wwPDB EM Validation Summary Report (i)

Feb 20, 2025 – 11:09 AM EST

|		
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

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	Percentile Ranks	Value
Clashscore		103
Ramachandran outliers		0.3%
Sidechain outliers		0

Worse　　　　　　　　　　　　　　　　　　　Better

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
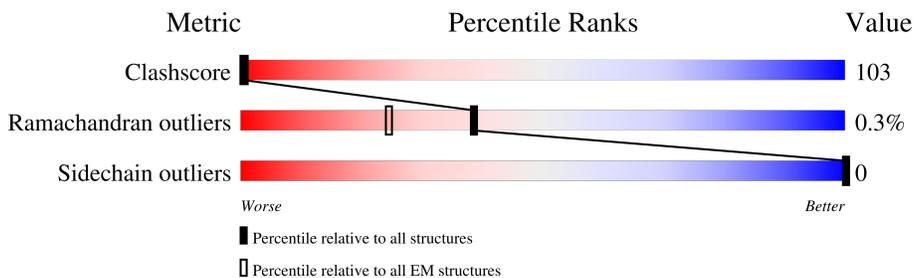
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	355	50% / 20% / 79% / •
1	B	355	51% / 21% / 79% / •
1	C	355	50% / 22% / 78% / •
1	D	355	50% / 21% / 79% / •

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
1	A	355	Total	C	H	N	O	S	0	0
			3642	1734	981	455	461	11		
1	B	355	Total	C	H	N	O	S	0	0
			3642	1734	981	455	461	11		
1	C	355	Total	C	H	N	O	S	0	0
			3642	1734	981	455	461	11		
1	D	355	Total	C	H	N	O	S	0	0
			3642	1734	981	455	461	11		

- 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.
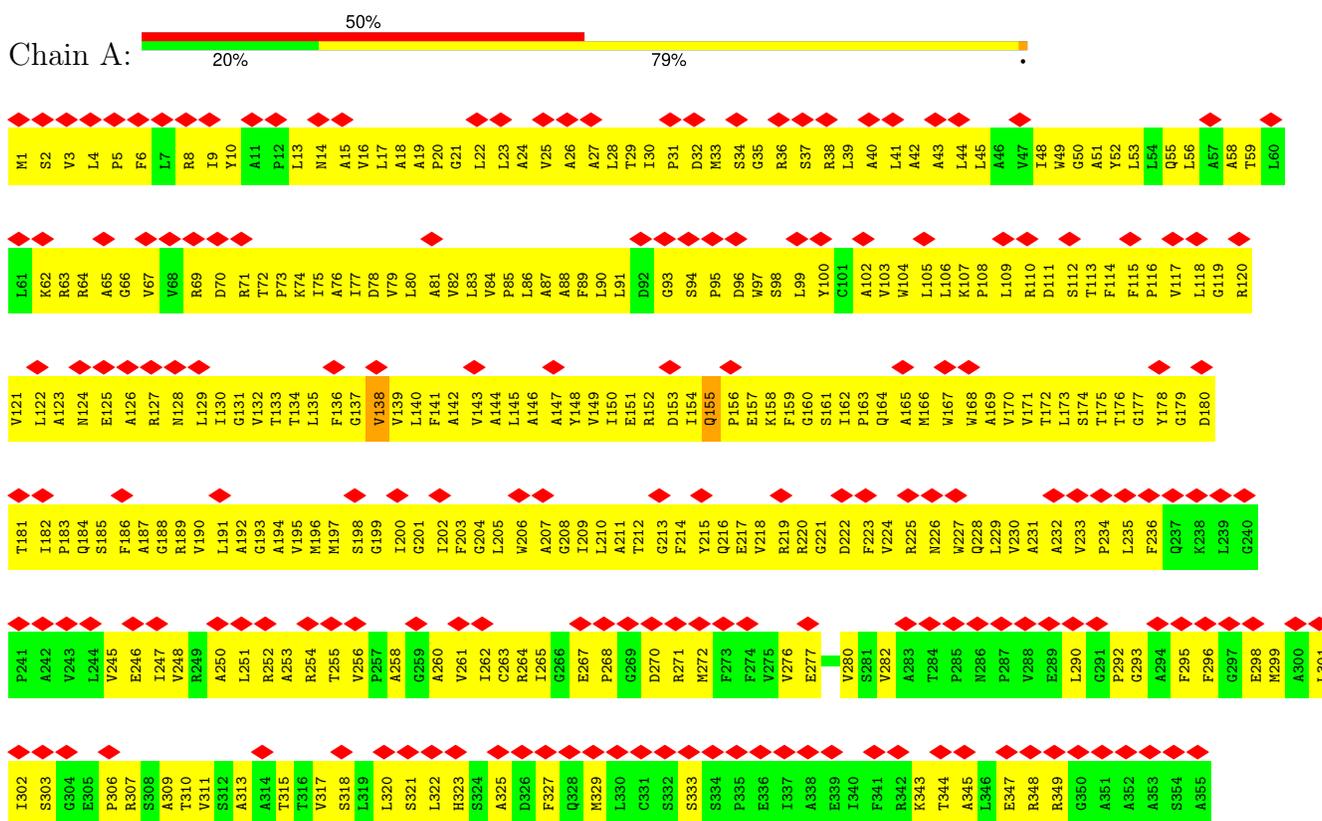
• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241


• Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

V121 L122 A123 N124 E125 A126 R127 N128 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 W167 W168 A169 V170 V171 T172 L173 S174 T175 T176 G177 Y178 G179 D180

T181 I182 P183 Q184 S185 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 S303 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

- Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

Chain C:

M1 S2 V3 L4 P5 F6 L7 R8 I9 Y10 A11 P12 L13 N14 A15 V16 L17 A18 A19 P20 G21 L22 L23 A24 V25 A26 A27 L28 T29 I30 P31 D32 M33 S34 G35 R36 S37 R38 L39 A40 L41 A42 A43 L44 L45 A46 V47 I48 W49 G50 A51 Y52 L53 L54 Q55 L56 A57 A58 T59 L60

L61 K62 R63 R64 A65 G66 V67 V68 R69 D70 R71 T72 P73 K74 I75 A76 I77 D78 V79 L80 A81 V82 L83 V84 P85 L86 A87 A88 F89 L90 L91 D92 G93 S94 P95 D96 W97 S98 L99 Y100 C101 A102 V103 W104 L105 L106 K107 P108 L109 R110 D111 S112 T113 F114 F115 P116 V117 L118 G119 R120

V121 L122 A123 N124 E125 A126 R127 N128 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 W167 W168 A169 V170 V171 T172 L173 S174 T175 T176 G177 Y178 G179 D180

T181 I182 P183 Q184 S185 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 S303 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

- Molecule 1: Cyclic nucleotide-gated potassium channel mll3241

Chain D:

M1 S2 V3 L4 P5 F6 L7 R8 I9 Y10 A11 P12 L13 N14 A15 V16 L17 A18 A19 P20 G21 L22 L23 A24 V25 A26 A27 L28 T29 I30 P31 D32 M33 S34 G35 R36 S37 R38 L39 A40 L41 A42 A43 L44 L45 I48 W49 G50 A51 Y52 L53 L54 Q55 L56 A57 A58 T59 L60 L61

K62 R63 R64 A65 G66 V67 V68 R69 D70 R71 T72 P73 K74 I75 A76 I77 D78 V79 L80 A81 V82 L83 V84 P85 L86 A87 A88 F89 L90 L91 D92 G93 S94 P95 D96 W97 S98 L99 Y100 C101 A102 V103 W104 L105 L106 K107 P108 L109 R110 D111 S112 T113 F114 F115 P116 V117 L118 G119 R120 V121

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	2D CRYSTAL, a=135 Å, b=135 Å, c=200 Å, γ=90°, 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 $(e^-/Å^2)$	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	Depositor
Map size (Å)	106.96, 106.96, 210.045	wwPDB
Map dimensions	112, 112, 201	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 1.045	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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(^{o})	Ideal(^{o})
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 ⓘ

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	1769
1	B	2661	981	2775	596	1254
1	C	2661	981	2775	600	1700
1	D	2661	981	2775	603	1383
2	C	2	0	0	0	0
All	All	10646	3924	11100	2240	3526

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

The worst 5 of 3526 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:C:173:LEU:C	1:D:200:ILE:C[7_556]	0.11	2.09
1:A:206:TRP:CZ3	1:C:170:VAL:C[7_556]	0.17	2.03
1:A:158:LYS:C	1:C:120:ARG:CZ[7_556]	0.21	1.99
1:A:117:VAL:CG2	1:C:147:ALA:O[7_556]	0.22	1.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PRO:N	1:C:122:LEU:CA[7_556]	0.25	1.95

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	37	72
1	B	353/355 (99%)	300 (85%)	52 (15%)	1 (0%)	37	72
1	C	353/355 (99%)	299 (85%)	53 (15%)	1 (0%)	37	72
1	D	353/355 (99%)	299 (85%)	53 (15%)	1 (0%)	37	72
All	All	1412/1420 (99%)	1197 (85%)	211 (15%)	4 (0%)	38	72

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 ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
1	D	323	HIS
1	D	55	GLN
1	B	55	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

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 ⓘ

6.1.1   Primary map

| X | Y | Z |
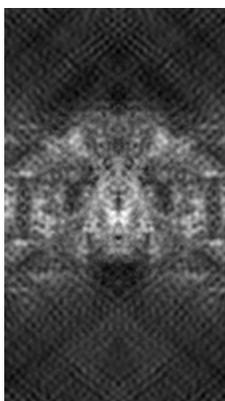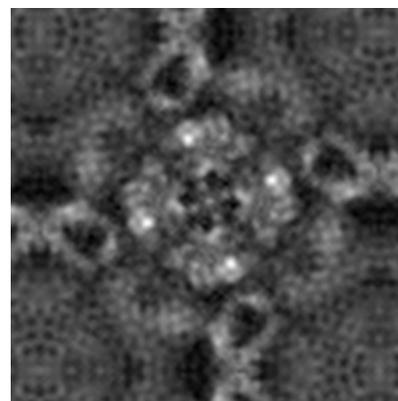
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
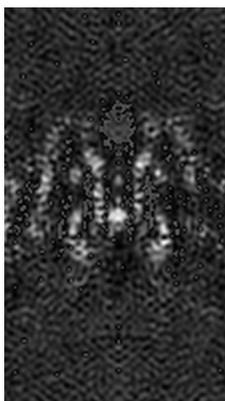
6.2.1   Primary map
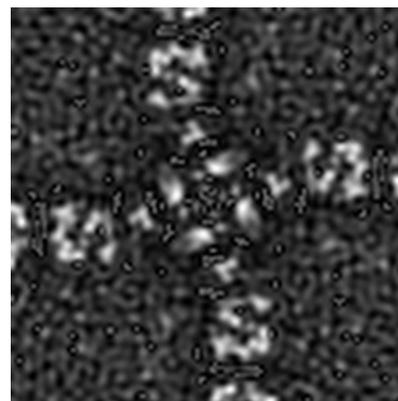
| X Index: 56 | Y Index: 56 | Z Index: 100 |

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

6.3 Largest variance slices ⓘ
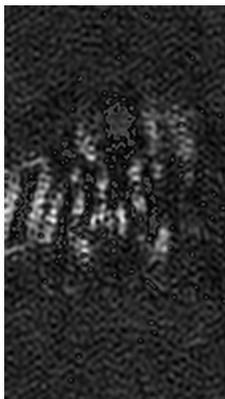
6.3.1 Primary map
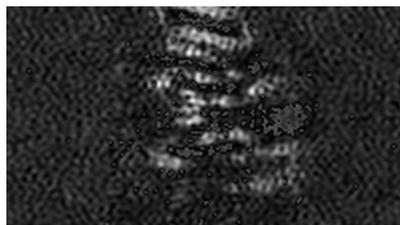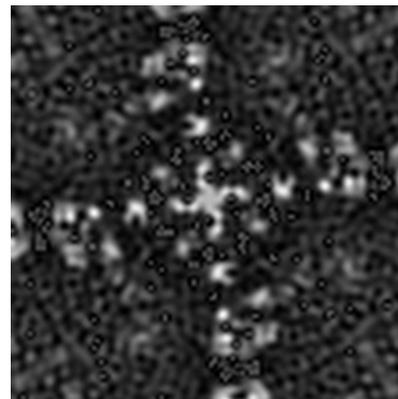
X Index: 59   Y Index: 60   Z Index: 96

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

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

6.4.1 Primary map

X   Y   Z
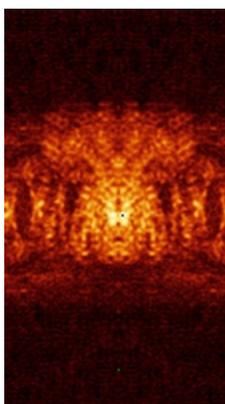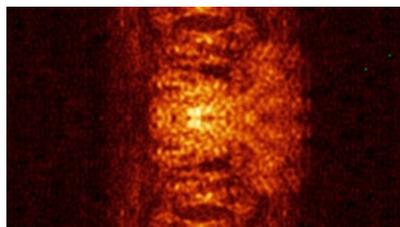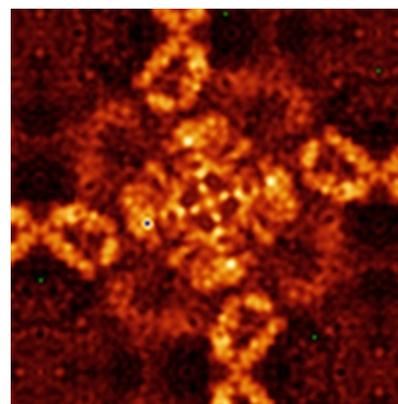
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ
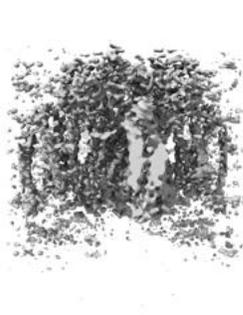
6.5.1 Primary map

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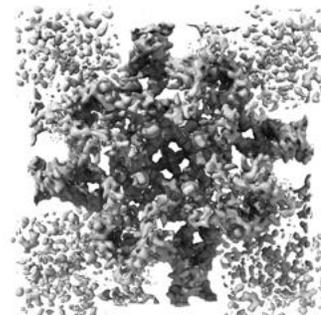
The images above show the 3D surface view of the map at the recommended contour level 600.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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 ⓘ
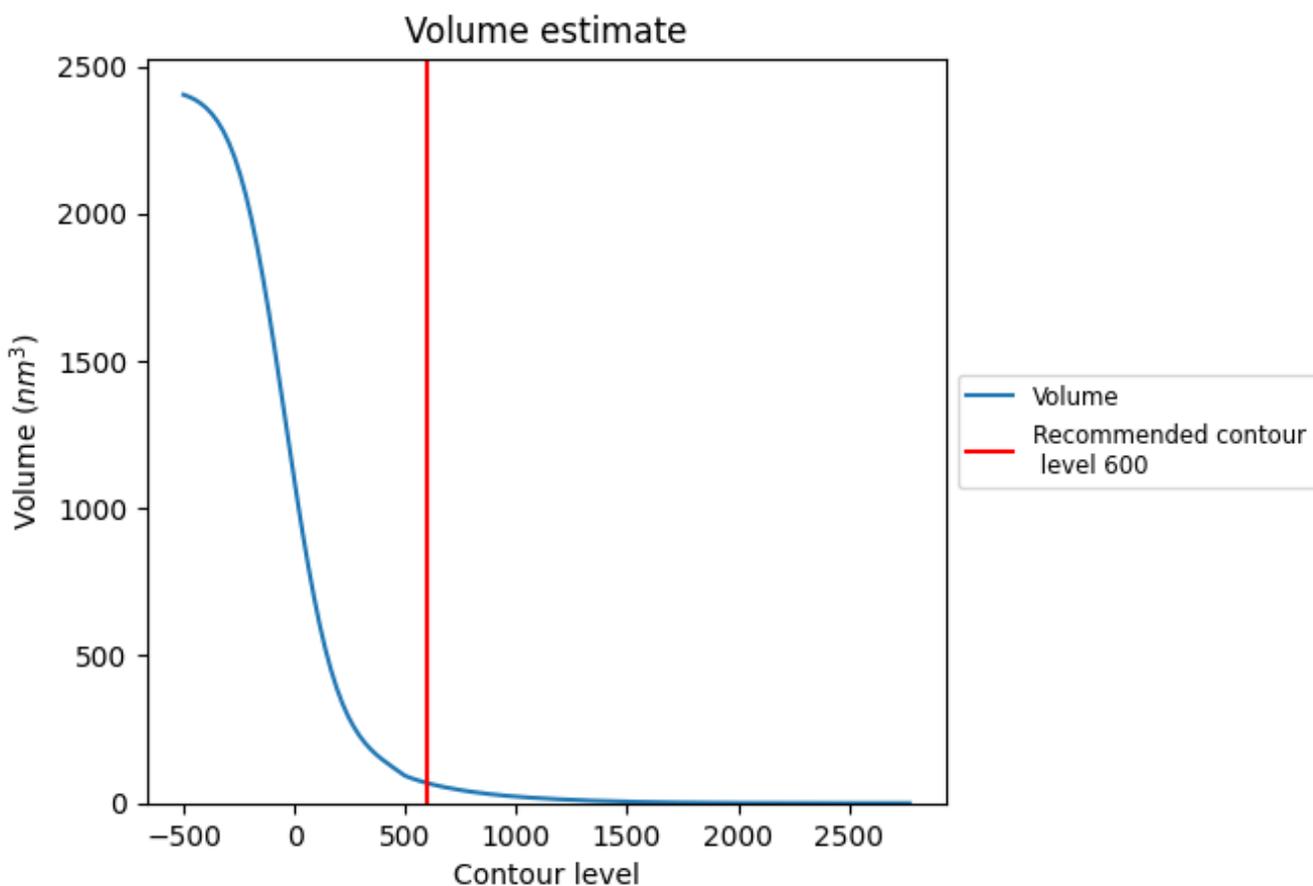
The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 61 kDa.

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 ⓘ

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-3907 and PDB model 6EO1. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ

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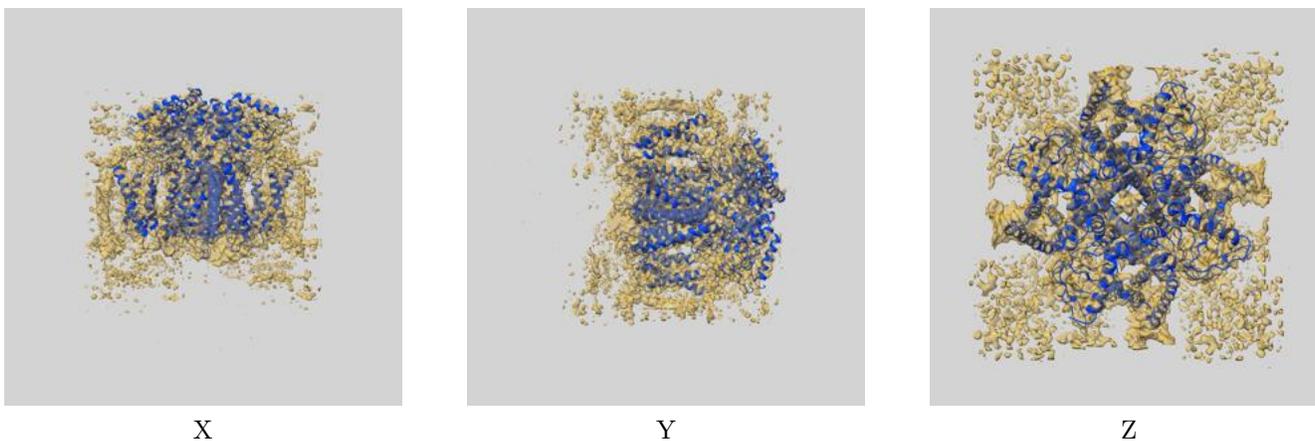
The images above show the 3D surface view of the map at the recommended contour level 600.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ
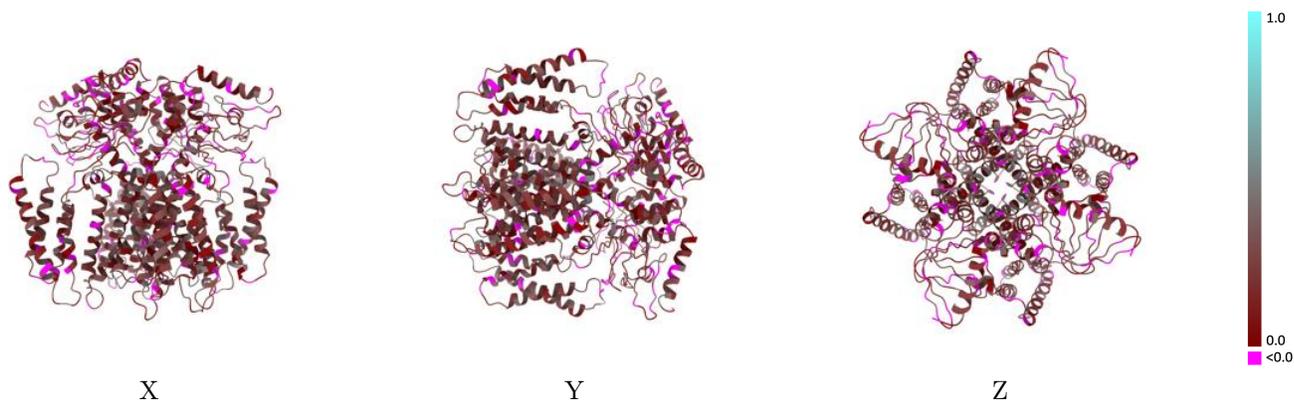
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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   ⓘ
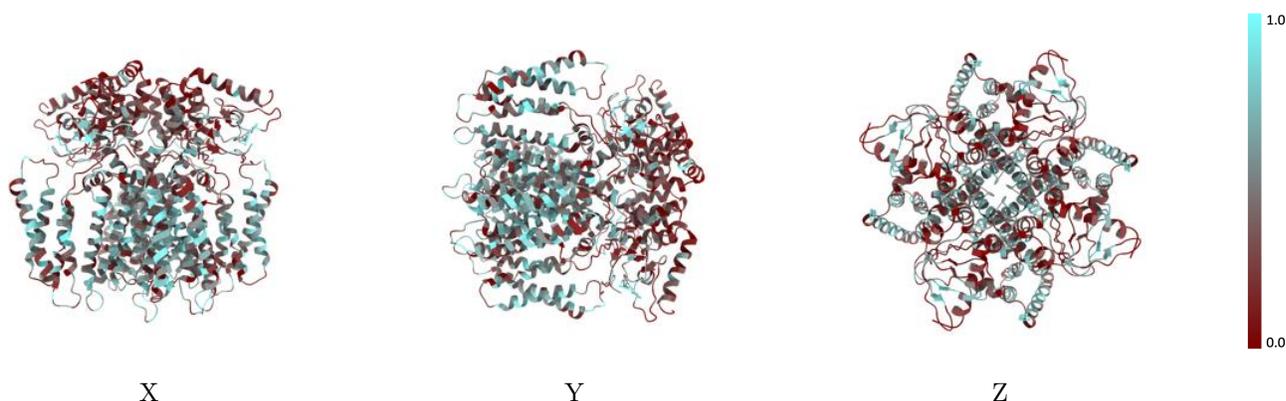
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (600).

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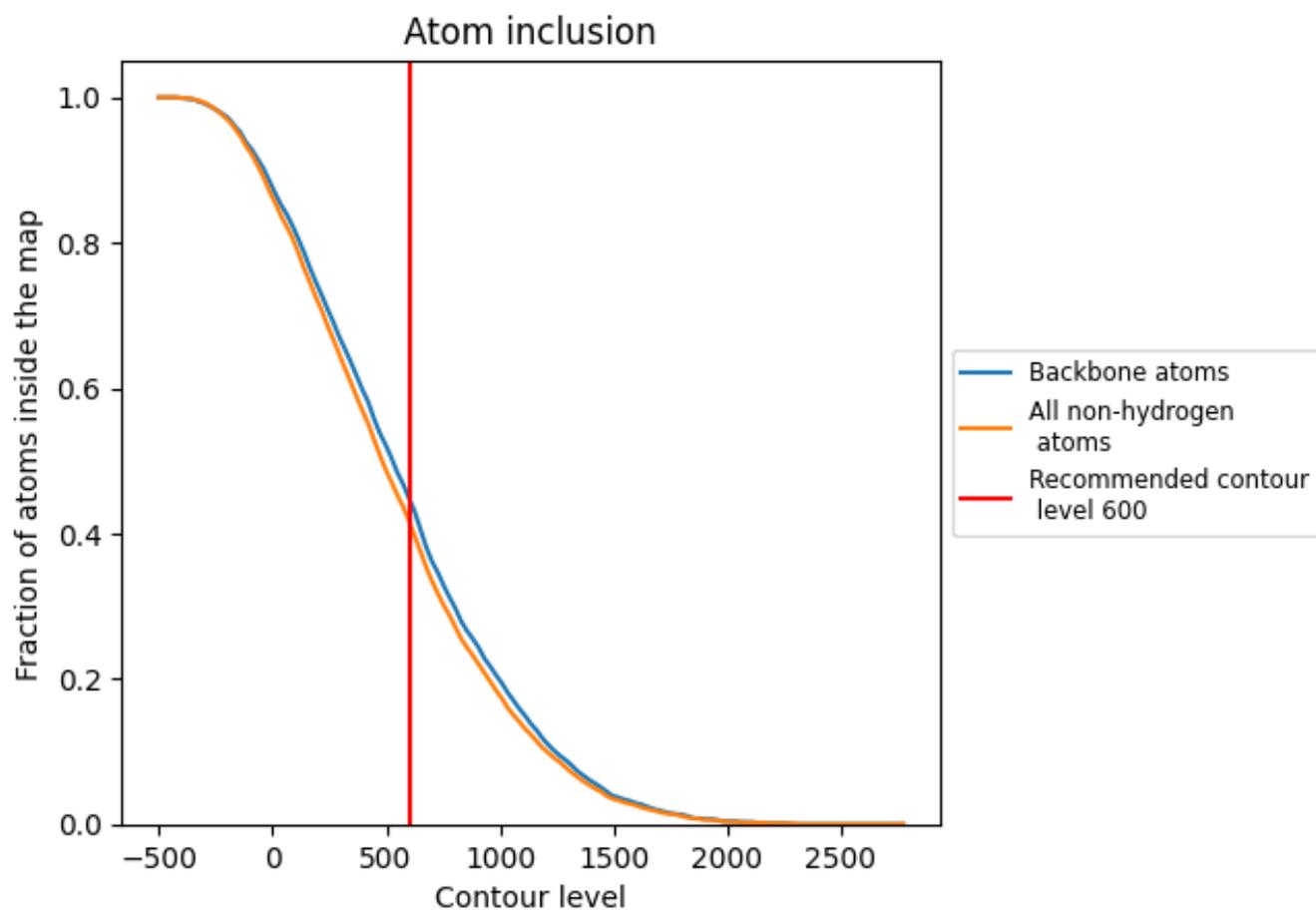
At the recommended contour level, 45% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (600) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4180	0.1840
A	0.4240	0.1830
B	0.4160	0.1830
C	0.4220	0.1870
D	0.4160	0.1820

1.0

0.0
<0.0