Full wwPDB EM Validation Report (i)

Sep 17, 2024 – 02:08 pm BST

PDB ID	:	8GY7
EMDB ID	:	EMD-34371
Title	:	Cryo-EM structure of ACTH-bound melanocortin-2 receptor in complex with MRAP1 and Gs protein
Authors	:	Luo, P.; Feng, W.B.; Ma, S.S.; Dai, A.T.; Yuan, Q.N.; Wu, K.; Yang, D.H.; Wang, M.W.; Xu, H.E.; Jiang, Y.
Deposited on	:	2022-09-21
Resolution	:	3.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

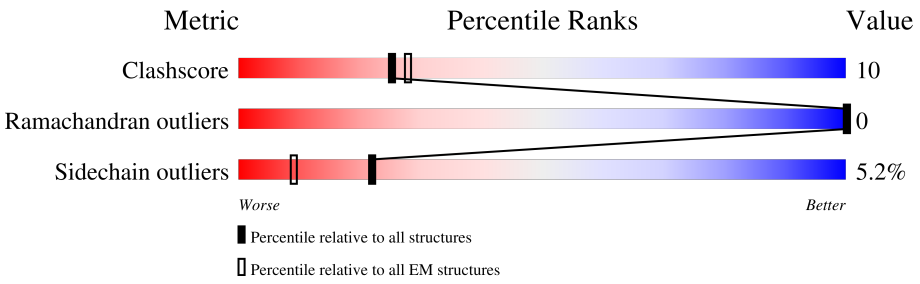
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 3.30 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	A	361	48% 14% • 36%
2	B	371	69% 21% • 9%
3	G	71	13% 61% 13% • 24%
4	M	18	89% 11%
5	P	184	25% • 72%
6	R	601	33% 11% • 54%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7661 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-3,Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLas.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	232	1920	1212	345	354	9	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	ASP	conflict	UNP P08754
A	21	LYS	ARG	conflict	UNP P08754
A	22	GLN	ASN	conflict	UNP P08754
A	24	GLN	ARG	conflict	UNP P08754
A	25	LYS	GLU	conflict	UNP P08754
A	27	LYS	GLY	conflict	UNP P08754
A	28	GLN	GLU	conflict	UNP P08754
A	29	VAL	LYS	conflict	UNP P08754
A	30	TYR	ALA	conflict	UNP P08754
A	31	ARG	ALA	conflict	UNP P08754
A	32	ALA	LYS	conflict	UNP P08754
A	33	THR	GLU	conflict	UNP P08754
A	34	HIS	VAL	conflict	UNP P08754
A	35	ARG	LYS	conflict	UNP P08754
A	42	ASP	GLY	conflict	UNP P08754
A	43	ASN	GLU	conflict	UNP P08754
A	54	ARG	LYS	conflict	UNP P08754
A	56	TYR	ILE	conflict	UNP P08754
A	58	VAL	GLU	conflict	UNP P08754
A	59	ASN	ASP	conflict	UNP P08754
A	64	GLU	ASP	conflict	UNP P08754
A	71	ALA	VAL	conflict	UNP P08754
A	97	ASP	GLU	conflict	UNP P08754
A	98	SER	ALA	conflict	UNP P08754
A	113	ALA	SER	conflict	UNP P08754
A	118	PHE	VAL	conflict	UNP P08754
A	121	ALA	PRO	conflict	UNP P08754

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Chain	Residue	Modelled	Actual	Comment	Reference
A	132	LYS	ARG	conflict	UNP P08754
A	134	SER	GLY	conflict	UNP P08754
A	141	ASN	SER	conflict	UNP P08754
A	153	ALA	SER	conflict	UNP P08754
A	163	ALA	SER	conflict	UNP P08754
A	165	PRO	SER	conflict	UNP P08754
A	182	SER	THR	conflict	UNP P08754
A	185	PHE	VAL	conflict	UNP P08754
A	188	LYS	HIS	conflict	UNP P08754
A	190	GLN	THR	conflict	UNP P08754
A	191	VAL	PHE	conflict	UNP P08754
A	192	ASP	LYS	conflict	UNP P08754
A	193	LYS	ASP	conflict	UNP P08754
A	194	VAL	LEU	conflict	UNP P08754
A	195	ASN	TYR	conflict	UNP P08754
A	197	HIS	LYS	conflict	UNP P08754
A	203	ALA	GLY	conflict	UNP P08754
A	206	ASP	SER	conflict	UNP P08754
A	209	ARG	LYS	conflict	UNP P08754
A	213	GLN	HIS	conflict	UNP P08754
A	216	ASN	GLU	conflict	UNP P08754
A	217	ASP	GLY	conflict	UNP P08754
A	224	VAL	CYS	conflict	UNP P08754
A	226	ASP	ALA	conflict	UNP P08754
A	227	SER	LEU	conflict	UNP P08754
A	239	ASP	LEU	conflict	UNP Q5JWF2
A	333	SER	ALA	conflict	UNP Q5JWF2
A	339	ALA	ILE	conflict	UNP Q5JWF2
A	342	ILE	VAL	conflict	UNP Q5JWF2

- 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	B	339	2604	1606	468	509	21	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P62873
B	2	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	-	expression tag	UNP P62873
B	4	LEU	-	expression tag	UNP P62873
B	5	LEU	-	expression tag	UNP P62873
B	6	GLN	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	SER	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	GLY	-	expression tag	UNP P62873
B	357	GLY	-	expression tag	UNP P62873
B	358	SER	-	expression tag	UNP P62873
B	359	SER	-	expression tag	UNP P62873
B	360	GLY	-	expression tag	UNP P62873
B	361	VAL	-	expression tag	UNP P62873
B	362	SER	-	expression tag	UNP P62873
B	363	GLY	-	expression tag	UNP P62873
B	364	TRP	-	expression tag	UNP P62873
B	365	ARG	-	expression tag	UNP P62873
B	366	LEU	-	expression tag	UNP P62873
B	367	PHE	-	expression tag	UNP P62873
B	368	LYS	-	expression tag	UNP P62873
B	369	LYS	-	expression tag	UNP P62873
B	370	ILE	-	expression tag	UNP P62873
B	371	SER	-	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
			Total	C	N	O	S		
3	G	54	411	258	73	77	3	0	0

- Molecule 4 is a protein called Corticotropin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	18	158	101	33	23	1	0	0

- Molecule 5 is a protein called Melanocortin-2 receptor accessory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	51	413	283	59	70	1	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-11	MET	-	initiating methionine	UNP Q8TCY5
P	-10	ASP	-	expression tag	UNP Q8TCY5
P	-9	TYR	-	expression tag	UNP Q8TCY5
P	-8	LYS	-	expression tag	UNP Q8TCY5
P	-7	ASP	-	expression tag	UNP Q8TCY5
P	-6	ASP	-	expression tag	UNP Q8TCY5
P	-5	ASP	-	expression tag	UNP Q8TCY5
P	-4	ASP	-	expression tag	UNP Q8TCY5
P	-3	LYS	-	expression tag	UNP Q8TCY5
P	-2	GLY	-	expression tag	UNP Q8TCY5
P	-1	SER	-	expression tag	UNP Q8TCY5
P	0	GLY	-	expression tag	UNP Q8TCY5

- Molecule 6 is a protein called Soluble cytochrome b562,Adrenocorticotropic hormone rece ptor,melanocortin-2 receptor,Adrenocorticotropic hormone receptor,Adrenocorticotropic hormone receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	274	2154	1430	344	359	21	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-130	MET	-	initiating methionine	UNP P0ABE7
R	-129	LYS	-	expression tag	UNP P0ABE7
R	-128	THR	-	expression tag	UNP P0ABE7
R	-127	ILE	-	expression tag	UNP P0ABE7
R	-126	ILE	-	expression tag	UNP P0ABE7
R	-125	ALA	-	expression tag	UNP P0ABE7
R	-124	LEU	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-123	SER	-	expression tag	UNP P0ABE7
R	-122	TYR	-	expression tag	UNP P0ABE7
R	-121	ILE	-	expression tag	UNP P0ABE7
R	-120	PHE	-	expression tag	UNP P0ABE7
R	-119	CYS	-	expression tag	UNP P0ABE7
R	-118	LEU	-	expression tag	UNP P0ABE7
R	-117	VAL	-	expression tag	UNP P0ABE7
R	-116	PHE	-	expression tag	UNP P0ABE7
R	-115	ALA	-	expression tag	UNP P0ABE7
R	-114	HIS	-	expression tag	UNP P0ABE7
R	-113	HIS	-	expression tag	UNP P0ABE7
R	-112	HIS	-	expression tag	UNP P0ABE7
R	-111	HIS	-	expression tag	UNP P0ABE7
R	-110	HIS	-	expression tag	UNP P0ABE7
R	-109	HIS	-	expression tag	UNP P0ABE7
R	-108	HIS	-	expression tag	UNP P0ABE7
R	-107	HIS	-	expression tag	UNP P0ABE7
R	-106	HIS	-	expression tag	UNP P0ABE7
R	-105	HIS	-	expression tag	UNP P0ABE7
R	-98	TRP	MET	conflict	UNP P0ABE7
R	-3	ILE	HIS	conflict	UNP P0ABE7
R	1	LEU	ARG	conflict	UNP P0ABE7

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

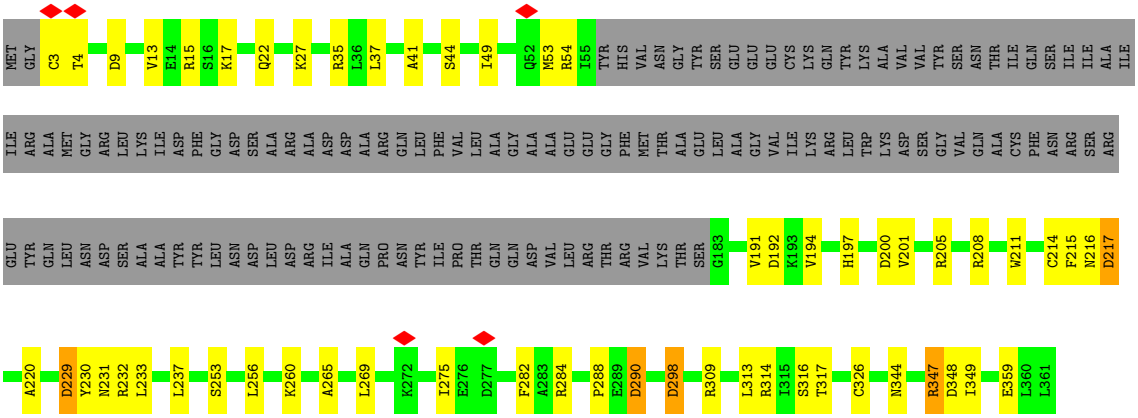
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
7	R	1	1	1	0

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.

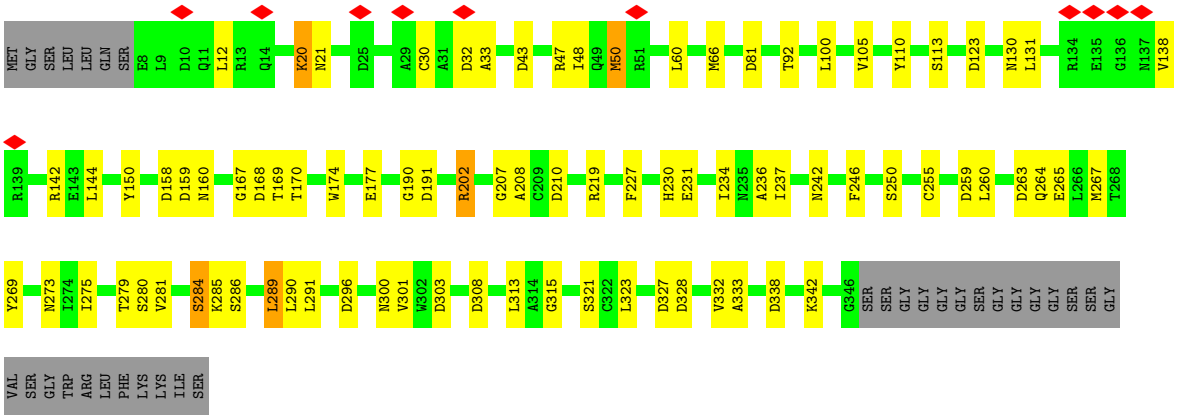
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-3,Guanine nucleotide-binding protein G(s) subunit alpha isoforms XLas

Chain A:



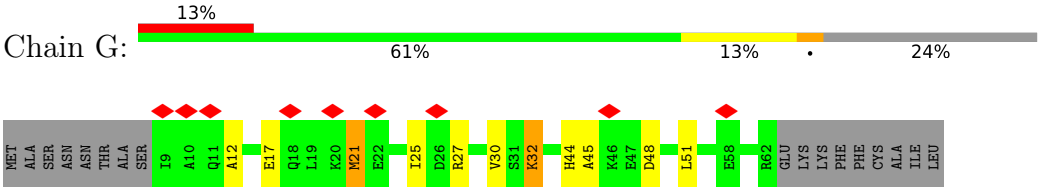
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



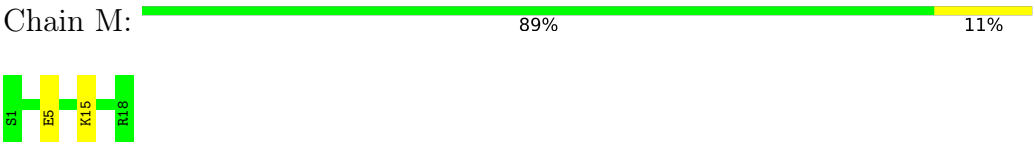
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



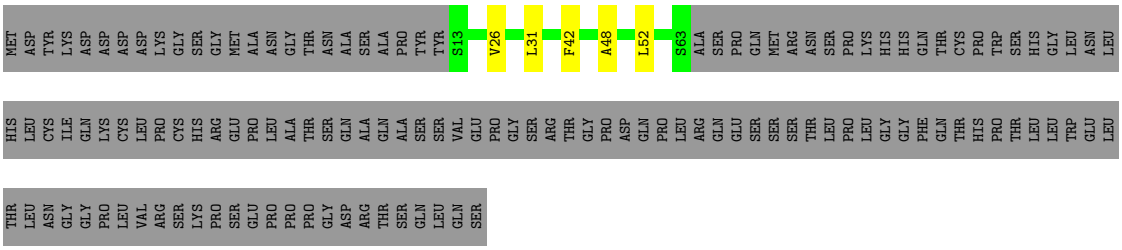
• Molecule 4: Corticotropin

Chain M:



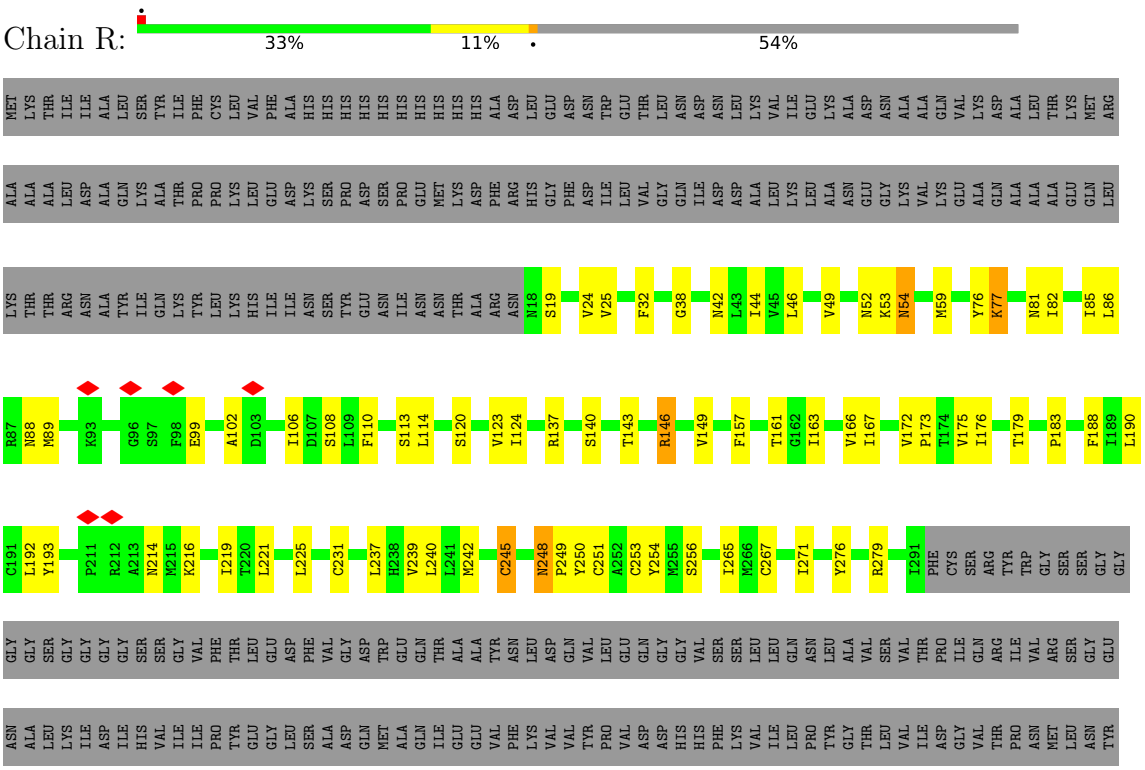
• Molecule 5: Melanocortin-2 receptor accessory protein

Chain P:



• Molecule 6: Soluble cytochrome b562,Adrenocorticotropic hormone receptor,melanocortin-2 receptor,Adrenocorticotropic hormone receptor,Adrenocorticotropic hormone receptor

Chain R:



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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.848	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	249.59999, 249.59999, 249.59999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.30	0/1957	0.58	1/2634 (0.0%)
2	B	0.28	0/2651	0.59	0/3594
3	G	0.28	0/417	0.51	0/563
4	M	0.30	0/163	0.60	0/214
5	P	0.28	0/426	0.42	0/581
6	R	0.33	0/2207	0.55	0/2999
All	All	0.30	0/7821	0.56	1/10585 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	PRO	CA-N-CD	-6.61	102.25	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1920	0	1900	37	0
2	B	2604	0	2508	66	0
3	G	411	0	416	8	0
4	M	158	0	162	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	413	0	409	5	0
6	R	2154	0	2222	49	0
7	R	1	0	0	0	0
All	All	7661	0	7617	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:143:THR:HG22	6:R:146:ARG:HD2	1.36	1.06
6:R:143:THR:HG22	6:R:146:ARG:CD	1.96	0.96
6:R:143:THR:CG2	6:R:146:ARG:HD2	1.99	0.90
3:G:25:ILE:HD11	3:G:27:ARG:NH1	2.08	0.69
6:R:143:THR:HG22	6:R:146:ARG:HD3	1.83	0.59
2:B:259:ASP:OD1	2:B:260:LEU:N	2.36	0.58
2:B:263:ASP:O	2:B:263:ASP:OD1	2.21	0.58
6:R:146:ARG:HA	6:R:149:VAL:HG12	1.86	0.58
1:A:22:GLN:HA	1:A:22:GLN:OE1	2.05	0.57
2:B:230:HIS:CD2	2:B:234:ILE:HG12	2.39	0.57
2:B:308:ASP:OD1	2:B:308:ASP:N	2.38	0.57
6:R:237:LEU:HD23	6:R:254:TYR:CZ	2.40	0.57
6:R:157:PHE:CE1	6:R:161:THR:HG21	2.40	0.56
6:R:76:TYR:CD1	6:R:106:ILE:HG22	2.41	0.56
1:A:41:ALA:O	1:A:44:SER:OG	2.22	0.56
6:R:245:CYS:O	6:R:245:CYS:SG	2.63	0.56
1:A:3:CYS:SG	1:A:4:THR:N	2.78	0.56
3:G:32:LYS:O	3:G:32:LYS:HD3	2.07	0.55
2:B:234:ILE:HD13	2:B:250:SER:HA	1.88	0.55
1:A:191:VAL:O	1:A:194:VAL:HG12	2.05	0.55
1:A:359:GLU:OE1	6:R:279:ARG:NH2	2.40	0.54
6:R:143:THR:HG23	6:R:146:ARG:H	1.72	0.54
4:M:5:GLU:HA	4:M:5:GLU:OE1	2.07	0.53
5:P:26:VAL:HG23	6:R:249:PRO:HB3	1.90	0.53
1:A:298:ASP:OD1	1:A:298:ASP:C	2.46	0.53
2:B:264:GLN:N	2:B:264:GLN:OE1	2.41	0.53
2:B:142:ARG:NH1	2:B:177:GLU:O	2.39	0.52
1:A:208:ARG:HG2	1:A:211:TRP:CZ2	2.44	0.52
2:B:47:ARG:O	2:B:47:ARG:HG3	2.09	0.52
1:A:313:LEU:O	1:A:317:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:SER:OG	3:G:48:ASP:OD2	2.24	0.52
1:A:230:TYR:CE2	1:A:275:ILE:HD13	2.45	0.52
2:B:168:ASP:O	2:B:168:ASP:OD1	2.28	0.51
6:R:248:ASN:OD1	6:R:250:TYR:N	2.43	0.51
2:B:273:ASN:N	2:B:273:ASN:OD1	2.44	0.51
2:B:279:THR:HG21	2:B:321:SER:HA	1.93	0.51
6:R:52:ASN:HB3	6:R:54:ASN:HD22	1.75	0.51
5:P:48:ALA:O	5:P:52:LEU:HD23	2.10	0.51
6:R:81:ASN:O	6:R:85:ILE:HD13	2.10	0.50
2:B:113:SER:OG	2:B:159:ASP:OD1	2.29	0.50
1:A:290:ASP:OD1	1:A:290:ASP:C	2.50	0.50
2:B:202:ARG:N	2:B:202:ARG:HD2	2.27	0.49
2:B:281:VAL:CG2	2:B:290:LEU:HD11	2.42	0.49
6:R:179:THR:O	6:R:183:PRO:HD2	2.13	0.49
1:A:284:ARG:HB2	1:A:284:ARG:NH1	2.28	0.49
2:B:231:GLU:OE2	2:B:231:GLU:HA	2.12	0.49
2:B:50:MET:SD	2:B:313:LEU:HD21	2.53	0.49
6:R:38:GLY:O	6:R:42:ASN:ND2	2.46	0.49
5:P:26:VAL:HG11	6:R:253:CYS:SG	2.52	0.49
1:A:217:ASP:OD1	1:A:217:ASP:C	2.52	0.48
2:B:144:LEU:HD12	2:B:144:LEU:N	2.28	0.48
2:B:207:GLY:HA3	2:B:234:ILE:HG21	1.95	0.48
1:A:37:LEU:HD22	1:A:215:PHE:CG	2.49	0.48
6:R:88:ASN:O	6:R:89:MET:HB3	2.14	0.48
6:R:102:ALA:O	6:R:106:ILE:HG12	2.14	0.48
2:B:291:LEU:HD22	2:B:332:VAL:HG11	1.96	0.47
1:A:35:ARG:NH1	1:A:217:ASP:OD1	2.47	0.47
6:R:231:CYS:O	6:R:265:ILE:HA	2.15	0.47
2:B:81:ASP:OD1	2:B:81:ASP:C	2.53	0.47
1:A:35:ARG:HA	1:A:197:HIS:HB2	1.97	0.47
6:R:110:PHE:CZ	6:R:114:LEU:HD11	2.50	0.47
2:B:100:LEU:HD13	2:B:105:VAL:HG21	1.95	0.47
6:R:157:PHE:O	6:R:161:THR:HG23	2.14	0.47
2:B:81:ASP:OD1	2:B:81:ASP:O	2.33	0.47
6:R:77:LYS:HA	6:R:77:LYS:HD3	1.58	0.47
1:A:284:ARG:HB2	1:A:284:ARG:CZ	2.45	0.47
6:R:175:VAL:HG13	6:R:239:VAL:HG12	1.97	0.47
2:B:12:LEU:HD13	3:G:12:ALA:CB	2.45	0.46
1:A:9:ASP:O	1:A:13:VAL:HG23	2.16	0.46
2:B:123:ASP:O	2:B:123:ASP:OD1	2.34	0.46
6:R:267:CYS:O	6:R:271:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:52:ASN:HB3	6:R:54:ASN:ND2	2.30	0.46
6:R:76:TYR:HD1	6:R:106:ILE:HG22	1.81	0.46
2:B:168:ASP:O	2:B:170:THR:N	2.48	0.46
6:R:216:LYS:HA	6:R:219:ILE:HG22	1.98	0.46
1:A:265:ALA:O	1:A:269:LEU:HD23	2.16	0.46
2:B:242:ASN:O	2:B:242:ASN:OD1	2.34	0.46
2:B:158:ASP:N	2:B:158:ASP:OD1	2.49	0.45
2:B:100:LEU:CD1	2:B:105:VAL:HG21	2.46	0.45
6:R:193:TYR:HB3	6:R:221:LEU:HD22	1.98	0.45
2:B:265:GLU:O	2:B:265:GLU:HG3	2.16	0.45
2:B:328:ASP:OD1	2:B:328:ASP:N	2.49	0.45
2:B:131:LEU:HA	2:B:138:VAL:HG12	1.98	0.45
5:P:42:PHE:CG	6:R:237:LEU:HD22	2.52	0.45
6:R:46:LEU:O	6:R:49:VAL:O	2.35	0.45
2:B:286:SER:HB2	3:G:44:HIS:HB2	1.98	0.45
2:B:323:LEU:O	2:B:323:LEU:HG	2.17	0.45
1:A:208:ARG:HG2	1:A:211:TRP:HZ2	1.80	0.44
2:B:130:ASN:OD1	2:B:130:ASN:C	2.55	0.44
6:R:124:ILE:HG21	6:R:276:TYR:CE1	2.52	0.44
3:G:45:ALA:O	3:G:51:LEU:HD23	2.17	0.44
2:B:60:LEU:HD12	2:B:81:ASP:OD2	2.17	0.44
6:R:24:VAL:HG12	6:R:256:SER:O	2.17	0.44
1:A:229:ASP:OD1	1:A:232:ARG:HB2	2.18	0.44
6:R:190:LEU:HD21	6:R:225:LEU:HD13	1.99	0.44
1:A:49:ILE:O	1:A:53:MET:HG2	2.18	0.44
1:A:344:ASN:OD1	1:A:347:ARG:NH2	2.51	0.44
2:B:169:THR:HG22	2:B:190:GLY:C	2.38	0.44
2:B:275:ILE:HG22	2:B:275:ILE:O	2.18	0.44
2:B:43:ASP:OD1	2:B:43:ASP:N	2.44	0.43
2:B:263:ASP:O	2:B:264:GLN:HG3	2.18	0.43
2:B:303:ASP:OD1	2:B:303:ASP:C	2.57	0.43
6:R:25:VAL:HG23	6:R:25:VAL:O	2.18	0.43
1:A:260:LYS:NZ	1:A:260:LYS:HB2	2.33	0.43
2:B:160:ASN:O	2:B:160:ASN:OD1	2.37	0.43
6:R:120:SER:HA	6:R:123:VAL:HG22	2.01	0.43
1:A:200:ASP:OD1	1:A:201:VAL:N	2.51	0.42
1:A:201:VAL:HG21	1:A:211:TRP:CH2	2.54	0.42
2:B:48:ILE:HG21	2:B:289:LEU:HD11	2.01	0.42
1:A:35:ARG:NH1	1:A:35:ARG:HB2	2.33	0.42
2:B:168:ASP:OD1	2:B:168:ASP:C	2.57	0.42
2:B:237:ILE:HD12	2:B:237:ILE:HA	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:O	1:A:54:ARG:HD2	2.19	0.42
1:A:275:ILE:HG21	1:A:282:PHE:HB2	2.01	0.42
2:B:150:TYR:O	2:B:167:GLY:N	2.51	0.42
2:B:255:CYS:O	2:B:269:TYR:N	2.47	0.42
2:B:338:ASP:OD1	2:B:338:ASP:C	2.57	0.42
6:R:24:VAL:HG13	6:R:24:VAL:O	2.20	0.42
1:A:314:ARG:HH11	1:A:314:ARG:HG3	1.85	0.42
2:B:255:CYS:SG	2:B:290:LEU:HD21	2.60	0.42
6:R:214:ASN:C	6:R:214:ASN:OD1	2.57	0.42
1:A:220:ALA:HB2	1:A:349:ILE:HD13	2.02	0.42
1:A:27:LYS:HB2	2:B:60:LEU:HD22	2.01	0.42
1:A:192:ASP:O	6:R:137:ARG:NH2	2.51	0.42
6:R:82:ILE:O	6:R:86:LEU:HD13	2.19	0.41
6:R:179:THR:HG21	6:R:240:LEU:HD11	2.02	0.41
1:A:232:ARG:HH11	1:A:232:ARG:HG2	1.86	0.41
1:A:233:LEU:O	1:A:237:LEU:HD23	2.20	0.41
2:B:144:LEU:HD23	2:B:174:TRP:CB	2.50	0.41
2:B:236:ALA:HB2	2:B:280:SER:HA	2.02	0.41
2:B:66:MET:SD	2:B:333:ALA:HB3	2.60	0.41
2:B:315:GLY:O	2:B:342:LYS:HE3	2.20	0.41
6:R:188:PHE:O	6:R:192:LEU:HD13	2.20	0.41
1:A:309:ARG:O	1:A:313:LEU:HD23	2.20	0.41
2:B:242:ASN:OD1	2:B:242:ASN:C	2.59	0.41
2:B:296:ASP:O	2:B:296:ASP:OD1	2.38	0.41
6:R:52:ASN:C	6:R:54:ASN:N	2.74	0.41
6:R:176:ILE:HD13	6:R:176:ILE:HA	1.84	0.41
2:B:20:LYS:HE3	2:B:21:ASN:N	2.36	0.41
2:B:32:ASP:O	2:B:33:ALA:C	2.59	0.41
2:B:208:ALA:HB3	2:B:210:ASP:OD1	2.21	0.41
2:B:281:VAL:HG22	2:B:290:LEU:HD11	2.03	0.41
6:R:163:ILE:O	6:R:167:ILE:HG23	2.20	0.41
6:R:248:ASN:O	6:R:251:CYS:HB2	2.21	0.41
1:A:205:ARG:NE	2:B:191:ASP:OD1	2.54	0.40
1:A:256:LEU:HD12	1:A:326:CYS:SG	2.61	0.40
5:P:26:VAL:HG23	5:P:31:LEU:HD11	2.03	0.40
2:B:92:THR:HG22	2:B:92:THR:O	2.21	0.40
3:G:17:GLU:O	3:G:21:MET:HG3	2.22	0.40
6:R:52:ASN:C	6:R:54:ASN:H	2.24	0.40
2:B:30:CYS:O	3:G:30:VAL:HG23	2.22	0.40
2:B:237:ILE:HD11	2:B:246:PHE:CD2	2.57	0.40
2:B:285:LYS:O	2:B:286:SER:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LEU:HD12	2:B:301:VAL:CG1	2.51	0.40
6:R:172:VAL:N	6:R:173:PRO:HD2	2.37	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	A	228/361 (63%)	222 (97%)	6 (3%)	0	100	100
2	B	337/371 (91%)	316 (94%)	21 (6%)	0	100	100
3	G	52/71 (73%)	52 (100%)	0	0	100	100
4	M	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
5	P	49/184 (27%)	45 (92%)	4 (8%)	0	100	100
6	R	272/601 (45%)	259 (95%)	13 (5%)	0	100	100
All	All	954/1606 (59%)	909 (95%)	45 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/315 (66%)	196 (94%)	13 (6%)	15	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	281/302 (93%)	270 (96%)	11 (4%)	27	55
3	G	42/58 (72%)	40 (95%)	2 (5%)	21	50
4	M	16/16 (100%)	15 (94%)	1 (6%)	15	41
5	P	44/162 (27%)	44 (100%)	0	100	100
6	R	242/523 (46%)	226 (93%)	16 (7%)	14	40
All	All	834/1376 (61%)	791 (95%)	43 (5%)	22	47

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	17	LYS
1	A	214	CYS
1	A	216	ASN
1	A	217	ASP
1	A	229	ASP
1	A	231	ASN
1	A	253	SER
1	A	290	ASP
1	A	298	ASP
1	A	316	SER
1	A	347	ARG
1	A	348	ASP
2	B	20	LYS
2	B	50	MET
2	B	110	TYR
2	B	202	ARG
2	B	219	ARG
2	B	227	PHE
2	B	267	MET
2	B	284	SER
2	B	289	LEU
2	B	300	ASN
2	B	327	ASP
3	G	21	MET
3	G	32	LYS
4	M	15	LYS
6	R	19	SER
6	R	32	PHE
6	R	44	ILE

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Mol	Chain	Res	Type
6	R	53	LYS
6	R	54	ASN
6	R	59	MET
6	R	77	LYS
6	R	99	GLU
6	R	108	SER
6	R	113	SER
6	R	140	SER
6	R	146	ARG
6	R	166	VAL
6	R	242	MET
6	R	245	CYS
6	R	248	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
6	R	54	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

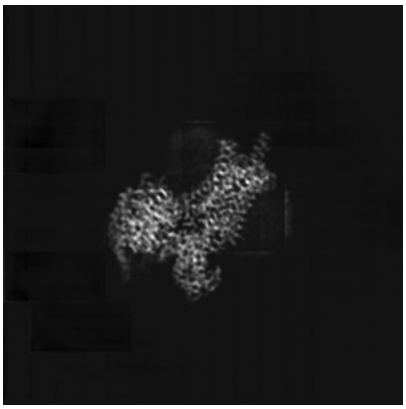
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-34371. 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.

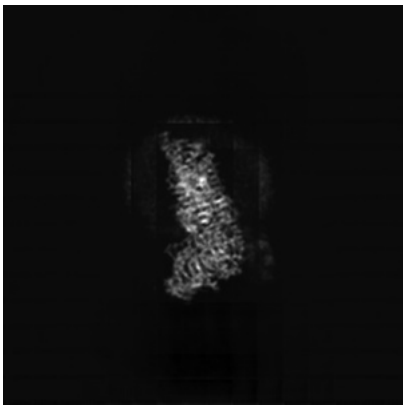
6.1 Orthogonal projections (i)

6.1.1 Primary map



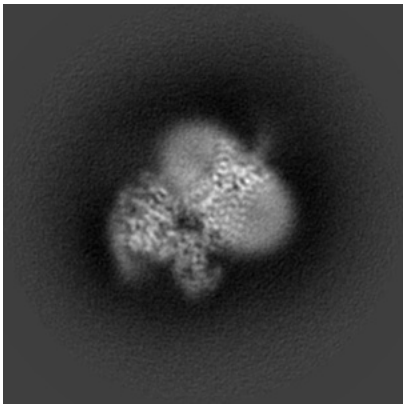
X

Y

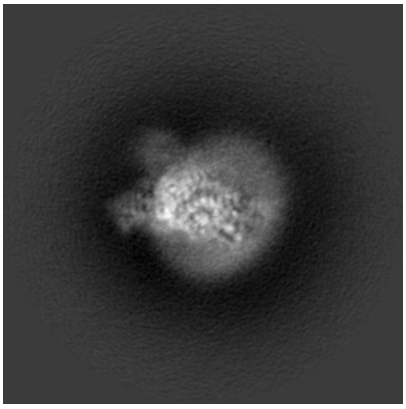


Z

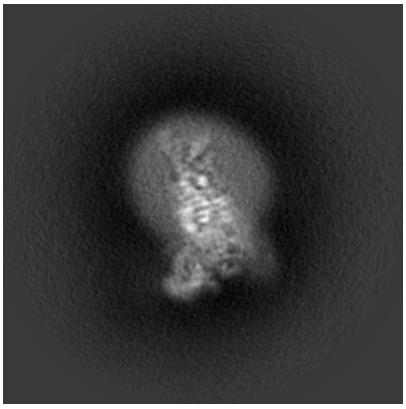
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

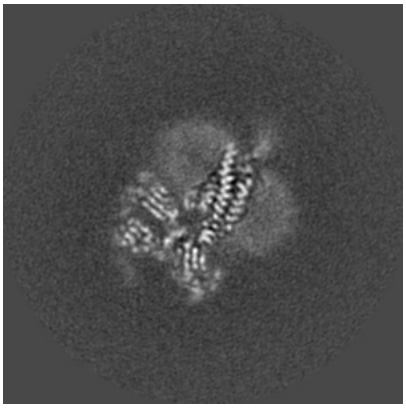
6.2.1 Primary map

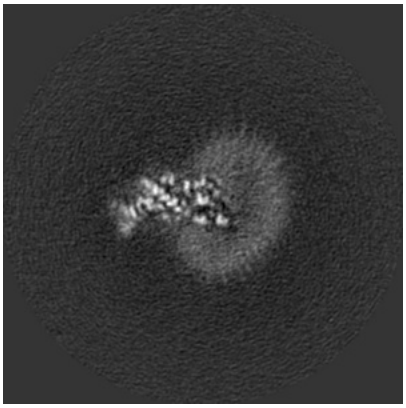
X Index: 120

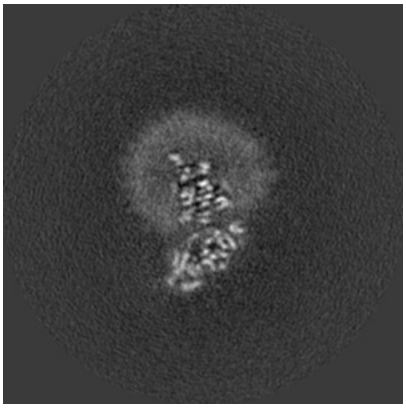
Y Index: 120

Z Index: 120

6.2.2 Raw map


X Index: 120


Y Index: 120


Z Index: 120

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

6.3 Largest variance slices (i)

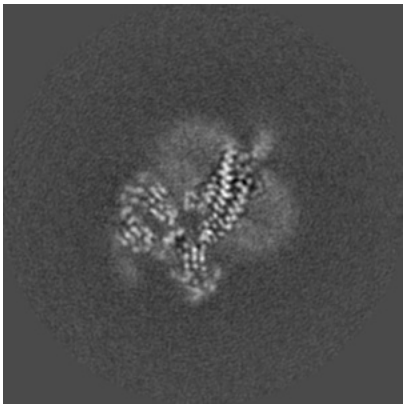
6.3.1 Primary map

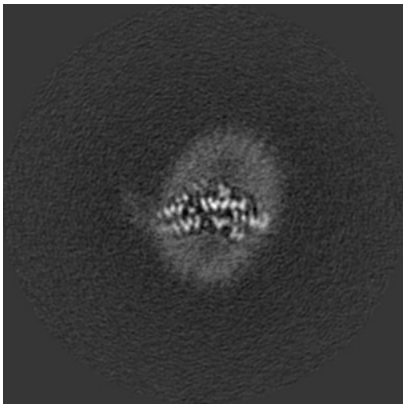
X Index: 118

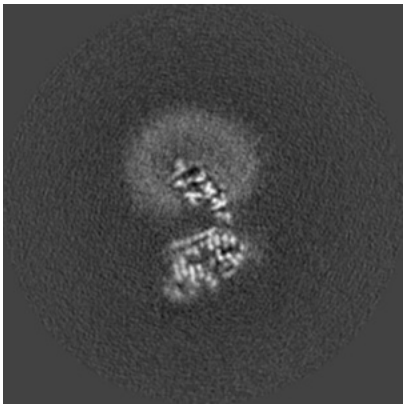
Y Index: 88

Z Index: 110

6.3.2 Raw map


X Index: 119

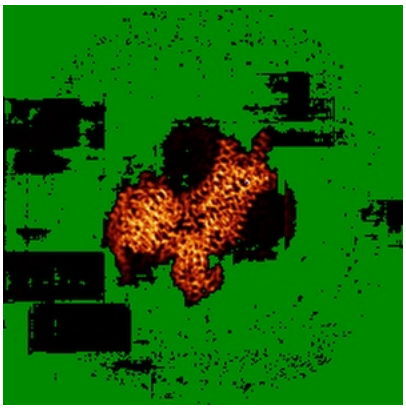

Y Index: 132

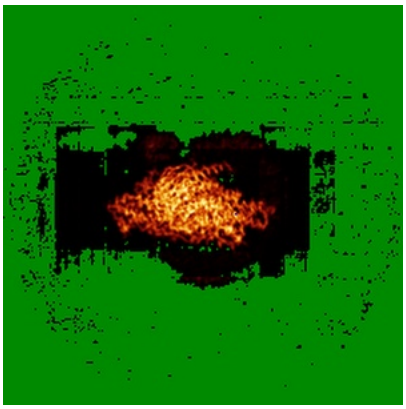

Z Index: 110

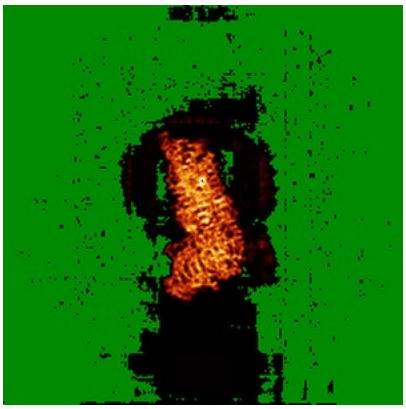
The images above show the largest variance slices of the map in three orthogonal directions.

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

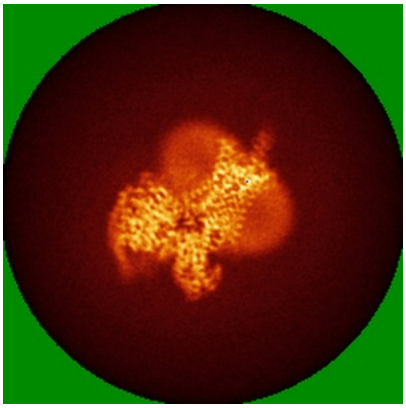
6.4.1 Primary map

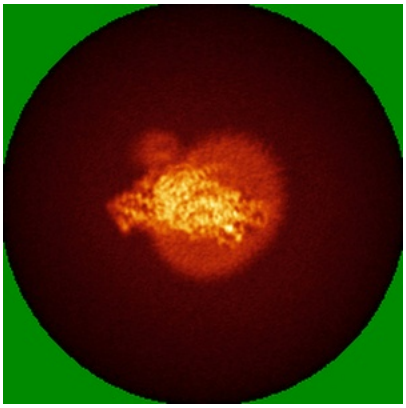

X

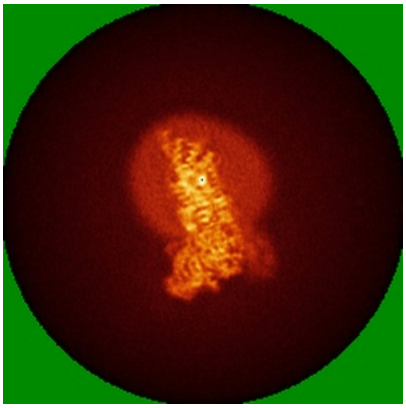

Y


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

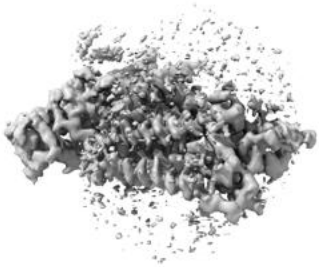
Y

Z

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

6.5.2 Raw map

X



Y

Z

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

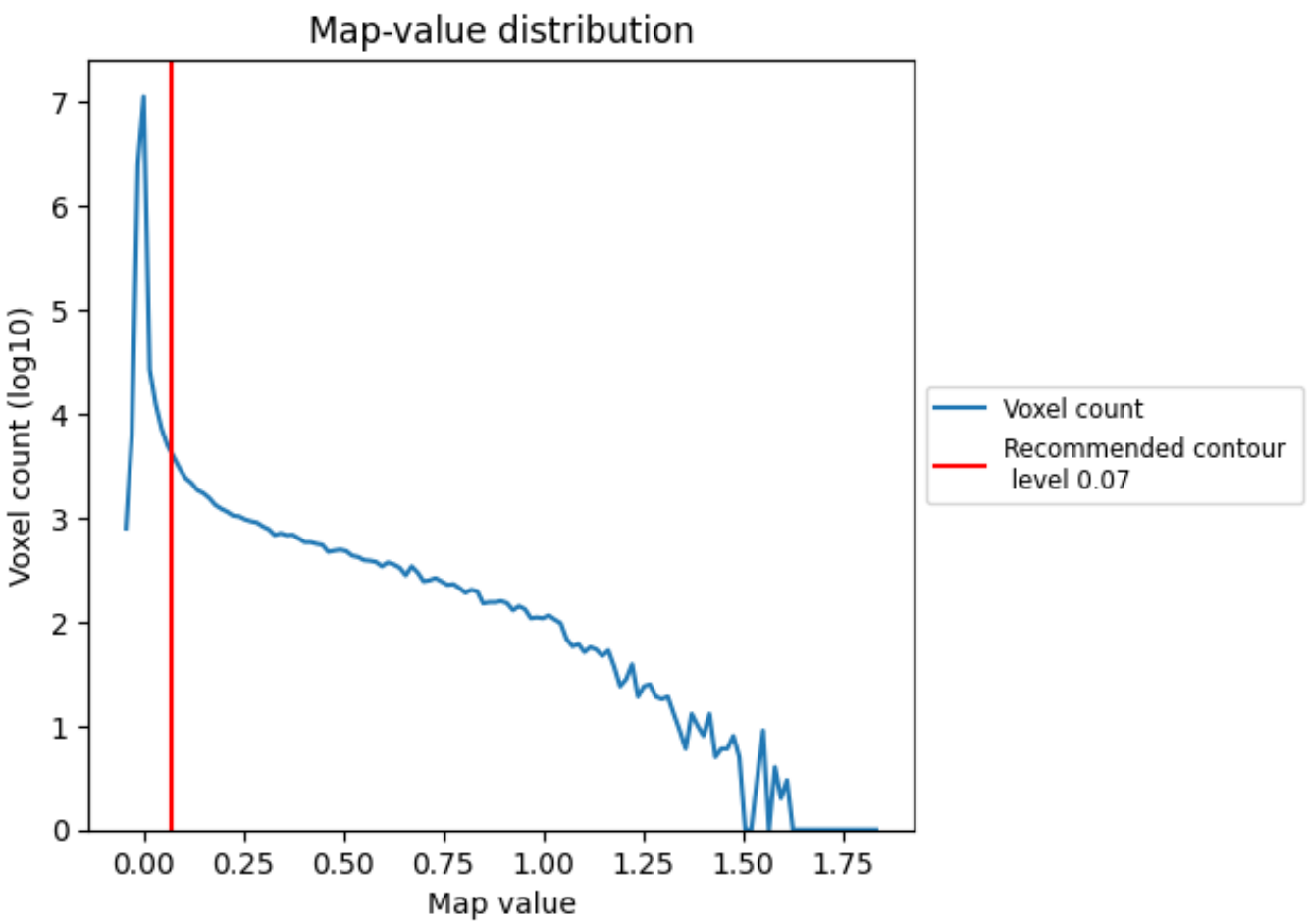
6.6 Mask visualisation (i)

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

7 Map analysis (i)

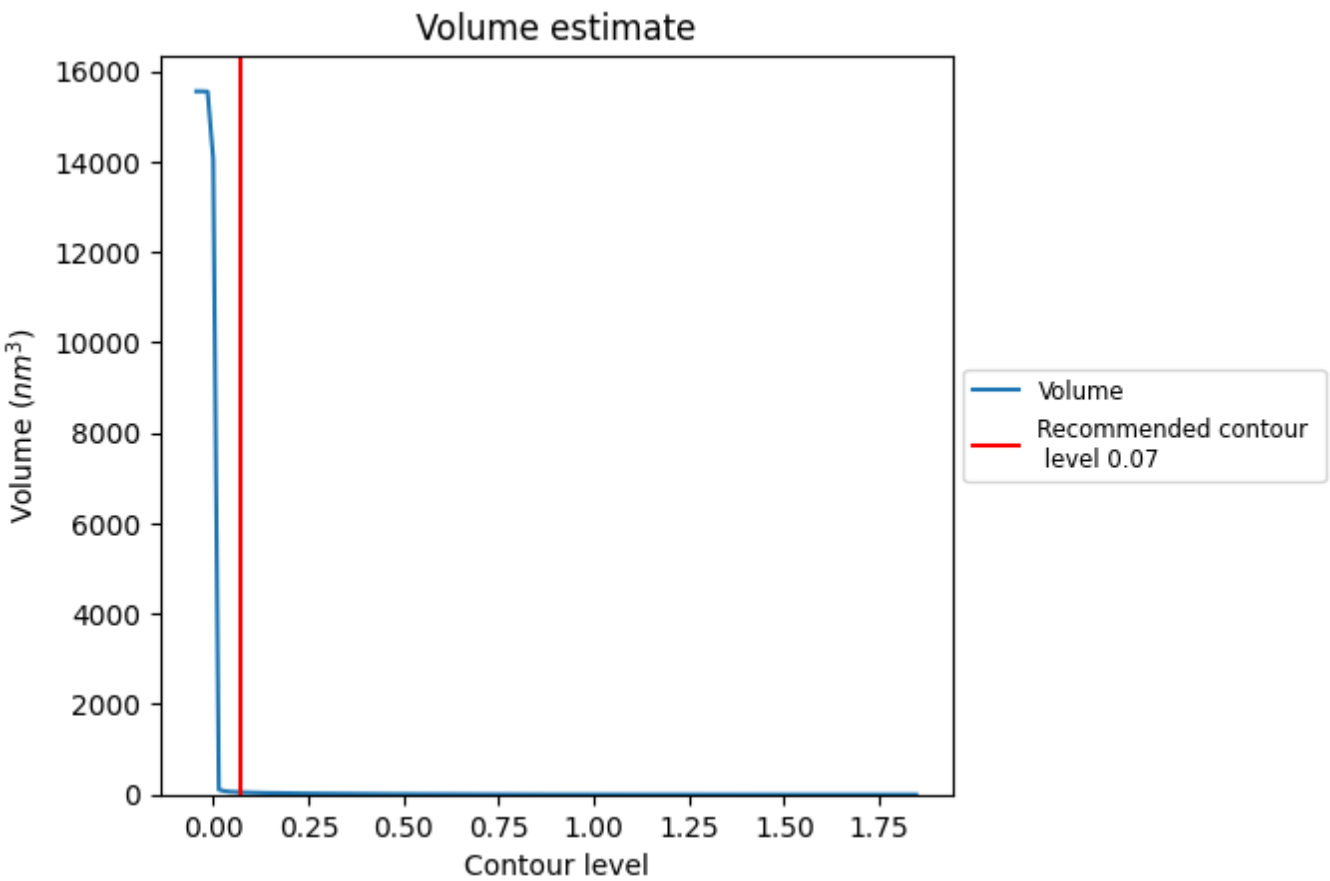
This section contains the results of statistical analysis of the map.

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.

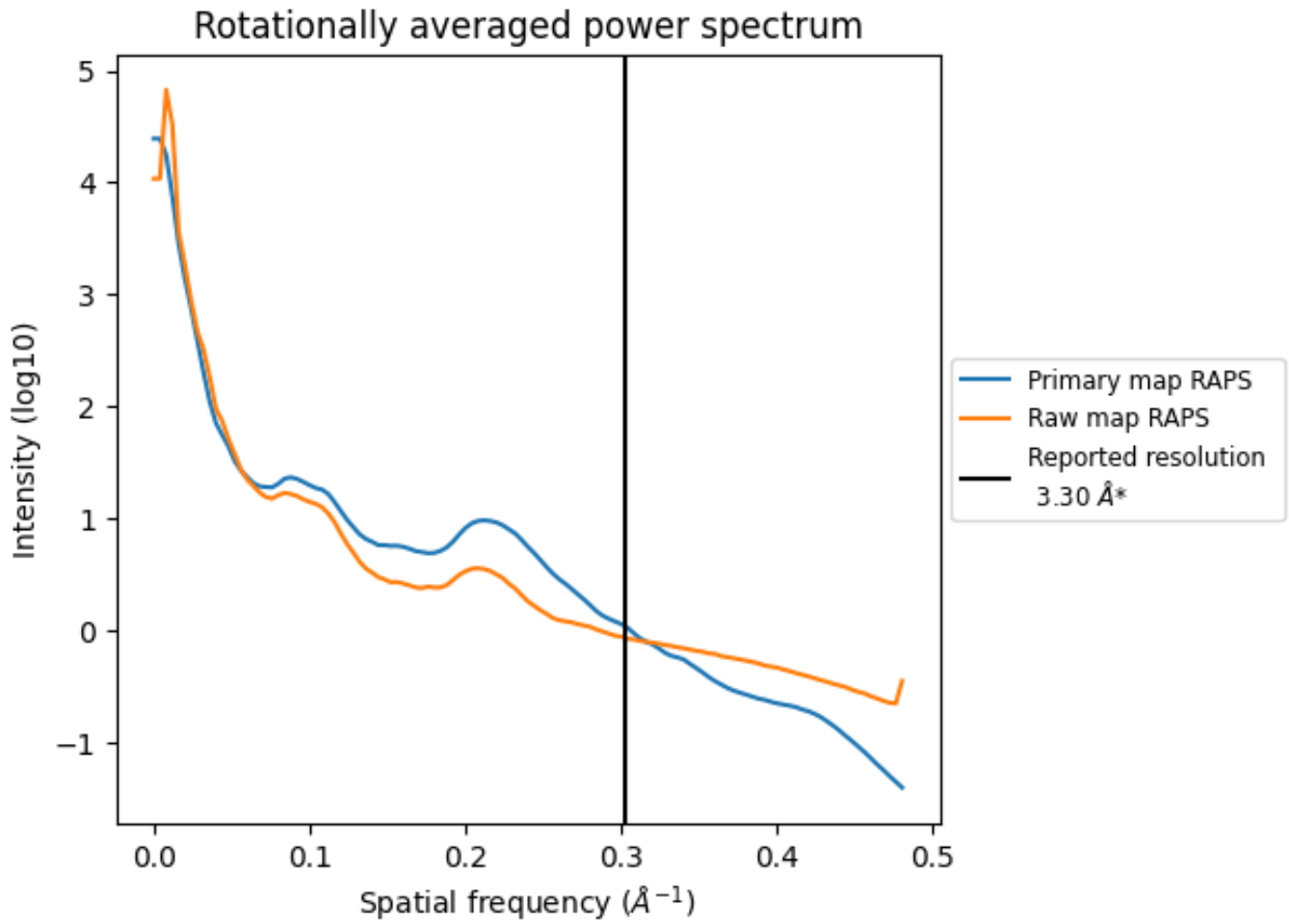
7.2 Volume estimate (i)



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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)

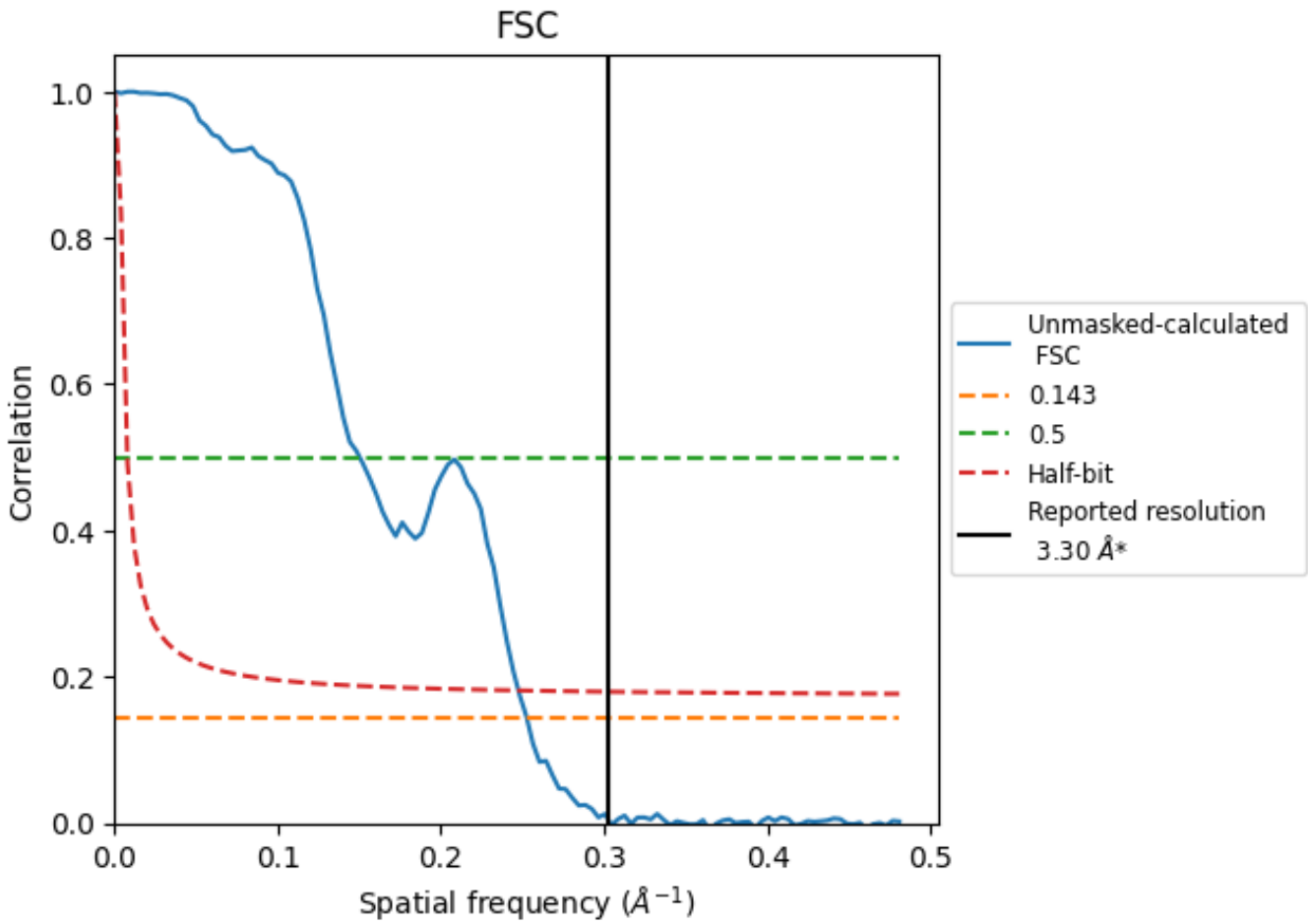


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

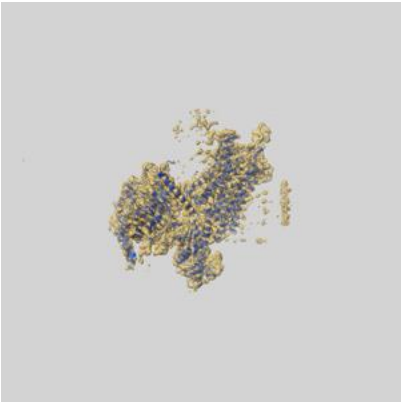
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	6.66	4.04

*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 3.96 differs from the reported value 3.3 by more than 10 %

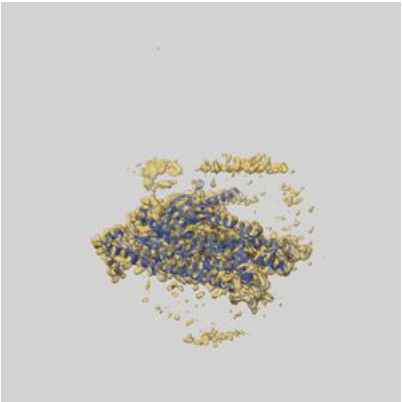
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34371 and PDB model 8GY7. Per-residue inclusion information can be found in section 3 on page 8.

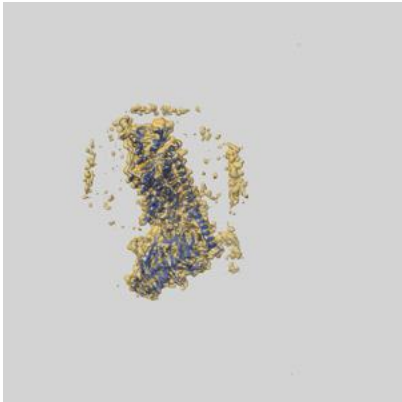
9.1 Map-model overlay (i)



X



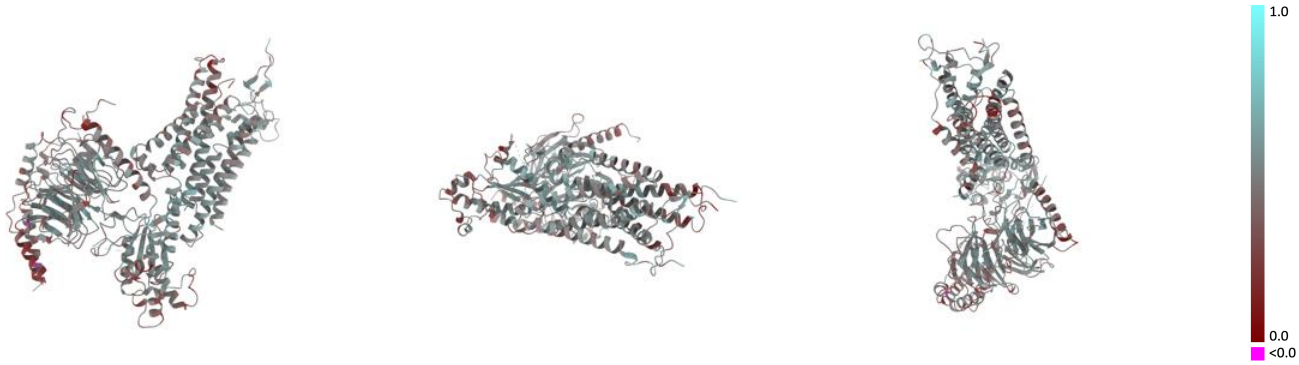
Y



Z

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

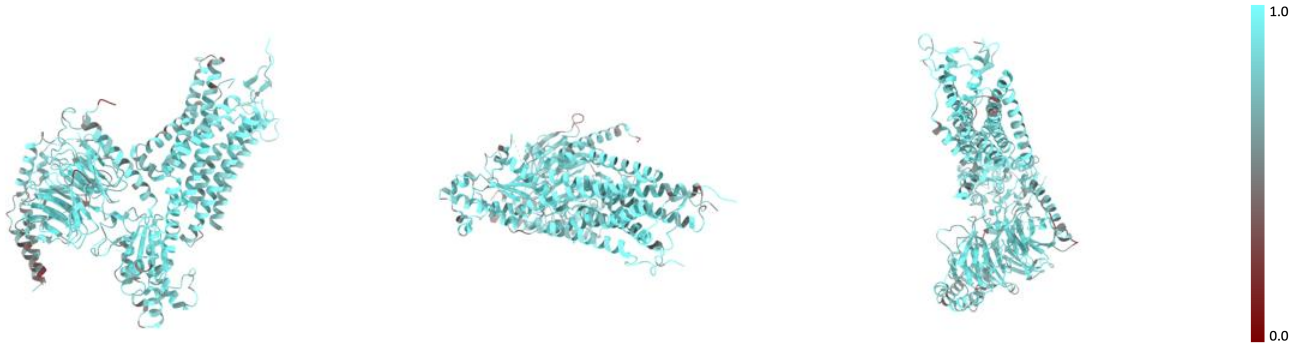
9.2 Q-score mapped to coordinate model (i)



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.

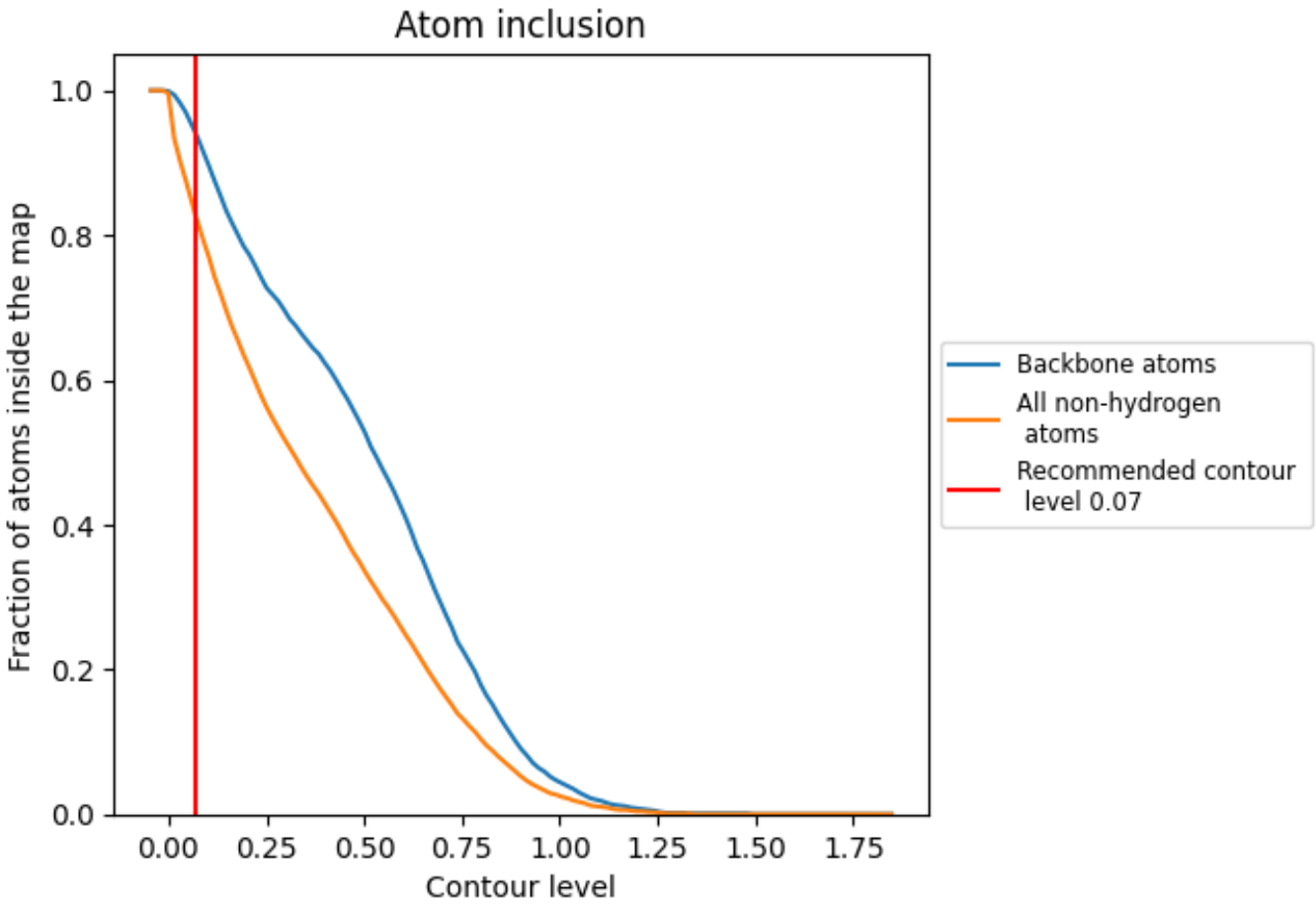
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.8250	0.4530
A	0.8320	0.4570
B	0.8180	0.4470
G	0.6630	0.3400
M	0.8200	0.4630
P	0.8400	0.4750
R	0.8560	0.4730