



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 07:59 am GMT

PDB ID : 7NJ1
EMDB ID : EMD-12369
Title : CryoEM structure of the human Separase-Securin complex
Authors : Yu, J.; Raia, P.; Ghent, C.M.; Raisch, T.; Sadian, Y.; Barford, D.; Raunser, S.; Morgan, D.O.; Boland, A.
Deposited on : 2021-02-14
Resolution : 2.90 Å(reported)

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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.dev43
MolProbity : 4.02b-467
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

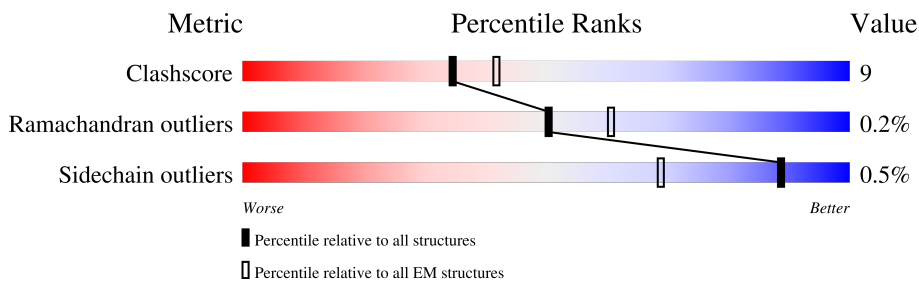
1 Overall quality at a glance

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)
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 $\leq 5\%$. 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	2160	 8% 53% 13% 33%
2	B	202	 7% 18% 8% 74%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11096 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 Separin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1448	10660	6755	1879	1975	51	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	ALA	conflict	UNP Q14674
A	116	VAL	ALA	conflict	UNP Q14674
A	693	ILE	MET	conflict	UNP Q14674
A	1329	SER	ARG	conflict	UNP Q14674
A	1561	GLN	ARG	conflict	UNP Q14674
A	2037	HIS	ARG	conflict	UNP Q14674
A	2121	SER	-	expression tag	UNP Q14674
A	2122	SER	-	expression tag	UNP Q14674
A	2123	LEU	-	expression tag	UNP Q14674
A	2124	ALA	-	expression tag	UNP Q14674
A	2125	GLU	-	expression tag	UNP Q14674
A	2126	GLU	-	expression tag	UNP Q14674
A	2127	ASN	-	expression tag	UNP Q14674
A	2128	LEU	-	expression tag	UNP Q14674
A	2129	TYR	-	expression tag	UNP Q14674
A	2130	PHE	-	expression tag	UNP Q14674
A	2131	GLN	-	expression tag	UNP Q14674
A	2132	SER	-	expression tag	UNP Q14674
A	2133	TRP	-	expression tag	UNP Q14674
A	2134	SER	-	expression tag	UNP Q14674
A	2135	HIS	-	expression tag	UNP Q14674
A	2136	PRO	-	expression tag	UNP Q14674
A	2137	GLN	-	expression tag	UNP Q14674
A	2138	PHE	-	expression tag	UNP Q14674
A	2139	GLU	-	expression tag	UNP Q14674
A	2140	LYS	-	expression tag	UNP Q14674
A	2141	GLY	-	expression tag	UNP Q14674
A	2142	GLY	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2143	GLY	-	expression tag	UNP Q14674
A	2144	SER	-	expression tag	UNP Q14674
A	2145	GLY	-	expression tag	UNP Q14674
A	2146	GLY	-	expression tag	UNP Q14674
A	2147	GLY	-	expression tag	UNP Q14674
A	2148	SER	-	expression tag	UNP Q14674
A	2149	GLY	-	expression tag	UNP Q14674
A	2150	GLY	-	expression tag	UNP Q14674
A	2151	GLY	-	expression tag	UNP Q14674
A	2152	SER	-	expression tag	UNP Q14674
A	2153	TRP	-	expression tag	UNP Q14674
A	2154	SER	-	expression tag	UNP Q14674
A	2155	HIS	-	expression tag	UNP Q14674
A	2156	PRO	-	expression tag	UNP Q14674
A	2157	GLN	-	expression tag	UNP Q14674
A	2158	PHE	-	expression tag	UNP Q14674
A	2159	GLU	-	expression tag	UNP Q14674
A	2160	LYS	-	expression tag	UNP Q14674

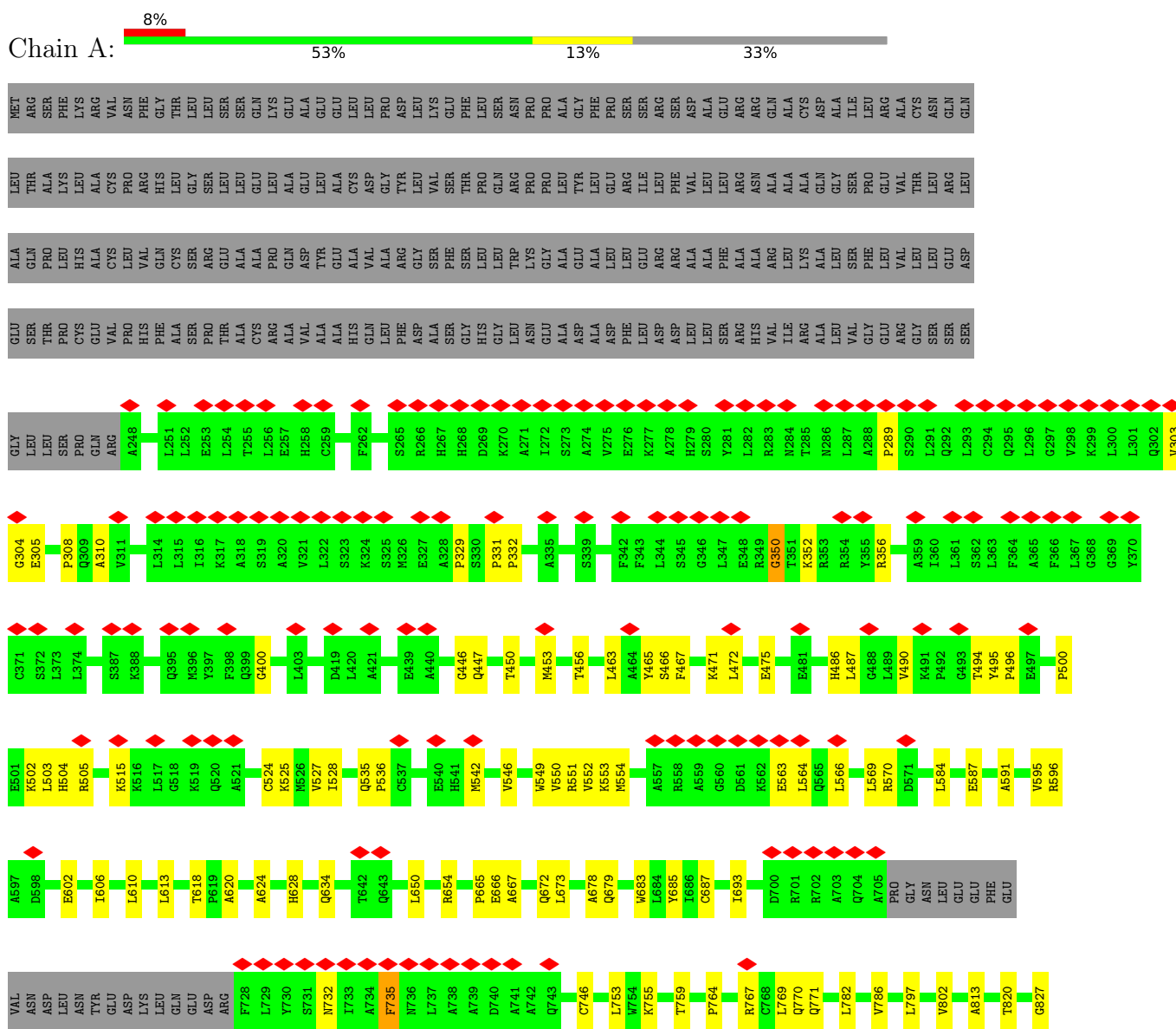
- Molecule 2 is a protein called Securin.

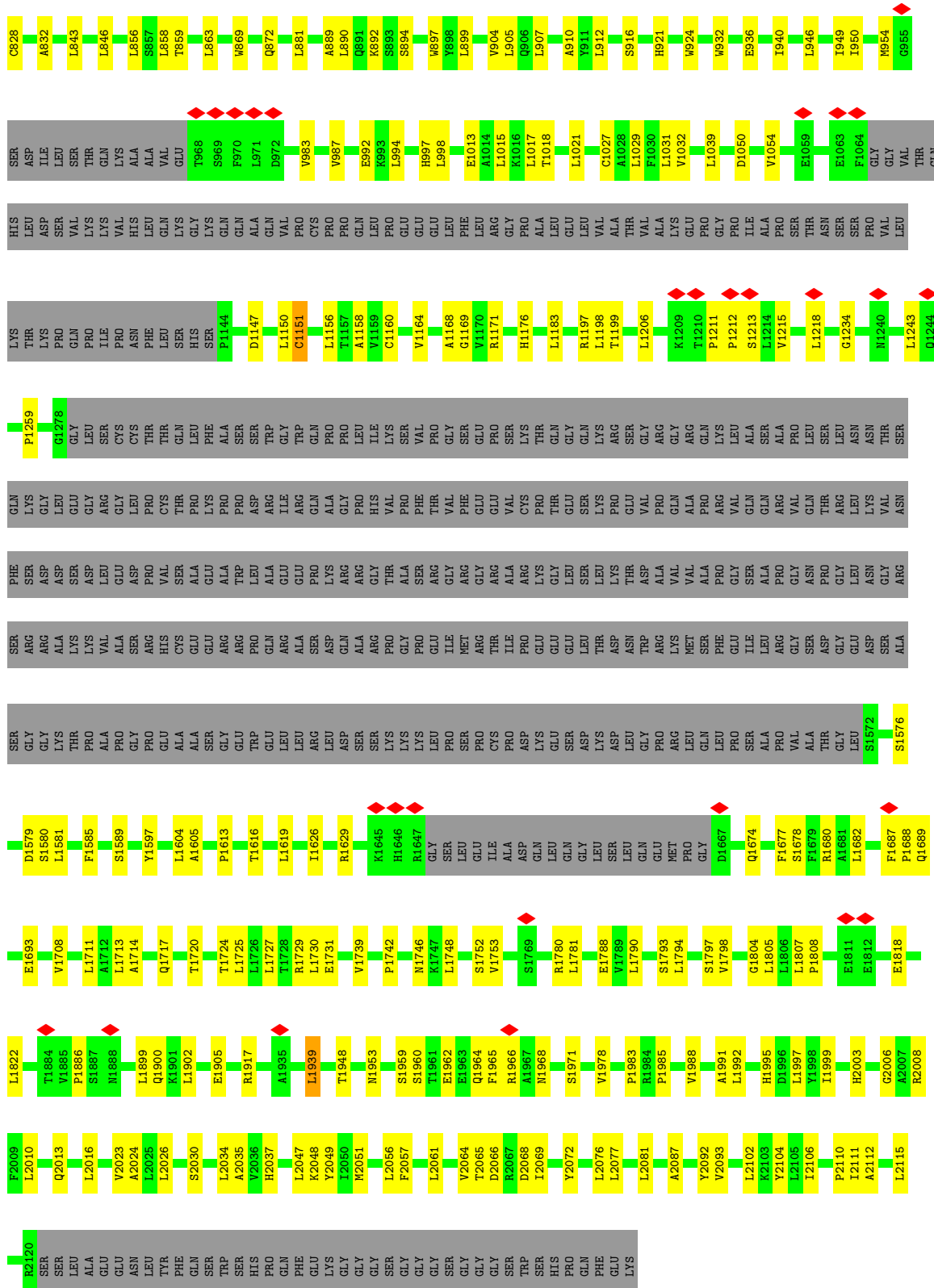
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	53	436	288	65	82	1	0	0

3 Residue-property plots

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: Separin





• Molecule 2: Securin



MET
ALA
THR
LEU
ILE
TYR
VAL
VAL
ASP
LYS
GLU
ASN
GLY
PRO
GLY
THR
ARG
VAL
VAL
ALA
LYS
GLY
LEU
LYS
LEU
GLY
SER
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SER
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ALA
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ALA
SER
SER
VAL
PRO
ALA
ASP
ASP
ALA
Y111
F120
N121
P122
L123
E126
S127
F128

D129
L130
P131
E132
I136
L141
I148
L149
D150
E151
E152
R153
E154
L155
E156
K157
L158
F159
Q160
L161
G162
P163
SER
PRO
VAL
LYS
MET
GLU
PRO
SER
PRO
PRO
TRP
GLU
SER
ASN
LEU
LEU
GLN
SER
PRO
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THR
LEU
ASP
VAL
GLU
LEU
PRO
PRO
VAL
CYS

ASP
ILE
ASP
ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	205300	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 ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.878	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	333.9, 333.9, 333.9	wwPDB
Map dimensions	318, 318, 318	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/10853	0.45	5/14786 (0.0%)
2	B	0.34	0/450	0.54	0/611
All	All	0.30	0/11303	0.45	5/15397 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	PRO	N-CA-CB	5.77	110.22	103.30
1	A	331	PRO	N-CA-CB	5.75	110.20	103.30
1	A	332	PRO	N-CA-CB	5.71	110.15	103.30
1	A	289	PRO	N-CA-CB	5.64	110.07	103.30
1	A	308	PRO	N-CA-CB	5.42	109.80	103.30

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	10660	0	10313	189	0
2	B	436	0	416	17	0
All	All	11096	0	10729	193	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 193 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:524:CYS:HG	1:A:549:TRP:HE1	1.18	0.88
1:A:527:VAL:HG11	1:A:549:TRP:HB2	1.64	0.78
1:A:453:MET:HA	1:A:456:THR:HG22	1.66	0.77
1:A:472:LEU:HD21	1:A:475:GLU:HB3	1.71	0.72
1:A:894:SER:HB3	1:A:897:TRP:HD1	1.55	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	1436/2160 (66%)	1328 (92%)	105 (7%)	3 (0%)	47 78
2	B	51/202 (25%)	46 (90%)	5 (10%)	0	100 100
All	All	1487/2362 (63%)	1374 (92%)	110 (7%)	3 (0%)	50 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	GLY
1	A	350	GLY
1	A	400	GLY

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	1052/1815 (58%)	1047 (100%)	5 (0%)	88	96
2	B	49/178 (28%)	49 (100%)	0	100	100
All	All	1101/1993 (55%)	1096 (100%)	5 (0%)	89	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	687	CYS
1	A	735	PHE
1	A	802	VAL
1	A	1151	CYS
1	A	1939	LEU

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12369. 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](#)

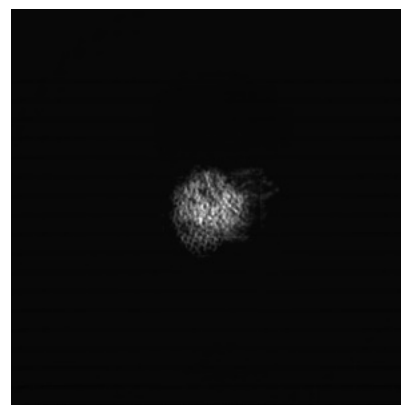
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

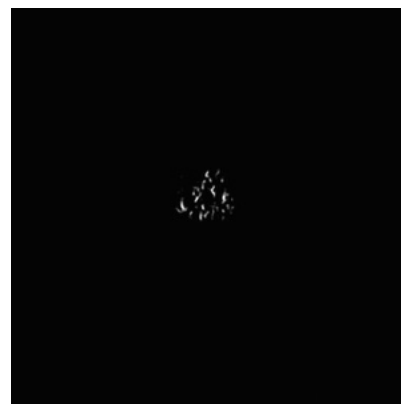
6.2.1 Primary map



X Index: 159



Y Index: 159



Z Index: 159

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

6.3 Largest variance slices [i](#)

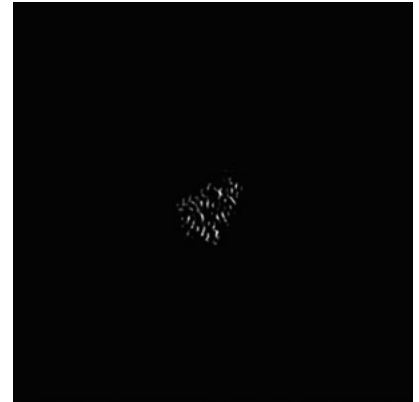
6.3.1 Primary map



X Index: 156



Y Index: 159



Z Index: 112

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

6.4 Orthogonal surface views [i](#)

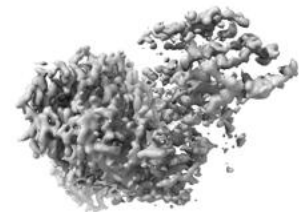
6.4.1 Primary map



X



Y



Z

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

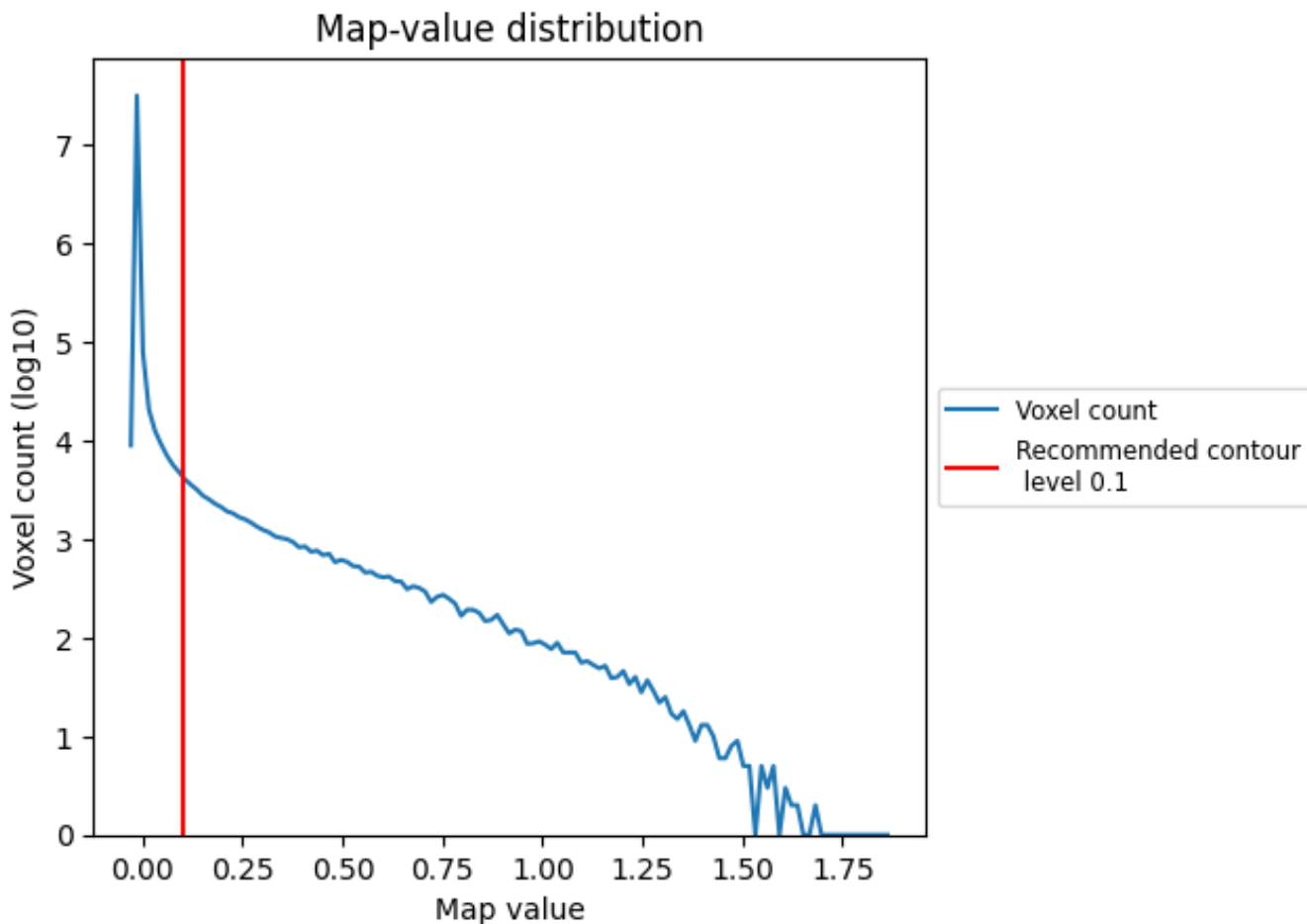
6.5 Mask visualisation

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

7 Map analysis [i](#)

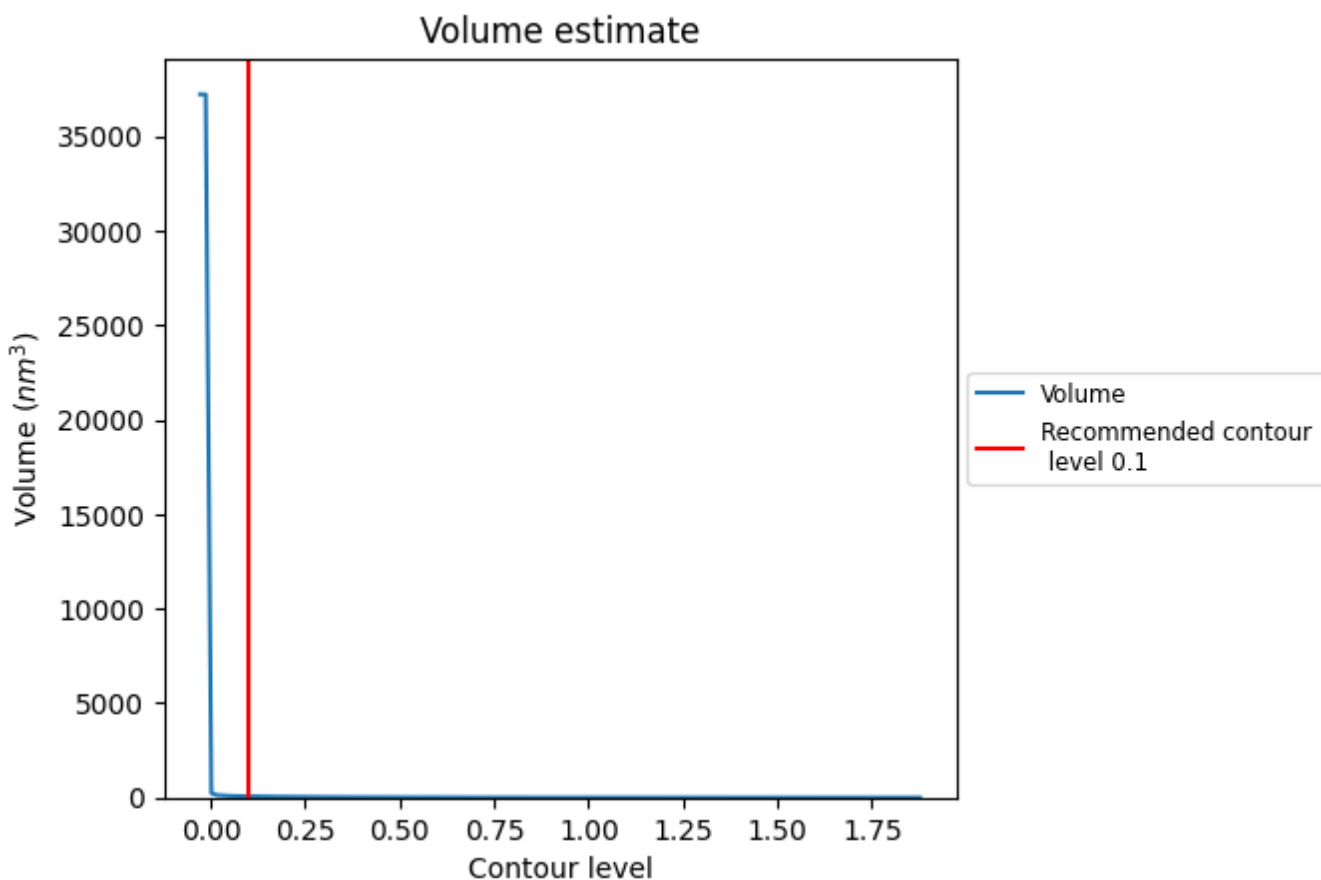
This section contains the results of statistical analysis of the map.

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.

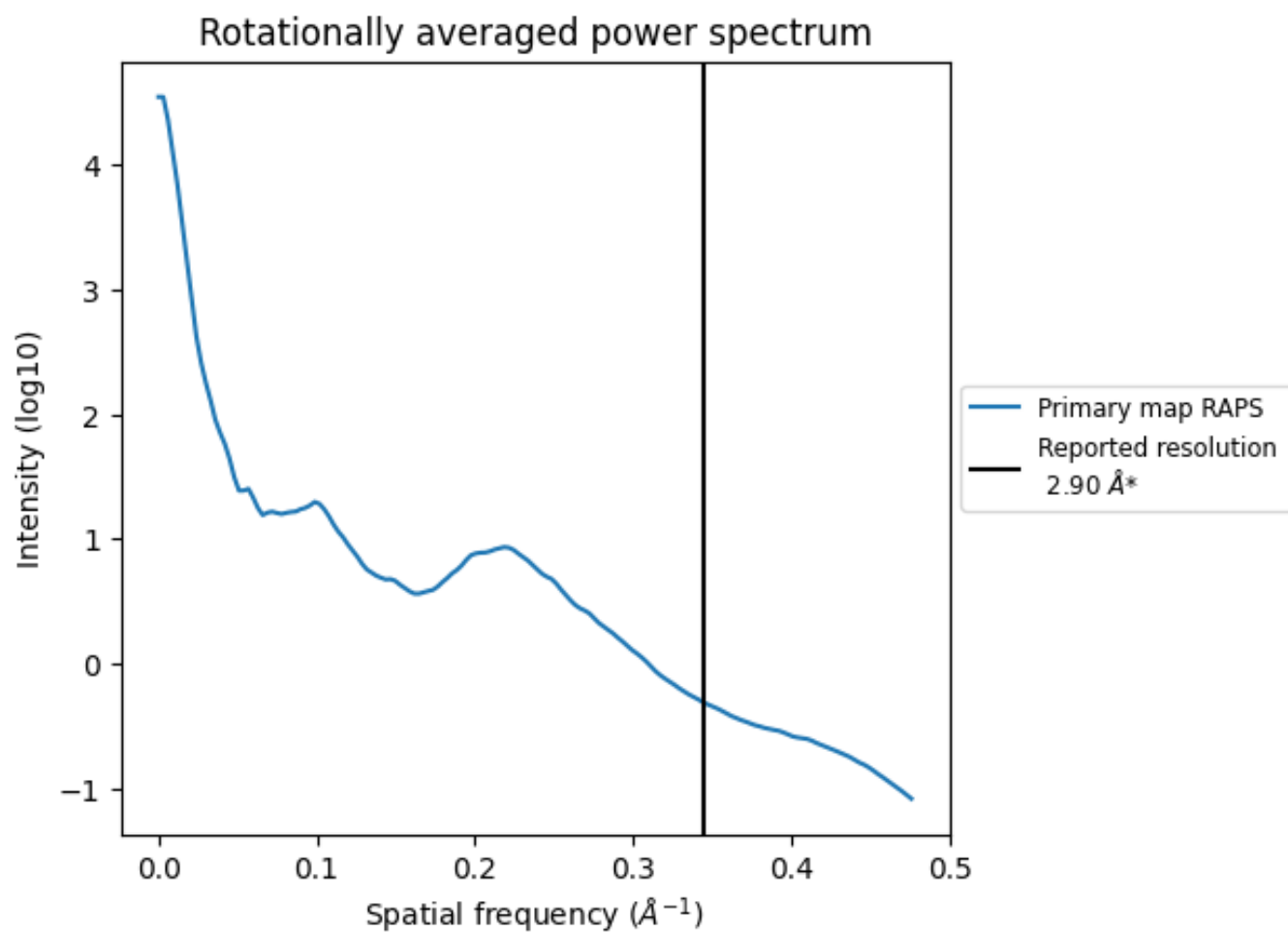
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm^3 ; this corresponds to an approximate mass of 58 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 \AA^{-1}

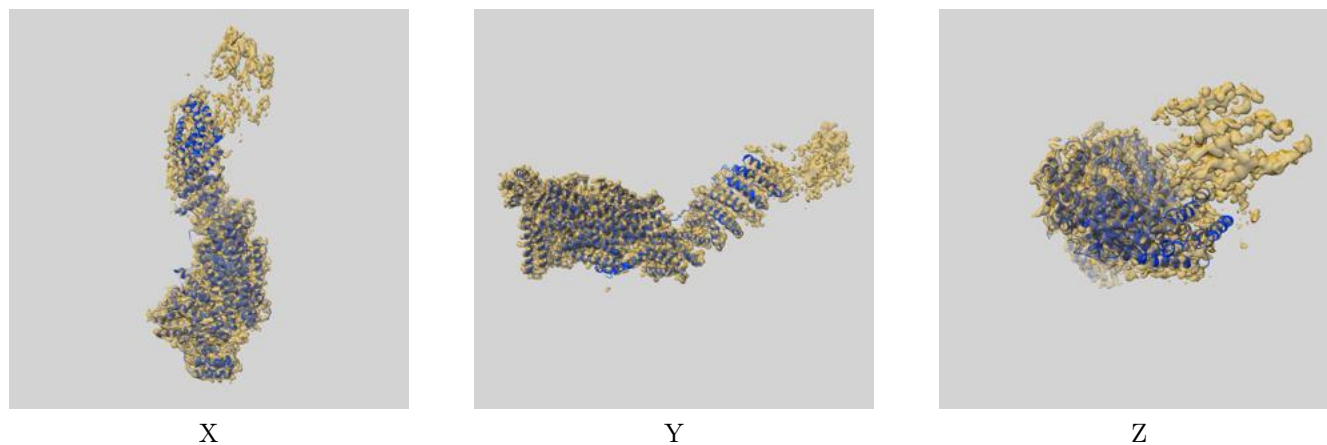
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

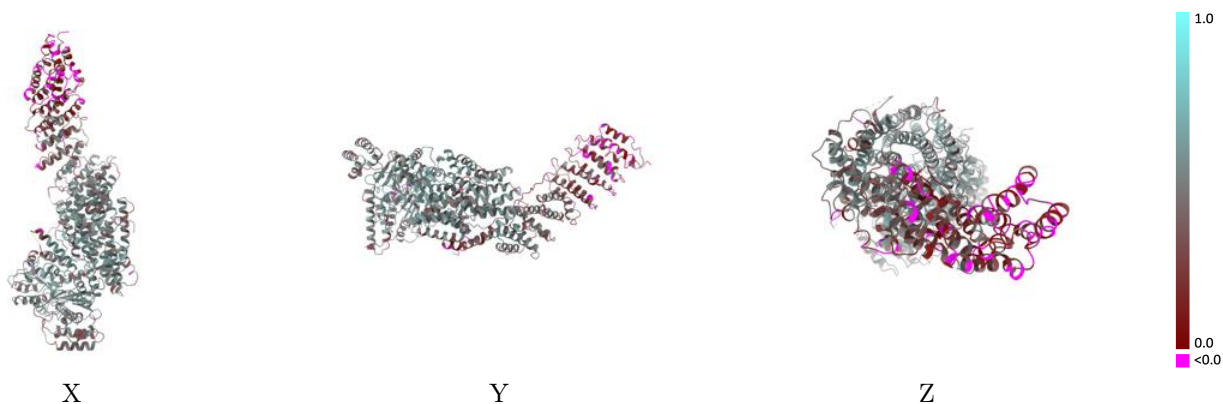
This section contains information regarding the fit between EMDB map EMD-12369 and PDB model 7NJ1. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



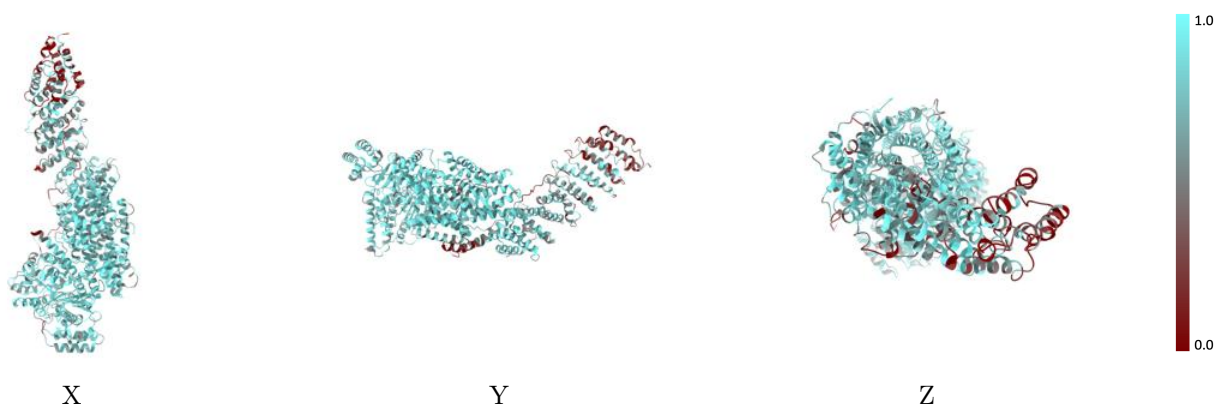
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



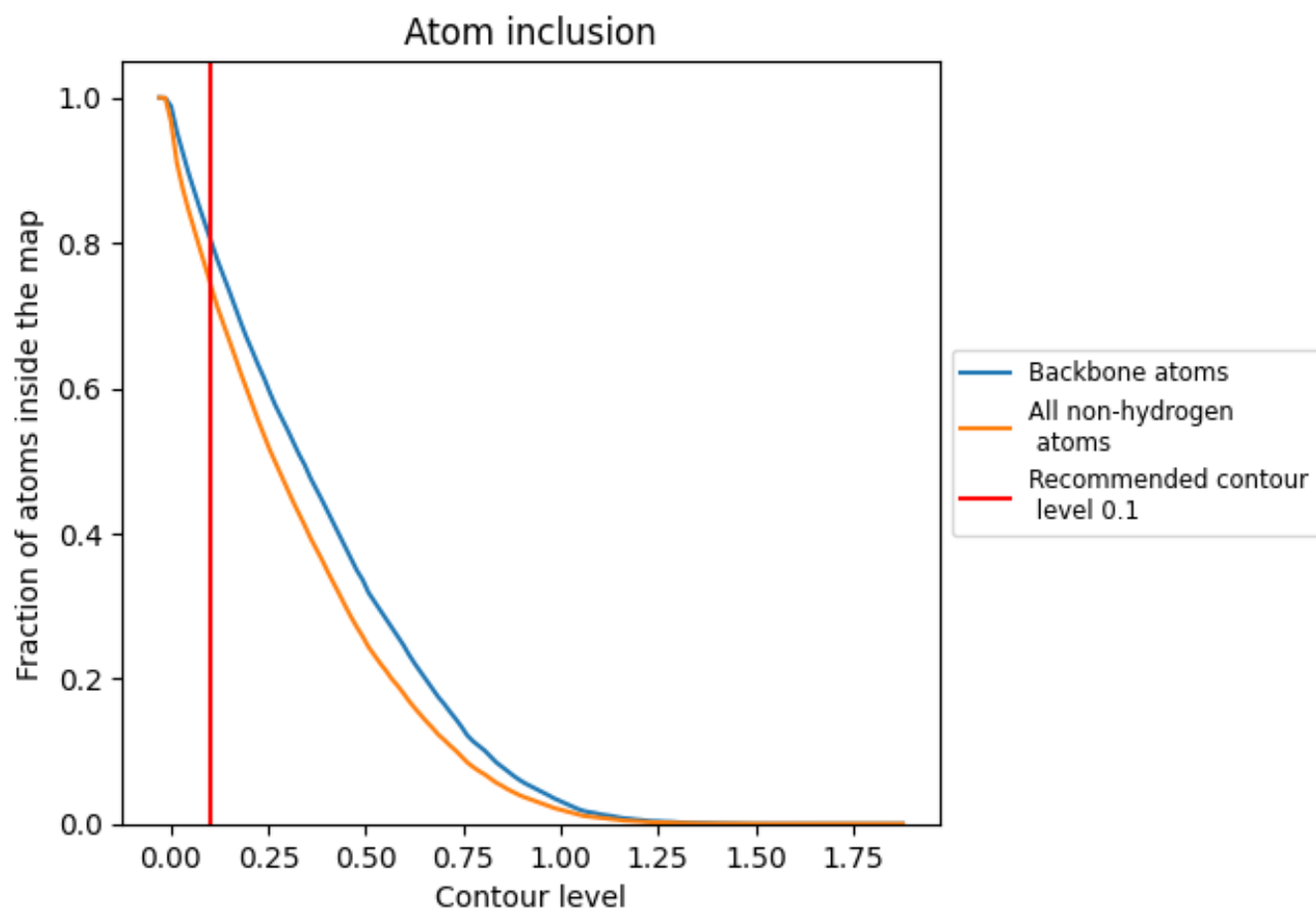
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7487	 0.4410
A	 0.7547	 0.4440
B	 0.6037	 0.3780

