



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:17 pm GMT

PDB ID : 6EO1
EMDB ID : EMD-3907
Title : The electron crystallography structure of the cAMP-bound potassium channel MloK1 (PCO-refined)
Authors : Kowal, J.; Biyani, N.; Chami, M.; Scherer, S.; Rzepiela, A.; Baumgartner, P.; Upadhyay, V.; Nimigean, C.; Stahlberg, H.
Deposited on : 2017-10-08
Resolution : 4.50 Å (reported)
Based on initial model : 4CHV

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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

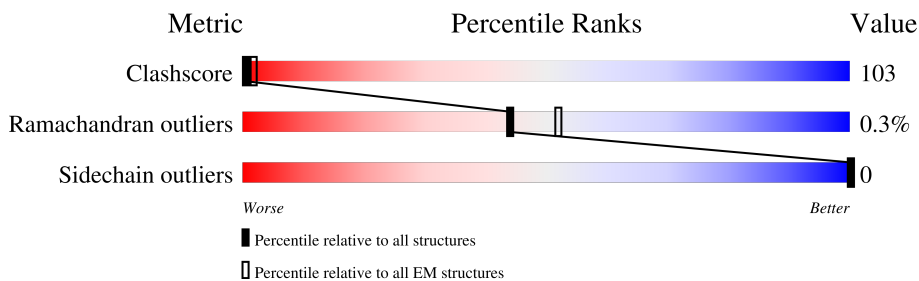
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 4.50 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 $\leq 5\%$. 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	355	
1	B	355	
1	C	355	
1	D	355	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14570 atoms, of which 3924 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 Cyclic nucleotide-gated potassium channel mll3241.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	355	3642	1734	981	455	461	11	0	0
1	B	355	3642	1734	981	455	461	11	0	0
1	C	355	3642	1734	981	455	461	11	0	0
1	D	355	3642	1734	981	455	461	11	0	0

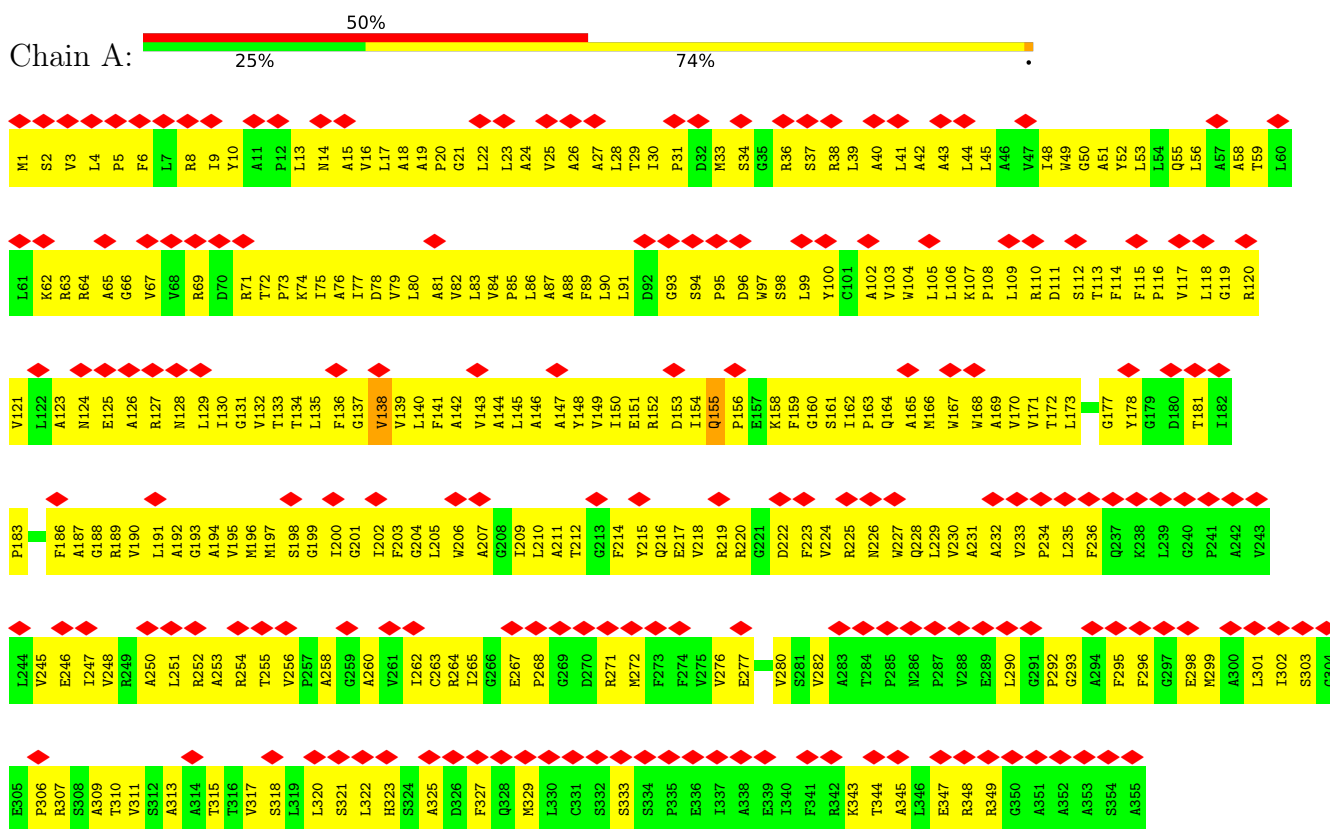
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
2	C	2	Total	K	0
			2	2	

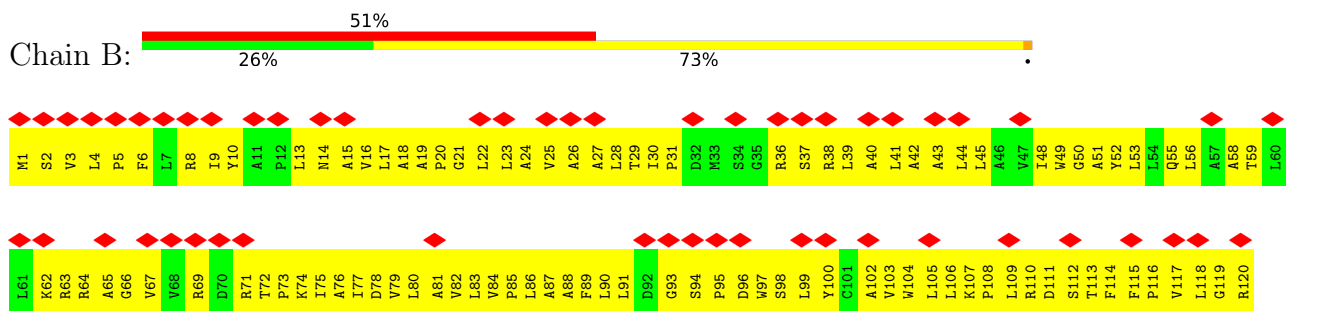
3 Residue-property plots

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: Cyclic nucleotide-gated potassium channel mll3241

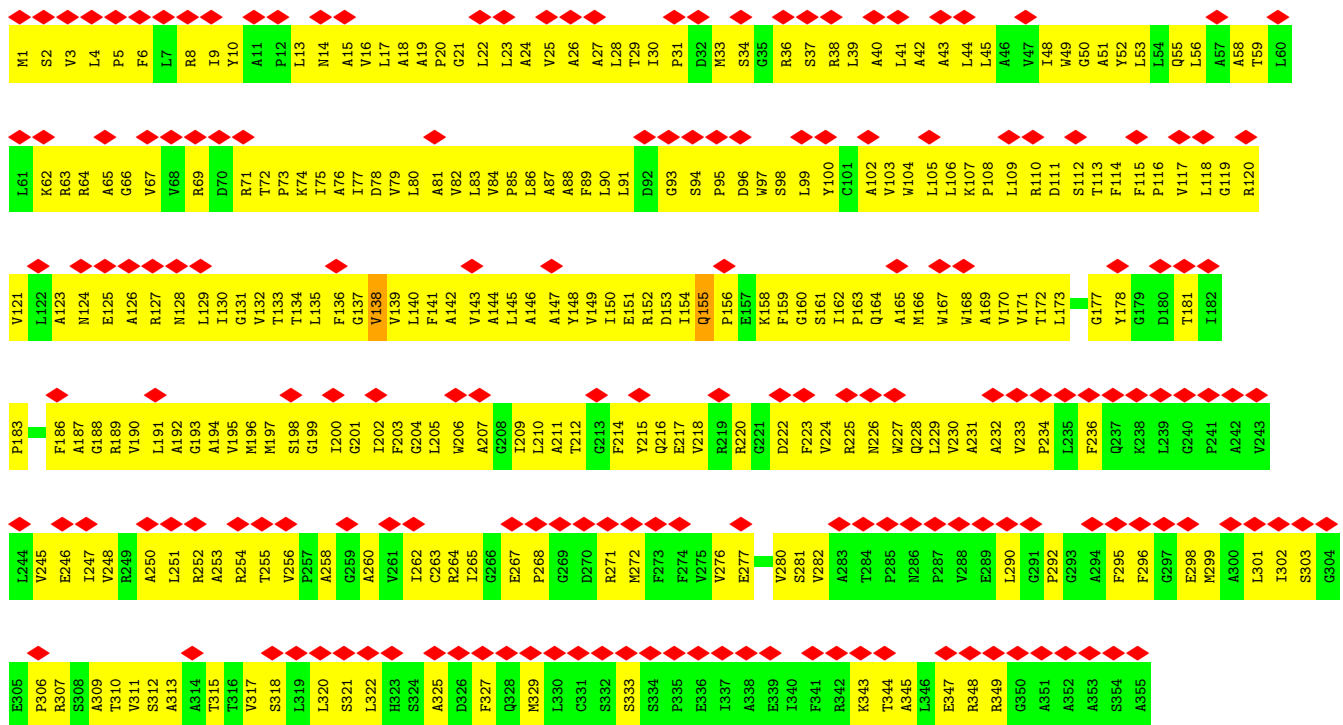


- Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

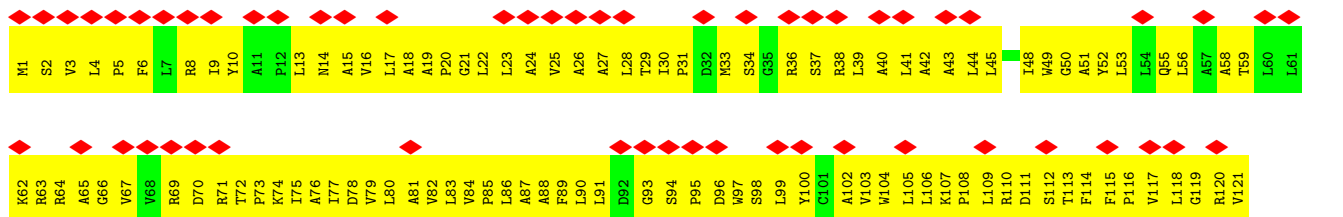




• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241



• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241



L122	A123	A124	E125	A126	R127	M128	L129	I130	G131	V132	T133	T134	L135	F136	G137	V138	V139	L140	F141	A142	V143	A144	L145	A146	A147	Y148	V149	I150	E151	R152	D153	I154	Q155	P156	E157	K158	F159	G160	S161	I162	P163	Q164	A165	M166	M167	W168	A169	V170	V171	T172	L173	G177	Y178	G179	D180	T181	I182	P183
F186	A187	G188	R189	V190	L191	A192	G193	A194	V195	M196	M197	S198	G199	I200	G201	I202	F203	G204	L205	W206	A207	G208	I209	L210	A211	T212	G213	F214	Y215	Q216	E217	V218	R219	R220	G221	D222	F223	V224	R225	N226	W227	Q228	L229	V230	A231	A232	V233	P234	L235	F236	Q237	K238	L239	G240	P241	A242	V243	L244
V245	E246	I247	V248	R249	A250	L251	R252	A253	R254	T255	V256	P257	A258	G259	A260	V261	I262	C263	R264	I265	G266	E267	P268	G269	D270	R271	M272	F273	F274	V275	V276	E277	V280	S281	V282	A283	T284	P285	N286	P287	V288	E289	L290	G291	P292	G293	A294	F295	F296	G297	E298	M299	A300	L301	I302	SS303	G304	E305
P306	R307	S308	A309	T310	V311	S312	A313	A314	T315	T316	V317	S318	L319	L320	S321	L322	H323	S324	A325	D326	F327	Q328	M329	L330	C331	S332	S333	S334	P335	E336	I337	A338	E339	I340	F341	R342	K343	T344	A345	L346	E347	R348	R349	G350	A351	A352	A353	S354	A355									

4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, $a=135 \text{ \AA}$, $b=135 \text{ \AA}$, $c=200 \text{ \AA}$, $\gamma=90^\circ$, space group=P 4 21 2	Depositor
Number of images used	Not provided	
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2773.677	Depositor
Minimum map value	-499.998	Depositor
Average map value	9.992	Depositor
Map value standard deviation	257.079	Depositor
Recommended contour level	600.0	Depositor
Map size (\AA)	106.96, 106.96, 210.045	wwPDB
Map dimensions	112, 112, 201	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.955, 0.955, 1.045	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	0.36	0/2720	0.58	0/3713
1	B	0.36	0/2720	0.58	1/3713 (0.0%)
1	C	0.36	0/2720	0.58	0/3713
1	D	0.36	0/2720	0.58	1/3713 (0.0%)
All	All	0.36	0/10880	0.58	2/14852 (0.0%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	D	189	ARG	NE-CZ-NH1	-5.06	117.77	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	GLN	Peptide
1	B	155	GLN	Peptide
1	C	155	GLN	Peptide
1	D	155	GLN	Peptide

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	2661	981	2775	607	0
1	B	2661	981	2775	596	0
1	C	2661	981	2775	600	0
1	D	2661	981	2775	603	0
2	C	2	0	0	0	0
All	All	10646	3924	11100	2240	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 103.

The worst 5 of 2240 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:B:206:TRP:HA	1:B:209:ILE:HD12	1.23	1.18
1:A:58:ALA:O	1:A:62:LYS:HB3	1.45	1.16
1:A:206:TRP:HA	1:A:209:ILE:HD12	1.23	1.16
1:D:58:ALA:O	1:D:62:LYS:HB3	1.45	1.16
1:D:206:TRP:HA	1:D:209:ILE:HD12	1.23	1.16

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	353/355 (99%)	299 (85%)	53 (15%)	1 (0%)	41	76
1	B	353/355 (99%)	300 (85%)	52 (15%)	1 (0%)	41	76
1	C	353/355 (99%)	299 (85%)	53 (15%)	1 (0%)	41	76
1	D	353/355 (99%)	299 (85%)	53 (15%)	1 (0%)	41	76
All	All	1412/1420 (99%)	1197 (85%)	211 (15%)	4 (0%)	44	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	VAL
1	B	138	VAL
1	C	138	VAL
1	D	138	VAL

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	273/273 (100%)	273 (100%)	0	100	100
1	B	273/273 (100%)	273 (100%)	0	100	100
1	C	273/273 (100%)	273 (100%)	0	100	100
1	D	273/273 (100%)	273 (100%)	0	100	100
All	All	1092/1092 (100%)	1092 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	226	ASN
1	C	323	HIS

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Continued from previous page...

Mol	Chain	Res	Type
1	D	323	HIS
1	D	55	GLN
1	B	55	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

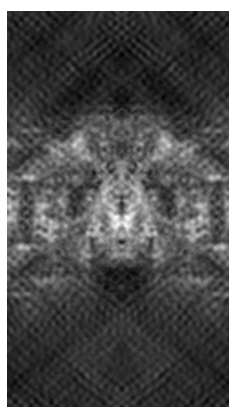
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3907. 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](#)

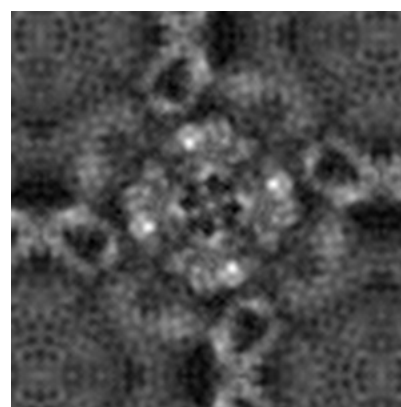
6.1.1 Primary map



X



Y

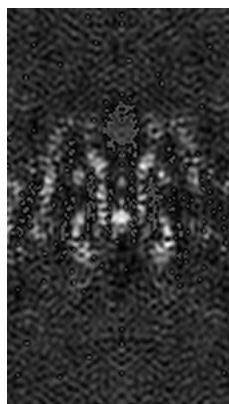


Z

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

6.2 Central slices [i](#)

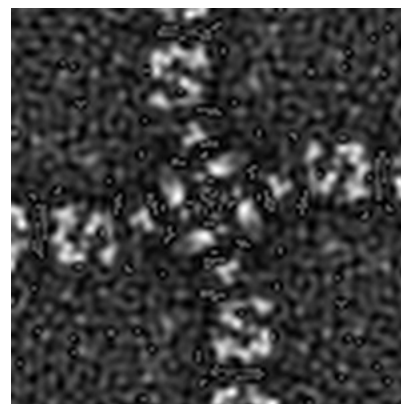
6.2.1 Primary map



X Index: 56



Y Index: 56

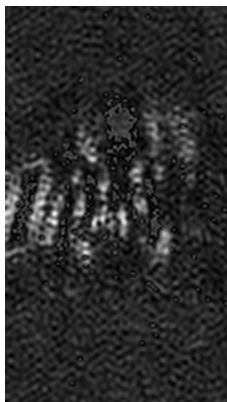


Z Index: 100

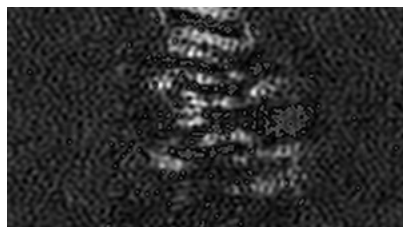
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

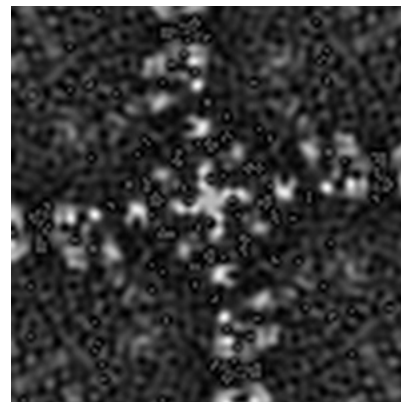
6.3.1 Primary map



X Index: 59



Y Index: 60

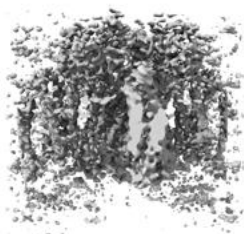


Z Index: 96

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

6.4 Orthogonal surface views [i](#)

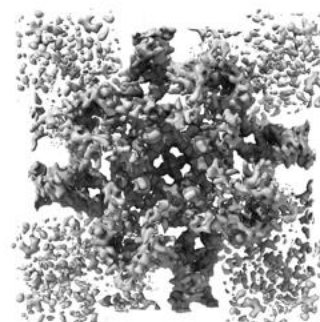
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 600.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

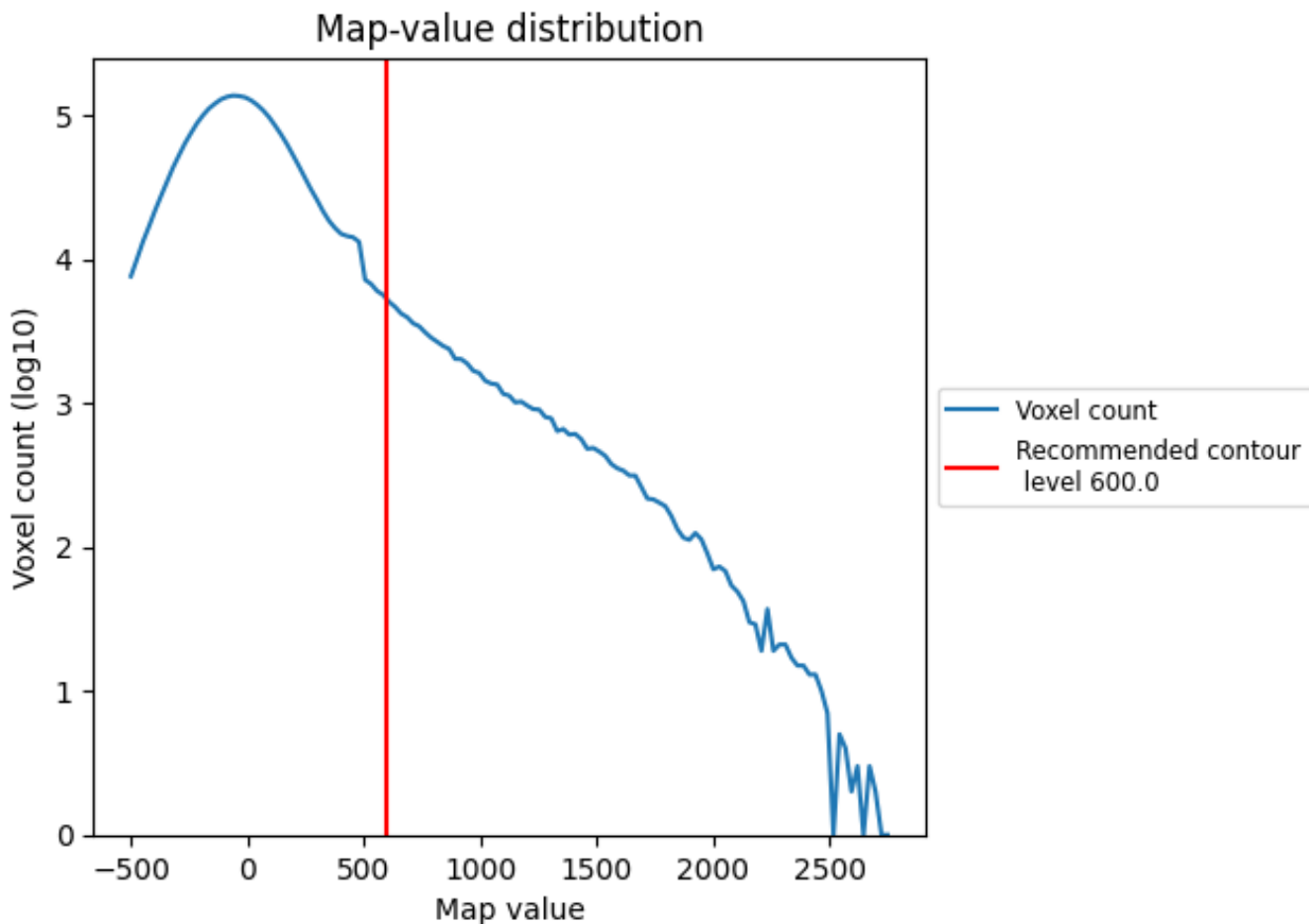
6.5 Mask visualisation

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

7 Map analysis [i](#)

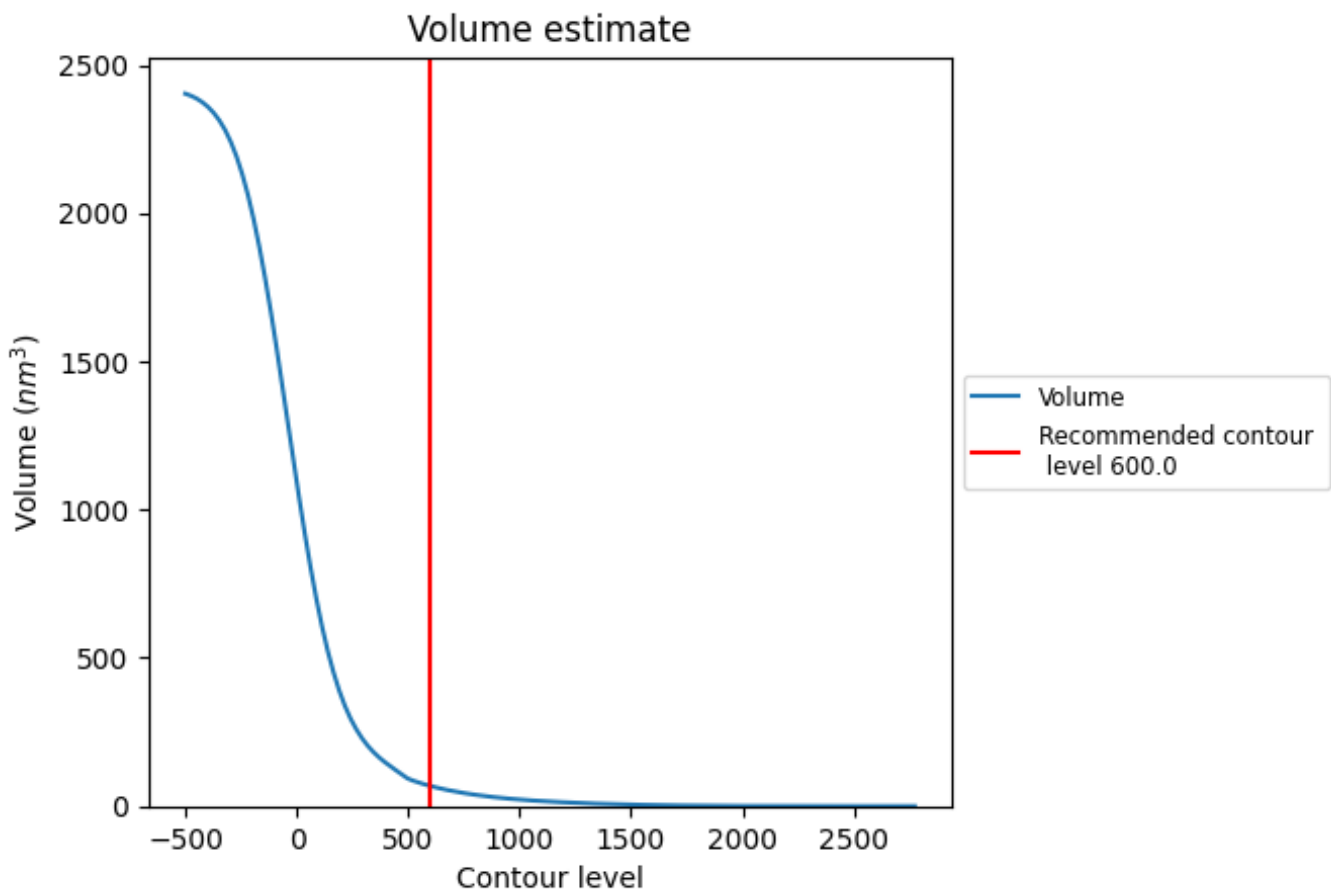
This section contains the results of statistical analysis of the map.

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 68 nm³; this corresponds to an approximate mass of 61 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](#)

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

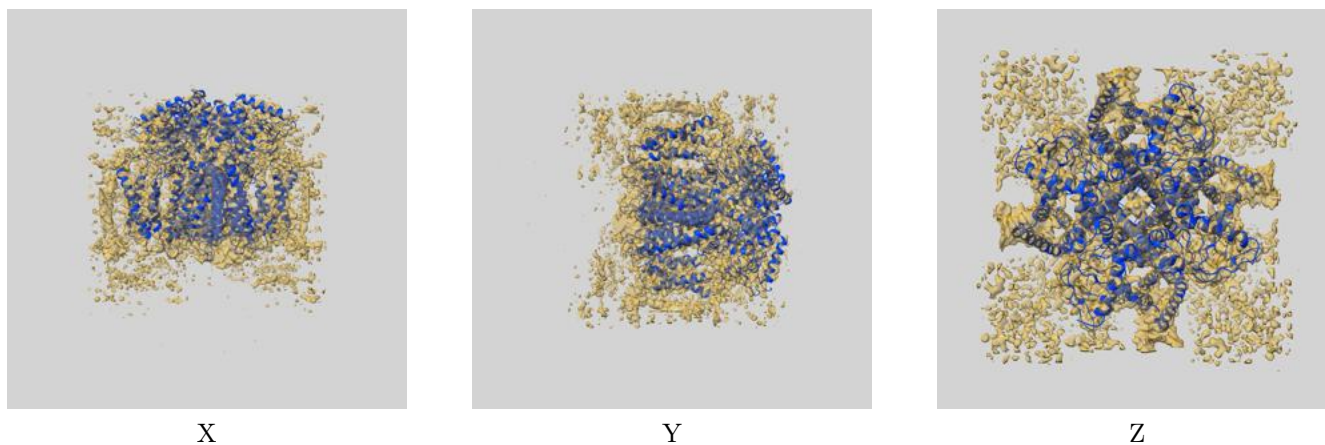
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

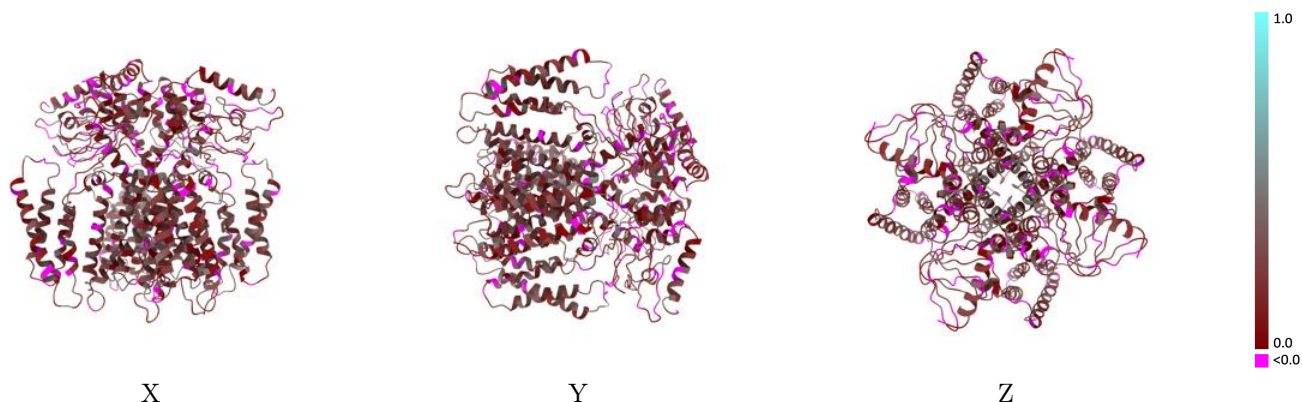
This section contains information regarding the fit between EMDB map EMD-3907 and PDB model 6EO1. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



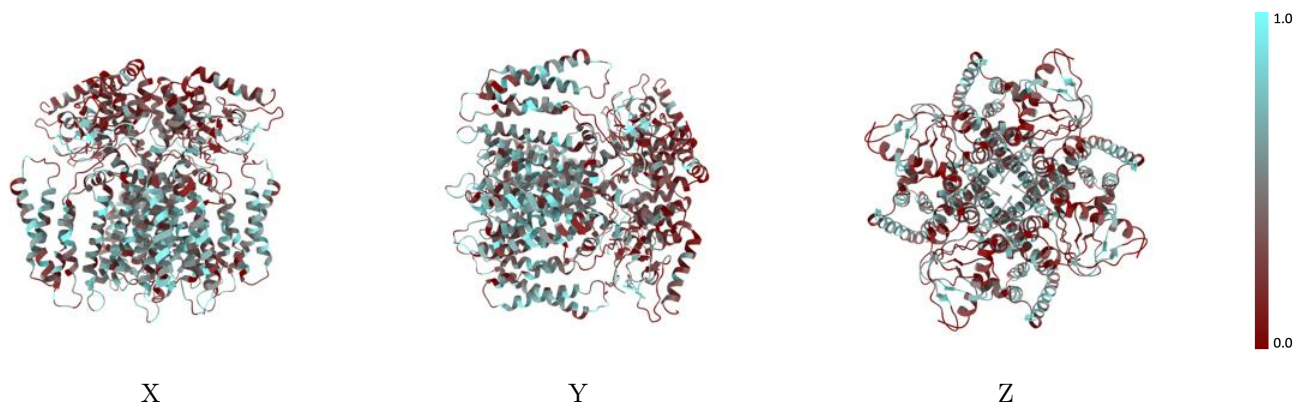
The images above show the 3D surface view of the map at the recommended contour level 600.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



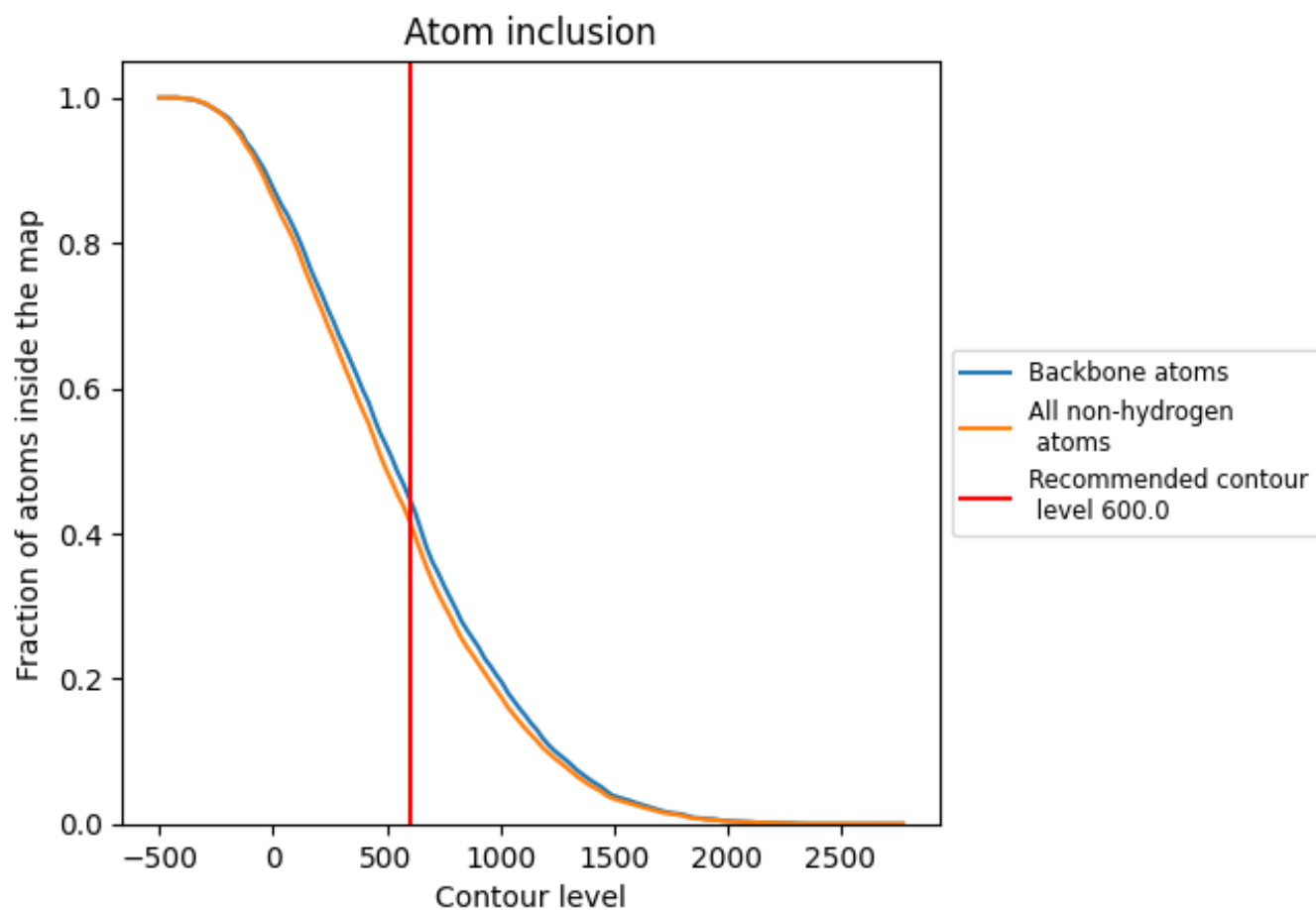
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (600.0).











9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (600.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4180	 0.1840
A	 0.4242	 0.1830
B	 0.4165	 0.1830
C	 0.4216	 0.1870
D	 0.4162	 0.1820

