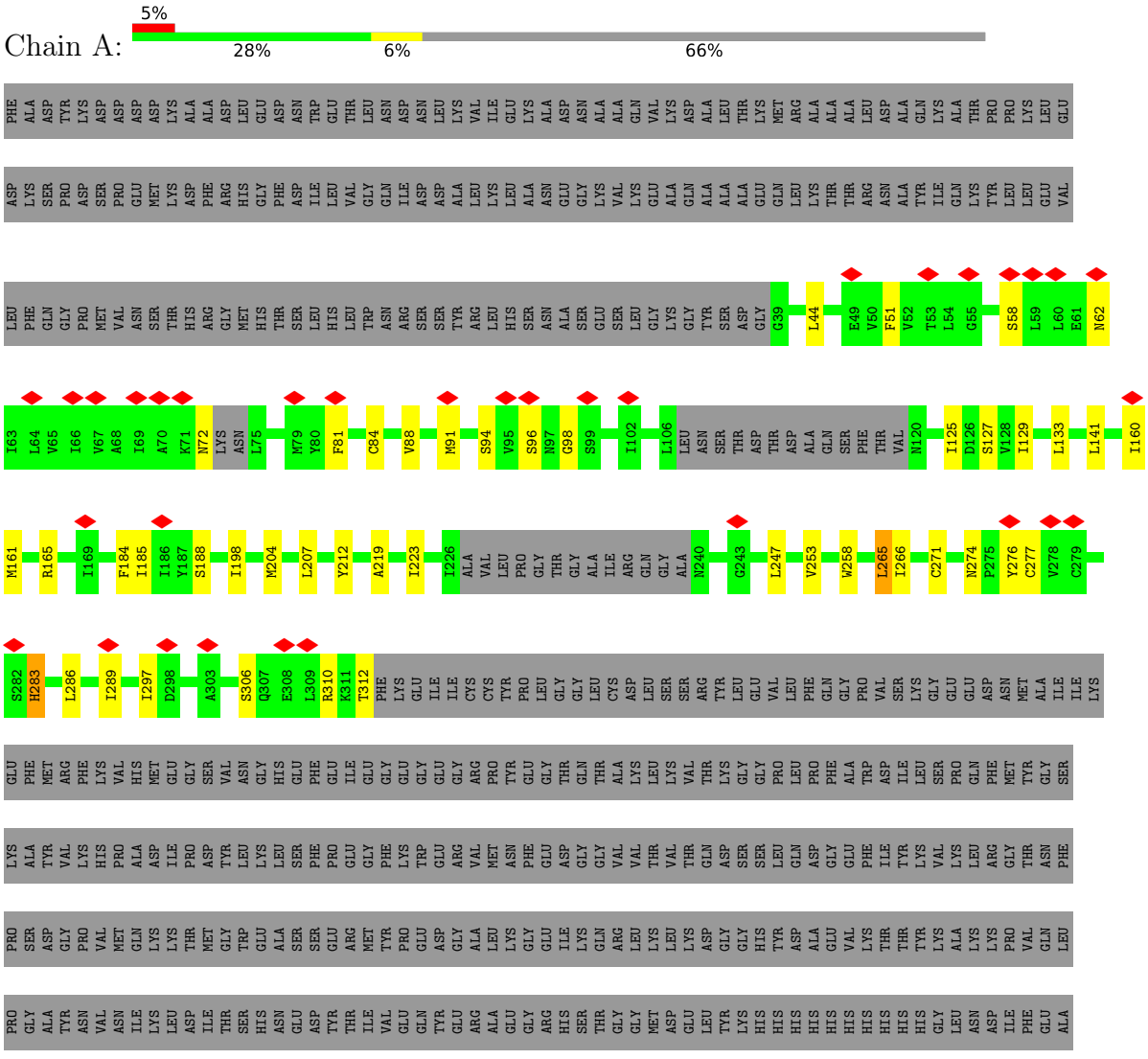
• Molecule 4: Nanobody-35

Chain N:



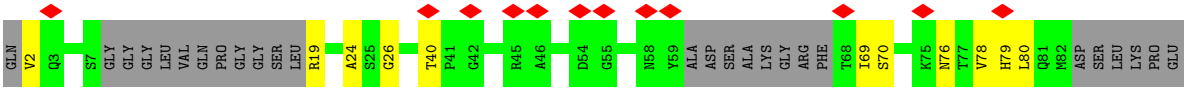
• Molecule 5: Soluble cytochrome b562,Melanocortin receptor 4,Red fluorescent protein drFP583

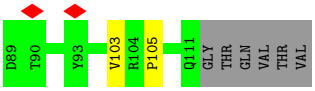
Chain A:



• Molecule 6: pN162

Chain D:





4 Experimental information (i)

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 ($e^-/Å^2$)	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.

All (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
6:D:70:SER:HB3	6:D:79:HIS:HB2	1.76	0.67
5:A:129:ILE:HG23	6:D:103:VAL:HG21	1.78	0.66
1:B:308:ILE:HD11	1:B:341:ILE:HD11	1.79	0.64
4:N:9:GLY:HA2	4:N:18:LEU:HD13	1.81	0.63
6:D:2:VAL:HG13	6:D:26:GLY:HA3	1.81	0.63
2:C:82:TRP:HE1	2:C:89:LYS:HG2	1.64	0.62
2:C:186:ASP:N	2:C:186:ASP:OD1	2.31	0.62
1:B:239:ASN:ND2	1:B:281:TRP:O	2.34	0.61
4:N:94:TYR:O	4:N:121:GLY:HA3	2.02	0.60
5:A:184:PHE:O	5:A:188:SER:OG	2.20	0.59
4:N:34:MET:HB3	4:N:79:LEU:HD11	1.86	0.58
5:A:160:ILE:HG13	5:A:161:MET:HG2	1.86	0.58
2:C:320:VAL:HG22	2:C:327:VAL:HG22	1.85	0.58
5:A:198:ILE:HD13	5:A:266:ILE:HG12	1.85	0.58
5:A:58:SER:O	5:A:62:ASN:ND2	2.38	0.57
2:C:197:ARG:HB3	2:C:198:LEU:HD12	1.86	0.57
2:C:95:LEU:HD13	2:C:100:VAL:HG21	1.85	0.56
2:C:34:THR:HG23	2:C:37:ILE:HD12	1.88	0.56
5:A:51:PHE:HE1	5:A:289:ILE:HG22	1.71	0.56
2:C:51:LEU:HB2	2:C:336:LEU:HB2	1.88	0.56
5:A:94:SER:O	5:A:98:GLY:N	2.38	0.56
2:C:48:ARG:HE	2:C:340:ASN:HB3	1.71	0.55
2:C:258:ASP:HB3	3:G:27:ARG:HD3	1.87	0.55
2:C:105:TYR:HE1	2:C:109:GLY:HA2	1.71	0.55
3:G:51:LEU:H	3:G:51:LEU:HD23	1.71	0.55
2:C:249:THR:HG22	2:C:265:SER:HB3	1.87	0.55
2:C:286:LEU:HG	2:C:296:VAL:HG22	1.89	0.55
5:A:274:ASN:O	5:A:276:TYR:N	2.41	0.54
2:C:119:ASN:ND2	2:C:144:GLY:O	2.40	0.54
5:A:127:SER:HB2	5:A:185:ILE:HG21	1.89	0.53
4:N:22:CYS:HB3	4:N:79:LEU:HB2	1.91	0.53
1:B:19:GLN:OE1	2:C:88:ASN:ND2	2.36	0.52
4:N:52:SER:HB2	4:N:57:SER:HB2	1.90	0.52
5:A:274:ASN:O	5:A:277:CYS:N	2.41	0.51
2:C:228:ASP:N	2:C:228:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:125:ILE:O	5:A:129:ILE:HG22	2.11	0.51
6:D:19:ARG:N	6:D:80:LEU:O	2.44	0.51
4:N:94:TYR:O	4:N:121:GLY:CA	2.59	0.50
2:C:125:ASN:OD1	2:C:126:LEU:N	2.43	0.50
6:D:69:ILE:HD11	6:D:78:VAL:HG13	1.93	0.50
1:B:394:LEU:HD22	5:A:223:ILE:HD11	1.94	0.49
5:A:253:VAL:HG21	5:A:297:ILE:HG21	1.94	0.49
5:A:265:LEU:HG	6:D:105:PRO:HG3	1.94	0.49
4:N:2:VAL:HG11	4:N:98:ARG:HH12	1.77	0.49
2:C:198:LEU:HD23	2:C:210:LEU:HD21	1.93	0.49
4:N:29:PHE:O	4:N:72:ARG:NH1	2.45	0.49
5:A:160:ILE:O	5:A:165:ARG:NH1	2.46	0.48
2:C:124:TYR:HE1	2:C:135:VAL:HG22	1.78	0.48
4:N:91:THR:HA	4:N:124:VAL:O	2.14	0.47
2:C:124:TYR:CE1	2:C:135:VAL:HG22	2.49	0.47
5:A:141:LEU:HD22	5:A:204:MET:HG3	1.95	0.47
1:B:338:LYS:HB3	1:B:363:PHE:HE1	1.81	0.46
2:C:161:SER:OG	2:C:163:ASP:OD1	2.24	0.46
2:C:82:TRP:NE1	2:C:89:LYS:HG2	2.31	0.46
2:C:316:SER:HB3	2:C:332:TRP:CD1	2.50	0.46
5:A:286:LEU:O	5:A:289:ILE:HG12	2.15	0.46
1:B:325:THR:HG22	1:B:335:THR:HG21	1.98	0.46
4:N:36:TRP:CD2	4:N:81:LEU:HD22	2.51	0.46
2:C:81:ILE:HB	2:C:91:HIS:HB2	1.98	0.46
5:A:88:VAL:O	5:A:91:MET:HG2	2.16	0.46
2:C:120:ILE:HD11	2:C:138:GLU:HB3	1.97	0.46
1:B:228:ARG:HH12	2:C:185:GLY:HA2	1.80	0.45
4:N:60:TYR:HB3	4:N:64:VAL:HG23	1.99	0.45
1:B:283:ARG:HD3	1:B:354:ASP:HB2	1.98	0.45
5:A:212:TYR:HB3	5:A:247:LEU:HD13	1.99	0.45
2:C:30:LEU:C	2:C:32:GLN:H	2.18	0.45
5:A:81:PHE:O	5:A:84:CYS:HB2	2.17	0.45
2:C:226:GLU:HG2	4:N:27:PHE:HB3	1.98	0.45
2:C:226:GLU:O	4:N:98:ARG:NH2	2.50	0.44
1:B:338:LYS:HB3	1:B:363:PHE:CE1	2.52	0.44
2:C:75:GLN:HE21	2:C:99:TRP:HE3	1.66	0.44
2:C:156:GLN:HA	2:C:169:TRP:O	2.18	0.43
1:B:34:LYS:HA	2:C:55:LEU:HD21	2.00	0.43
2:C:254:ASP:HB2	2:C:261:LEU:HD11	1.99	0.43
4:N:47:TRP:HZ2	4:N:50:ASP:HB2	1.83	0.43
5:A:96:SER:HB3	5:A:129:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASN:HA	1:B:364:THR:O	2.19	0.43
2:C:37:ILE:HD11	3:G:38:MET:SD	2.58	0.43
1:B:50:GLU:HB3	1:B:292:ASN:ND2	2.33	0.42
5:A:62:ASN:HB2	5:A:91:MET:HB3	2.02	0.42
5:A:306:SER:O	5:A:310:ARG:HG3	2.20	0.42
1:B:394:LEU:C	5:A:219:ALA:HB1	2.40	0.42
2:C:54:HIS:ND1	2:C:74:SER:HB2	2.35	0.41
1:B:204:THR:OG1	1:B:205:SER:N	2.51	0.41
1:B:266:LEU:HD23	1:B:266:LEU:HA	1.91	0.41
2:C:79:LEU:HD11	2:C:103:CYS:SG	2.61	0.41
5:A:271:CYS:HB2	5:A:274:ASN:HB2	2.01	0.41
5:A:72:ASN:OD1	5:A:312:THR:OG1	2.38	0.41
2:C:338:ILE:HG21	3:G:61:PHE:CE2	2.56	0.40
5:A:133:LEU:HD22	5:A:258:TRP:CH2	2.56	0.40
5:A:271:CYS:HB2	5:A:274:ASN:CB	2.52	0.40
1:B:280:LYS:HA	1:B:283:ARG:HH12	1.86	0.40
1:B:44:LEU:HD22	1:B:238:PHE:CG	2.57	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	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

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	331	ASP
1	B	357	HIS
1	B	367	VAL
1	B	394	LEU
2	C	59	TYR
2	C	82	TRP
2	C	119	ASN
2	C	186	ASP
2	C	190	LEU
2	C	228	ASP
2	C	234	PHE
2	C	263	THR
2	C	278	PHE
2	C	321	THR
3	G	59	ASN
4	N	91	THR
5	A	207	LEU
5	A	265	LEU
5	A	283	HIS

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Mol	Chain	Res	Type
6	D	40	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	ASN
2	C	44	GLN
2	C	220	GLN
4	N	39	GLN
5	A	283	HIS
5	A	285	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

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

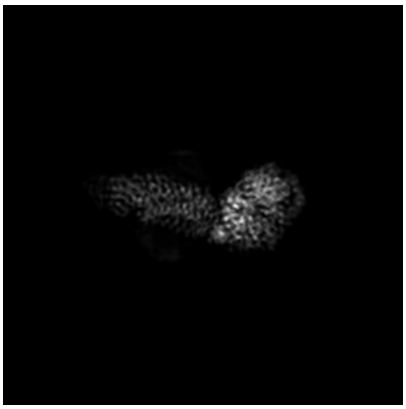
This section contains visualisations of the EMDB entry EMD-18442. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

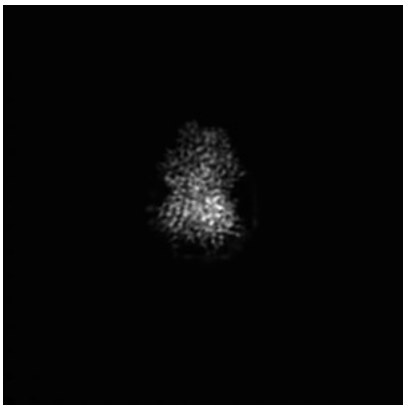
6.1 Orthogonal projections

6.1.1 Primary map

X

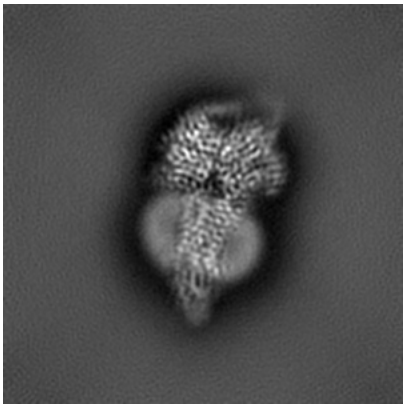


Y

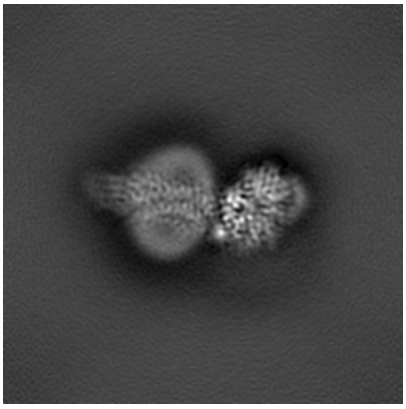


Z

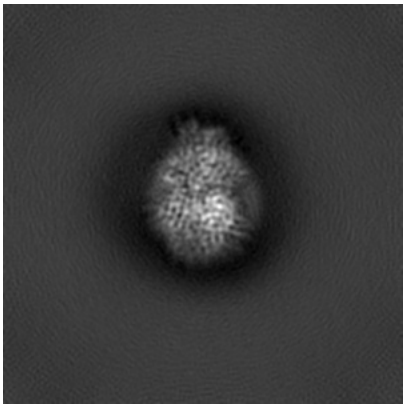
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

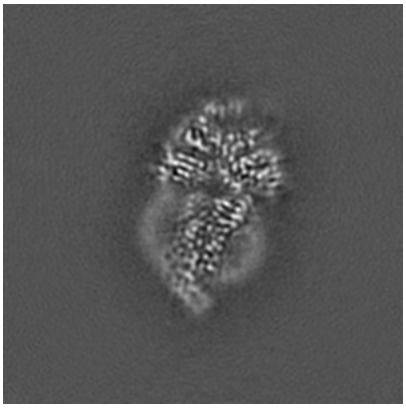
6.2.1 Primary map

X Index: 90

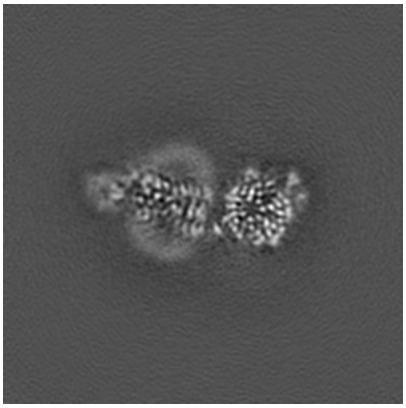
Y Index: 90

Z Index: 90

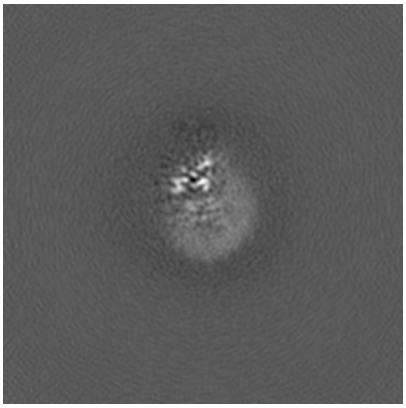
6.2.2 Raw map



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)

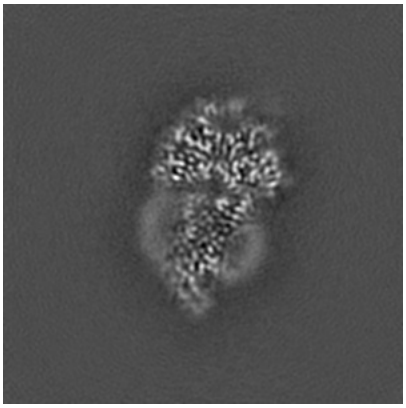
6.3.1 Primary map

X Index: 92

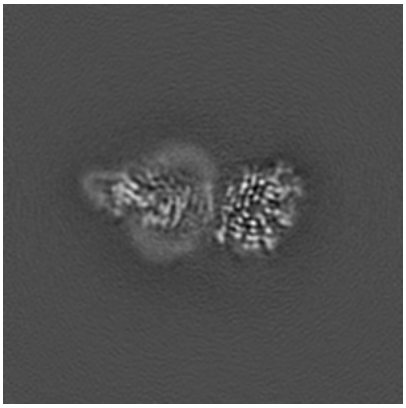
Y Index: 85

Z Index: 111

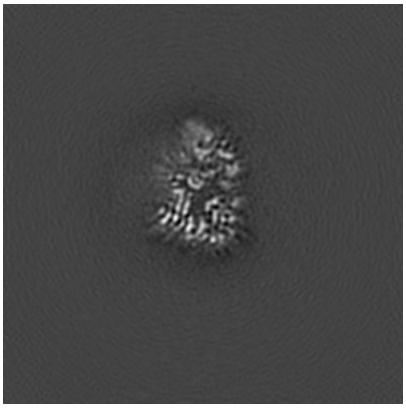
6.3.2 Raw map



X Index: 91



Y Index: 85



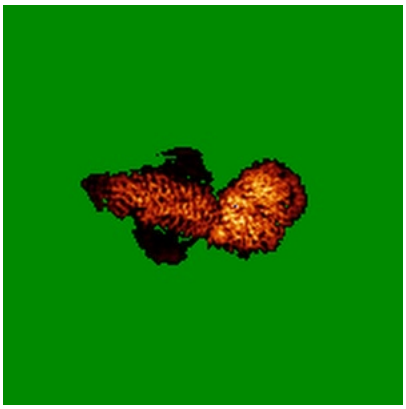
Z Index: 111

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

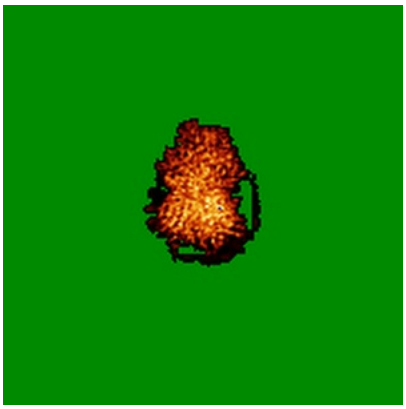
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

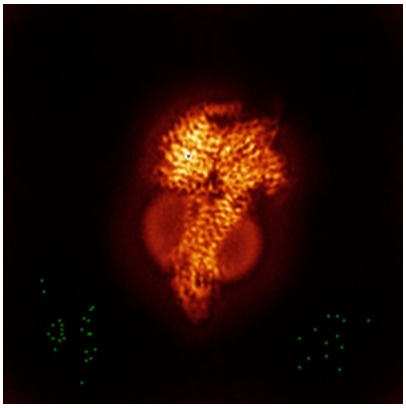


Y

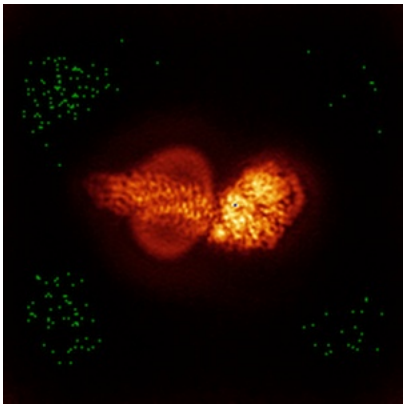


Z

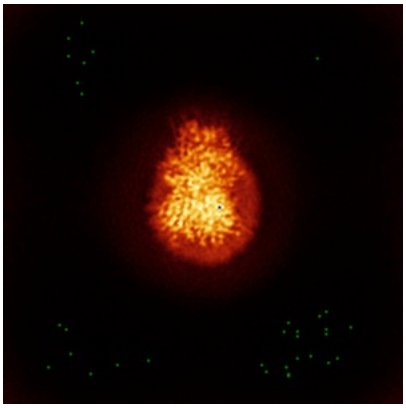
6.4.2 Raw map



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.

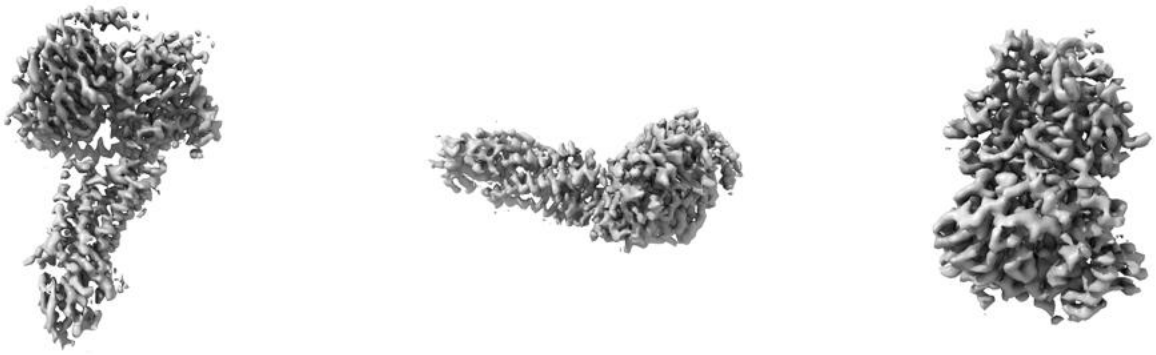
6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

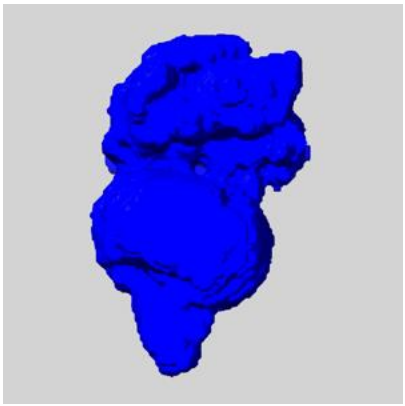
6.6 Mask visualisation (i)

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

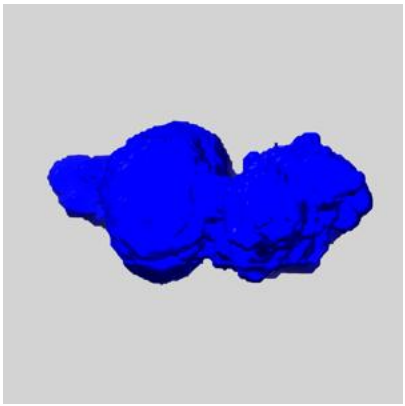
A mask typically either:

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

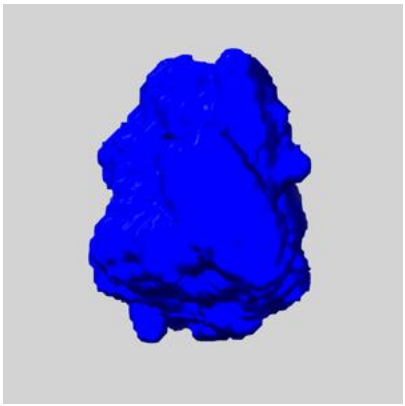
6.6.1 emd_18442_msk_1.map (i)



X



Y

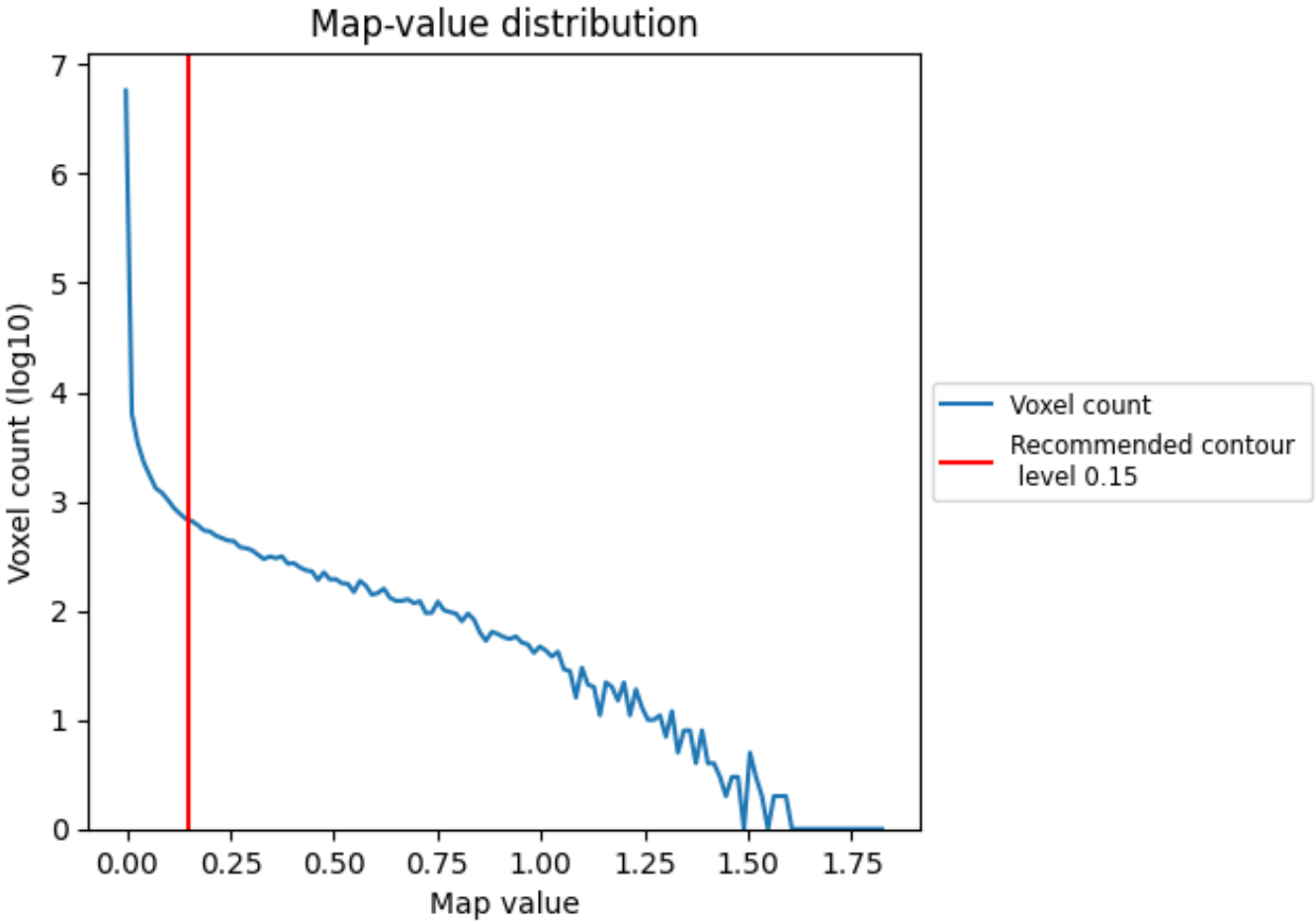


Z

7 Map analysis

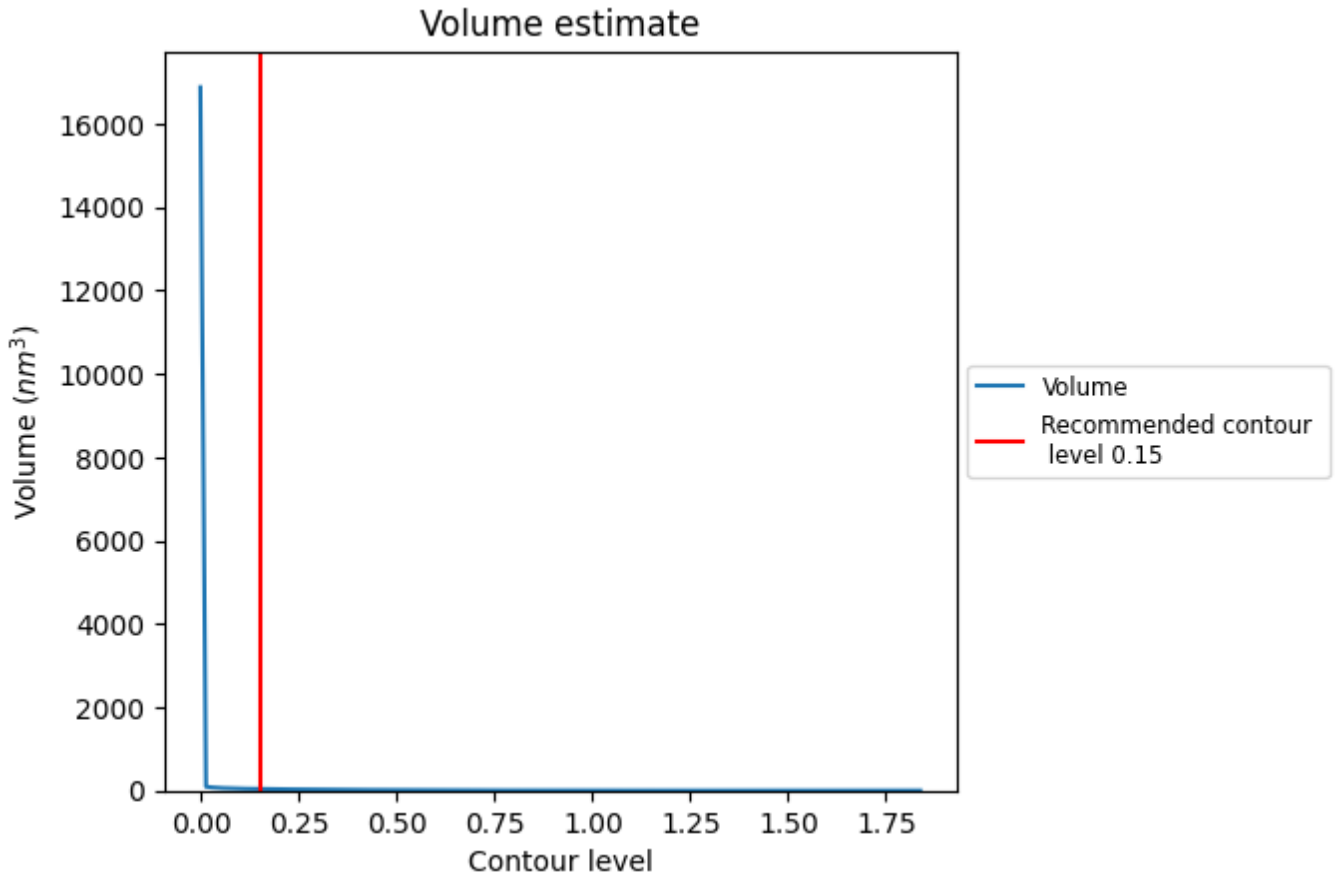
This section contains the results of statistical analysis of the map.

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.

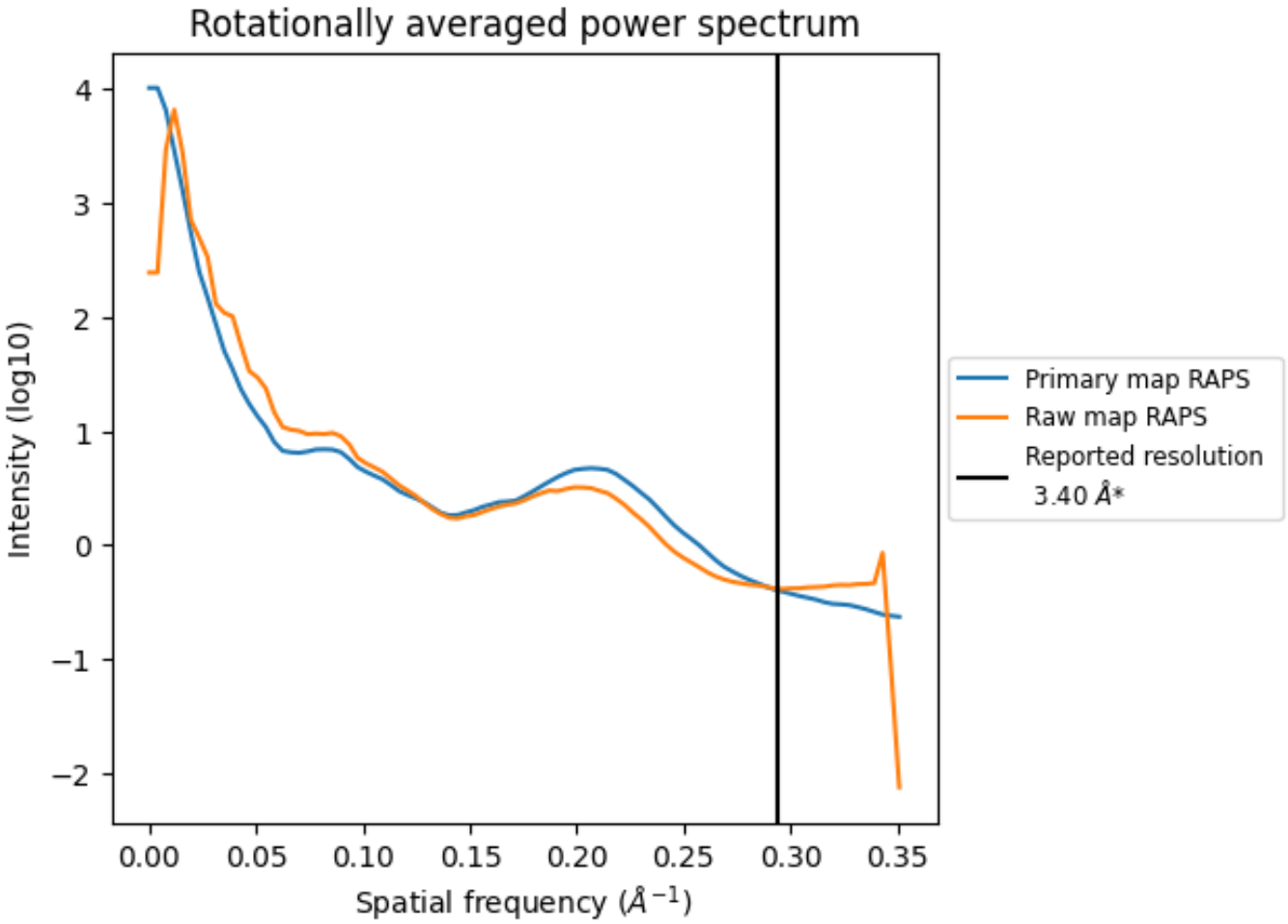
7.2 Volume estimate



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 (i)

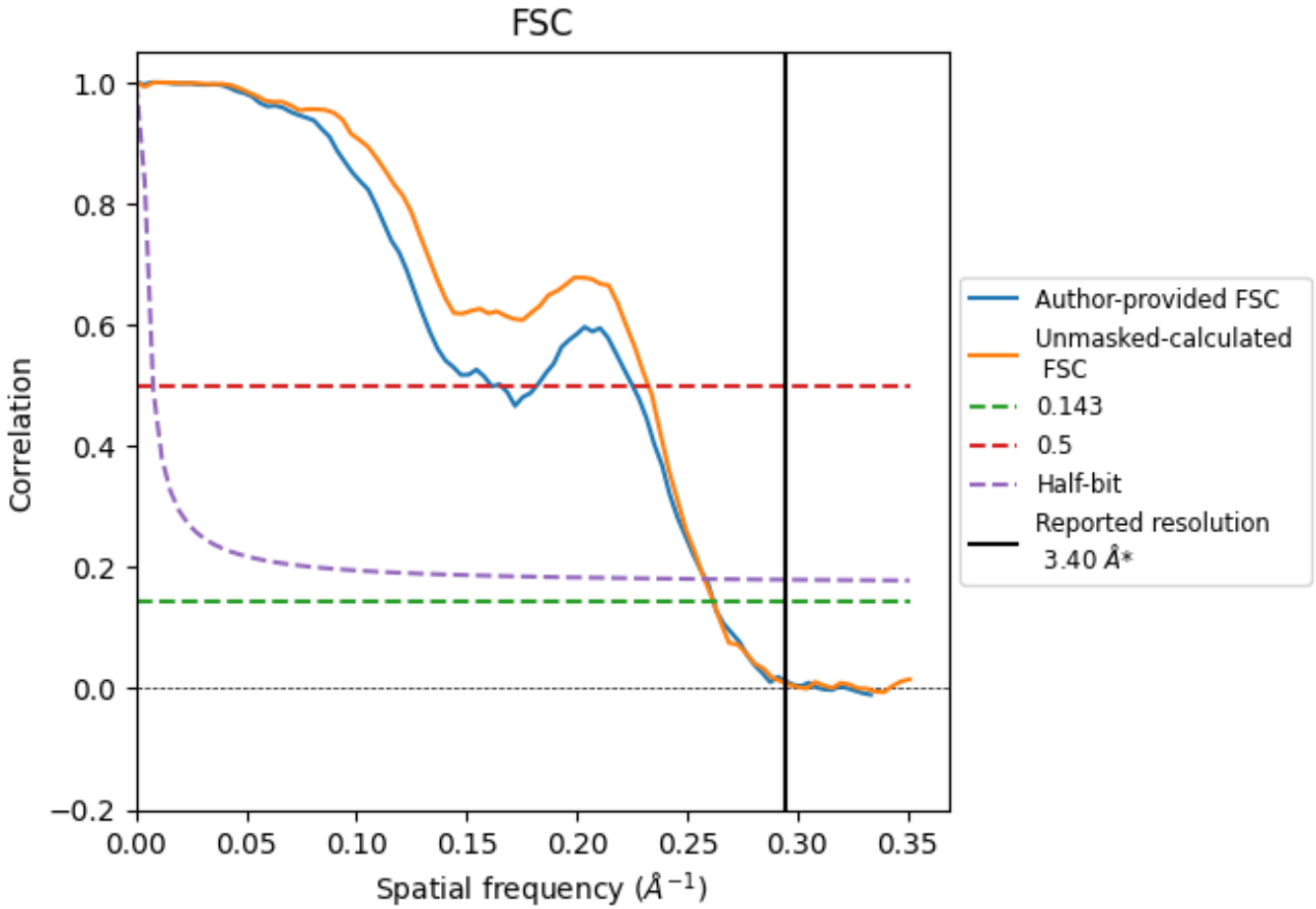


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 (i)

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

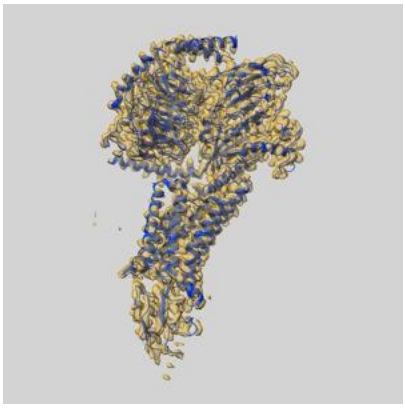
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.4 by more than 10 %

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 %

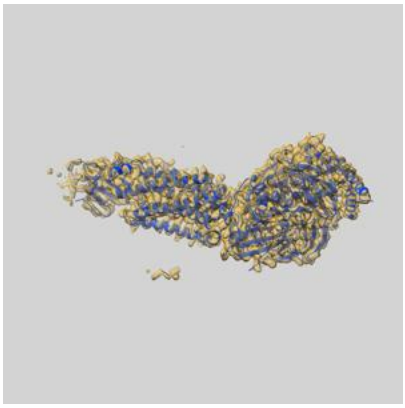
9 Map-model fit

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.

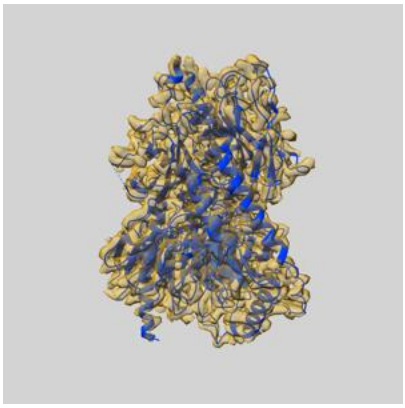
9.1 Map-model overlay



X



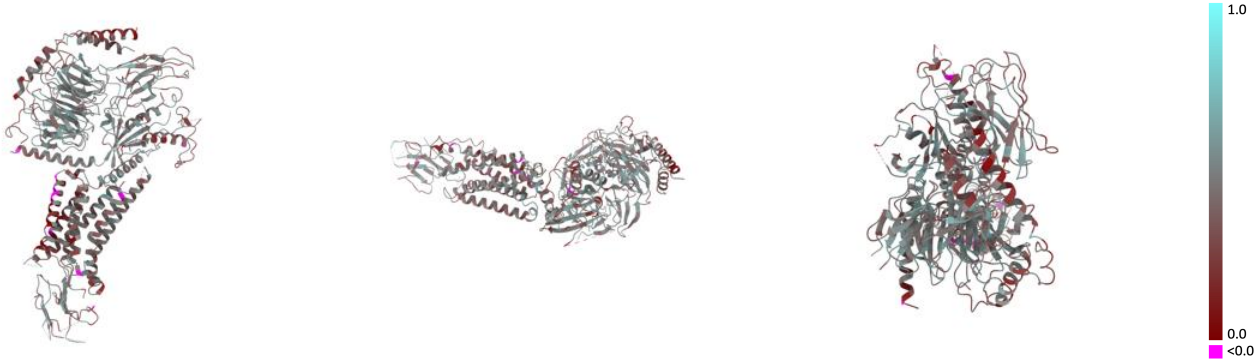
Y



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.

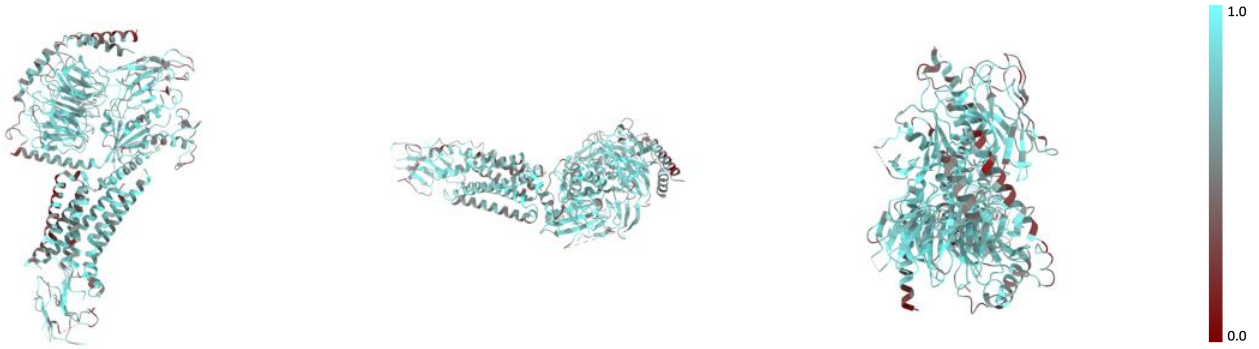
9.2 Q-score mapped to coordinate model (i)



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.

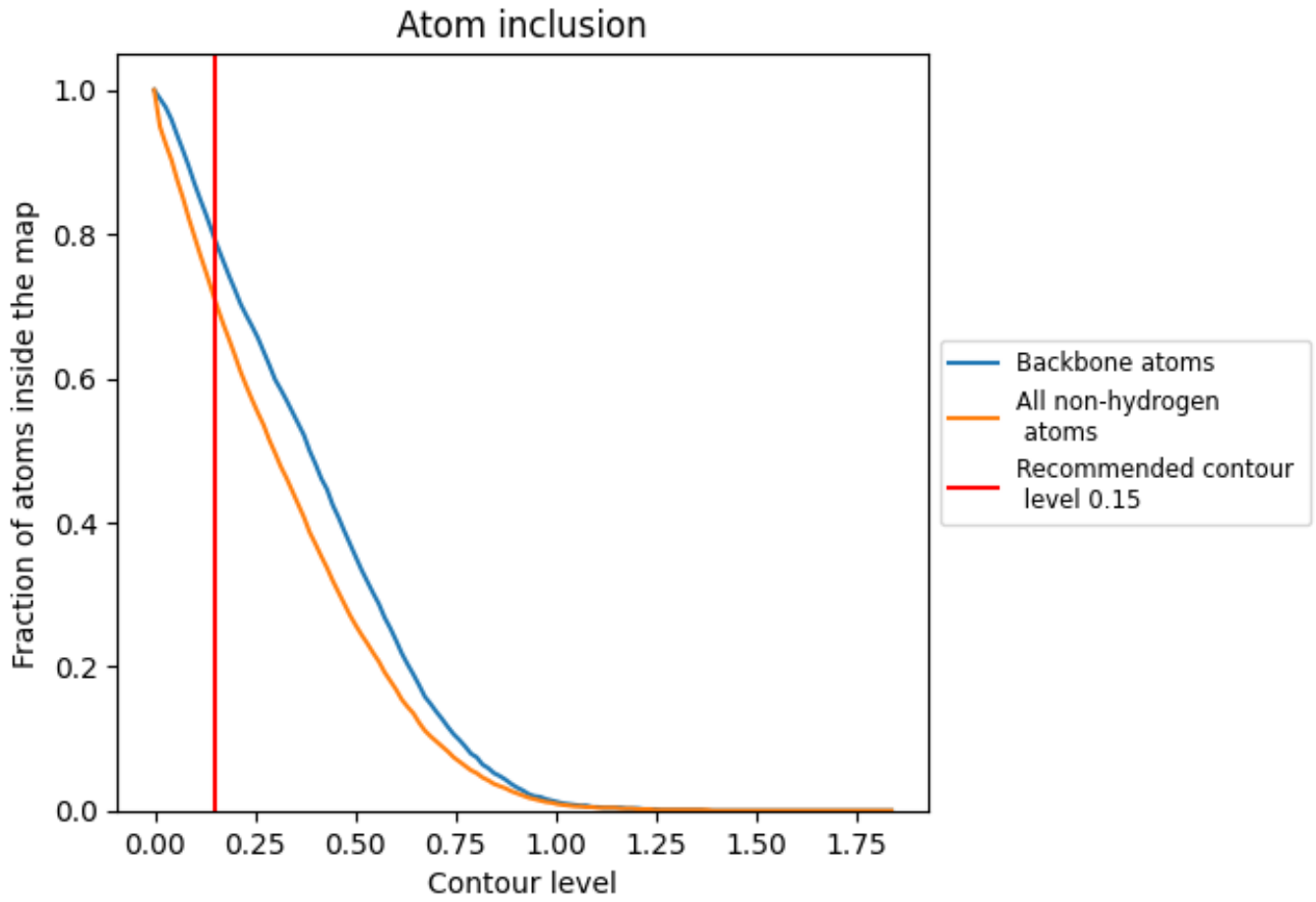
9.3 Atom inclusion mapped to coordinate model (i)



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