



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 04:13 AM EST

PDB ID : 6WDO
EMDB ID : EMD-21643
Title : Cryo-EM structure of mitochondrial calcium uniporter holocomplex in high Ca²⁺
Authors : Feng, L.; Zhang, J.; Fan, M.
Deposited on : 2020-04-01
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

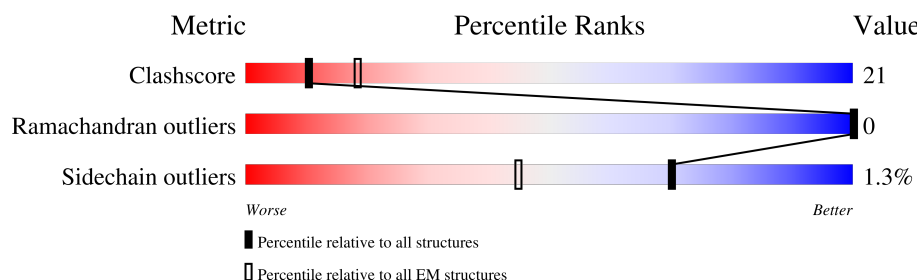
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.





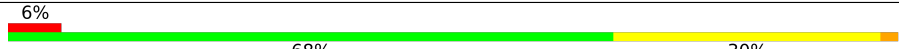
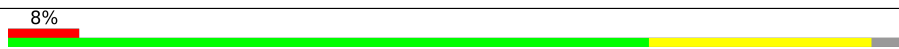

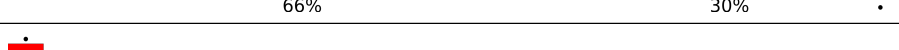
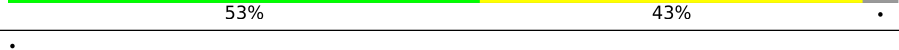

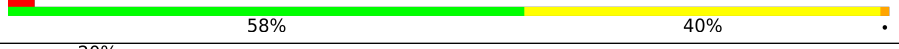
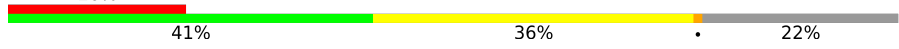

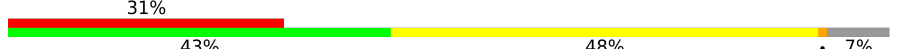
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	273	
1	E	273	
1	G	273	
1	I	273	
1	M	273	
1	O	273	
2	B	53	
2	D	53	

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Mol	Chain	Length	Quality of chain
2	F	53	
2	H	53	
2	J	53	
2	L	53	
2	N	53	
2	P	53	
3	C	268	
3	K	268	
4	Q	339	
4	S	339	
5	R	310	
5	T	310	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29867 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 Calcium uniporter protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	255	Total	C	N	O	S	0	0
			2102	1349	363	382	8		
1	A	273	Total	C	N	O	S	0	0
			2254	1444	393	409	8		
1	E	270	Total	C	N	O	S	0	0
			2226	1427	386	405	8		
1	I	273	Total	C	N	O	S	0	0
			2254	1444	393	409	8		
1	O	255	Total	C	N	O	S	0	0
			2102	1349	363	382	8		
1	M	270	Total	C	N	O	S	0	0
			2226	1427	386	405	8		

- Molecule 2 is a protein called Essential MCU regulator, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	51	Total	C	N	O	S	0	0
			400	271	63	65	1		
2	D	51	Total	C	N	O	S	0	0
			400	271	63	65	1		
2	B	53	Total	C	N	O	S	0	0
			414	281	65	67	1		
2	F	50	Total	C	N	O	S	0	0
			389	262	62	64	1		
2	J	53	Total	C	N	O	S	0	0
			414	281	65	67	1		
2	L	51	Total	C	N	O	S	0	0
			400	271	63	65	1		
2	P	51	Total	C	N	O	S	0	0
			400	271	63	65	1		
2	N	51	Total	C	N	O	S	0	0
			400	271	63	65	1		

- Molecule 3 is a protein called Calcium uniporter protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	268	Total	C	N	O	S	0	0
			2211	1416	384	403	8		
3	K	268	Total	C	N	O	S	0	0
			2211	1416	384	403	8		

- Molecule 4 is a protein called Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	264	Total	C	N	O	S	0	0
			2136	1367	357	401	11		
4	S	264	Total	C	N	O	S	0	0
			2136	1367	357	401	11		

- Molecule 5 is a protein called Calcium uptake protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	287	Total	C	N	O	S	0	0
			2395	1540	404	436	15		
5	T	287	Total	C	N	O	S	0	0
			2395	1540	404	436	15		

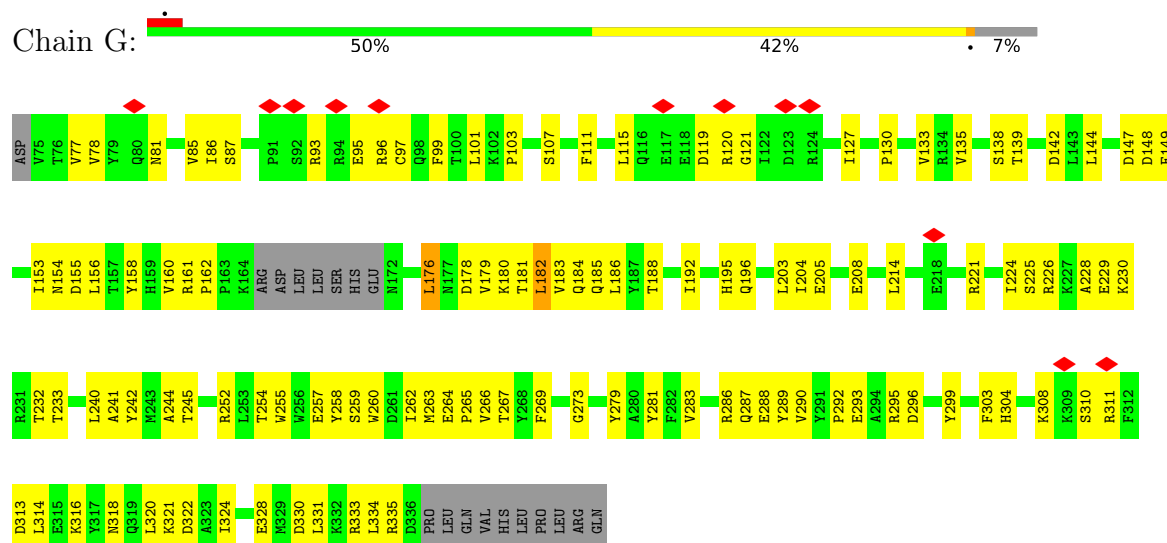
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	

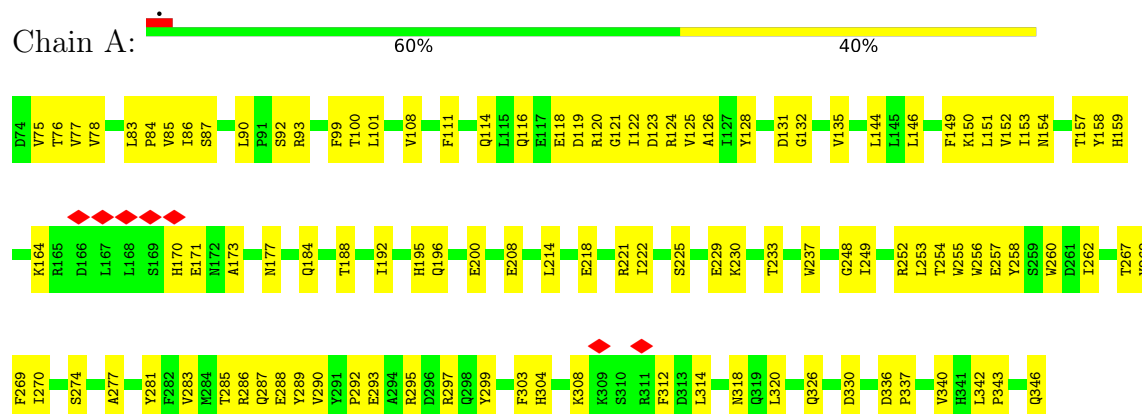
3 Residue-property plots

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: Calcium uniporter protein, mitochondrial

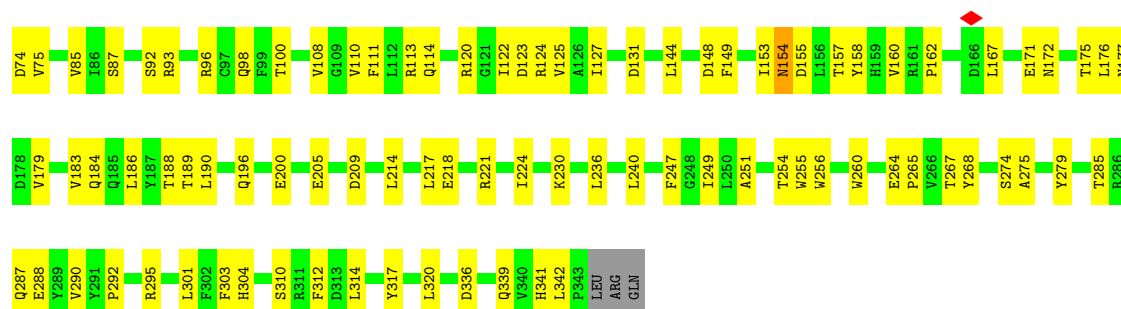


- Molecule 1: Calcium uniporter protein, mitochondrial



- Molecule 1: Calcium uniporter protein, mitochondrial

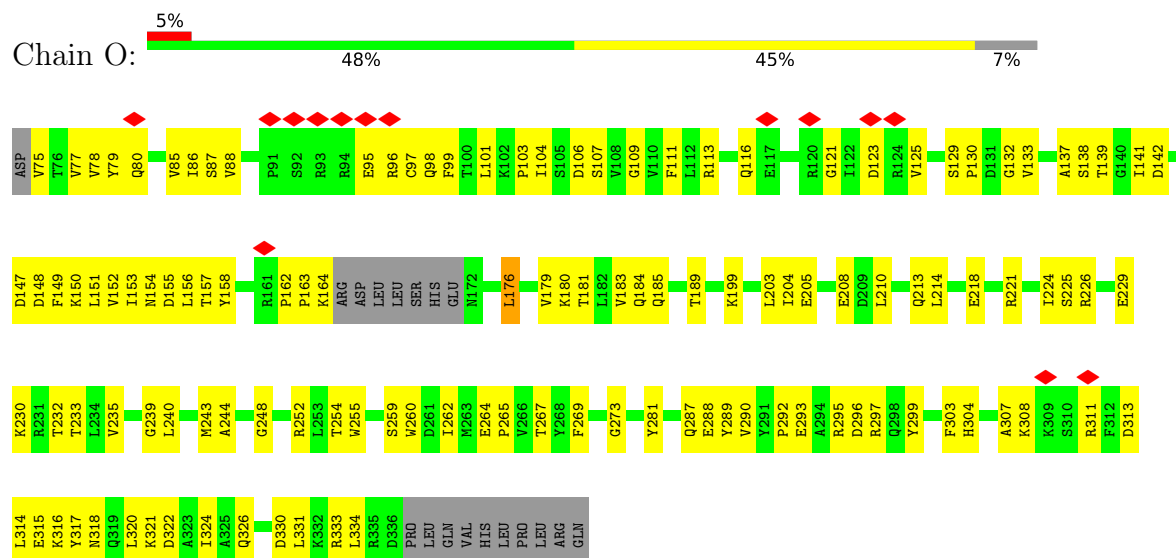




- Molecule 1: Calcium uniporter protein, mitochondrial

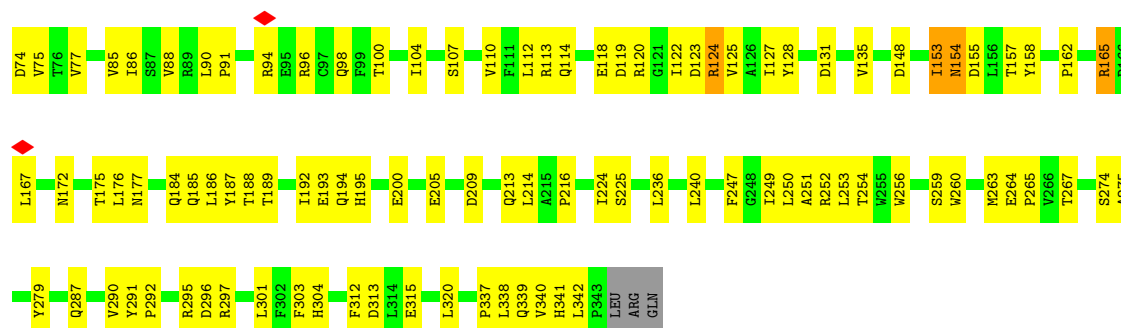


- Molecule 1: Calcium uniporter protein, mitochondrial



- Molecule 1: Calcium uniporter protein, mitochondrial

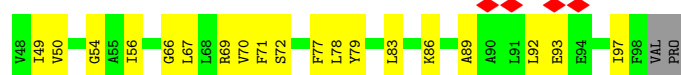




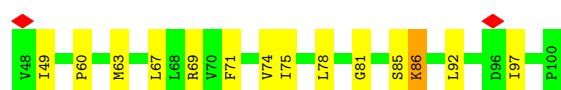
- Molecule 2: Essential MCU regulator, mitochondrial



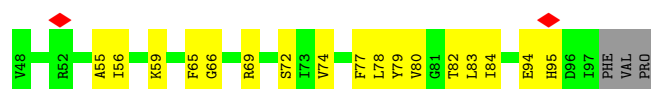
- Molecule 2: Essential MCU regulator, mitochondrial



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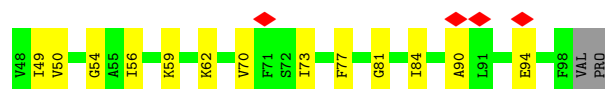
- Molecule 2: Essential MCU regulator, mitochondrial



- Molecule 2: Essential MCU regulator, mitochondrial



- Molecule 2: Essential MCU regulator, mitochondrial



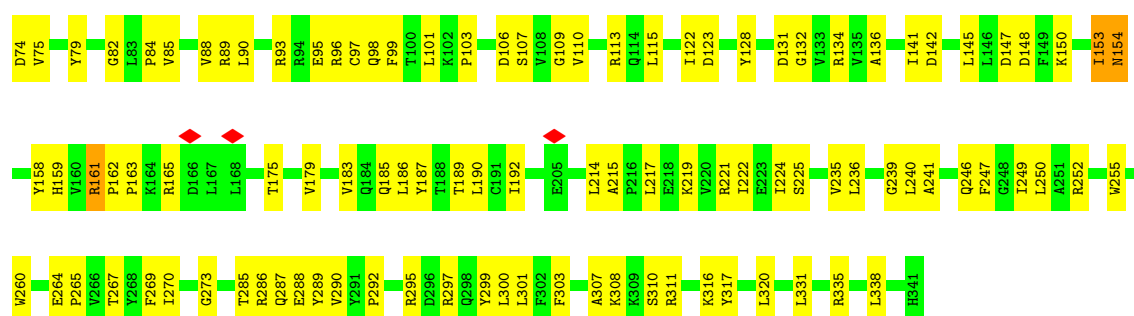
- Molecule 2: Essential MCU regulator, mitochondrial



- Molecule 2: Essential MCU regulator, mitochondrial

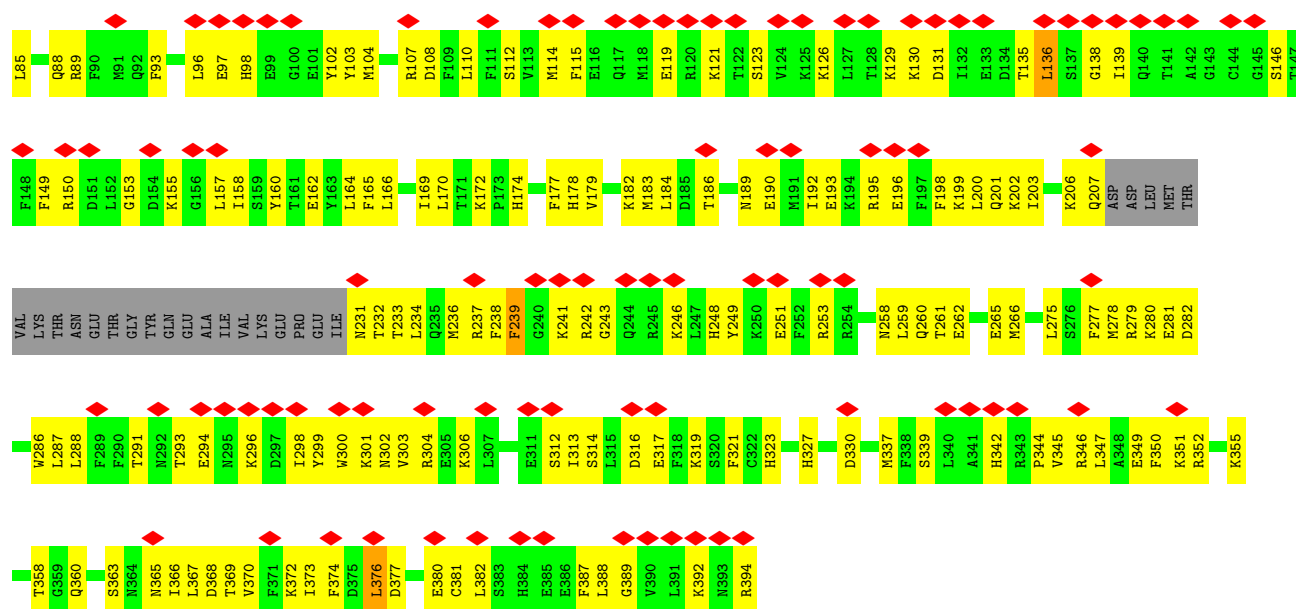
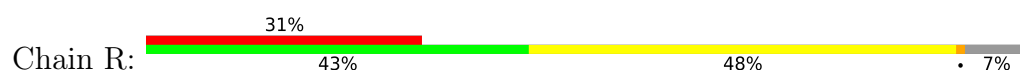


- Molecule 3: Calcium uniporter protein, mitochondrial

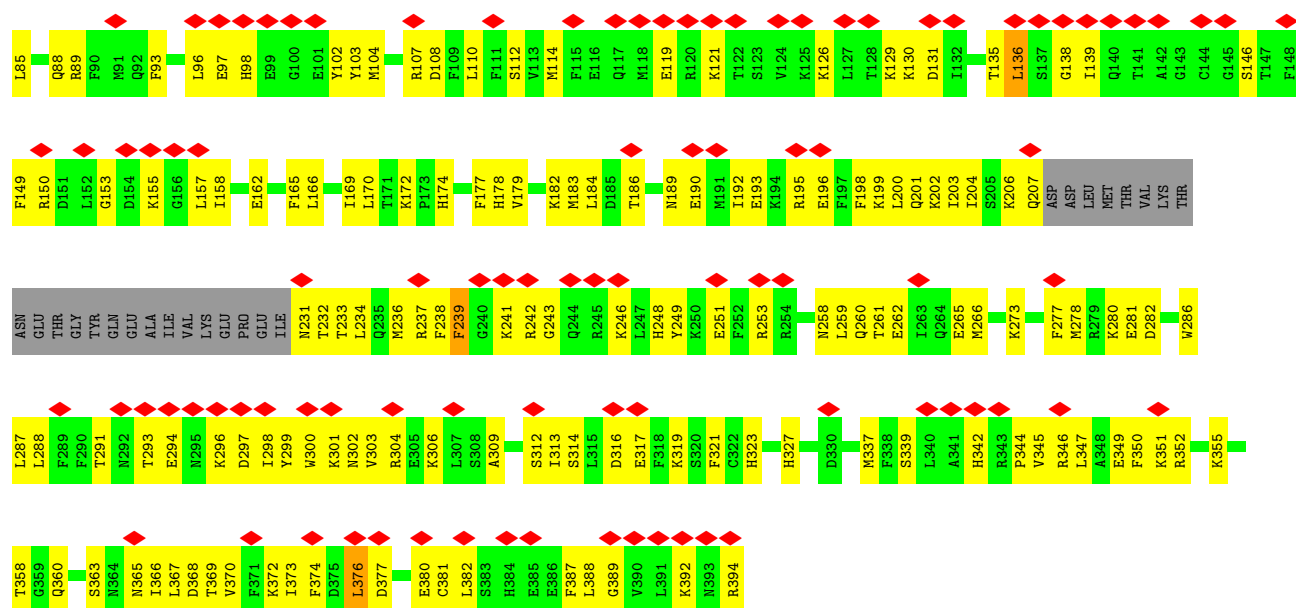
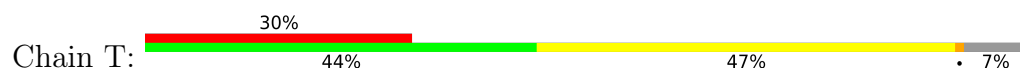


- Molecule 3: Calcium uniporter protein, mitochondrial





• Molecule 5: Calcium uptake protein 2, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	128221	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.588	Depositor
Minimum map value	-0.733	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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	0.35	0/2300	0.46	0/3114
1	E	0.36	0/2272	0.46	0/3077
1	G	0.34	0/2143	0.48	0/2898
1	I	0.34	0/2300	0.43	0/3114
1	M	0.36	0/2272	0.44	0/3077
1	O	0.33	0/2143	0.47	0/2898
2	B	0.29	0/424	0.42	0/576
2	D	0.28	0/409	0.43	0/554
2	F	0.30	0/397	0.44	0/538
2	H	0.29	0/409	0.42	0/554
2	J	0.29	0/424	0.46	0/576
2	L	0.27	0/409	0.43	0/554
2	N	0.32	0/409	0.46	0/554
2	P	0.33	0/409	0.61	0/554
3	C	0.35	0/2256	0.46	0/3054
3	K	0.35	0/2256	0.45	0/3054
4	Q	0.27	0/2175	0.49	3/2919 (0.1%)
4	S	0.27	0/2175	0.49	3/2919 (0.1%)
5	R	0.28	0/2445	0.43	0/3265
5	T	0.28	0/2445	0.43	0/3265
All	All	0.32	0/30472	0.46	6/41114 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	107	ARG	NE-CZ-NH2	6.40	123.50	120.30
4	S	107	ARG	NE-CZ-NH2	6.34	123.47	120.30
4	S	391	LEU	CA-CB-CG	5.87	128.80	115.30
4	Q	391	LEU	CA-CB-CG	5.86	128.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	107	ARG	CG-CD-NE	5.31	122.96	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2287	95	0
1	E	2226	0	2255	97	0
1	G	2102	0	2133	114	0
1	I	2254	0	2287	108	0
1	M	2226	0	2255	109	0
1	O	2102	0	2133	95	0
2	B	414	0	448	15	0
2	D	400	0	432	13	0
2	F	389	0	423	16	0
2	H	400	0	432	17	0
2	J	414	0	448	17	0
2	L	400	0	432	11	0
2	N	400	0	432	17	0
2	P	400	0	432	19	0
3	C	2211	0	2237	92	0
3	K	2211	0	2237	96	0
4	Q	2136	0	2083	96	0
4	S	2136	0	2083	99	0
5	R	2395	0	2373	163	0
5	T	2395	0	2373	162	0
6	A	1	0	0	0	0
6	I	1	0	0	0	0
All	All	29867	0	30215	1272	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 21.

The worst 5 of 1272 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)
1:I:197:LEU:HD13	1:M:104:ILE:CD1	1.59	1.33
5:R:193:GLU:HG2	5:R:239:PHE:CD1	1.66	1.31
1:G:176:LEU:HB2	1:E:167:LEU:O	1.37	1.23
1:M:153:ILE:HD11	1:M:158:TYR:CD2	1.76	1.21
5:R:193:GLU:HA	5:R:239:PHE:CE1	1.78	1.18

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	271/273 (99%)	244 (90%)	27 (10%)	0	100	100
1	E	268/273 (98%)	244 (91%)	24 (9%)	0	100	100
1	G	251/273 (92%)	230 (92%)	21 (8%)	0	100	100
1	I	271/273 (99%)	244 (90%)	27 (10%)	0	100	100
1	M	268/273 (98%)	243 (91%)	25 (9%)	0	100	100
1	O	251/273 (92%)	226 (90%)	25 (10%)	0	100	100
2	B	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
2	D	49/53 (92%)	45 (92%)	4 (8%)	0	100	100
2	F	48/53 (91%)	45 (94%)	3 (6%)	0	100	100
2	H	49/53 (92%)	45 (92%)	4 (8%)	0	100	100
2	J	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
2	L	49/53 (92%)	41 (84%)	8 (16%)	0	100	100
2	N	49/53 (92%)	45 (92%)	4 (8%)	0	100	100
2	P	49/53 (92%)	47 (96%)	2 (4%)	0	100	100
3	C	266/268 (99%)	235 (88%)	31 (12%)	0	100	100
3	K	266/268 (99%)	237 (89%)	29 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	256/339 (76%)	225 (88%)	31 (12%)	0	100	100
4	S	256/339 (76%)	225 (88%)	31 (12%)	0	100	100
5	R	283/310 (91%)	259 (92%)	24 (8%)	0	100	100
5	T	283/310 (91%)	259 (92%)	24 (8%)	0	100	100
All	All	3585/3896 (92%)	3234 (90%)	351 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/245 (100%)	245 (100%)	0	100	100
1	E	242/245 (99%)	238 (98%)	4 (2%)	60	82
1	G	227/245 (93%)	221 (97%)	6 (3%)	46	74
1	I	245/245 (100%)	245 (100%)	0	100	100
1	M	242/245 (99%)	238 (98%)	4 (2%)	60	82
1	O	227/245 (93%)	225 (99%)	2 (1%)	78	90
2	B	47/47 (100%)	46 (98%)	1 (2%)	53	78
2	D	45/47 (96%)	45 (100%)	0	100	100
2	F	44/47 (94%)	44 (100%)	0	100	100
2	H	45/47 (96%)	45 (100%)	0	100	100
2	J	47/47 (100%)	46 (98%)	1 (2%)	53	78
2	L	45/47 (96%)	45 (100%)	0	100	100
2	N	45/47 (96%)	45 (100%)	0	100	100
2	P	45/47 (96%)	44 (98%)	1 (2%)	52	77
3	C	240/240 (100%)	237 (99%)	3 (1%)	69	86
3	K	240/240 (100%)	235 (98%)	5 (2%)	53	78
4	Q	232/301 (77%)	229 (99%)	3 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	S	232/301 (77%)	229 (99%)	3 (1%)	69	86
5	R	262/283 (93%)	257 (98%)	5 (2%)	57	80
5	T	262/283 (93%)	257 (98%)	5 (2%)	57	80
All	All	3259/3494 (93%)	3216 (99%)	43 (1%)	70	86

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	213	THR
4	S	107	ARG
4	Q	440	ARG
5	R	239	PHE
4	S	440	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	K	172	ASN
1	O	318	ASN
5	T	260	GLN
3	K	194	GLN
1	O	287	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

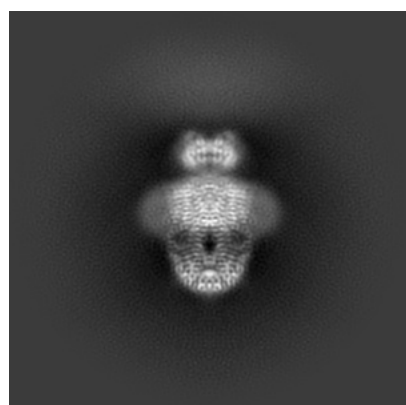
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21643. These allow visual inspection of the internal detail of the map and identification of artifacts.

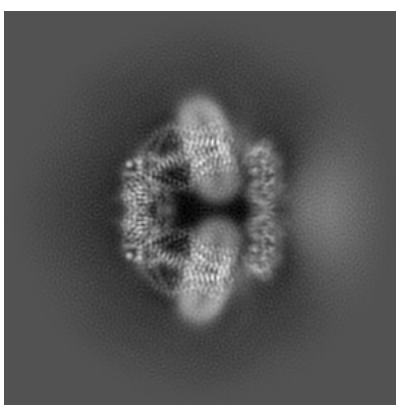
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

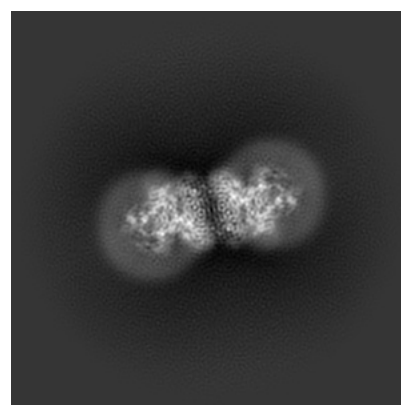
6.1.1 Primary map



X



Y

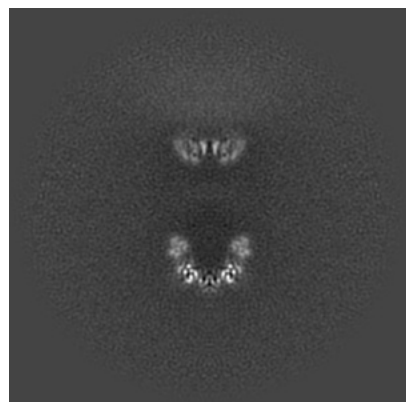


Z

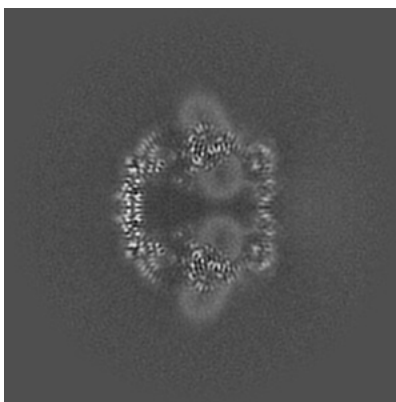
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

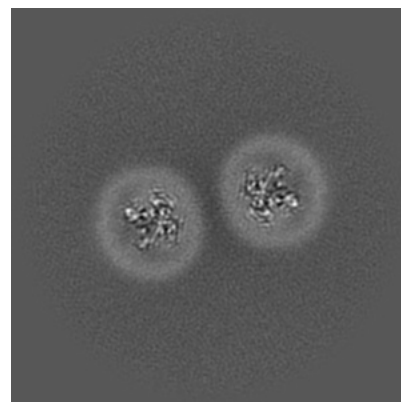
6.2.1 Primary map



X Index: 180



Y Index: 180

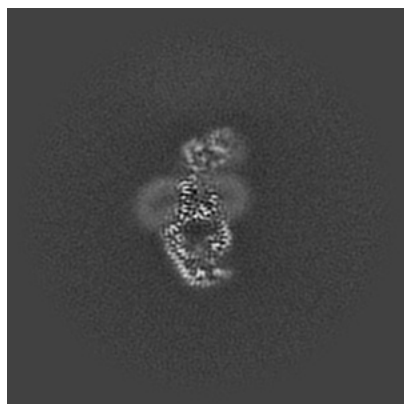


Z Index: 180

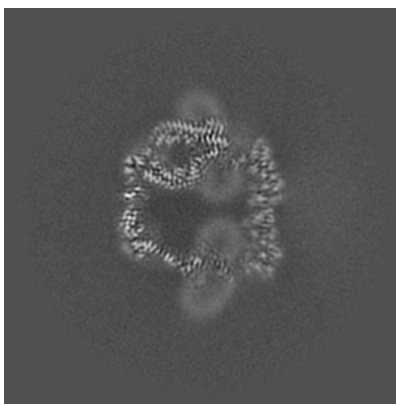
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

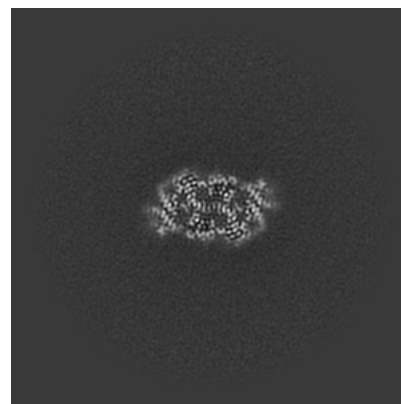
6.3.1 Primary map



X Index: 136



Y Index: 189



Z Index: 122

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

6.4 Orthogonal surface views [i](#)

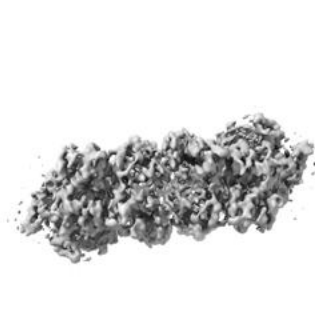
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

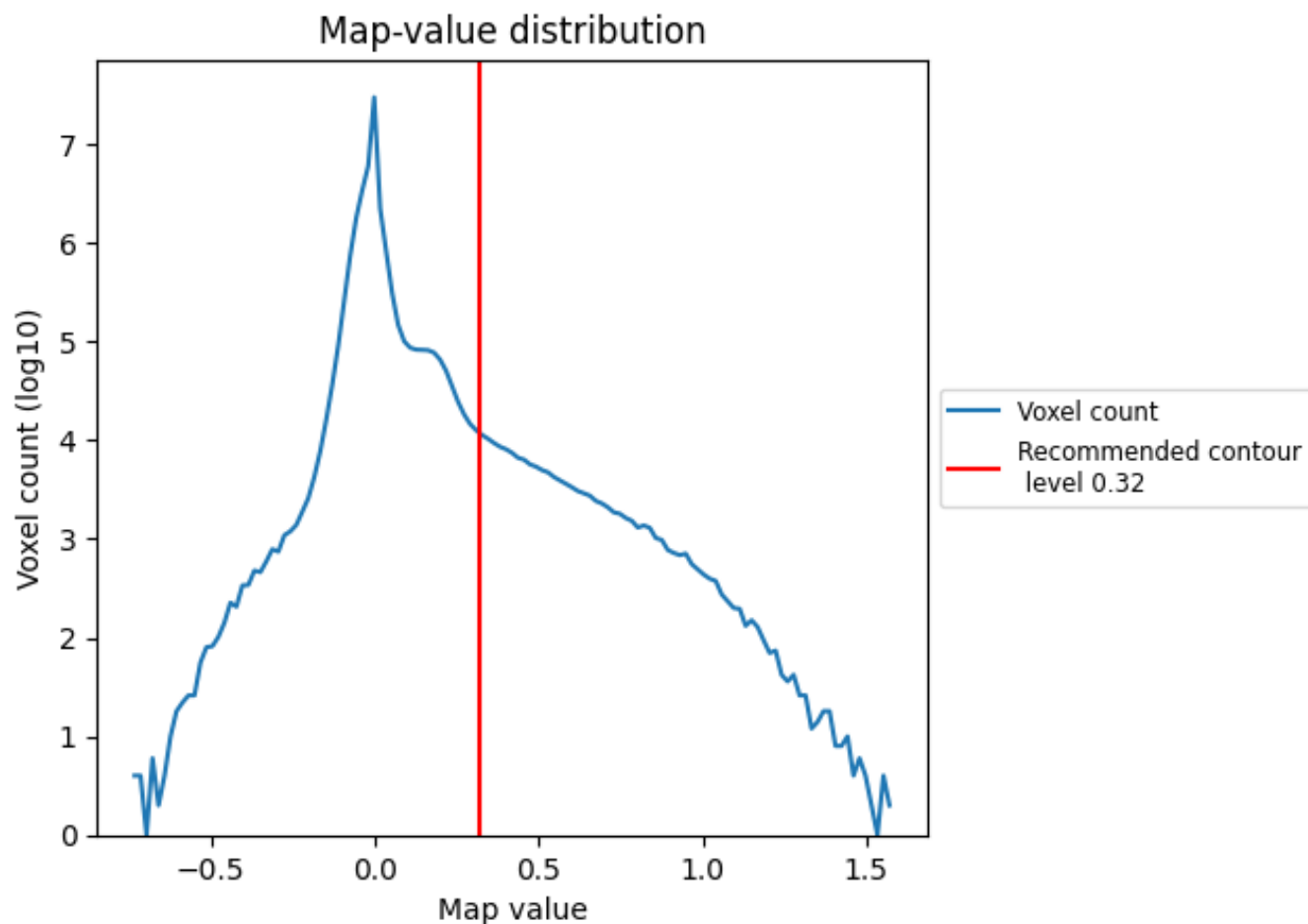
6.5 Mask visualisation

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

7 Map analysis [i](#)

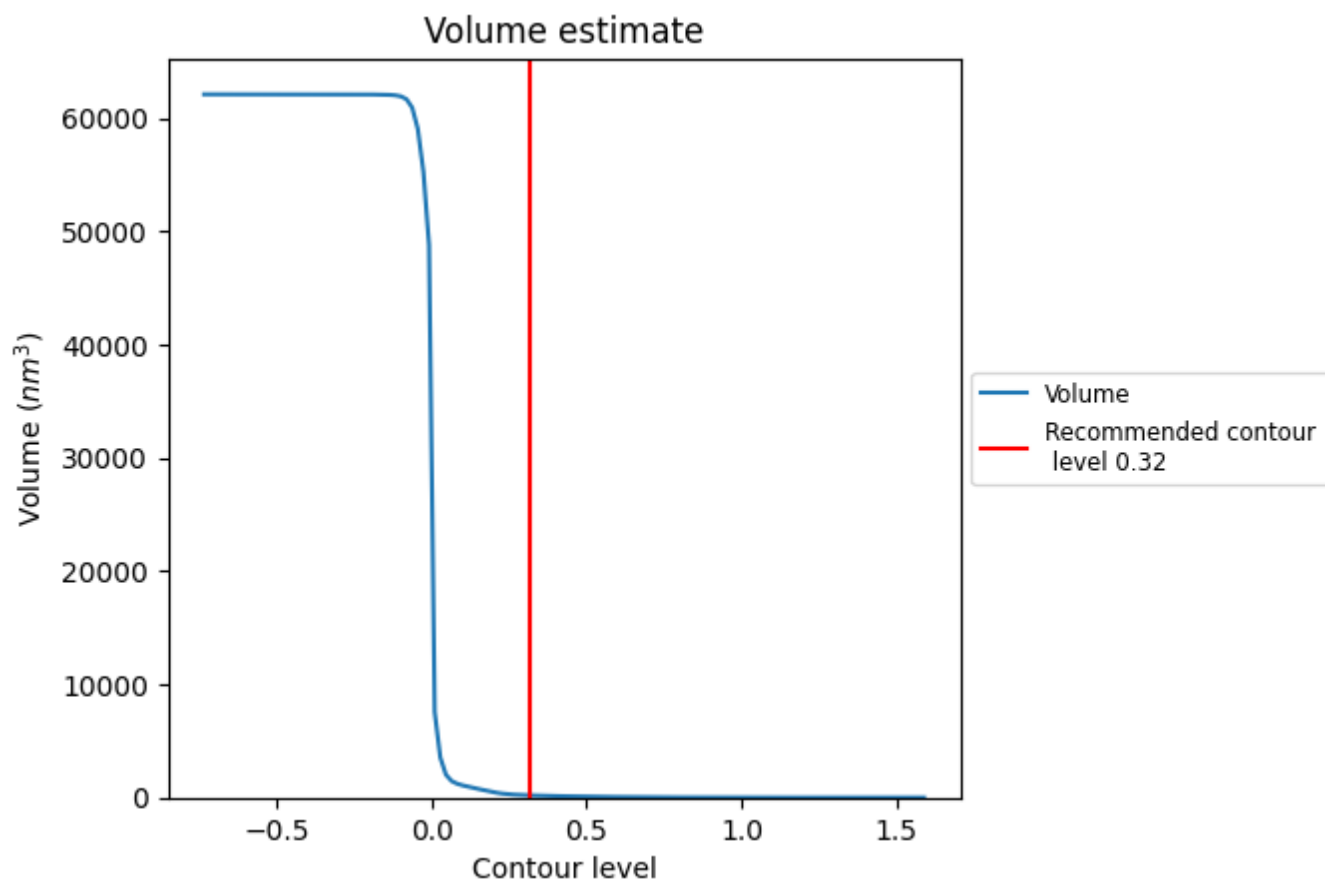
This section contains the results of statistical analysis of the map.

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.

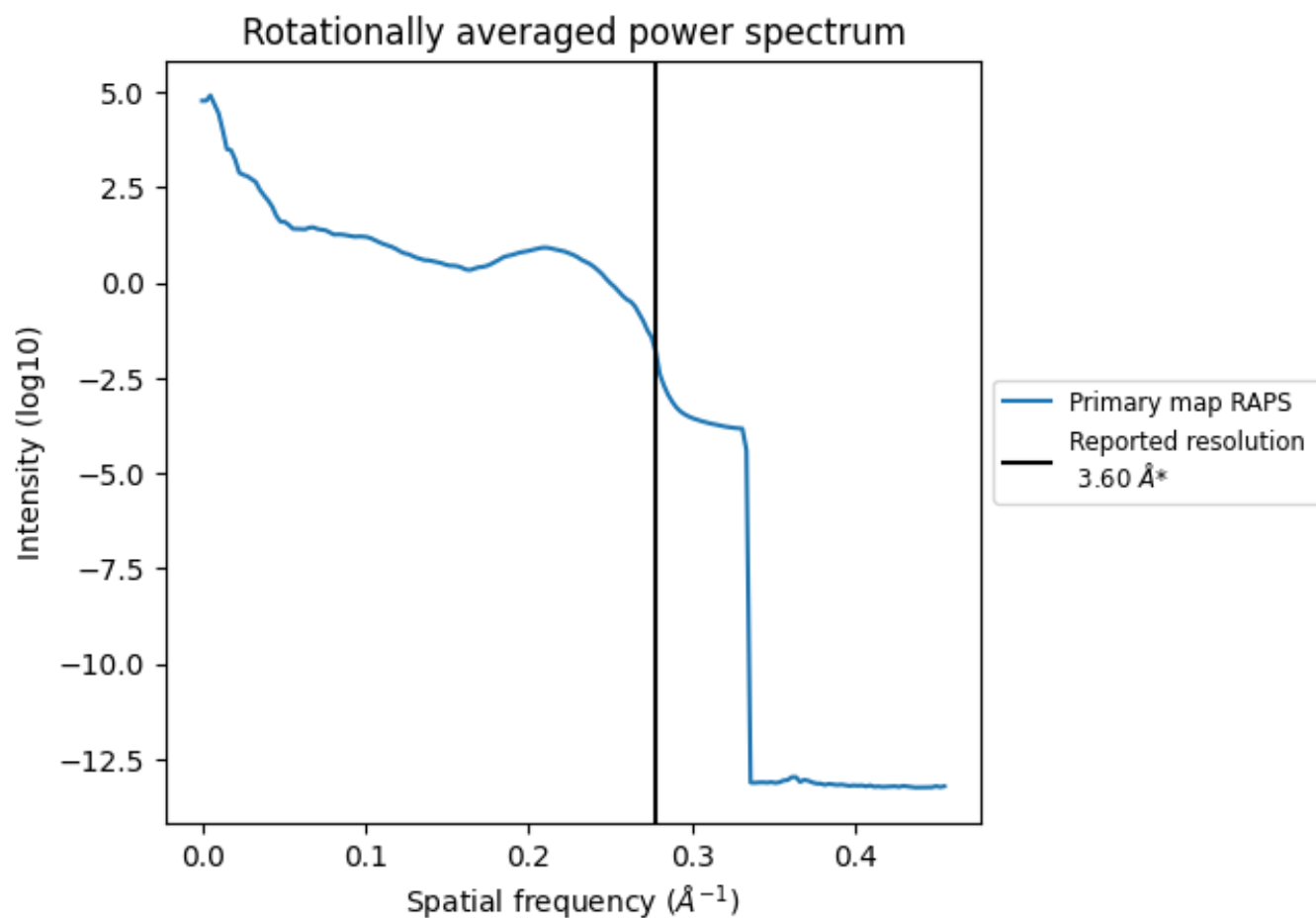
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 173 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 0.278 Å⁻¹

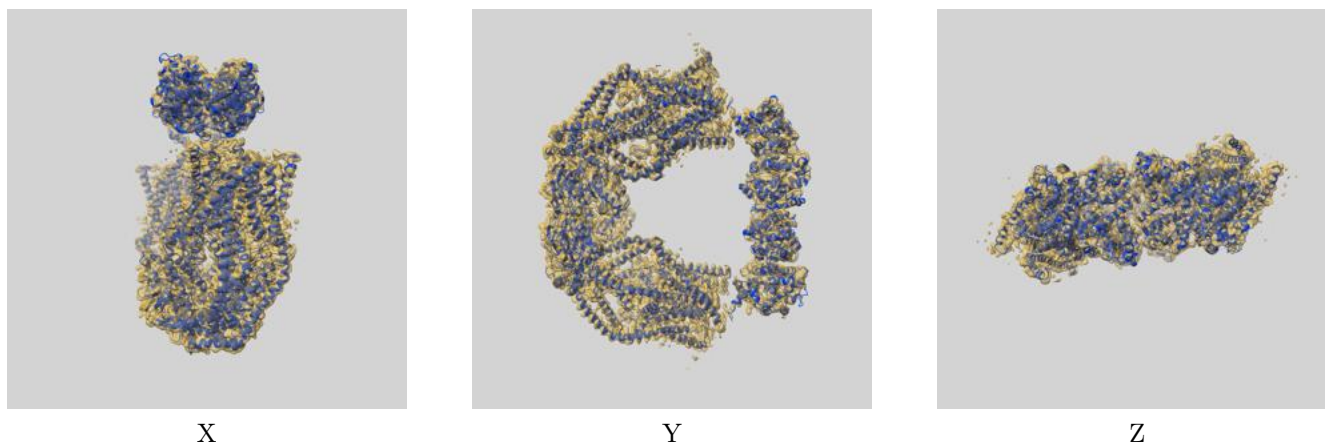
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

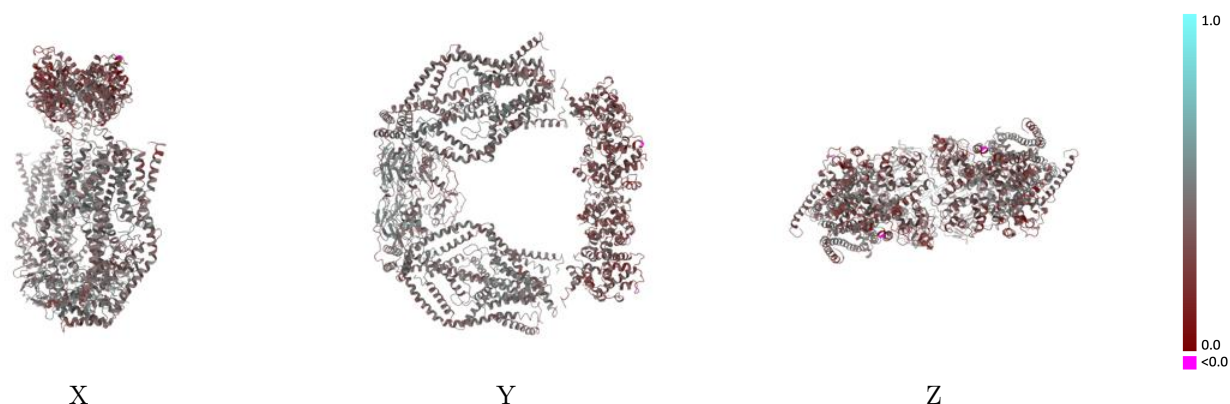
This section contains information regarding the fit between EMDB map EMD-21643 and PDB model 6WDO. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



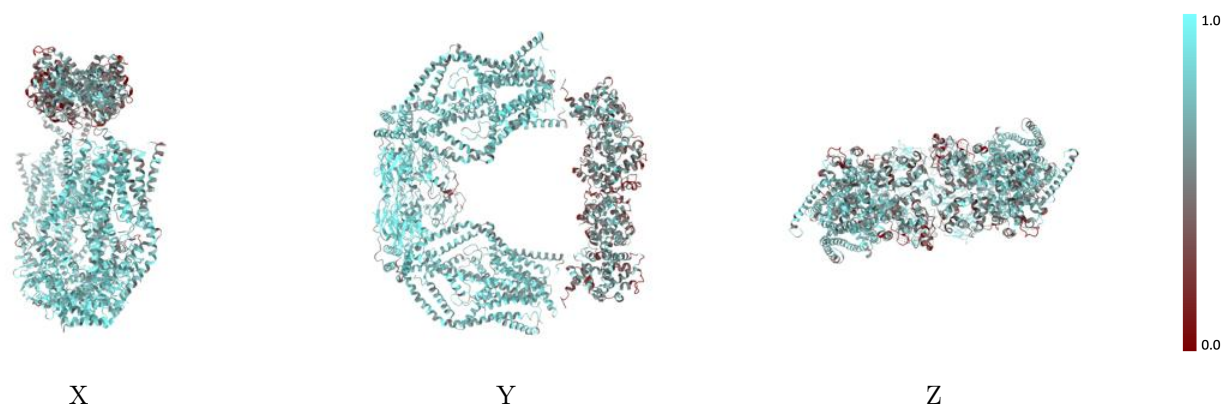
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



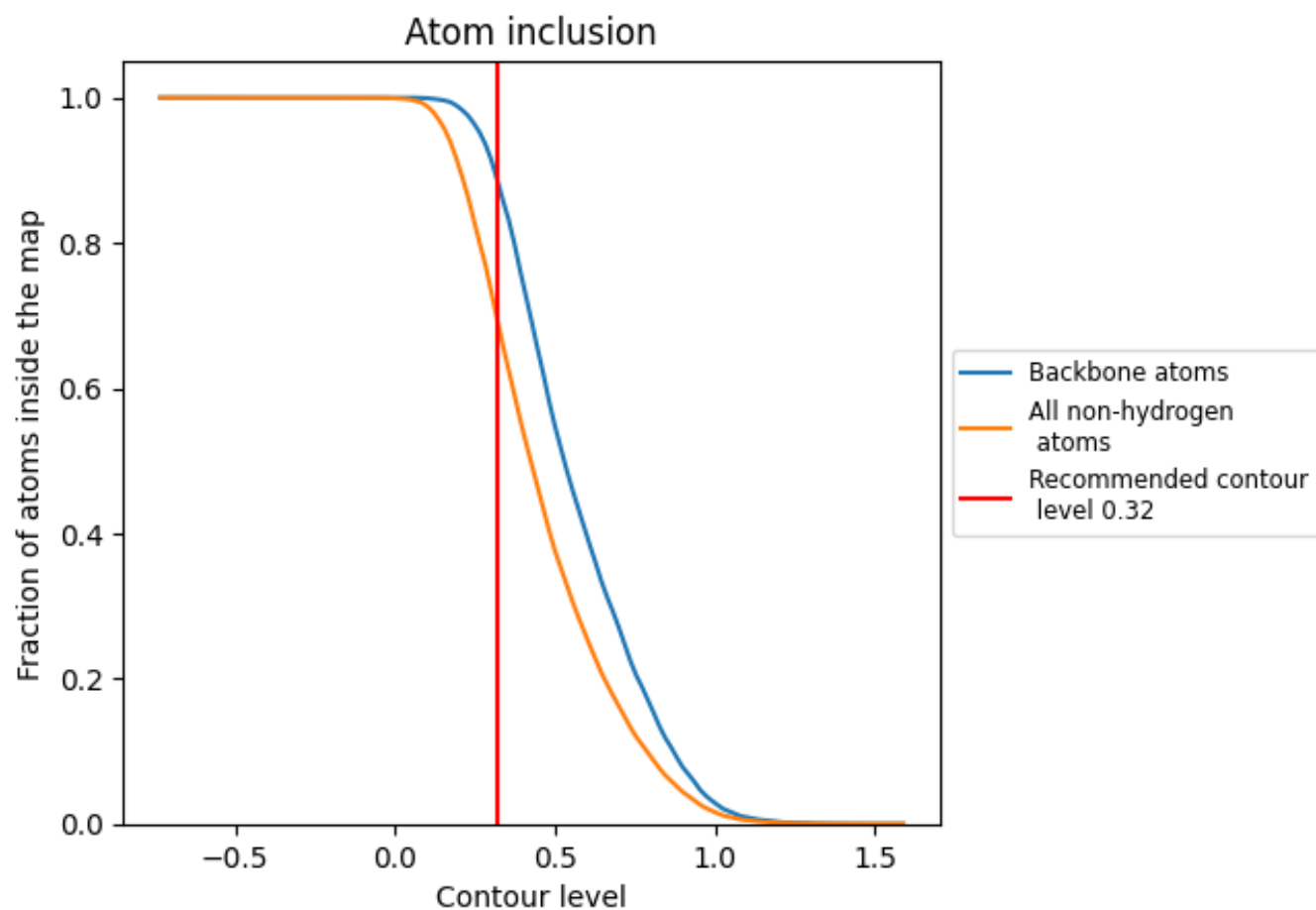
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 70% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6953	 0.4020
A	 0.7960	 0.4440
B	 0.6699	 0.4310
C	 0.7934	 0.4360
D	 0.6228	 0.4020
E	 0.8299	 0.4530
F	 0.7266	 0.4320
G	 0.7493	 0.4080
H	 0.7038	 0.4180
I	 0.7951	 0.4470
J	 0.6748	 0.4260
K	 0.7929	 0.4370
L	 0.6405	 0.4020
M	 0.8332	 0.4530
N	 0.7266	 0.4330
O	 0.7395	 0.4100
P	 0.6911	 0.4170
Q	 0.5462	 0.3280
R	 0.4858	 0.3300
S	 0.5505	 0.3280
T	 0.4845	 0.3260

