wwPDB EM Validation Summary Report (i)

Aug 25, 2026 – 01:27 am BST

PDB ID	:	9FR0 / pdb_00009fr0
EMDB ID	:	EMD-50674
Title	:	Triangle state of ACS found in the as-isolated state
Authors	:	Ruickoldt, J.; Wendler, P.; Dobbek, H.
Deposited on	:	2024-06-18
Resolution	:	3.42 Å(reported)

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

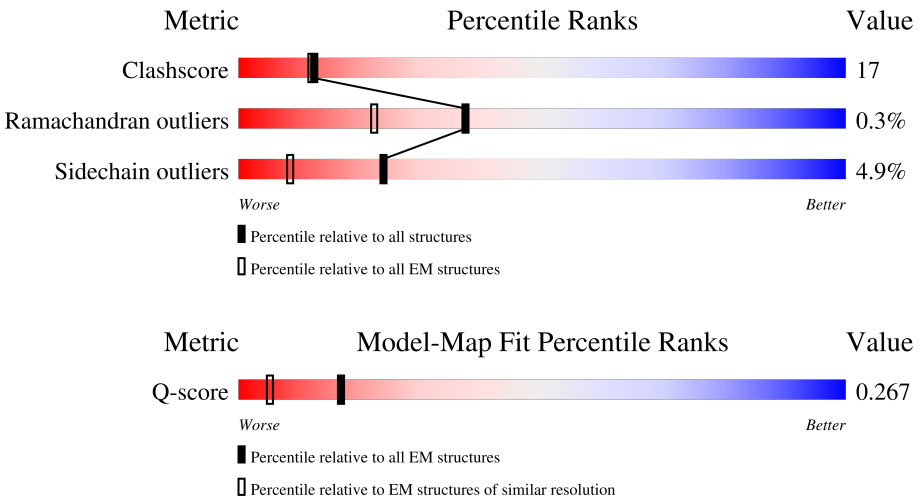
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.42 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13959 (2.92 - 3.92)

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	732	5% 36% 19% • 43%
1	B	732	11% 38% 19% 43%
1	C	732	10% 40% 16% • 42%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	A	803	-	-	X	-
3	SF4	B	803	-	-	X	-
3	SF4	C	803	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10123 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 CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	419	3315	2109	562	624	20	0	0
1	B	420	3322	2113	563	626	20	0	0
1	C	421	3330	2119	564	627	20	0	0

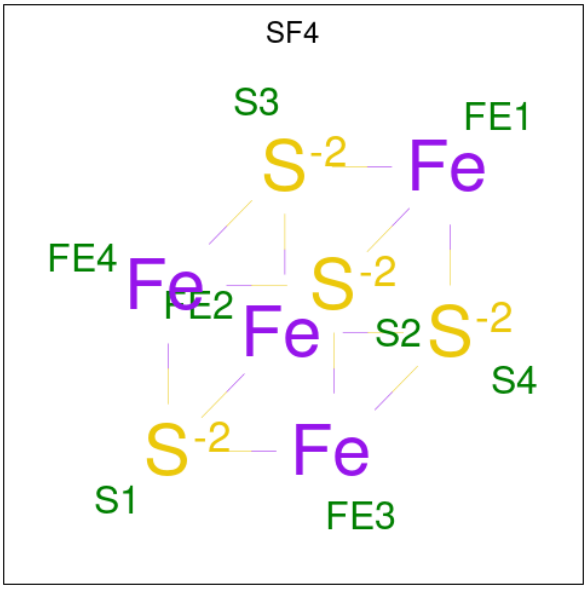
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	733	ARG	-	expression tag	UNP P83789
A	734	SER	-	expression tag	UNP P83789
A	735	HIS	-	expression tag	UNP P83789
A	736	HIS	-	expression tag	UNP P83789
B	733	ARG	-	expression tag	UNP P83789
B	734	SER	-	expression tag	UNP P83789
B	735	HIS	-	expression tag	UNP P83789
B	736	HIS	-	expression tag	UNP P83789
C	733	ARG	-	expression tag	UNP P83789
C	734	SER	-	expression tag	UNP P83789
C	735	HIS	-	expression tag	UNP P83789
C	736	HIS	-	expression tag	UNP P83789

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ni	
2	A	2	2	2	0
2	B	2	2	2	0
2	C	2	2	2	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
3	A	1	8	4	4	0
3	B	1	8	4	4	0
3	C	1	8	4	4	0

- Molecule 4 is water.

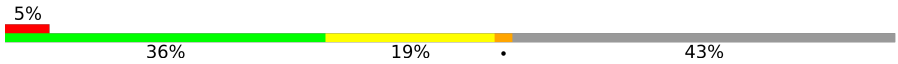
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
4	A	42	42	42	0
4	B	45	45	45	0
4	C	39	39	39	0

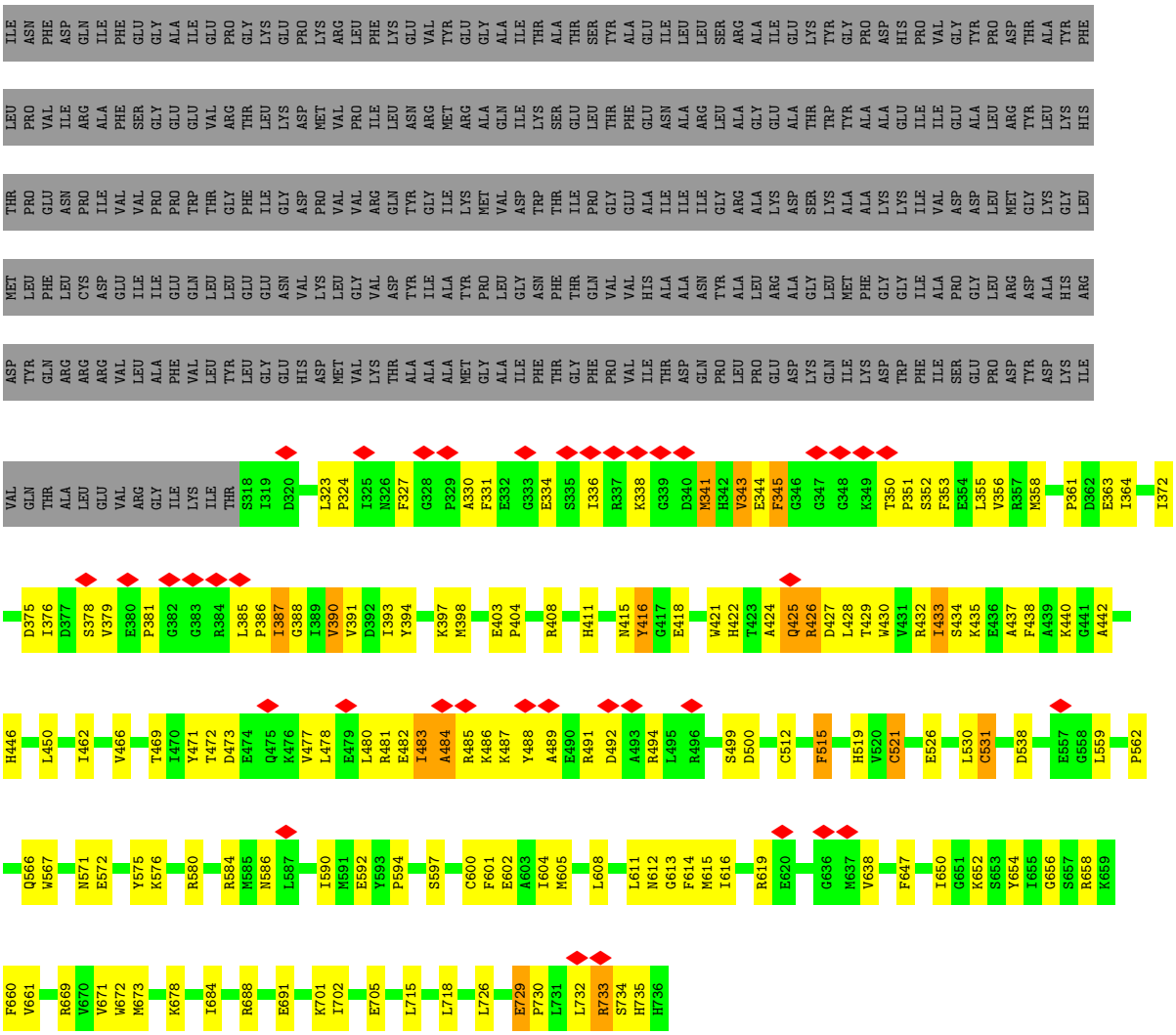
3 Residue-property plots (i)

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: CO-methylating acetyl-CoA synthase

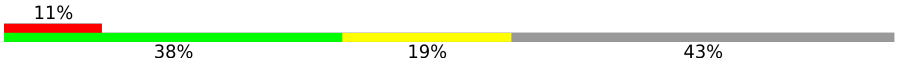
Chain A:

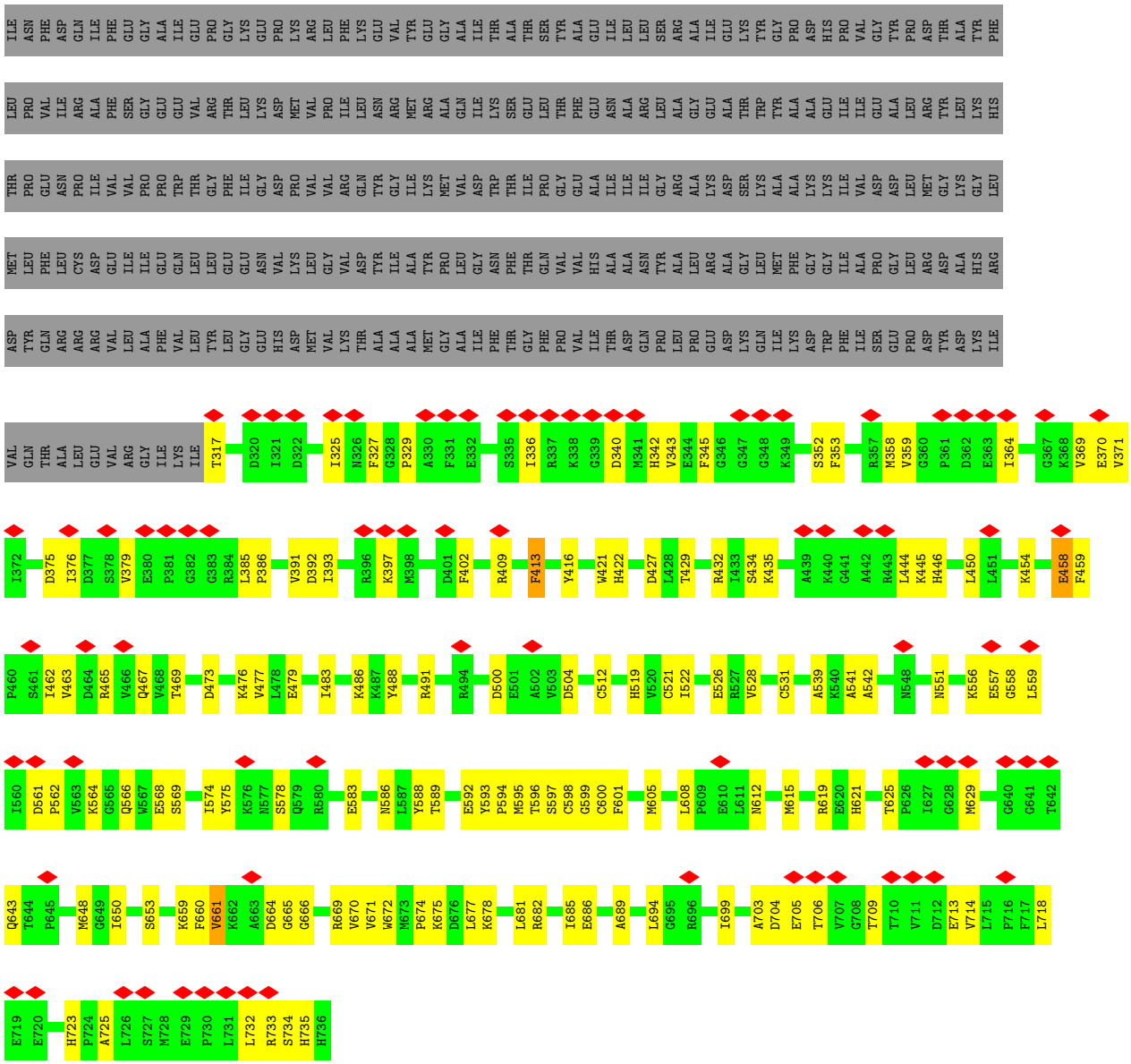




• Molecule 1: CO-methylating acetyl-CoA synthase

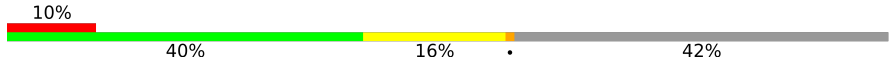
Chain B:

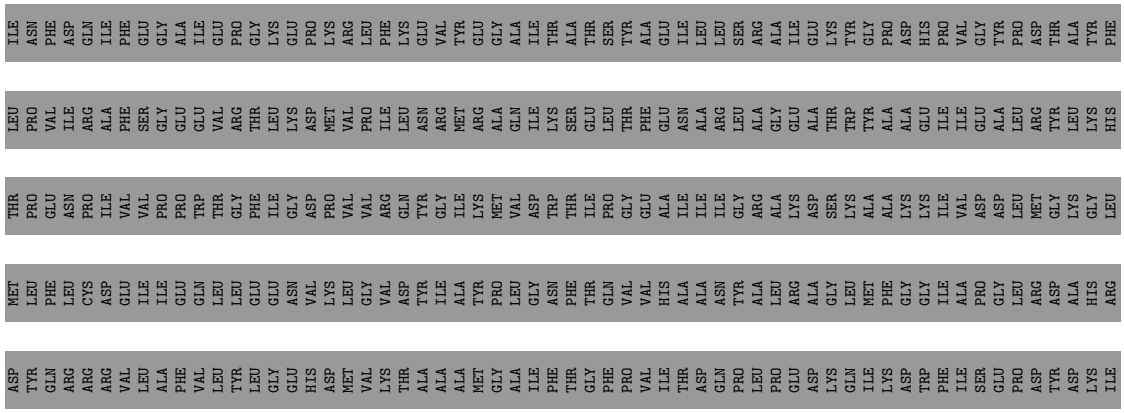


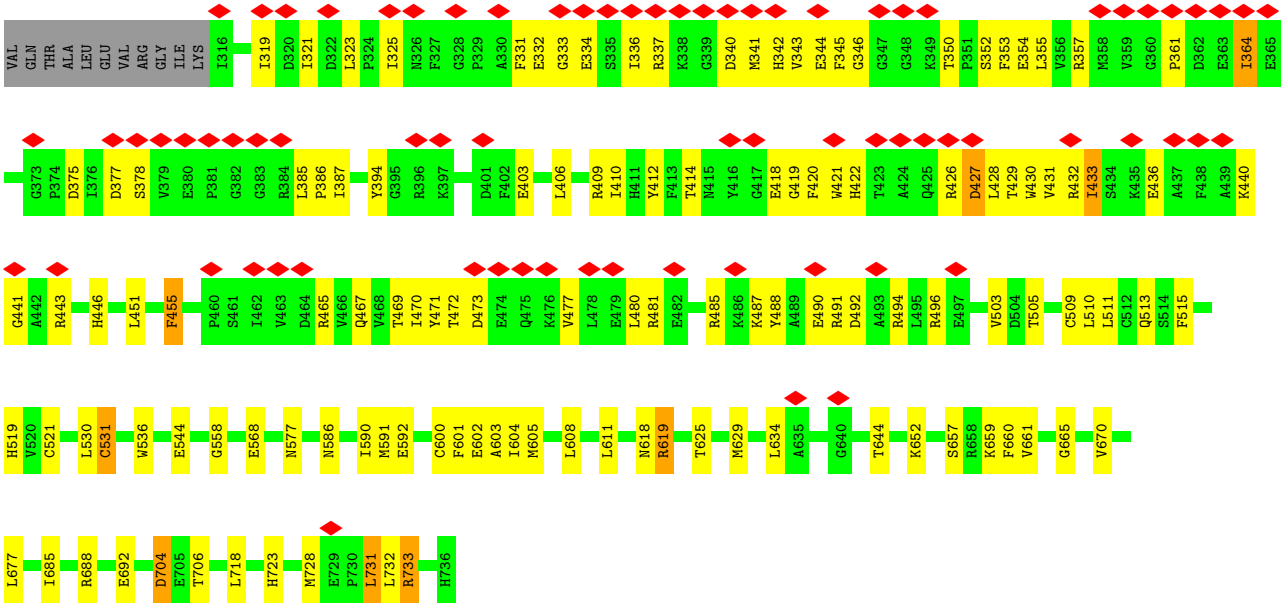


- Molecule 1: CO-methylating acetyl-CoA synthase

Chain C:






VAL GLN THR ALA LEU GLU VAL ARG GLY ILE LYS I316 I319 D320 I321 D322 L323 P324 I325 N326 F327 G328 P329 A330 F331 E332 G333 E334 S335 I336 R337 K338 G339 D340 M341 H342 V343 E344 F345 G346 G347 G348 K349 T350 P351 S352 F353 E354 L355 V356 R357 M358 V359 G360 P361 D362 E363 I364 E365
G373 P374 D375 I376 D377 S378 V379 E380 P381 G382 G383 R384 L385 P386 I387 Y394 G395 R396 K397 D401 F402 E403 L406 R409 I410 H411 Y412 F413 T414 M415 Y416 G417 E418 G419 F420 W421 H422 T423 A424 Q425 R426 D427 L428 T429 W430 V431 R432 I433 S434 K435 E436 A437 F438 A439 K440
G441 A442 R443 H446 L451 F455 P460 S461 I462 V463 D464 R465 V466 Q467 V468 T469 I470 Y471 T472 D473 E474 Q475 K476 V477 L478 E479 L480 R481 E482 R485 K486 K487 Y488 A489 E490 R491 D492 A493 R494 L495 R496 E497 V503 D504 T505 C509 L510 L511 C512 Q513 S514 F515
H519 V520 C521 L530 C531 W536 E544 G558 E568 N577 N586 I590 M591 E592 C600 F601 E602 A603 I604 M605 L608 L611 N618 R619 T625 M629 L634 A635 G640 T644 K652 S657 R658 K659 F660 V661 G665 V670
L677 I685 R688 E692 D704 E705 T706 L718 H723 M728 E729 P730 L731 L732 R733 H736

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.060	Depositor
Minimum map value	-0.264	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	369.0, 369.0, 369.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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: NI, SF4

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	0.15	0/3391	0.38	1/4581 (0.0%)
1	B	1.19	7/3398 (0.2%)	0.38	3/4591 (0.1%)
1	C	0.12	0/3406	0.31	0/4602
All	All	0.69	7/10195 (0.1%)	0.36	4/13774 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	GLU	CG-CD	46.13	2.67	1.52
1	B	413	PHE	CE2-CZ	23.28	2.08	1.38
1	B	413	PHE	CD1-CE1	22.76	2.06	1.38
1	B	413	PHE	CD2-CE2	22.56	2.06	1.38
1	B	413	PHE	CE1-CZ	21.68	2.03	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	458	GLU	CB-CG-CD	11.19	131.62	112.60
1	B	458	GLU	OE1-CD-OE2	-9.84	99.29	122.90
1	B	458	GLU	CG-CD-OE1	5.85	131.87	118.40
1	A	484	ALA	N-CA-C	5.17	120.34	112.54

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	3315	0	3263	123	0
1	B	3322	0	3269	122	0
1	C	3330	0	3281	92	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	8	0	0	2	0
3	B	8	0	0	4	0
3	C	8	0	0	2	0
4	A	42	0	0	0	0
4	B	45	0	0	2	0
4	C	39	0	0	3	0
All	All	10123	0	9813	335	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 17.

The worst 5 of 335 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:413:PHE:CE1	1:B:413:PHE:CZ	2.03	1.44
1:B:413:PHE:CE2	1:B:413:PHE:CD2	2.06	1.42
1:B:413:PHE:CZ	1:B:413:PHE:CE2	2.08	1.41
1:B:413:PHE:CE1	1:B:413:PHE:CD1	2.06	1.40
1:B:413:PHE:CE2	1:B:458:GLU:CD	2.23	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	417/732 (57%)	385 (92%)	31 (7%)	1 (0%)	43	71
1	B	418/732 (57%)	393 (94%)	23 (6%)	2 (0%)	24	54
1	C	419/732 (57%)	393 (94%)	25 (6%)	1 (0%)	43	71
All	All	1254/2196 (57%)	1171 (93%)	79 (6%)	4 (0%)	37	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	LEU
1	B	661	VAL
1	C	661	VAL
1	A	661	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	356/614 (58%)	332 (93%)	24 (7%)	15	40
1	B	357/614 (58%)	351 (98%)	6 (2%)	53	67
1	C	358/614 (58%)	336 (94%)	22 (6%)	17	42
All	All	1071/1842 (58%)	1019 (95%)	52 (5%)	24	48

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	593	TYR
1	C	433	ILE
1	C	704	ASP
1	B	670	VAL
1	C	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	571	ASN
1	B	618	ASN
1	C	449	GLN
1	C	326	ASN
1	B	457	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	SF4	C	803	1	0,12,12	-	-	-		
3	SF4	A	803	1	0,12,12	-	-	-		
3	SF4	B	803	1	0,12,12	-	-	-		

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
3	SF4	C	803	1	-	-	0/6/5/5
3	SF4	A	803	1	-	-	0/6/5/5
3	SF4	B	803	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

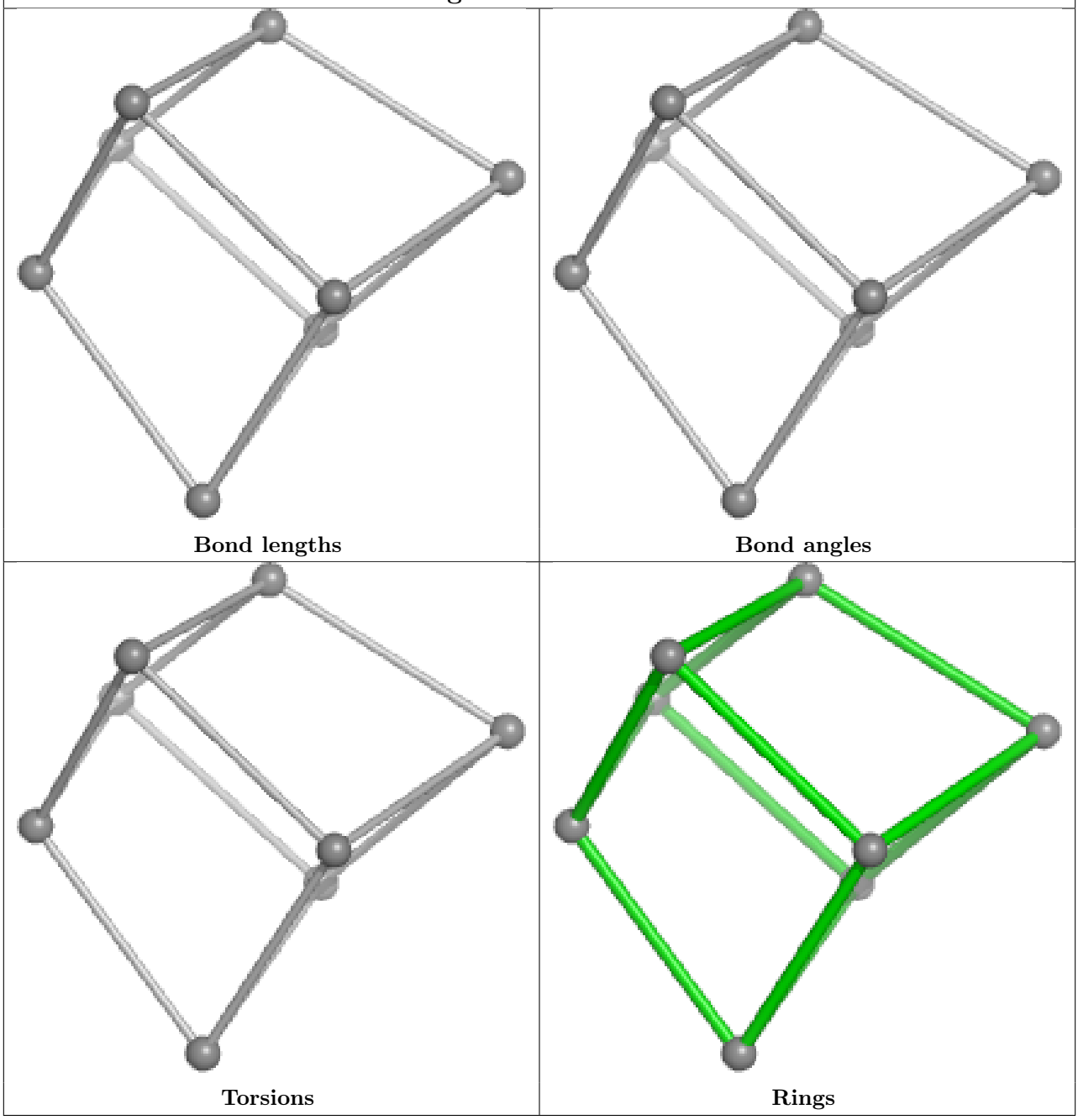
There are no ring outliers.

3 monomers are involved in 8 short contacts:

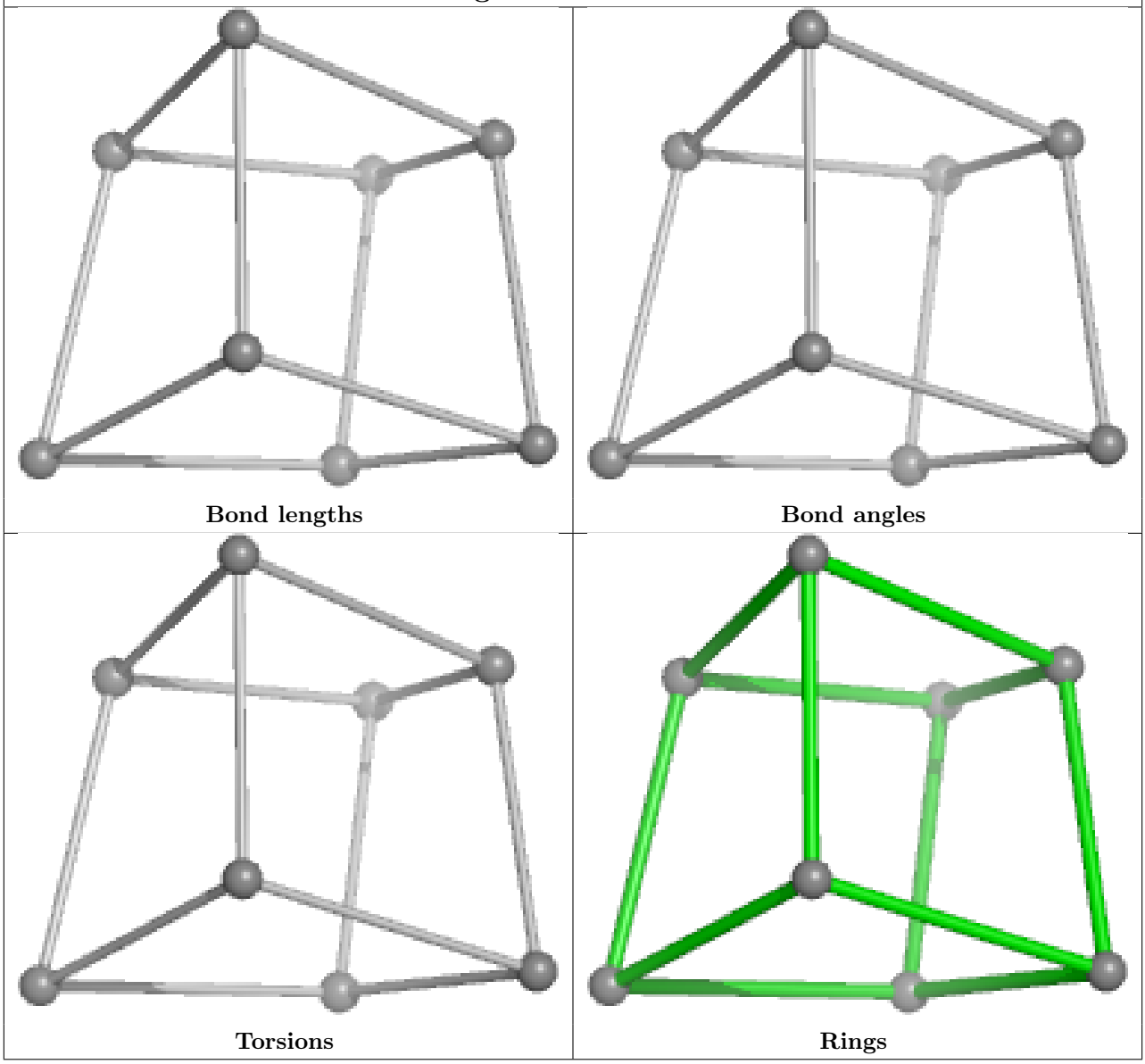
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	803	SF4	2	0
3	A	803	SF4	2	0
3	B	803	SF4	4	0

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.

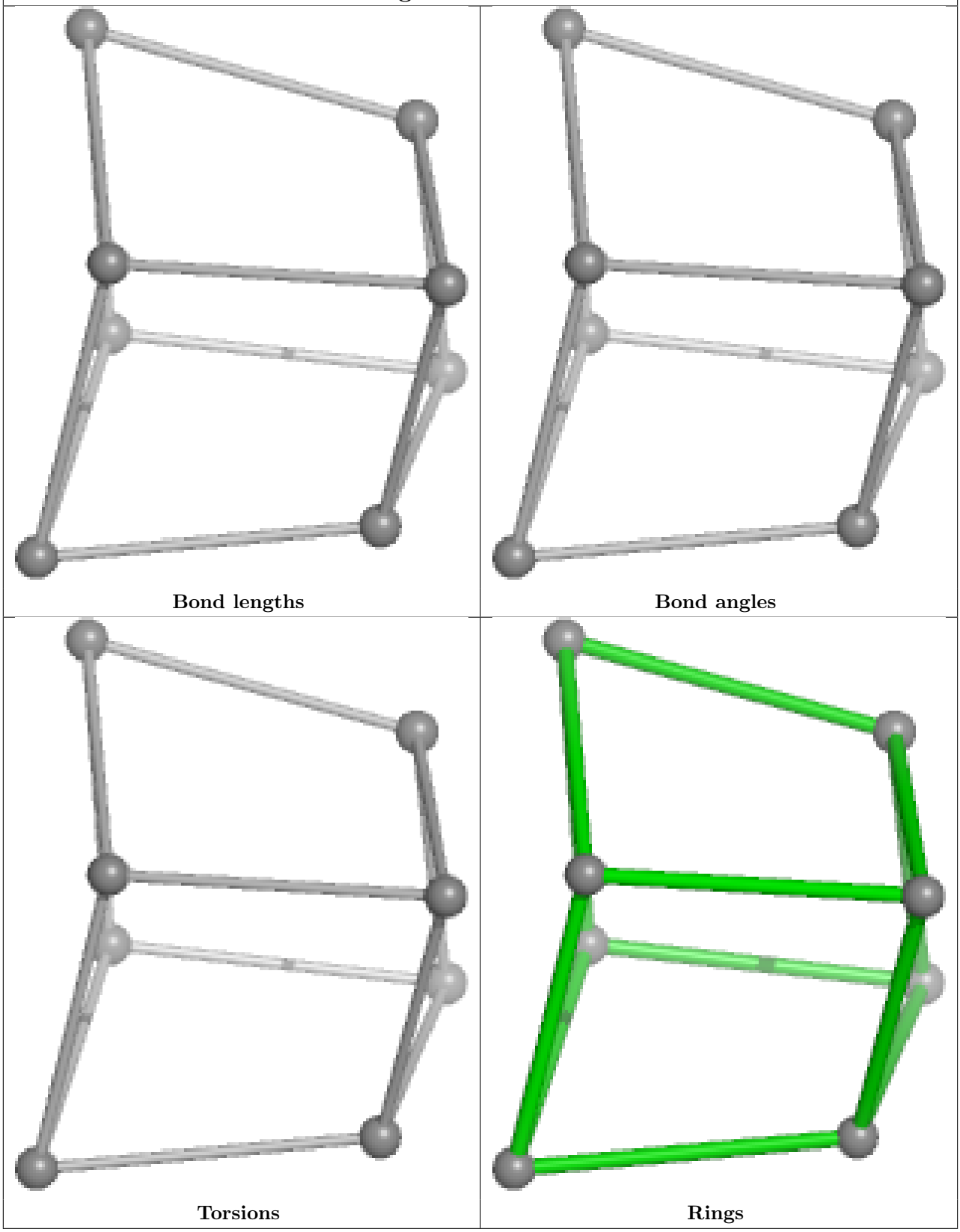
Ligand SF4 C 803



Ligand SF4 A 803



Ligand SF4 B 803



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.

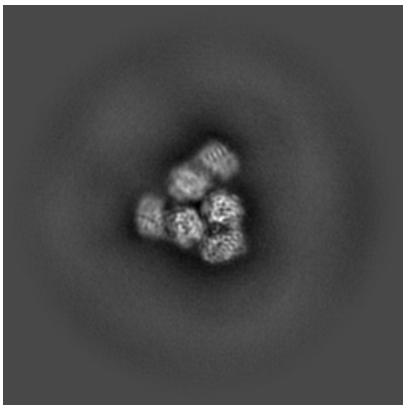
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-50674. These allow visual inspection of the internal detail of the map and identification of artifacts.

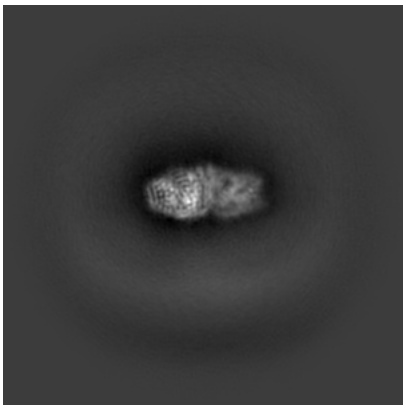
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

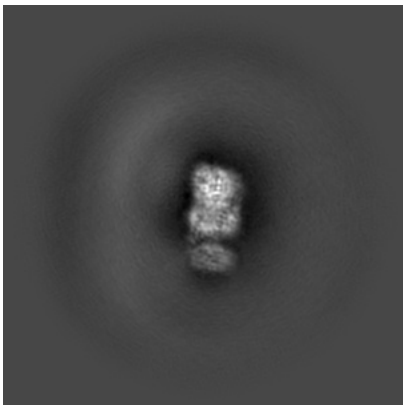
6.1.1 Primary map



X

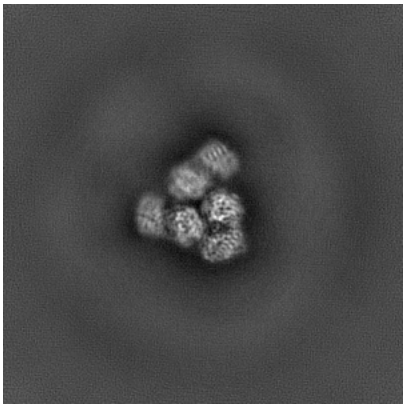


Y

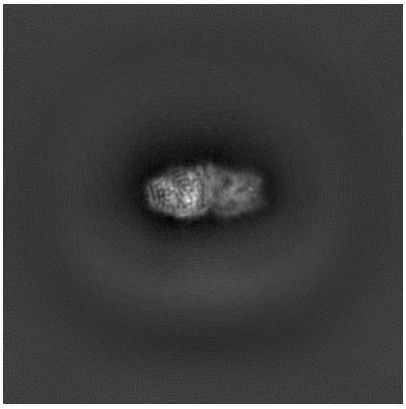


Z

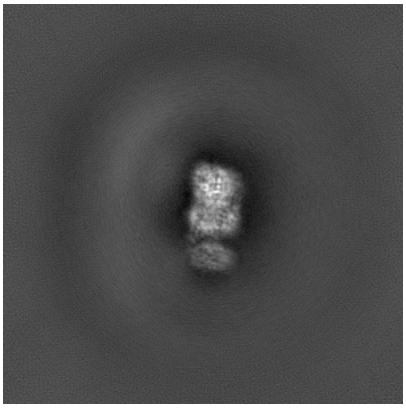
6.1.2 Raw map



X



Y



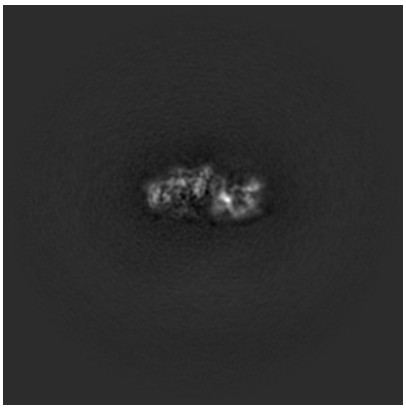
Z

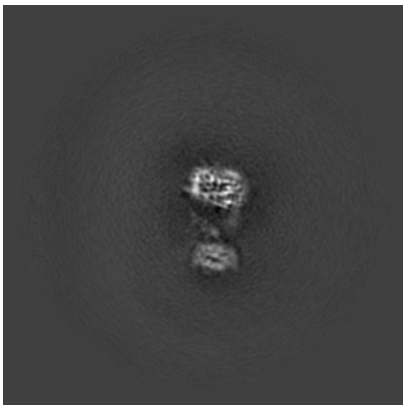
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

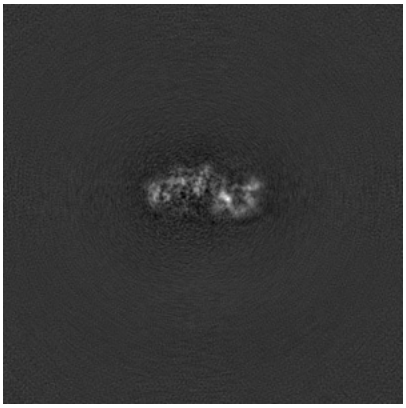
X Index: 150

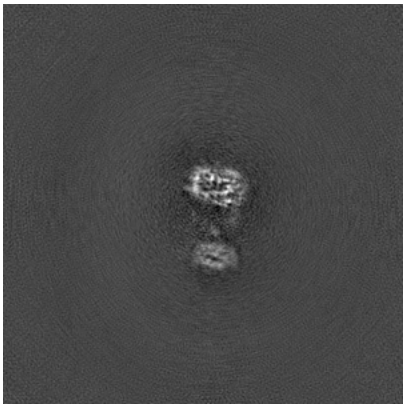

Y Index: 150


Z Index: 150

6.2.2 Raw map

X Index: 150

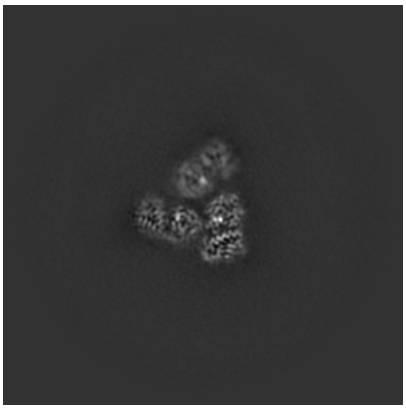

Y Index: 150


Z Index: 150

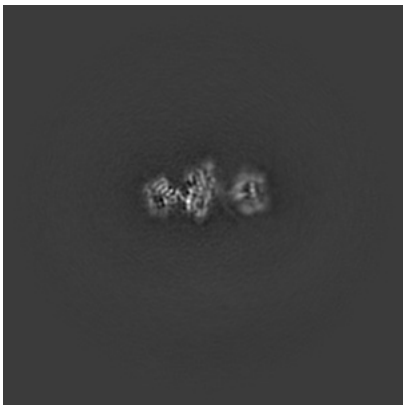
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



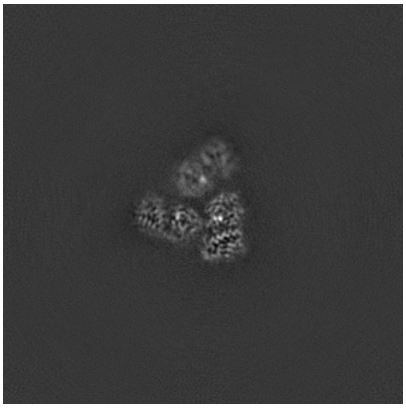
X Index: 153



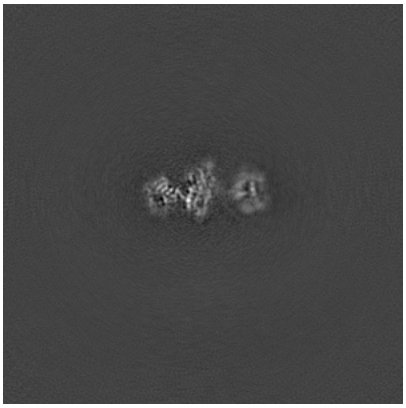
Y Index: 159

Z Index: 139

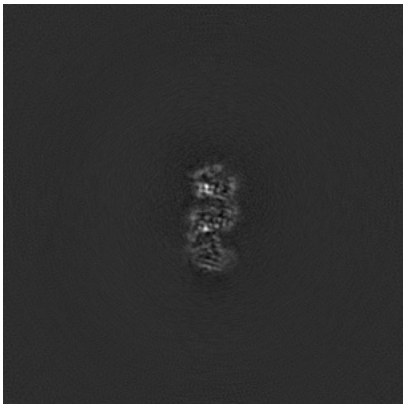
6.3.2 Raw map



X Index: 153



Y Index: 159

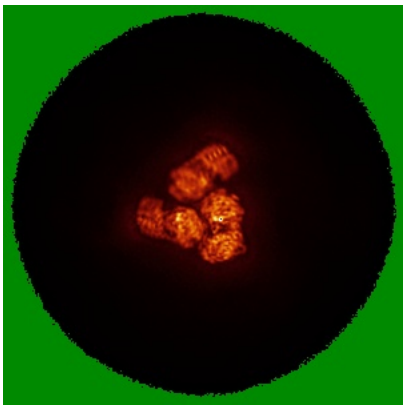


Z Index: 139

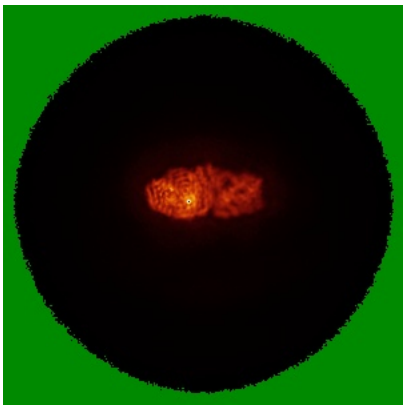
The images above show the largest variance slices of the map in three orthogonal directions.

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

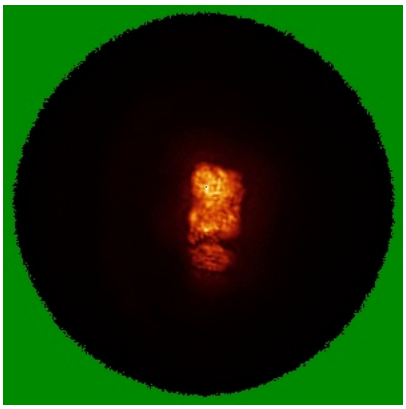
6.4.1 Primary map



X

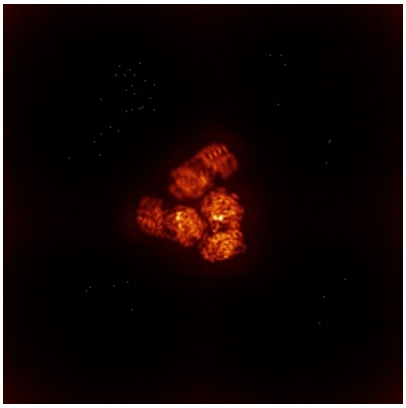


Y

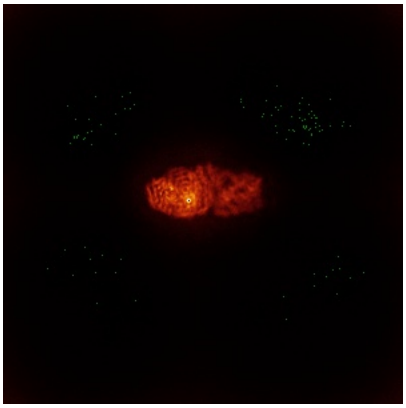


Z

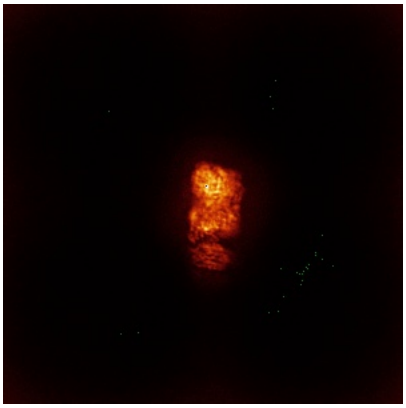
6.4.2 Raw map



X



Y

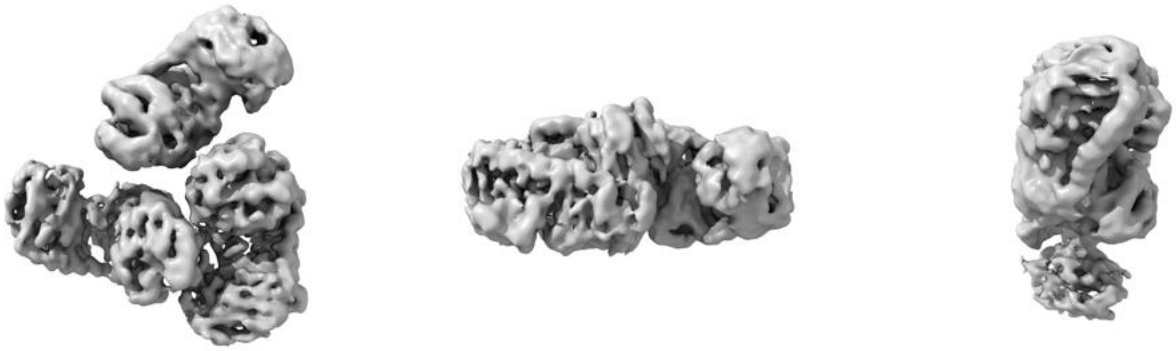


Z

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 (i)

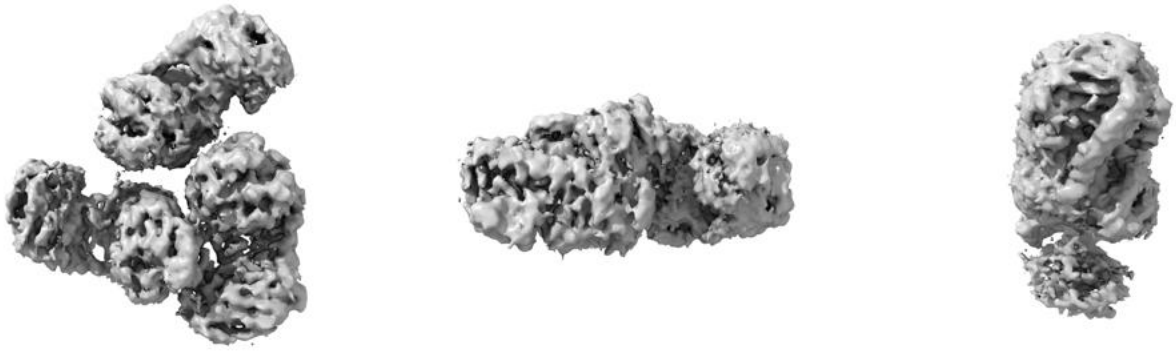
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

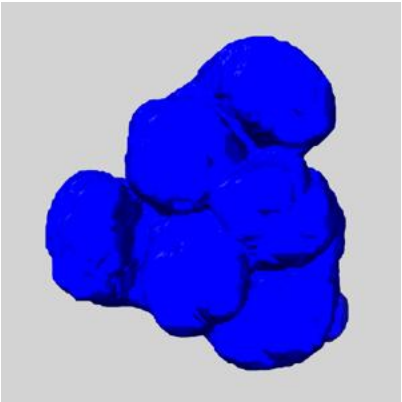
6.6 Mask visualisation (i)

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

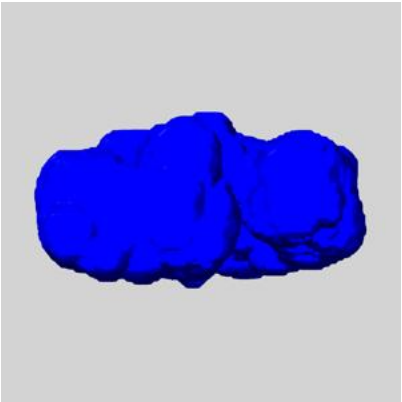
A mask typically either:

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

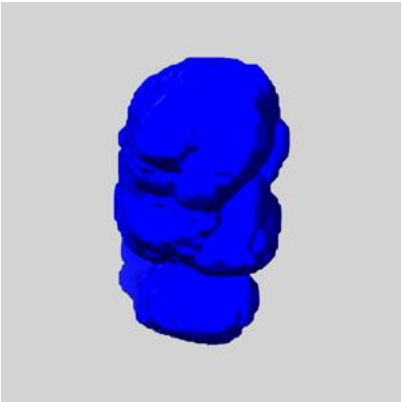
6.6.1 emd_50674_msk_1.map (i)



X



Y

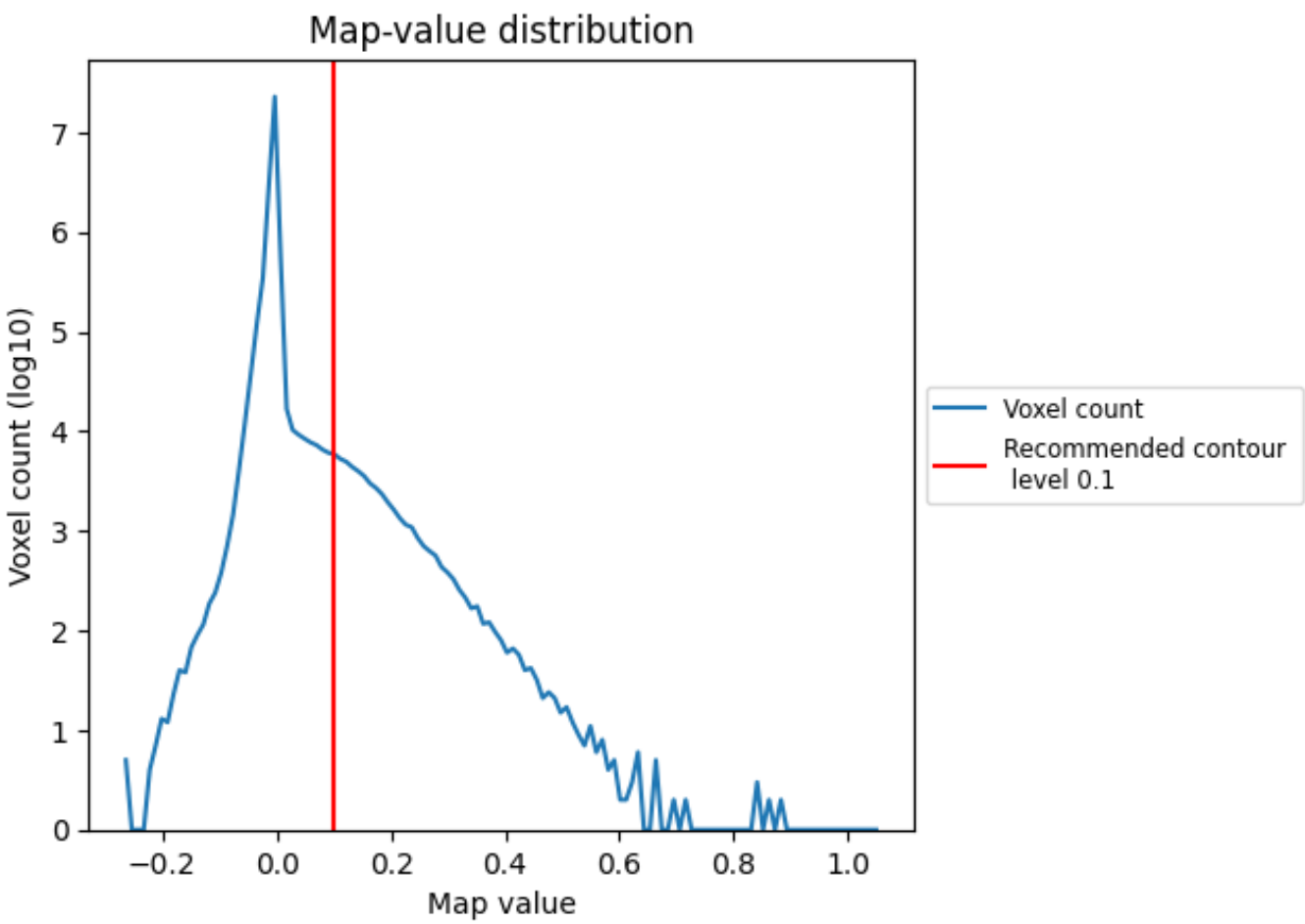


Z

7 Map analysis (i)

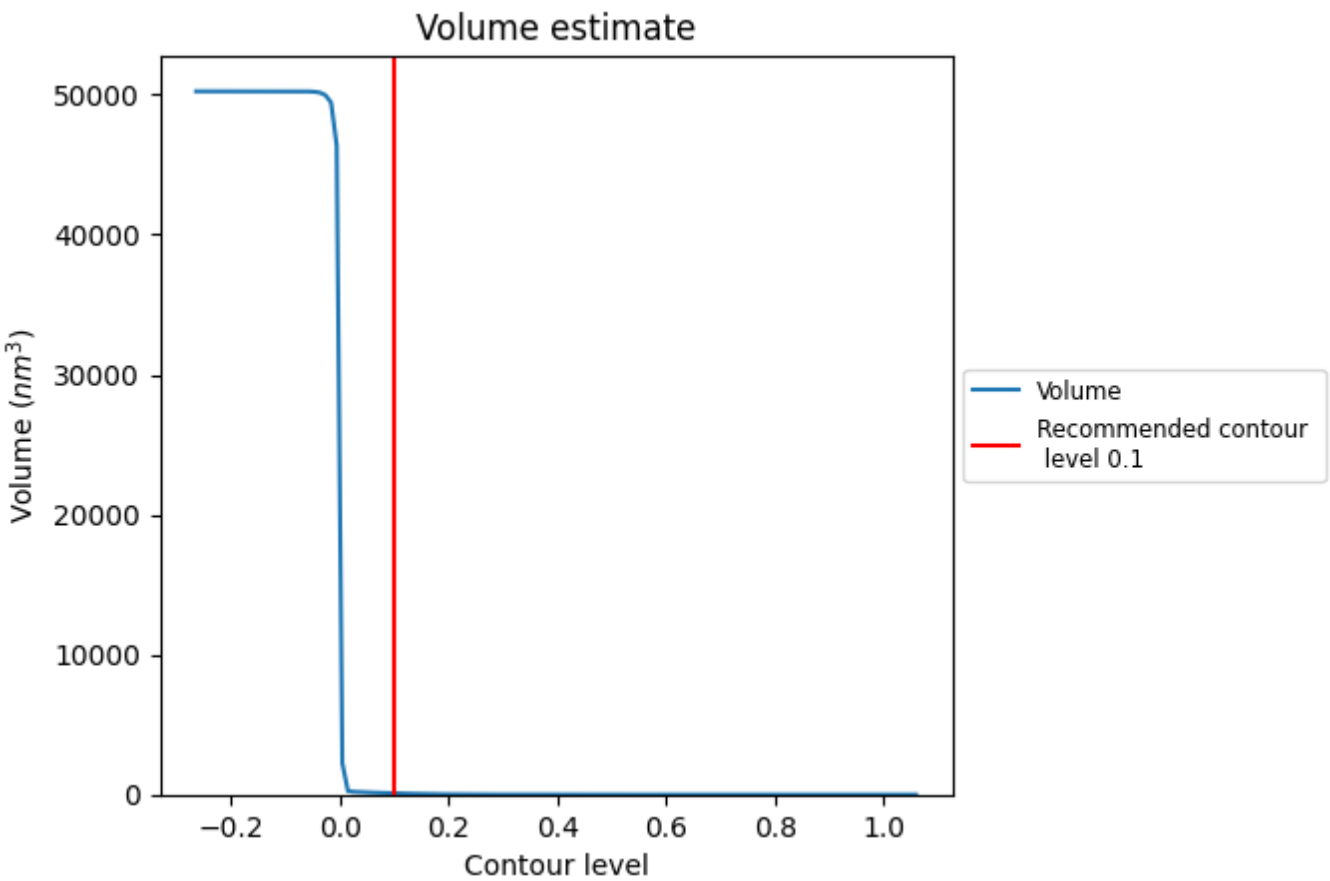
This section contains the results of statistical analysis of the map.

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.

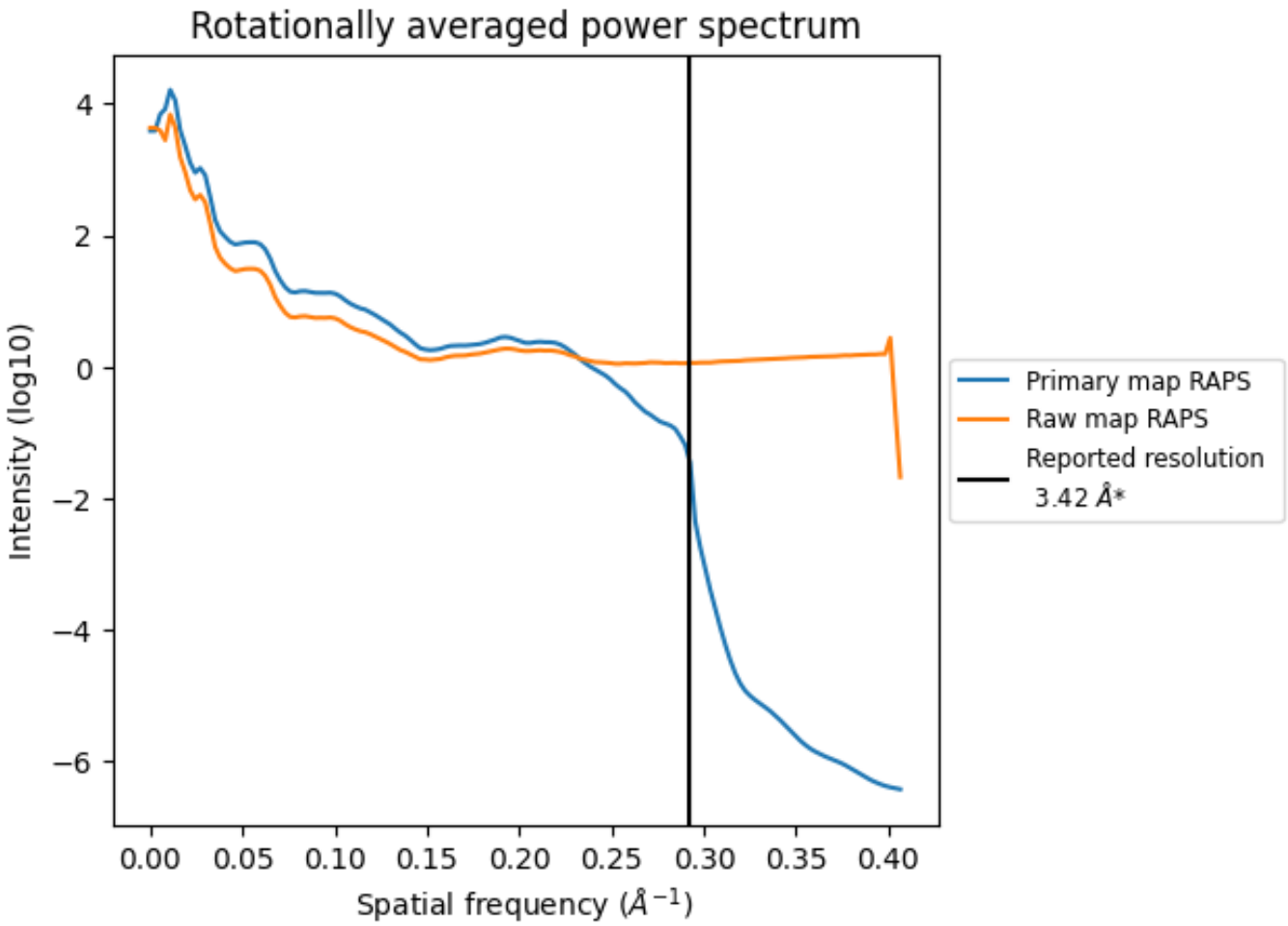
7.2 Volume estimate (i)



The volume at the recommended contour level is 92 nm^3; this corresponds to an approximate mass of 83 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)

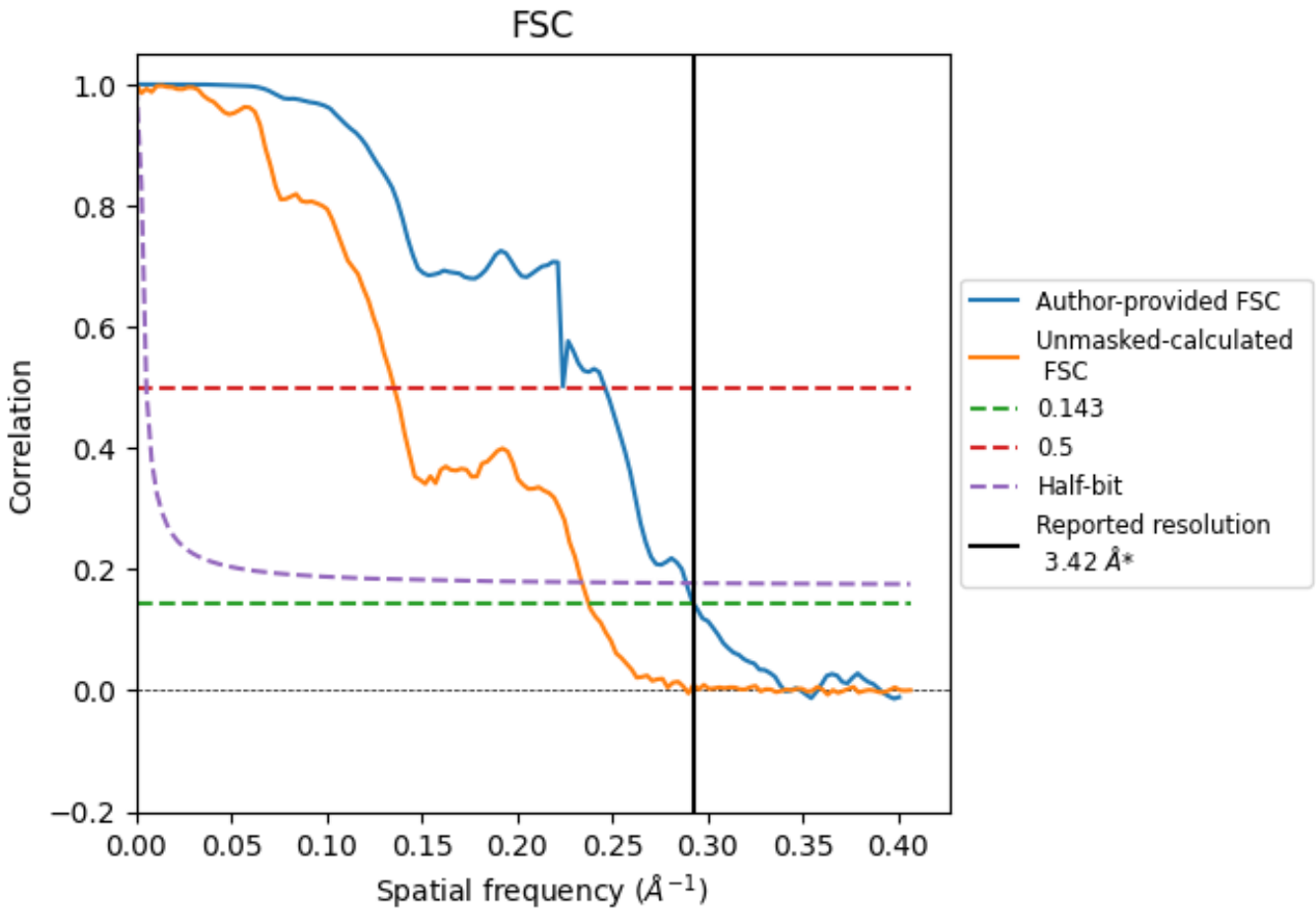


*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

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 0.292 Å^{-1}

8.2 Resolution estimates (i)

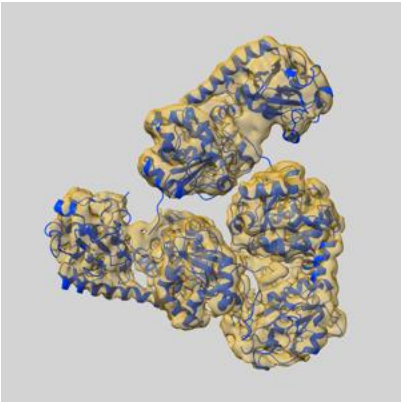
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	4.06	3.46
Unmasked-calculated*	4.21	7.39	4.27

*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 4.21 differs from the reported value 3.42 by more than 10 %

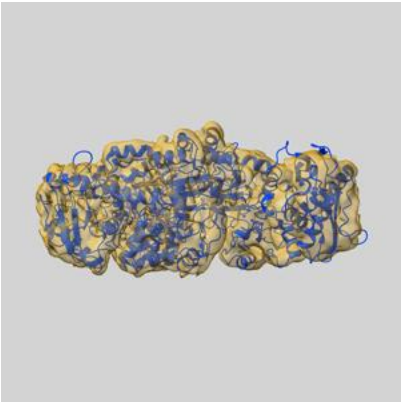
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-50674 and PDB model 9FR0. Per-residue inclusion information can be found in section 3 on page 6.

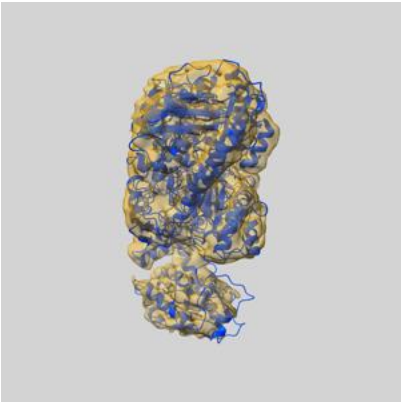
9.1 Map-model overlay (i)



X



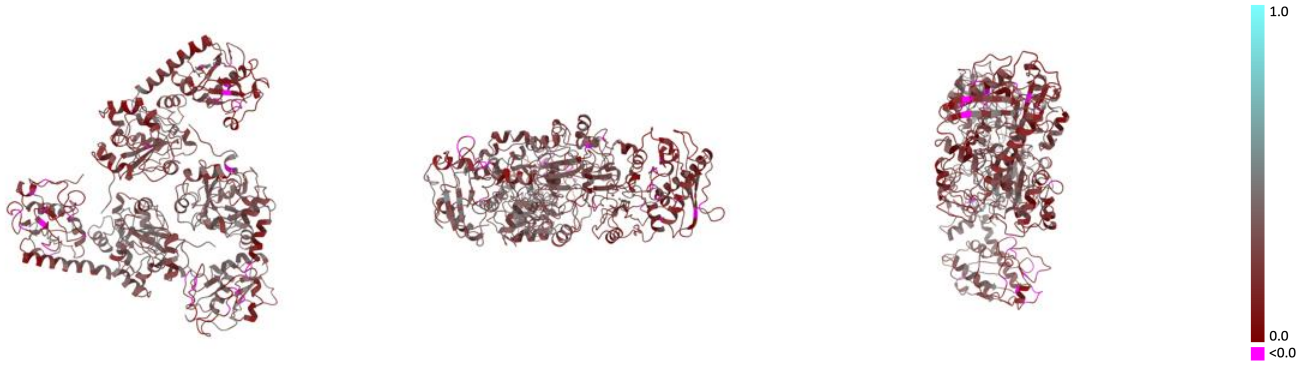
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

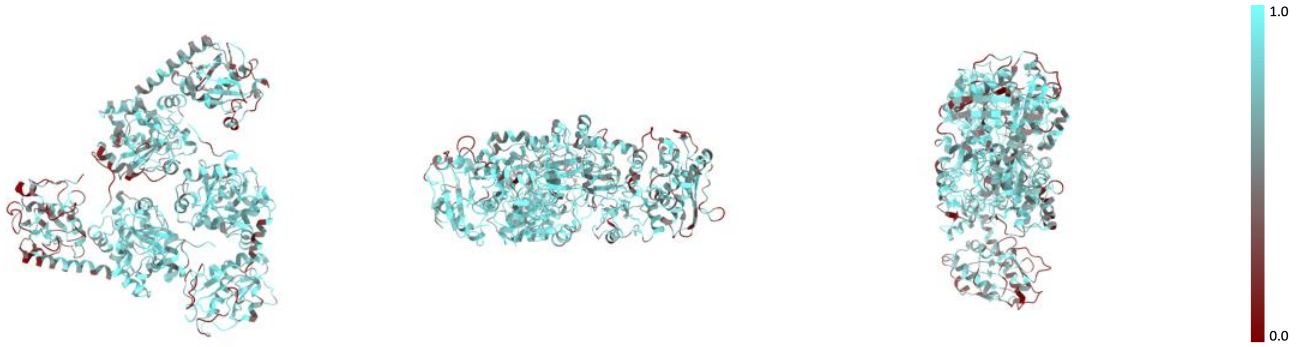
9.2 Q-score mapped to coordinate model (i)



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.

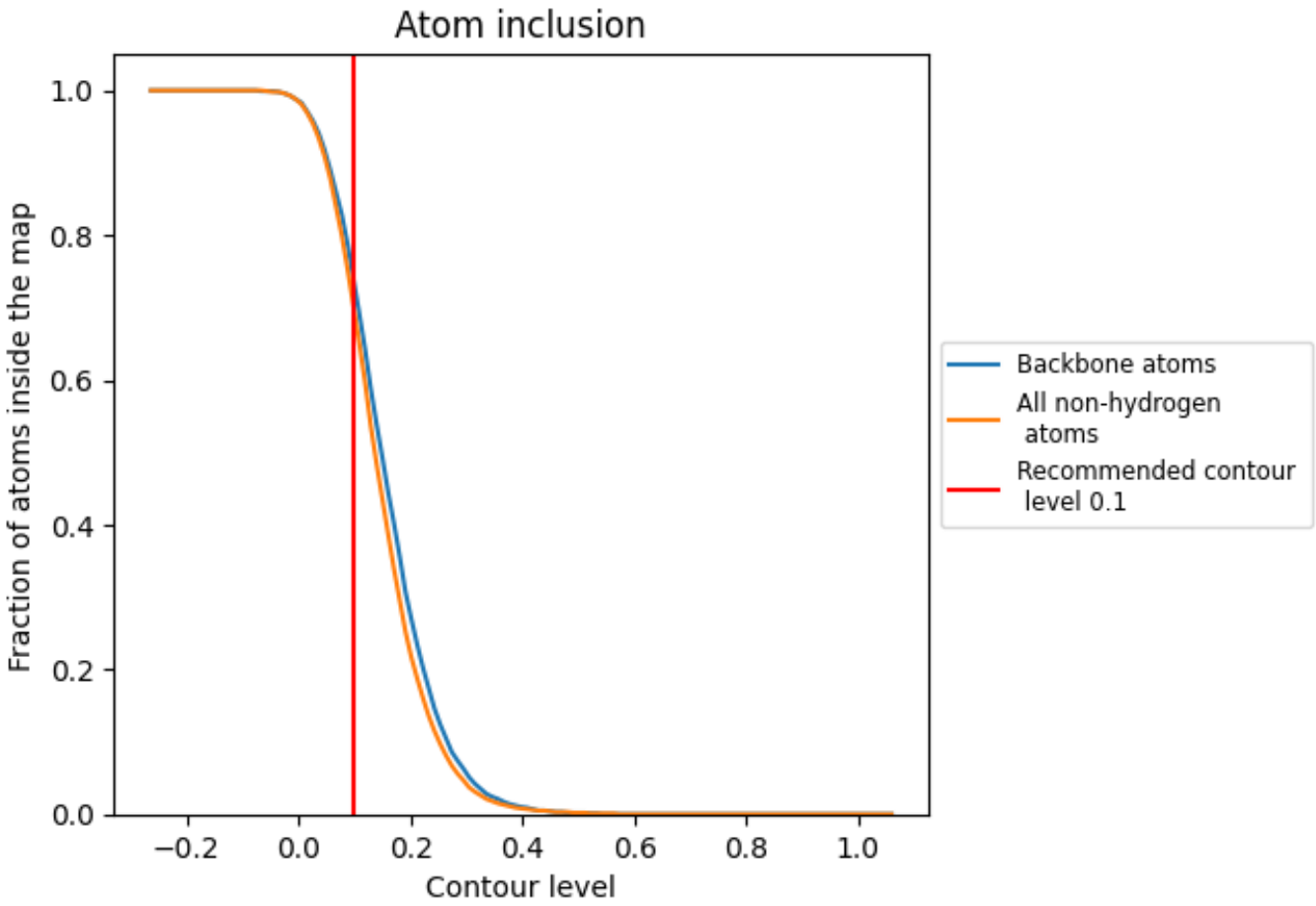
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 69% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.2670
A	0.7700	0.3000
B	0.6510	0.2100
C	0.6750	0.2920