



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2025 – 07:39 PM JST

PDB ID : 9ITM
EMDB ID : EMD-60871
Title : Chloroflexus aurantiacus ATP synthase, state 1, focused refinement of FO
Authors : Zhang, X.; Wu, J.; Xu, X.
Deposited on : 2024-07-20
Resolution : 3.16 Å(reported)

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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) : 2.41.2

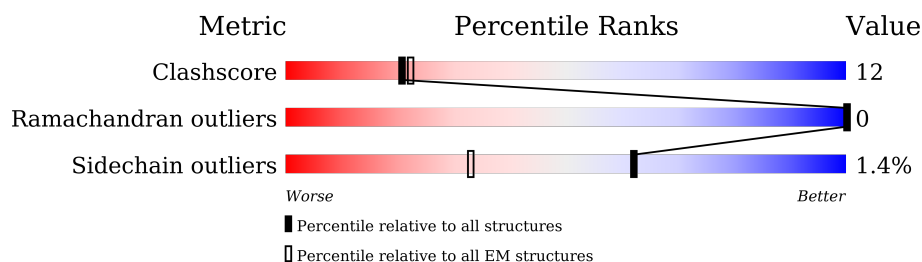
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 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 $\leq 5\%$. 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	H	76	67% 28% 5%
1	I	76	66% 29% 5%
1	J	76	59% 36% 5%
1	K	76	59% 36% 5%
1	L	76	67% 28% 5%
1	M	76	53% 42% 5%
1	N	76	68% 26% 5%
1	O	76	74% 21% 5%

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Mol	Chain	Length	Quality of chain
1	P	76	 71%24%5%
1	Q	76	 59%36%5%
2	T	312	 63%22%15%
2	Z	312	 65%18%16%
3	U	164	 23%6%71%
3	V	164	 15%8%76%
3	X	164	 18%8%74%
3	Y	164	 26%71%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10692 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 ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	72	Total	C	N	O	S	0	0
			506	336	82	87	1		
1	I	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	J	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	K	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	L	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	M	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	N	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	O	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	P	72	Total	C	N	O	S	0	0
			513	340	82	89	2		
1	Q	72	Total	C	N	O	S	0	0
			513	340	82	89	2		

- Molecule 2 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	266	Total	C	N	O	S	0	0
			2064	1405	317	336	6		
2	Z	261	Total	C	N	O	S	0	0
			2038	1392	312	328	6		

- Molecule 3 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	48	Total	C	N	O	S	0	0
			396	261	68	65	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	40	Total	C	N	O	S	0	0
			335	224	60	50	1		
3	X	42	Total	C	N	O	S	0	0
			348	233	62	52	1		
3	Y	47	Total	C	N	O	S	0	0
			388	256	67	64	1		

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.

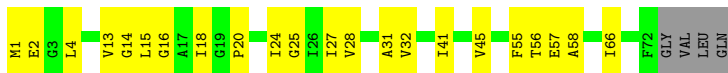
- Molecule 1: ATP synthase subunit c

Chain H: 



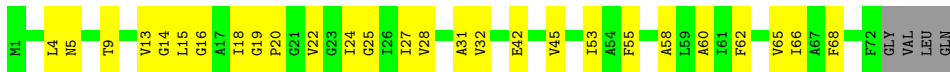
- Molecule 1: ATP synthase subunit c

Chain I: 



- Molecule 1: ATP synthase subunit c

Chain J: 



- Molecule 1: ATP synthase subunit c

Chain K: 



- Molecule 1: ATP synthase subunit c

Chain L: 



- Molecule 1: ATP synthase subunit c

M1		L4	N5	T9	A10	L11	A12	V13	G14	L15	G16	A17	L18	G19	P20		I24	G25	I26	I27	V28		A31		I35	N38	I41	E42		V45		I51	G52	I53	A54	F55	T56	E57	A58	L59	A60	T61	F62	G63		I66		F72	GLY	VAL	LEU
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- Chain N:  68% 26% 5%

#1	N5	T9	V13	G14	L15	I18	G19	P20	I24	I27	V28	A31	V32	I35	I41	V45	F55	A58	F62	V65	I66	F72	G73	V74	L75	I76	G77	V78	L79	I80	G81	V82	L83	I84	G85	V86	L87	I88	G89	V90	L91	I92	G93	V94	L95	I96	G97	V98	L99	I100	G101	V102	L103	I104	G105	V106	L107	I108	G109	V110	L111	I112	G113	V114	L115	I116	G117	V118	L119	I120	G121	V122	L123	I124	G125	V126	L127	I128	G129	V130	L131	I132	G133	V134	L135	I136	G137	V138	L139	I140	G141	V142	L143	I144	G145	V146	L147	I148	G149	V150	L151	I152	G153	V154	L155	I156	G157	V158	L159	I160	G161	V162	L163	I164	G165	V166	L167	I168	G169	V170	L171	I172	G173	V174	L175	I176	G177	V178	L179	I180	G181	V182	L183	I184	G185	V186	L187	I188	G189	V190	L191	I192	G193	V194	L195	I196	G197	V198	L199	I200	G201	V202	L203	I204	G205	V206	L207	I208	G209	V210	L211	I212	G213	V214	L215	I216	G217	V218	L219	I220	G221	V222	L223	I224	G225	V226	L227	I228	G229	V230	L231	I232	G233	V234	L235	I236	G237	V238	L239	I240	G241	V242	L243	I244	G245	V246	L247	I248	G249	V250	L251	I252	G253	V254	L255	I256	G257	V258	L259	I260	G261	V262	L263	I264	G265	V266	L267	I268	G269	V270	L271	I272	G273	V274	L275	I276	G277	V278	L279	I280	G281	V282	L283	I284	G285	V286	L287	I288	G289	V290	L291	I292	G293	V294	L295	I296	G297	V298	L299	I300	G301	V302	L303	I304	G305	V306	L307	I308	G309	V310	L311	I312	G313	V314	L315	I316	G317	V318	L319	I320	G321	V322	L323	I324	G325	V326	L327	I328	G329	V330	L331	I332	G333	V334	L335	I336	G337	V338	L339	I340	G341	V342	L343	I344	G345	V346	L347	I348	G349	V350	L351	I352	G353	V354	L355	I356	G357	V358	L359	I360	G361	V362	L363	I364	G365	V366	L367	I368	G369	V370	L371	I372	G373	V374	L375	I376	G377	V378	L379	I380	G381	V382	L383	I384	G385	V386	L387	I388	G389	V390	L391	I392	G393	V394	L395	I396	G397	V398	L399	I400	G401	V402	L403	I404	G405	V406	L407	I408	G409	V410	L411	I412	G413	V414	L415	I416	G417	V418	L419	I420	G421	V422	L423	I424	G425	V426	L427	I428	G429	V430	L431	I432	G433	V434	L435	I436	G437	V438	L439	I440	G441	V442	L443	I444	G445	V446	L447	I448	G449	V450	L451	I452	G453	V454	L455	I456	G457	V458	L459	I460	G461	V462	L463	I464	G465	V466	L467	I468	G469	V470	L471	I472	G473	V474	L475	I476	G477	V478	L479	I480	G481	V482	L483	I484	G485	V486	L487	I488	G489	V490	L491	I492	G493	V494	L495	I496	G497	V498	L499	I500	G501	V502	L503	I504	G505	V506	L507	I508	G509	V510	L511	I512	G513	V514	L515	I516	G517	V518	L519	I520	G521	V522	L523	I524	G525	V526	L527	I528	G529	V530	L531	I532	G533	V534	L535	I536	G537	V538	L539	I540	G541	V542	L543	I544	G545	V546	L547	I548	G549	V550	L551	I552	G553	V554	L555	I556	G557	V558	L559	I560	G561	V562	L563	I564	G565	V566	L56
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- Chain 0:  74% 21% 5%

M1		L4	N5	L6	V13	G14	L15	I18	G19	G25	I26	I27	V32	I35	G36	I41	E42	R43	R44	V45	F72	GLY	VAL	LEU	GIN
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- Chain P:  71% 24% 5%

M1	V7	G14	L15	G16	A17	L18	G19	P20	G25	L26	L27	A31	V32	N38	L41	E42	F65	A58	L59	A60	V65	I66	F72	GLY	VAL	LEU	GLN
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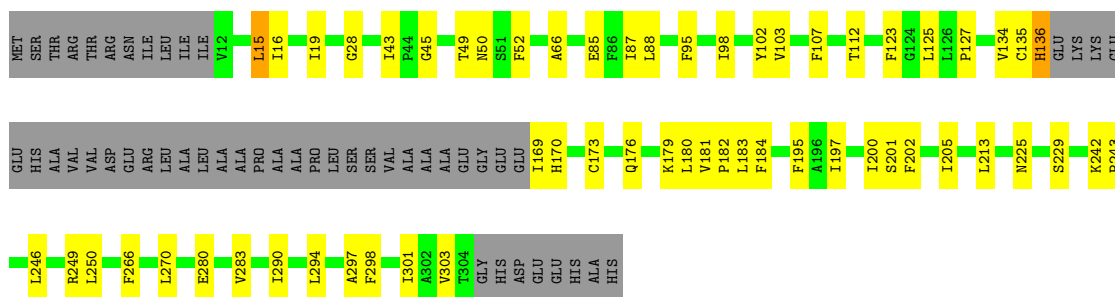
- Chain Q:  59% 36% 5%

F1		N5	T9	A12	V13	G14	L15	G16	G19	P20	G23	I24	G25	I26	I27	V28	V32	I35	G36	R37	I41	E42	Y48	I51	T56	E57	A58	I61	I66	A67	F72	GLY	VAL	LEU	ILE
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- Chain T:  63% 22% • 15%

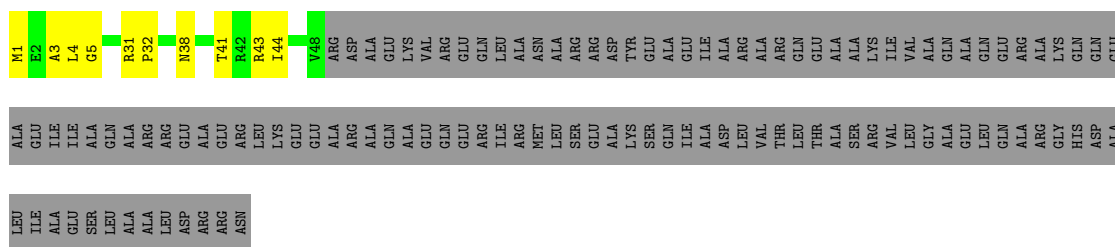
[illegible]

- Chain Z: 65% 18% 16%



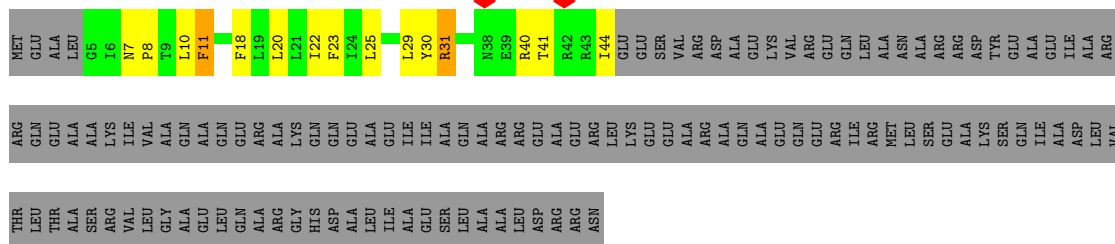
• Molecule 3: ATP synthase subunit b

Chain U: 23% 6% 71%



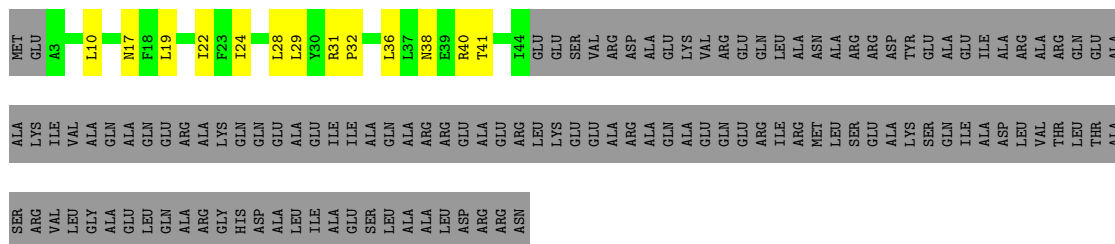
• Molecule 3: ATP synthase subunit b

Chain V: 15% 8% . 76%



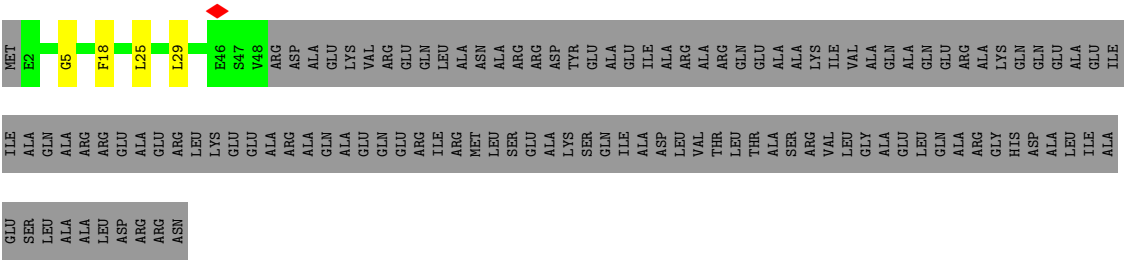
• Molecule 3: ATP synthase subunit b

Chain X: 18% 8% 74%



• Molecule 3: ATP synthase subunit b

Chain Y: 26% . 71%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	231462	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.644	Depositor
Minimum map value	-0.292	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	H	0.32	0/513	0.45	0/698
1	I	0.33	0/520	0.46	0/706
1	J	0.32	0/520	0.46	0/706
1	K	0.32	0/520	0.45	0/706
1	L	0.33	0/520	0.46	0/706
1	M	0.32	0/520	0.45	0/706
1	N	0.32	0/520	0.46	0/706
1	O	0.32	0/520	0.46	0/706
1	P	0.30	0/520	0.45	0/706
1	Q	0.32	0/520	0.47	0/706
2	T	0.28	0/2125	0.46	0/2898
2	Z	0.29	0/2098	0.44	0/2861
3	U	0.24	0/401	0.47	0/542
3	V	0.25	0/340	0.51	0/460
3	X	0.26	0/353	0.50	0/478
3	Y	0.24	0/393	0.48	0/532
All	All	0.30	0/10903	0.46	0/14823

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 [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	H	506	0	535	18	0
1	I	513	0	546	20	0
1	J	513	0	546	25	0
1	K	513	0	546	22	0
1	L	513	0	546	19	0
1	M	513	0	546	29	0
1	N	513	0	546	20	0
1	O	513	0	546	17	0
1	P	513	0	546	18	0
1	Q	513	0	546	25	0
2	T	2064	0	2113	52	0
2	Z	2038	0	2102	46	0
3	U	396	0	433	6	0
3	V	335	0	373	12	0
3	X	348	0	389	10	0
3	Y	388	0	421	3	0
All	All	10692	0	11280	259	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 12.

The worst 5 of 259 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:M:56:THR:HG22	1:N:24:ILE:HG13	1.61	0.82
1:P:66:ILE:HG13	1:Q:13:VAL:HG21	1.64	0.80
1:H:19:GLY:HA3	1:I:18:ILE:HA	1.66	0.78
1:L:66:ILE:HG13	1:M:13:VAL:HG21	1.68	0.76
1:I:27:ILE:HG13	1:J:25:GLY:HA2	1.68	0.76

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
1	I	70/76 (92%)	68 (97%)	2 (3%)	0	100	100
1	J	70/76 (92%)	67 (96%)	3 (4%)	0	100	100
1	K	70/76 (92%)	65 (93%)	5 (7%)	0	100	100
1	L	70/76 (92%)	67 (96%)	3 (4%)	0	100	100
1	M	70/76 (92%)	69 (99%)	1 (1%)	0	100	100
1	N	70/76 (92%)	70 (100%)	0	0	100	100
1	O	70/76 (92%)	66 (94%)	4 (6%)	0	100	100
1	P	70/76 (92%)	69 (99%)	1 (1%)	0	100	100
1	Q	70/76 (92%)	69 (99%)	1 (1%)	0	100	100
2	T	262/312 (84%)	243 (93%)	19 (7%)	0	100	100
2	Z	257/312 (82%)	242 (94%)	15 (6%)	0	100	100
3	U	46/164 (28%)	45 (98%)	1 (2%)	0	100	100
3	V	38/164 (23%)	37 (97%)	1 (3%)	0	100	100
3	X	40/164 (24%)	40 (100%)	0	0	100	100
3	Y	45/164 (27%)	43 (96%)	2 (4%)	0	100	100
All	All	1388/2040 (68%)	1328 (96%)	60 (4%)	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	H	48/53 (91%)	48 (100%)	0	100	100
1	I	50/53 (94%)	50 (100%)	0	100	100
1	J	50/53 (94%)	49 (98%)	1 (2%)	50	72
1	K	50/53 (94%)	49 (98%)	1 (2%)	50	72
1	L	50/53 (94%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	50/53 (94%)	50 (100%)	0	100	100
1	N	50/53 (94%)	50 (100%)	0	100	100
1	O	50/53 (94%)	50 (100%)	0	100	100
1	P	50/53 (94%)	50 (100%)	0	100	100
1	Q	50/53 (94%)	49 (98%)	1 (2%)	50	72
2	T	213/251 (85%)	208 (98%)	5 (2%)	45	69
2	Z	212/251 (84%)	209 (99%)	3 (1%)	62	80
3	U	44/131 (34%)	43 (98%)	1 (2%)	45	69
3	V	37/131 (28%)	34 (92%)	3 (8%)	9	32
3	X	38/131 (29%)	38 (100%)	0	100	100
3	Y	43/131 (33%)	43 (100%)	0	100	100
All	All	1085/1556 (70%)	1070 (99%)	15 (1%)	62	80

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	277	TYR
2	Z	136	HIS
3	U	43	ARG
2	Z	195	PHE
3	V	31	ARG

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

Mol	Chain	Res	Type
2	T	253	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

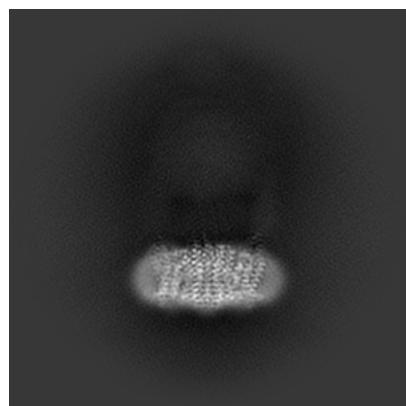
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60871. These allow visual inspection of the internal detail of the map and identification of artifacts.

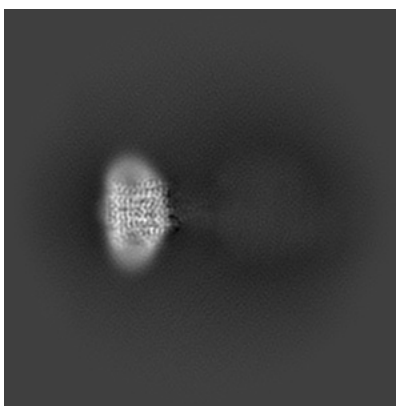
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

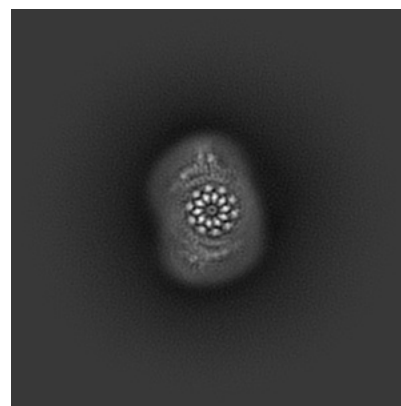
6.1.1 Primary map



X

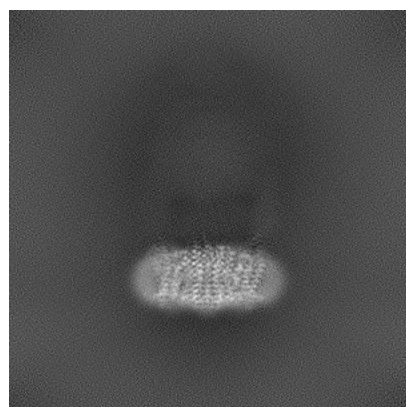


Y

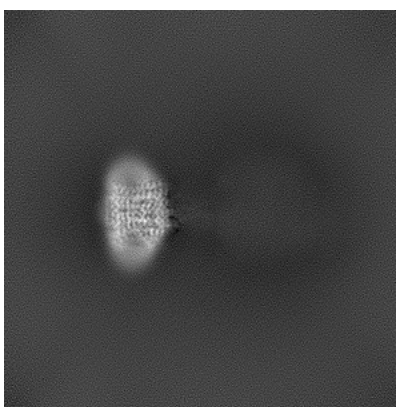


Z

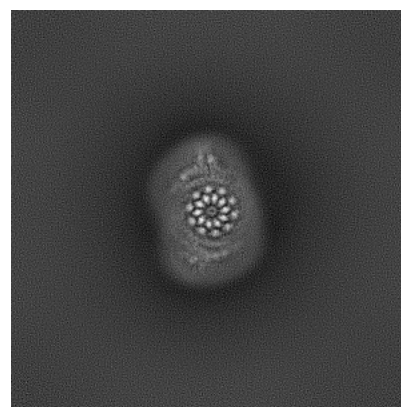
6.1.2 Raw map



X



Y

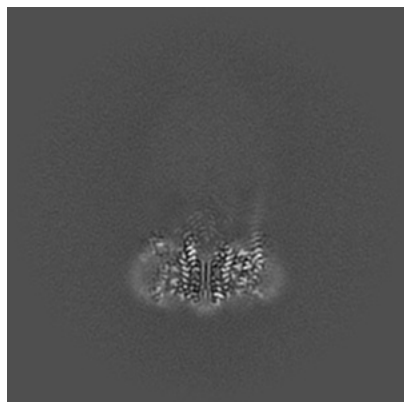


Z

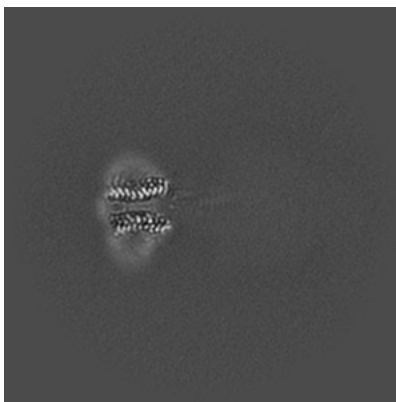
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

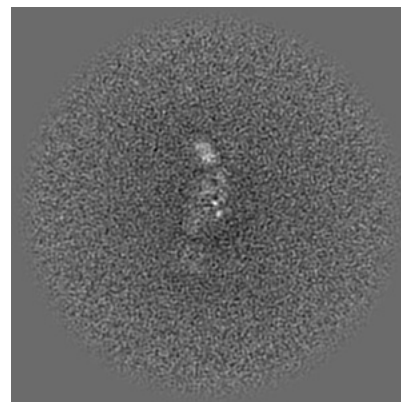
6.2.1 Primary map



X Index: 200

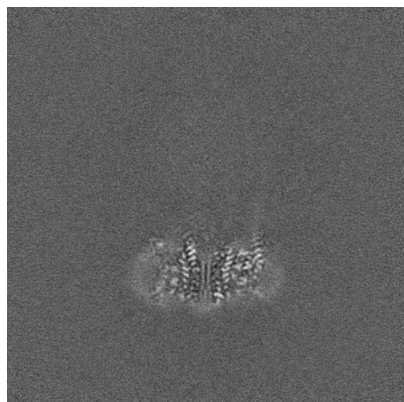


Y Index: 200

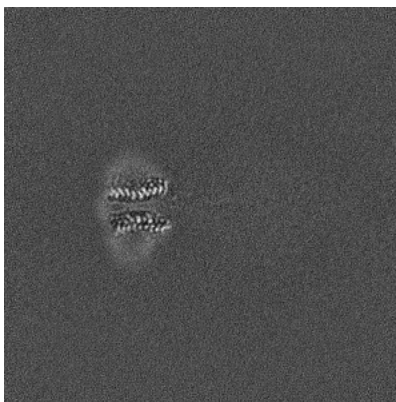


Z Index: 200

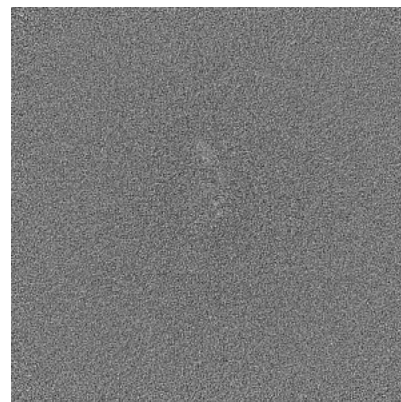
6.2.2 Raw map



X Index: 200



Y Index: 200

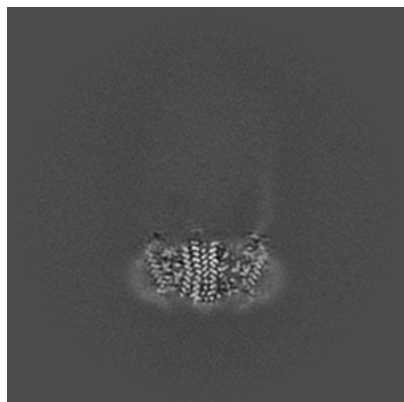


Z Index: 200

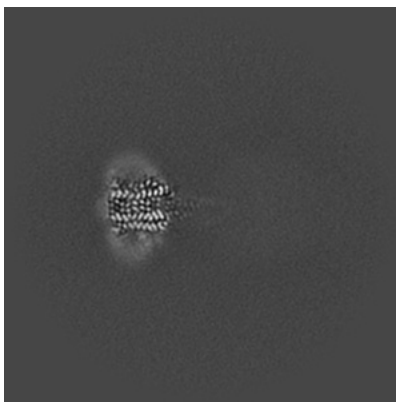
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

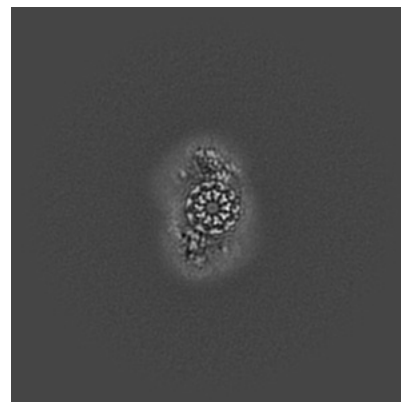
6.3.1 Primary map



X Index: 189

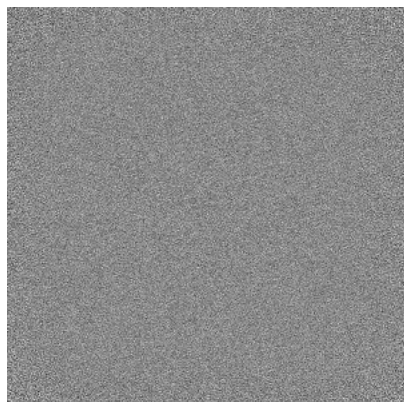


Y Index: 190

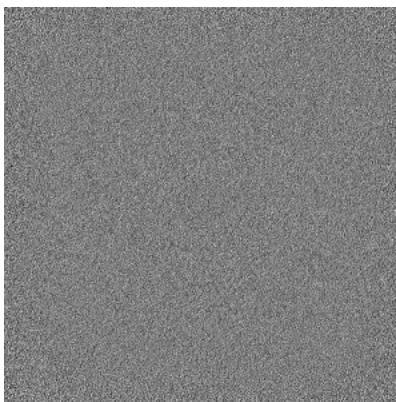


Z Index: 145

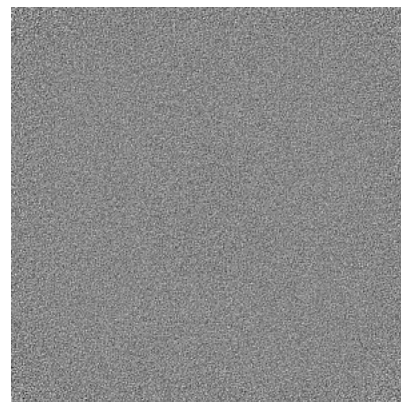
6.3.2 Raw map



X Index: 0



Y Index: 0

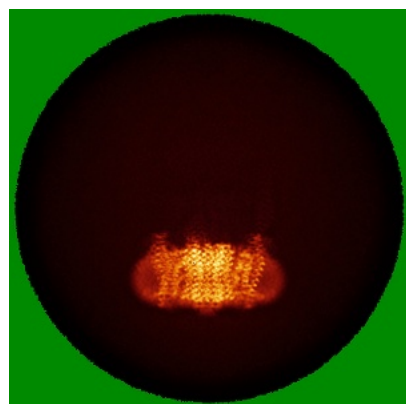


Z Index: 0

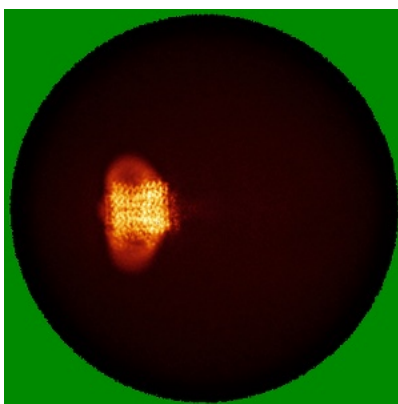
The images above show the largest variance slices of the map in three orthogonal directions.

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

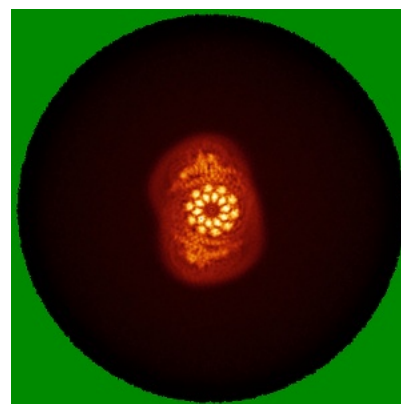
6.4.1 Primary map



X

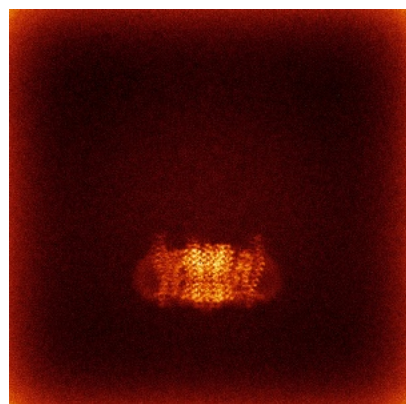


Y

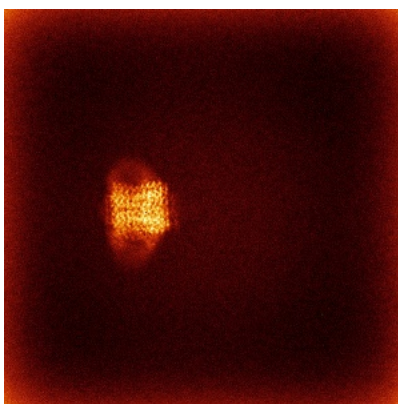


Z

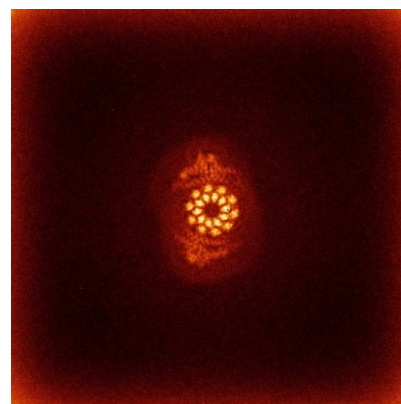
6.4.2 Raw map



X



Y

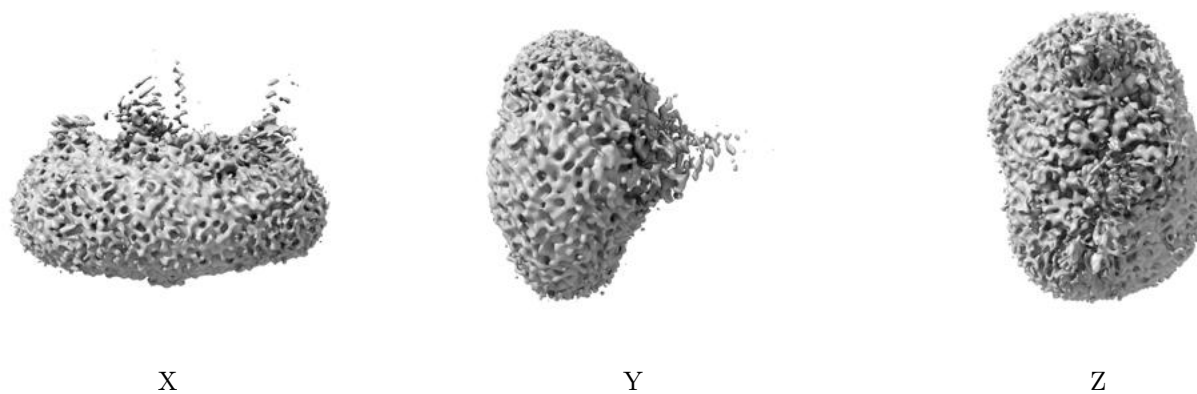


Z

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

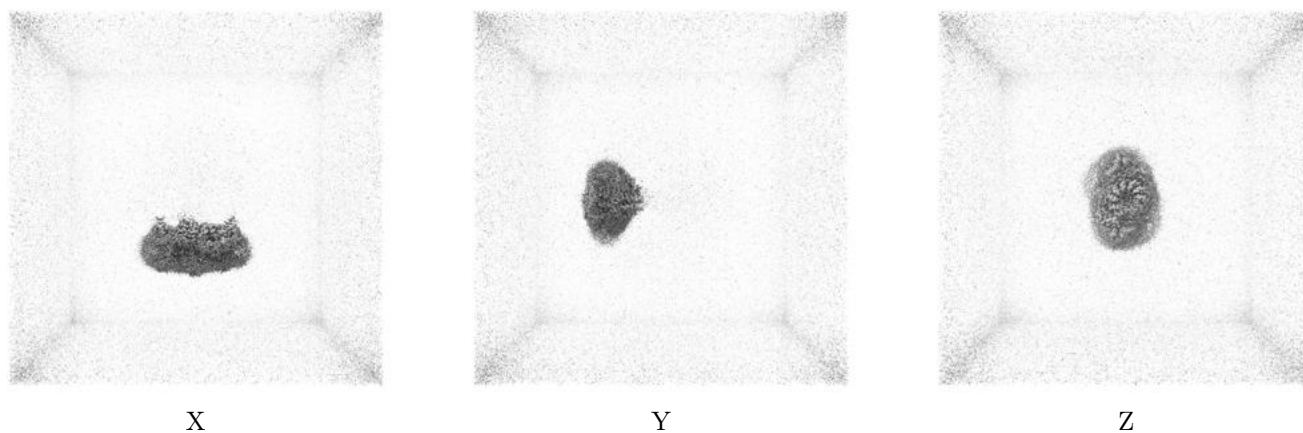
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

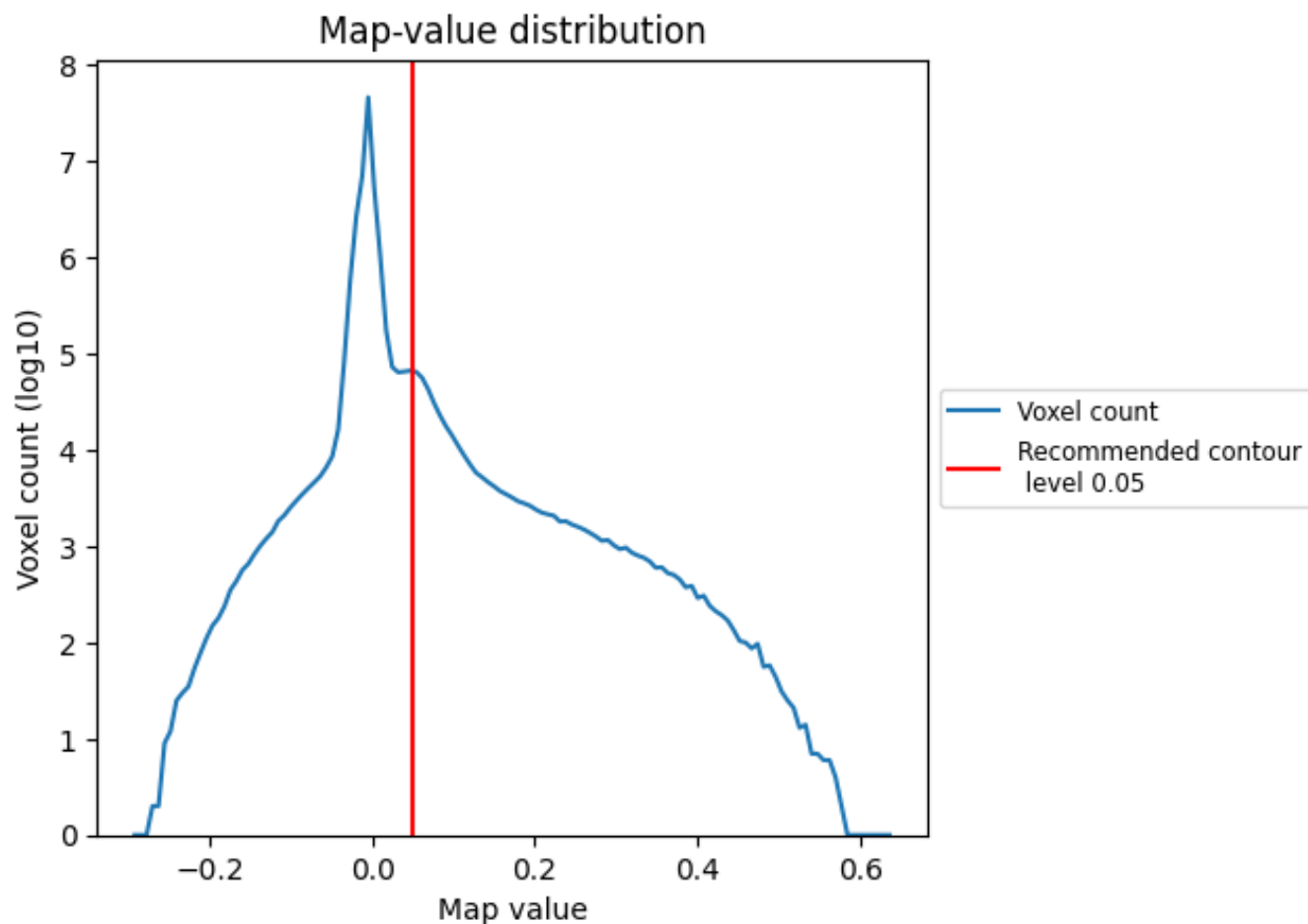
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

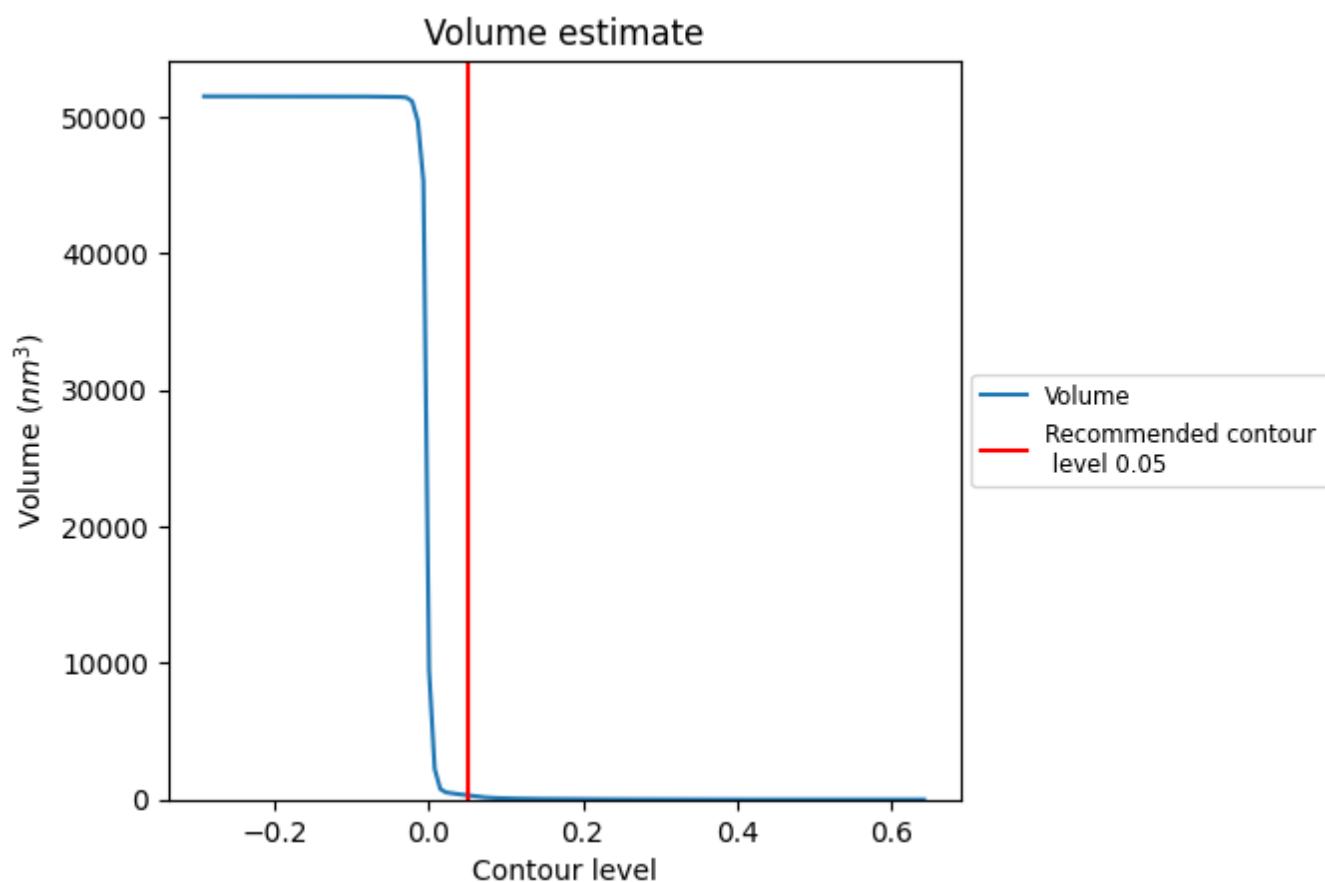
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

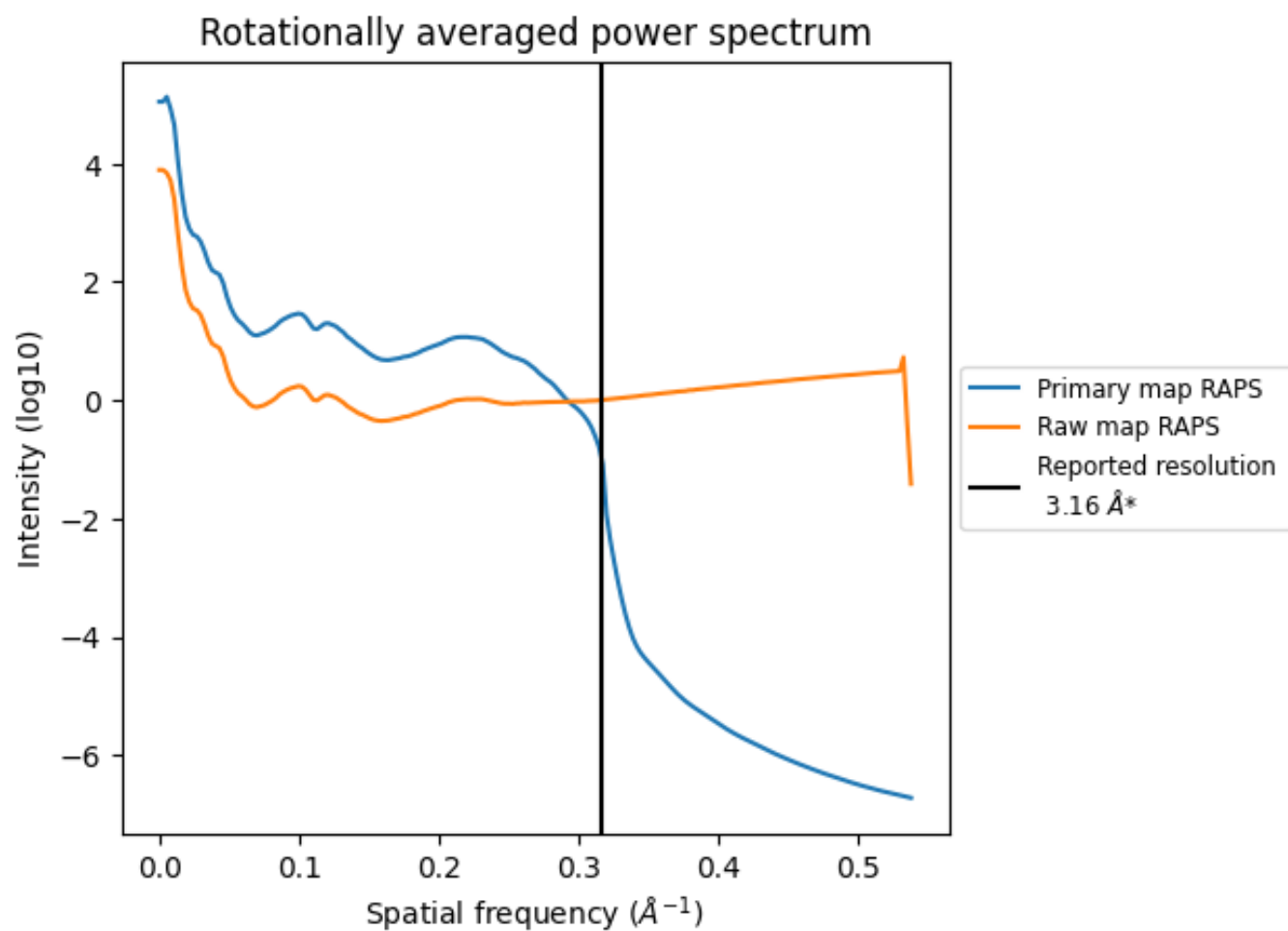
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm³; this corresponds to an approximate mass of 281 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 ⓘ

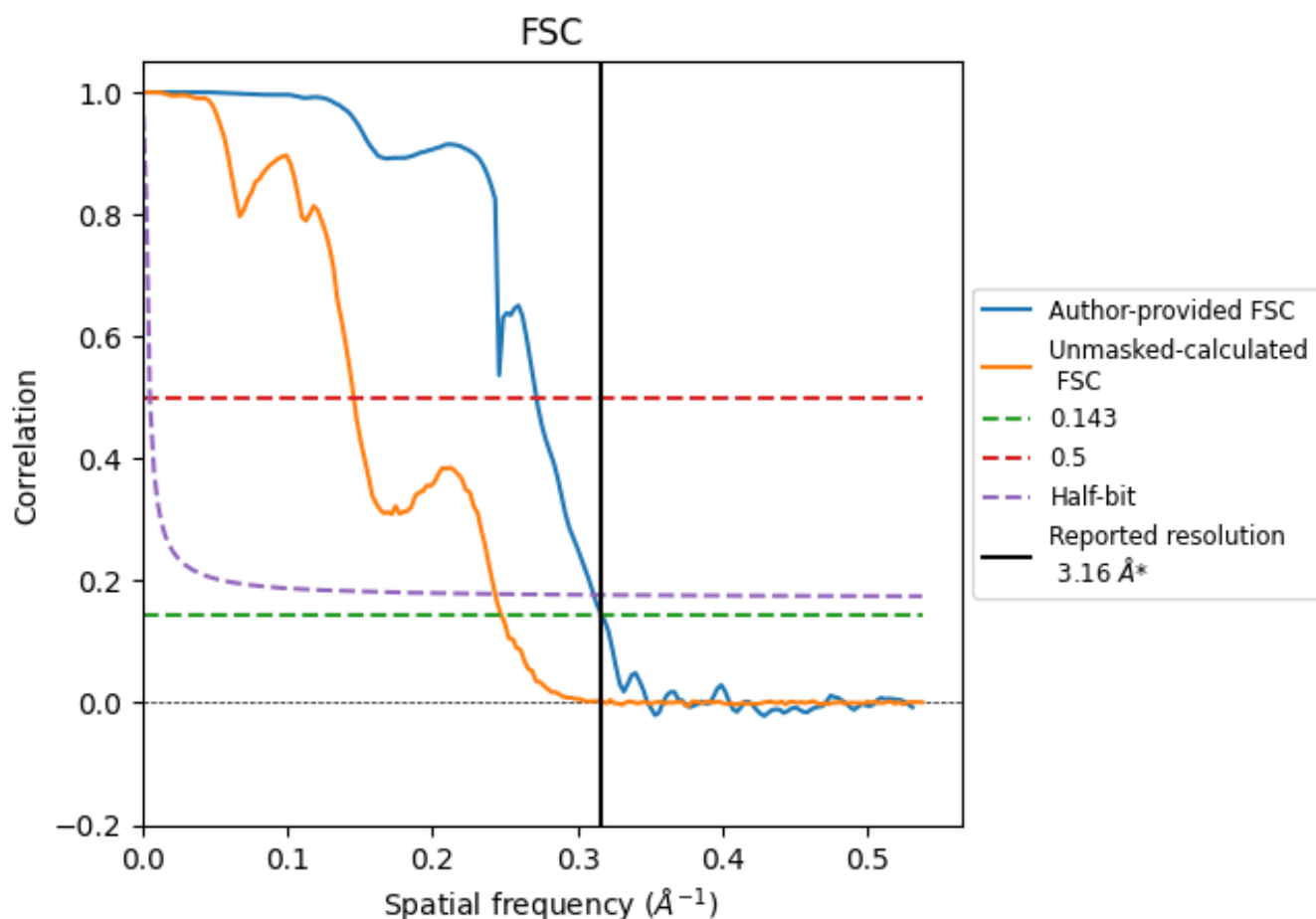


*Reported resolution corresponds to spatial frequency of 0.316 \AA^{-1}

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 0.316 \AA^{-1}

8.2 Resolution estimates [i](#)

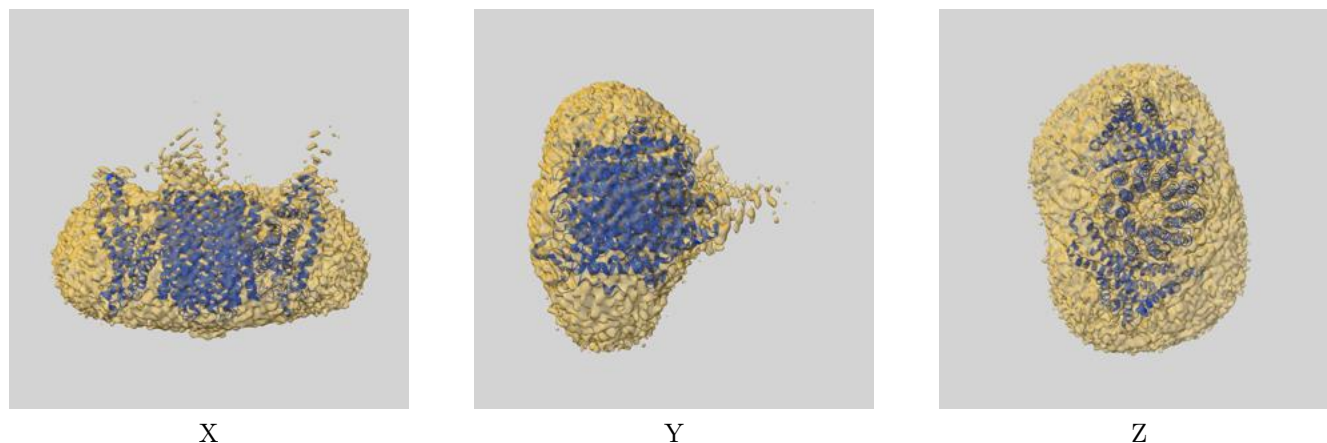
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.68	3.21
Unmasked-calculated*	4.04	6.86	4.11

*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 4.04 differs from the reported value 3.16 by more than 10 %

9 Map-model fit [i](#)

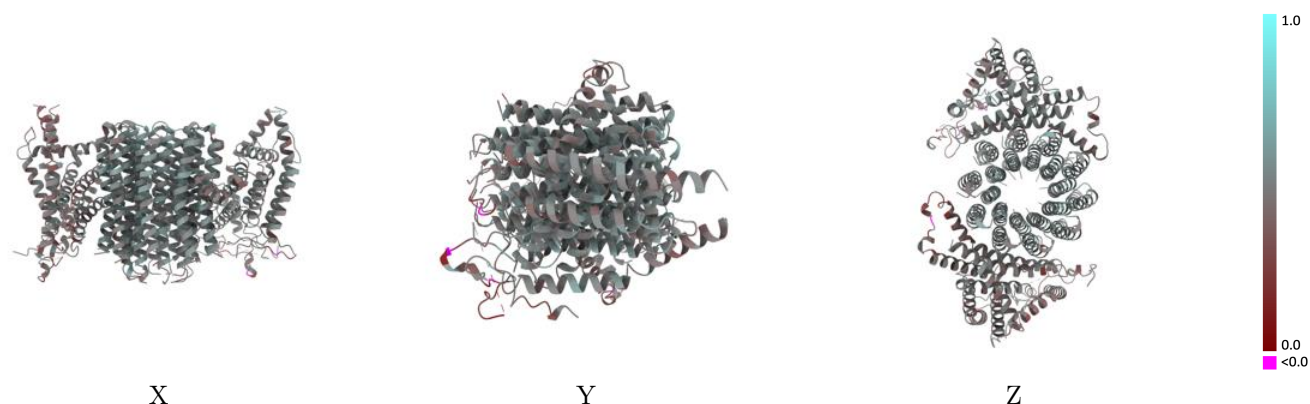
This section contains information regarding the fit between EMDB map EMD-60871 and PDB model 9ITM. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



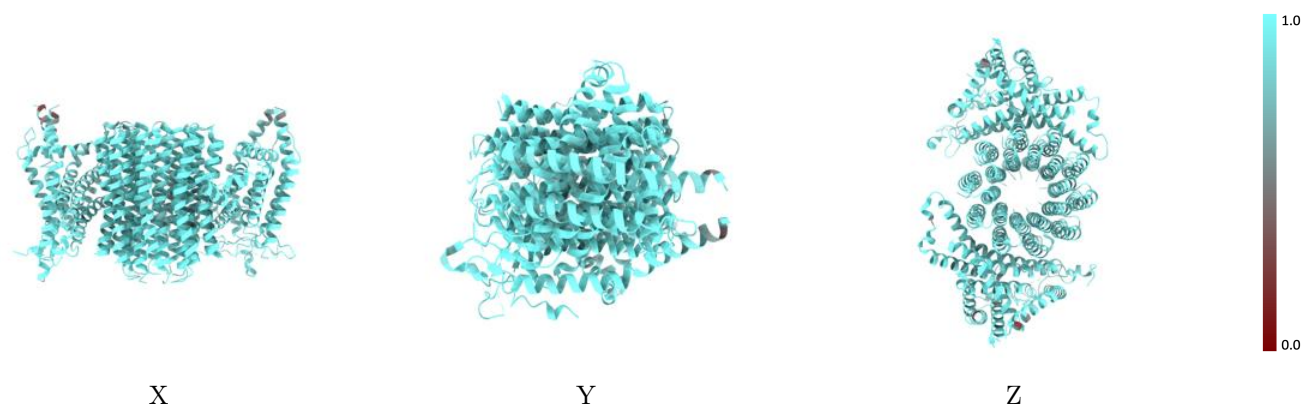
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



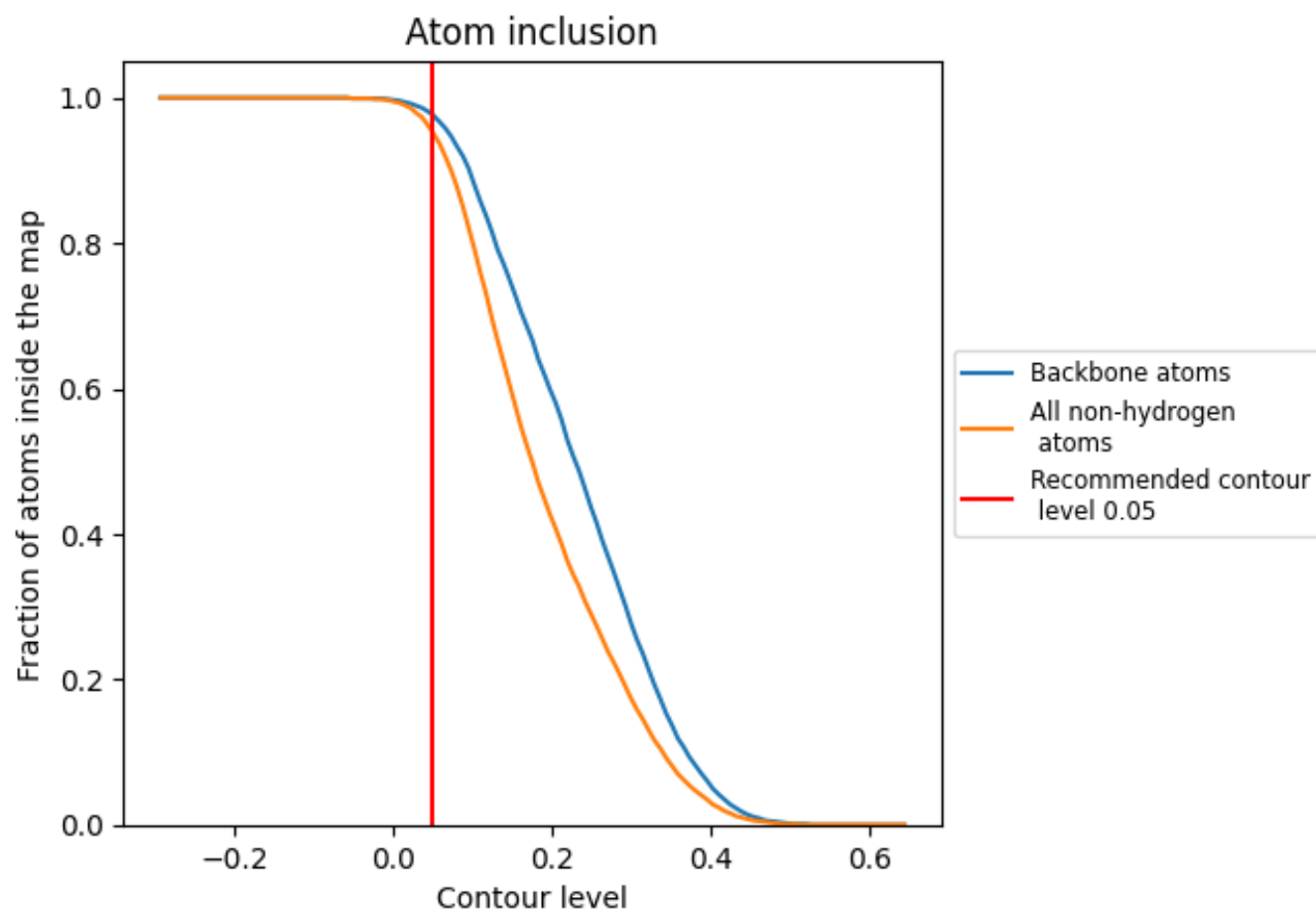
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4740
H	 0.9740	 0.5150
I	 0.9670	 0.5110
J	 0.9690	 0.5100
K	 0.9610	 0.5090
L	 0.9690	 0.5130
M	 0.9610	 0.5090
N	 0.9720	 0.5040
O	 0.9740	 0.5040
P	 0.9720	 0.5080
Q	 0.9740	 0.5090
T	 0.9640	 0.4550
U	 0.9250	 0.4730
V	 0.8670	 0.4210
X	 0.9080	 0.4690
Y	 0.9070	 0.4350
Z	 0.9360	 0.4240

