



wwPDB EM Validation Summary Report ⓘ

Dec 6, 2020 – 01:24 am GMT

PDB ID : 5ARE
EMDB ID : EMD-3165
Title : Bovine mitochondrial ATP synthase state 1b
Authors : Zhou, A.; Rohou, A.; Schep, D.G.; Bason, J.V.; Montgomery, M.G.; Walker, J.E.; Grigorieff, N.; Rubinstein, J.L.
Deposited on : 2015-09-24
Resolution : 7.40 Å (reported)
Based on initial models : 2CLY, 2XND, 2WSS

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

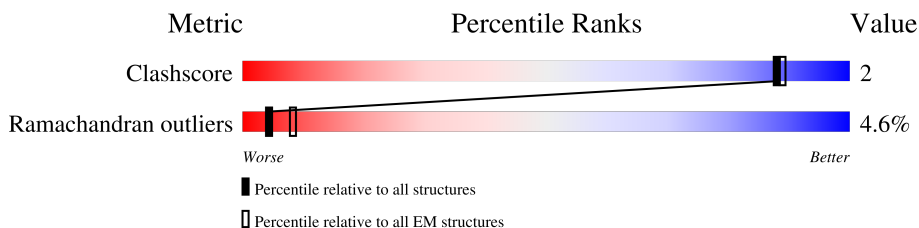
EMDB validation analysis : 0.0.0.dev61
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.15.1

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 7.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	273	
4	H	146	
5	I	50	

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Mol	Chain	Length	Quality of chain
6	J	72	 97%
6	K	72	 99%
6	L	72	 100%
6	M	72	 97%
6	N	72	 100%
6	O	72	 99%
6	P	72	 99%
6	Q	72	 97%
7	S	190	 56% 25% 6% 12%
8	T	174	 87% 11%
9	U	124	 78% 17%
10	V	77	 62% 21% 13%
11	W	217	 96%

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 18545 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 ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	509	2035	1018	509	508	0	0
1	B	480	1918	960	480	478	0	0
1	C	487	1947	974	487	486	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	467	1867	934	467	466	0	0
2	E	466	1863	932	466	465	0	0
2	F	466	1863	932	466	465	0	0

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	264	1053	528	264	261	0	0

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	H	131	523	262	131	130	0	0

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	I	47	187	94	47	46	0	0

- Molecule 6 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	J	72	288	144	72	72	0	0
6	K	72	288	144	72	72	0	0
6	L	72	288	144	72	72	0	0
6	M	72	288	144	72	72	0	0
6	N	72	288	144	72	72	0	0
6	O	72	288	144	72	72	0	0
6	P	72	288	144	72	72	0	0
6	Q	72	288	144	72	72	0	0

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	S	168	669	334	168	167	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	129	THR	ALA	conflict	UNP P13621

- Molecule 8 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	T	174	697	348	174	175	0	0

- Molecule 9 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	U	122	485	242	122	121	0	1

- Molecule 10 is a protein called ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	V	67	265	132	67	66	0	1

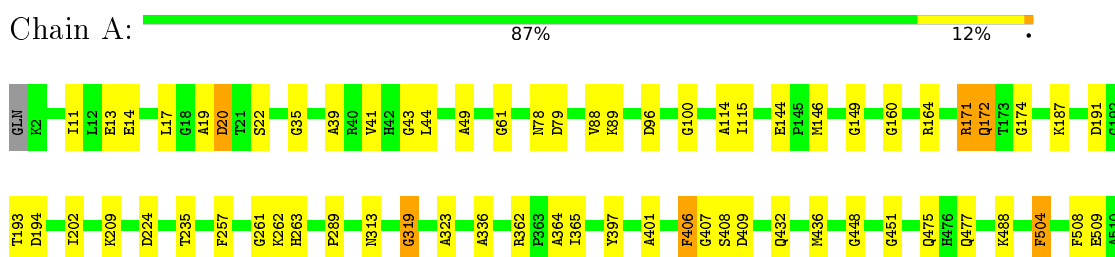
- Molecule 11 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	217	869	434	217	218	0	0

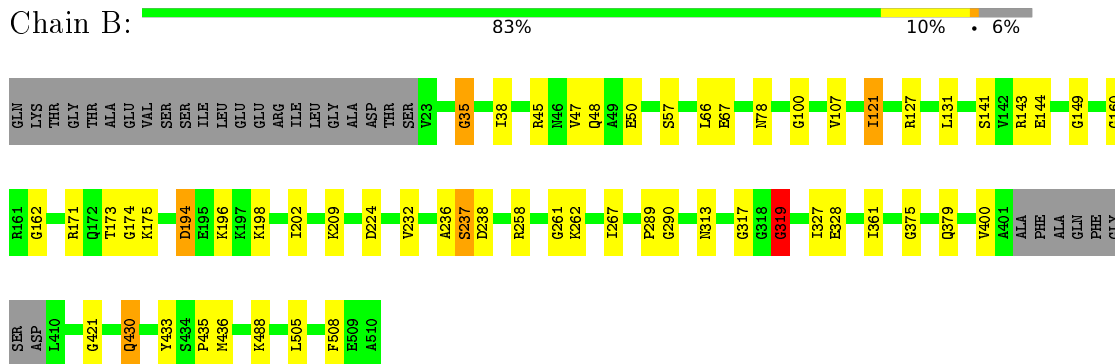
3 Residue-property plots [i](#)

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.

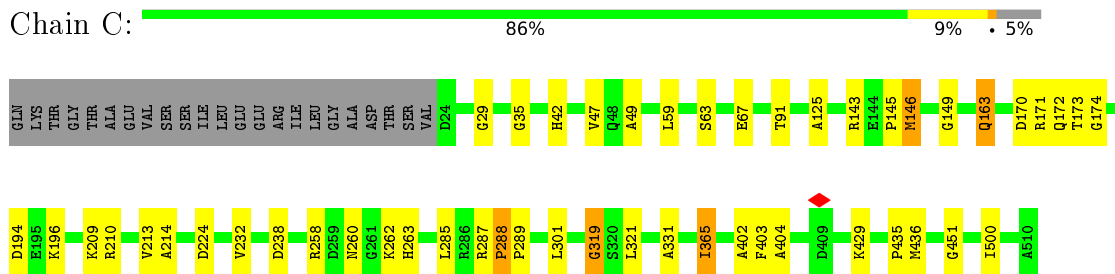
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



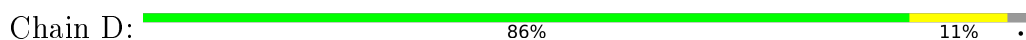
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

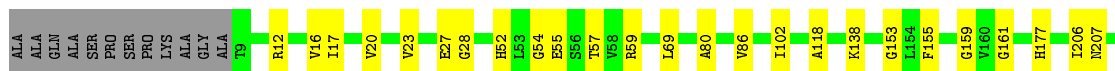


- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

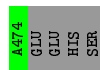
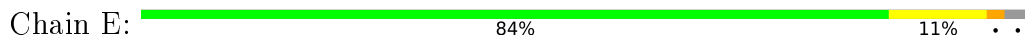


- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

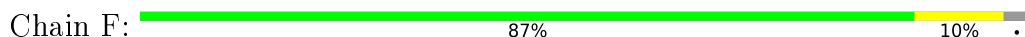




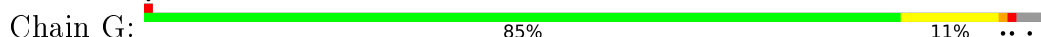
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



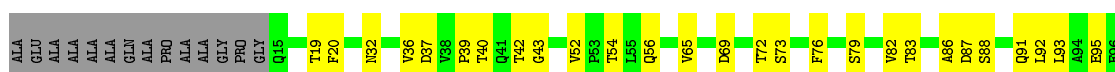
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL




• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

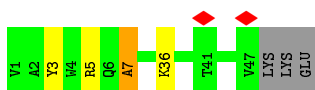


• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



- Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I:  86% 6% 6%



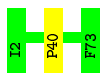
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain J:  97%



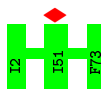
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain K:  99%



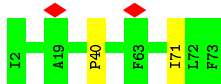
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain L:  100%



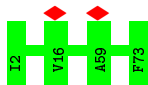
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain M:  97%



- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain N:  100%



- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O:  99%



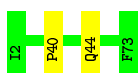
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain P: 99%



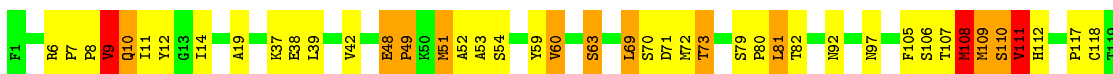
- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q: 97%



- Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

Chain S: 56% 25% 6% 12%



- Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL

Chain T: 87% 11%



- Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

Chain U: 78% 17%



- Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL

Chain V: 62% 21% 13%



- Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain W:  96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22935	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.3	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	30487	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.411	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	419.84, 419.84, 419.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.64, 1.64, 1.64	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	A	1.82	6/2034 (0.3%)	1.48	22/2541 (0.9%)
1	B	1.85	4/1916 (0.2%)	1.53	21/2392 (0.9%)
1	C	1.76	6/1946 (0.3%)	1.50	16/2431 (0.7%)
2	D	1.77	5/1866 (0.3%)	1.51	27/2331 (1.2%)
2	E	1.78	3/1862 (0.2%)	1.56	30/2326 (1.3%)
2	F	1.78	5/1862 (0.3%)	1.49	23/2326 (1.0%)
3	G	1.68	2/1050 (0.2%)	1.52	13/1308 (1.0%)
4	H	1.93	0/522	1.83	16/651 (2.5%)
5	I	1.68	0/186	1.35	1/231 (0.4%)
6	J	0.30	0/287	0.42	0/357
6	K	0.30	0/287	0.42	0/357
6	L	0.30	0/287	0.45	0/357
6	M	0.29	0/287	0.44	0/357
6	N	0.28	0/287	0.40	0/357
6	O	0.30	0/287	0.41	0/357
6	P	0.30	0/287	0.42	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.01	5/668 (0.7%)	1.79	16/834 (1.9%)
8	T	0.87	2/696 (0.3%)	1.05	3/867 (0.3%)
9	U	0.77	0/484	1.18	1/604 (0.2%)
10	V	0.78	0/264	1.31	1/329 (0.3%)
11	W	0.44	0/868	0.72	1/1082 (0.1%)
All	All	1.55	38/18520 (0.2%)	1.39	191/23109 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	5
2	F	0	4
3	G	0	5
4	H	0	2
7	S	0	38
8	T	0	16
9	U	0	30
10	V	0	16
11	W	0	5
All	All	0	132

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	93	ASP	N-CA	9.53	1.65	1.46
2	D	429	GLY	CA-C	-7.32	1.40	1.51
7	S	6	ARG	CA-C	6.89	1.70	1.52
1	C	35	GLY	CA-C	-6.80	1.41	1.51
7	S	6	ARG	C-N	6.77	1.47	1.34

The worst 5 of 191 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	48	GLU	O-C-N	13.96	147.63	121.10
7	S	48	GLU	CA-C-N	-11.40	85.17	117.10
7	S	6	ARG	CA-C-O	-9.20	100.79	120.10
7	S	108	MET	CA-C-O	-9.10	100.99	120.10
1	A	407	GLY	N-CA-C	-9.02	90.54	113.10

There are no chirality outliers.

5 of 132 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	406	PHE	Mainchain,Peptide
1	A	408	SER	Mainchain
1	A	509	GLU	Mainchain
1	B	379	GLN	Peptide
1	B	78	ASN	Mainchain

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	2035	0	589	10	0
1	B	1918	0	553	7	0
1	C	1947	0	562	8	0
2	D	1867	0	533	3	0
2	E	1863	0	532	8	0
2	F	1863	0	532	1	0
3	G	1053	0	283	1	0
4	H	523	0	140	1	0
5	I	187	0	53	0	0
6	J	288	0	92	0	0
6	K	288	0	92	0	0
6	L	288	0	92	0	0
6	M	288	0	92	0	0
6	N	288	0	92	0	0
6	O	288	0	92	0	0
6	P	288	0	92	0	0
6	Q	288	0	92	0	0
7	S	669	0	179	6	0
8	T	697	0	182	0	0
9	U	485	0	121	0	0
10	V	265	0	68	1	0
11	W	869	0	226	1	0
All	All	18545	0	5289	44	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 2.

The worst 5 of 44 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:A:17:LEU:CA	7:S:81:LEU:O	2.45	0.64
7:S:108:MET:O	7:S:112:HIS:CA	2.51	0.58
4:H:65:VAL:H	4:H:73:SER:H	1.55	0.55
7:S:106:SER:CA	7:S:109:MET:H	2.20	0.54
1:B:261:GLY:HA2	1:B:317:GLY:HA3	1.90	0.53

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	507/510 (99%)	441 (87%)	42 (8%)	24 (5%)	2	21
1	B	476/510 (93%)	420 (88%)	31 (6%)	25 (5%)	2	19
1	C	485/510 (95%)	433 (89%)	34 (7%)	18 (4%)	3	24
2	D	465/482 (96%)	404 (87%)	44 (10%)	17 (4%)	3	24
2	E	464/482 (96%)	413 (89%)	31 (7%)	20 (4%)	2	22
2	F	464/482 (96%)	414 (89%)	33 (7%)	17 (4%)	3	24
3	G	258/273 (94%)	204 (79%)	35 (14%)	19 (7%)	1	13
4	H	129/146 (88%)	110 (85%)	8 (6%)	11 (8%)	1	12
5	I	45/50 (90%)	34 (76%)	7 (16%)	4 (9%)	1	11
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	4	29
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11	46
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100	100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	4	29
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100	100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11	46
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	11	46
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	4	29
7	S	166/190 (87%)	112 (68%)	28 (17%)	26 (16%)	0	3
8	T	172/174 (99%)	156 (91%)	9 (5%)	7 (4%)	3	22
9	U	120/124 (97%)	103 (86%)	10 (8%)	7 (6%)	1	18
10	V	65/77 (84%)	49 (75%)	10 (15%)	6 (9%)	1	11
11	W	215/217 (99%)	192 (89%)	20 (9%)	3 (1%)	11	46
All	All	4591/4803 (96%)	3982 (87%)	396 (9%)	213 (5%)	4	21

5 of 213 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	224	ASP
1	A	262	LYS
1	A	365	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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-3165. These allow visual inspection of the internal detail of the map and identification of artifacts.

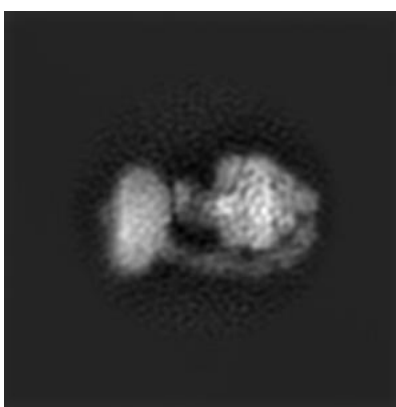
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

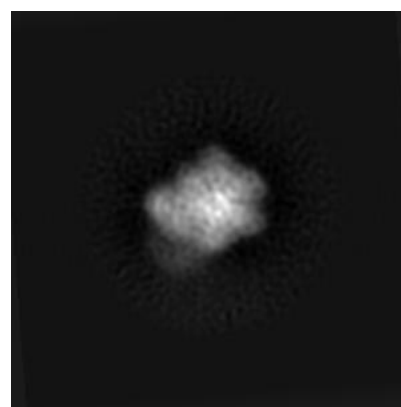
6.1.1 Primary map



X



Y

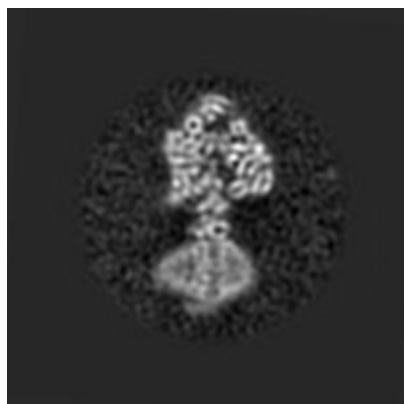


Z

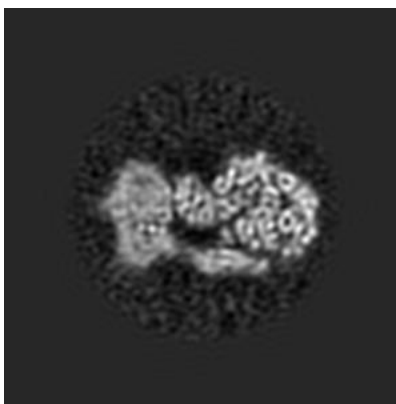
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

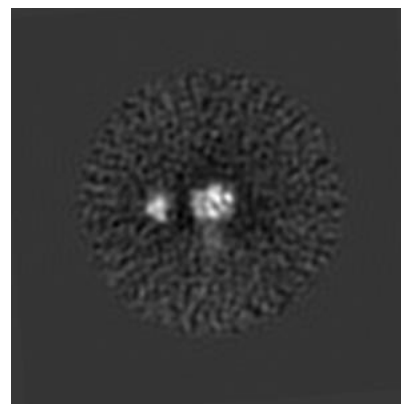
6.2.1 Primary map



X Index: 128



Y Index: 128

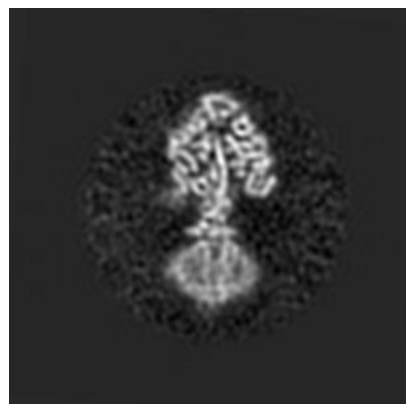


Z Index: 128

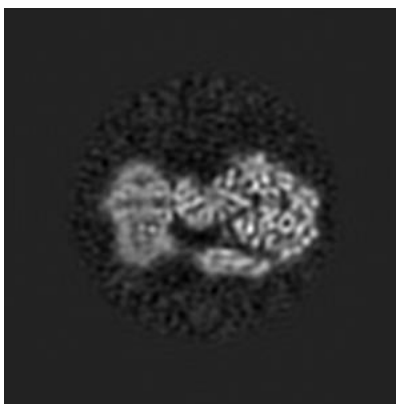
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

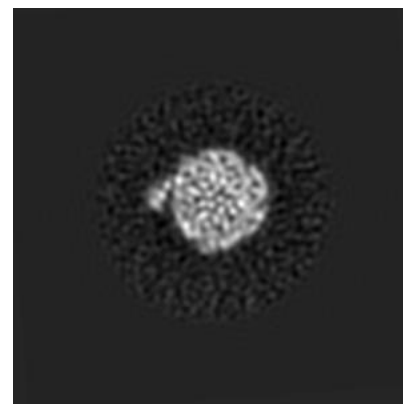
6.3.1 Primary map



X Index: 133



Y Index: 130

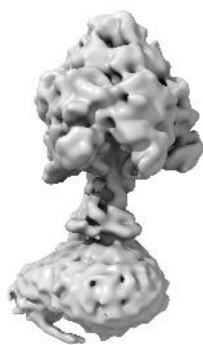


Z Index: 167

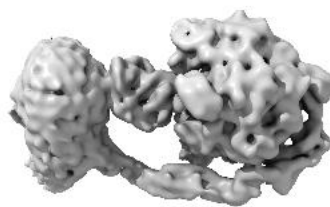
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

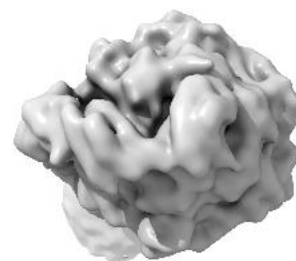
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

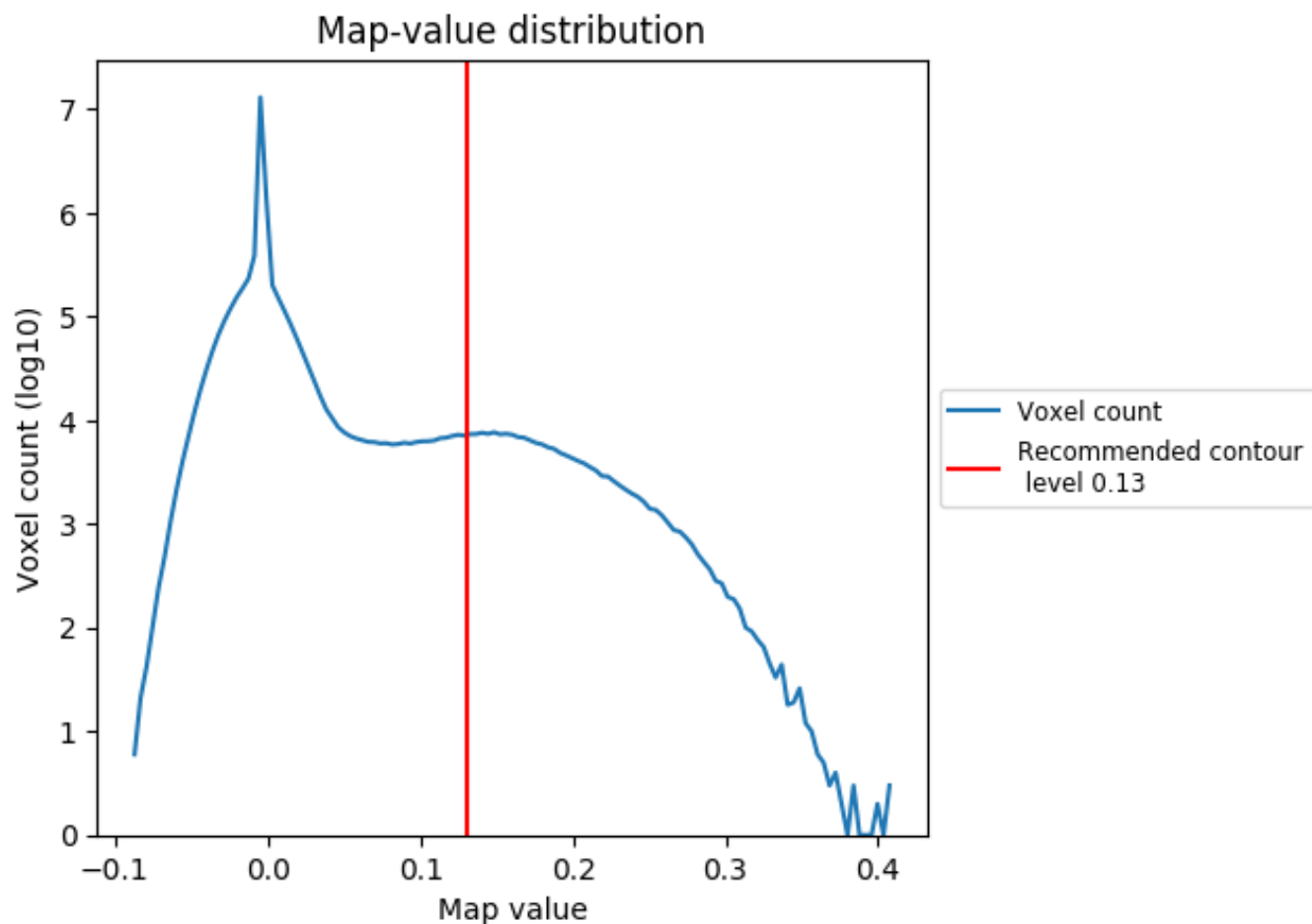
6.5 Mask visualisation

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

7 Map analysis [i](#)

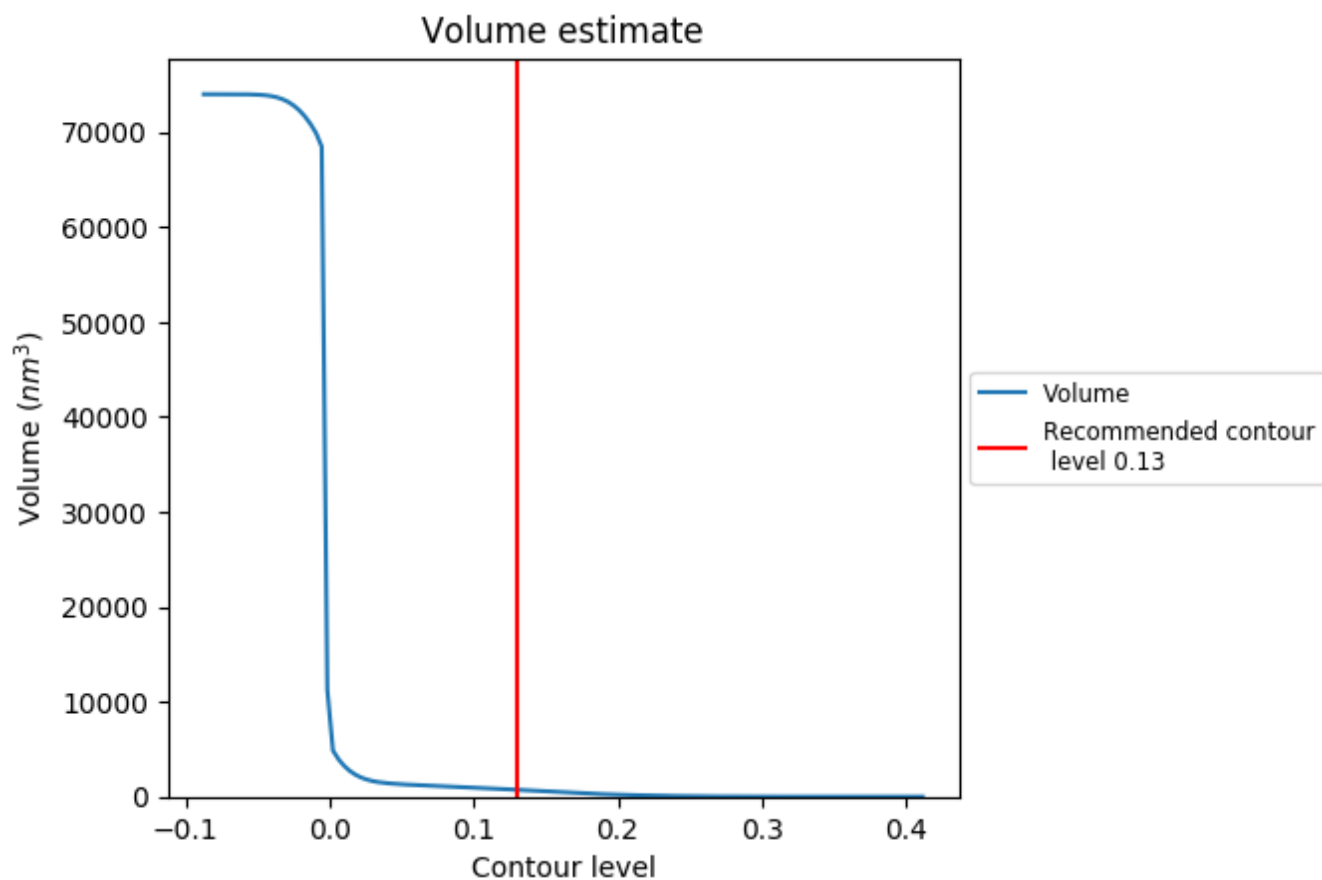
This section contains the results of statistical analysis of the map.

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.

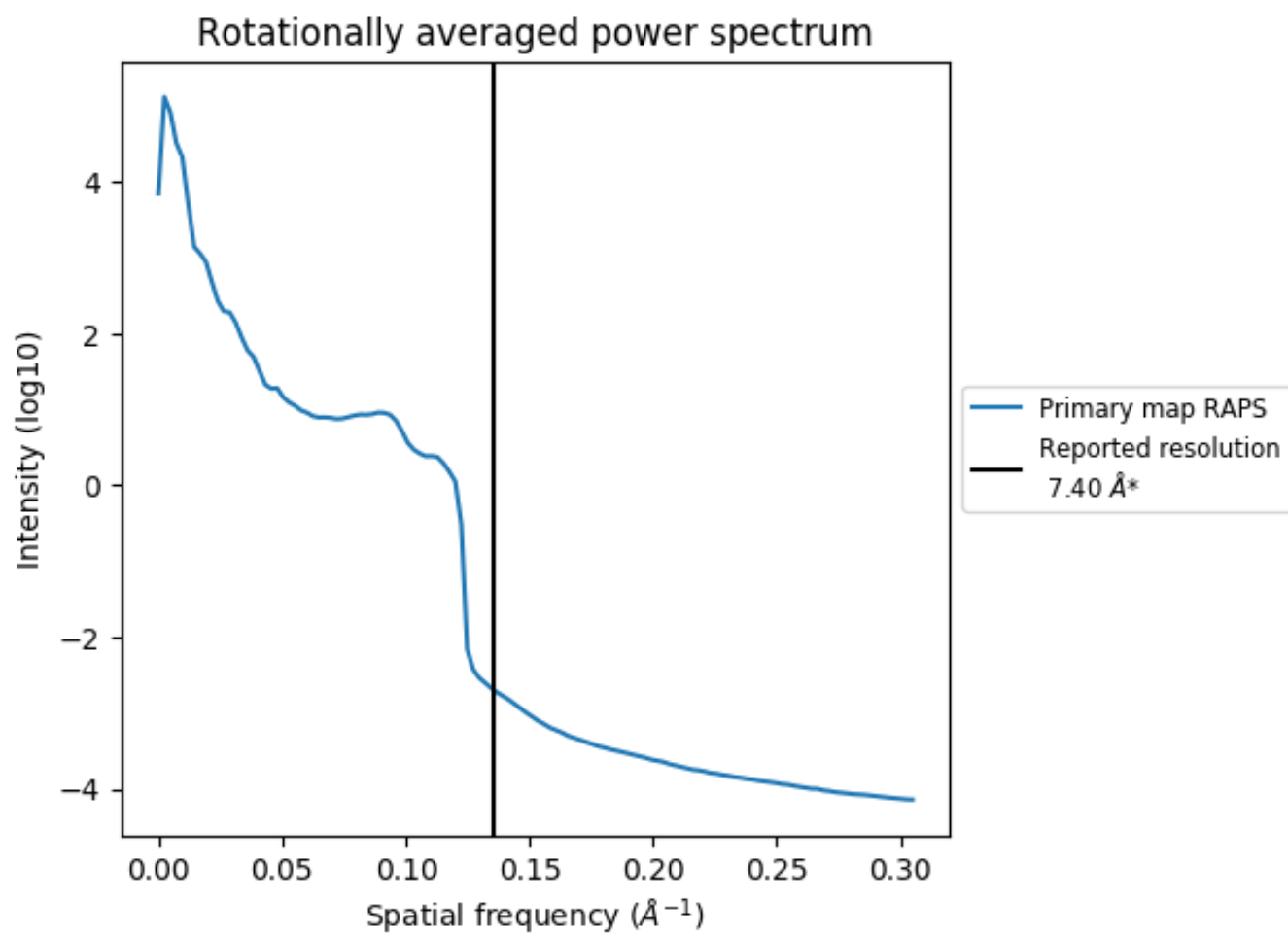
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 727 nm³; this corresponds to an approximate mass of 656 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 0.135\AA^{-1}

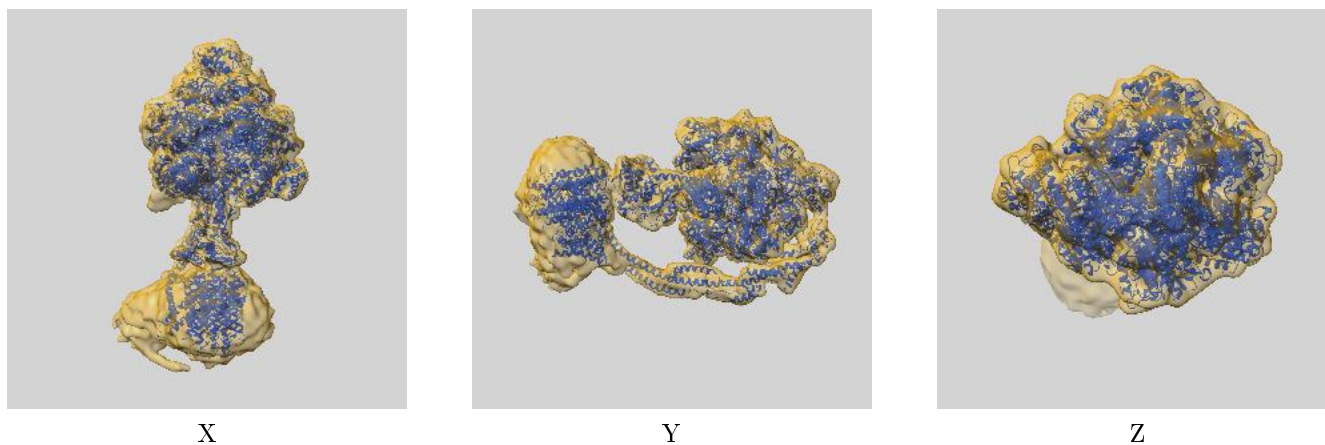
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

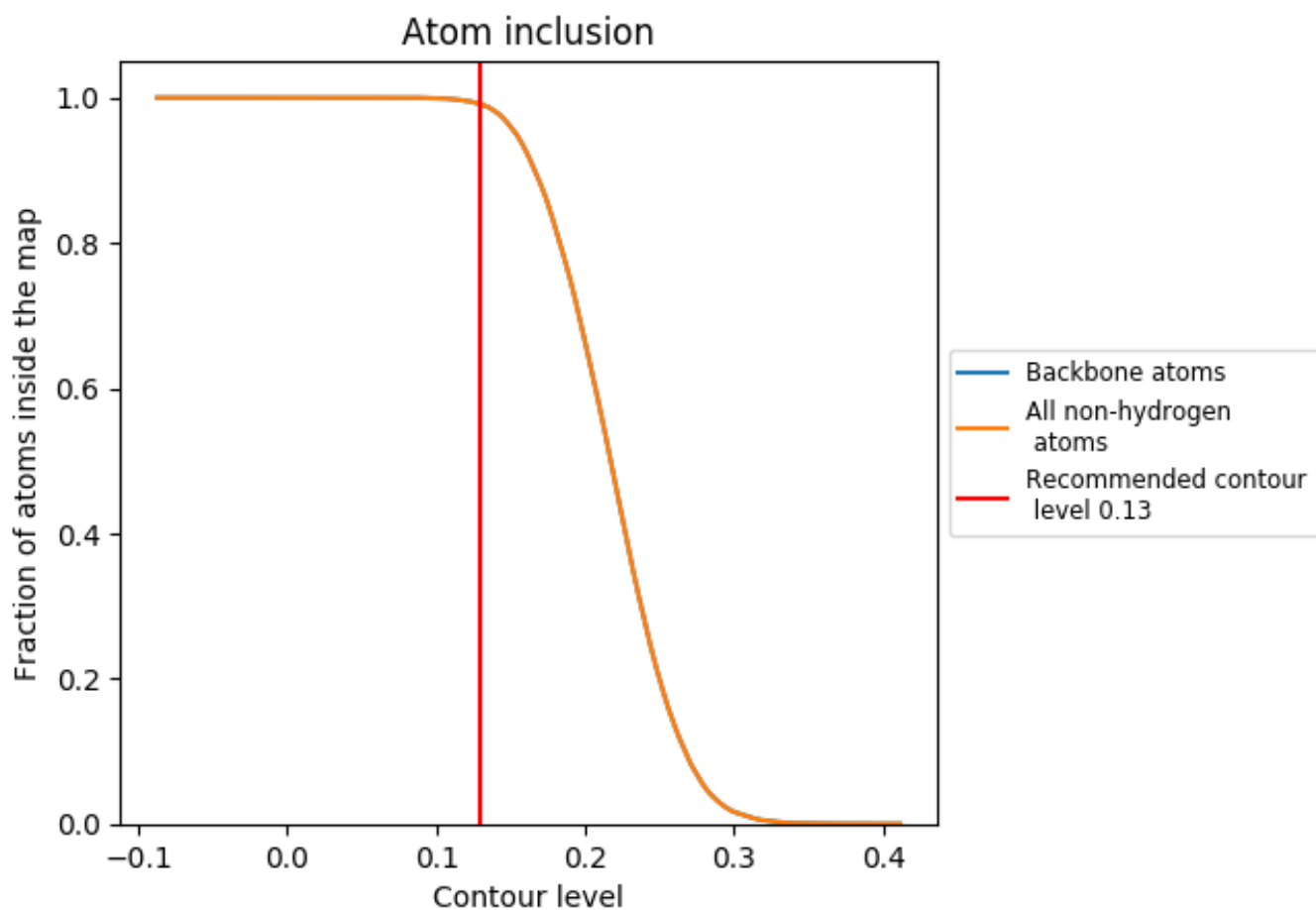
This section contains information regarding the fit between EMDB map EMD-3165 and PDB model 5ARE. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.13 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 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.