Full wwPDB EM Validation Report

Nov 12, 2022 – 09:29 AM EST

PDB ID	:	6PKR
EMDB ID	:	EMD-20364
Title	:	MicroED structure of proteinase K from a platinum-coated, polished, single lamella at 1.79A resolution (#13)
Authors	:	Martynowycz, M.W.; Zhao, W.; Hattne, J.; Jensen, G.J.; Gonen, T.
Deposited on	:	2019-06-29
Resolution	:	1.79 Å(reported)
Based on initial model	:	6CL7

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 (i) 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 (i)) were used in the production of this report:

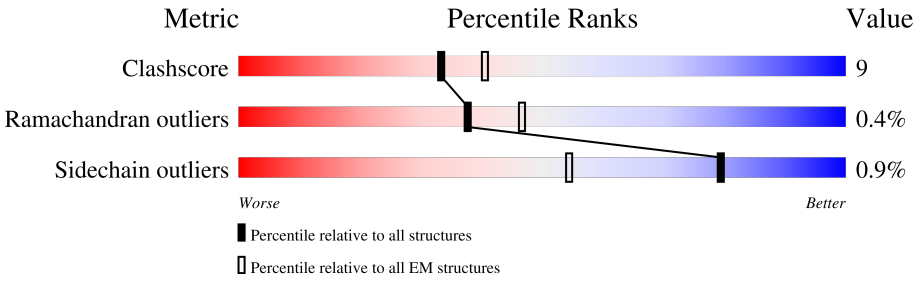
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 1.79 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	279	81% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2100 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 Proteinase K.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	279	Total	C	N	O	S	0	0
			2029	1247	357	415	10		

- Molecule 2 is water.

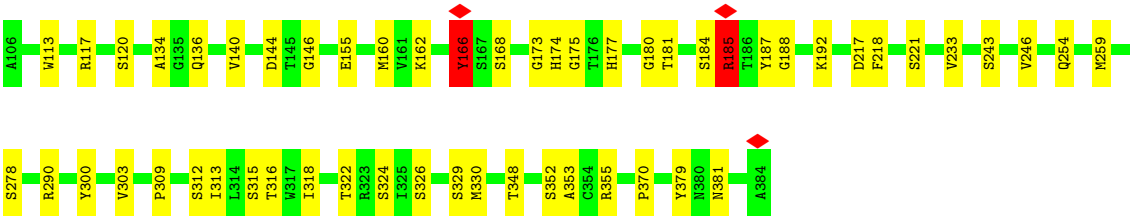
Mol	Chain	Residues	Atoms		AltConf
2	A	71	Total	O	0
			71	71	

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: Proteinase K

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a=67.1 Å, b=67.1 Å, c=107.0 Å, α=90°, β=90°, γ=90°, space group=96	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose (e^-/Å^2)	0.03	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI CETA (4k x 4k)	Depositor
Maximum map value	2.159	Depositor
Minimum map value	-0.770	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.323	Depositor
Recommended contour level	0.48507	Depositor
Map size (Å)	70.93369, 70.93369, 70.59928	wwPDB
Map dimensions	203, 203, 211	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.34942704, 0.34942704, 0.33459374	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	0.81	10/2068 (0.5%)	0.84	11/2810 (0.4%)

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	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	TYR	CD2-CE2	-13.98	1.18	1.39
1	A	166	TYR	CB-CG	-13.54	1.31	1.51
1	A	185	ARG	CB-CG	11.90	1.84	1.52
1	A	166	TYR	CD1-CE1	-10.47	1.23	1.39
1	A	185	ARG	CZ-NH1	8.42	1.44	1.33
1	A	185	ARG	CG-CD	6.93	1.69	1.51
1	A	166	TYR	CE2-CZ	-6.50	1.30	1.38
1	A	185	ARG	CD-NE	5.72	1.56	1.46
1	A	185	ARG	NE-CZ	5.46	1.40	1.33
1	A	166	TYR	CZ-OH	-5.22	1.28	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	TYR	CB-CG-CD2	-20.38	108.78	121.00
1	A	185	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	A	166	TYR	CB-CG-CD1	6.92	125.15	121.00
1	A	185	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
1	A	185	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	185	ARG	CA-CB-CG	6.40	127.47	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ARG	CG-CD-NE	6.02	124.44	111.80
1	A	166	TYR	CE1-CZ-CE2	5.90	129.25	119.80
1	A	166	TYR	CD1-CE1-CZ	-5.82	114.56	119.80
1	A	166	TYR	CB-CA-C	-5.64	99.11	110.40
1	A	185	ARG	CB-CG-CD	5.57	126.07	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Sidechain,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	2029	0	1932	36	1
2	A	71	0	0	7	0
All	All	2100	0	1932	36	1

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 9.

All (36) 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:185:ARG:CB	1:A:185:ARG:CG	1.84	1.50
1:A:180:GLY:HA2	1:A:184:SER:HB3	1.48	0.94
1:A:221:SER:HB3	2:A:404:HOH:O	1.82	0.80
1:A:330:MET:SD	2:A:405:HOH:O	2.40	0.79
1:A:312:SER:O	2:A:402:HOH:O	2.01	0.77
1:A:173:GLY:HA2	1:A:318:ILE:HG23	1.72	0.71
1:A:217:ASP:O	2:A:404:HOH:O	2.11	0.66
1:A:187:TYR:OH	1:A:322:THR:HG21	2.00	0.62
1:A:326:SER:N	2:A:403:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLY:CA	1:A:184:SER:HB3	2.29	0.58
1:A:177:HIS:CD2	1:A:315:SER:HB3	2.42	0.55
1:A:259:MET:HG3	1:A:353:ALA:HB3	1.88	0.54
1:A:290:ARG:NH2	2:A:401:HOH:O	2.01	0.54
1:A:155:GLU:CD	1:A:185:ARG:HG3	2.27	0.54
1:A:278:SER:HA	1:A:303:VAL:HG21	1.90	0.53
1:A:254:GLN:NE2	2:A:419:HOH:O	2.43	0.51
1:A:174:HIS:HE1	1:A:329:SER:HB2	1.73	0.51
1:A:166:TYR:N	1:A:166:TYR:CD1	2.80	0.48
1:A:174:HIS:CE1	1:A:329:SER:HB2	2.49	0.48
1:A:140:VAL:HG22	1:A:233:VAL:HB	1.97	0.46
1:A:348:THR:HG1	1:A:352:SER:HG	1.59	0.46
1:A:117:ARG:NH1	1:A:120:SER:O	2.48	0.46
1:A:300:TYR:CG	1:A:370:PRO:HG2	2.51	0.46
1:A:113:TRP:CH2	1:A:309:PRO:HB3	2.51	0.46
1:A:312:SER:N	1:A:326:SER:OG	2.41	0.45
1:A:134:ALA:HB3	1:A:192:LYS:HG3	1.97	0.45
1:A:181:THR:O	1:A:188:GLY:HA2	2.19	0.43
1:A:162:LYS:HB2	1:A:218:PHE:CZ	2.54	0.42
1:A:155:GLU:OE2	1:A:185:ARG:HG3	2.19	0.42
1:A:136:GLN:HB2	1:A:192:LYS:HE2	2.02	0.41
1:A:146:GLY:O	1:A:175:GLY:HA3	2.21	0.41
1:A:243:SER:HB3	1:A:246:VAL:HB	2.02	0.41
1:A:160:MET:HG3	1:A:168:SER:HB3	2.02	0.41
1:A:313:ILE:O	1:A:324:SER:HA	2.21	0.41
1:A:379:TYR:CZ	1:A:381:ASN:HA	2.55	0.41
1:A:315:SER:OG	1:A:316:THR:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:OH	1:A:185:ARG:O[4_545]	1.55	0.65

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	277/279 (99%)	263 (95%)	13 (5%)	1 (0%)	34 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ASP

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	213/213 (100%)	211 (99%)	2 (1%)	78 75

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

Mol	Chain	Res	Type
1	A	185	ARG
1	A	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

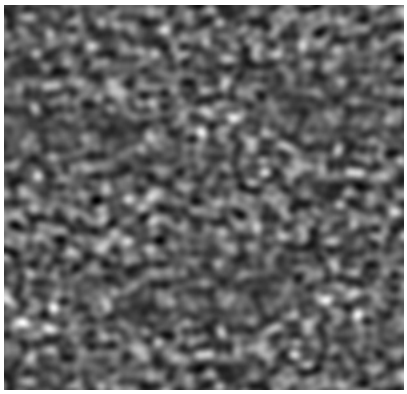
This section contains visualisations of the EMDB entry EMD-20364. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

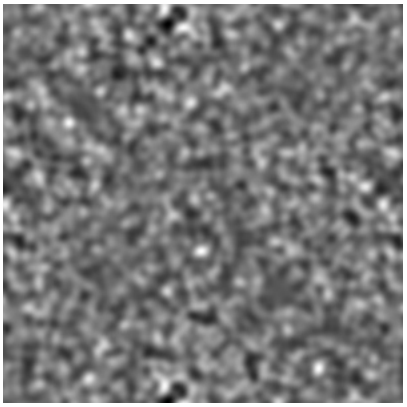
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

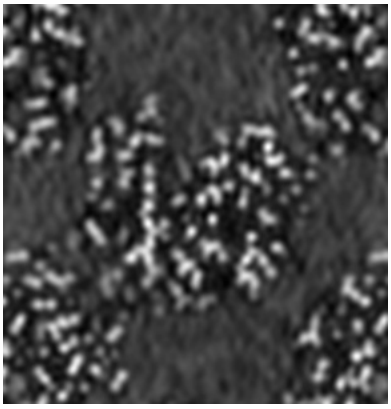


Z

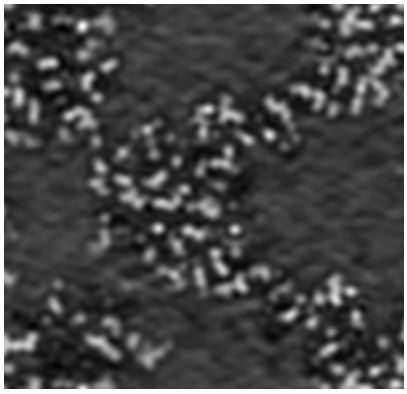
The images above show the map projected in three orthogonal directions.

6.2 Central slices

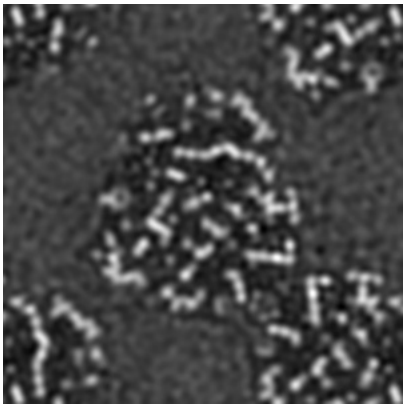
6.2.1 Primary map



X Index: 101



Y Index: 101

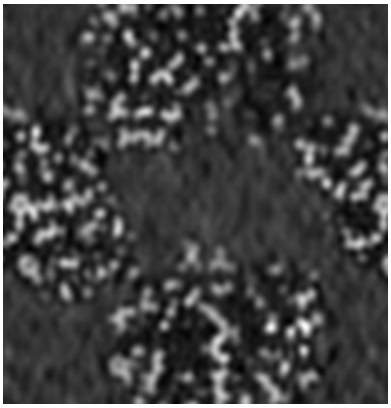


Z Index: 105

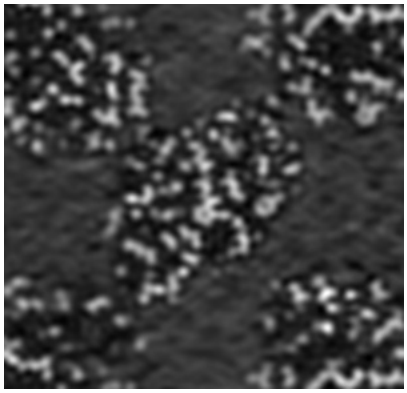
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

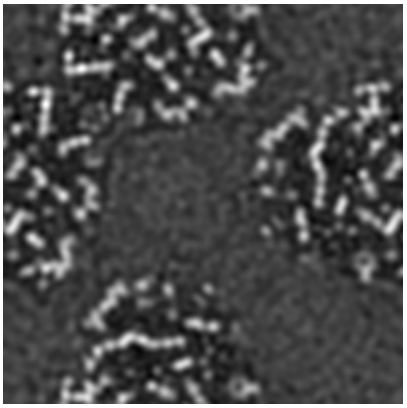
6.3.1 Primary map



X Index: 18



Y Index: 127

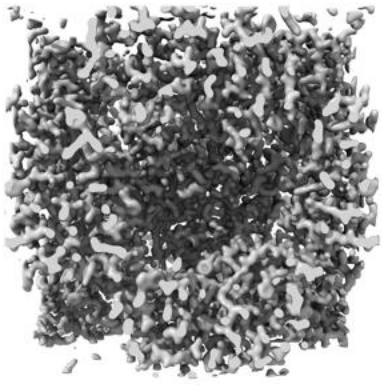


Z Index: 25

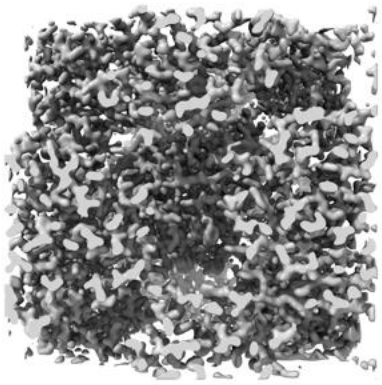
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

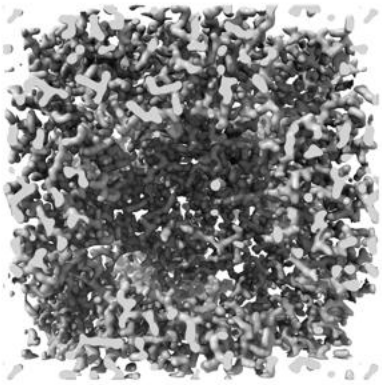
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.48507. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

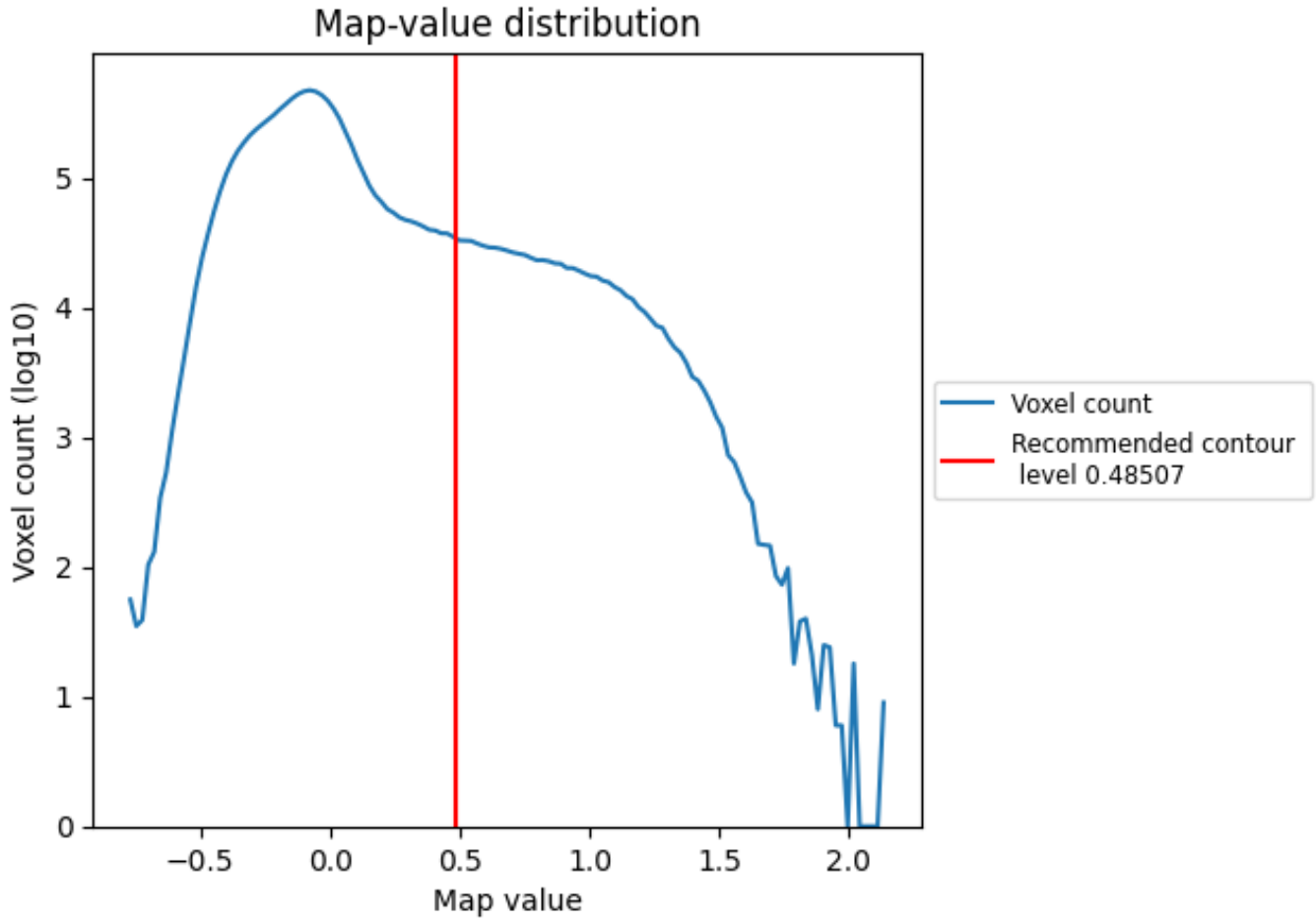
6.5 Mask visualisation (i)

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

7 Map analysis

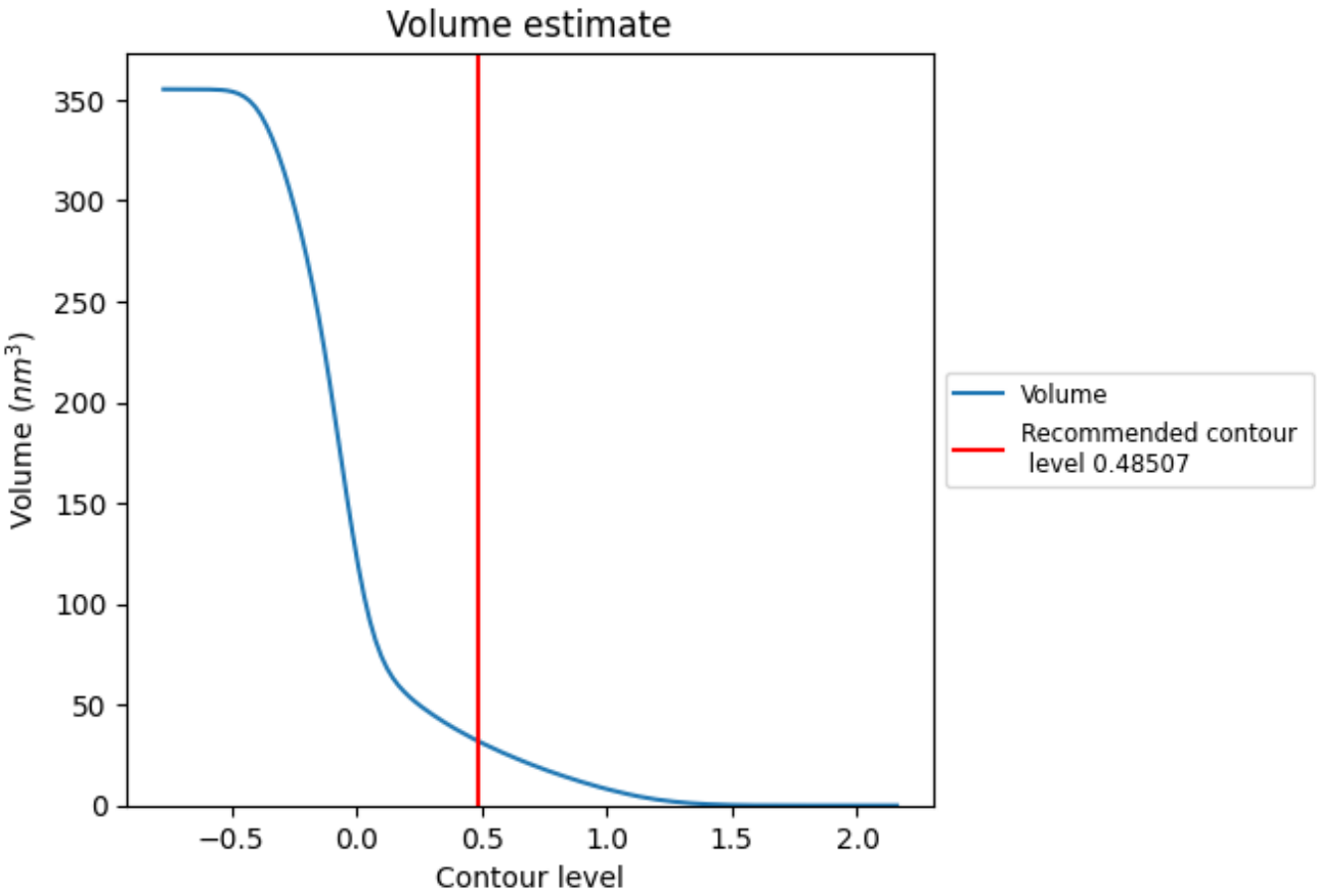
This section contains the results of statistical analysis of the map.

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 32 nm^3; this corresponds to an approximate mass of 29 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

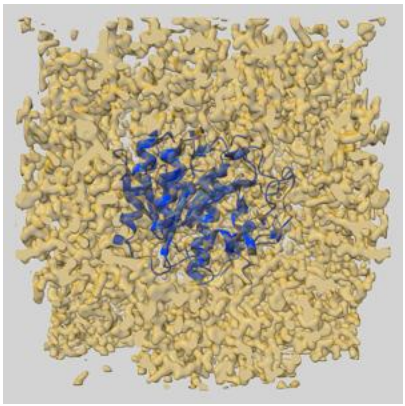
8 Fourier-Shell correlation (i)

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

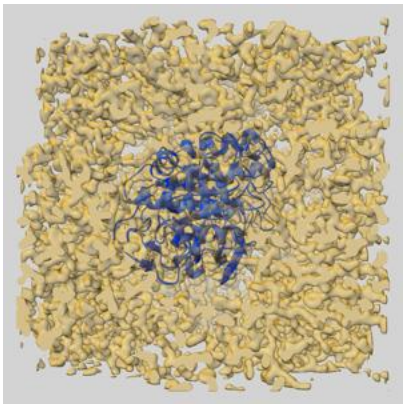
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20364 and PDB model 6PKR. Per-residue inclusion information can be found in section 3 on page 4.

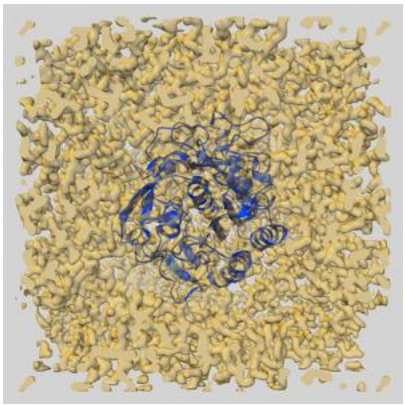
9.1 Map-model overlay



X



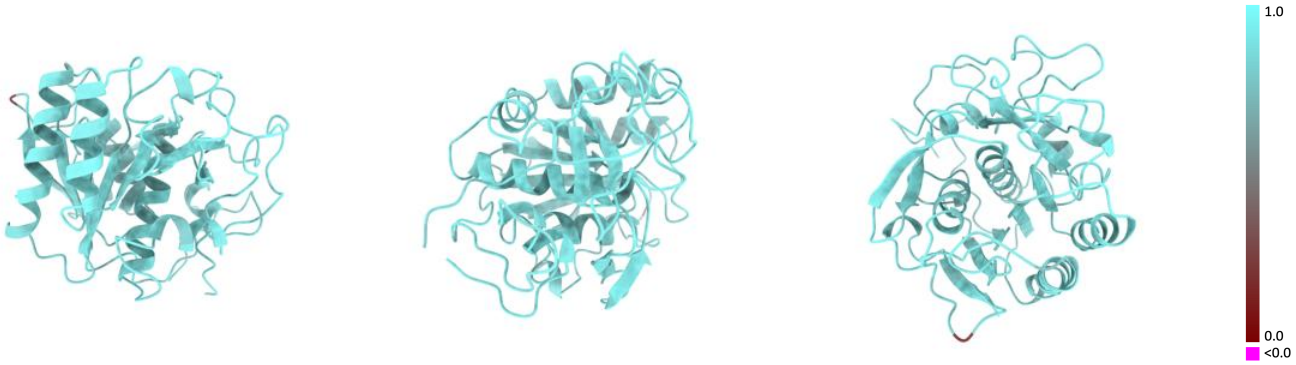
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.48507 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.

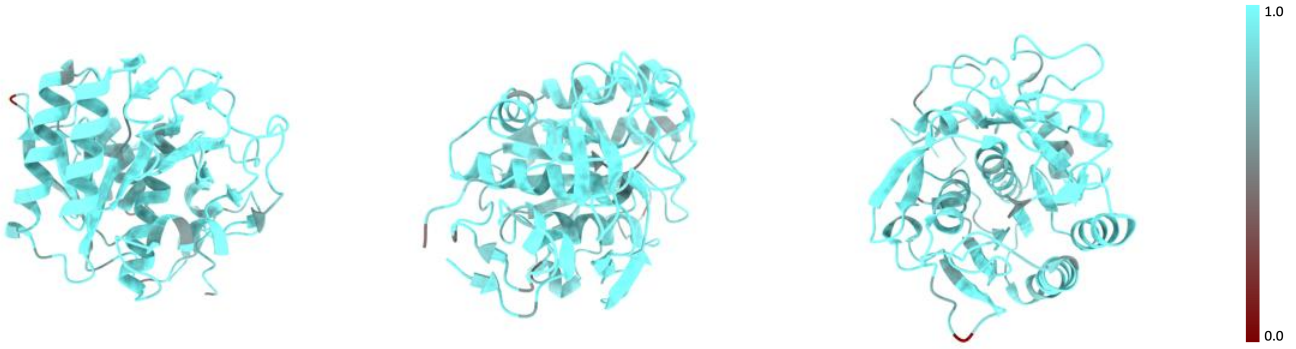
9.2 Q-score mapped to coordinate model



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.

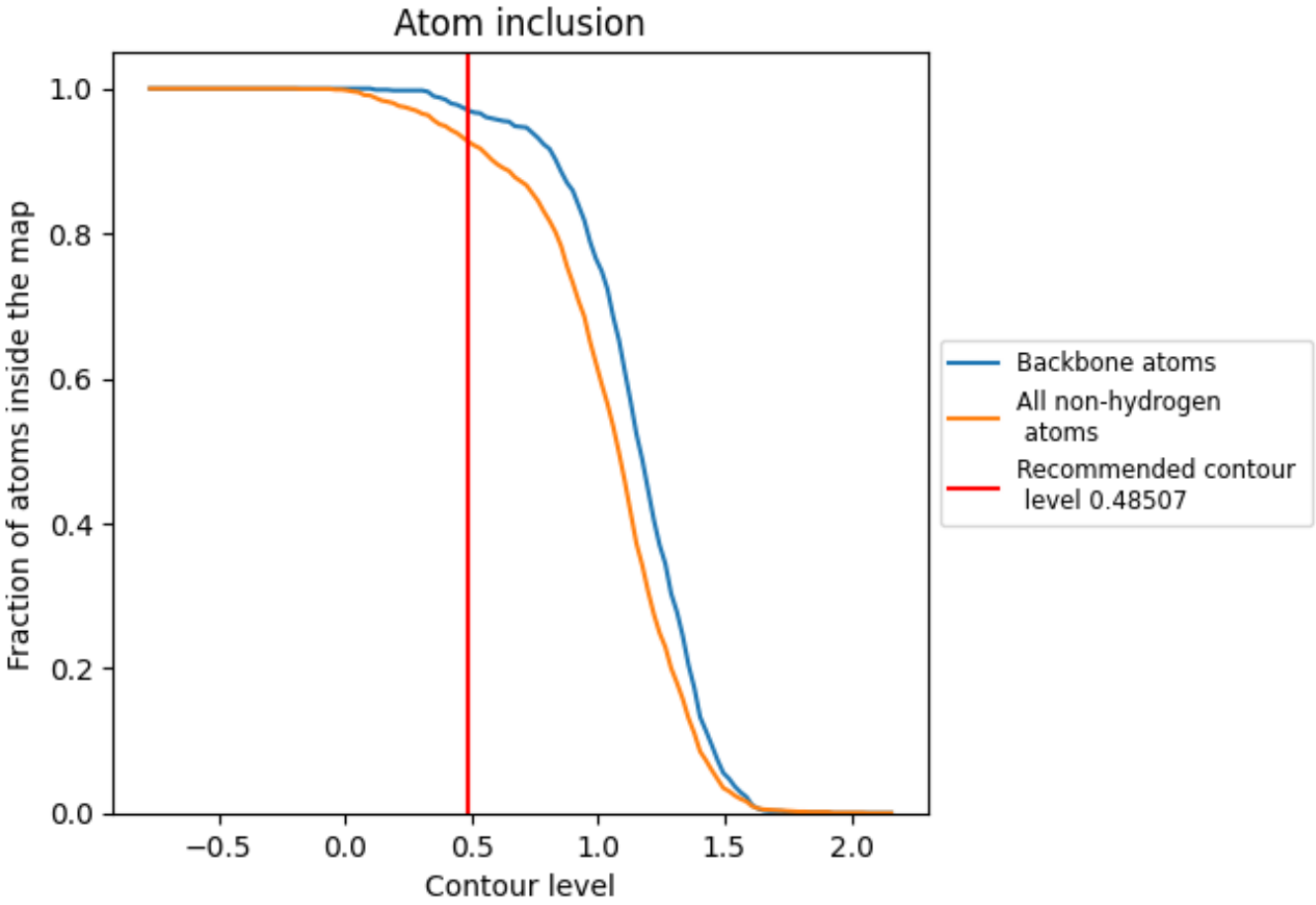
9.3 Atom inclusion mapped to coordinate model



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 (0.48507).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.48507) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9270	0.8070
A	0.9270	0.8070