wwPDB EM Validation Summary Report

Mar 8, 2026 – 03:19 AM UTC

PDB ID	:	6O7U / pdb_00006o7u
EMDB ID	:	EMD-0645
Title	:	Saccharomyces cerevisiae V-ATPase Stv1-VO
Authors	:	Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.
Deposited on	:	2019-03-08
Resolution	:	3.10 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:

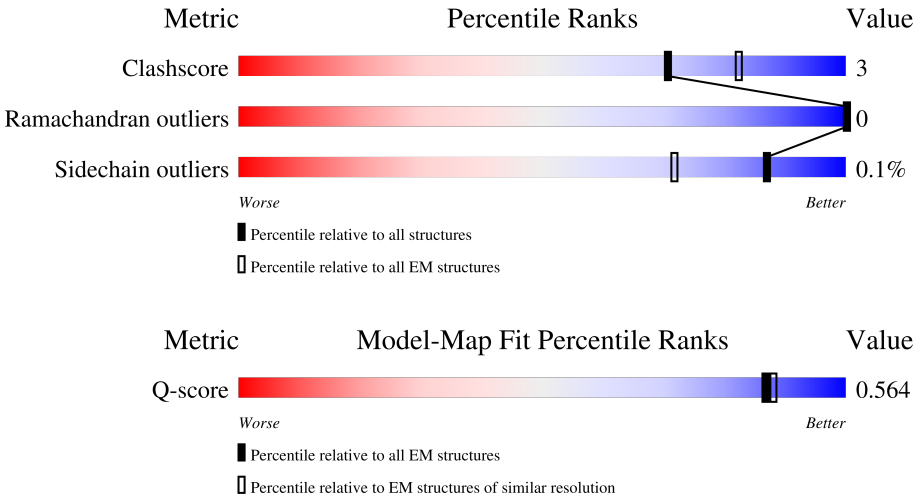
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	912	71% 7% 22%
2	b	265	16% 83%
3	c	213	79% 14% 8%
4	d	345	6% 90% 9%

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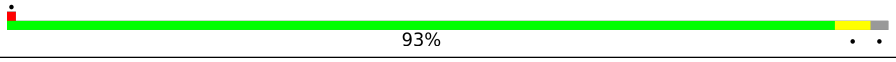
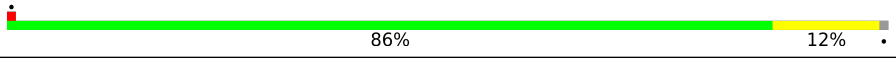
Mol	Chain	Length	Quality of chain
5	e	73	
6	f	85	
7	g	160	
7	h	160	
7	i	160	
7	j	160	
7	k	160	
7	l	160	
7	m	160	
7	n	160	
8	o	164	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21268 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 V-type proton ATPase subunit a, Golgi isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	713	5665	3710	917	1001	37	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	891	ASP	-	SEE REMARK 999	UNP P37296
a	892	TYR	-	SEE REMARK 999	UNP P37296
a	893	LYS	-	SEE REMARK 999	UNP P37296
a	894	ASP	-	SEE REMARK 999	UNP P37296
a	895	HIS	-	SEE REMARK 999	UNP P37296
a	896	ASP	-	SEE REMARK 999	UNP P37296
a	897	GLY	-	SEE REMARK 999	UNP P37296
a	898	ASP	-	SEE REMARK 999	UNP P37296
a	899	TYR	-	SEE REMARK 999	UNP P37296
a	900	LYS	-	SEE REMARK 999	UNP P37296
a	901	ASP	-	SEE REMARK 999	UNP P37296
a	902	HIS	-	SEE REMARK 999	UNP P37296
a	903	ASP	-	SEE REMARK 999	UNP P37296
a	904	ILE	-	SEE REMARK 999	UNP P37296
a	905	ASP	-	SEE REMARK 999	UNP P37296
a	906	TYR	-	SEE REMARK 999	UNP P37296
a	907	LYS	-	SEE REMARK 999	UNP P37296
a	908	ASP	-	SEE REMARK 999	UNP P37296
a	909	ASP	-	SEE REMARK 999	UNP P37296
a	910	ASP	-	SEE REMARK 999	UNP P37296
a	911	ASP	-	SEE REMARK 999	UNP P37296
a	912	LYS	-	SEE REMARK 999	UNP P37296

- Molecule 2 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	44	Total	C	N	O	S	0	0
			330	224	47	57	2		

- Molecule 3 is a protein called V-type proton ATPase subunit c".

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	197	Total	C	N	O	S	0	0
			1466	977	227	255	7		

- Molecule 4 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	343	Total	C	N	O	S	0	0
			2720	1732	450	527	11		

- Molecule 5 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	64	Total	C	N	O	S	0	0
			512	344	83	79	6		

- Molecule 6 is a protein called Putative protein YPR170W-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	61	Total	C	N	O	S	0	0
			463	307	71	82	3		

- Molecule 7 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	153	Total	C	N	O	S	0	0
			1094	723	176	188	7		
7	h	157	Total	C	N	O	S	0	0
			1125	742	180	196	7		
7	i	157	Total	C	N	O	S	0	0
			1125	742	180	196	7		
7	j	156	Total	C	N	O	S	0	0
			1116	737	179	193	7		
7	k	158	Total	C	N	O	S	0	0
			1132	746	181	198	7		
7	l	157	Total	C	N	O	S	0	0
			1125	742	180	196	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	158	Total	C	N	O	S	0	0
			1131	745	181	197	8		
7	n	158	Total	C	N	O	S	0	0
			1131	745	181	197	8		

- Molecule 8 is a protein called V-type proton ATPase subunit c'.

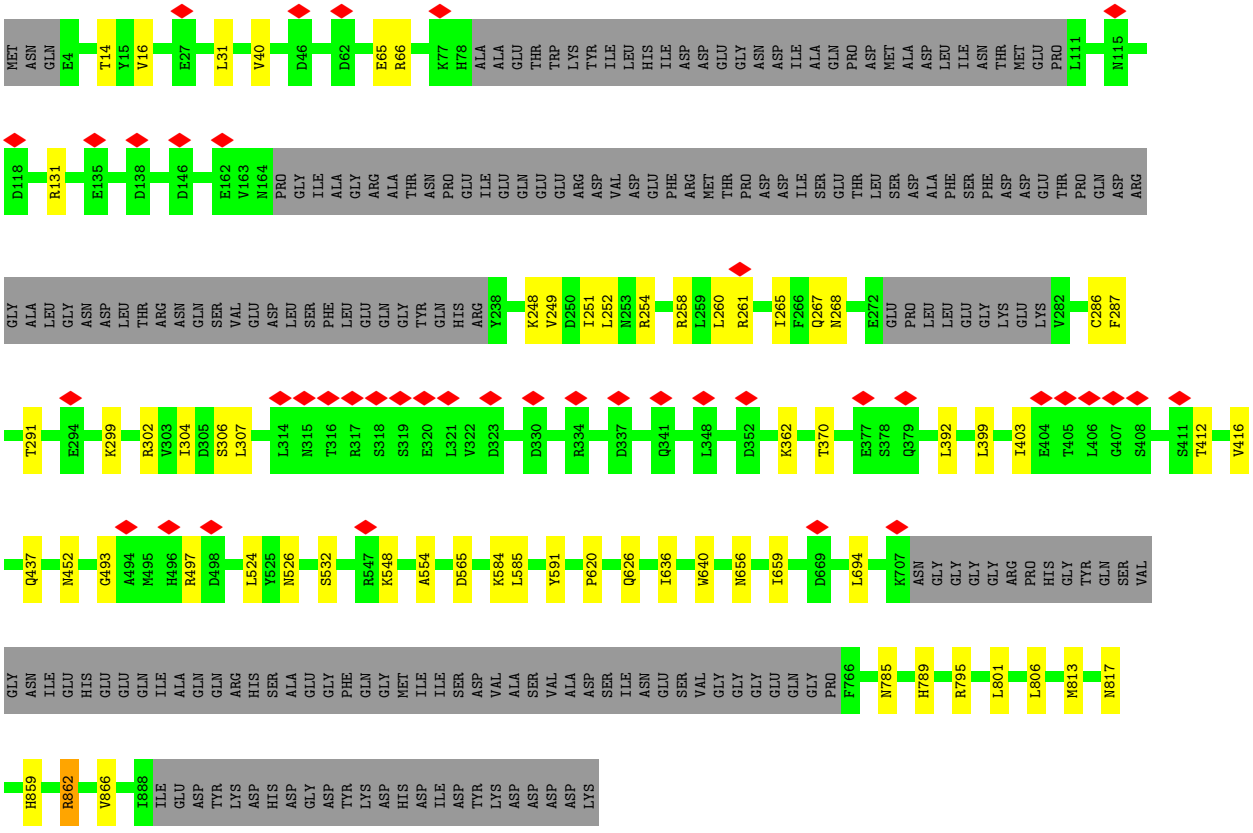
Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	156	Total	C	N	O	S	0	0
			1133	750	178	193	12		

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.

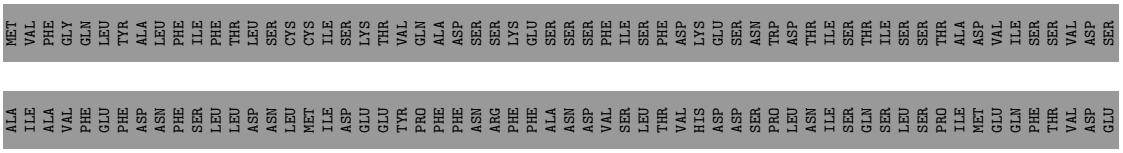
• Molecule 1: V-type proton ATPase subunit a, Golgi isoform

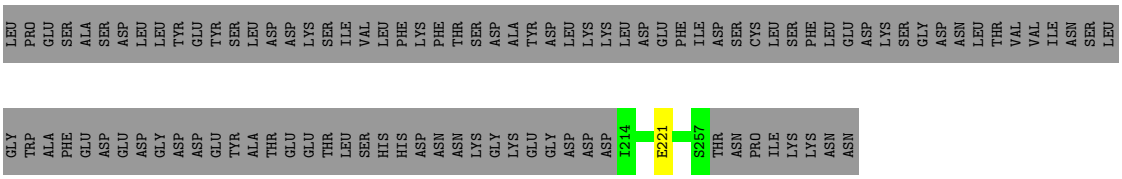
Chain a:



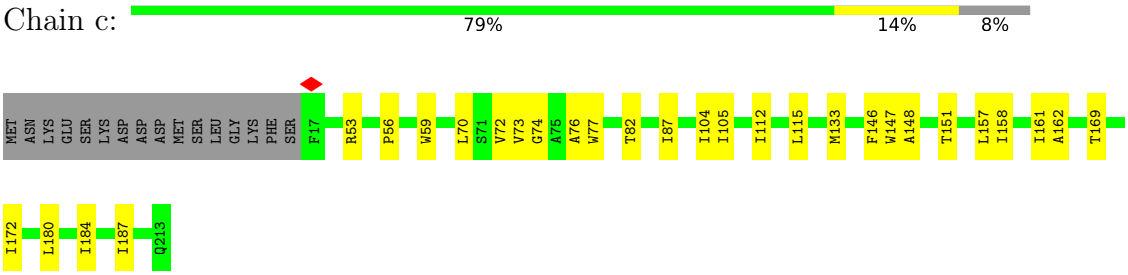
• Molecule 2: V0 assembly protein 1

Chain b:

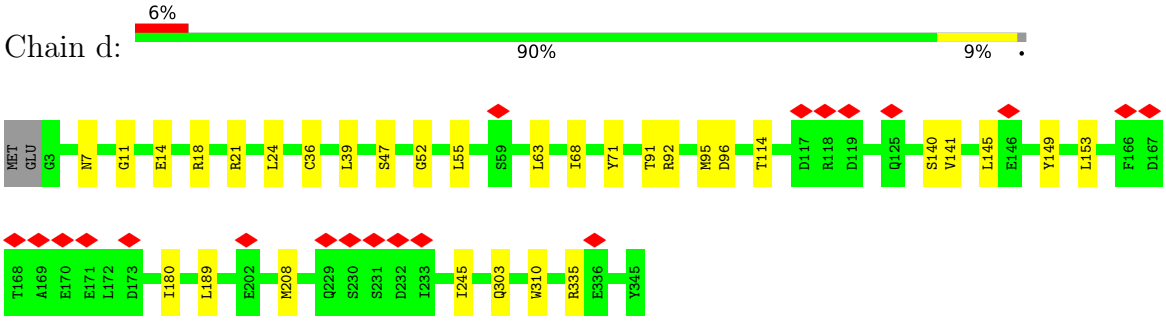




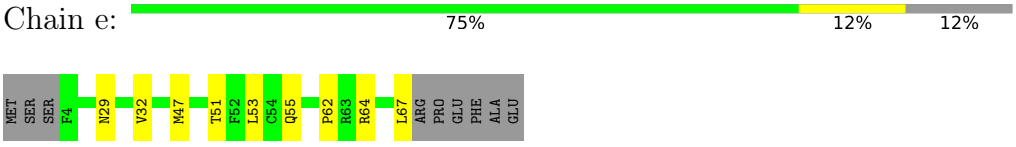
• Molecule 3: V-type proton ATPase subunit c"



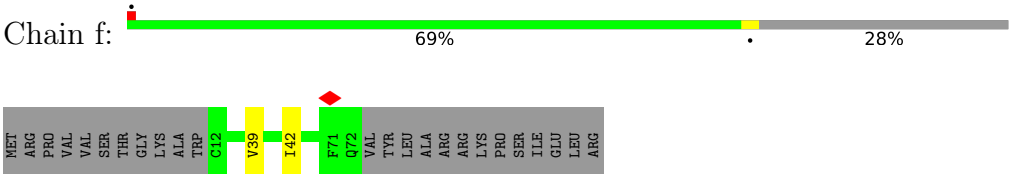
• Molecule 4: V-type proton ATPase subunit d



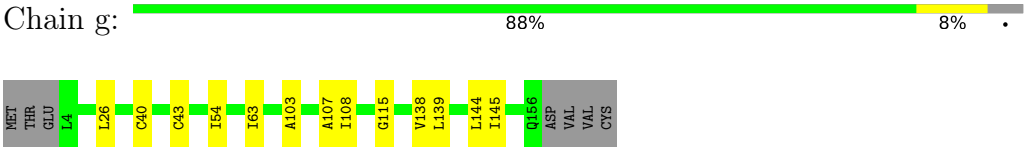
• Molecule 5: V-type proton ATPase subunit e



• Molecule 6: Putative protein YPR170W-B

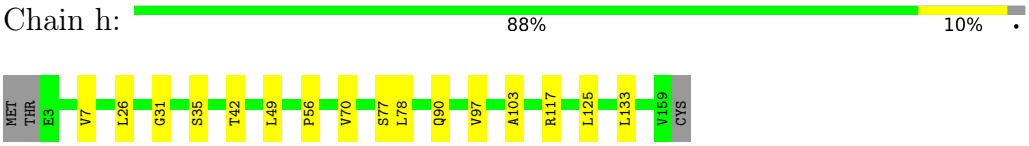


• Molecule 7: V-type proton ATPase subunit c



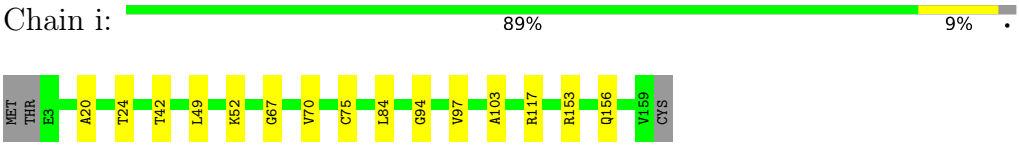
• Molecule 7: V-type proton ATPase subunit c

Chain h:



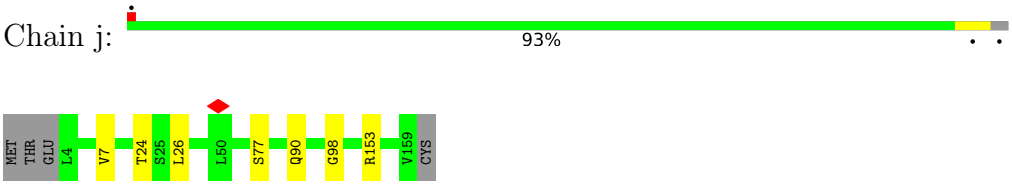
• Molecule 7: V-type proton ATPase subunit c

Chain i:



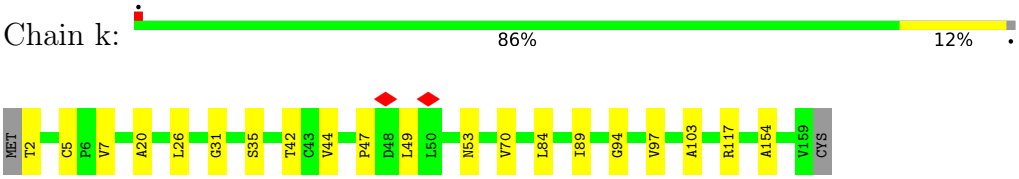
• Molecule 7: V-type proton ATPase subunit c

Chain j:



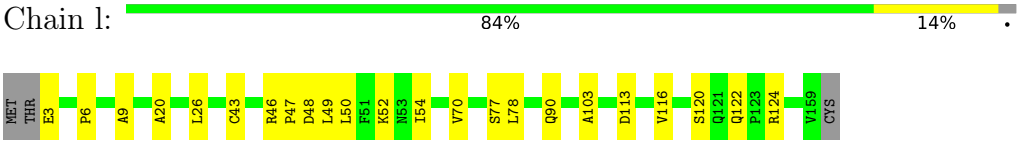
• Molecule 7: V-type proton ATPase subunit c

Chain k:



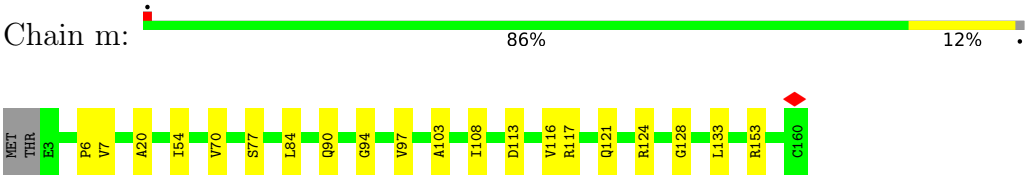
• Molecule 7: V-type proton ATPase subunit c

Chain l:



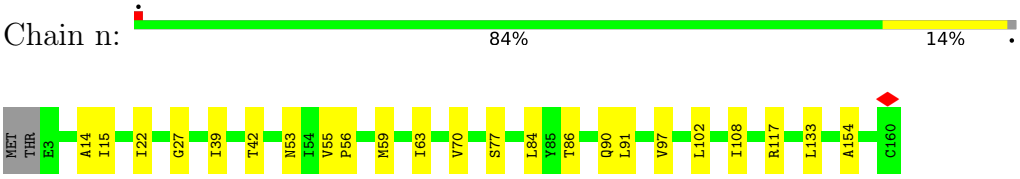
• Molecule 7: V-type proton ATPase subunit c

Chain m:



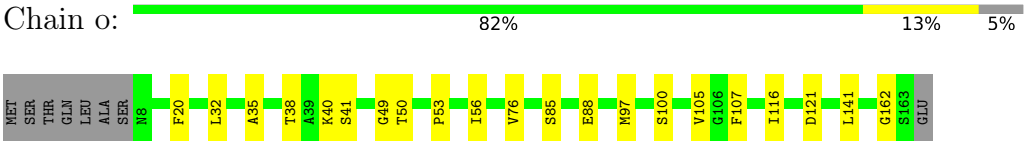
• Molecule 7: V-type proton ATPase subunit c

Chain n:



• Molecule 8: V-type proton ATPase subunit c'

Chain o:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163024	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 ($e^-/Å^2$)	42.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	9.957	Depositor
Minimum map value	-6.642	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.366	Depositor
Recommended contour level	1.3	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.22	0/5797	0.54	0/7856
2	b	0.23	0/335	0.48	0/459
3	c	0.26	0/1496	0.58	0/2033
4	d	0.23	0/2778	0.52	0/3777
5	e	0.21	0/527	0.50	0/720
6	f	0.17	0/476	0.51	1/652 (0.2%)
7	g	0.31	0/1112	0.61	2/1511 (0.1%)
7	h	0.25	0/1143	0.57	0/1554
7	i	0.29	0/1143	0.67	2/1554 (0.1%)
7	j	0.24	0/1134	0.53	0/1542
7	k	0.24	0/1150	0.55	0/1564
7	l	0.25	0/1143	0.63	2/1554 (0.1%)
7	m	0.26	0/1149	0.61	2/1562 (0.1%)
7	n	0.26	0/1149	0.60	0/1562
8	o	0.27	0/1156	0.58	0/1567
All	All	0.24	0/21688	0.56	9/29467 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	l	54	ILE	CA-C-N	8.16	125.38	120.24
7	l	54	ILE	C-N-CA	8.16	125.38	120.24
7	m	54	ILE	CA-C-N	5.80	123.89	120.24
7	m	54	ILE	C-N-CA	5.80	123.89	120.24
6	f	39	VAL	N-CA-C	-5.51	108.13	113.53

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	5665	0	5612	38	0
2	b	330	0	349	1	0
3	c	1466	0	1535	23	0
4	d	2720	0	2574	19	0
5	e	512	0	530	7	0
6	f	463	0	448	1	0
7	g	1094	0	1167	11	0
7	h	1125	0	1195	11	0
7	i	1125	0	1195	9	0
7	j	1116	0	1189	5	0
7	k	1132	0	1202	13	0
7	l	1125	0	1195	16	0
7	m	1131	0	1200	12	0
7	n	1131	0	1200	13	0
8	o	1133	0	1189	16	0
All	All	21268	0	21780	150	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 3.

The worst 5 of 150 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)
8:o:76:VAL:HG21	8:o:105:VAL:HG11	1.75	0.69
1:a:437:GLN:HE22	1:a:452:ASN:HD21	1.43	0.66
1:a:251:ILE:HG22	1:a:254:ARG:HH21	1.61	0.65
8:o:49:GLY:HA2	8:o:56:ILE:HD11	1.79	0.65
4:d:7:ASN:HD22	4:d:11:GLY:HA2	1.64	0.62

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	703/912 (77%)	675 (96%)	28 (4%)	0	100	100
2	b	42/265 (16%)	42 (100%)	0	0	100	100
3	c	195/213 (92%)	189 (97%)	6 (3%)	0	100	100
4	d	341/345 (99%)	327 (96%)	14 (4%)	0	100	100
5	e	62/73 (85%)	62 (100%)	0	0	100	100
6	f	59/85 (69%)	59 (100%)	0	0	100	100
7	g	151/160 (94%)	149 (99%)	2 (1%)	0	100	100
7	h	155/160 (97%)	154 (99%)	1 (1%)	0	100	100
7	i	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
7	j	154/160 (96%)	152 (99%)	2 (1%)	0	100	100
7	k	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
7	l	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
7	m	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
7	n	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
8	o	154/164 (94%)	152 (99%)	2 (1%)	0	100	100
All	All	2794/3337 (84%)	2729 (98%)	65 (2%)	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	604/805 (75%)	603 (100%)	1 (0%)	87 89
2	b	36/244 (15%)	36 (100%)	0	100 100
3	c	153/168 (91%)	153 (100%)	0	100 100
4	d	287/309 (93%)	287 (100%)	0	100 100
5	e	56/65 (86%)	56 (100%)	0	100 100
6	f	51/72 (71%)	51 (100%)	0	100 100
7	g	112/119 (94%)	112 (100%)	0	100 100
7	h	116/119 (98%)	115 (99%)	1 (1%)	70 80
7	i	116/119 (98%)	116 (100%)	0	100 100
7	j	115/119 (97%)	115 (100%)	0	100 100
7	k	117/119 (98%)	117 (100%)	0	100 100
7	l	116/119 (98%)	116 (100%)	0	100 100
7	m	117/119 (98%)	117 (100%)	0	100 100
7	n	117/119 (98%)	117 (100%)	0	100 100
8	o	118/125 (94%)	118 (100%)	0	100 100
All	All	2231/2740 (81%)	2229 (100%)	2 (0%)	87 90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	862	ARG
7	h	49	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
7	h	82	GLN
7	l	90	GLN
7	h	90	GLN
7	k	82	GLN
7	m	53	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

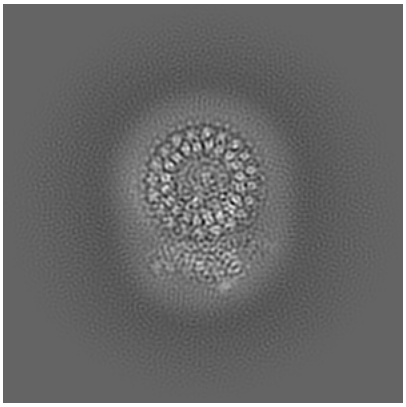
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0645. These allow visual inspection of the internal detail of the map and identification of artifacts.

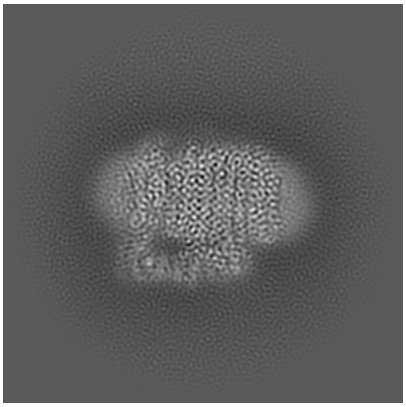
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

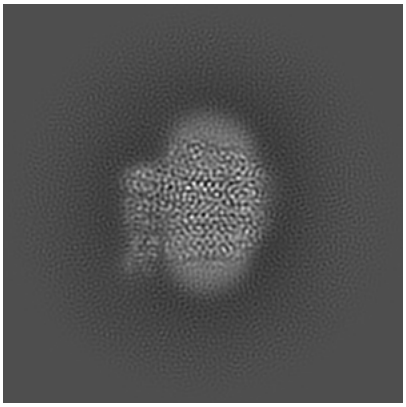
6.1.1 Primary map



X



Y

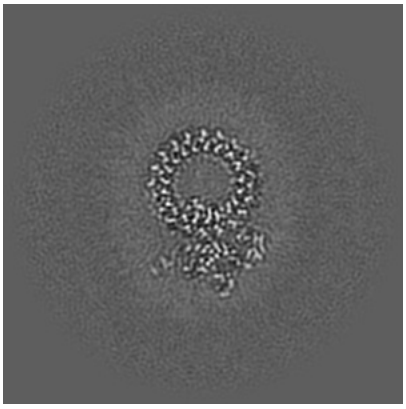


Z

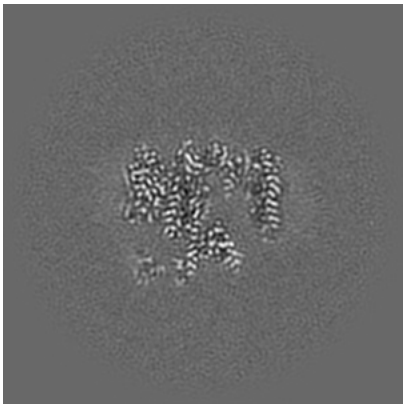
The images above show the map projected in three orthogonal directions.

6.2 Central slices

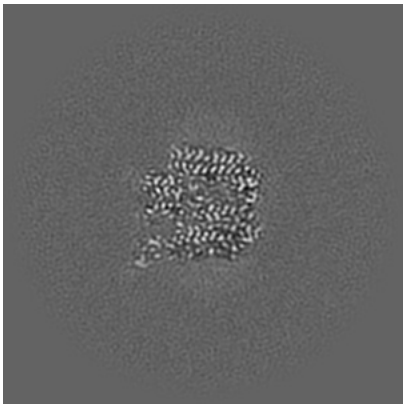
6.2.1 Primary map



X Index: 128



Y Index: 128

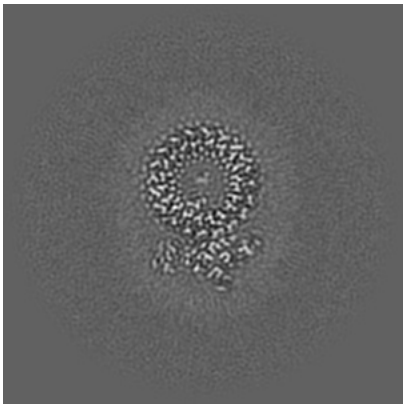


Z Index: 128

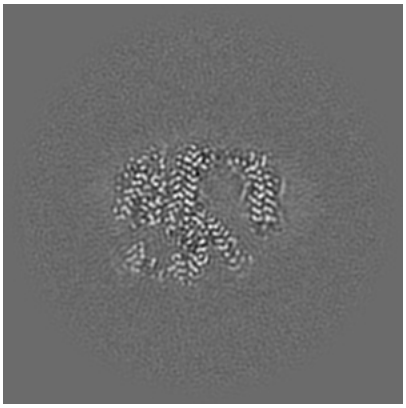
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

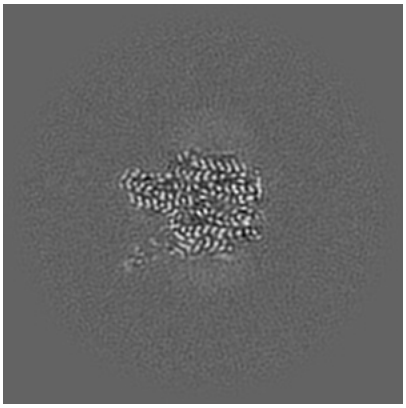
6.3.1 Primary map



X Index: 137



Y Index: 137

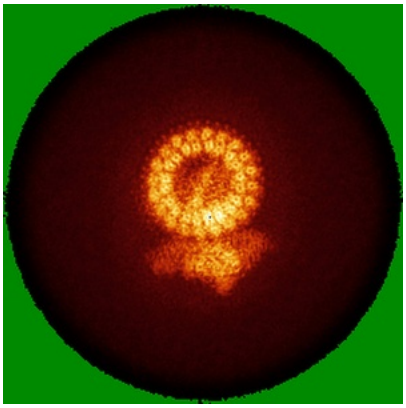


Z Index: 122

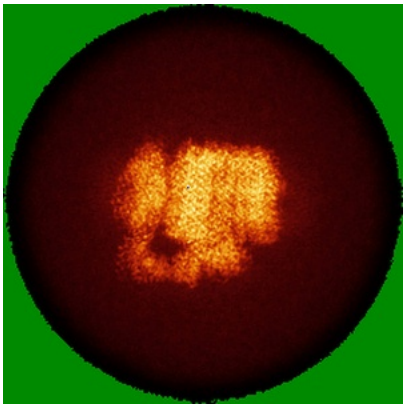
The images above show the largest variance slices of the map in three orthogonal directions.

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

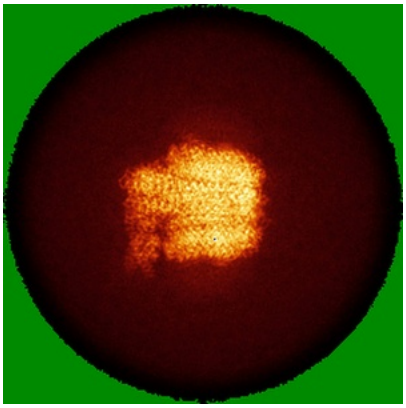
6.4.1 Primary map



X



Y



Z

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)

This section was not generated.

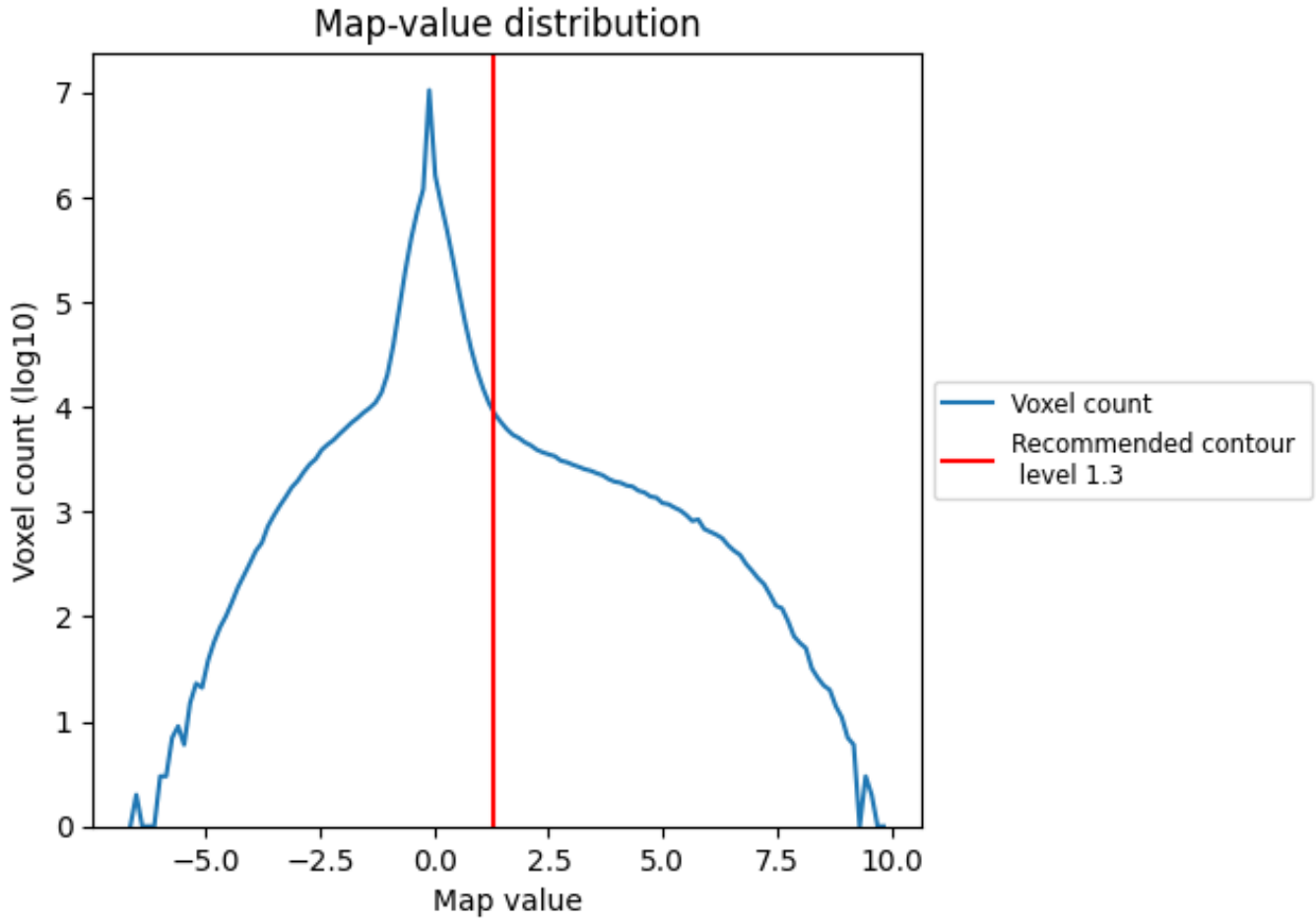
6.6 Mask visualisation (i)

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

7 Map analysis

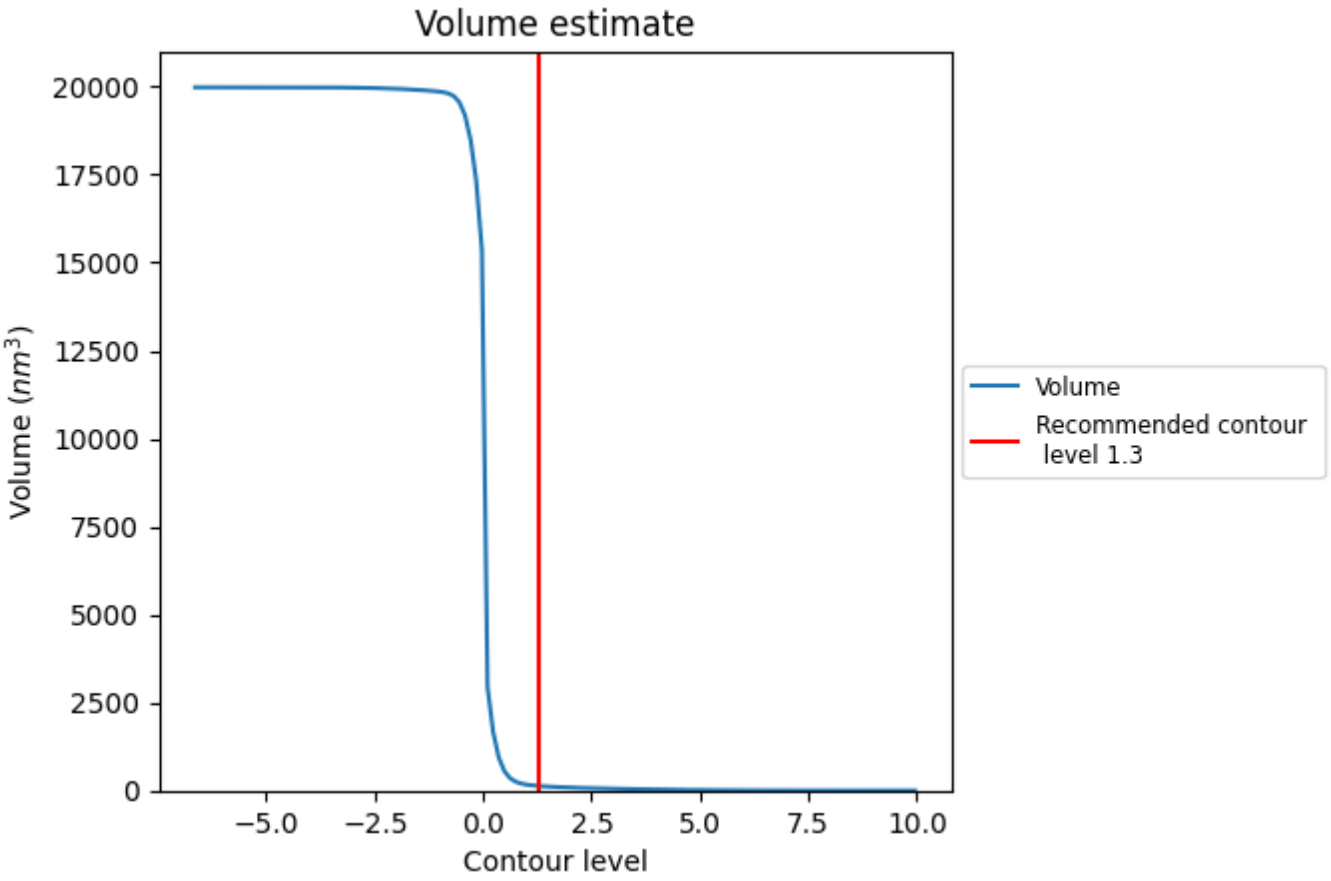
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

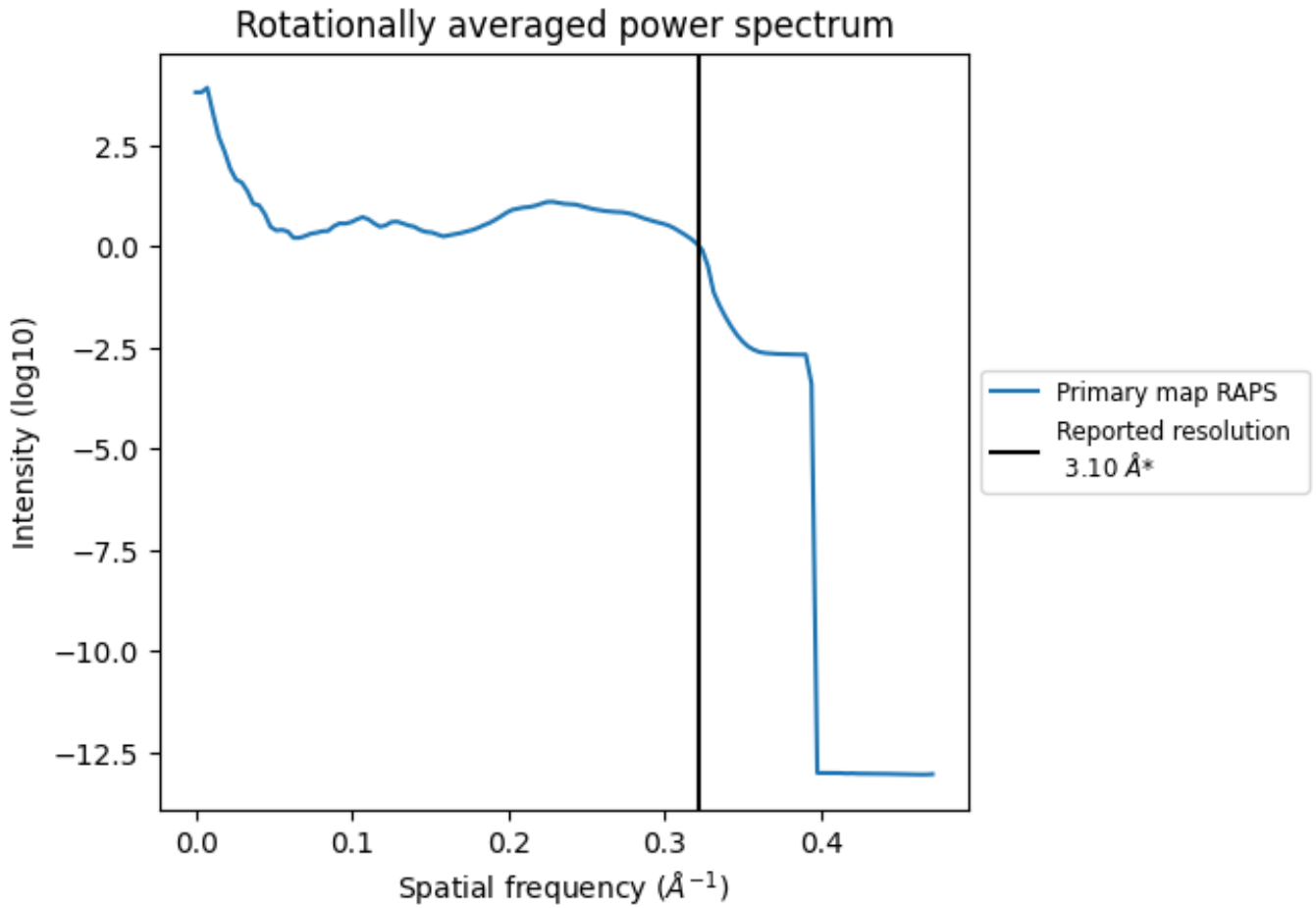
7.2 Volume estimate (i)



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 115 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 0.323 $Å^{-1}$

8 Fourier-Shell correlation (i)

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

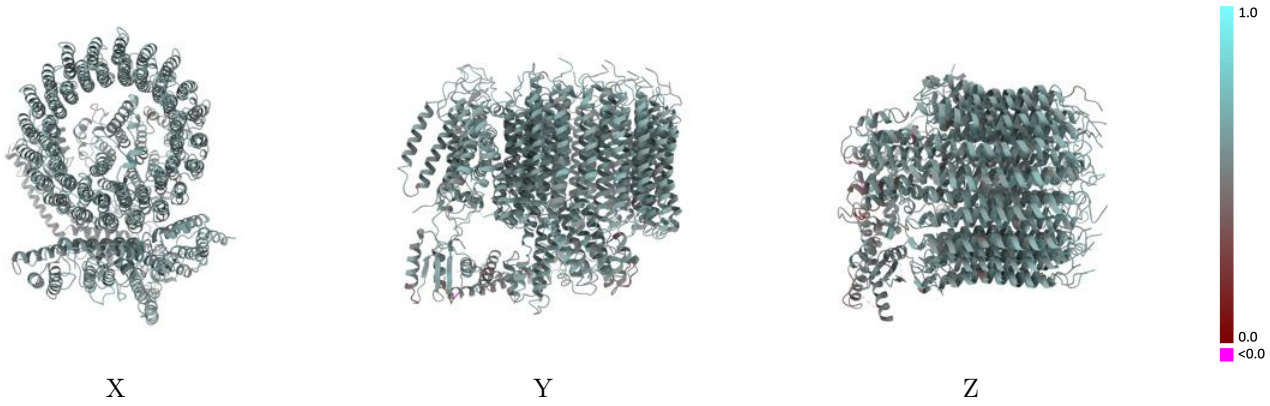
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0645 and PDB model 6O7U. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay

This section was not generated.

9.2 Q-score mapped to coordinate model



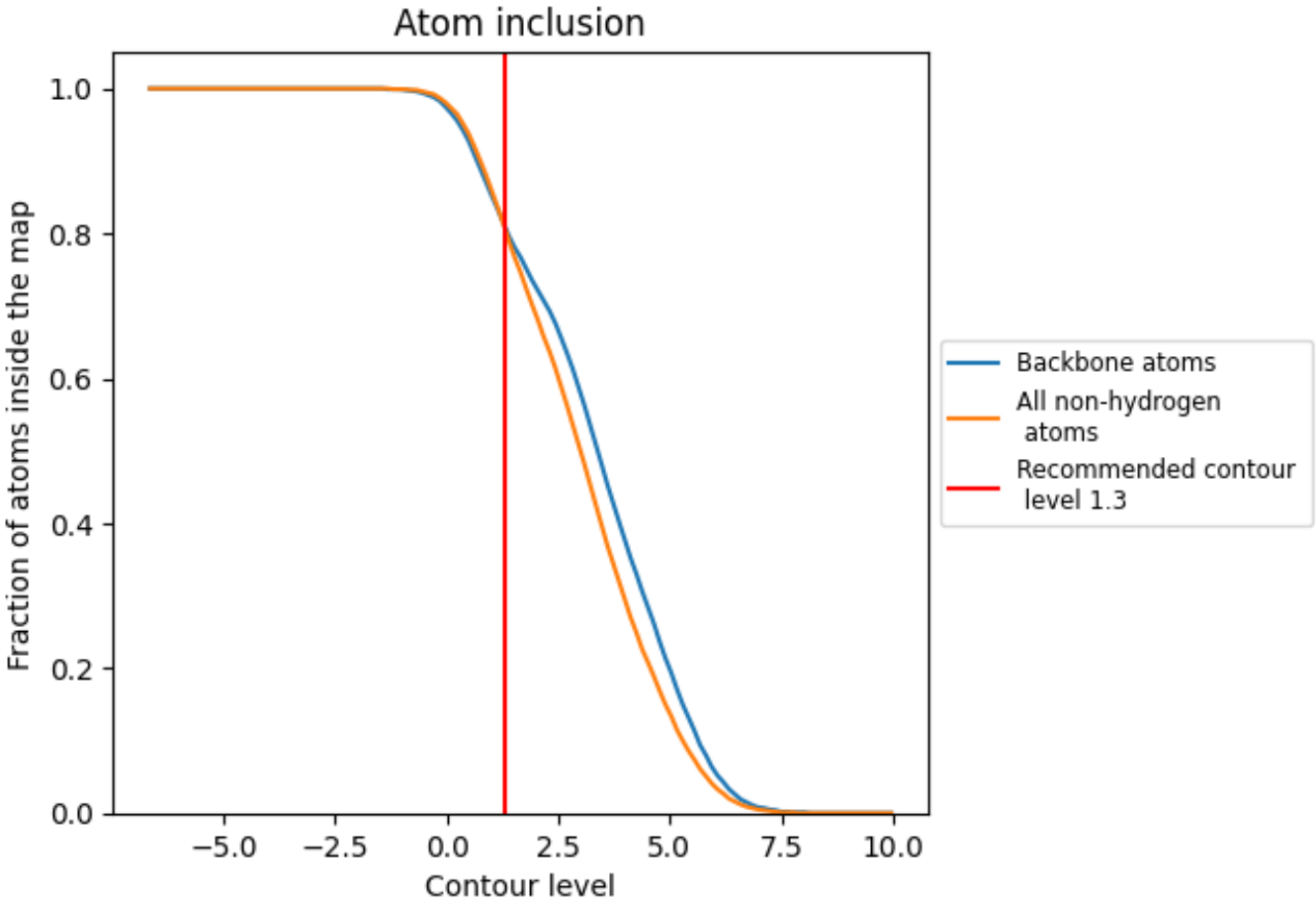
X Y Z

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

9.3 Atom inclusion mapped to coordinate model

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.5640
a	0.7520	0.5440
b	0.8440	0.5860
c	0.8380	0.5780
d	0.7800	0.5530
e	0.8070	0.5530
f	0.7270	0.5390
g	0.8670	0.5850
h	0.8590	0.5840
i	0.8610	0.5740
j	0.8260	0.5730
k	0.8060	0.5700
l	0.8270	0.5740
m	0.8420	0.5740
n	0.8410	0.5730
o	0.8660	0.5800