wwPDB EM Validation Summary Report

May 15, 2024 – 12:28 PM EDT

PDB ID	:	8T45
EMDB ID	:	EMD-41020
Title	:	Cryo-EM Analysis of AE1 Structure in 100 mM NaHCO3 Buffer: Form2
Authors	:	Su, C.C.
Deposited on	:	2023-06-08
Resolution	:	2.99 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 ⓘ 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:

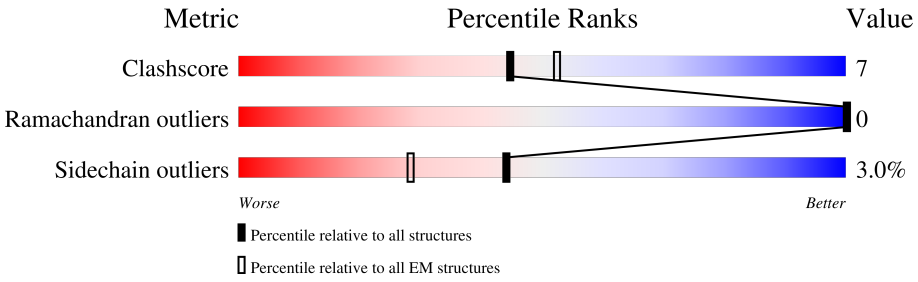
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.99 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	911	40% 10% 50%
1	B	911	40% 10% 50%

2 Entry composition (i)

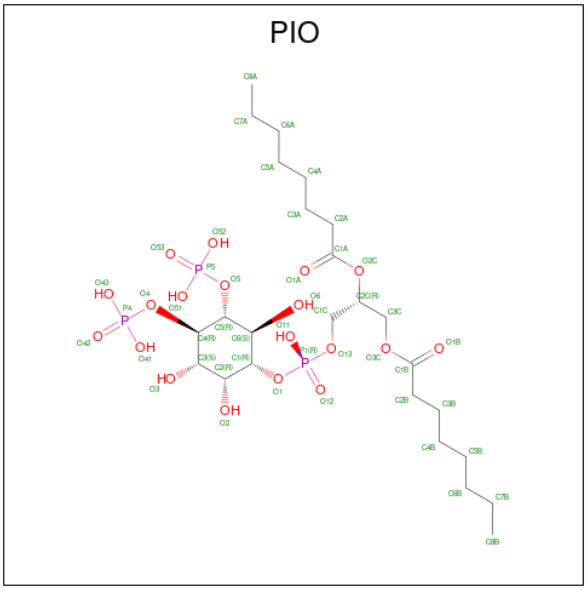
There are 4 unique types of molecules in this entry. The entry contains 7475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Band 3 anion transport protein.

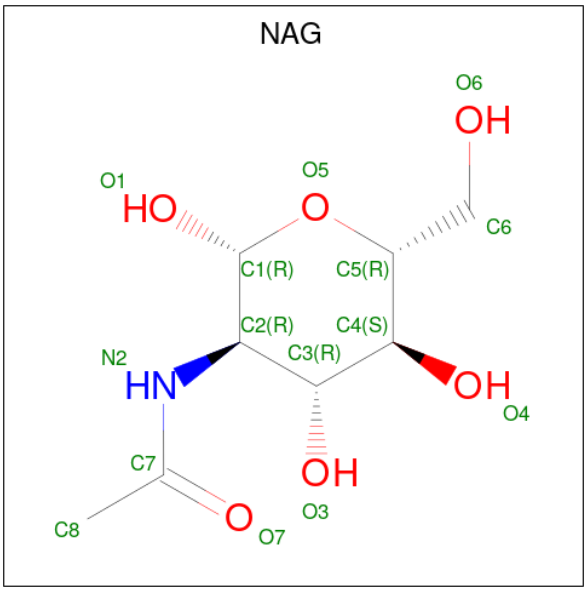
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3611	2428	570	597	16		
1	B	457	Total	C	N	O	S	0	0
			3607	2427	570	594	16		

- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: $C_{25}H_{49}O_{19}P_3$).



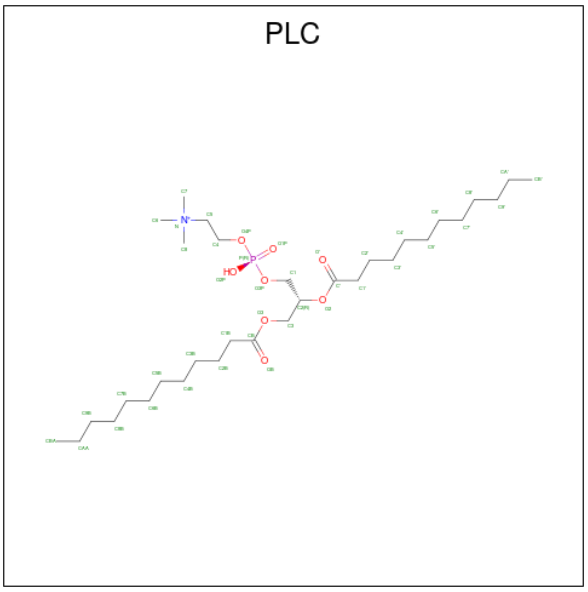
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			47	25	19	3	
2	B	1	Total	C	O	P	0
			44	22	19	3	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0

- Molecule 4 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O P 37 28 8 1	0

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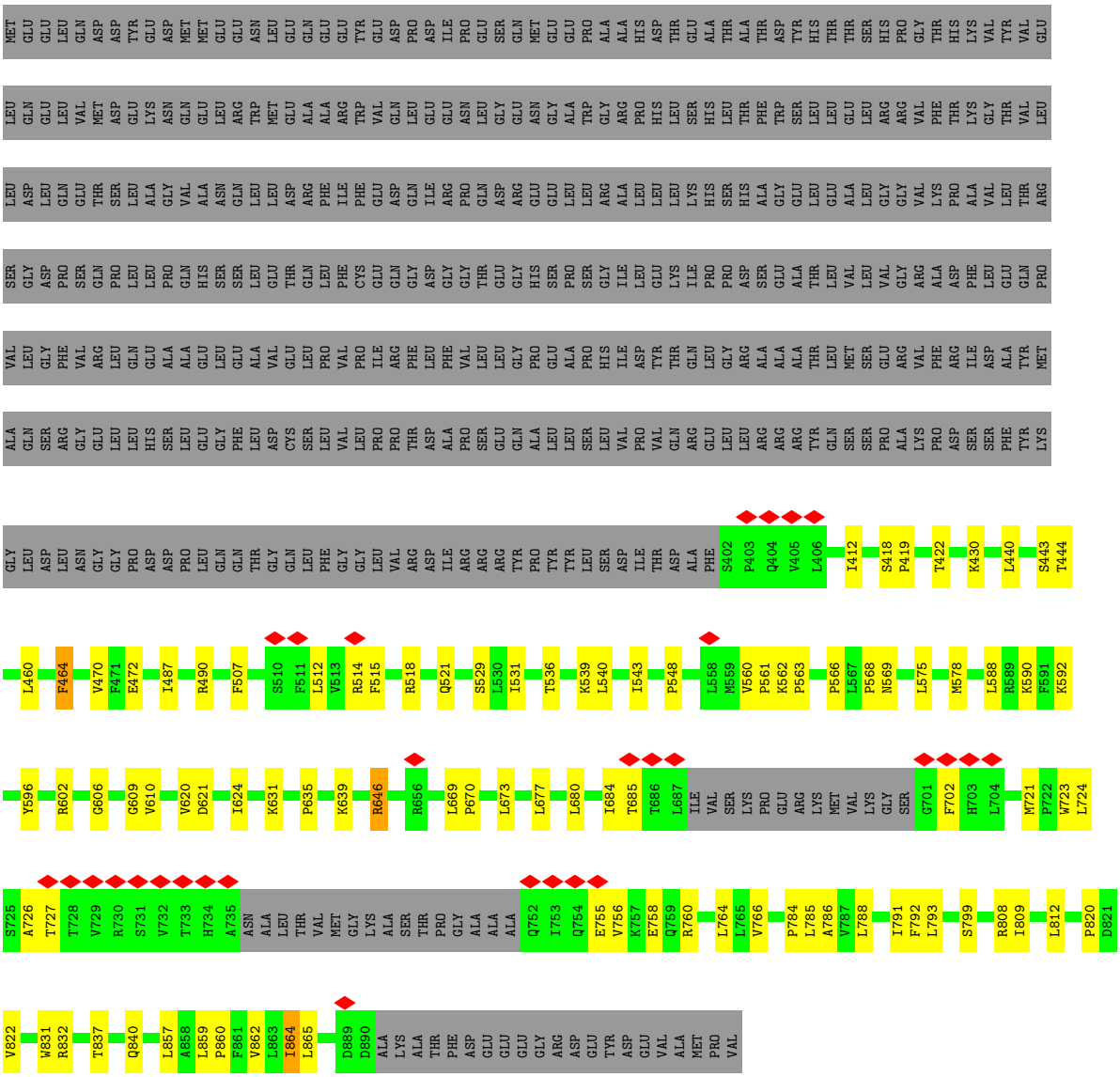
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			36	27	8	1	
4	B	1	Total	C	O	P	0
			36	27	8	1	
4	B	1	Total	C	O	P	0
			29	20	8	1	

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: Band 3 anion transport protein

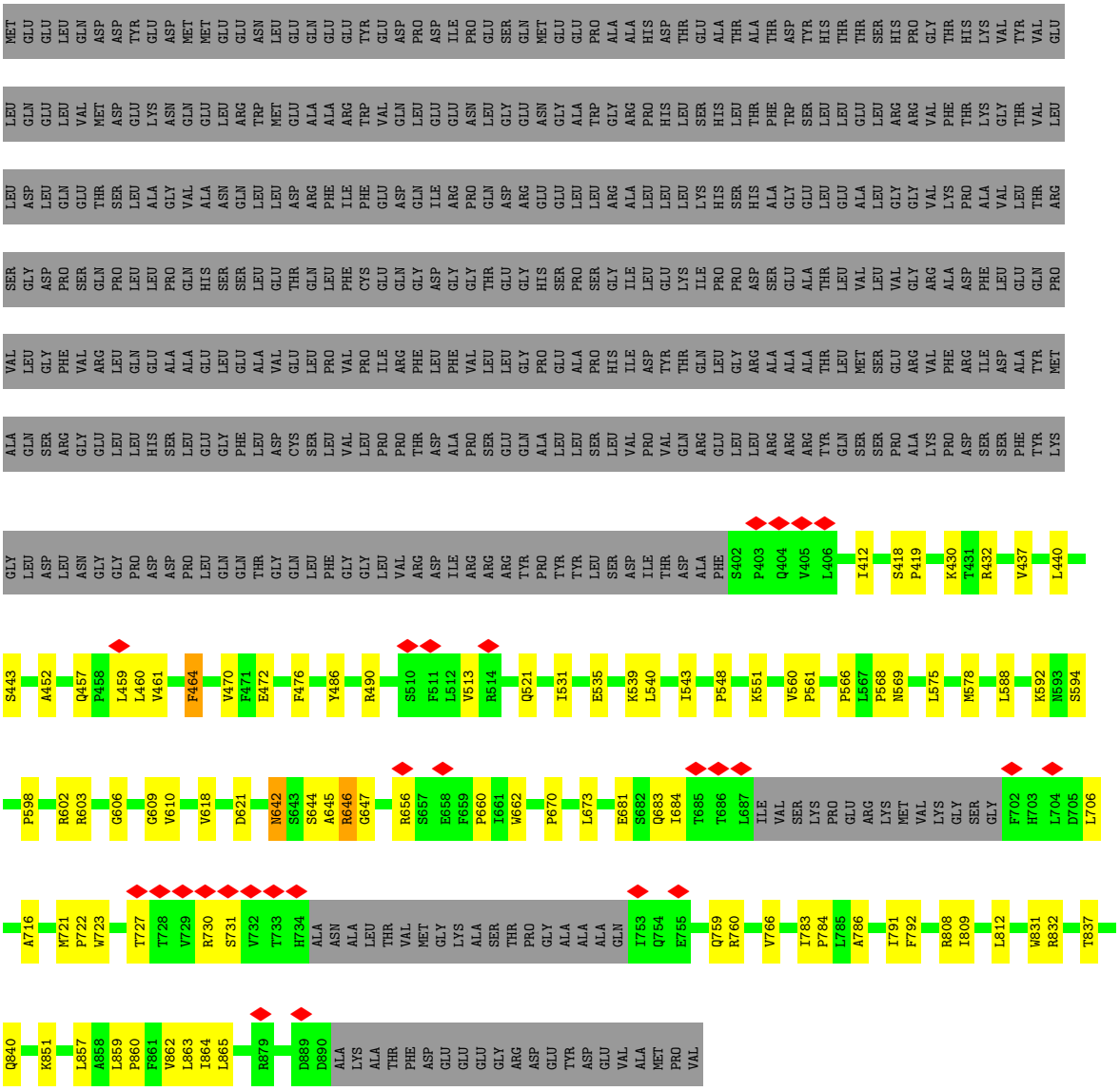
Chain A:



• Molecule 1: Band 3 anion transport protein

Chain B:


40%
10%
50%


MET GLU GLU LEU GLN ASP ASP TYR GLU ASP MET MET GLU GLU ASN LEU GLU GLN GLU GLU TYR GLU ASP PRO ASP ILE PRO GLU SER GLN MET GLU GLU PRO ALA ALA HIS ASP THR GLU ALA THR ALA THR ASP TYR HIS THR THR SER HIS PRO GLY THR HIS LYS VAL TYR VAL GLU
LEU GLN GLU LEU VAL MET ASP GLU LYS ASN GLN GLU LEU ARG TRP MET GLU ALA ALA ARG TRP VAL GLN LEU GLU GLU ILE ARG PRO GLN ASP ARG GLU GLU LEU LEU ARG ALA LEU LEU LYS HIS SER HIS ALA GLY GLU LEU GLU ALA LEU LEU GLY GLY VAL LYS PRO ALA VAL LEU THR ARG
LEU ASP LEU GLN LEU GLU THR SER LEU ALA GLY VAL ALA ASN GLN LEU LEU ASP ARG PHE ILE PHE GLU ASP GLN ILE ARG PRO GLN ASP ARG GLU GLU LEU LEU ARG ALA LEU LEU LEU LYS HIS SER HIS ALA GLY GLU LEU GLU ALA LEU LEU GLY GLY VAL LYS PRO ALA VAL LEU THR ARG
SER GLY ASP PRO SER GLN PRO LEU LEU PRO GLN HIS SER SER LEU GLU THR GLN LEU PHE CYS GLU GLN GLY ASP GLY GLY THR GLU GLY HIS SER PRO SER GLY ILE LEU GLU LEU LYS ILE PRO PRO ASP SER GLU ALA THR LEU VAL LEU VAL GLY GLY ARG VAL ARG ASP PHE LEU GLU PRO
VAL LEU GLY PHE VAL ARG LEU GLN GLU ALA ALA GLU LEU GLU ALA VAL GLU LEU PRO VAL PRO ILE ARG PHE LEU PHE VAL LEU LEU GLY PRO GLU ALA PRO HIS ILE ASP TYR THR GLN LEU GLY ARG ALA ALA ALA THR LEU MET SER GLU ARG VAL PHE ARG ILE ASP ALA TYR MET
ALA GLN SER ARG GLY GLU LEU LEU HIS SER LEU GLU GLY PHE LEU ASP CYS SER LEU VAL LEU PRO PRO THR ASP ALA PRO SER GLU GLN GLN ALA LEU LEU LEU SER LEU VAL PRO VAL GLN ARG GLU LEU LEU ARG ARG ARG TYR GLN SER SER PRO ALA LYS PRO ASP SER SER PHE TYR LYS
GLY LEU ASP LEU ASN GLY GLY PRO ASP PRO LEU GLN GLN THR GLY GLN LEU PHE GLY GLY LEU VAL ARG ASP ILE ARG ARG ARG TYR PRO TYR TYR LEU SER ASP ILE THR ASP ALA PHE S402 P403 Q404 V405 L406 I412 S418 P419 K430 T431 R432 V437 L440
S443 A452 Q457 P458 L459 L460 V461 F464 V470 F471 E472 F476 Y486 R490 S510 F511 L512 V513 R514 Q521 I531 E535 K539 L540 I543 P548 K551 V560 P561 P566 L567 P568 N569 L575 M578 L588 K592 N593 S594
P598 R602 R603 G606 G609 V610 V618 D621 N642 S643 S644 A645 R646 G647 R656 S657 E658 F659 P660 I661 W662 P670 L673 E681 S682 Q683 I684 T685 T686 L687 ILE VAL SER LYS PRO GLU ARG LYS MET VAL LYS GLY SER GLY F702 H703 L704 D705 L706
A716 M721 P722 W723 T727 T728 V729 R730 S731 V732 T733 H734 ALA ASN ALA LEU THR VAL MET GLY LYS ALA SER THR PRO GLY ALA ALA ALA GLN I753 Q754 E755 Q759 R760 V766 I783 P784 L785 A786 I791 F792 R808 I809 L812 W831 R832 T837
Q840 K851 L857 A858 L859 P860 F861 V862 L863 I864 L865 R879 D889 D890 ALA LYS ALA THR PHE ASP GLU GLU GLU GLY ARG ASP GLU TYR ASP GLU VAL ALA MET PRO VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.013	Depositor
Minimum map value	-1.814	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PIO, NAG, PLC

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	0.25	0/3704	0.42	0/5041
1	B	0.25	0/3700	0.43	0/5035
All	All	0.25	0/7404	0.42	0/10076

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

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	3611	0	3788	53	0
1	B	3607	0	3803	50	0
2	A	47	0	44	2	0
2	B	44	0	35	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	73	0	102	1	0
4	B	65	0	85	2	0
All	All	7475	0	7883	105	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 105 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:646:ARG:NH1	1:B:647:GLY:O	2.25	0.70
1:B:443:SER:HB2	1:B:721:MET:HB3	1.74	0.69
1:B:490:ARG:NH2	1:B:721:MET:O	2.26	0.68
1:A:673:LEU:HB3	1:A:860:PRO:HG2	1.75	0.68
1:B:592:LYS:HB2	1:B:606:GLY:HA3	1.79	0.65

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	454/911 (50%)	445 (98%)	9 (2%)	0	100	100
1	B	451/911 (50%)	437 (97%)	14 (3%)	0	100	100
All	All	905/1822 (50%)	882 (98%)	23 (2%)	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	396/786 (50%)	383 (97%)	13 (3%)	38	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	399/786 (51%)	388 (97%)	11 (3%)	43 77
All	All	795/1572 (51%)	771 (97%)	24 (3%)	44 75

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	464	PHE
1	B	646	ARG
1	B	642	ASN
1	B	706	LEU
1	A	723	TRP

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

Mol	Chain	Res	Type
1	B	683	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)

8 ligands are 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	$\#\|Z\| > 2$
3	NAG	A	1002	1	14,14,15	0.21	0	17,19,21	0.43	0
2	PIO	B	1002	-	44,44,47	1.22	6 (13%)	58,62,65	1.04	3 (5%)
3	NAG	B	1001	1	14,14,15	0.40	0	17,19,21	0.43	0
4	PLC	A	1004	-	35,35,41	0.64	1 (2%)	39,40,49	1.08	3 (7%)
4	PLC	A	1003	-	36,36,41	0.53	0	39,41,49	0.51	0
2	PIO	A	1001	-	47,47,47	1.17	6 (12%)	61,65,65	0.97	3 (4%)
4	PLC	B	1004	-	28,28,41	0.72	1 (3%)	32,33,49	1.13	2 (6%)
4	PLC	B	1003	-	35,35,41	0.66	1 (2%)	39,40,49	1.01	2 (5%)

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	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	PIO	B	1002	-	-	13/41/65/68	0/1/1/1
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
4	PLC	A	1004	-	-	11/37/37/45	-
4	PLC	A	1003	-	-	9/40/40/45	-
2	PIO	A	1001	-	-	26/44/68/68	0/1/1/1
4	PLC	B	1004	-	-	9/30/30/45	-
4	PLC	B	1003	-	-	4/37/37/45	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	PIO	P5-O5	3.16	1.65	1.59
2	B	1002	PIO	P5-O5	3.14	1.65	1.59
2	B	1002	PIO	P4-O4	3.11	1.65	1.59
2	A	1001	PIO	P4-O4	3.09	1.65	1.59
4	A	1004	PLC	P-O4P	2.70	1.65	1.54

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1004	PLC	O4P-P-O3P	-4.98	93.49	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1004	PLC	O4P-P-O3P	-4.97	93.51	106.73
4	B	1003	PLC	O4P-P-O3P	-4.96	93.53	106.73
2	B	1002	PIO	O2C-C1A-C2A	4.32	120.82	111.50
2	A	1001	PIO	O2C-C1A-C2A	3.60	119.26	111.50

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PIO	C2-C1-O1-P1
2	A	1001	PIO	C1-O1-P1-O11
2	A	1001	PIO	C5-O5-P5-O53
2	B	1002	PIO	O1A-C1A-O2C-C2C
2	B	1002	PIO	C2A-C1A-O2C-C2C

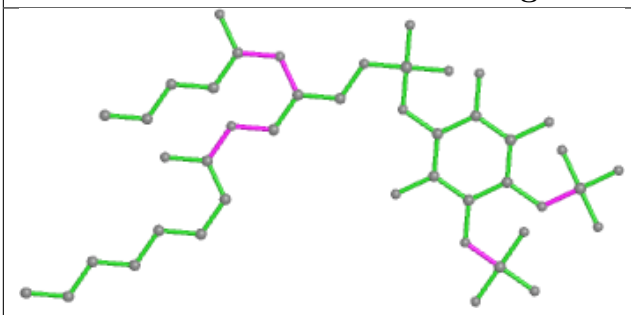
There are no ring outliers.

4 monomers are involved in 6 short contacts:

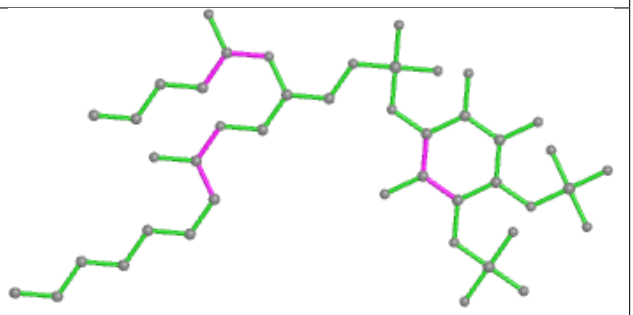
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	PIO	1	0
4	A	1003	PLC	1	0
2	A	1001	PIO	2	0
4	B	1003	PLC	2	0

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.

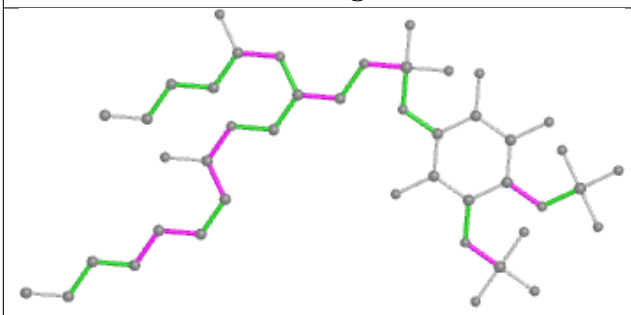
Ligand PIO B 1002



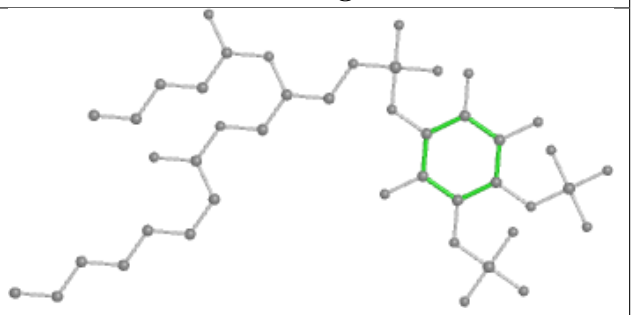
Bond lengths



Bond angles

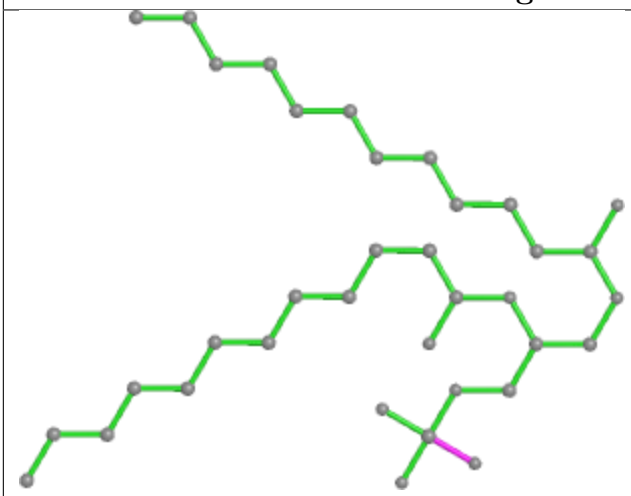


Torsions

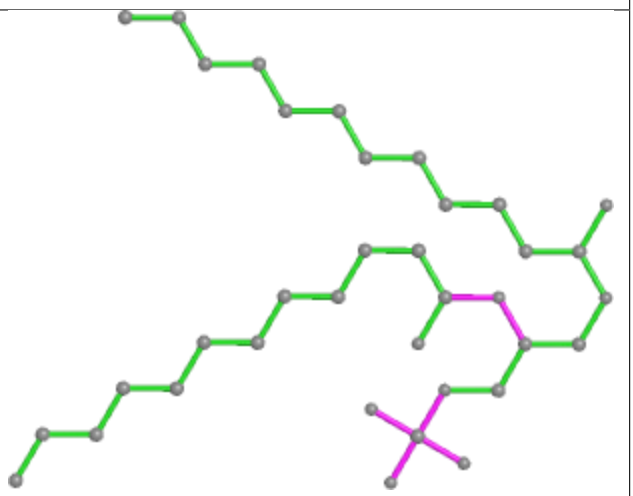


Rings

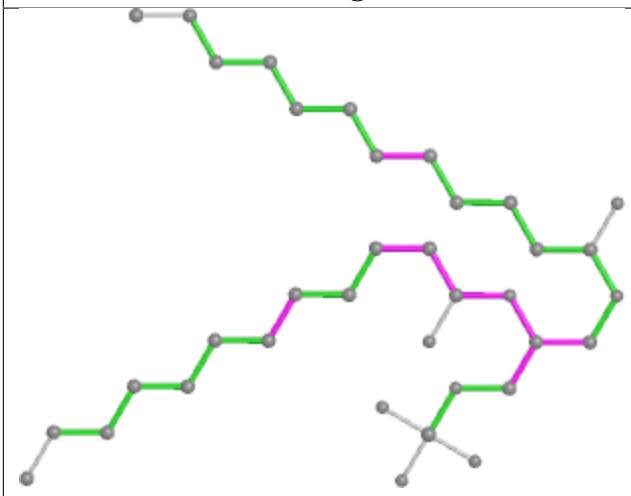
Ligand PLC A 1004



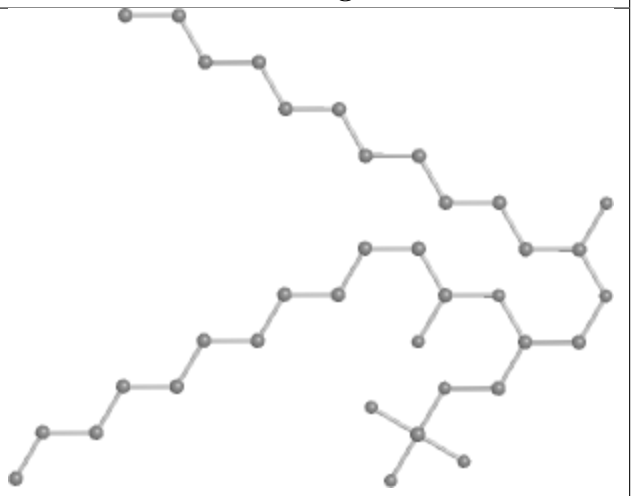
Bond lengths



Bond angles

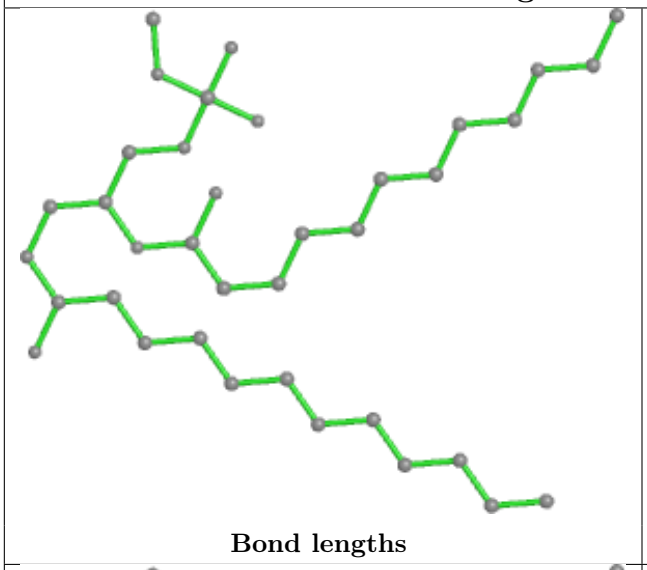


Torsions

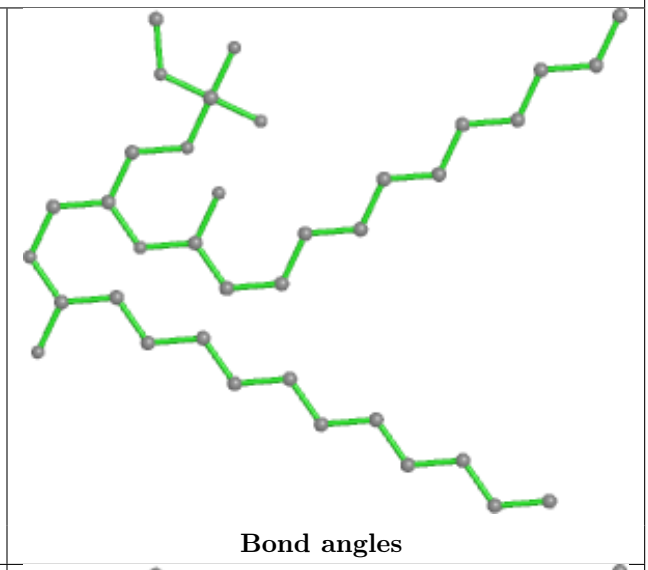


Rings

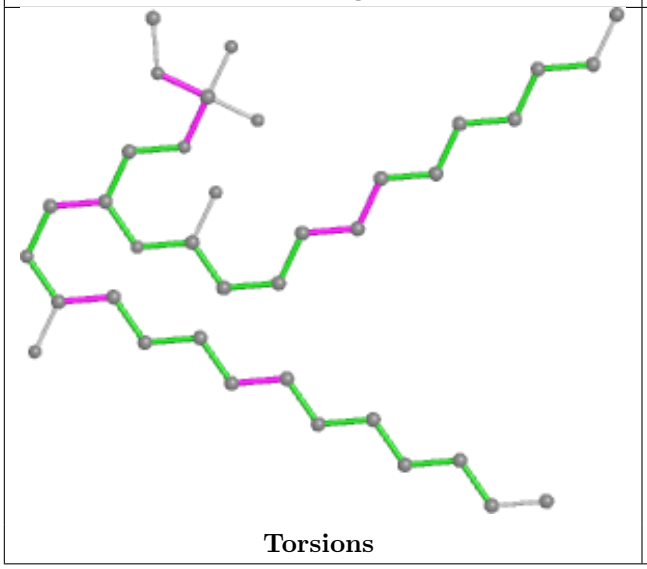
Ligand PLC A 1003



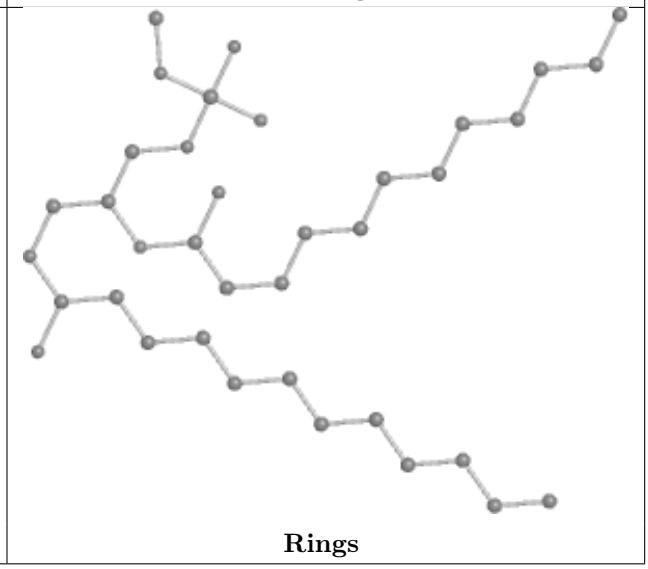
Bond lengths



Bond angles

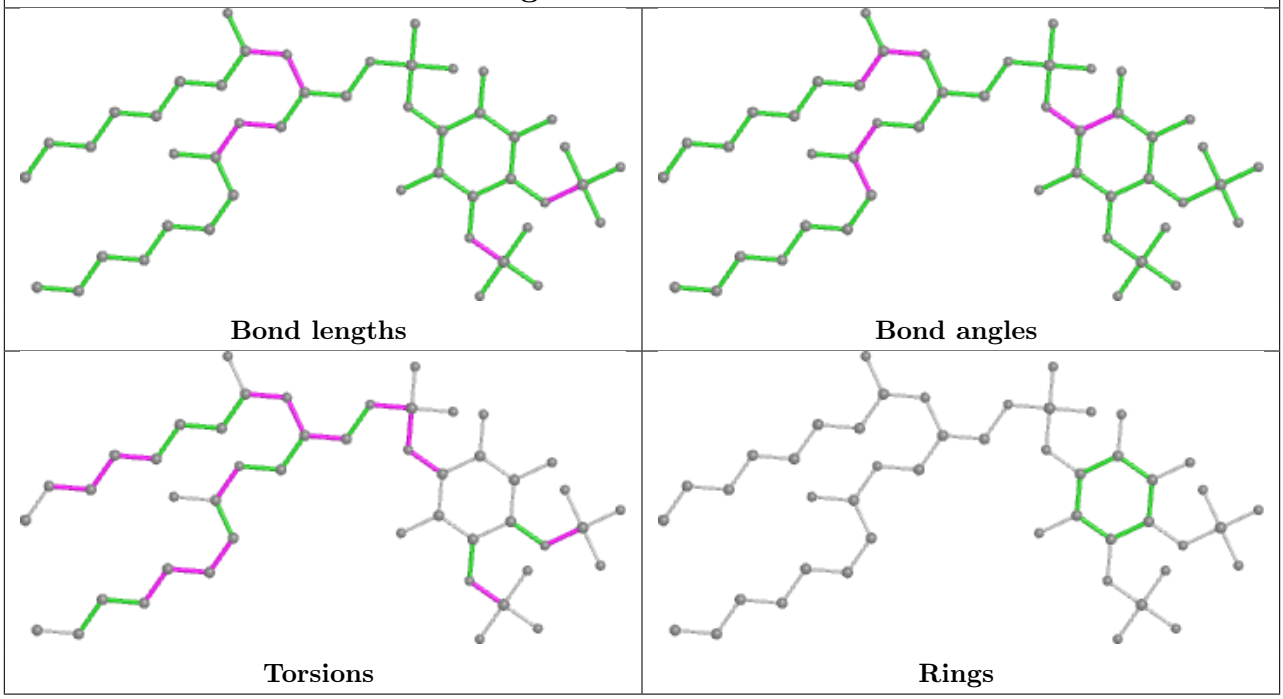


Torsions

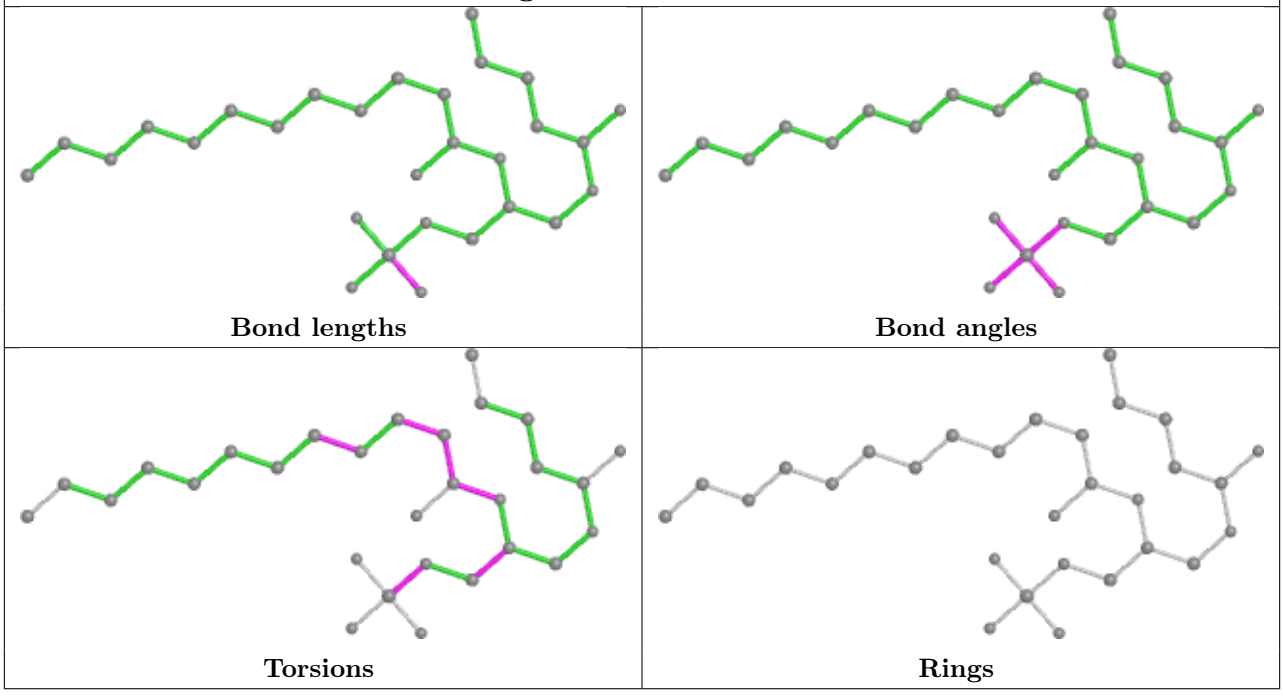


Rings

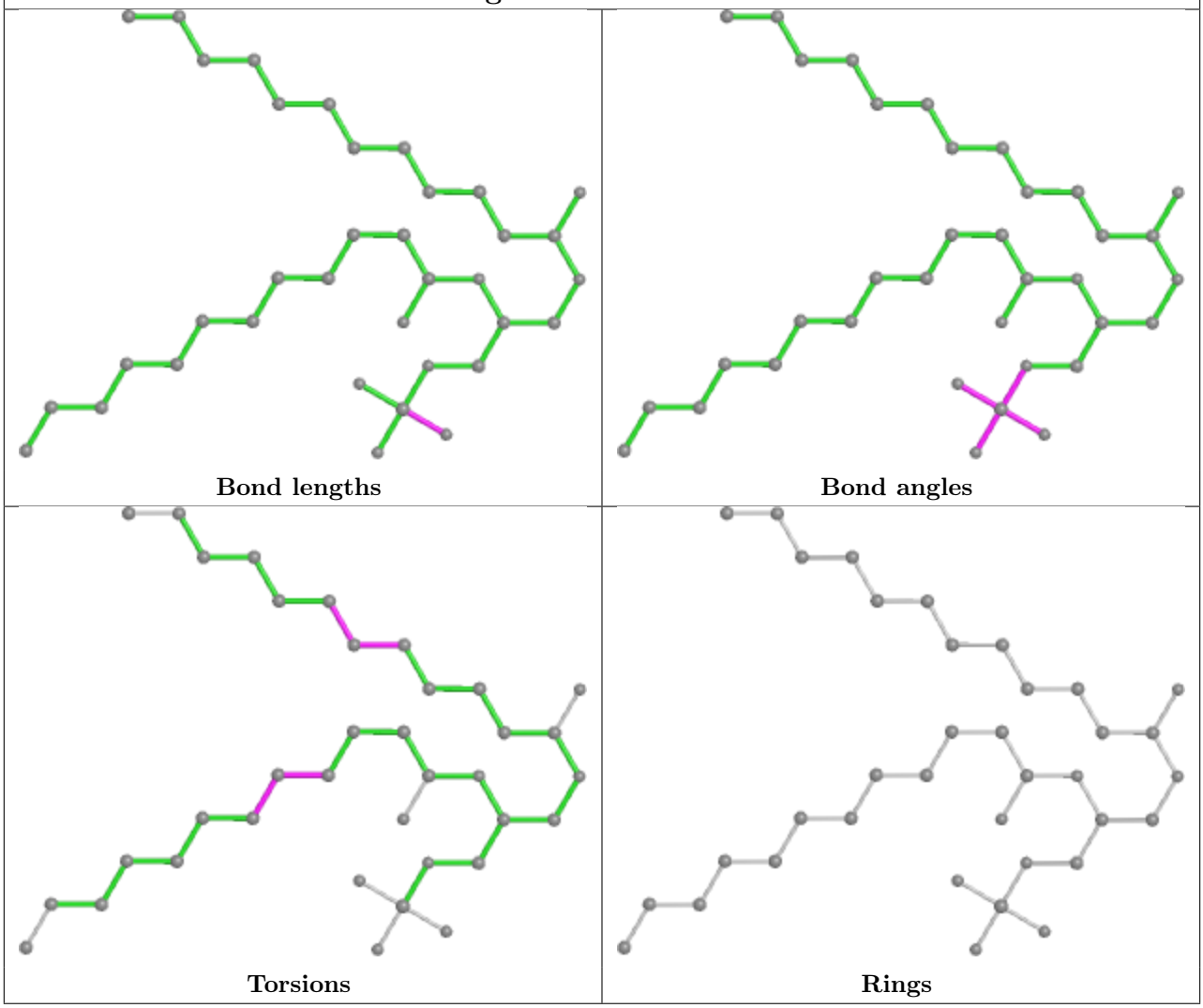
Ligand PIO A 1001



Ligand PLC B 1004



Ligand PLC B 1003



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

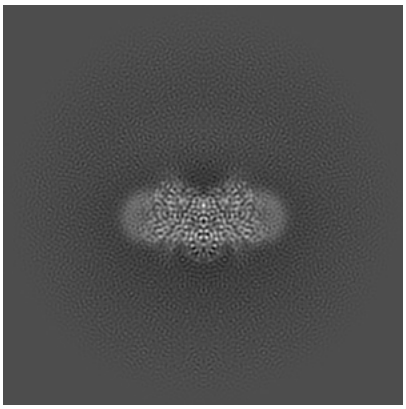
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41020. These allow visual inspection of the internal detail of the map and identification of artifacts.

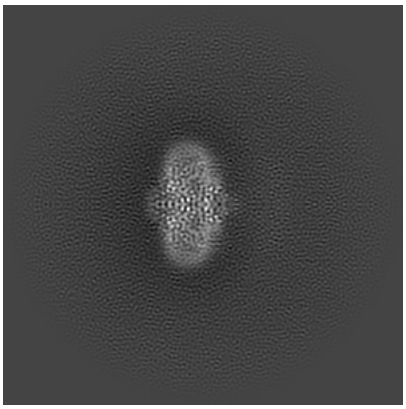
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

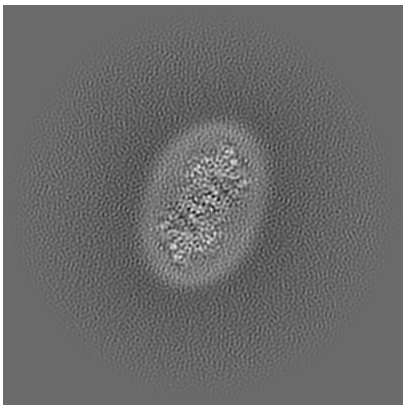
6.1.1 Primary map



X

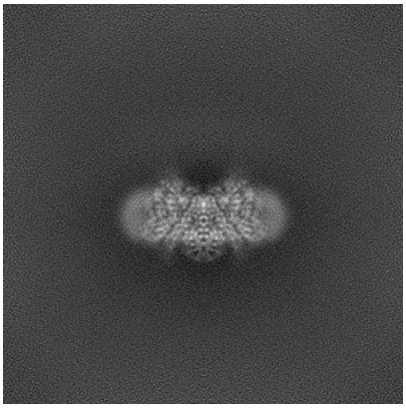


Y

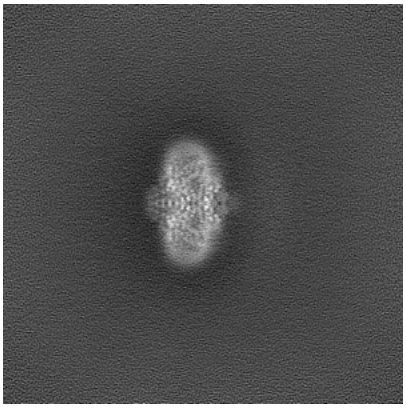


Z

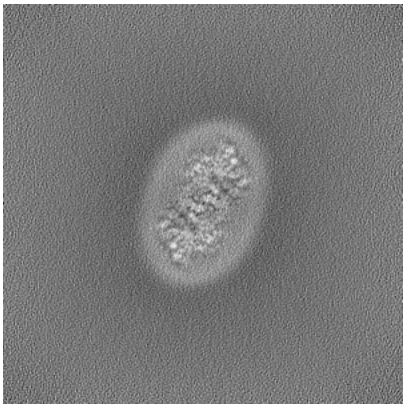
6.1.2 Raw map



X



Y

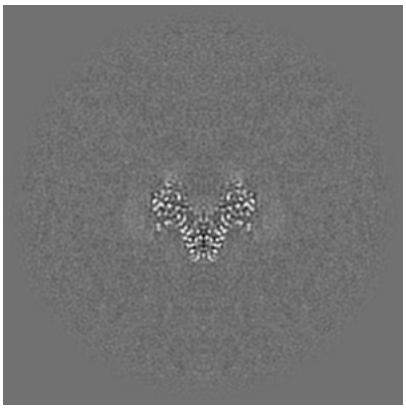


Z

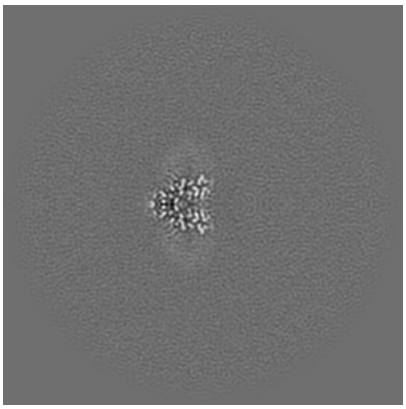
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

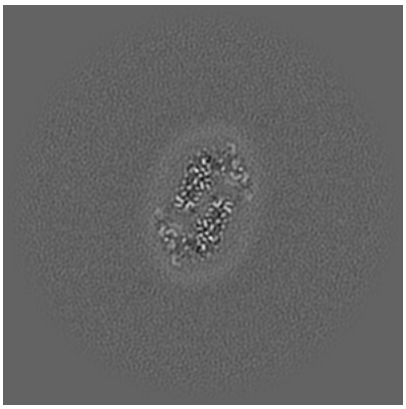
6.2.1 Primary map



X Index: 150

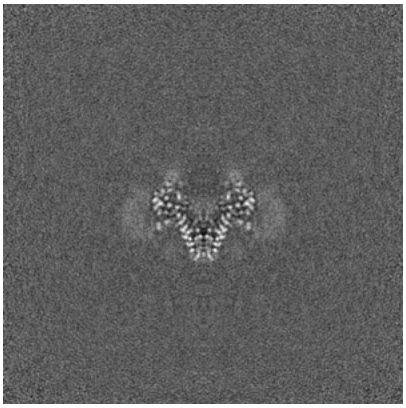


Y Index: 150

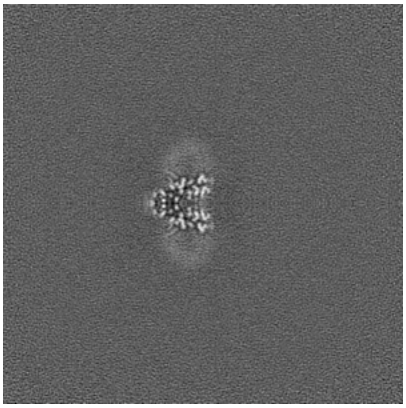


Z Index: 150

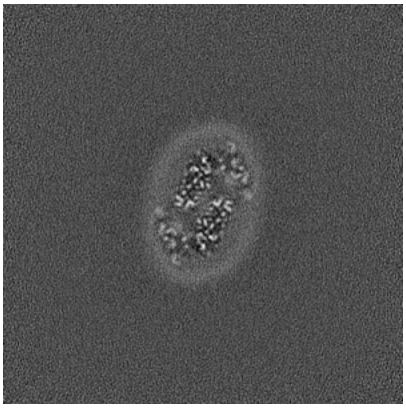
6.2.2 Raw map



X Index: 150



Y Index: 150

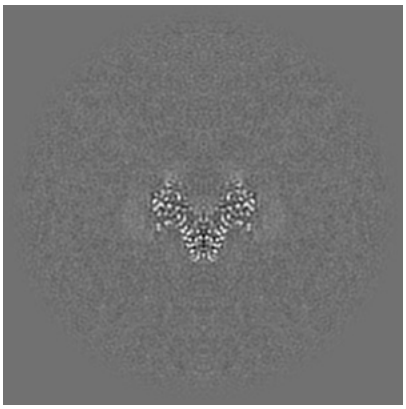


Z Index: 150

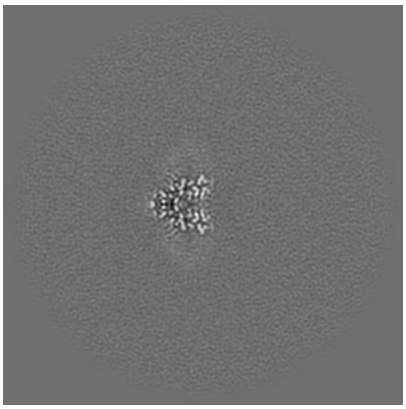
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

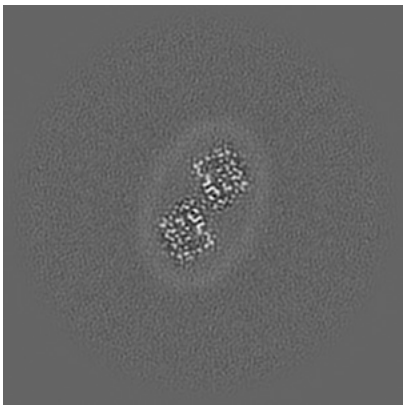
6.3.1 Primary map



X Index: 150

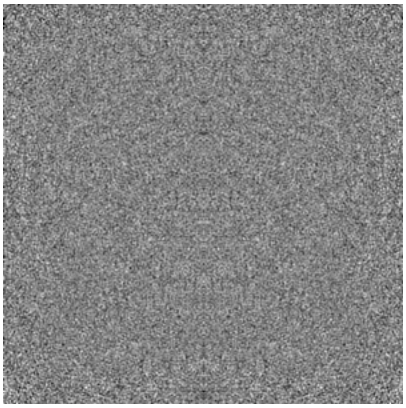


Y Index: 150

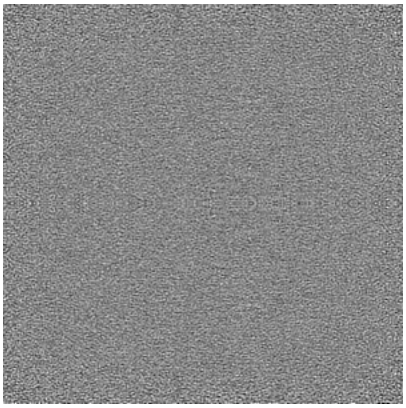


Z Index: 138

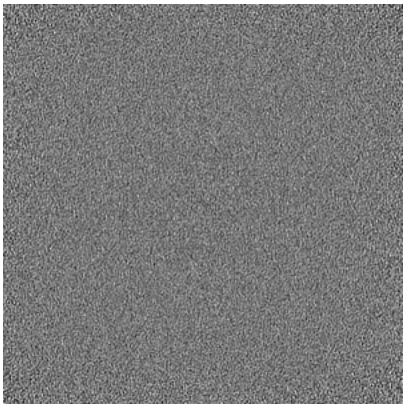
6.3.2 Raw map



X Index: 0



Y Index: 0

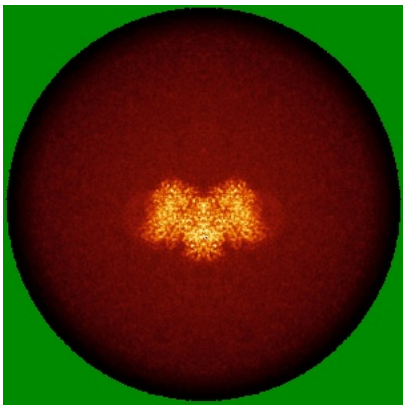


Z Index: 0

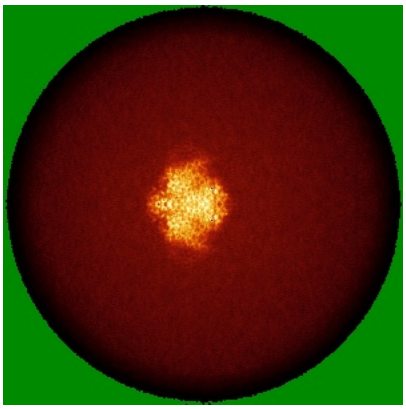
The images above show the largest variance slices of the map in three orthogonal directions.

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

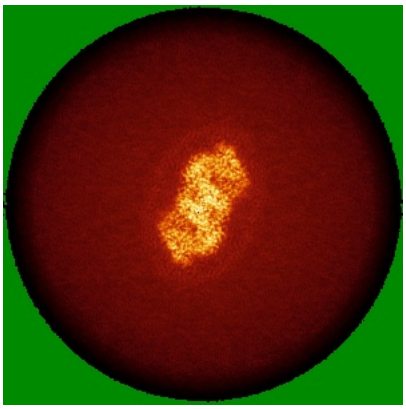
6.4.1 Primary map



X

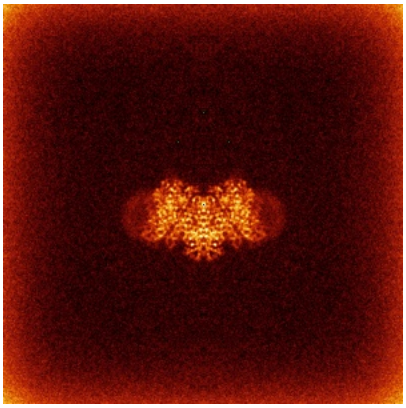


Y

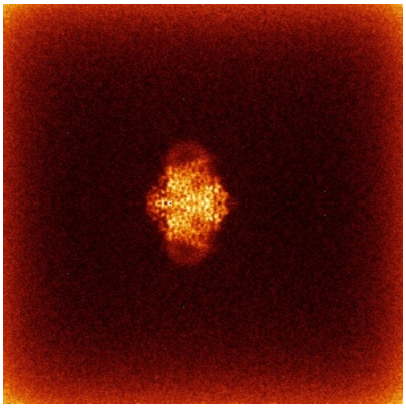


Z

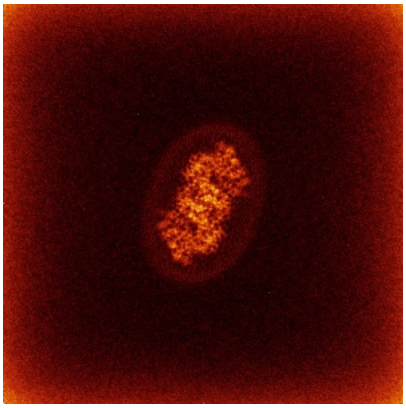
6.4.2 Raw map



X



Y

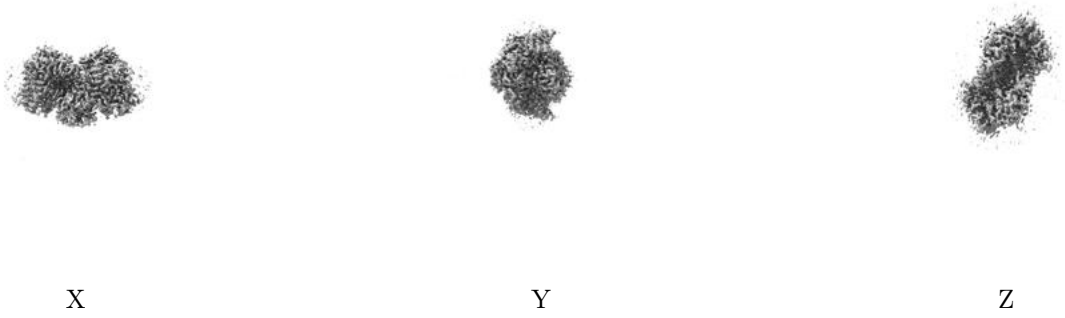


Z

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)

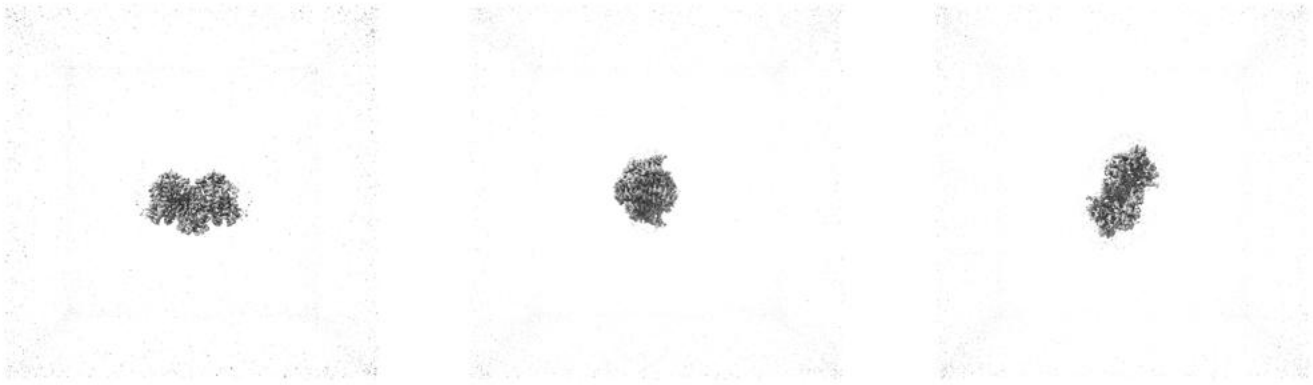
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

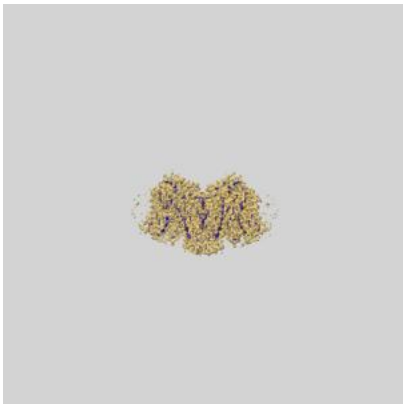
6.6 Mask visualisation (i)

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

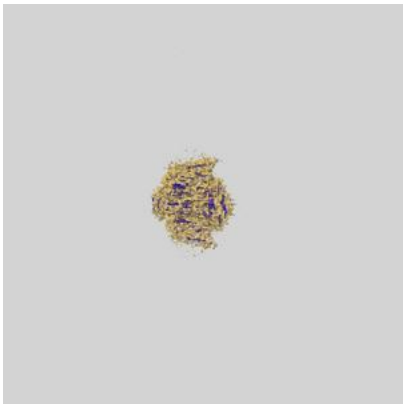
A mask typically either:

- 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_41020_msk_1.map (i)



X



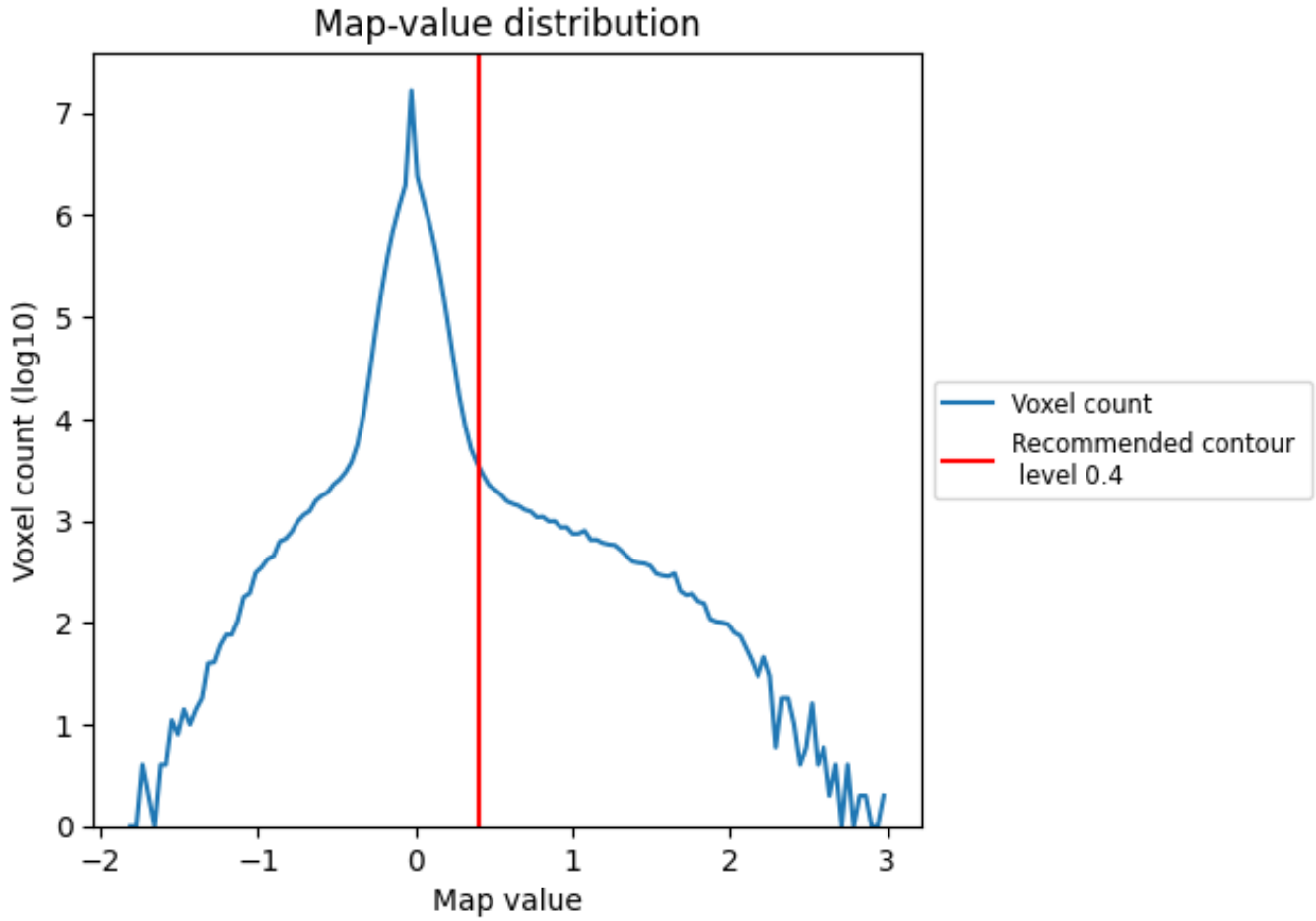
Y

Z

7 Map analysis

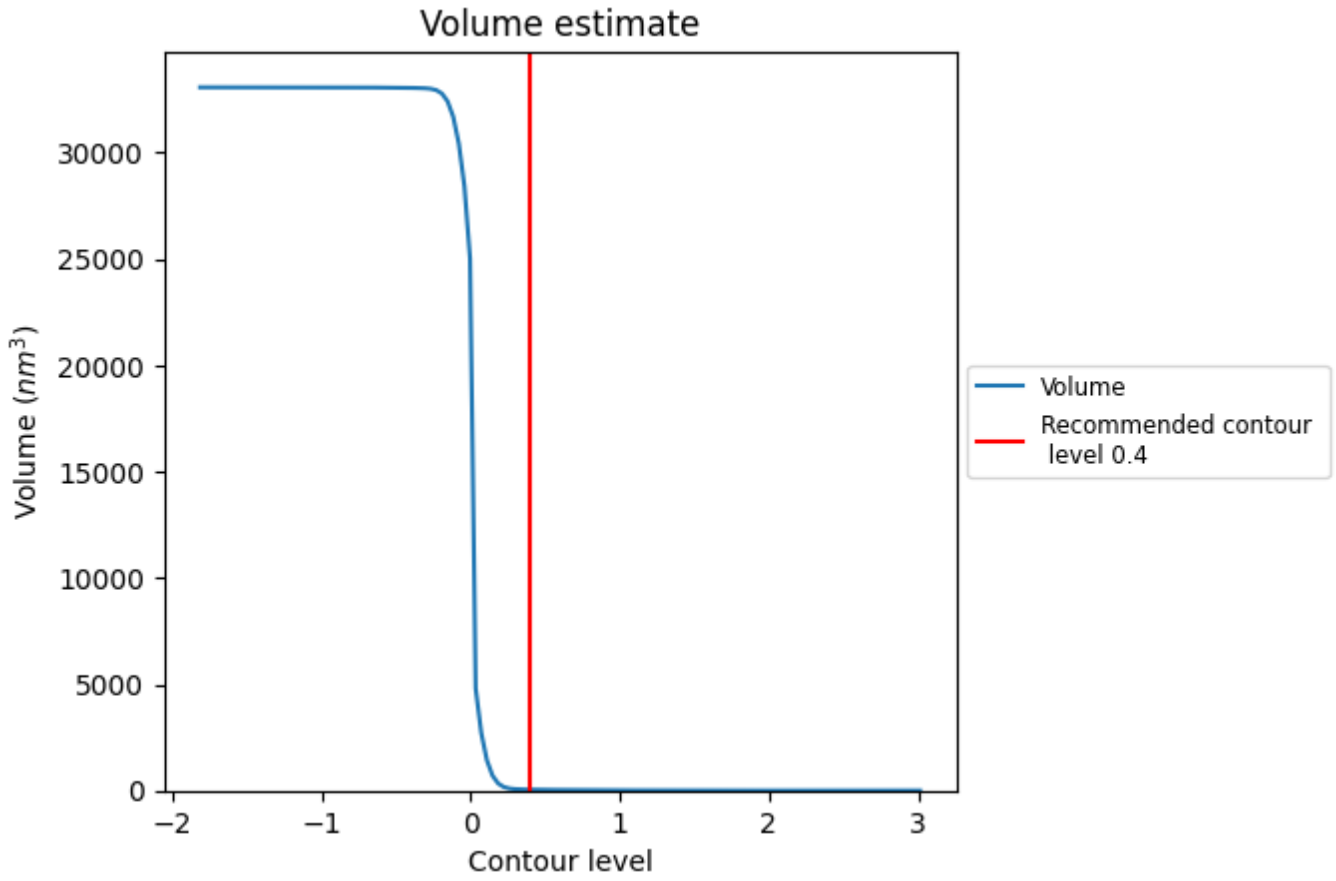
This section contains the results of statistical analysis of the map.

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.

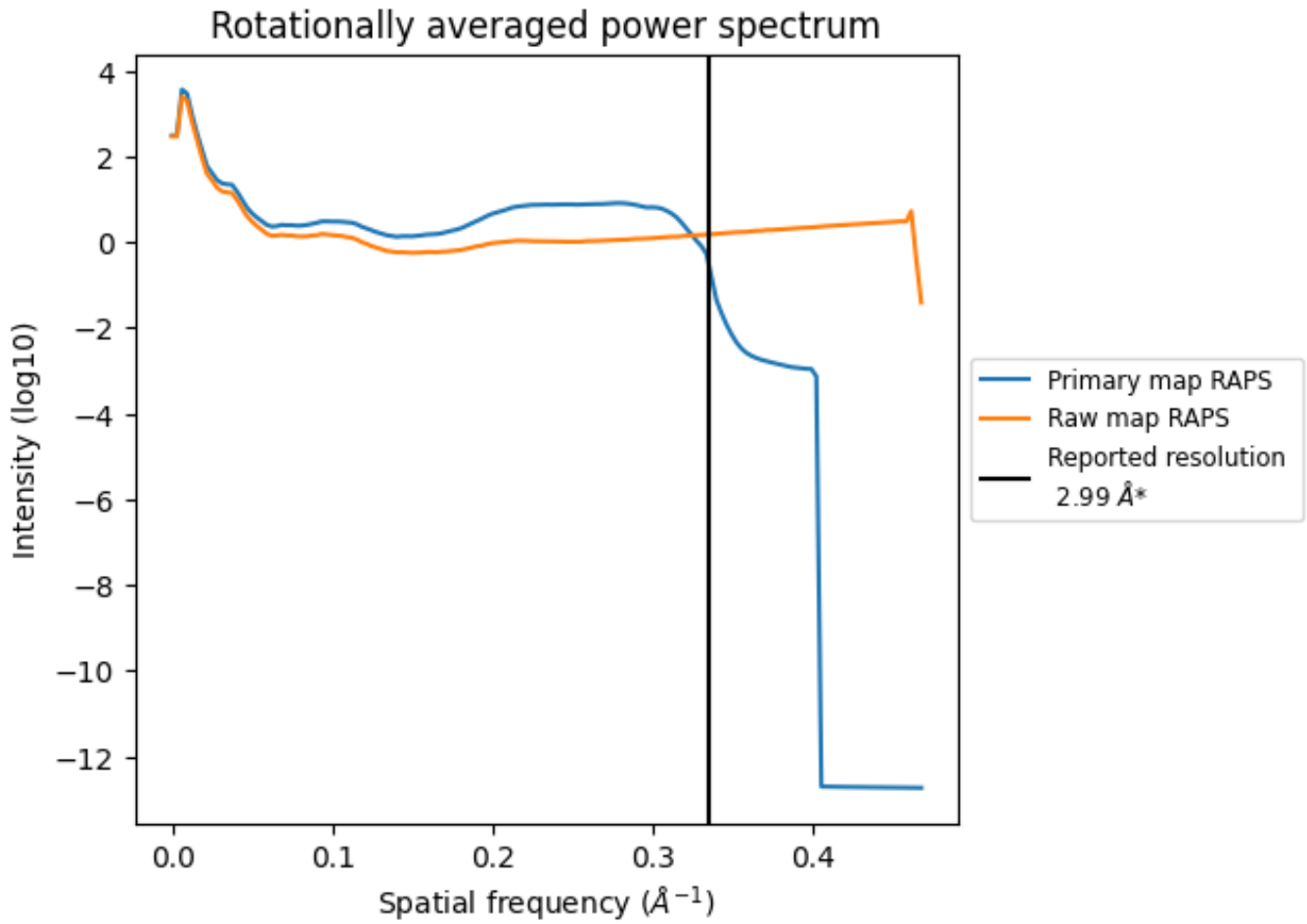
7.2 Volume estimate (i)



The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 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)

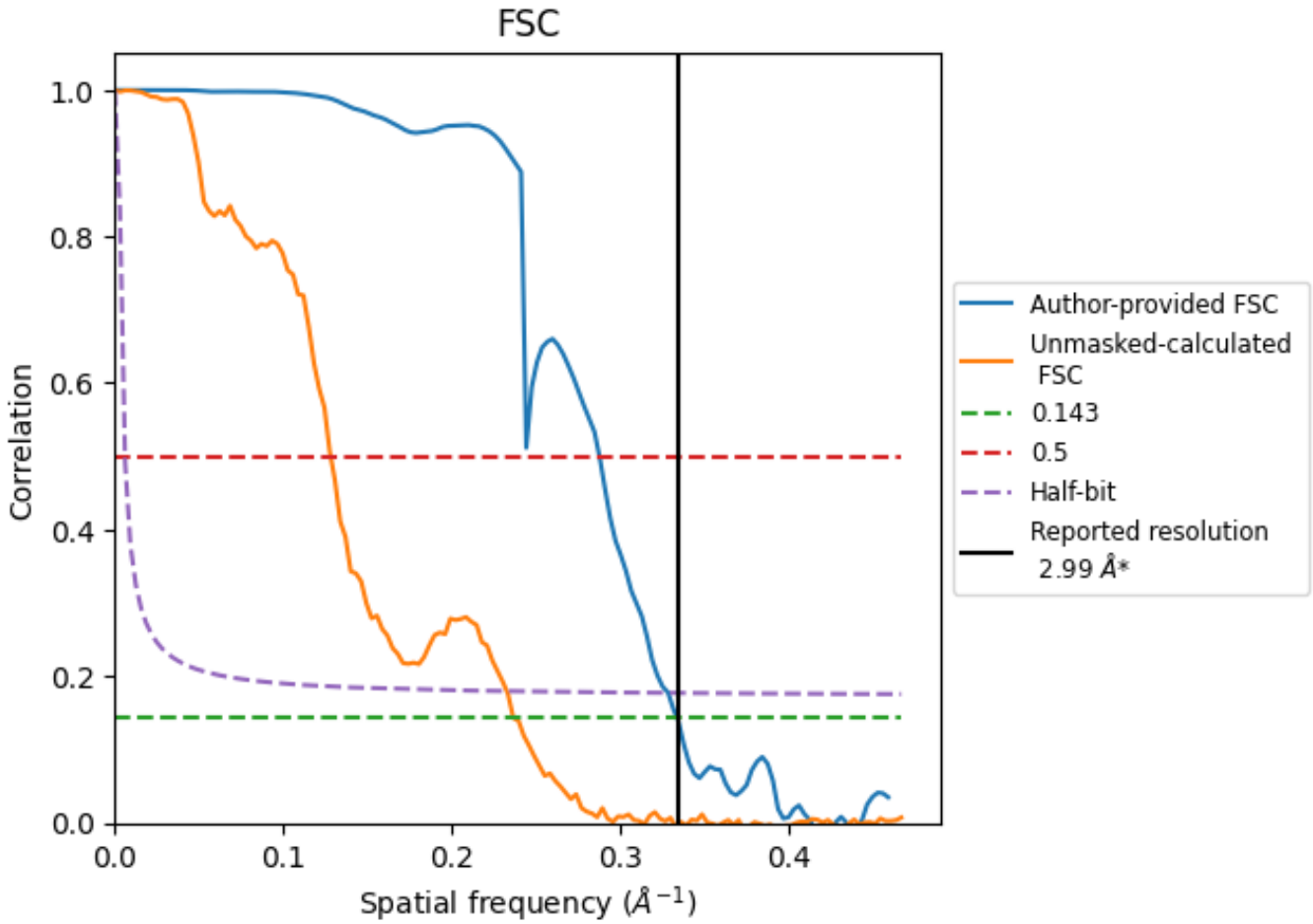


*Reported resolution corresponds to spatial frequency of 0.334 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.334 Å^{-1}

8.2 Resolution estimates (i)

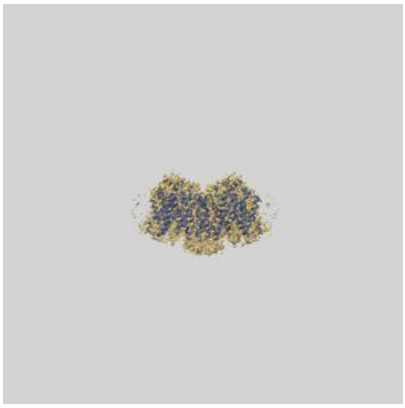
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.47	3.04
Unmasked-calculated*	4.22	7.79	4.29

*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 4.22 differs from the reported value 2.99 by more than 10 %

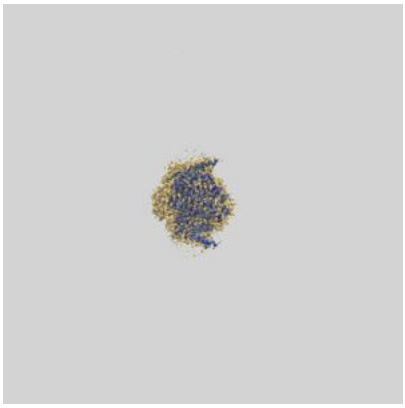
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41020 and PDB model 8T45. Per-residue inclusion information can be found in section 3 on page 6.

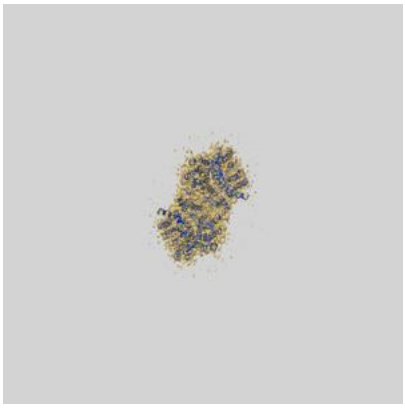
9.1 Map-model overlay



X



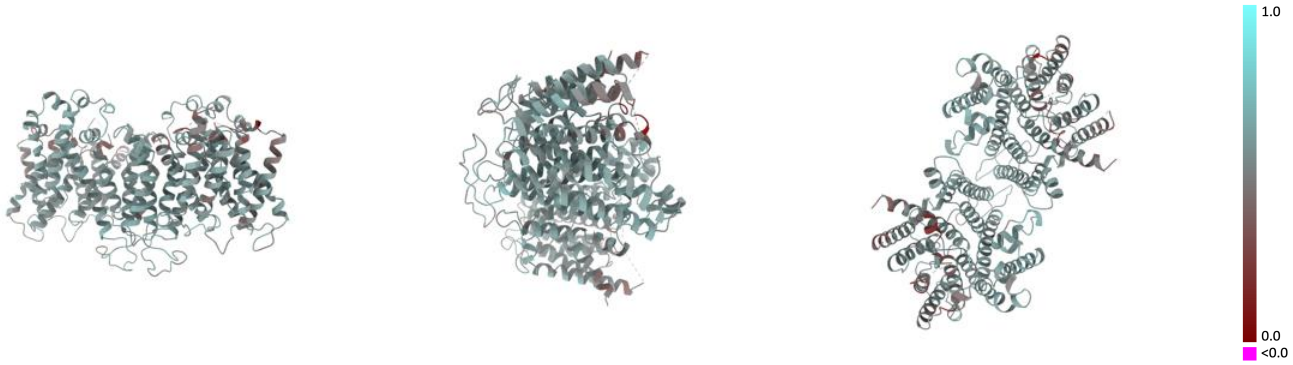
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

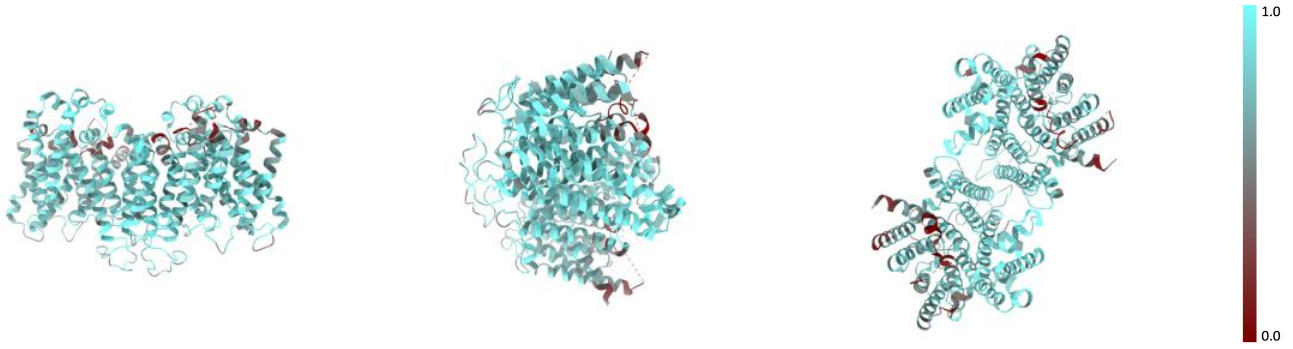
9.2 Q-score mapped to coordinate model



X Y Z

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

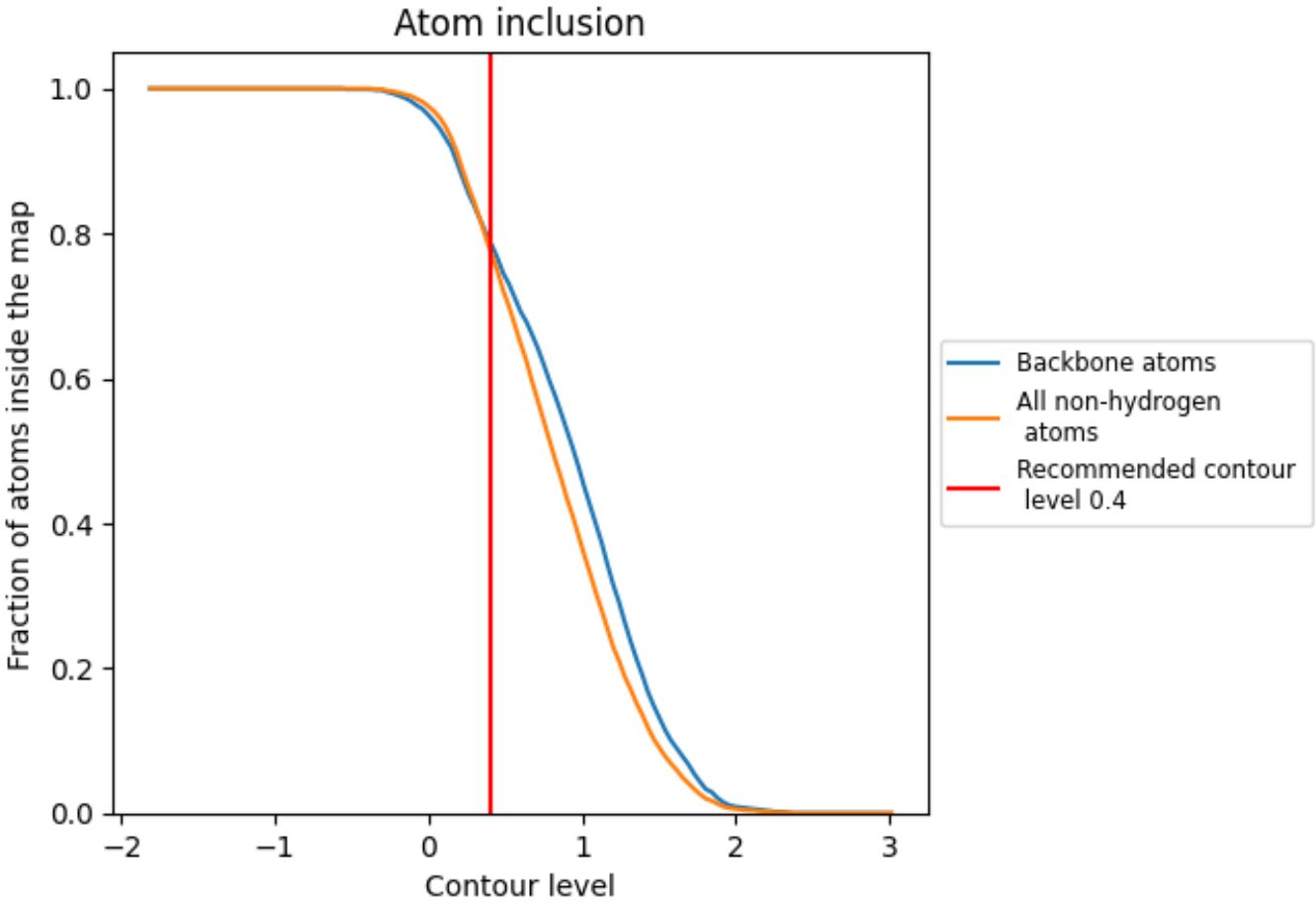
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.5460
A	0.7730	0.5450
B	0.7810	0.5460