wwPDB EM Validation Summary Report (i)

Oct 3, 2026 – 10:07 am BST

PDB ID	:	31XJ / pdb_000031xj
EMDB ID	:	EMD-58705
Title	:	Disulfide linked complex of T. ramosa IgA peptidase (IgAse2-4) with human IgA2 Fab' in precatalytic conformation
Authors	:	Ramirez-Larrota, J.S.; Gragera, M.; Eckhard, U.; Gomis-Ruth, F.X.
Deposited on	:	2026-06-26
Resolution	:	2.90 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 (1)) were used in the production of this report:

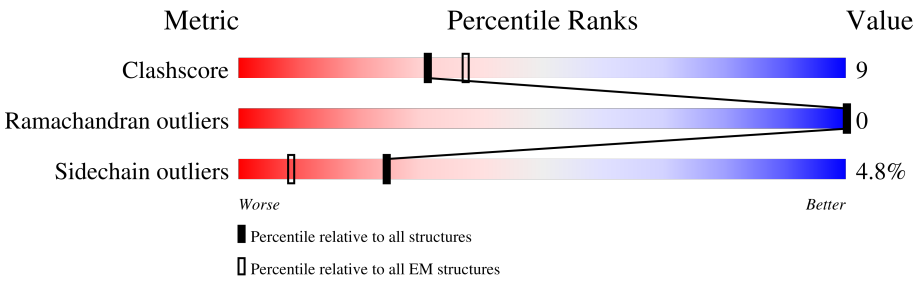
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

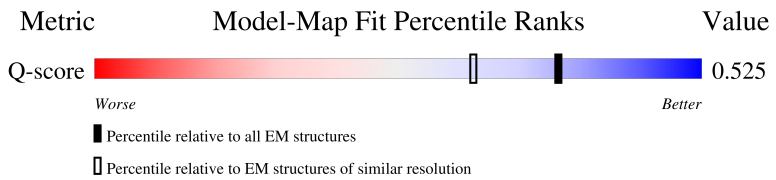
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	E	559	67% 17% • 15%
2	H	238	• 66% 26% • 5%
3	L	217	• 72% 24% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7450 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 IgA protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	477	3920	2490	658	757	15	10	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	326	MET	-	initiating methionine	UNP Q9AES2
E	327	GLY	-	expression tag	UNP Q9AES2
E	414	SER	CYS	engineered mutation	UNP Q9AES2
E	434	CYS	ASP	engineered mutation	UNP Q9AES2
E	476	SER	CYS	engineered mutation	UNP Q9AES2
E	540	ALA	GLU	engineered mutation	UNP Q9AES2
E	591	SER	CYS	engineered mutation	UNP Q9AES2
E	877	LEU	-	expression tag	UNP Q9AES2
E	878	GLU	-	expression tag	UNP Q9AES2
E	879	HIS	-	expression tag	UNP Q9AES2
E	880	HIS	-	expression tag	UNP Q9AES2
E	881	HIS	-	expression tag	UNP Q9AES2
E	882	HIS	-	expression tag	UNP Q9AES2
E	883	HIS	-	expression tag	UNP Q9AES2
E	884	HIS	-	expression tag	UNP Q9AES2

- Molecule 2 is a protein called IgA2(m1) Immunoglobulin Heavy Alpha Chain domains 1 and 2 including the hinge region (Q1-P226)..

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	226	1724	1080	294	342	8	1	0

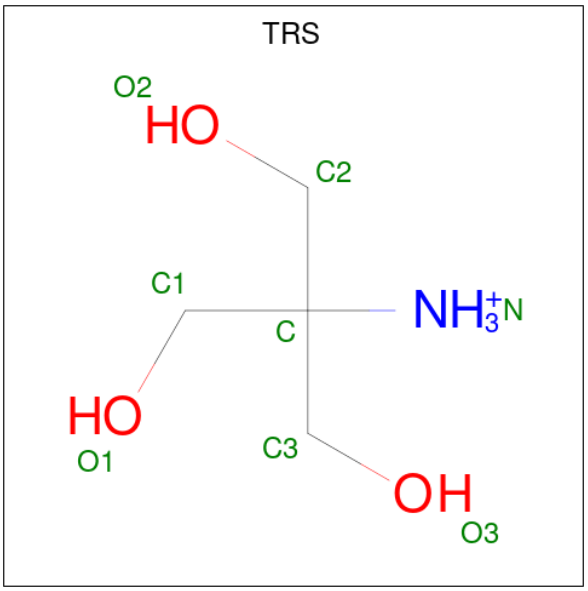
- Molecule 3 is a protein called IgA Immunoglobulin Lambda Light Chain domains 1 and 2 (S2-T214).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	214	1609	1014	270	320	5	3	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	E	2	2	2	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	E	1	8	4	1	3	0
5	H	1	8	4	1	3	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
6	H	2	2	2	0
6	L	1	1	1	0

- Molecule 7 is water.

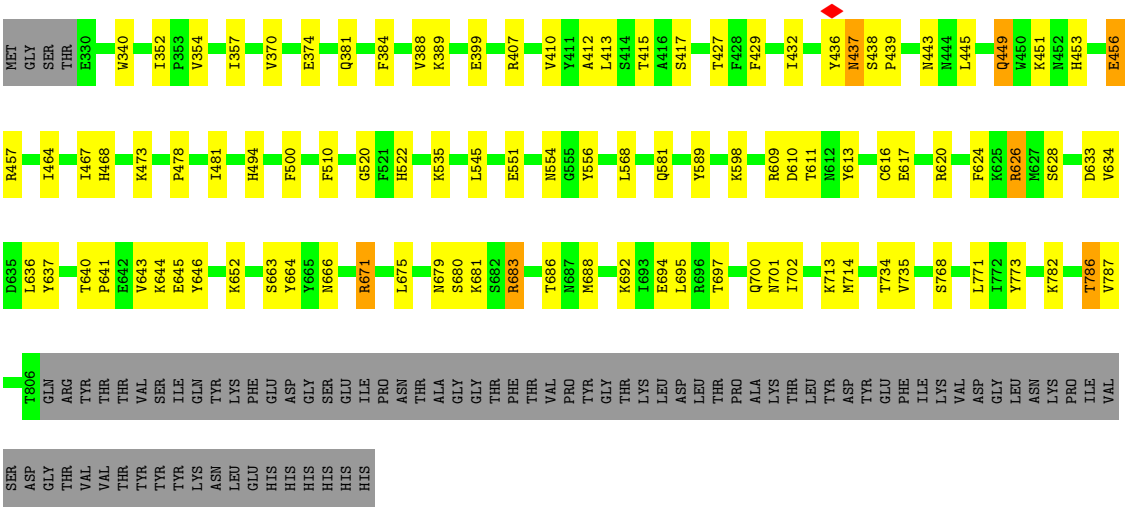
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
7	E	60	60	60	0
			Total	O	
7	H	63	63	63	0
			Total	O	
7	L	53	53	53	0

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.

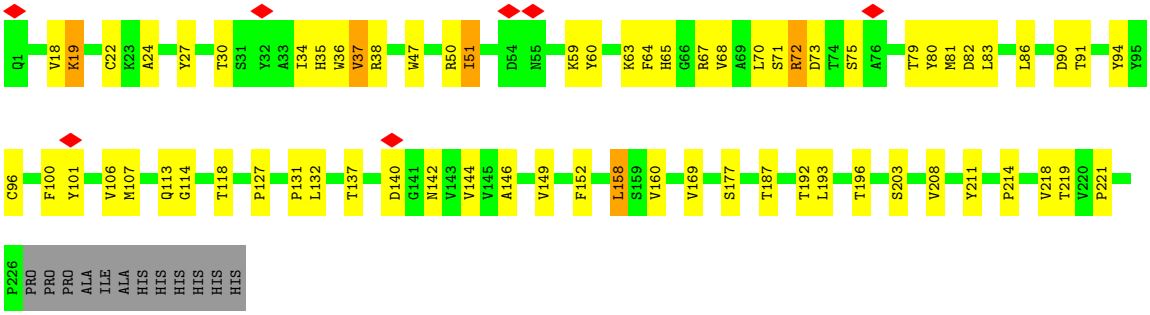
• Molecule 1: IgA protease

Chain E:



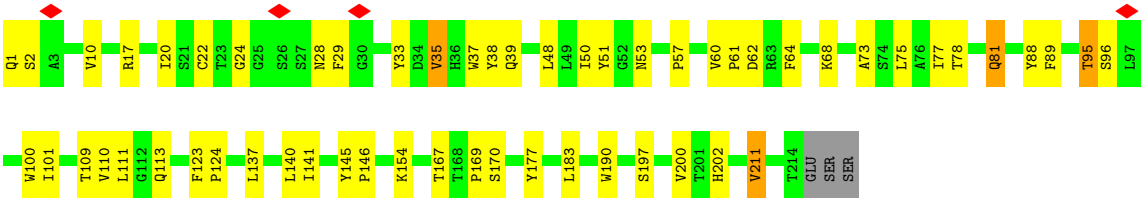
• Molecule 2: IgA2(m1) Immunoglobulin Heavy Alpha Chain domains 1 and 2 including the hinge region (Q1-P226).

Chain H:



• Molecule 3: IgA Immunoglobulin Lambda Light Chain domains 1 and 2 (S2-T214)

Chain L:


Q1
S2
A3
V10
R17
I20
S21
C22
T23
G24
G25
S26
S27
N28
F29
G30
Y33
D34
V35
H36
W37
Y38
Q39
L48
L49
I50
Y51
G52
N53
P57
V60
P61
D62
R63
F64
K68
A73
S74
L75
A76
I77
T78
Q81
Y88
F89
T95
S96
L97
W100
I101
T109
V110
L111
G112
Q113
F123
P124
L137
L140
I141
Y145
P146
K154
T167
T168
P169
S170
Y177
L183
W190
S197
V200
T201
H202
V211
T214
GLU
SER
SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105795	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.008	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000819	Depositor
Map size (Å)	262.80002, 262.80002, 262.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7300001, 0.7300001, 0.7300001	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: TRS, CL, ZN

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	E	0.19	0/4052	0.38	2/5486 (0.0%)
2	H	0.19	0/1775	0.36	0/2431
3	L	0.20	0/1662	0.40	0/2269
All	All	0.19	0/7489	0.38	2/10186 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	436	TYR	N-CA-C	10.19	122.39	111.28
1	E	436	TYR	CA-C-O	-5.74	114.47	120.55

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	E	3920	0	3755	57	0
2	H	1724	0	1640	41	0
3	L	1609	0	1555	34	0
4	E	2	0	0	0	0
5	E	8	0	12	0	0
5	H	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	2	0	0	1	0
6	L	1	0	0	1	0
7	E	60	0	0	0	0
7	H	63	0	0	0	0
7	L	53	0	0	0	0
All	All	7450	0	6974	126	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 126 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:E:551:GLU:HA	1:E:568:LEU:HD21	1.67	0.76
1:E:494[B]:HIS:CE1	1:E:522:HIS:HB3	2.22	0.74
1:E:680:SER:O	1:E:683[B]:ARG:HB3	1.89	0.72
1:E:449:GLN:HE21	1:E:449:GLN:H	1.40	0.69
2:H:94:TYR:O	2:H:114:GLY:HA2	1.93	0.69

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	E	485/559 (87%)	473 (98%)	12 (2%)	0	100	100
2	H	225/238 (94%)	211 (94%)	14 (6%)	0	100	100
3	L	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
All	All	925/1014 (91%)	890 (96%)	35 (4%)	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	E	436/499 (87%)	417 (96%)	19 (4%)	25	59
2	H	196/205 (96%)	185 (94%)	11 (6%)	19	50
3	L	178/178 (100%)	168 (94%)	10 (6%)	19	50
All	All	810/882 (92%)	770 (95%)	40 (5%)	24	54

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	211[A]	TYR
3	L	81	GLN
2	H	211[B]	TYR
3	L	62	ASP
3	L	101	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	150	GLN
2	H	155	GLN
3	L	174	ASN
3	L	91	GLN
3	L	172	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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TRS	H	301	-	7,7,7	0.35	0	9,9,9	0.76	0
5	TRS	E	903	4	7,7,7	0.36	0	9,9,9	0.66	0

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
5	TRS	H	301	-	-	7/9/9/9	-
5	TRS	E	903	4	-	4/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	903	TRS	C1-C-C2-O2
5	E	903	TRS	C3-C-C2-O2
5	E	903	TRS	N-C-C2-O2
5	H	301	TRS	C3-C-C2-O2
5	H	301	TRS	C2-C-C1-O1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	TRS	2	0

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.

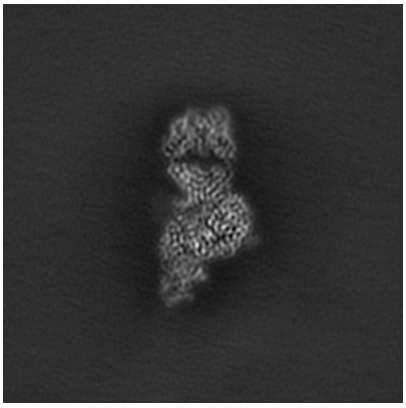
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-58705. These allow visual inspection of the internal detail of the map and identification of artifacts.

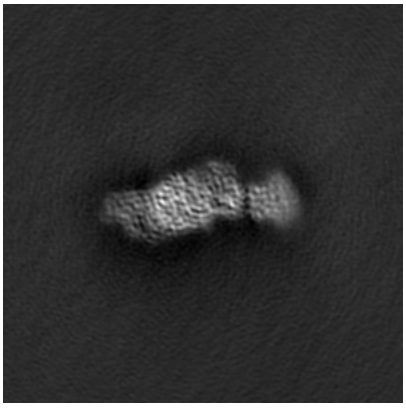
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

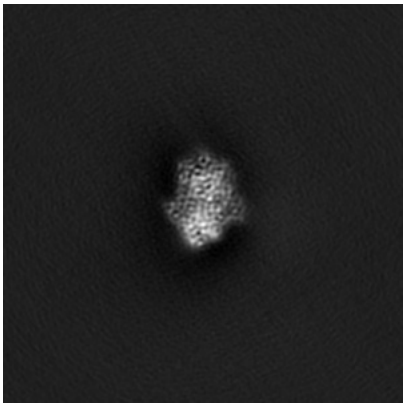
6.1.1 Primary map



X



Y

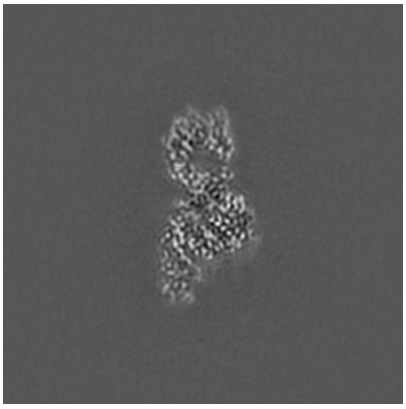


Z

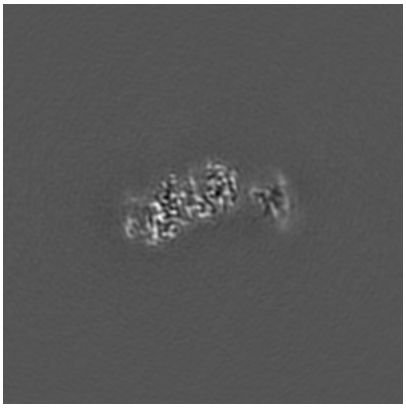
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

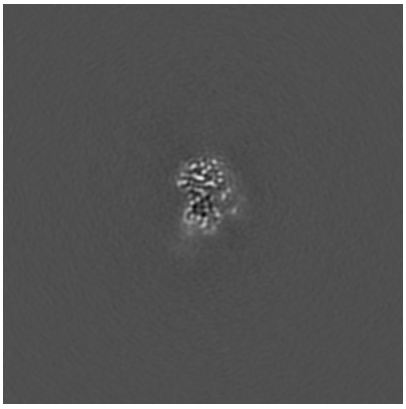
6.2.1 Primary map



X Index: 180



Y Index: 180

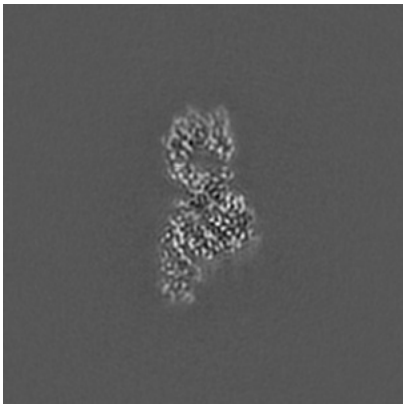


Z Index: 180

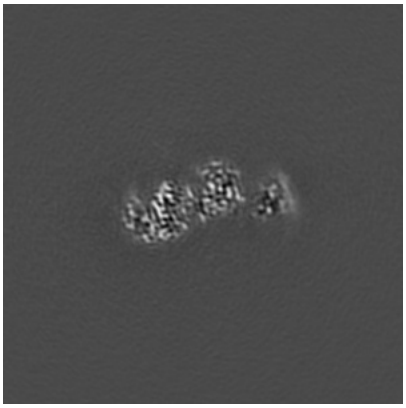
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

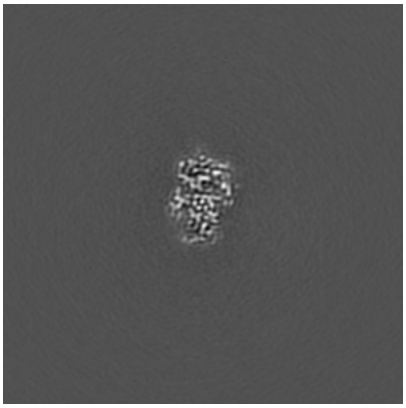
6.3.1 Primary map



X Index: 180



Y Index: 174

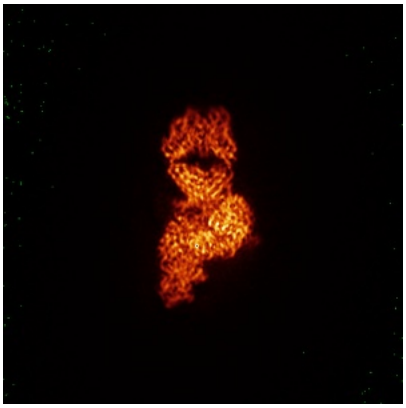


Z Index: 153

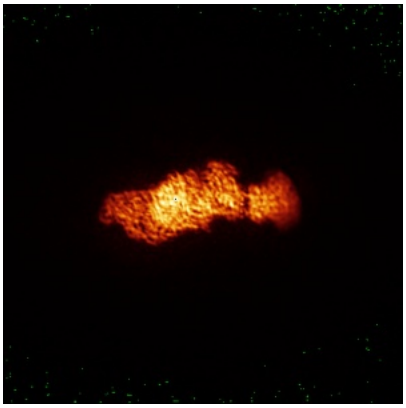
The images above show the largest variance slices of the map in three orthogonal directions.

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

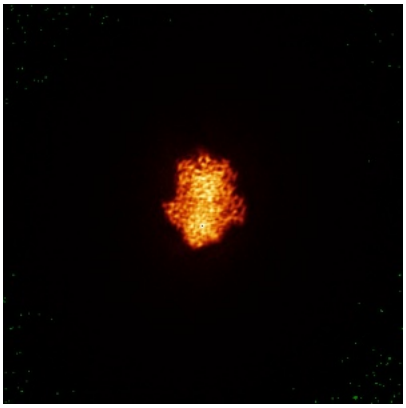
6.4.1 Primary map



X



Y



Z

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 0.000819. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

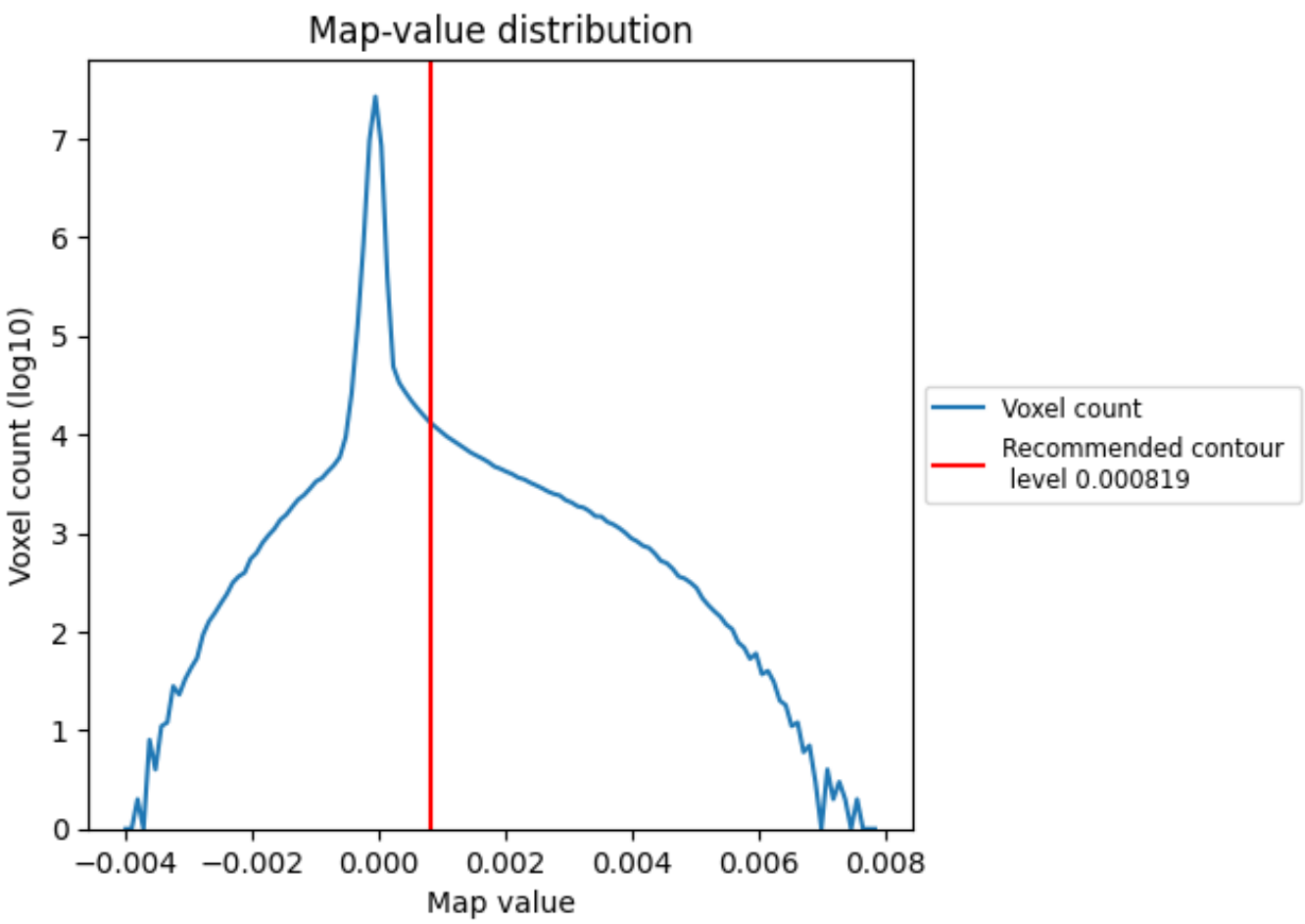
6.6 Mask visualisation (i)

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

7 Map analysis (i)

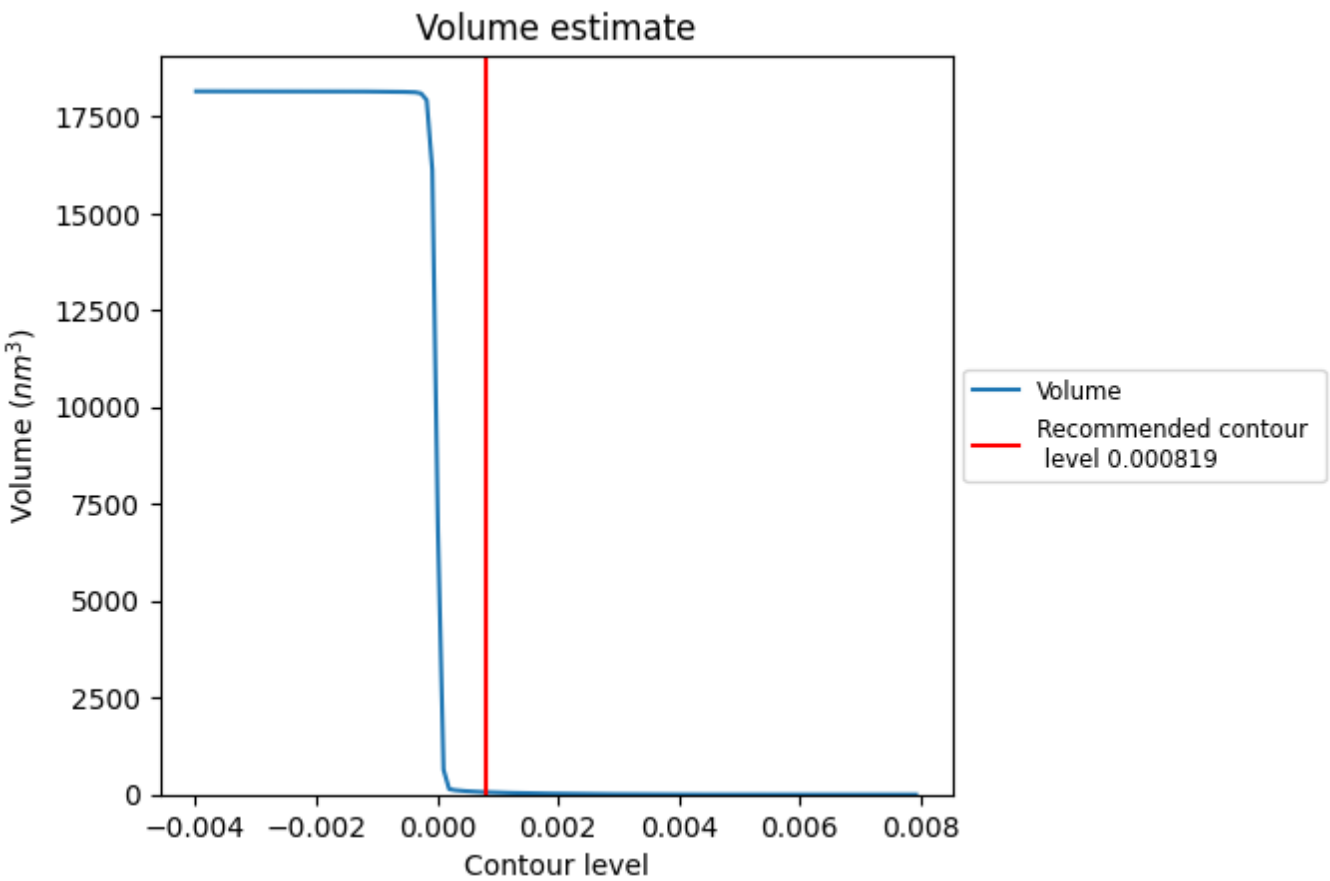
This section contains the results of statistical analysis of the map.

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.

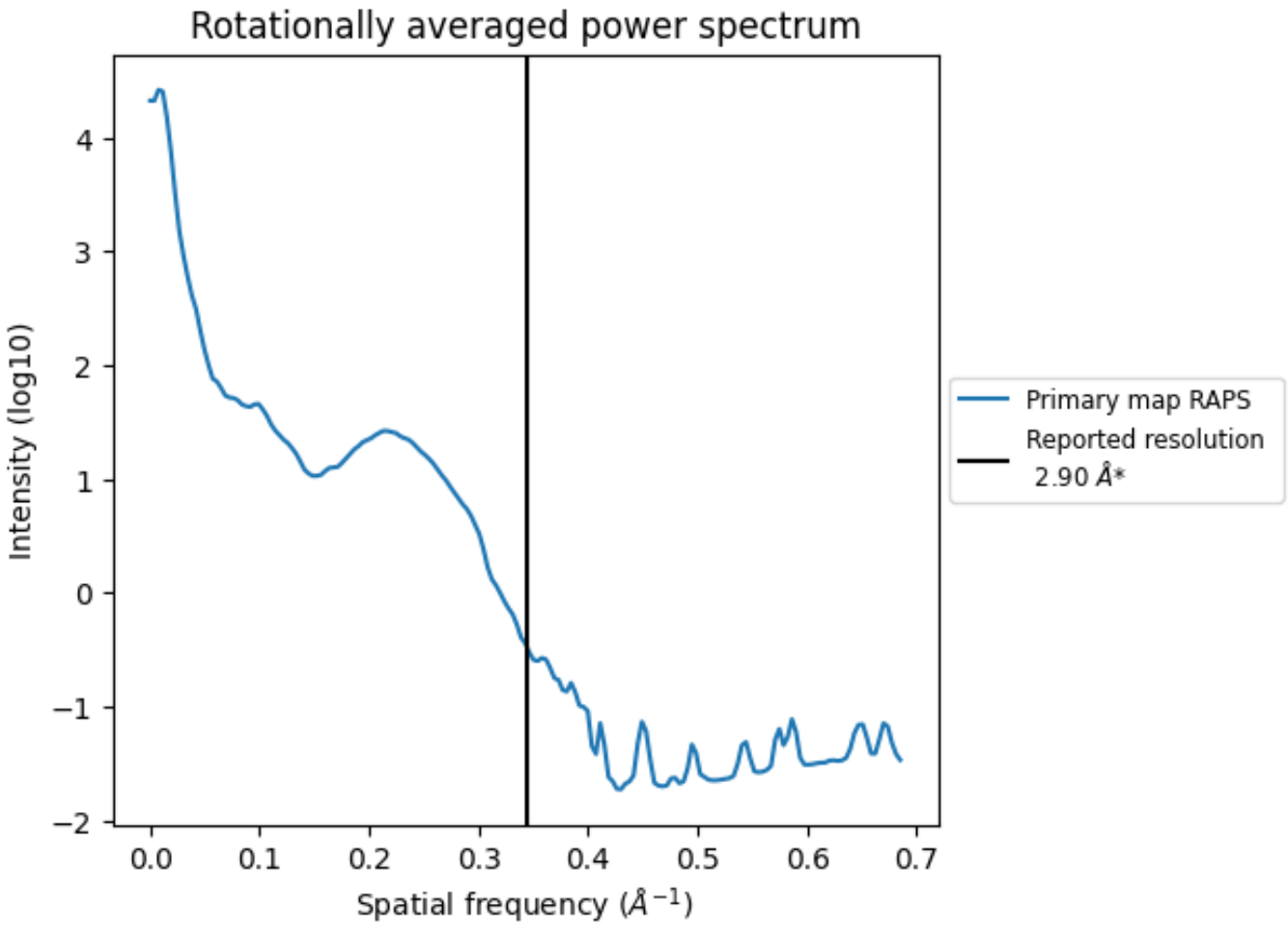
7.2 Volume estimate (i)



The volume at the recommended contour level is 61 nm^3; this corresponds to an approximate mass of 55 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 0.345 Å^{-1}

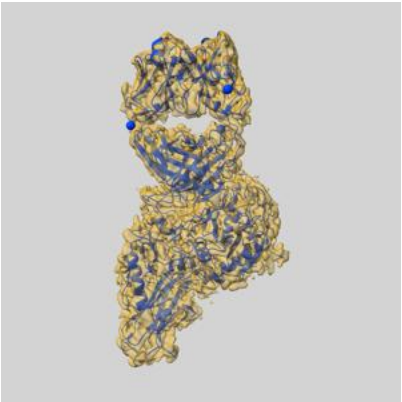
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

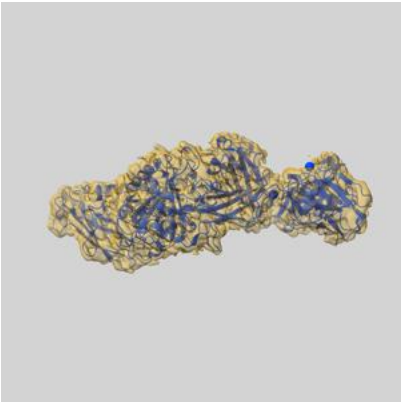
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-58705 and PDB model 31XJ. Per-residue inclusion information can be found in section 3 on page 6.

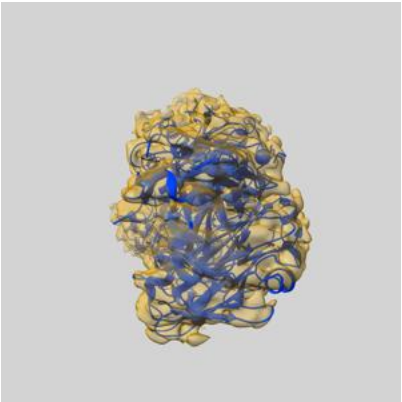
9.1 Map-model overlay (i)



X



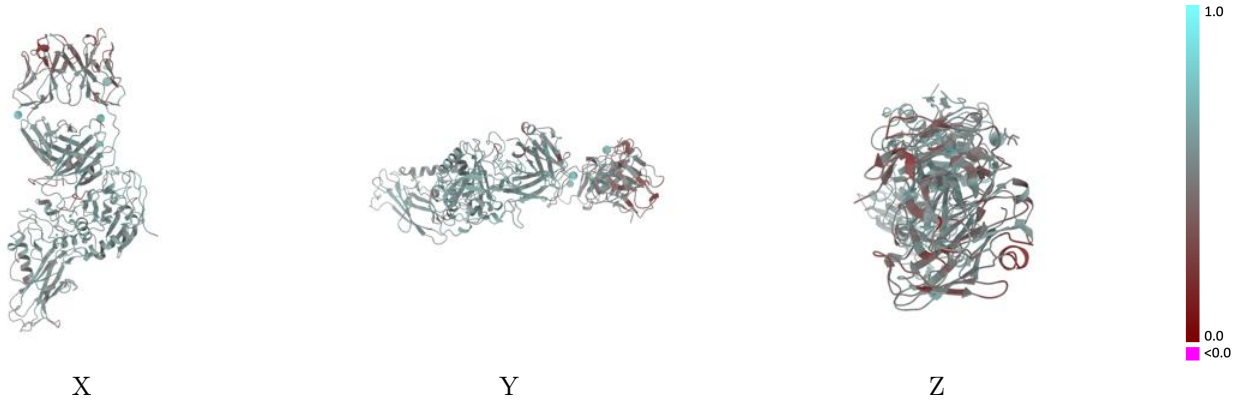
Y



Z

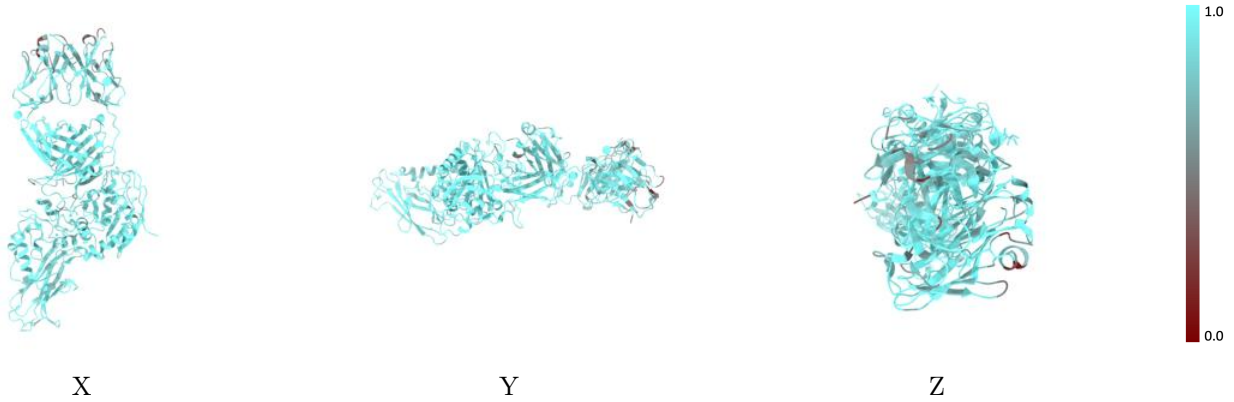
The images above show the 3D surface view of the map at the recommended contour level 0.000819 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



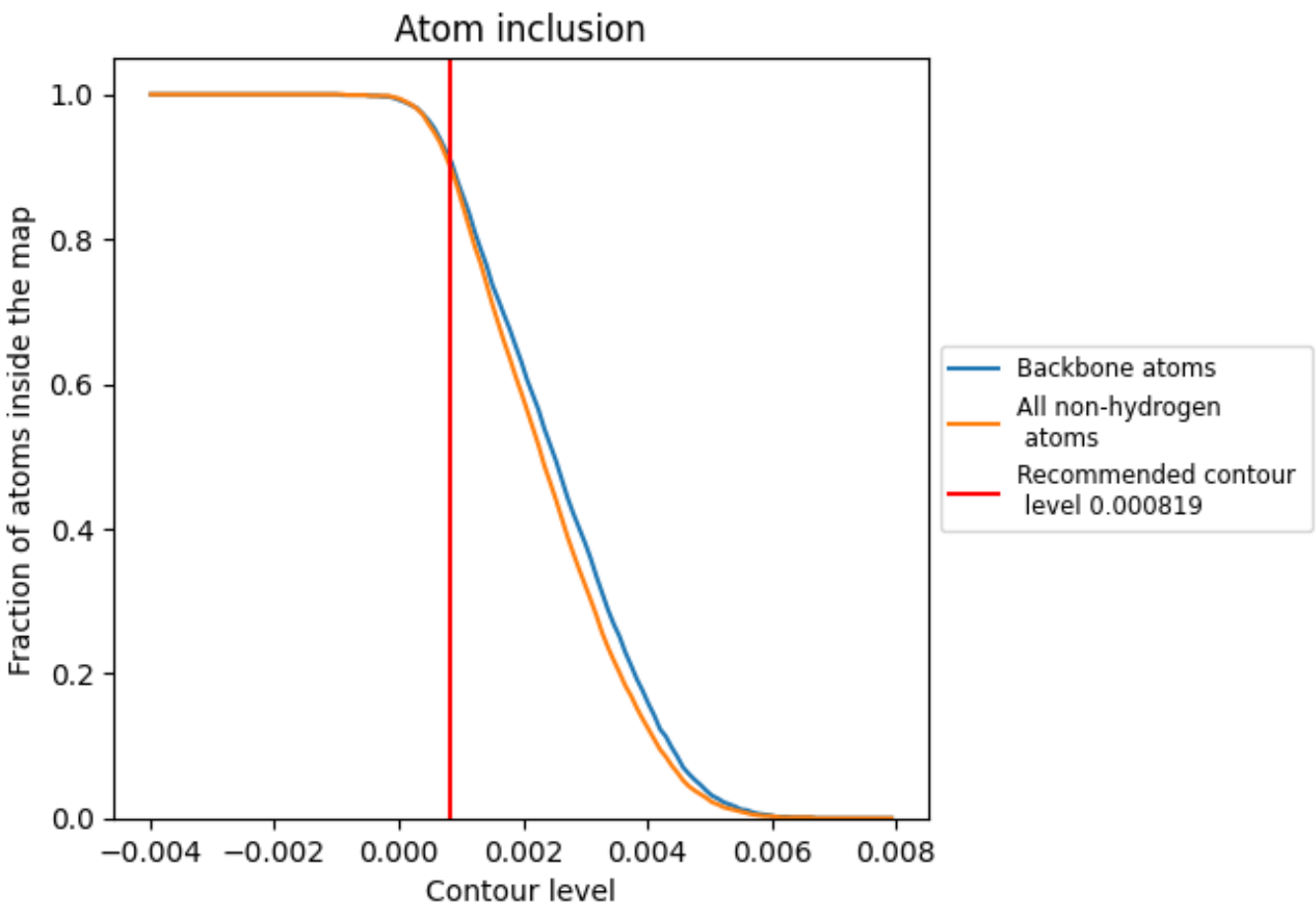
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.000819).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.000819) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.5250
E	0.9380	0.5570
H	0.8590	0.4930
L	0.8740	0.4800