wwPDB EM Validation Summary Report (i)

Nov 23, 2022 – 04:07 AM JST

PDB ID	:	7FD9
EMDB ID	:	EMD-31537
Title	:	Thermostabilised full length human mGluR5-5M with orthosteric antagonist, LY341495
Authors	:	Vinothkumar, K.R.; Cannone, G.; Lebon, G.
Deposited on	:	2021-07-16
Resolution	:	4.00 Å(reported)
Based on initial models	:	6N52, 7P2L

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:

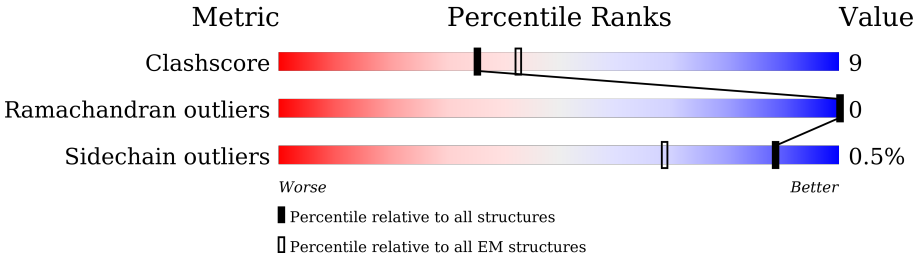
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.00 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	862	7% 72% 16% 11%
1	B	862	7% 72% 17% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11476 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 Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	767	5698	3664	956	1023	55	0	0
1	B	767	5698	3664	956	1023	55	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ASP	-	expression tag	UNP P41594
A	-4	TYR	-	expression tag	UNP P41594
A	-3	LYS	-	expression tag	UNP P41594
A	-2	ASP	-	expression tag	UNP P41594
A	-1	ASP	-	expression tag	UNP P41594
A	0	ASP	-	expression tag	UNP P41594
A	1	ASP	-	expression tag	UNP P41594
A	2	LYS	-	expression tag	UNP P41594
A	3	HIS	-	expression tag	UNP P41594
A	4	HIS	-	expression tag	UNP P41594
A	5	HIS	-	expression tag	UNP P41594
A	6	HIS	-	expression tag	UNP P41594
A	7	HIS	-	expression tag	UNP P41594
A	8	HIS	-	expression tag	UNP P41594
A	9	HIS	-	expression tag	UNP P41594
A	10	HIS	-	expression tag	UNP P41594
A	11	HIS	-	expression tag	UNP P41594
A	12	HIS	-	expression tag	UNP P41594
A	13	LEU	-	expression tag	UNP P41594
A	14	GLU	-	expression tag	UNP P41594
A	15	VAL	-	expression tag	UNP P41594
A	16	LEU	-	expression tag	UNP P41594
A	17	PHE	-	expression tag	UNP P41594
A	18	GLN	-	expression tag	UNP P41594
A	19	GLY	-	expression tag	UNP P41594
A	20	PRO	-	expression tag	UNP P41594

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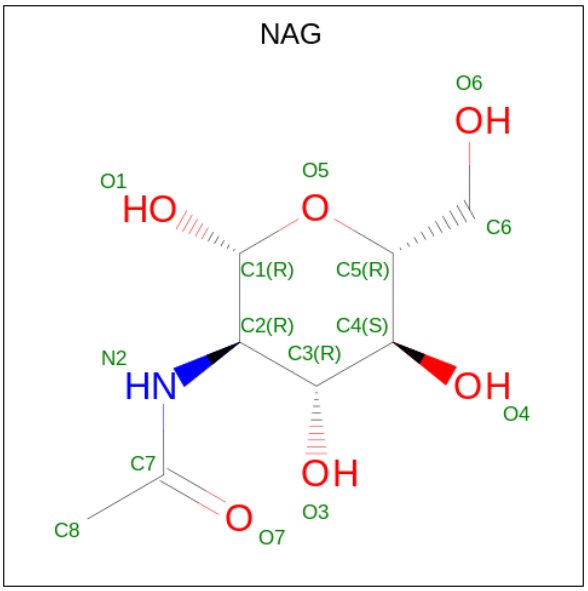
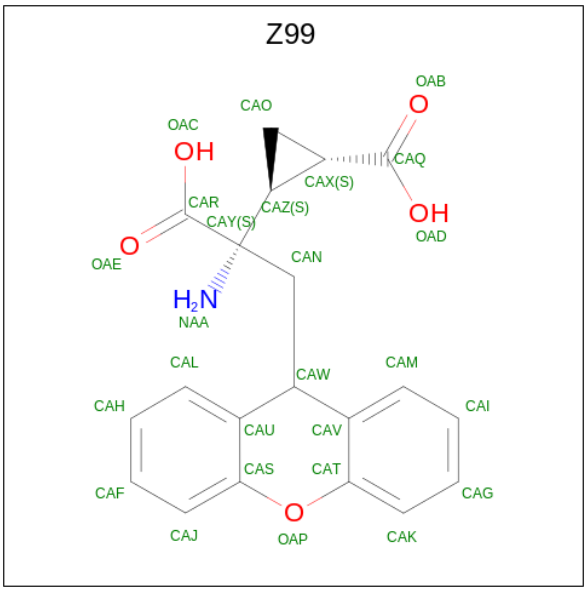
Chain	Residue	Modelled	Actual	Comment	Reference
A	350	LEU	HIS	engineered mutation	UNP P41594
A	445	ALA	ASN	engineered mutation	UNP P41594
A	742	ALA	THR	engineered mutation	UNP P41594
A	753	ALA	SER	engineered mutation	UNP P41594
A	777	ALA	THR	engineered mutation	UNP P41594
A	799	ALA	ILE	engineered mutation	UNP P41594
A	813	LEU	ALA	engineered mutation	UNP P41594
B	-5	ASP	-	expression tag	UNP P41594
B	-4	TYR	-	expression tag	UNP P41594
B	-3	LYS	-	expression tag	UNP P41594
B	-2	ASP	-	expression tag	UNP P41594
B	-1	ASP	-	expression tag	UNP P41594
B	0	ASP	-	expression tag	UNP P41594
B	1	ASP	-	expression tag	UNP P41594
B	2	LYS	-	expression tag	UNP P41594
B	3	HIS	-	expression tag	UNP P41594
B	4	HIS	-	expression tag	UNP P41594
B	5	HIS	-	expression tag	UNP P41594
B	6	HIS	-	expression tag	UNP P41594
B	7	HIS	-	expression tag	UNP P41594
B	8	HIS	-	expression tag	UNP P41594
B	9	HIS	-	expression tag	UNP P41594
B	10	HIS	-	expression tag	UNP P41594
B	11	HIS	-	expression tag	UNP P41594
B	12	HIS	-	expression tag	UNP P41594
B	13	LEU	-	expression tag	UNP P41594
B	14	GLU	-	expression tag	UNP P41594
B	15	VAL	-	expression tag	UNP P41594
B	16	LEU	-	expression tag	UNP P41594
B	17	PHE	-	expression tag	UNP P41594
B	18	GLN	-	expression tag	UNP P41594
B	19	GLY	-	expression tag	UNP P41594
B	20	PRO	-	expression tag	UNP P41594
B	350	LEU	HIS	engineered mutation	UNP P41594
B	445	ALA	ASN	engineered mutation	UNP P41594
B	742	ALA	THR	engineered mutation	UNP P41594
B	753	ALA	SER	engineered mutation	UNP P41594
B	777	ALA	THR	engineered mutation	UNP P41594
B	799	ALA	ILE	engineered mutation	UNP P41594
B	813	LEU	ALA	engineered mutation	UNP P41594

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



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

- Molecule 3 is 2-[(1S,2S)-2-carboxycyclopropyl]-3-(9H-xanthen-9-yl)-D-alanine (three-letter code: Z99) (formula: $C_{20}H_{19}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	26	20	1	5	0

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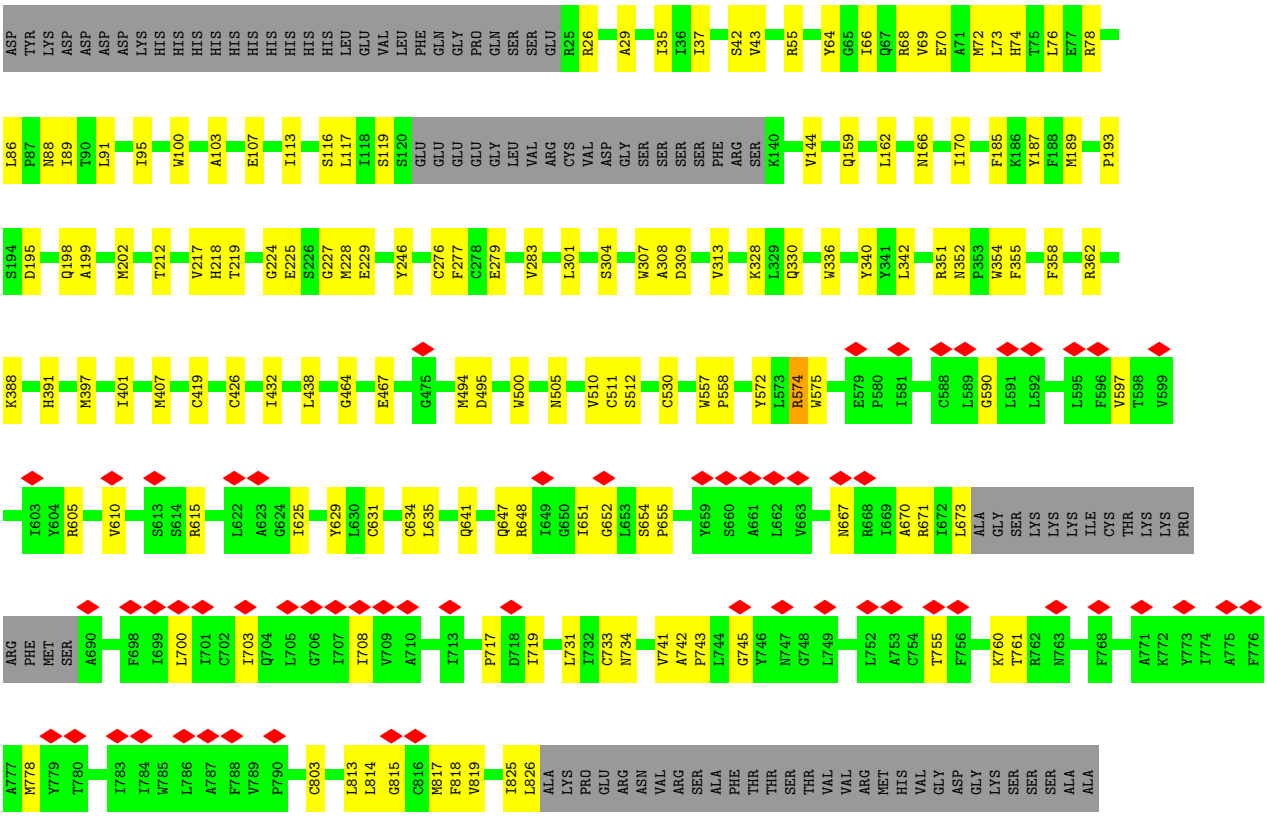
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	26	20	1	5	0

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.

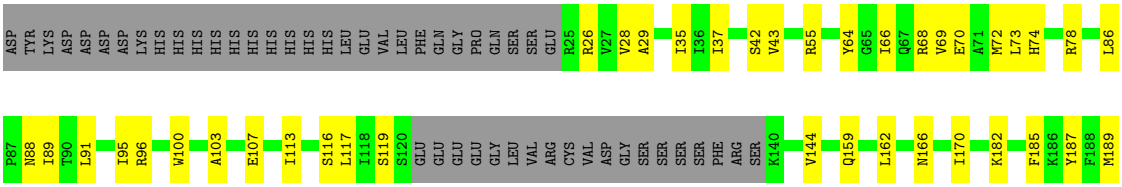
• Molecule 1: Metabotropic glutamate receptor 5

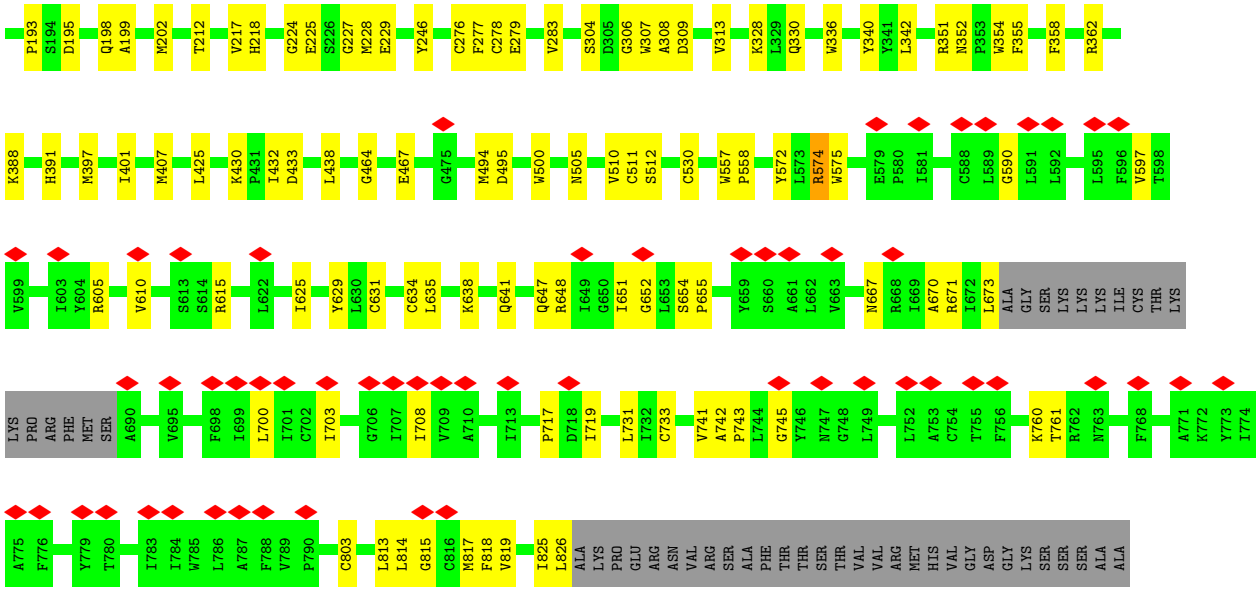
Chain A:



• Molecule 1: Metabotropic glutamate receptor 5

Chain B:




P193 S194 D195 Q198 A199 M202 T212 V217 H218 G224 E225 S226 G227 M228 E229 Y246 C276 F277 C278 E279 V283 S304 D305 G306 W307 A308 D309 V313 K328 L329 Q330 W336 Y340 Y341 L342 R351 N352 P353 W354 F355 F358 R362
K388 H391 M397 I401 M407 L425 K430 P431 I432 D433 L438 G464 E467 G475 M494 D495 W500 N505 V510 C511 S512 C530 W557 P558 Y572 L573 R574 W575 E579 P580 I581 C588 L589 G590 L591 L592 L595 F596 V597 T598
V599 I603 Y604 R605 V610 S613 S614 R615 L622 I625 Y629 I630 C631 C634 L635 K638 Q641 Q647 R648 I649 G650 I651 G652 I653 S654 P655 Y659 S660 A661 L662 V663 N667 R668 I669 A670 R671 I672 L673 ALA GLY SER LYS LYS LYS ILE CYS THR LYS
LYS PRO ARG PHE MET SER A690 V695 F698 I699 L700 I701 C702 I703 G706 I707 I708 V709 A710 I713 P717 D718 I719 L731 I732 C733 V741 A742 P743 L744 G745 Y746 N747 G748 L749 L752 A753 C754 T755 F756 K760 T761 R762 M763 F768 A771 K772 Y773 I774
A775 F776 Y779 T780 I783 I784 W785 L786 A787 F788 V789 P790 C803 L813 L814 G815 C816 M817 F818 V819 I825 L826 ALA LYS PRO GLU ARG ASN VAL ARG SER ALA PHE THR THR SER THR VAL VAL ARG MET HIS VAL GLY ASP GLY LYS SER SER SER ALA ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	142191	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 ($e^-/Å^2$)	49.9	Depositor
Minimum defocus (nm)	1200.0	Depositor
Maximum defocus (nm)	2800.0	Depositor
Magnification	44500	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0095	Depositor
Map size (Å)	267.0, 267.0, 267.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89, 0.89, 0.89	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: NAG, Z99

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	0.26	0/5828	0.53	0/7939
1	B	0.26	0/5828	0.53	0/7939
All	All	0.26	0/11656	0.53	0/15878

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	5698	0	5389	95	0
1	B	5698	0	5389	98	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
All	All	11476	0	10836	191	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 9.

The worst 5 of 191 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:A:69:VAL:HG23	1:A:95:ILE:HG13	1.64	0.79
1:B:69:VAL:HG23	1:B:95:ILE:HG13	1.64	0.78
1:B:166:ASN:HA	1:B:187:TYR:CE2	2.24	0.73
1:A:166:ASN:HA	1:A:187:TYR:CE2	2.24	0.72
1:B:66:ILE:HA	1:B:69:VAL:HG12	1.73	0.71

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	761/862 (88%)	713 (94%)	48 (6%)	0	100	100
1	B	761/862 (88%)	712 (94%)	49 (6%)	0	100	100
All	All	1522/1724 (88%)	1425 (94%)	97 (6%)	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	566/748 (76%)	563 (100%)	3 (0%)	88	93
1	B	566/748 (76%)	563 (100%)	3 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1132/1496 (76%)	1126 (100%)	6 (0%)	89 93

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88	ASN
1	B	362	ARG
1	B	574	ARG
1	A	362	ARG
1	A	88	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

4 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	Z99	B	902	-	26,29,29	1.92	7 (26%)	36,44,44	3.48	19 (52%)
2	NAG	B	901	1	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
3	Z99	A	902	-	26,29,29	1.93	7 (26%)	36,44,44	3.48	19 (52%)
2	NAG	A	901	1	14,14,15	0.68	0	17,19,21	1.01	1 (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	Z99	B	902	-	-	4/15/38/38	0/4/4/4
2	NAG	B	901	1	-	2/6/23/26	0/1/1/1
3	Z99	A	902	-	-	4/15/38/38	0/4/4/4
2	NAG	A	901	1	-	2/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	Z99	CAS-CAU	4.44	1.48	1.39
3	B	902	Z99	CAS-CAU	4.41	1.48	1.39
3	A	902	Z99	CAT-CAV	4.28	1.48	1.39
3	B	902	Z99	CAT-CAV	4.25	1.48	1.39
3	A	902	Z99	CAU-CAW	-4.20	1.45	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	902	Z99	CAY-CAN-CAW	9.05	131.39	117.06
3	A	902	Z99	CAY-CAN-CAW	9.02	131.35	117.06
3	A	902	Z99	CAT-CAV-CAW	-8.94	106.06	119.99
3	B	902	Z99	CAT-CAV-CAW	-8.90	106.11	119.99
3	A	902	Z99	CAS-CAU-CAW	-8.01	107.50	119.99

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	Z99	CAY-CAN-CAW-CAV
3	A	902	Z99	CAW-CAN-CAY-CAR

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Mol	Chain	Res	Type	Atoms
3	A	902	Z99	CAR-CAY-CAZ-CAO
3	B	902	Z99	CAY-CAN-CAW-CAV
3	B	902	Z99	CAW-CAN-CAY-CAR

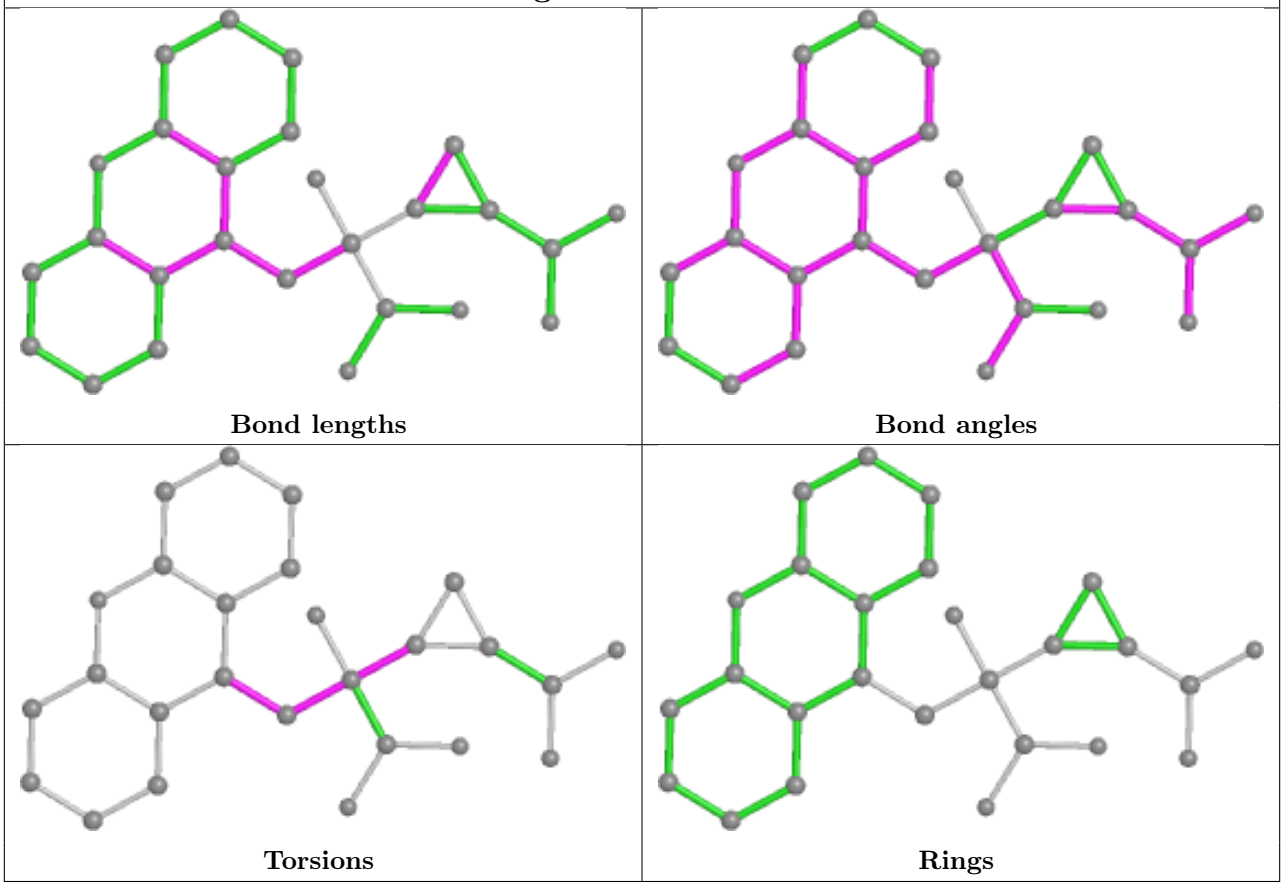
There are no ring outliers.

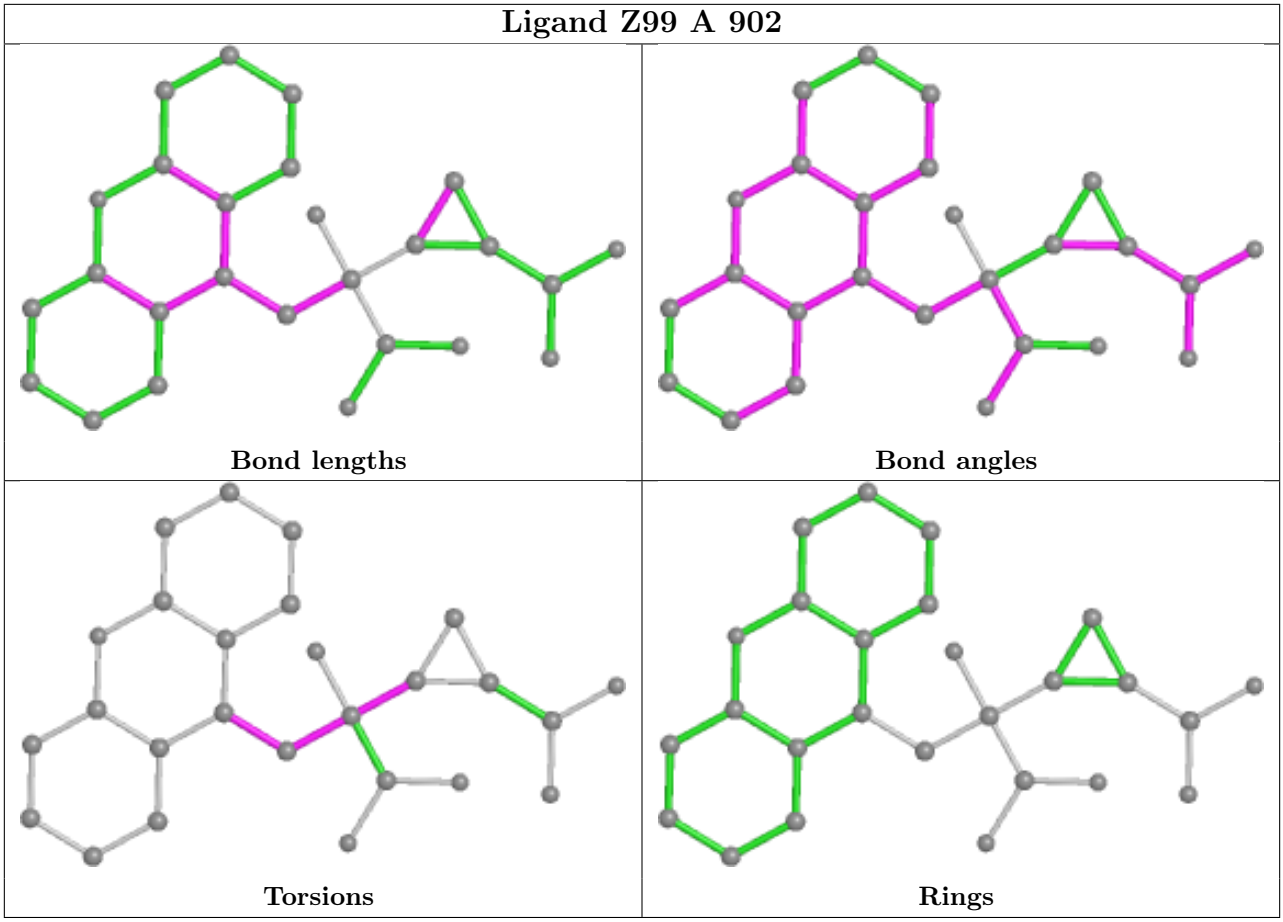
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	Z99	1	0
3	A	902	Z99	1	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 Z99 B 902





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.

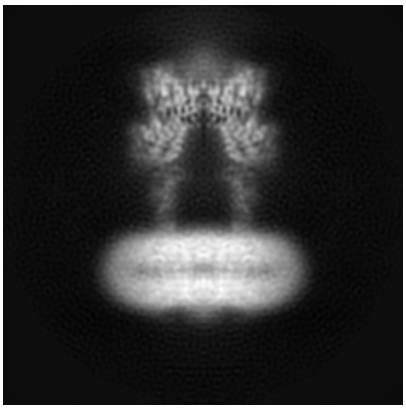
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31537. These allow visual inspection of the internal detail of the map and identification of artifacts.

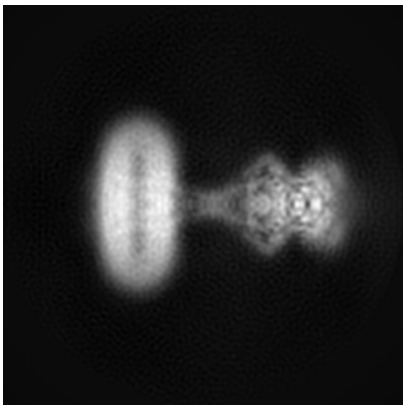
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

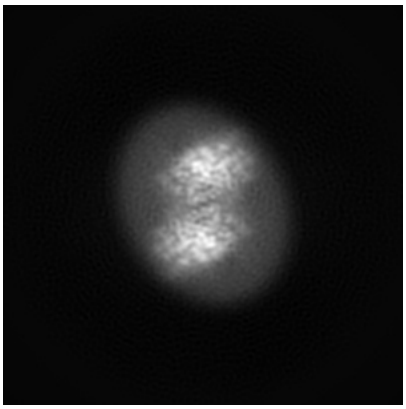
6.1.1 Primary map



X

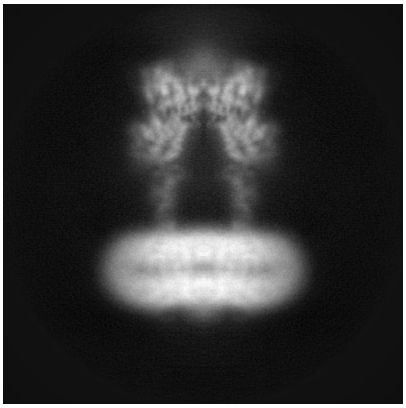


Y

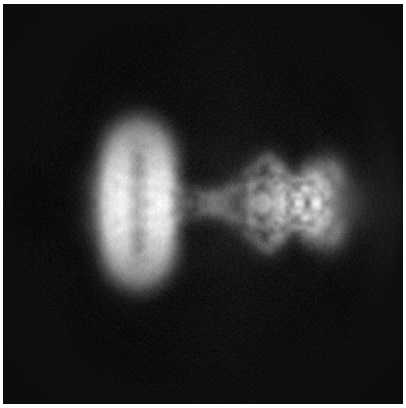


Z

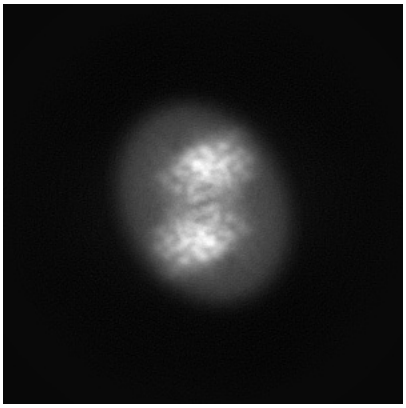
6.1.2 Raw map



X



Y

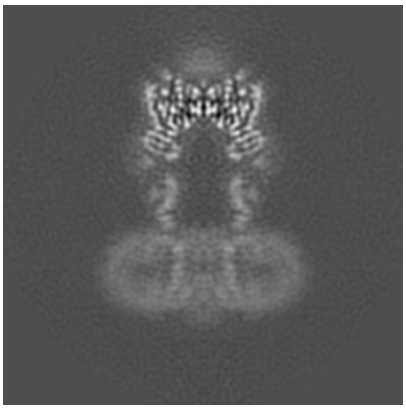


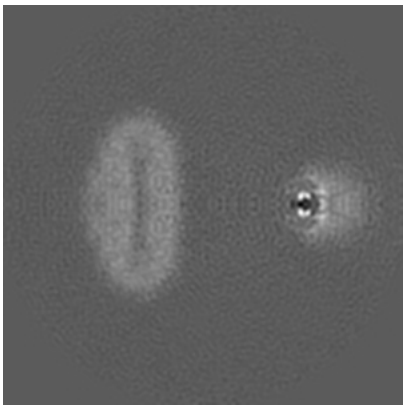
Z

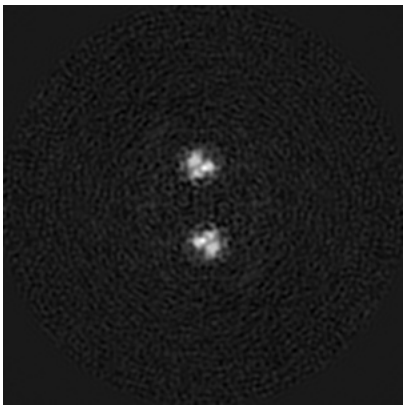
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

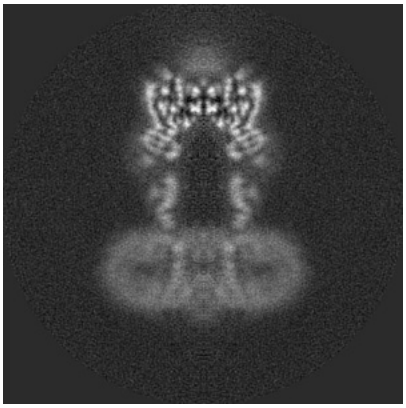
6.2.1 Primary map

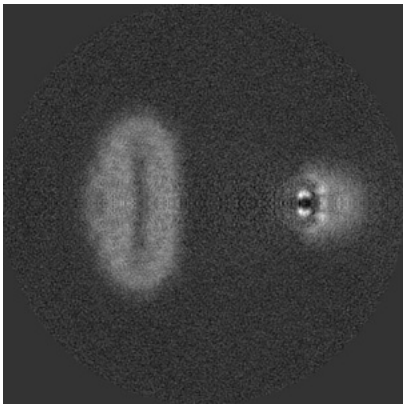

X Index: 150

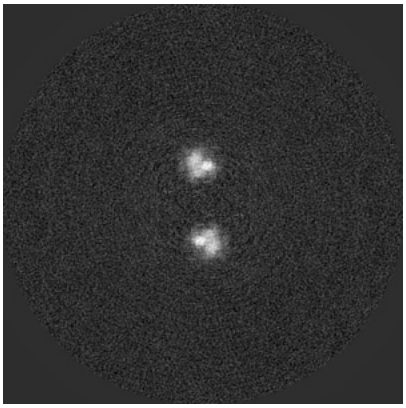

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

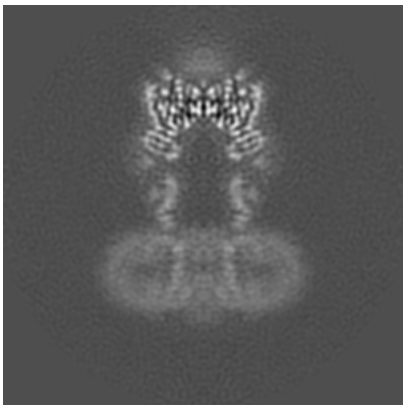

Y Index: 150

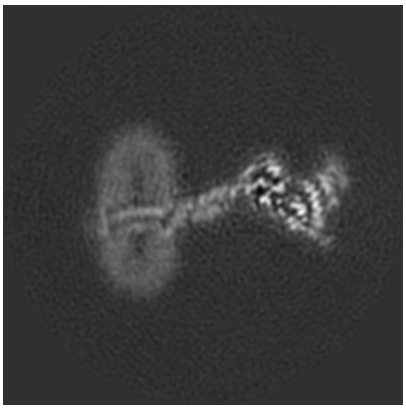

Z Index: 150

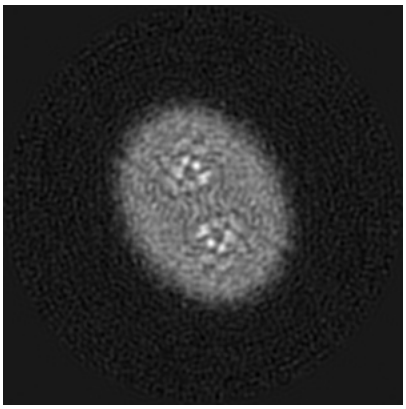
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

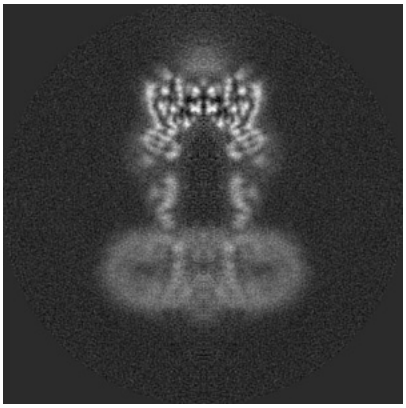
6.3.1 Primary map

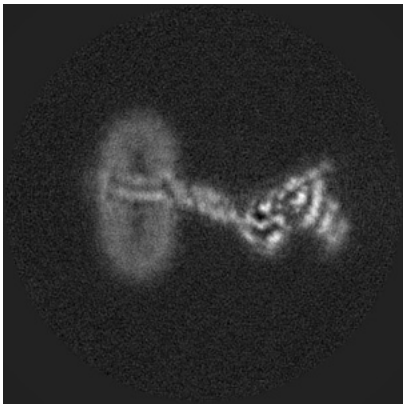

X Index: 150

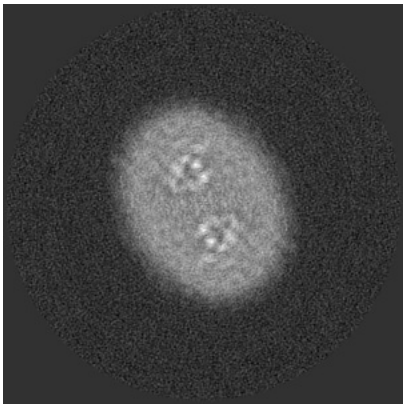

Y Index: 179


Z Index: 116

6.3.2 Raw map


X Index: 150

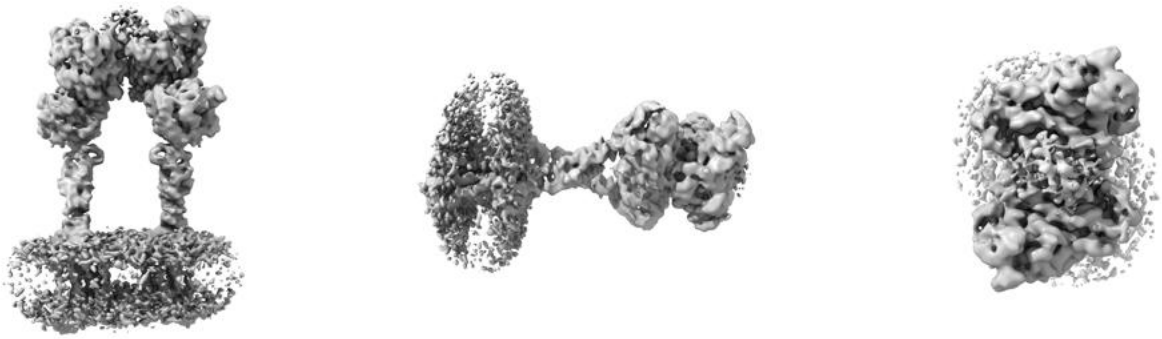

Y Index: 121


Z Index: 117

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

6.4 Orthogonal surface views (i)

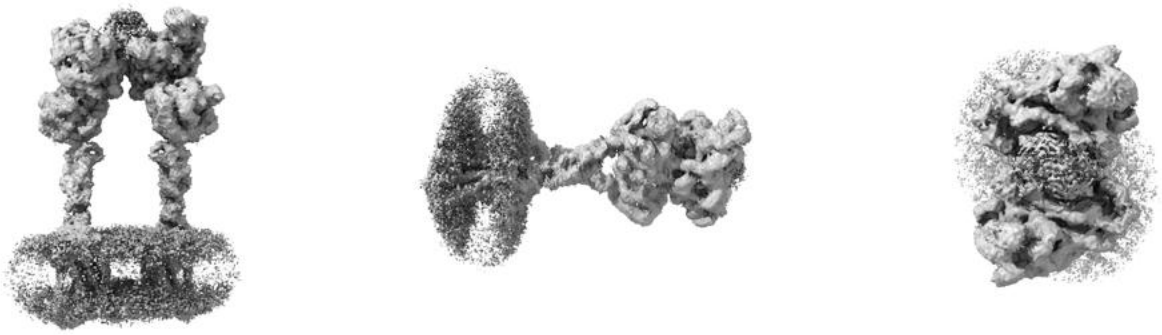
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0095. 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.

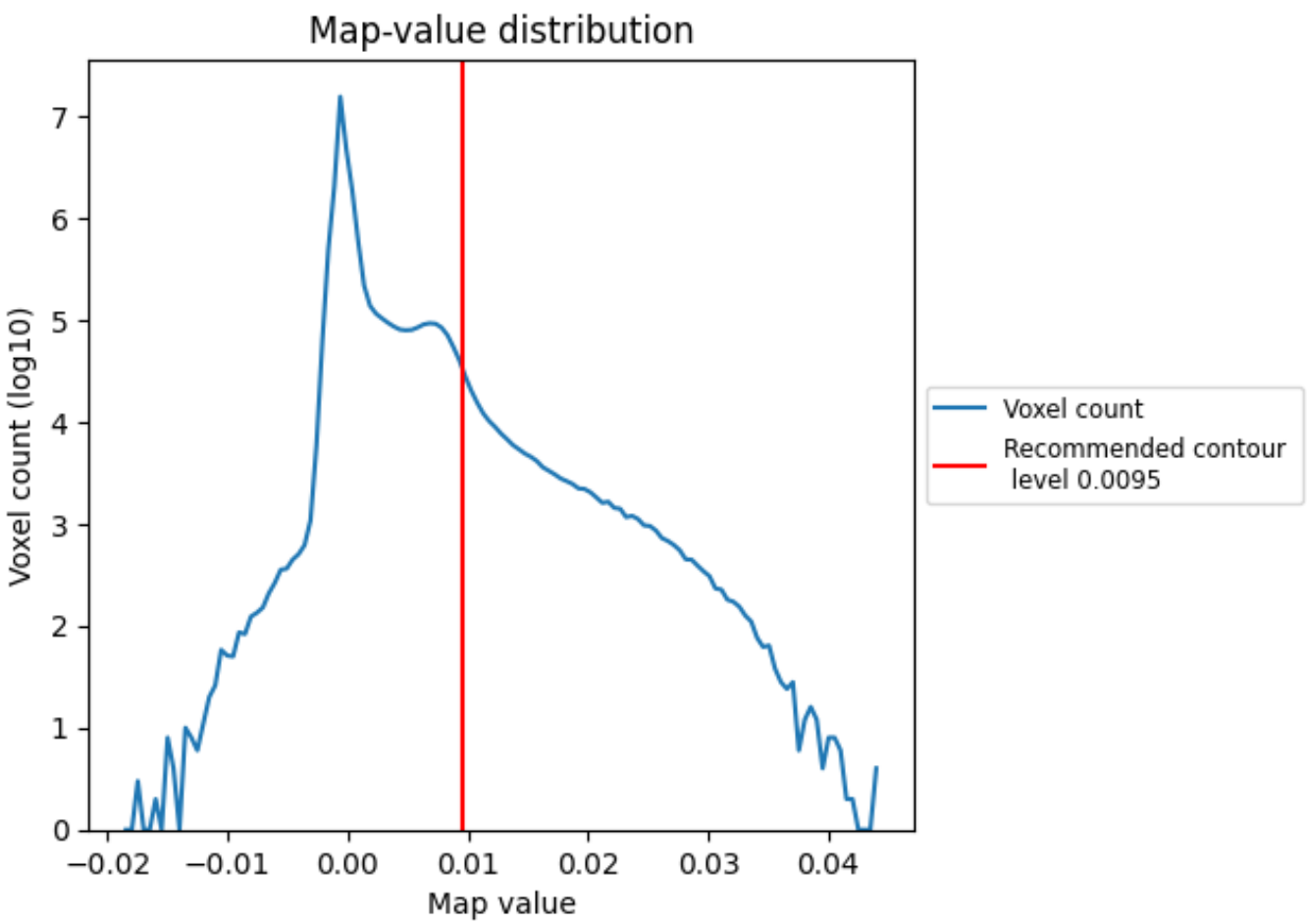
6.5 Mask visualisation (i)

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

7 Map analysis (i)

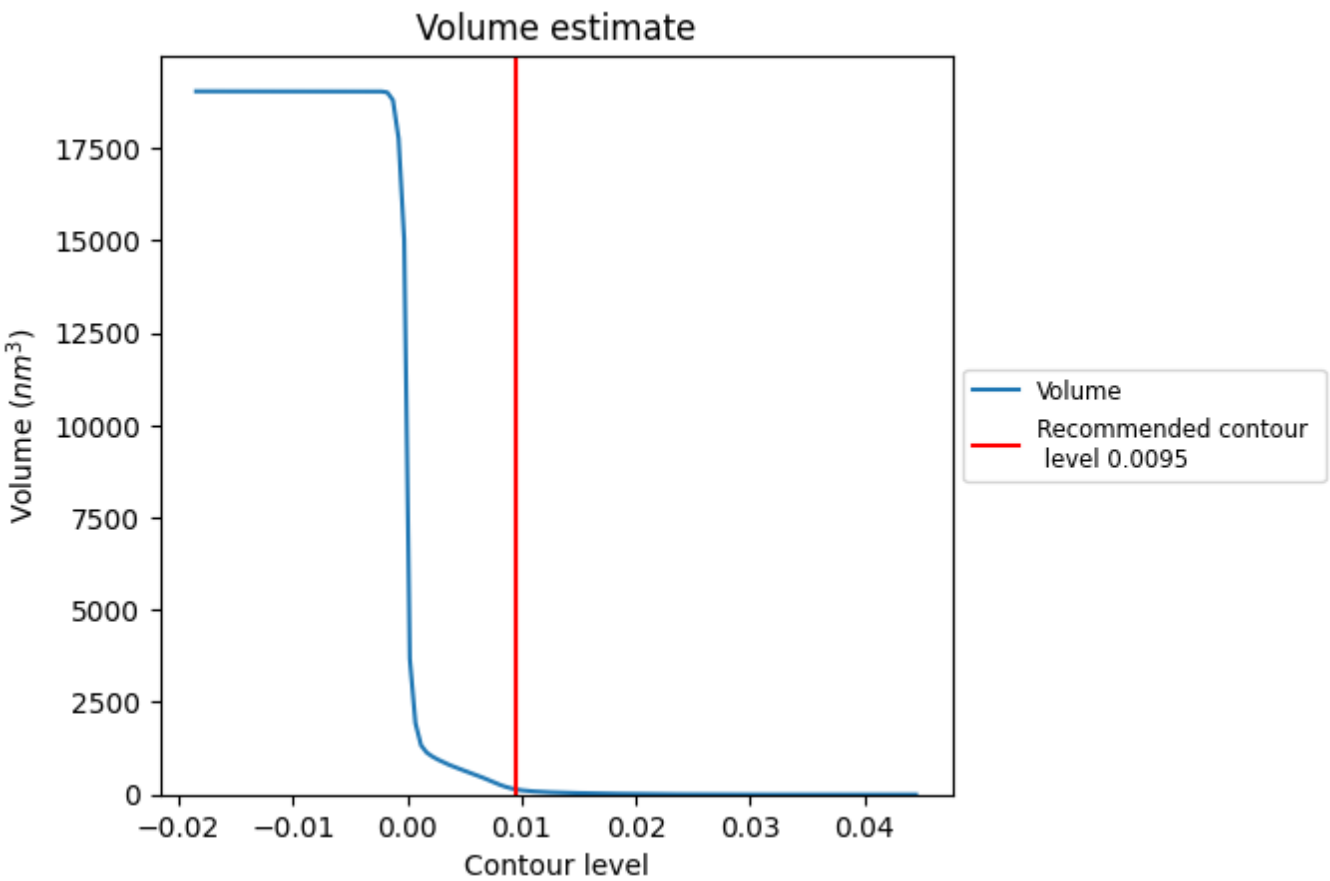
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

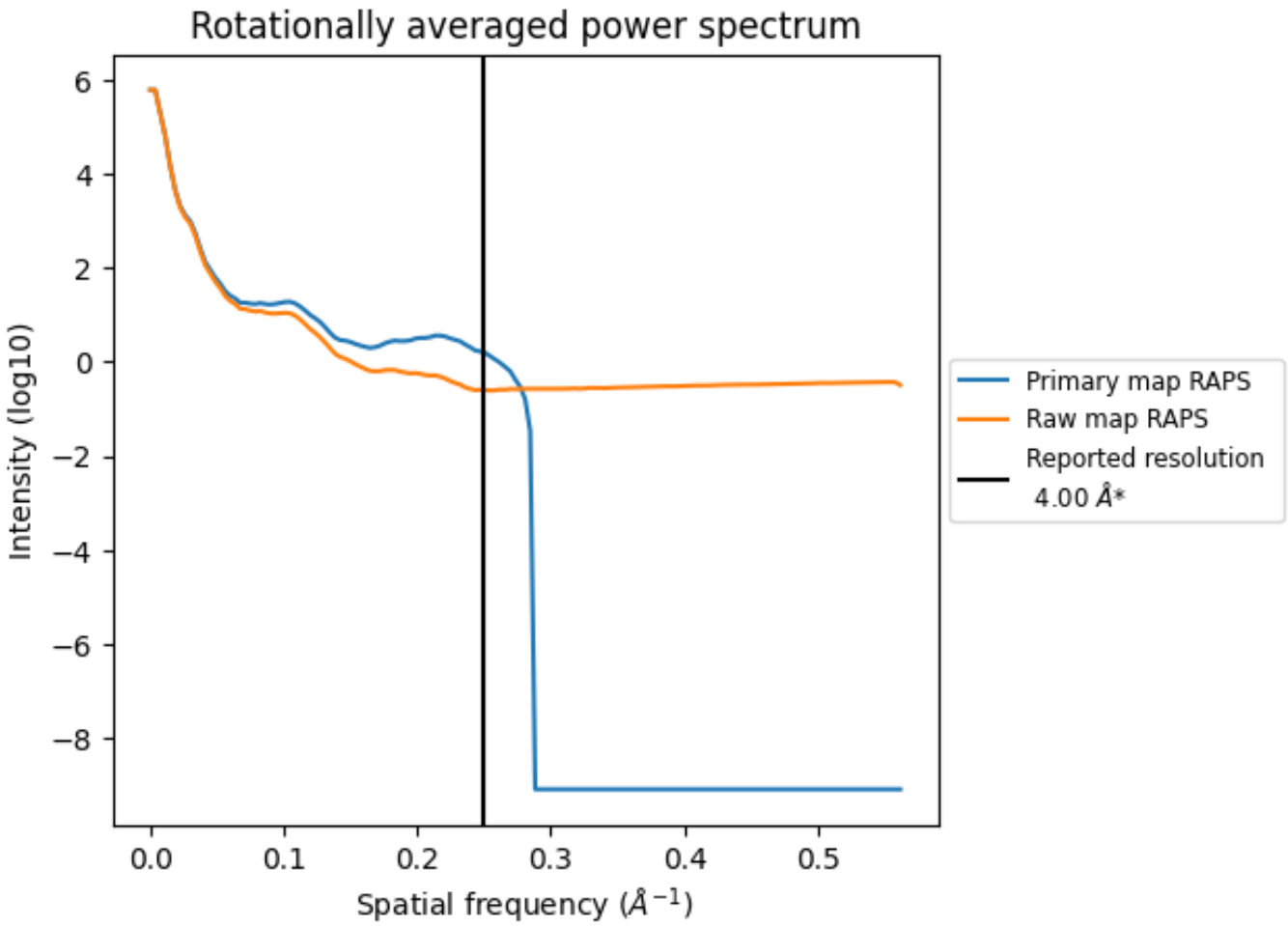
7.2 Volume estimate (i)



The volume at the recommended contour level is 141 nm^3; this corresponds to an approximate mass of 127 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)

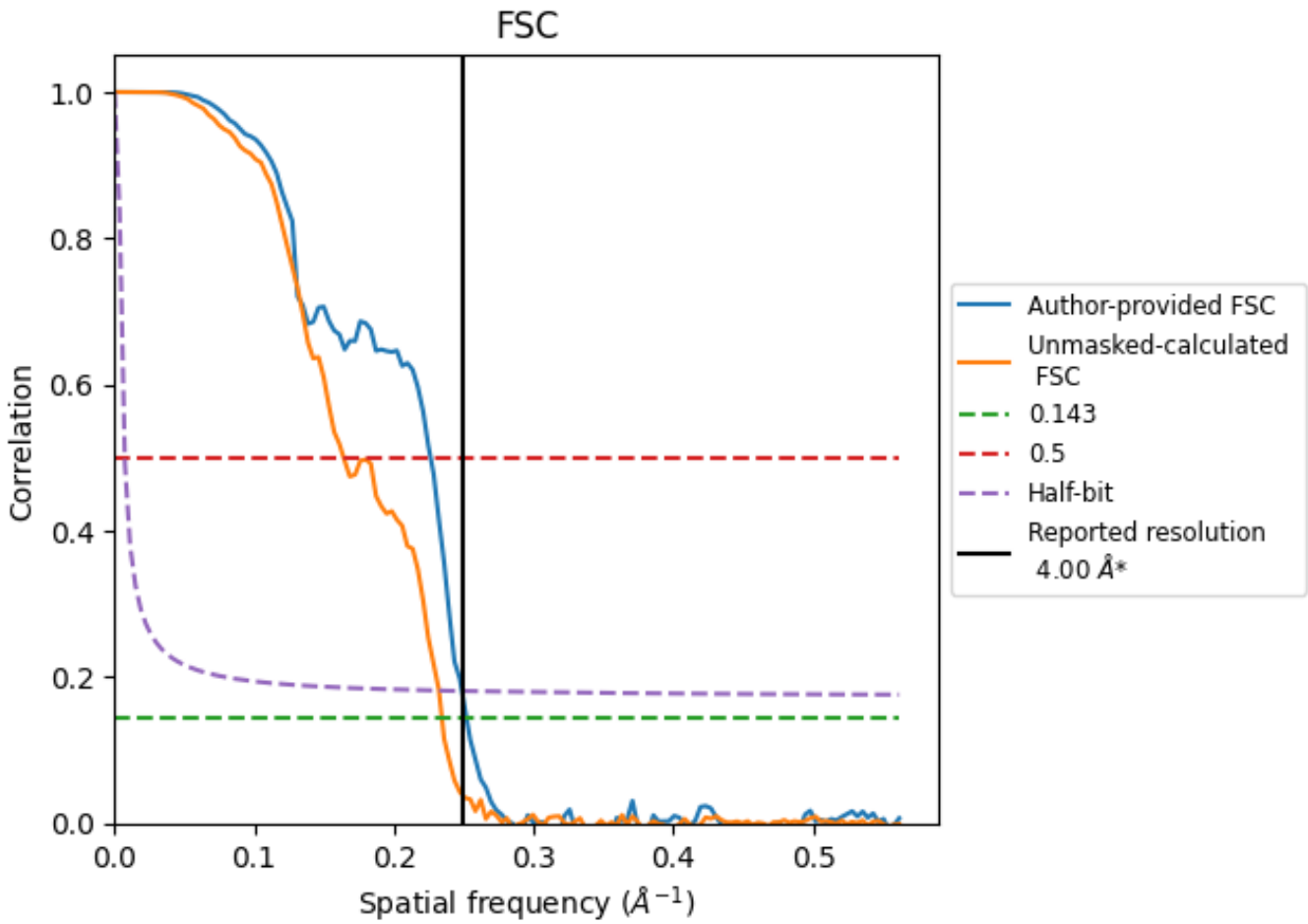


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

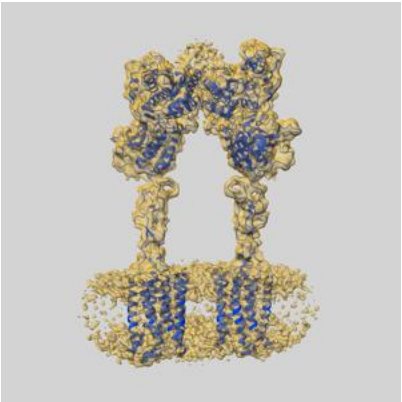
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.42	4.02
Unmasked-calculated*	4.27	6.09	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

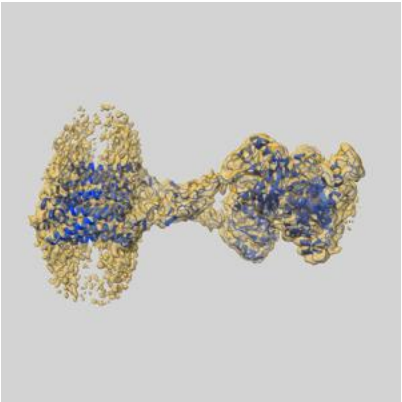
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31537 and PDB model 7FD9. Per-residue inclusion information can be found in section 3 on page 7.

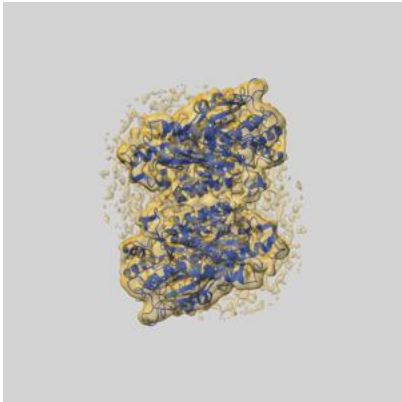
9.1 Map-model overlay (i)



X



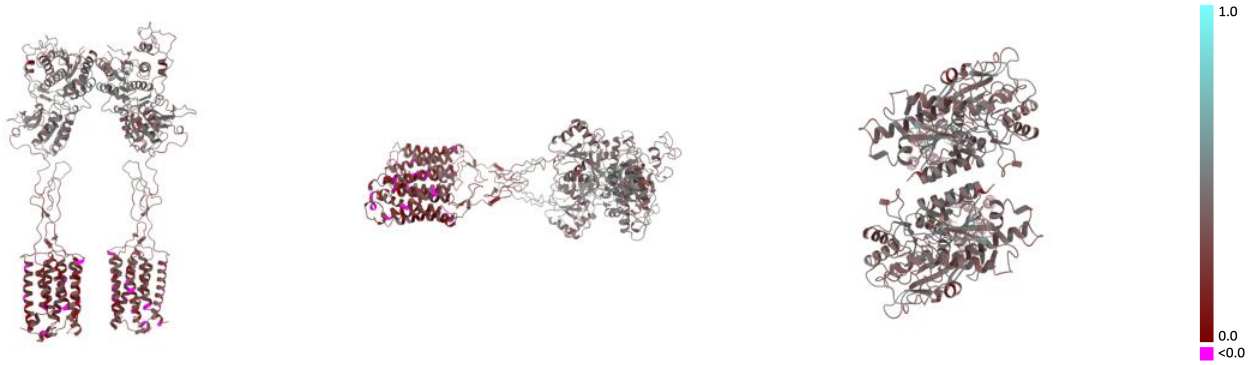
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0095 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.

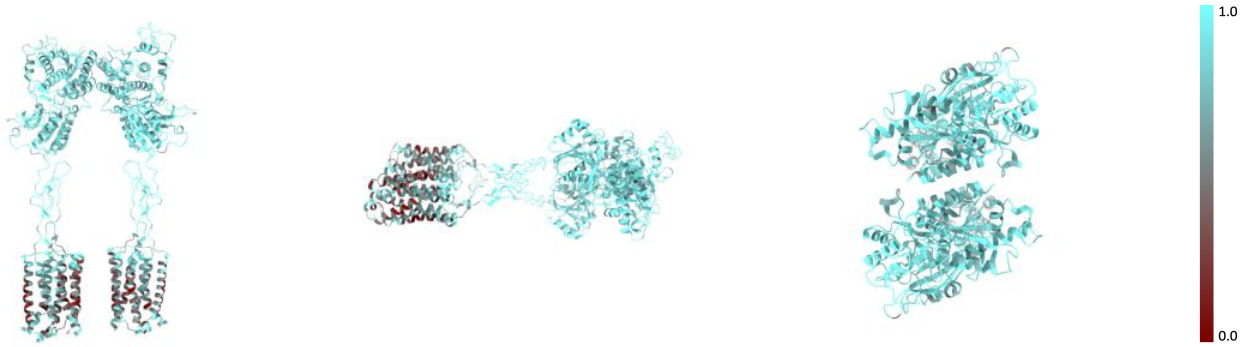
9.2 Q-score mapped to coordinate model (i)



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.

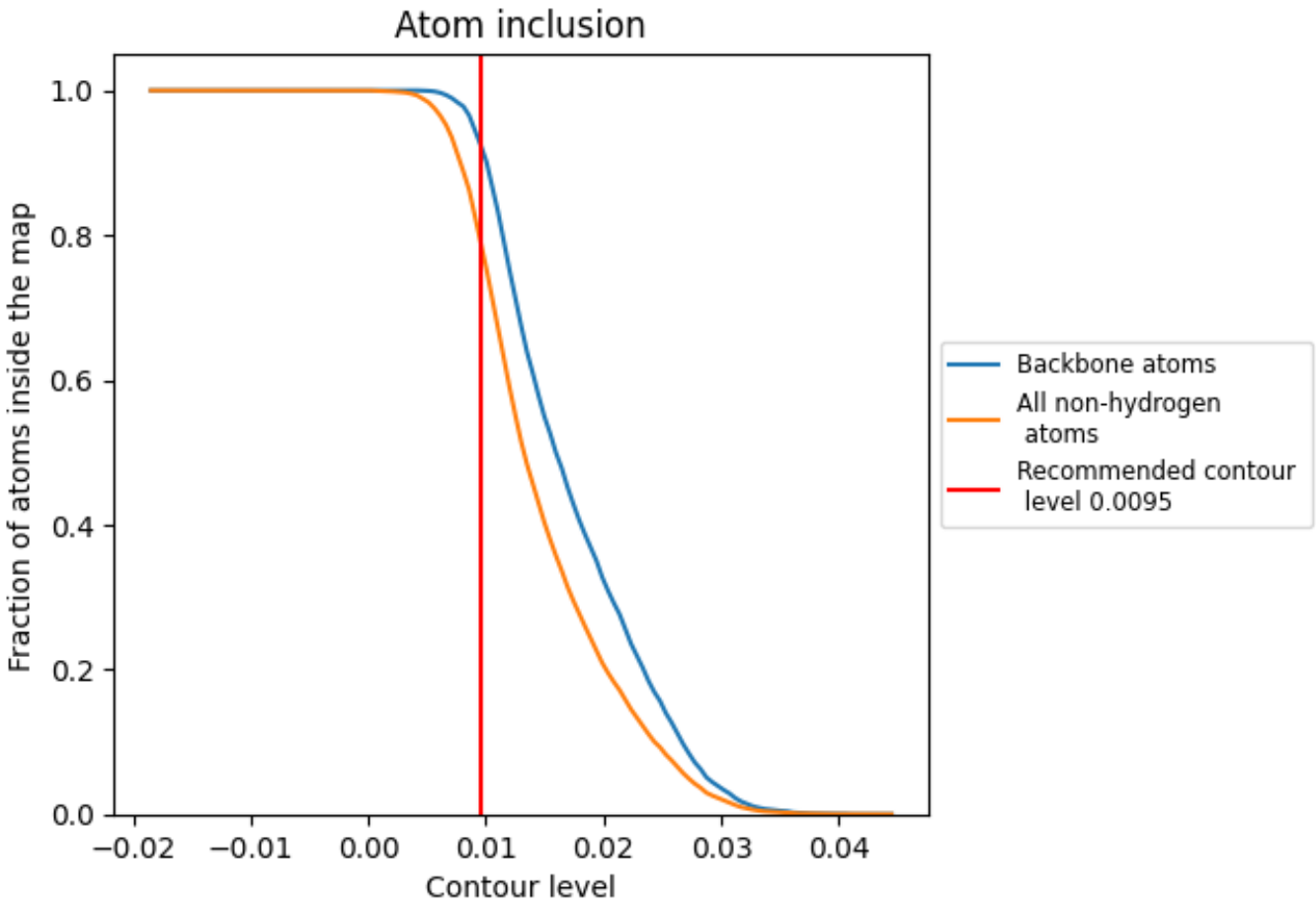
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0095).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 79% 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 (0.0095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7937	0.3530
A	0.7953	0.3540
B	0.7921	0.3520