Full wwPDB EM Validation Report

Nov 5, 2022 – 07:44 AM EDT

PDB ID	:	5VCA
EMDB ID	:	EMD-8659
Title	:	VCP like ATPase from T. acidophilum (VAT)-Substrate bound conformation
Authors	:	Ripstein, Z.A.; Huang, R.; Augustyniak, R.; Kay, L.E.; Rubinstein, J.L.
Deposited on	:	2017-03-31
Resolution	:	4.80 Å(reported)
Based on initial model	:	5VC7

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

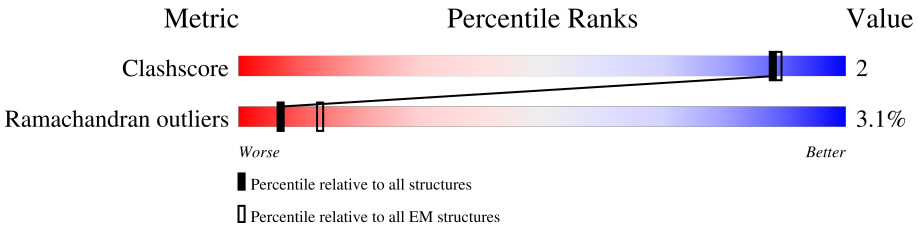
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.80 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 <=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	M	564	91% 5%
1	N	564	91% 5%
1	O	564	91%
1	P	564	7% 91% 5%
1	Q	564	91% 5%
1	R	564	6% 91% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16080 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 VCP-like ATPase.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	P	544	Total 2680	C 1593	N 544	O 543	0	0
1	M	544	Total 2680	C 1593	N 544	O 543	0	0
1	N	544	Total 2680	C 1593	N 544	O 543	0	0
1	O	544	Total 2680	C 1593	N 544	O 543	0	0
1	Q	544	Total 2680	C 1593	N 544	O 543	0	0
1	R	544	Total 2680	C 1593	N 544	O 543	0	0

There are 6 discrepancies between the modelled and reference sequences:

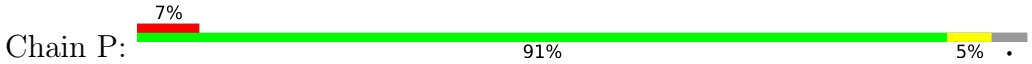
Chain	Residue	Modelled	Actual	Comment	Reference
P	182	MET	-	expression tag	UNP O05209
M	182	MET	-	expression tag	UNP O05209
N	182	MET	-	expression tag	UNP O05209
O	182	MET	-	expression tag	UNP O05209
Q	182	MET	-	expression tag	UNP O05209
R	182	MET	-	expression tag	UNP O05209

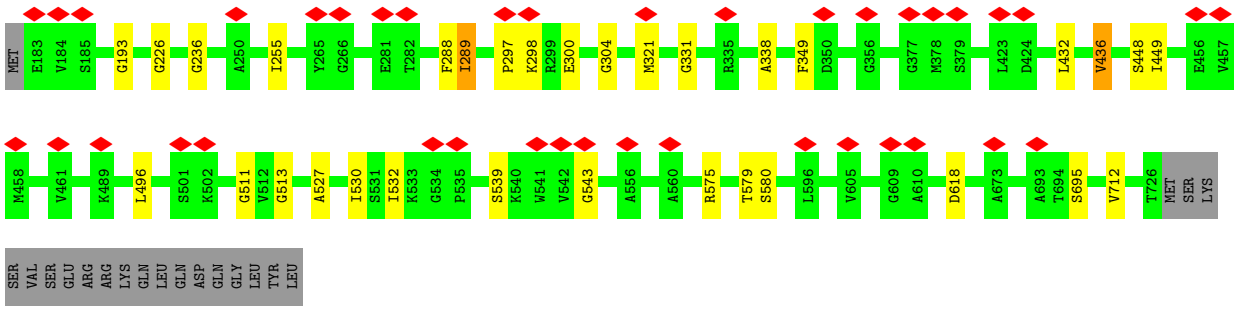
3 Residue-property plots (i)

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: VCP-like ATPase

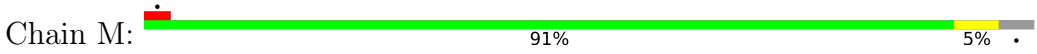
Chain P:

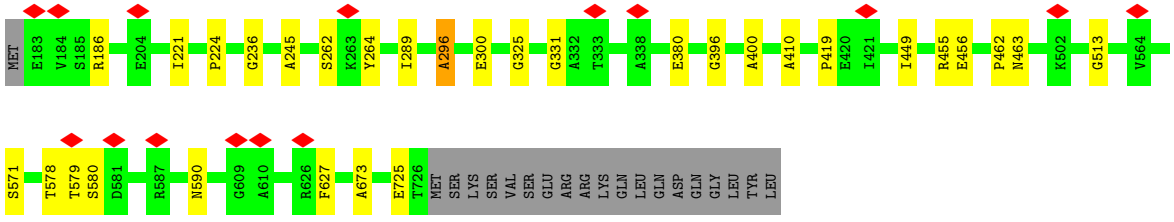




• Molecule 1: VCP-like ATPase

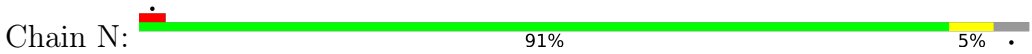
Chain M:

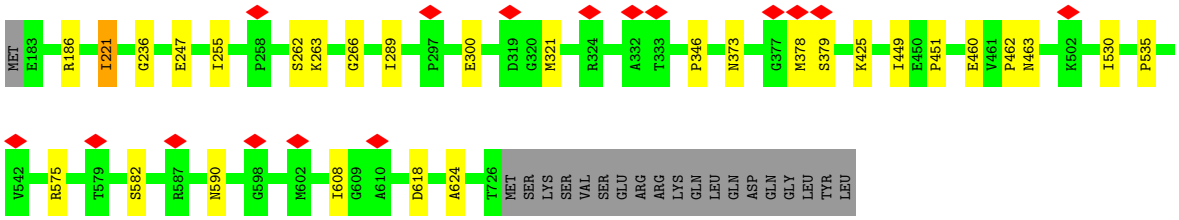




• Molecule 1: VCP-like ATPase

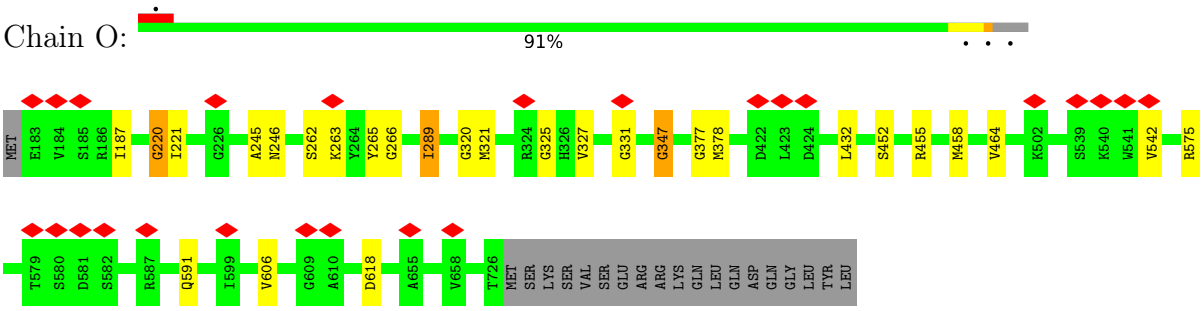
Chain N:





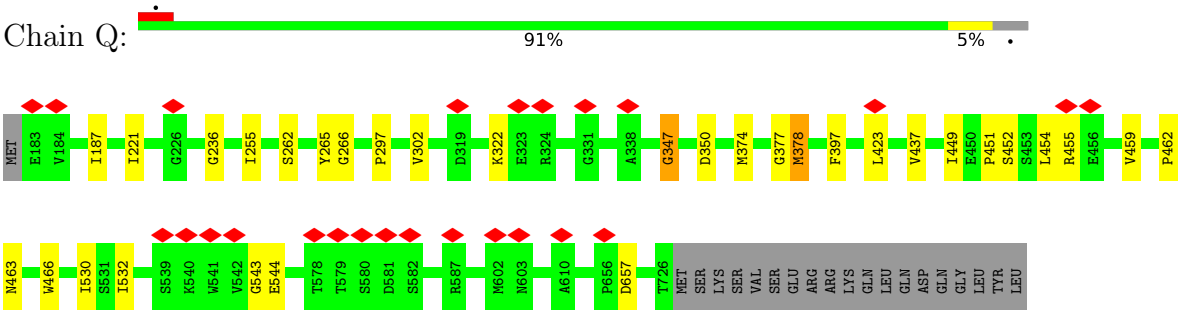
• Molecule 1: VCP-like ATPase

Chain O:



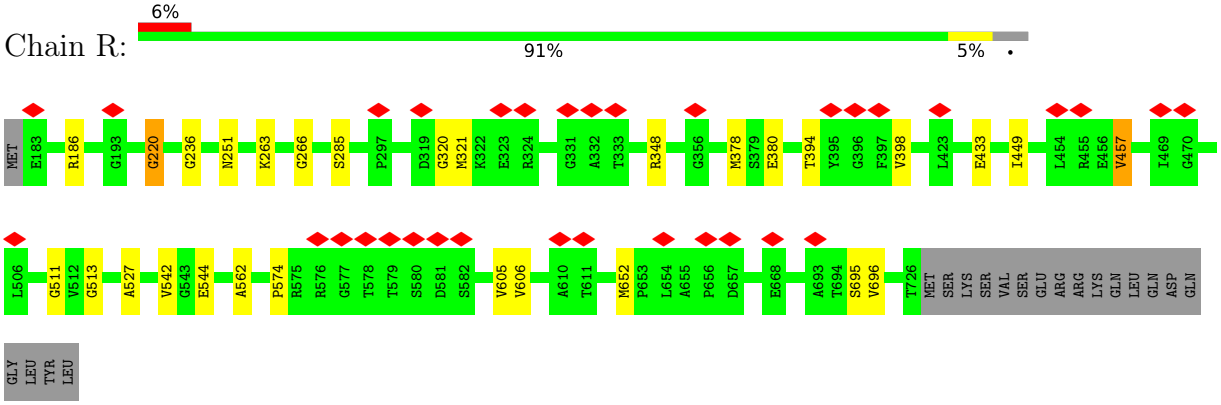
• Molecule 1: VCP-like ATPase

Chain Q:



• Molecule 1: VCP-like ATPase

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.743	Depositor
Minimum map value	-0.411	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.137	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	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	M	0.94	0/2679	1.18	4/3726 (0.1%)
1	N	0.99	0/2679	1.18	5/3726 (0.1%)
1	O	0.99	0/2679	1.19	4/3726 (0.1%)
1	P	0.96	0/2679	1.18	9/3726 (0.2%)
1	Q	0.98	0/2679	1.17	8/3726 (0.2%)
1	R	0.97	0/2679	1.17	6/3726 (0.2%)
All	All	0.97	0/16074	1.18	36/22356 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	457	VAL	N-CA-C	-6.81	92.61	111.00
1	P	236	GLY	N-CA-C	-6.75	96.22	113.10
1	M	396	GLY	N-CA-C	-6.58	96.65	113.10
1	M	513	GLY	N-CA-C	-6.55	96.72	113.10
1	M	296	ALA	N-CA-CB	6.44	119.11	110.10
1	P	436	VAL	N-CA-C	-5.96	94.90	111.00
1	O	347	GLY	N-CA-C	-5.94	98.26	113.10
1	M	725	GLU	N-CA-C	-5.91	95.05	111.00
1	Q	530	ILE	N-CA-C	-5.84	95.24	111.00
1	P	289	ILE	N-CA-C	-5.79	95.38	111.00
1	Q	532	ILE	N-CA-C	-5.75	95.47	111.00
1	N	255	ILE	N-CA-C	-5.74	95.49	111.00
1	Q	322	LYS	N-CA-C	-5.71	95.59	111.00
1	P	288	PHE	N-CA-C	-5.69	95.65	111.00
1	N	530	ILE	N-CA-C	-5.55	96.01	111.00
1	R	394	THR	N-CA-C	-5.54	96.04	111.00
1	R	513	GLY	N-CA-C	-5.47	99.42	113.10
1	Q	255	ILE	N-CA-C	-5.47	96.24	111.00
1	Q	466	TRP	CB-CA-C	-5.45	99.49	110.40
1	R	320	GLY	C-N-CA	5.45	135.32	121.70
1	R	695	SER	N-CA-C	-5.39	96.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	532	ILE	N-CA-C	-5.38	96.46	111.00
1	O	320	GLY	C-N-CA	5.38	135.15	121.70
1	O	289	ILE	N-CA-C	-5.36	96.53	111.00
1	P	513	GLY	N-CA-C	-5.26	99.96	113.10
1	N	449	ILE	N-CA-C	-5.25	96.82	111.00
1	R	606	VAL	N-CA-C	-5.24	96.86	111.00
1	N	289	ILE	N-CA-C	-5.22	96.91	111.00
1	P	530	ILE	N-CA-C	-5.12	97.17	111.00
1	O	606	VAL	N-CA-C	-5.10	97.22	111.00
1	P	255	ILE	N-CA-C	-5.09	97.25	111.00
1	Q	378	MET	N-CA-CB	5.08	119.75	110.60
1	Q	452	SER	N-CA-C	-5.07	97.31	111.00
1	Q	347	GLY	N-CA-C	-5.05	100.48	113.10
1	P	226	GLY	N-CA-C	-5.04	100.49	113.10
1	N	608	ILE	N-CA-C	-5.01	97.47	111.00

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	M	2680	0	1205	15	0
1	N	2680	0	1205	14	0
1	O	2680	0	1205	11	0
1	P	2680	0	1205	14	0
1	Q	2680	0	1205	11	0
1	R	2680	0	1205	14	0
All	All	16080	0	7230	45	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.

All (45) 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:N:262:SER:CB	1:O:266:GLY:O	1.66	1.43
1:P:579:THR:CB	1:R:542:VAL:CB	1.98	1.39
1:O:262:SER:CA	1:Q:266:GLY:HA3	1.66	1.26
1:O:262:SER:HA	1:Q:266:GLY:CA	1.62	1.25
1:P:579:THR:CB	1:R:542:VAL:HA	1.84	1.07
1:P:579:THR:CB	1:R:542:VAL:CA	2.33	1.06
1:P:539:SER:CB	1:M:590:ASN:CB	2.37	1.03
1:Q:262:SER:CB	1:R:266:GLY:O	2.08	1.02
1:Q:262:SER:HA	1:R:266:GLY:HA3	1.40	1.01
1:P:580:SER:HA	1:M:579:THR:HA	1.42	0.99
1:P:496:LEU:O	1:R:652:MET:HA	1.69	0.92
1:M:580:SER:O	1:N:582:SER:CB	2.13	0.87
1:P:580:SER:CB	1:M:578:THR:O	2.24	0.86
1:Q:262:SER:HA	1:R:266:GLY:CA	2.07	0.84
1:O:262:SER:O	1:Q:265:TYR:O	1.97	0.81
1:M:400:ALA:HB1	1:N:346:PRO:O	1.79	0.81
1:M:673:ALA:CB	1:N:624:ALA:HB3	2.16	0.75
1:P:579:THR:CA	1:R:542:VAL:CB	2.67	0.72
1:M:673:ALA:HB1	1:N:624:ALA:HB3	1.76	0.66
1:P:580:SER:HA	1:M:579:THR:CA	2.21	0.64
1:M:673:ALA:HB3	1:N:624:ALA:HB3	1.81	0.61
1:N:535:PRO:CB	1:O:591:GLN:CB	2.84	0.56
1:P:579:THR:HA	1:R:542:VAL:CB	2.37	0.55
1:O:262:SER:HA	1:Q:266:GLY:HA3	0.71	0.54
1:P:289:ILE:O	1:P:331:GLY:HA2	2.07	0.54
1:N:575:ARG:HA	1:N:618:ASP:HA	1.90	0.53
1:Q:347:GLY:H	1:Q:350:ASP:HA	1.75	0.51
1:Q:377:GLY:HA3	1:Q:437:VAL:H	1.75	0.51
1:M:262:SER:CB	1:N:266:GLY:O	2.59	0.51
1:M:289:ILE:O	1:M:331:GLY:HA2	2.13	0.48
1:N:262:SER:HA	1:O:266:GLY:HA3	1.97	0.47
1:Q:262:SER:CA	1:R:266:GLY:O	2.62	0.47
1:P:496:LEU:O	1:R:652:MET:CA	2.54	0.46
1:P:580:SER:HA	1:M:579:THR:CB	2.47	0.44
1:M:571:SER:CB	1:N:590:ASN:CB	2.95	0.44
1:P:575:ARG:HA	1:P:618:ASP:HA	2.00	0.44
1:M:410:ALA:CB	1:N:221:ILE:CB	2.95	0.44
1:R:562:ALA:O	1:R:605:VAL:HA	2.18	0.44
1:Q:374:MET:CB	1:R:220:GLY:HA2	2.48	0.43
1:O:289:ILE:O	1:O:331:GLY:HA2	2.18	0.43
1:M:673:ALA:HB1	1:N:624:ALA:CB	2.47	0.42
1:N:373:ASN:O	1:O:220:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:251:ASN:H	1:R:285:SER:HA	1.86	0.41
1:O:325:GLY:C	1:O:327:VAL:H	2.24	0.41
1:O:575:ARG:HA	1:O:618:ASP:HA	2.03	0.41

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	M	542/564 (96%)	482 (89%)	43 (8%)	17 (3%)	4	30
1	N	542/564 (96%)	488 (90%)	40 (7%)	14 (3%)	5	34
1	O	542/564 (96%)	489 (90%)	36 (7%)	17 (3%)	4	30
1	P	542/564 (96%)	486 (90%)	39 (7%)	17 (3%)	4	30
1	Q	542/564 (96%)	494 (91%)	30 (6%)	18 (3%)	4	29
1	R	542/564 (96%)	488 (90%)	37 (7%)	17 (3%)	4	30
All	All	3252/3384 (96%)	2927 (90%)	225 (7%)	100 (3%)	7	30

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	297	PRO
1	P	321	MET
1	P	338	ALA
1	P	449	ILE
1	P	712	VAL
1	M	449	ILE
1	M	455	ARG
1	M	456	GLU
1	M	627	PHE

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Mol	Chain	Res	Type
1	O	187	ILE
1	O	221	ILE
1	O	321	MET
1	O	378	MET
1	O	432	LEU
1	O	455	ARG
1	O	464	VAL
1	Q	221	ILE
1	Q	454	LEU
1	Q	657	ASP
1	R	321	MET
1	R	348	ARG
1	R	380	GLU
1	R	433	GLU
1	P	193	GLY
1	P	511	GLY
1	P	527	ALA
1	M	186	ARG
1	M	264	TYR
1	M	462	PRO
1	M	463	ASN
1	N	186	ARG
1	N	221	ILE
1	N	321	MET
1	N	379	SER
1	O	265	TYR
1	O	458	MET
1	O	542	VAL
1	Q	187	ILE
1	Q	297	PRO
1	Q	378	MET
1	Q	459	VAL
1	Q	463	ASN
1	Q	544	GLU
1	R	263	LYS
1	R	378	MET
1	R	511	GLY
1	R	696	VAL
1	P	298	LYS
1	P	432	LEU
1	P	695	SER
1	M	236	GLY

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Mol	Chain	Res	Type
1	N	263	LYS
1	N	300	GLU
1	N	451	PRO
1	N	460	GLU
1	O	220	GLY
1	O	245	ALA
1	O	452	SER
1	Q	236	GLY
1	Q	423	LEU
1	Q	543	GLY
1	R	527	ALA
1	R	544	GLU
1	P	300	GLU
1	M	221	ILE
1	M	296	ALA
1	M	300	GLU
1	N	236	GLY
1	N	378	MET
1	N	462	PRO
1	N	463	ASN
1	O	246	ASN
1	Q	449	ILE
1	Q	451	PRO
1	R	236	GLY
1	R	398	VAL
1	P	349	PHE
1	P	448	SER
1	M	245	ALA
1	M	380	GLU
1	N	247	GLU
1	N	425	LYS
1	Q	397	PHE
1	Q	462	PRO
1	R	186	ARG
1	R	574	PRO
1	P	304	GLY
1	M	224	PRO
1	M	325	GLY
1	O	263	LYS
1	Q	455	ARG
1	P	543	GLY
1	O	377	GLY

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Mol	Chain	Res	Type
1	R	449	ILE
1	R	457	VAL
1	R	220	GLY
1	O	347	GLY
1	Q	302	VAL
1	P	436	VAL
1	M	419	PRO

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.

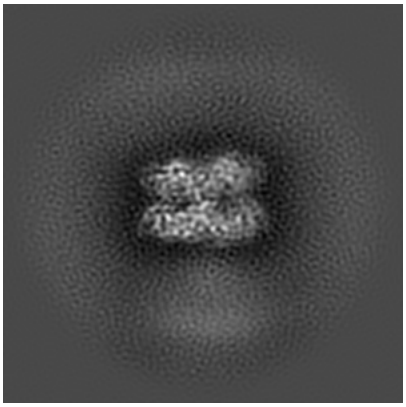
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8659. These allow visual inspection of the internal detail of the map and identification of artifacts.

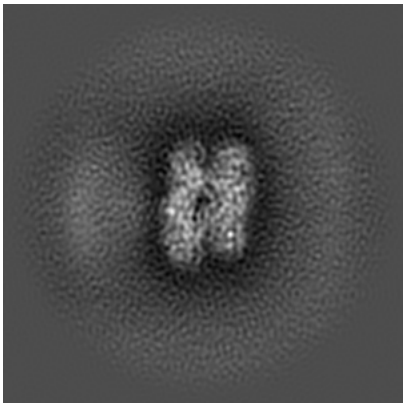
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

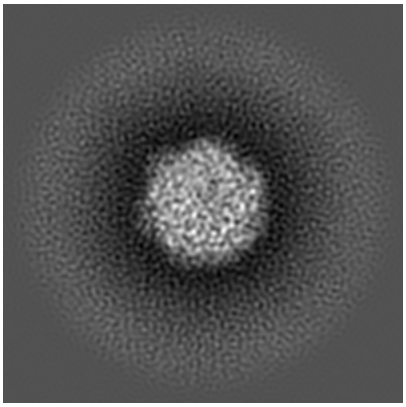
6.1.1 Primary map



X



Y

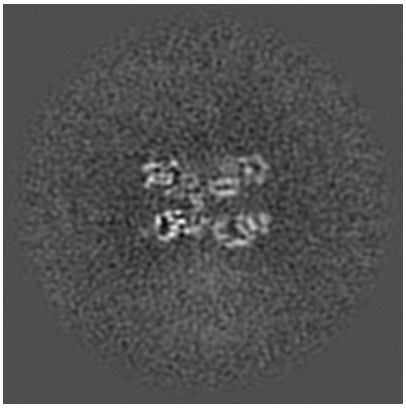


Z

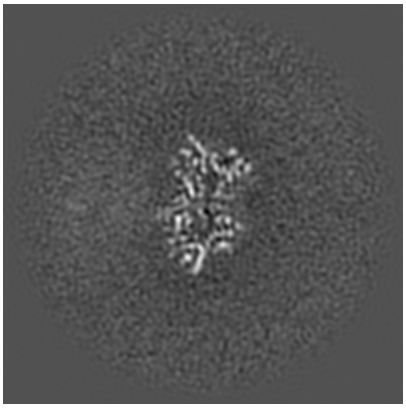
The images above show the map projected in three orthogonal directions.

6.2 Central slices

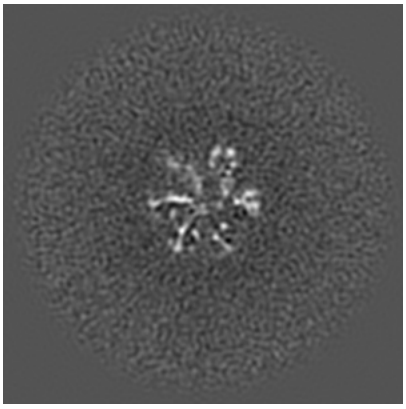
6.2.1 Primary map



X Index: 128



Y Index: 128

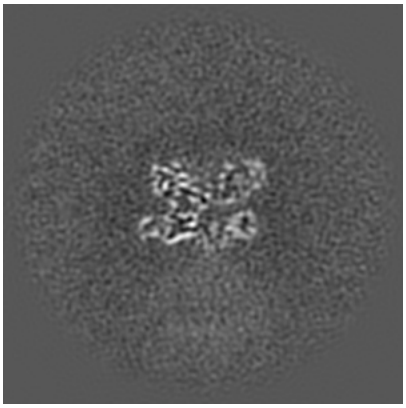


Z Index: 128

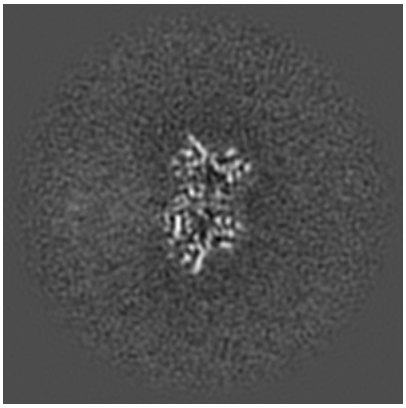
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

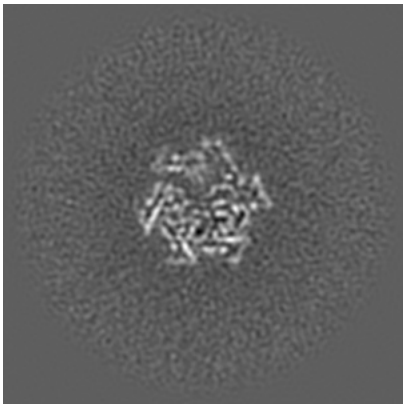
6.3.1 Primary map



X Index: 123



Y Index: 127

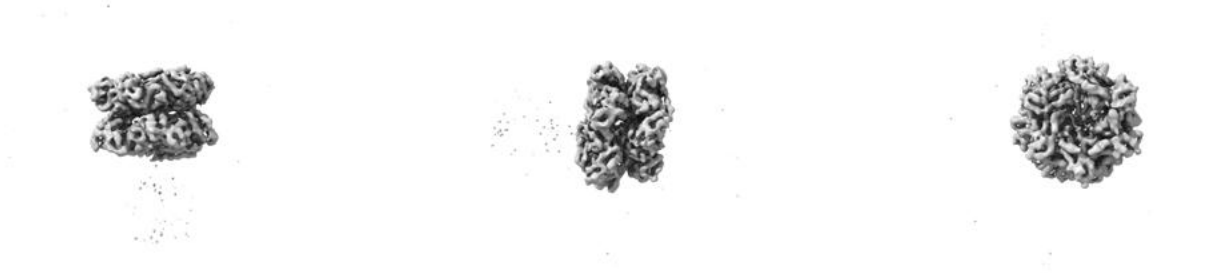


Z Index: 119

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 0.137. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

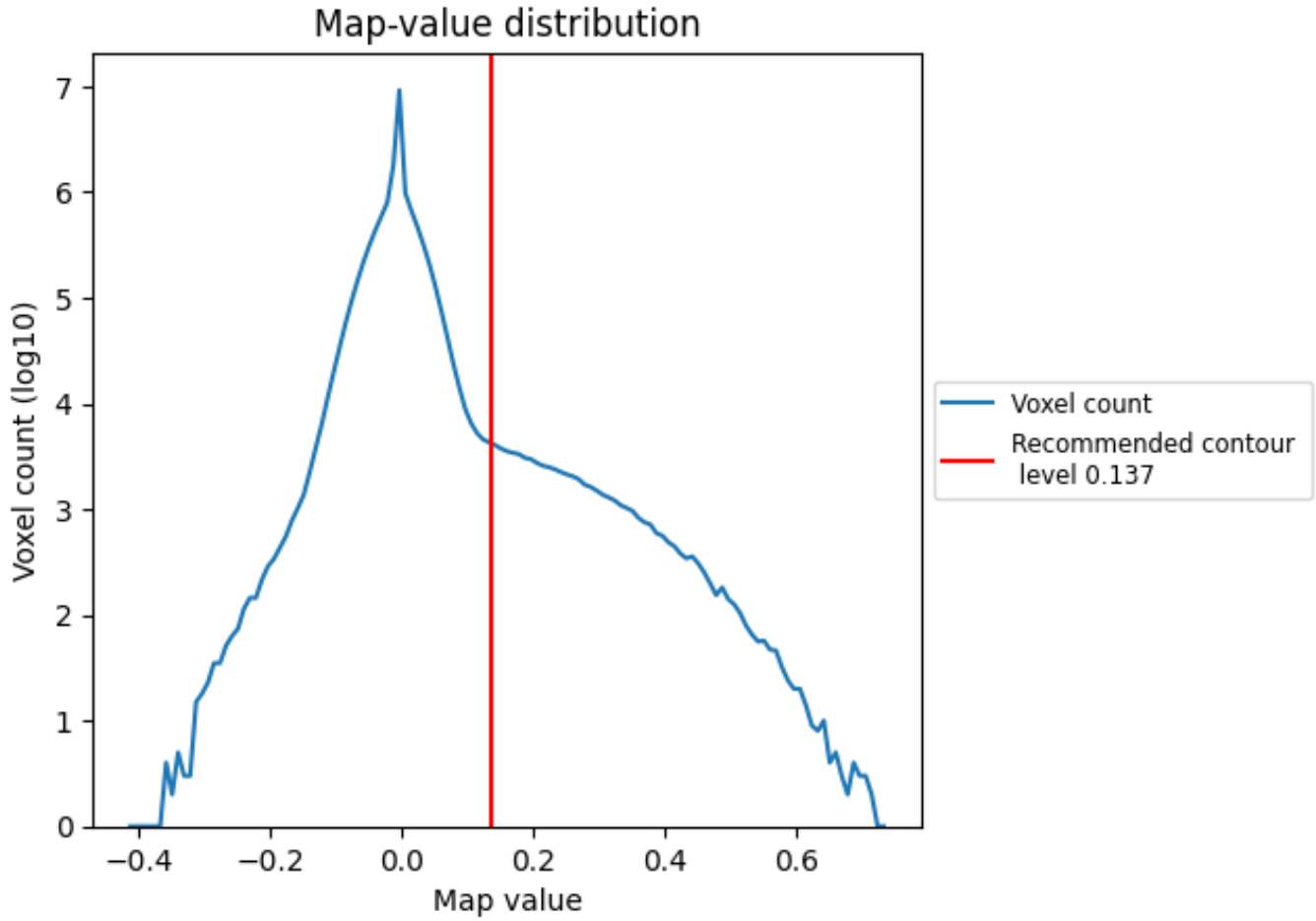
6.5 Mask visualisation (i)

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

7 Map analysis

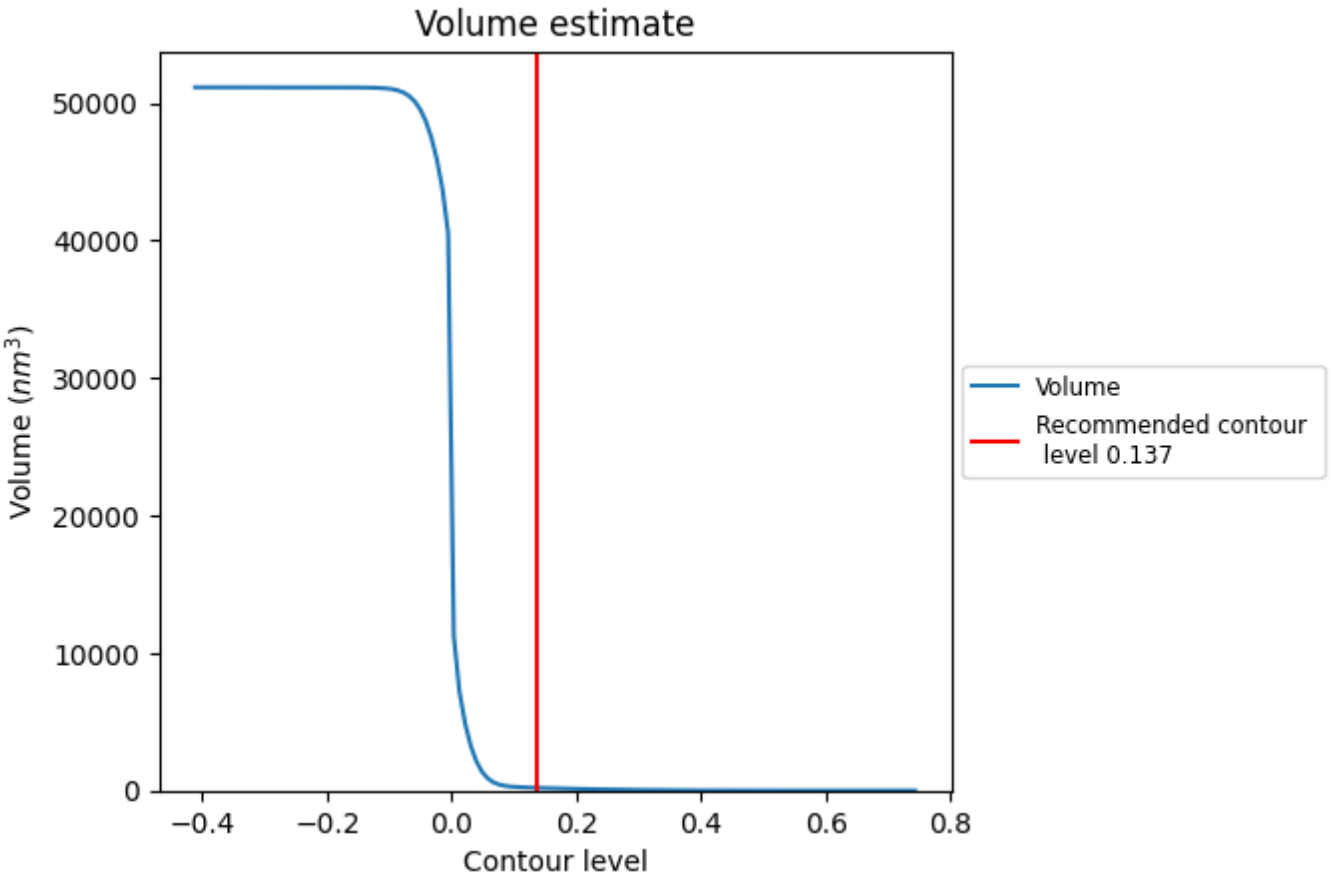
This section contains the results of statistical analysis of the map.

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.

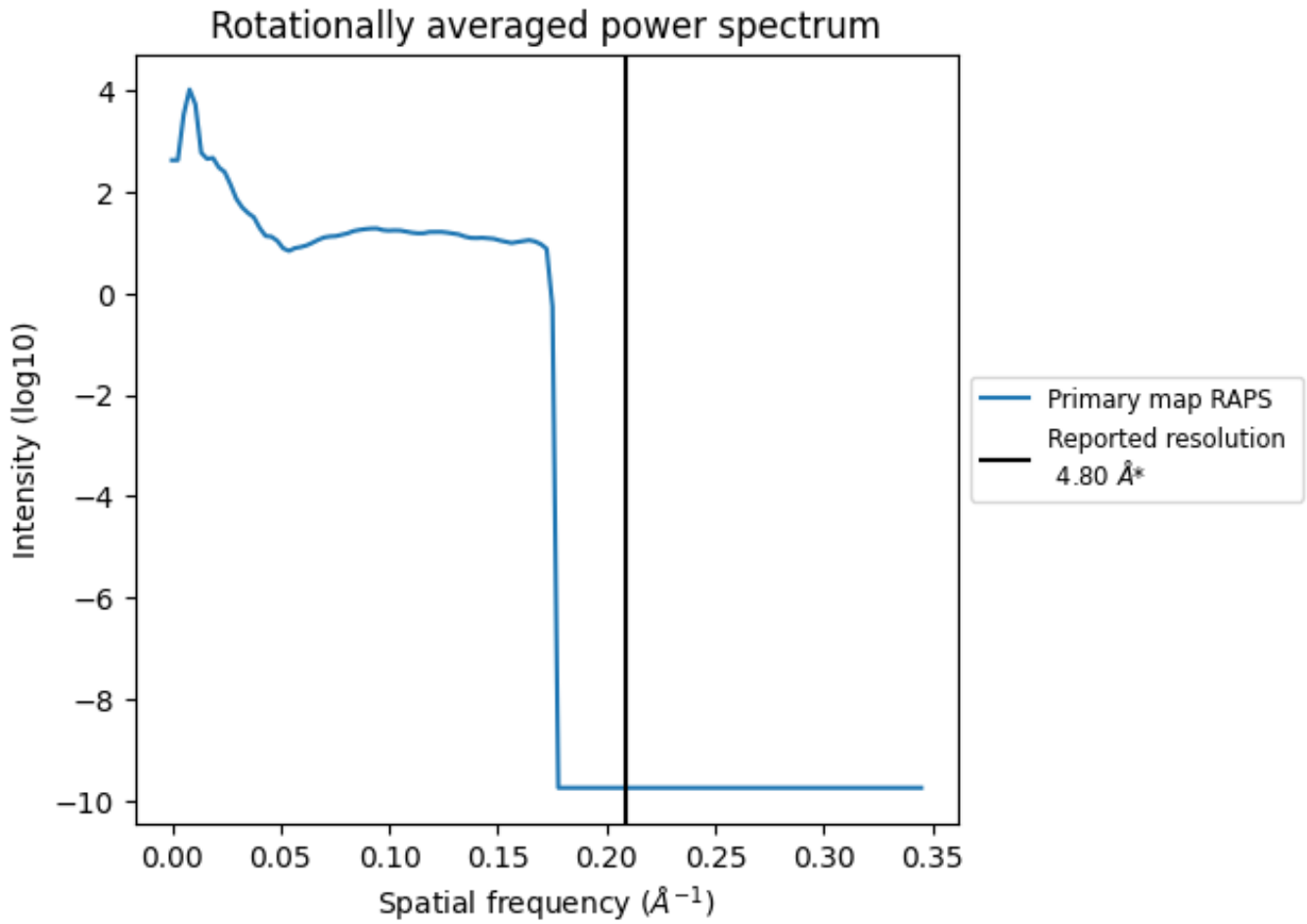
7.2 Volume estimate



The volume at the recommended contour level is 197 nm^3; this corresponds to an approximate mass of 178 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 0.208 Å^{-1}

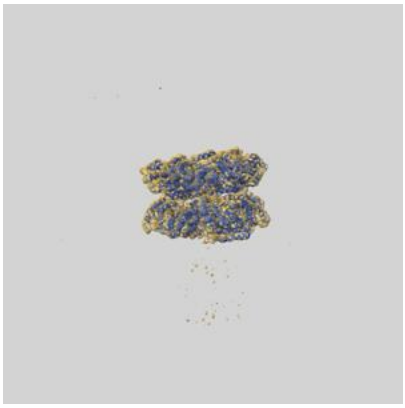
8 Fourier-Shell correlation (i)

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

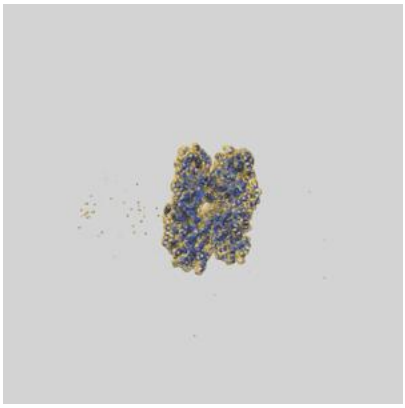
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8659 and PDB model 5VCA. Per-residue inclusion information can be found in section 3 on page 4.

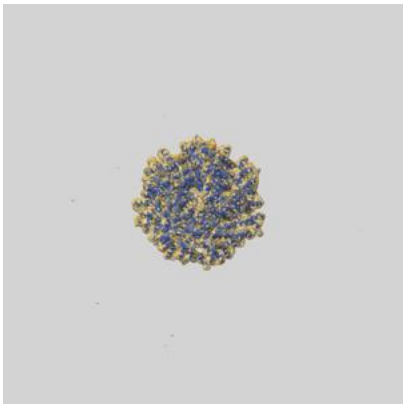
9.1 Map-model overlay



X



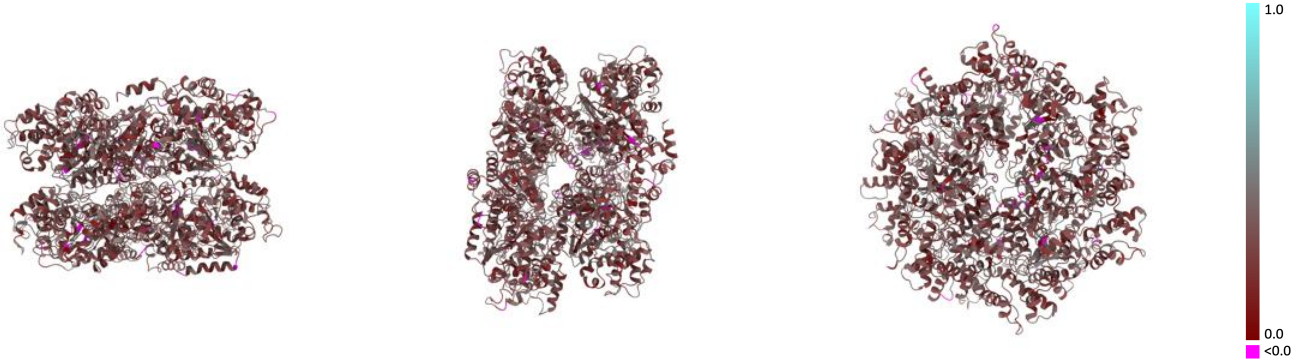
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.137 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.

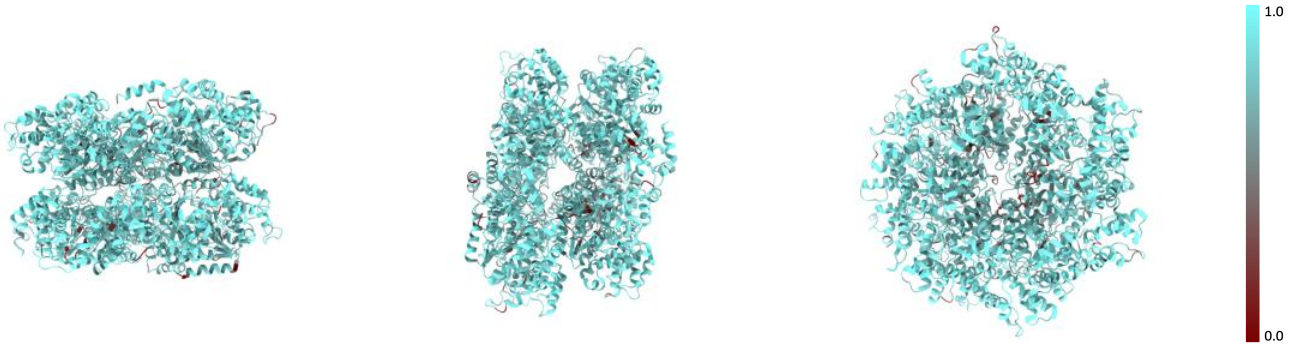
9.2 Q-score mapped to coordinate model



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.

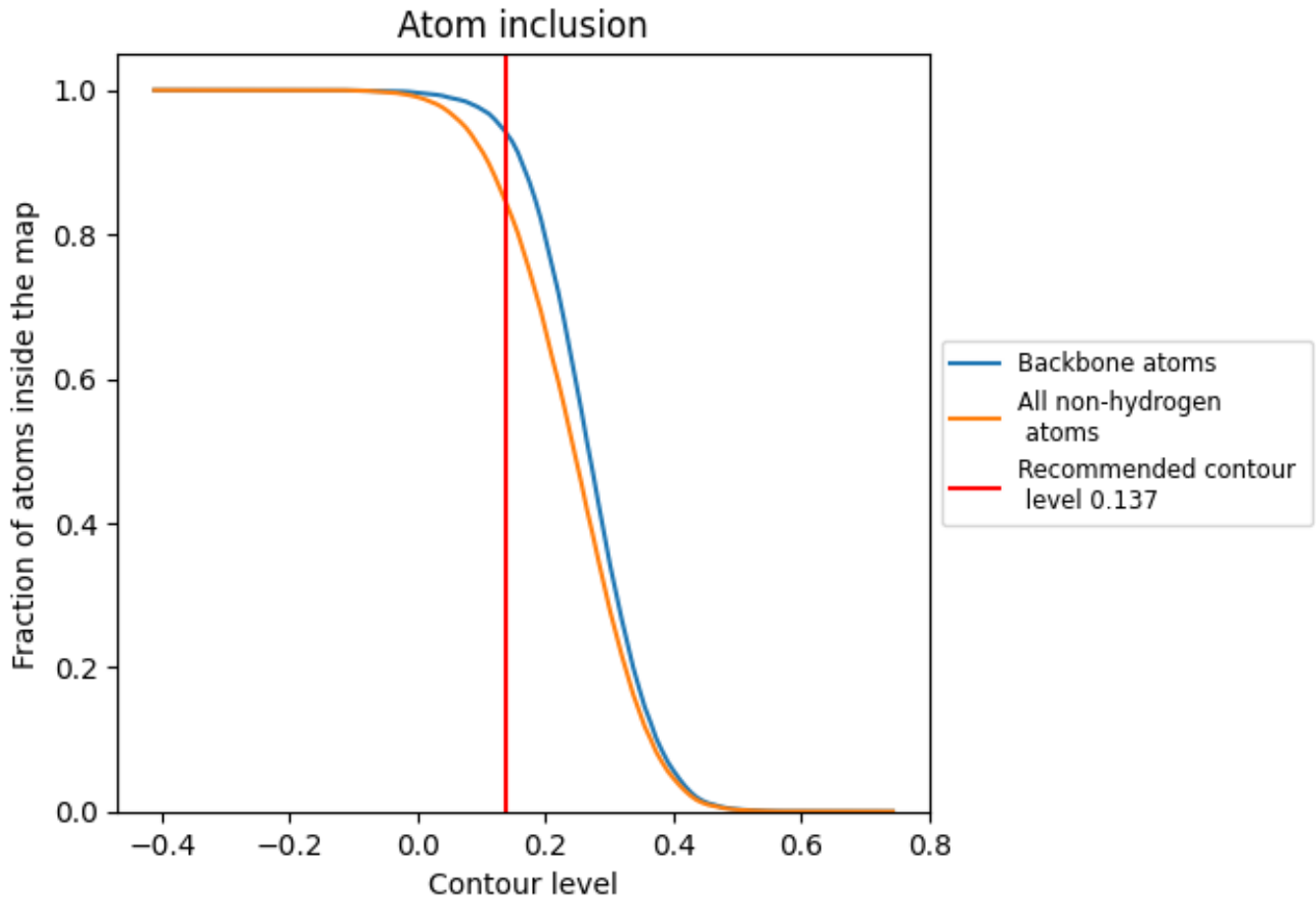
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.137).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.137) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8469	0.2980
M	0.8608	0.3030
N	0.8690	0.3040
O	0.8616	0.3020
P	0.8108	0.2890
Q	0.8500	0.2990
R	0.8291	0.2900