wwPDB EM Validation Summary Report (i)

Nov 10, 2022 – 03:18 pm GMT

PDB ID	:	7ZRI
EMDB ID	:	EMD-14915
Title	:	Cryo-EM structure of the KdpFABC complex in a nucleotide-free E1 conformation loaded with K+
Authors	:	Hielkema, L.; Stock, C.; Silberberg, J.M.; Corey, R.A.; Wunnicke, D.; Stansfeld, P.J.; Haenelt, I.; Paulino, C.
Deposited on	:	2022-05-04
Resolution	:	3.50 Å(reported)
Based on initial model	:	6HRA

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

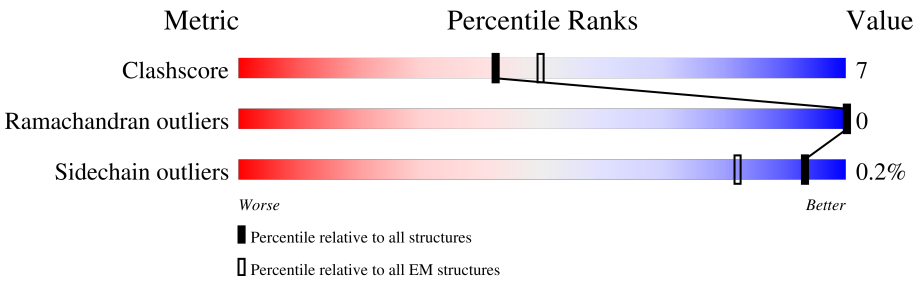
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 MICROSCOPY

The reported resolution of this entry is 3.50 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 <=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	557	82% 18%
2	C	190	82% 18%
3	D	27	100%
4	B	682	29% 80% 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11014 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 Potassium-transporting ATPase potassium-binding subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	557	4155	2715	679	726	35	0	0

- Molecule 2 is a protein called Potassium-transporting ATPase KdpC subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	190	1431	913	248	268	2	0	0

- Molecule 3 is a protein called Potassium-transporting ATPase KdpF subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	27	200	137	28	34	1	0	0

- Molecule 4 is a protein called Potassium-transporting ATPase ATP-binding subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
4	B	676	5021	3196	867	933	1	24	0	0

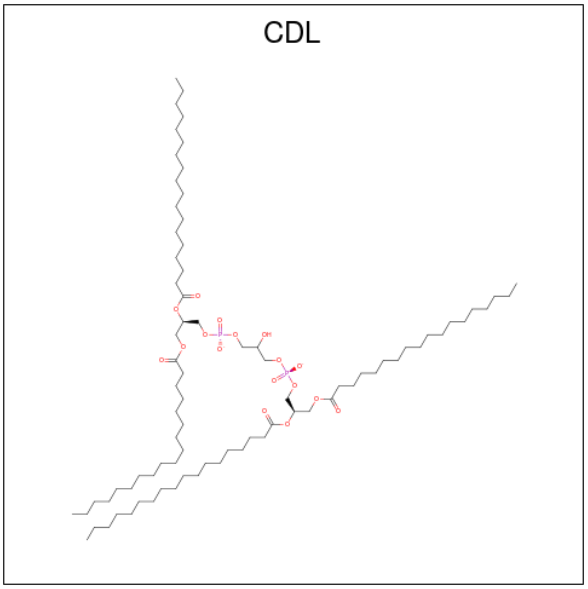
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	307	ASN	ASP	engineered mutation	UNP P03960

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
5	A	5	5	5	0
5	B	2	2	2	0

- Molecule 6 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



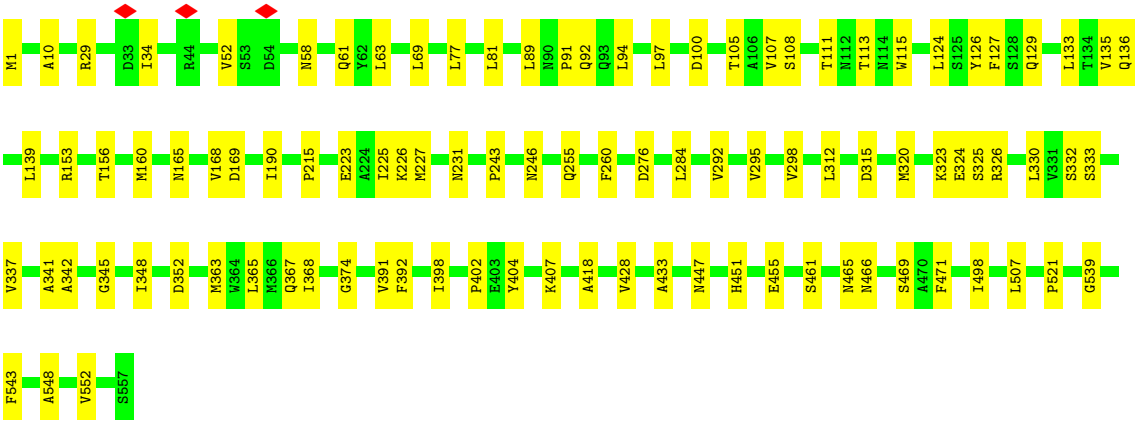
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
6	A	1	100	81	17	2	0
			Total	C	O	P	
6	B	1	100	81	17	2	0

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.

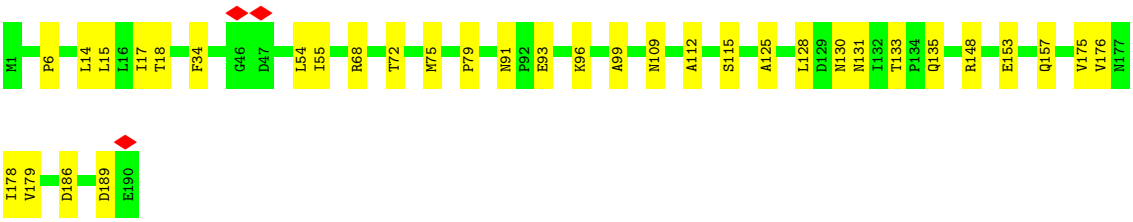
• Molecule 1: Potassium-transporting ATPase potassium-binding subunit

Chain A: 82% 18%



• Molecule 2: Potassium-transporting ATPase KdpC subunit

Chain C: 82% 18%



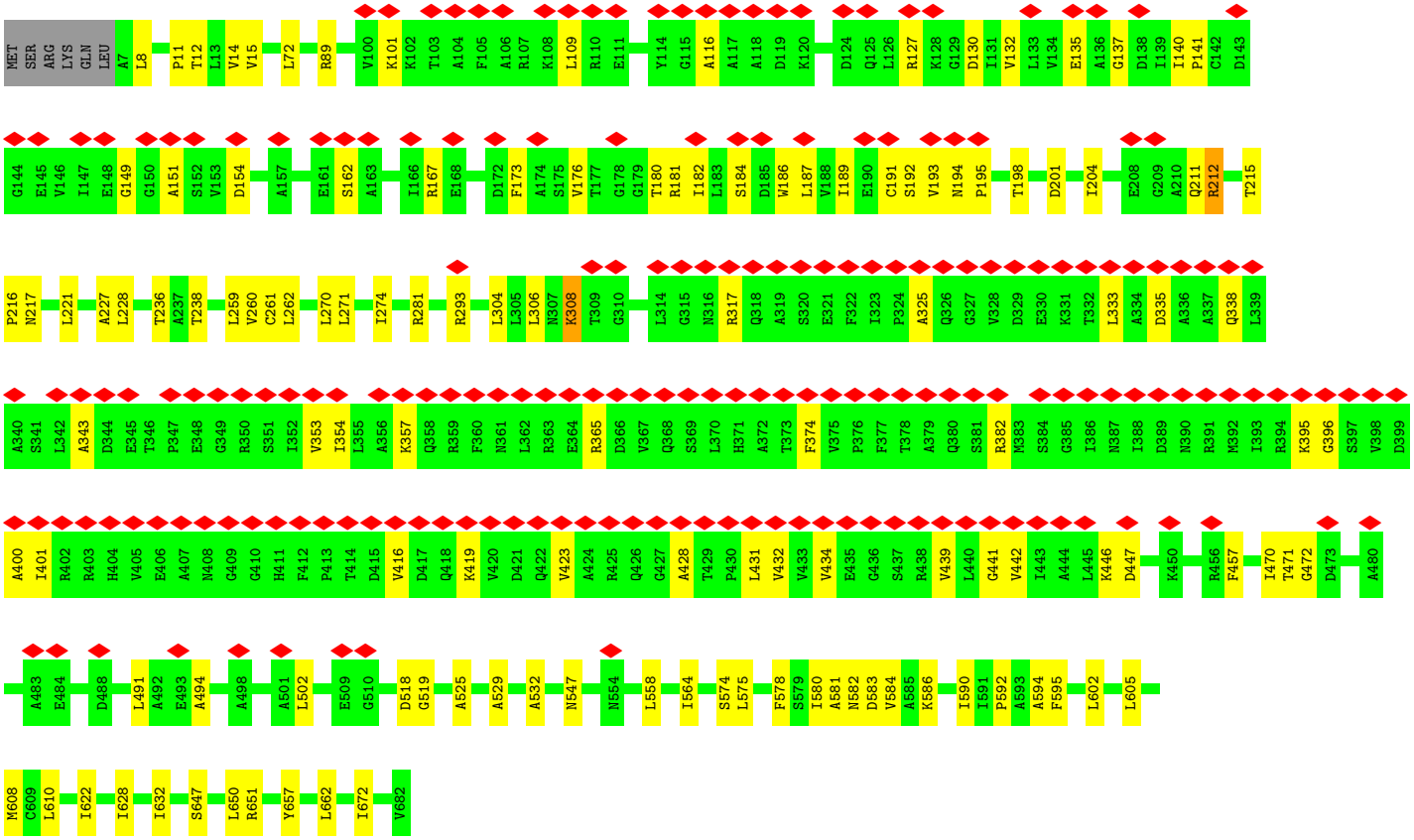
• Molecule 3: Potassium-transporting ATPase KdpF subunit

Chain D: 100%

There are no outlier residues recorded for this chain.

• Molecule 4: Potassium-transporting ATPase ATP-binding subunit

Chain B: 29% 80% 19%


MET SER ARG LYS GLN LEU A7 L8 P11 T12 L13 V14 V15 L72 R89 V100 K101 K102 T103 A104 F105 A106 R107 K108 L109 R110 E111 Y114 G115 A116 A117 A118 D119 K120 D124 Q125 L126 R127 K128 G129 D130 I131 V132 L133 V134 E135 A136 G137 D138 I139 I140 P141 C142 D143
G144 E145 V146 I147 E148 G149 G150 A151 S152 V153 D154 A157 E161 S162 A163 I166 R167 E168 D172 F173 A174 S175 V176 T177 G178 G179 T180 R181 I182 L183 S184 D185 W186 L187 V188 I189 E190 C191 S192 V193 N194 P195 T198 D201 I204 E208 G209 A210 Q211 R212 T215
P216 N217 L221 A227 L228 T236 A237 T238 L259 V260 C261 L262 L270 L271 I274 R281 R293 L304 L305 L306 N307 K308 T309 G310 L314 G315 N316 R317 Q318 A319 S320 E321 F322 I323 P324 A325 Q326 G327 V328 D329 E330 K331 T332 L333 A334 D335 A336 A337 Q338 L339
A340 S341 L342 A343 D344 E345 T346 P347 E348 G349 R350 S351 I352 V353 I354 L355 A356 K357 Q358 R359 F360 N361 L362 R363 E364 R365 D366 V367 Q368 S369 L370 H371 A372 T373 F374 V375 P376 F377 T378 A379 Q380 S381 R382 M383 S384 G385 I386 N387 I388 D389 N390 R391 M392 I393 R394 K395 G396 S397 V398 D399
A400 I401 R402 R403 H404 V405 E406 A407 N408 G409 G410 H411 F412 P413 T414 D415 V416 D417 Q418 K419 V420 D421 Q422 V423 A424 R425 Q426 G427 A428 T429 P430 L431 V432 V433 V434 E435 G436 S437 R438 V439 L440 G441 V442 I443 A444 L445 K446 D447 K450 R456 F457 I470 T471 G472 D473 A480
A483 E484 D488 L491 A492 E493 A494 A498 A501 L502 E509 G510 D518 G519 A525 A529 A532 N547 N554 L558 I564 S574 L575 F578 S579 I580 A581 N582 D583 V584 A585 K586 I590 I591 P592 A593 A594 F595 L602 L605
M608 C609 L610 I622 I628 I632 S647 L650 R651 Y657 L662 I672 V682

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75711	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	49407	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0323	Depositor
Map size (Å)	242.87999, 242.87999, 242.87999	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.012, 1.012, 1.012	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, SEP, CDL

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	0.29	0/4247	0.53	0/5782
2	C	0.27	0/1462	0.54	0/2000
3	D	0.25	0/202	0.50	0/275
4	B	0.26	0/5085	0.53	0/6907
All	All	0.27	0/10996	0.53	0/14964

There are no bond length outliers.

There are no bond angle outliers.

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	A	4155	0	4281	65	0
2	C	1431	0	1448	26	0
3	D	200	0	221	0	0
4	B	5021	0	5212	79	0
5	A	5	0	0	0	0
5	B	2	0	0	0	0
6	A	100	0	156	7	0
6	B	100	0	156	3	0
All	All	11014	0	11474	161	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 7.

The worst 5 of 161 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)
4:B:578:PHE:O	4:B:582:ASN:HB2	1.80	0.81
4:B:261:CYS:HB3	4:B:586:LYS:HG2	1.68	0.76
1:A:77:LEU:HD22	1:A:136:GLN:HG3	1.72	0.69
4:B:151:ALA:HB1	4:B:184:SER:HB3	1.76	0.66
4:B:130:ASP:H	4:B:191:CYS:HB2	1.62	0.64

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	555/557 (100%)	530 (96%)	25 (4%)	0	100	100
2	C	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
3	D	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
4	B	673/682 (99%)	642 (95%)	31 (5%)	0	100	100
All	All	1441/1456 (99%)	1375 (95%)	66 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	439/439 (100%)	439 (100%)	0	100	100
2	C	151/151 (100%)	151 (100%)	0	100	100
3	D	21/21 (100%)	21 (100%)	0	100	100
4	B	524/530 (99%)	522 (100%)	2 (0%)	91	96
All	All	1135/1141 (100%)	1133 (100%)	2 (0%)	93	98

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

Mol	Chain	Res	Type
4	B	212	ARG
4	B	308	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SEP	B	162	4	8,9,10	1.55	1 (12%)	8,12,14	1.64	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SEP	B	162	4	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	162	SEP	P-O1P	3.38	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	162	SEP	P-OG-CB	-3.12	109.69	118.30
4	B	162	SEP	OG-CB-CA	2.87	110.94	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	162	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CDL	B	702	-	99,99,99	1.01	6 (6%)	105,111,111	1.09	4 (3%)
6	CDL	A	606	-	99,99,99	1.01	6 (6%)	105,111,111	1.10	4 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CDL	B	702	-	-	61/110/110/110	-
6	CDL	A	606	-	-	48/110/110/110	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	702	CDL	OB8-CB7	3.21	1.42	1.33
6	A	606	CDL	OB8-CB7	3.17	1.42	1.33
6	A	606	CDL	OA8-CA7	3.14	1.42	1.33
6	B	702	CDL	OA8-CA7	3.01	1.42	1.33
6	B	702	CDL	OA6-CA5	2.98	1.42	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	702	CDL	OA6-CA5-C11	4.41	121.01	111.50
6	B	702	CDL	OB6-CB5-C51	4.12	120.39	111.50
6	A	606	CDL	OA6-CA5-C11	4.02	120.17	111.50
6	A	606	CDL	OB6-CB5-C51	3.94	119.99	111.50
6	A	606	CDL	OA8-CA7-C31	3.04	121.44	111.91

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	606	CDL	CB2-C1-CA2-OA2
6	A	606	CDL	CA2-OA2-PA1-OA3
6	A	606	CDL	CA2-OA2-PA1-OA4
6	A	606	CDL	CA3-OA5-PA1-OA4
6	A	606	CDL	C11-CA5-OA6-CA4

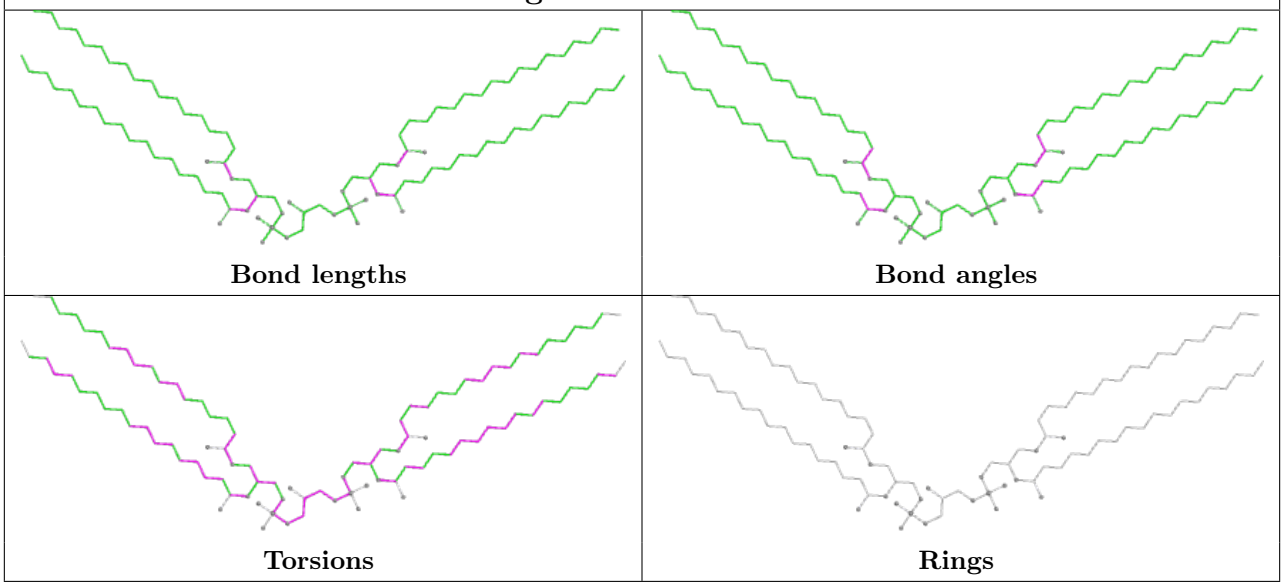
There are no ring outliers.

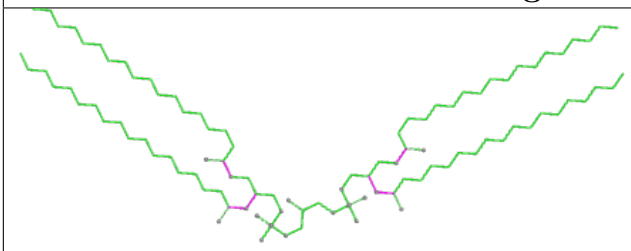
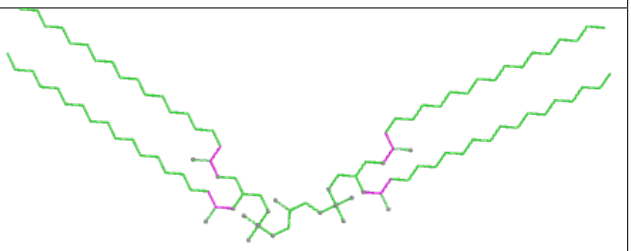
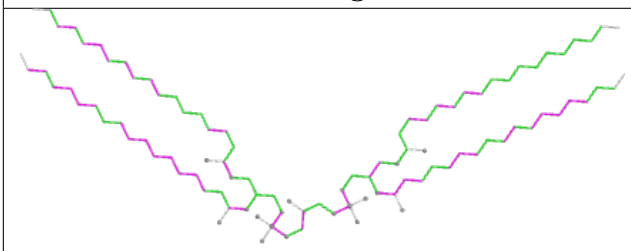
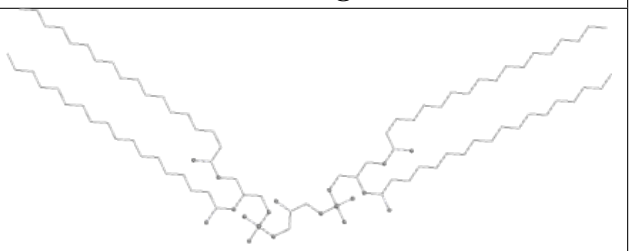
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	702	CDL	3	0
6	A	606	CDL	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CDL B 702



Ligand CDL A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

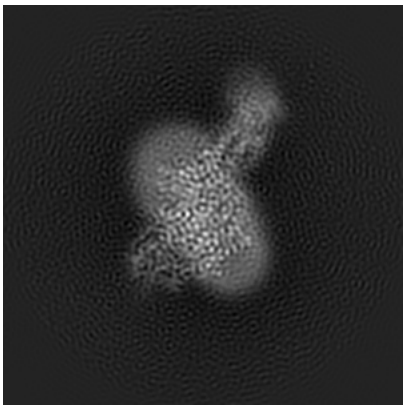
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14915. These allow visual inspection of the internal detail of the map and identification of artifacts.

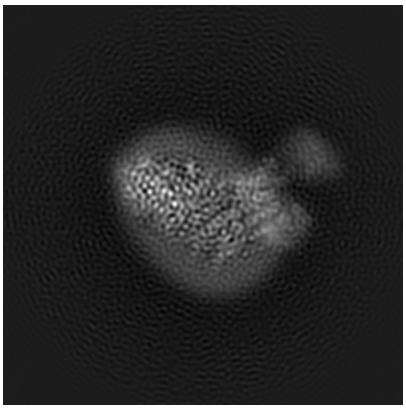
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

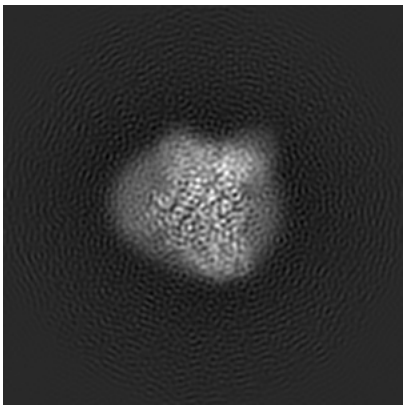
6.1.1 Primary map



X

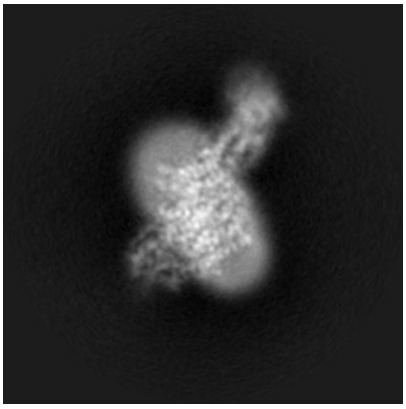


Y

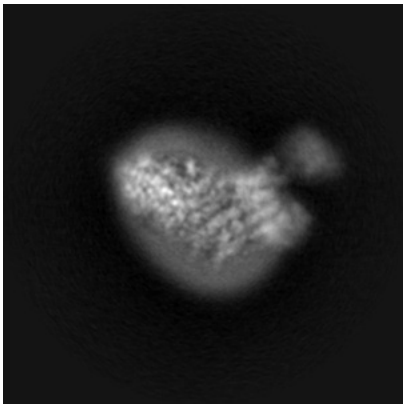


Z

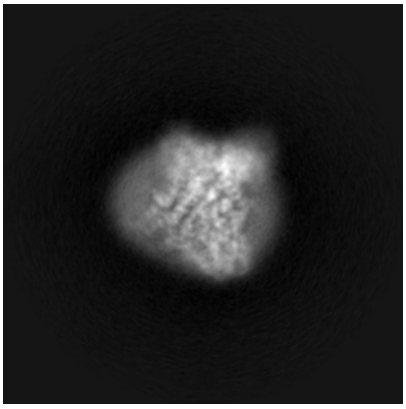
6.1.2 Raw map



X



Y

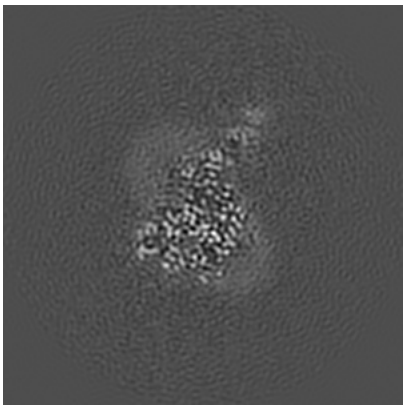


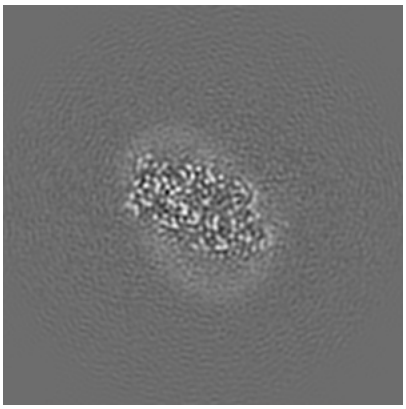
Z

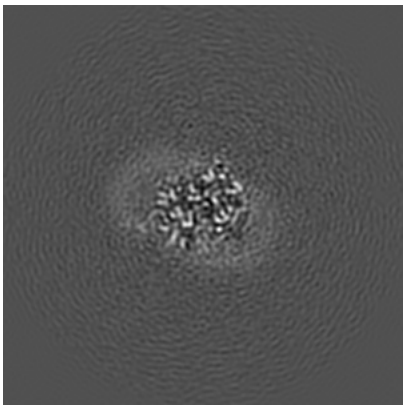
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

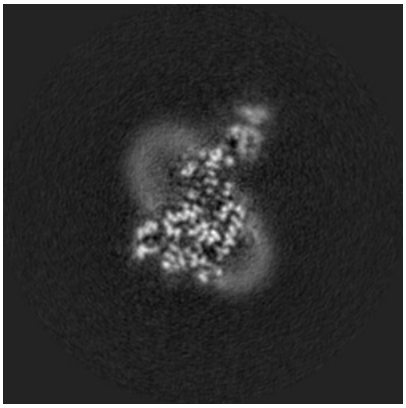
6.2.1 Primary map

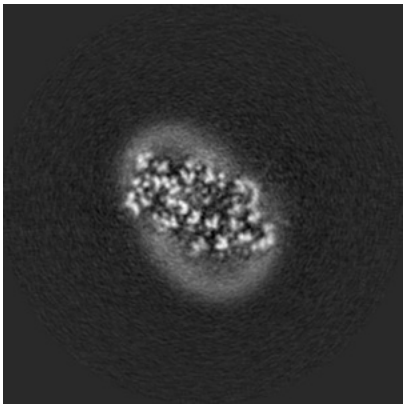

X Index: 120

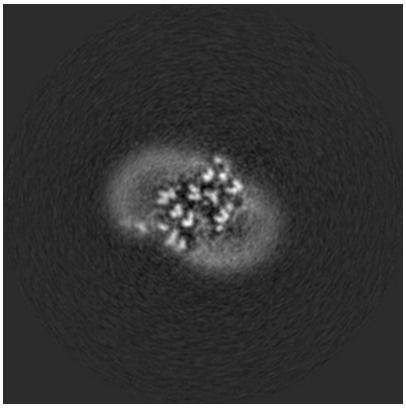

Y Index: 120


Z Index: 120

6.2.2 Raw map


X Index: 120

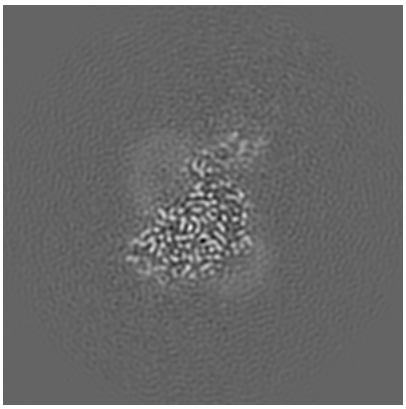

Y Index: 120


Z Index: 120

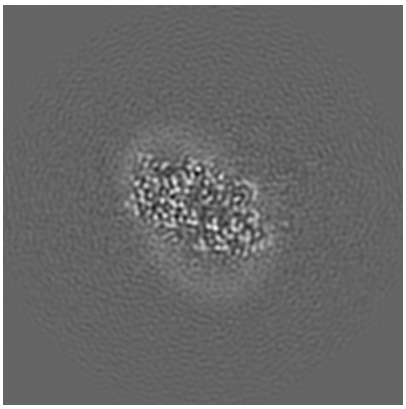
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

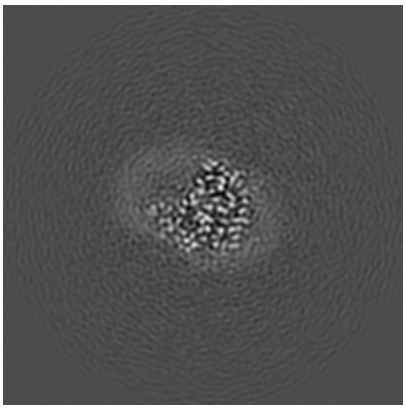
6.3.1 Primary map



X Index: 127

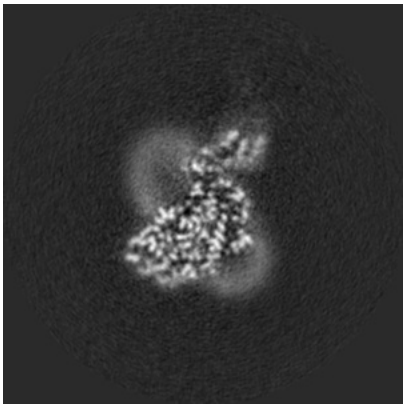


Y Index: 121

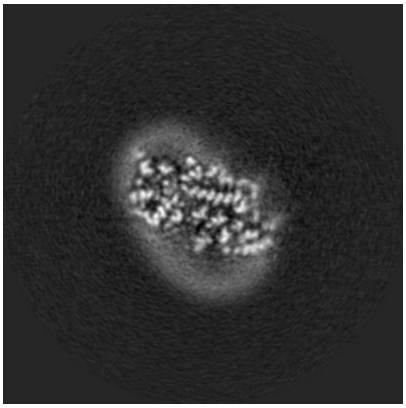


Z Index: 114

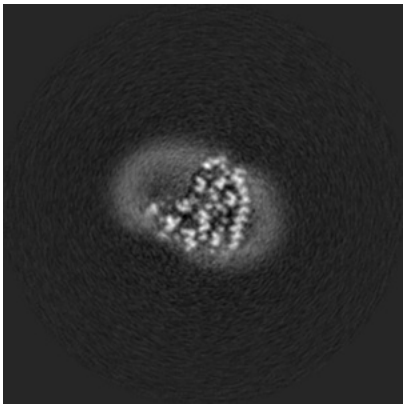
6.3.2 Raw map



X Index: 127



Y Index: 123



Z Index: 113

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 0.0323. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

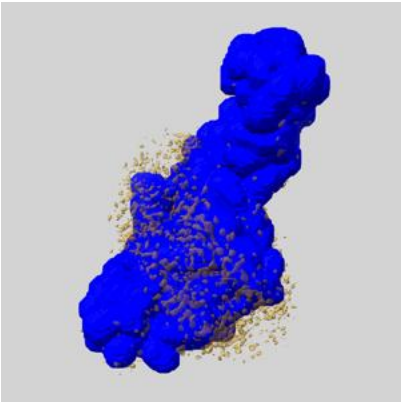
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

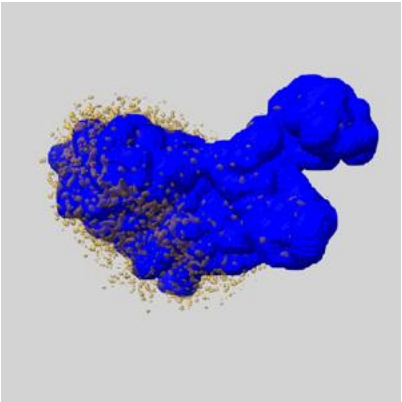
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

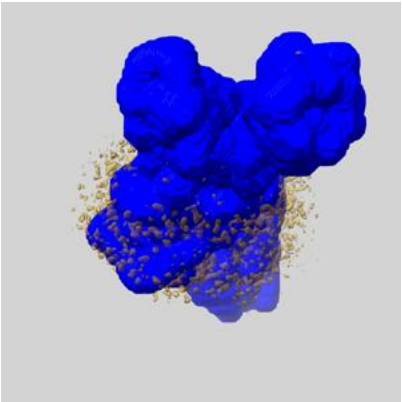
6.5.1 emd_14915_msk_1.map (i)



X



Y

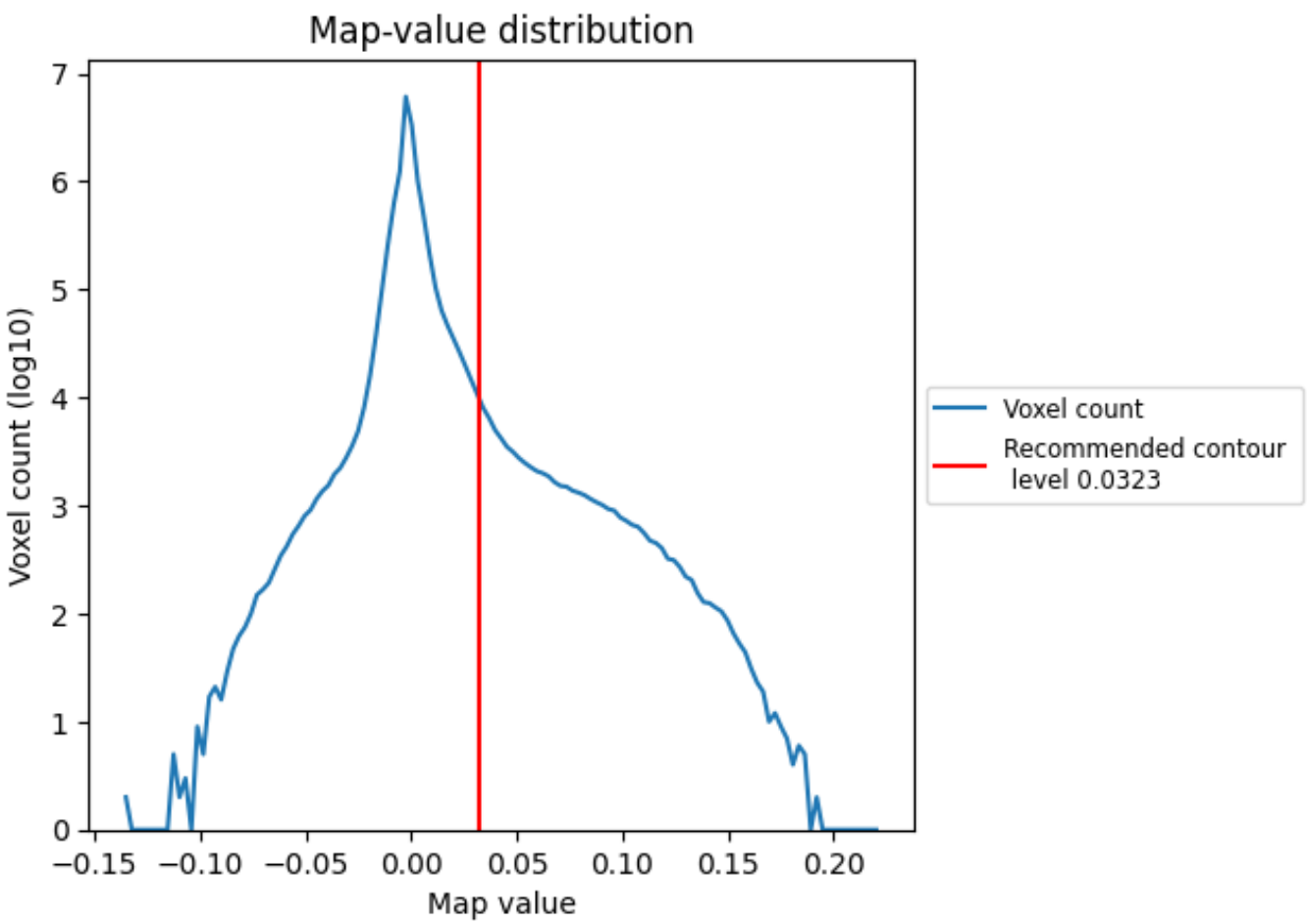


Z

7 Map analysis (i)

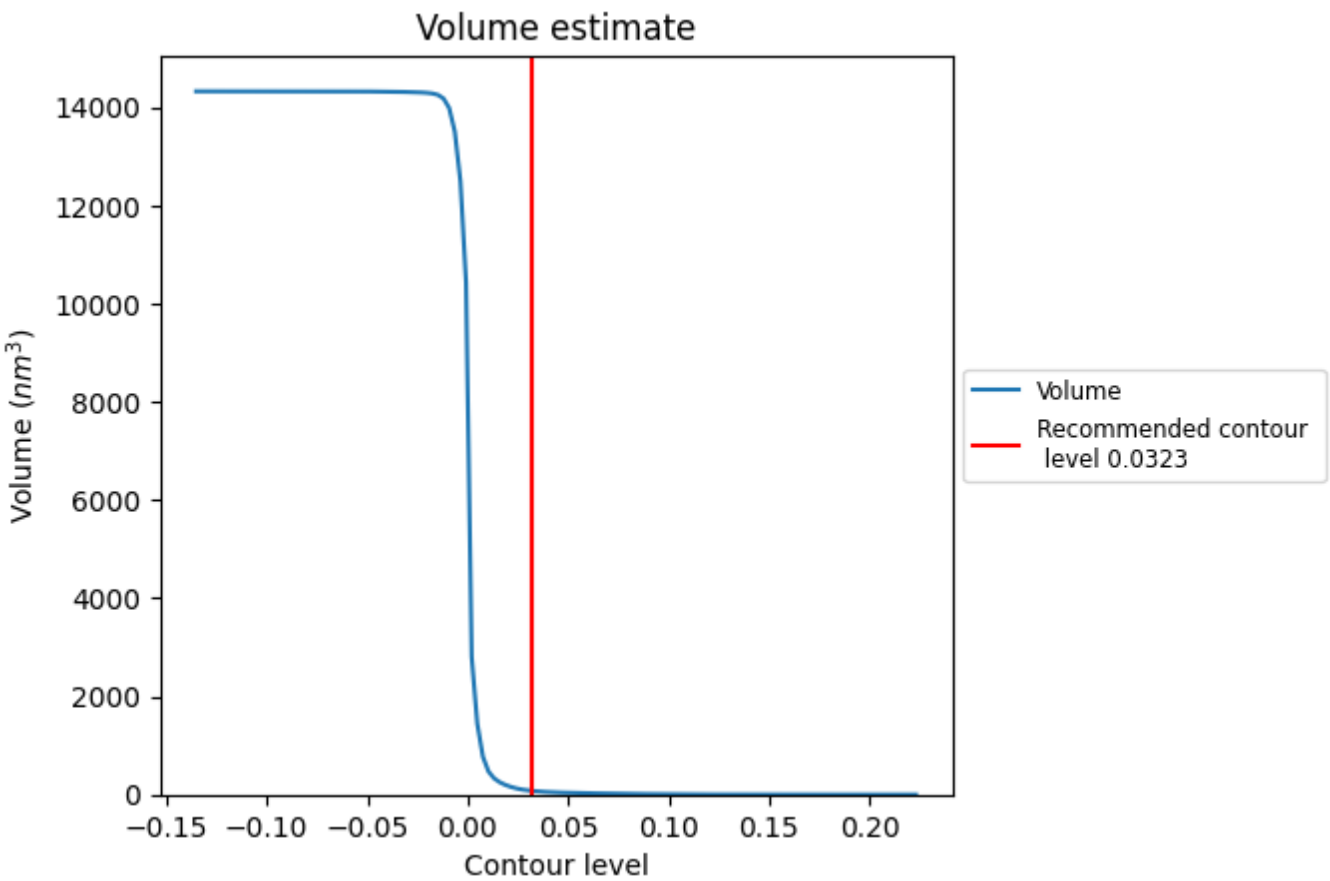
This section contains the results of statistical analysis of the map.

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.

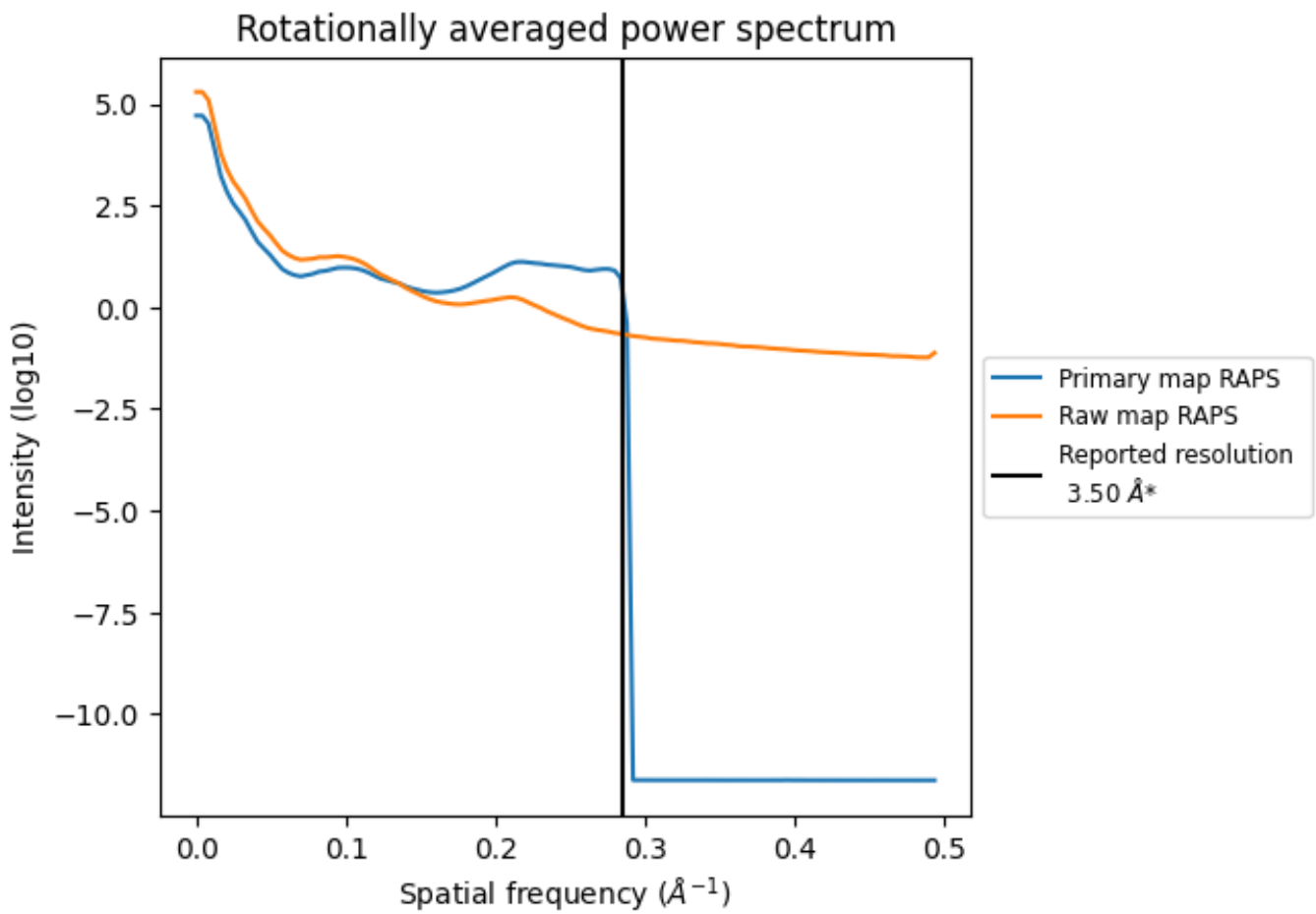
7.2 Volume estimate (i)



The volume at the recommended contour level is 74 nm^3; this corresponds to an approximate mass of 67 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)

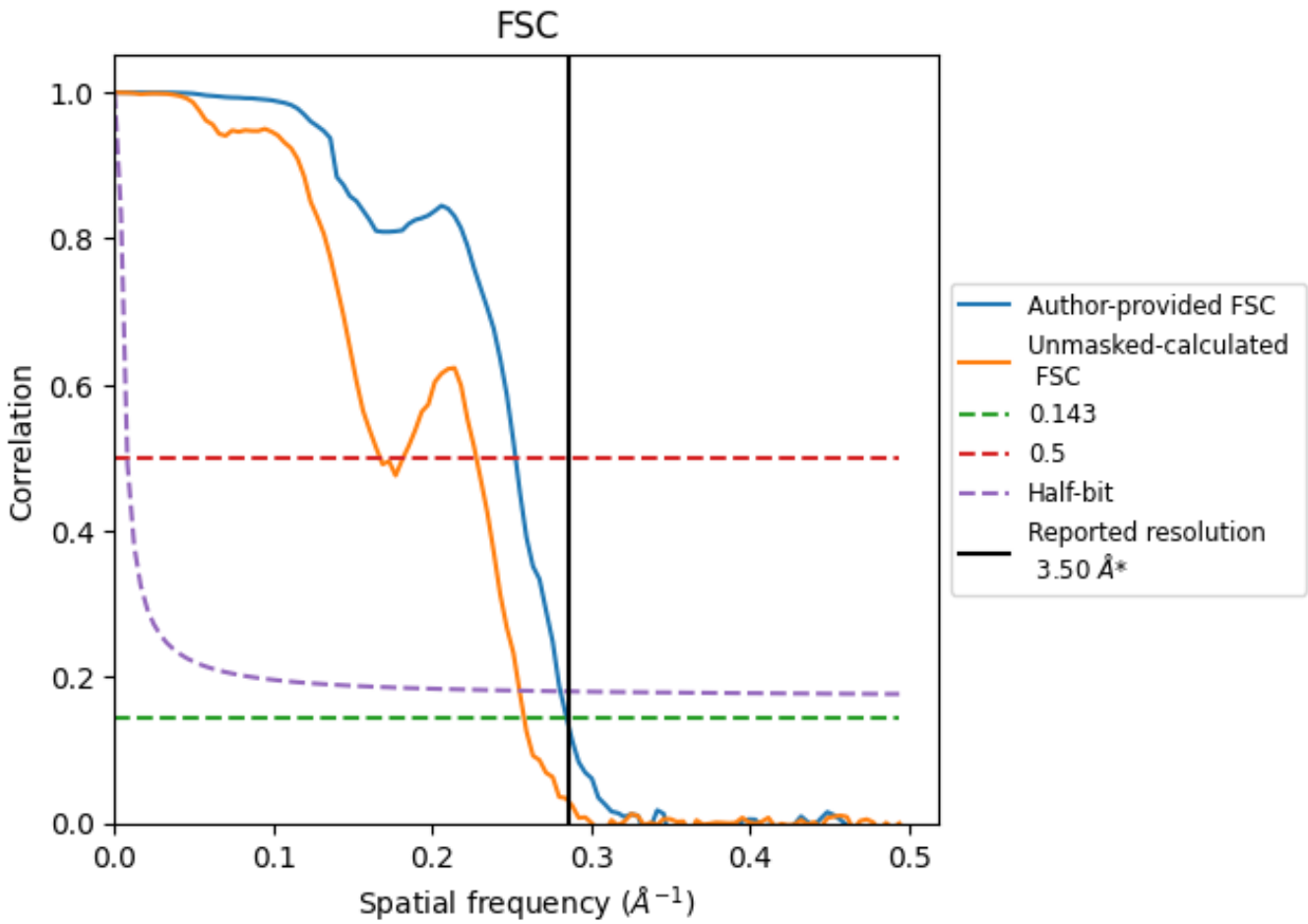


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

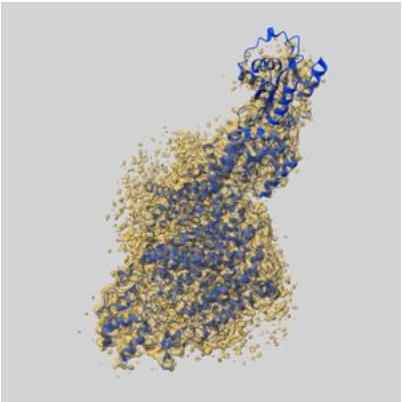
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.96	3.56
Unmasked-calculated*	3.88	5.98	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.5 by more than 10 %

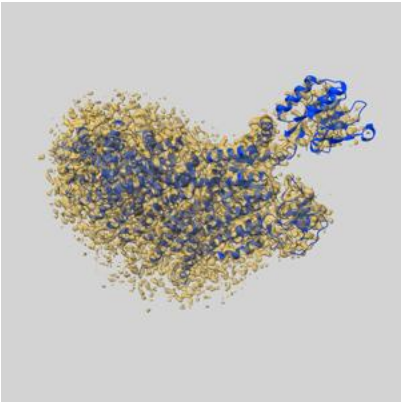
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14915 and PDB model 7ZRI. Per-residue inclusion information can be found in section 3 on page 5.

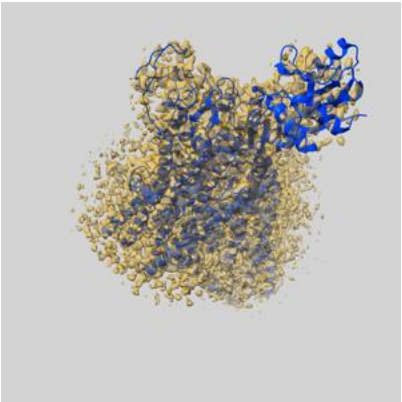
9.1 Map-model overlay (i)



X



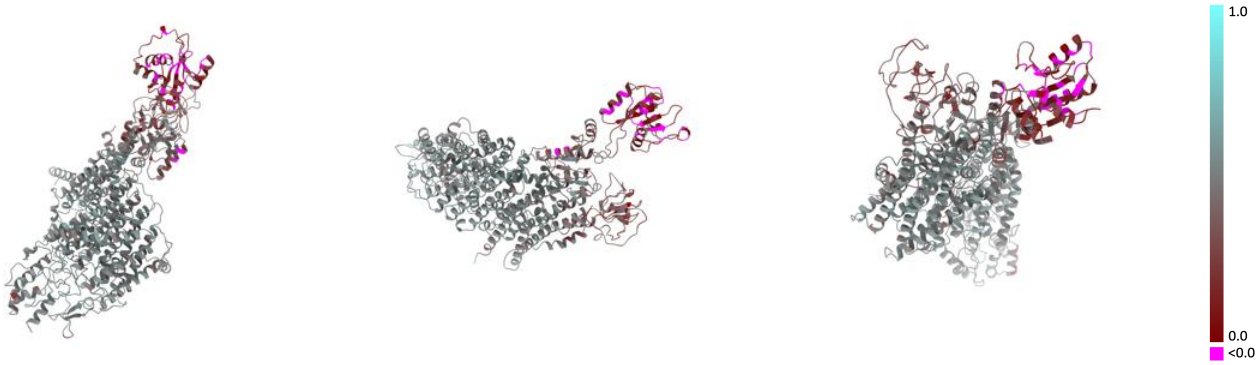
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0323 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.

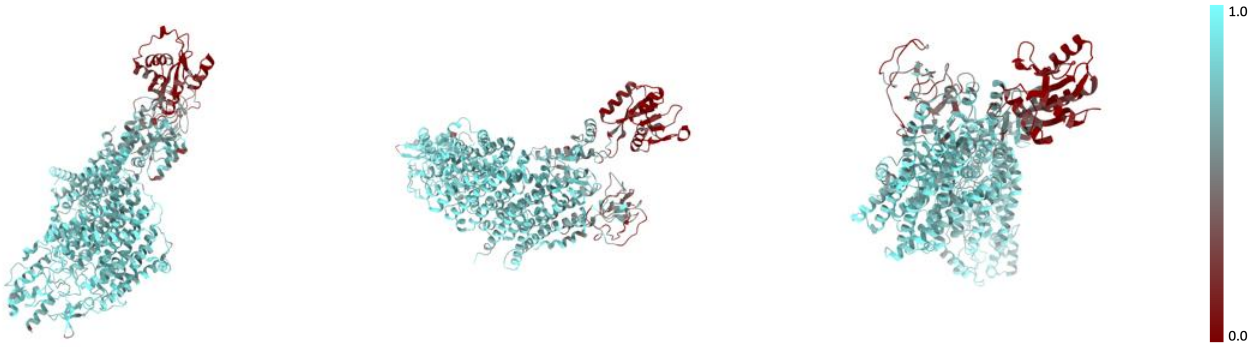
9.2 Q-score mapped to coordinate model (i)



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.

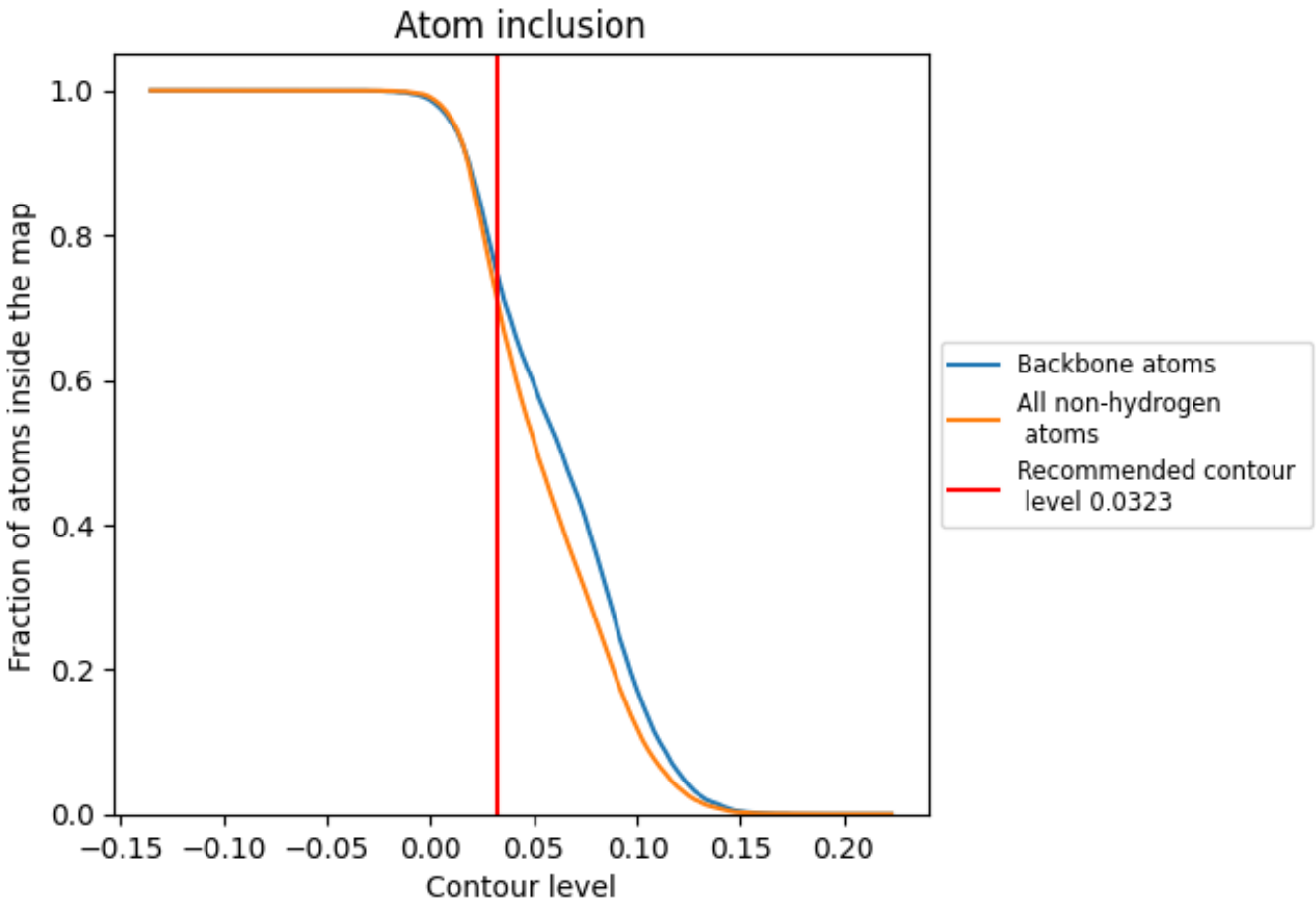
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0323).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 71% 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 (0.0323) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7112	0.4570
A	0.8392	0.5190
B	0.5726	0.3900
C	0.8158	0.5080
D	0.7778	0.4850