



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 10:00 am GMT

PDB ID : 7NIL
EMDB ID : EMD-12362
Title : 1918 H1N1 Viral influenza polymerase heterotrimer with Nb8190 core
Authors : Keown, J.R.; Carrique, L.; Fodor, E.; Grimes, J.M.
Deposited on : 2021-02-12
Resolution : 5.01 Å (reported)
Based on initial model : 7HNA

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:

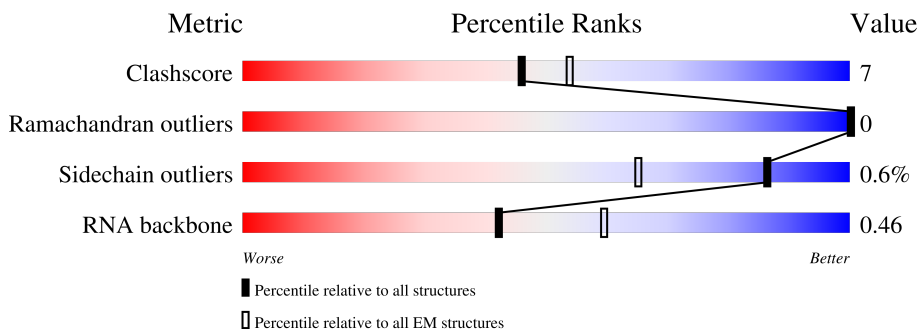
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 5.01 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
RNA backbone	4643	859

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	716	 20% 17% 61% 11% 28%
2	B	757	 17% 21% 80% 17% 5%
3	C	905	 12% 29% 6% 72% 21%
4	E	17	 60% 18% 7% 15%
5	D	15	 66% 9% 25%
6	F	133	 66% 9% 25%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 25558 atoms, of which 12260 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	517	8270	2631	4118	702	790	29	0	0

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	735	11704	3691	5833	1028	1106	46	0	0

- Molecule 3 is a protein called Polymerase basic protein 2,Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	249	4075	1271	2058	361	369	16	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLU	-	linker	UNP Q3HM41
C	761	ASN	-	linker	UNP Q3HM41
C	762	LEU	-	linker	UNP Q3HM41
C	763	TYR	-	linker	UNP Q3HM41
C	764	PHE	-	linker	UNP Q3HM41
C	765	GLN	-	linker	UNP Q3HM41
C	766	GLY	-	linker	UNP Q3HM41
C	767	GLU	-	linker	UNP Q3HM41
C	768	LEU	-	linker	UNP Q3HM41
C	769	LYS	-	linker	UNP Q3HM41
C	770	THR	-	linker	UNP Q3HM41
C	771	ALA	-	linker	UNP Q3HM41
C	772	ALA	-	linker	UNP Q3HM41
C	773	LEU	-	linker	UNP Q3HM41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	774	ALA	-	linker	UNP Q3HM41
C	775	GLN	-	linker	UNP Q3HM41
C	776	HIS	-	linker	UNP Q3HM41
C	777	ASP	-	linker	UNP Q3HM41
C	778	GLU	-	linker	UNP Q3HM41
C	779	ALA	-	linker	UNP Q3HM41
C	780	VAL	-	linker	UNP Q3HM41
C	781	ASP	-	linker	UNP Q3HM41
C	782	ASN	-	linker	UNP Q3HM41
C	783	LYS	-	linker	UNP Q3HM41
C	797	HIS	ASN	conflict	UNP P38507
C	798	LEU	MET	conflict	UNP P38507
C	808	ALA	GLY	conflict	UNP P38507
C	832	ASP	GLU	conflict	UNP P38507
C	833	ALA	SER	conflict	UNP P38507
C	838	VAL	ALA	conflict	UNP P38507
C	866	ALA	GLY	conflict	UNP P38507
C	873	ALA	ASP	conflict	UNP P38507
C	890	GLY	ASP	conflict	UNP P38507
C	896	VAL	ALA	conflict	UNP P38507
C	898	ALA	-	expression tag	UNP P38507
C	899	ASN	-	expression tag	UNP P38507
C	900	SER	-	expression tag	UNP P38507
C	901	ALA	-	expression tag	UNP P38507
C	902	GLY	-	expression tag	UNP P38507
C	903	LYS	-	expression tag	UNP P38507
C	904	SER	-	expression tag	UNP P38507
C	905	THR	-	expression tag	UNP P38507

- Molecule 4 is a RNA chain called RNA (5'-R(P*GP*GP*CP*CP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
4	E	8	255	75	86	28	58	8	0	0

- Molecule 5 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP*AP*GP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
5	D	15	491	146	165	66	99	15	0	0

- Molecule 6 is a protein called Nanobody8190 core.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	763	475	134	150	4	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: Polymerase acidic protein

Chain A: 

MET
GLU
ASP
PHE
VAL
ARG
GLN
CYS
PHE
ASN
ALA
ASN
LEU
MET
ILE
VAL
LEU
ALA
GLU
GLY
LYS
ALA
MET
LYS
GLU
GLY
SER
THR
GLY
GLY
LEU
ASP
TRP
PHE
THR
VAL
ILE
GLY
THR
SER
ASN
PHE
CYS
PHE
ALA
ALA
ILE
CYS
THR
HIS
LEU
LEU
VAL
VAL
CYS
PHE
MET
TYR
SER
ASP
PHE
HIS
TYR
LEU
ASN
ARG
GLU
GLY
SER

ILE
ILE
VAL
GLU
SER
GLY
ASP
PRO
ASN
ALA
LEU
LEU
LEU
HIS
ARG
PHE
GLU
ILE
ILE
GLY
SER
GLY
THR
THR
HIS
HIS
ILE
PHE
TRP
THR
VAL
VAL
ASN
GLY
SER
ILE
GLU
MET
CYS
ASN
THR
THR
GLY
ALA
ALA
ASP
ALA
TYR
LEU
PRO
LYS
PHE
PHE
LEU
MET
TYR
ASP
LEU
TYR
ASP
TYR
HIS
PHE
GLY
ASN
ASN
GLU
ARG
PHE
ILE
ILE
ILE

GLY
VAL
THR
ARG
ARG
GLY
VAL
HIS
ILE
PHE
TYR
TYR
PRO
LEU
GLU
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ALA
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SER
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THR
THR
GLY
SER
GLY
THR
HIS
HIS
ILE
PHE
TRP
THR
VAL
THR
THR
GLY
GLY
GLU
MET
MET
ALA
THR
LYS
ALA
ASP
THR
THR
LEU
LEU
VAL
GLU
GLU
SER
SER
ARG
ARG
ALA
ILE
LYS
THR
THR
LEU
PHE
THR
ILE
ARG
GLN


GLU
MET
ALA
SER
ARG
ARG
GLY
LEU
TRP
ASP
SER
PHE
PRO
ARG
GLN
SER
GLU
ARG
GLY
GLU
SER
GLU
GLY
GLY
SER
T200
I201
E202
M211
E227
R230
E243
L246
S277
Q278
L283
D286
H297
E298
G299
E300
M311
R312
T313
L345
T348
E349
N350
E351
T354
K358
N359

K360
K361
K362
L366
K367
G371
A404
S405
W406
I407
Q408
M412
D426
E427
H437
M441
R442
F446
A455
K461
C474
A475
A476
M477
D478
F480
S487
K488
Y501
I505
K506
E510
L511
R512
N513
D514
V521
S522
M523
S526
P530

K536
M537
V542
I545
S552
A553
I554
S555
M561
V565
S578
M579
E580
R583
C584
L586
Q587
S588
L589
I592
E593
A598
S601
V602
K603
E604
K605
D606
M607
T608
K609
F612
E613
M614
K615
L640
L641
E661
L676
Q679
E692

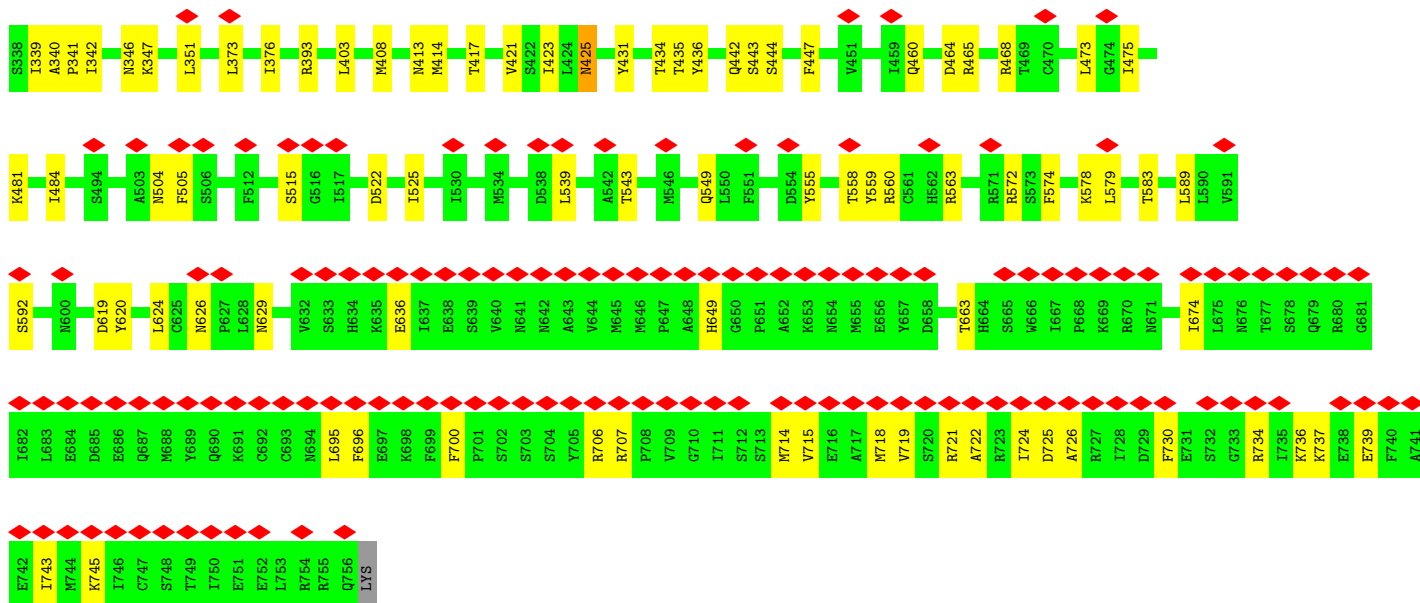
D697
V700
L715
R716

- Molecule 2: RNA-directed RNA polymerase catalytic subunit

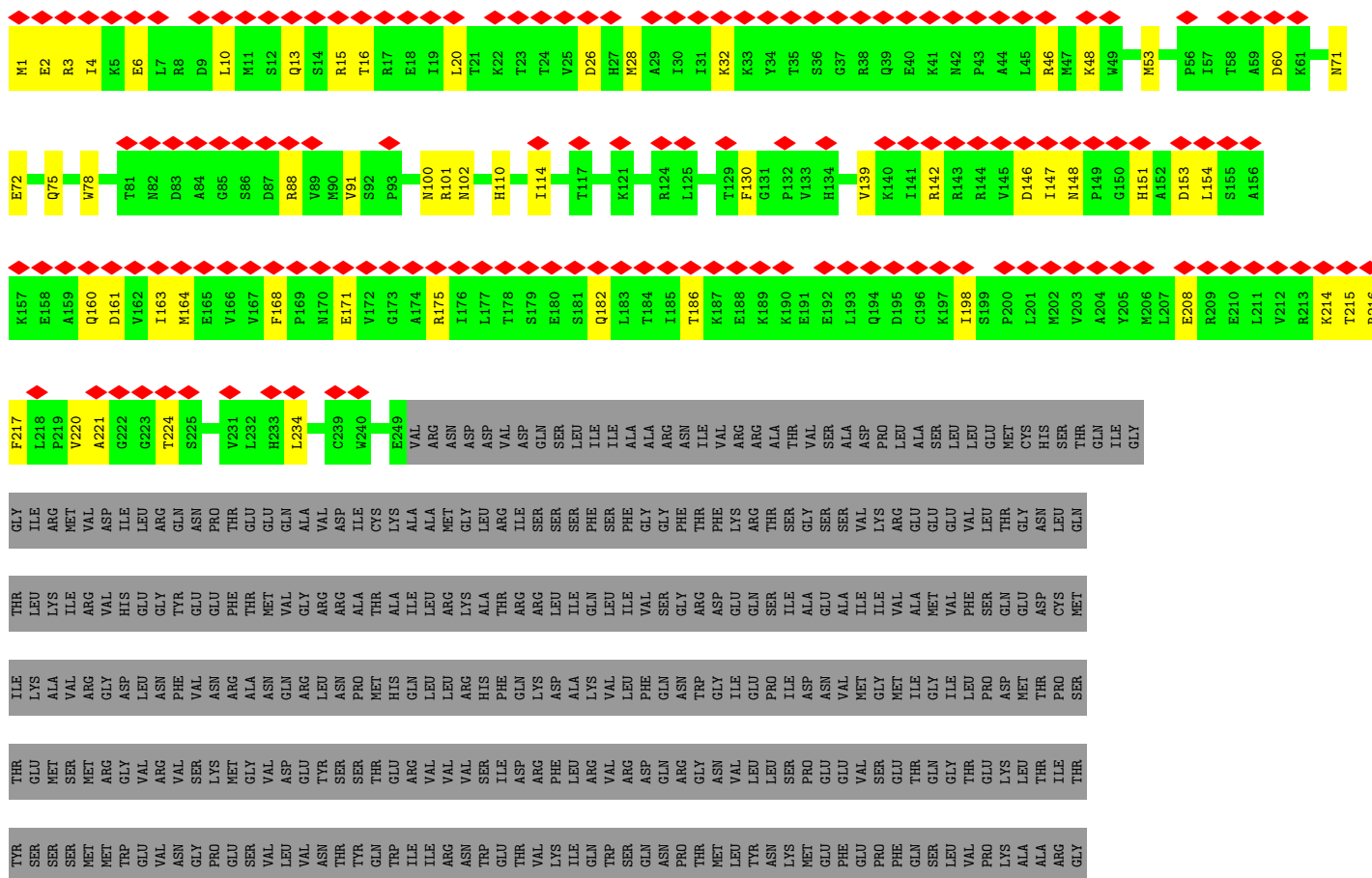
Chain B: 

M1
A14
M40
M44
S50
T57
E60
L66
D86
C87
V88
S98
I102
F103
E104
N105
E109
T110
M111
V114
R118
V119
D120
R126
Q127
T128
Y129
M134
R135
N136
A139
A142
T146
V170
S173
I181
T182
T183
H184

F185
GLN
ARG
LYS
ARG
ARG
VAL
ARG
ASP
ASN
MET
THR
THR
LYS
LYS
MET
VAL
THR
GLN
ARG
THR
ILE
GLY
K207
R215
L222
N225
E232
R239
A242
F251
L258
L266
S269
G270
L271
P272
K278
N292
D295
D305
N306
M317
V336
L337



● Molecule 3: Polymerase basic protein 2,Immunoglobulin G-binding protein A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	9.532	Depositor
Minimum map value	-5.892	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.181	Depositor
Recommended contour level	1.15	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	170, 170, 170	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0, 2.0, 2.0	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	0.25	0/4241	0.48	0/5722
2	B	0.25	0/5987	0.49	0/8075
3	C	0.26	0/2057	0.51	0/2773
4	E	0.19	0/187	0.75	0/289
5	D	0.20	0/366	0.71	0/569
6	F	0.72	0/774	1.05	3/1041 (0.3%)
All	All	0.30	0/13612	0.55	3/18469 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	68	PHE	CB-CG-CD1	7.62	126.14	120.80
6	F	68	PHE	CB-CG-CD2	-6.32	116.38	120.80
6	F	72	ARG	NE-CZ-NH1	5.48	123.04	120.30

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	4152	4118	4123	54	0
2	B	5871	5833	5847	91	0
3	C	2017	2058	2058	44	0
4	E	169	86	87	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	326	165	165	2	0
6	F	763	0	733	3	0
All	All	13298	12260	13013	173	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 173 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)
2:B:522:ASP:OD2	2:B:559:TYR:OH	1.91	0.88
5:D:5:G:OP2	5:D:5:G:N2	2.10	0.83
1:A:300:GLU:O	1:A:488:LYS:NZ	2.17	0.76
1:A:476:ALA:O	1:A:506:LYS:NZ	2.19	0.76
1:A:350:ASN:OD1	1:A:351:GLU:N	2.19	0.76

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	515/716 (72%)	495 (96%)	20 (4%)	0	100	100
2	B	731/757 (97%)	709 (97%)	22 (3%)	0	100	100
3	C	247/905 (27%)	233 (94%)	14 (6%)	0	100	100
6	F	92/133 (69%)	90 (98%)	2 (2%)	0	100	100
All	All	1585/2511 (63%)	1527 (96%)	58 (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	A	462/640 (72%)	462 (100%)	0	100	100
2	B	648/669 (97%)	644 (99%)	4 (1%)	86	92
3	C	223/788 (28%)	223 (100%)	0	100	100
6	F	78/107 (73%)	74 (95%)	4 (5%)	24	50
All	All	1411/2204 (64%)	1403 (99%)	8 (1%)	86	92

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	82	GLN
6	F	76	LYS
6	F	12	VAL
2	B	745	LYS
6	F	65	LYS

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	7/17 (41%)	1 (14%)	0
5	D	14/15 (93%)	4 (28%)	0
All	All	21/32 (65%)	5 (23%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	2	G
5	D	6	A
5	D	8	A
5	D	11	A

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Mol	Chain	Res	Type
5	D	15	C

There are no RNA pucker outliers to report.

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 [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12362. 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](#)

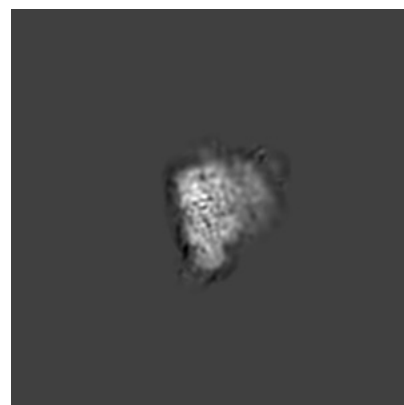
6.1.1 Primary map



X



Y



Z

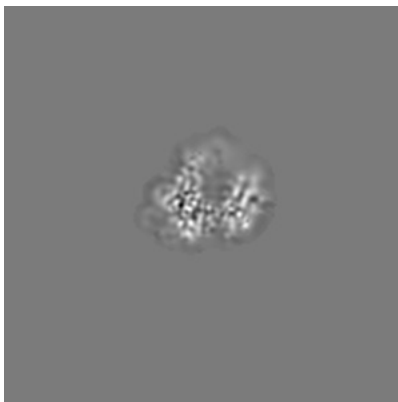
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 85



Y Index: 85

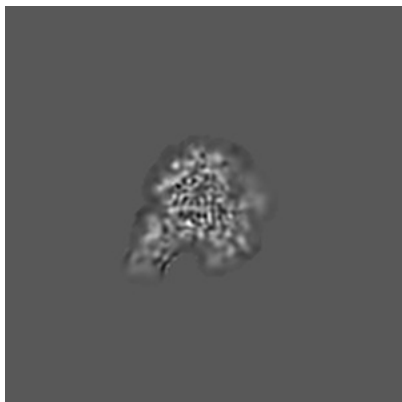


Z Index: 85

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: 81



Y Index: 90

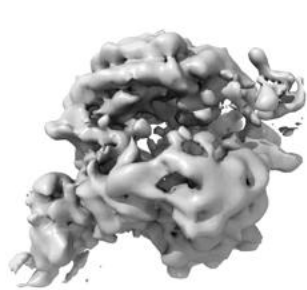


Z Index: 78

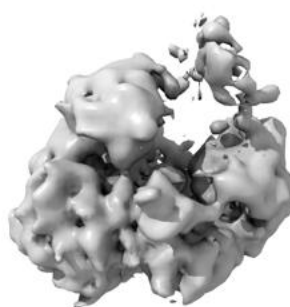
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

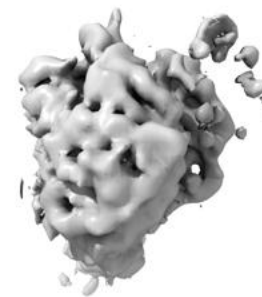
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

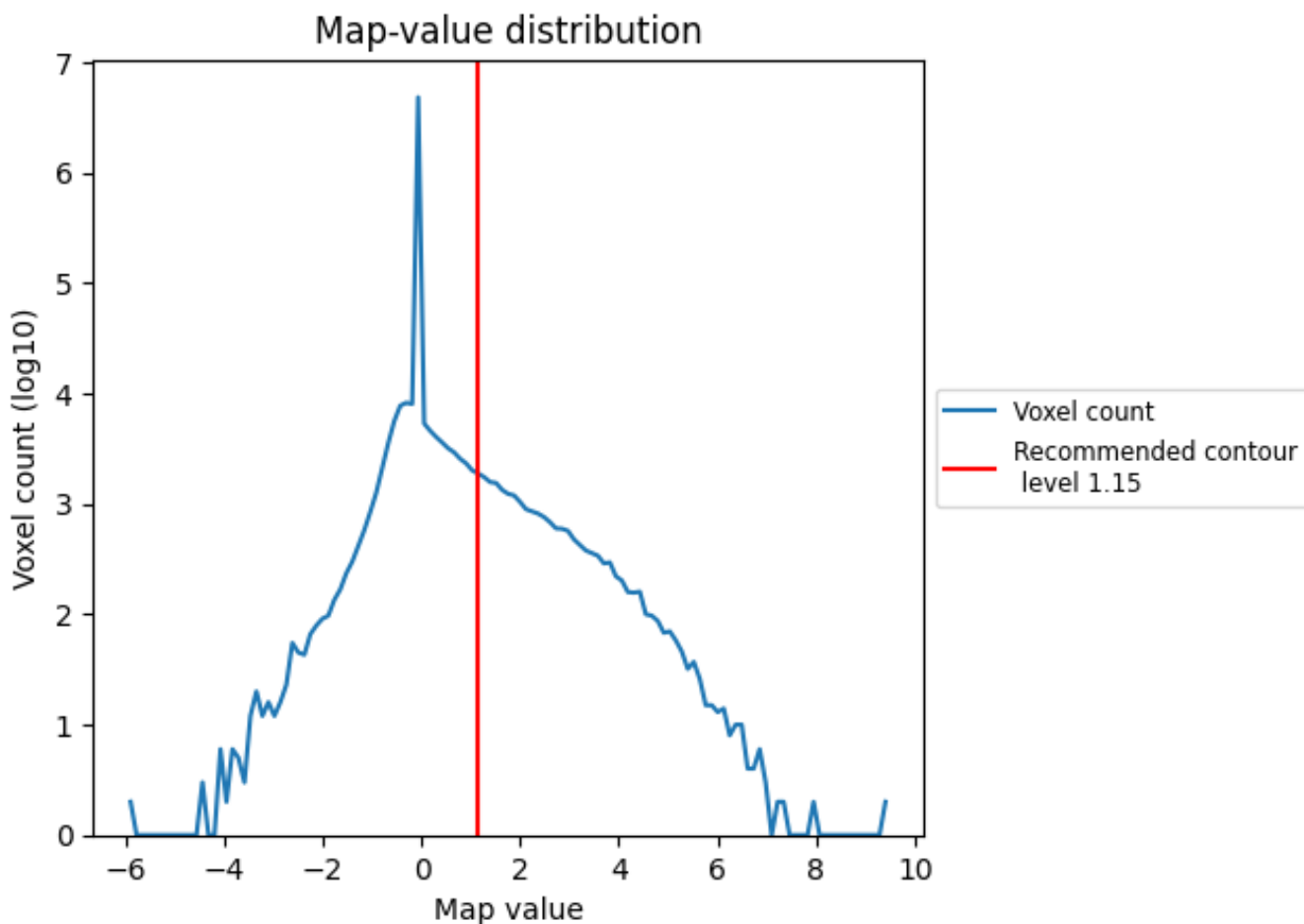
6.5 Mask visualisation

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

7 Map analysis [i](#)

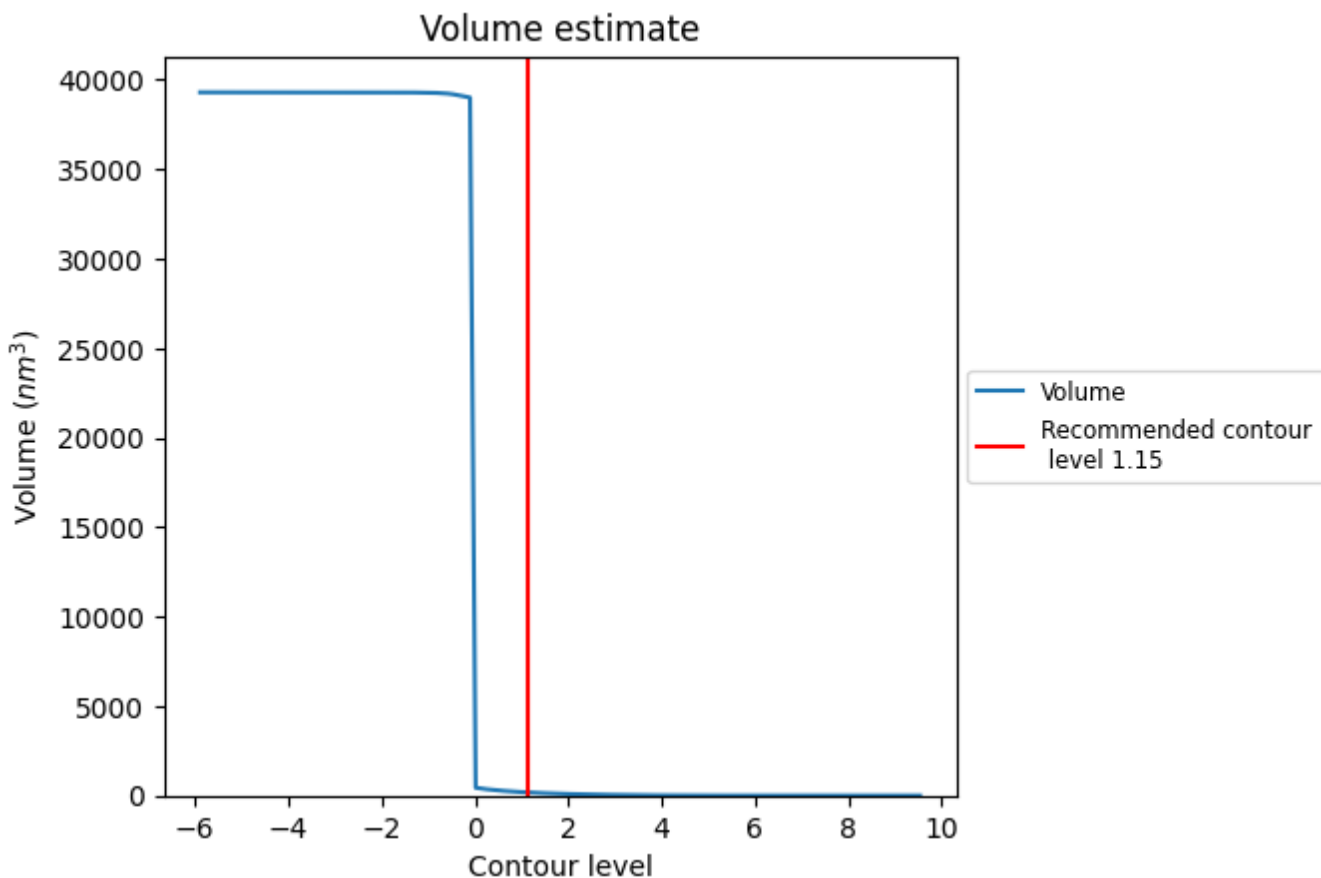
This section contains the results of statistical analysis of the map.

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.

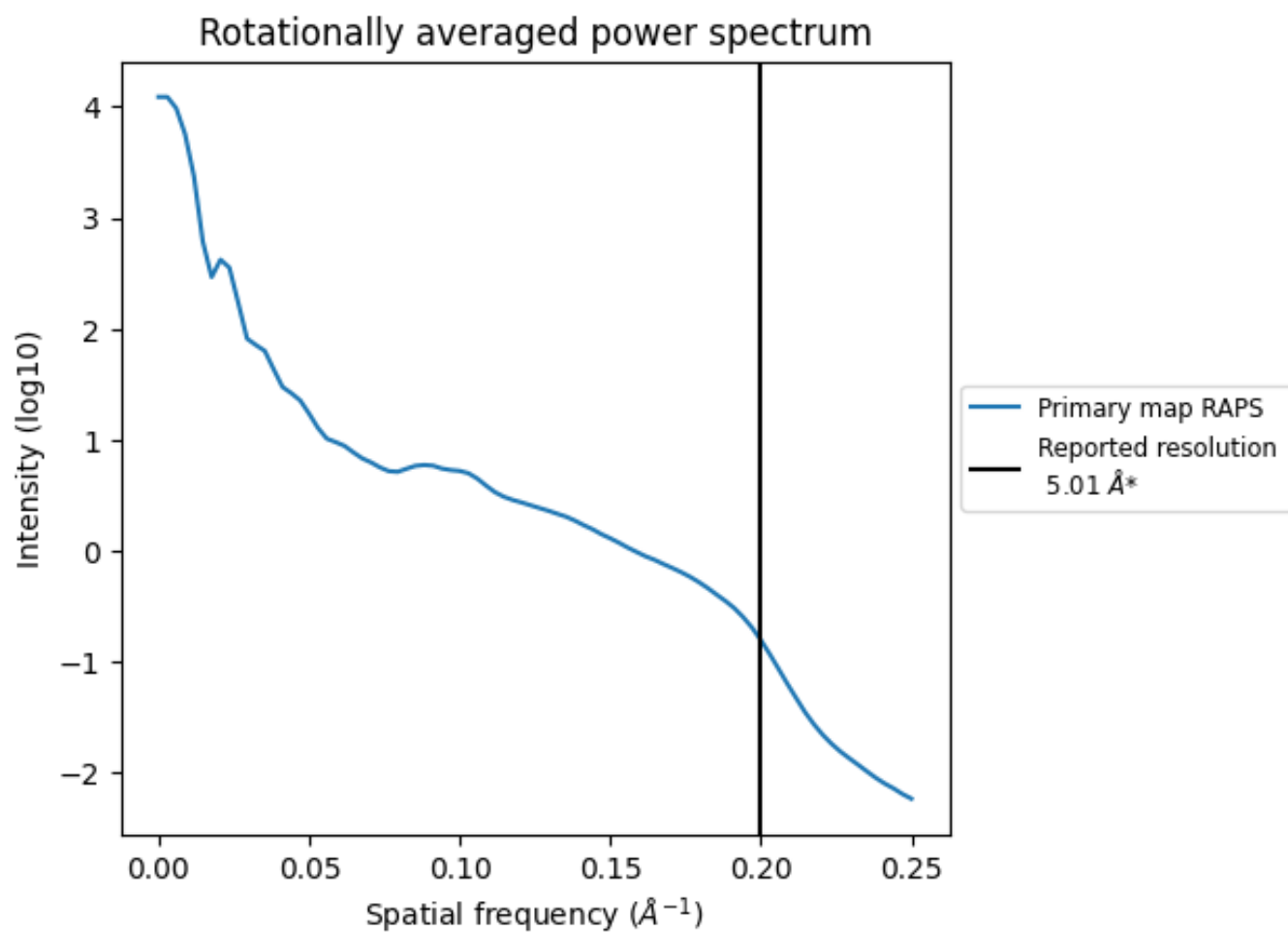
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 156 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 0.200 Å⁻¹

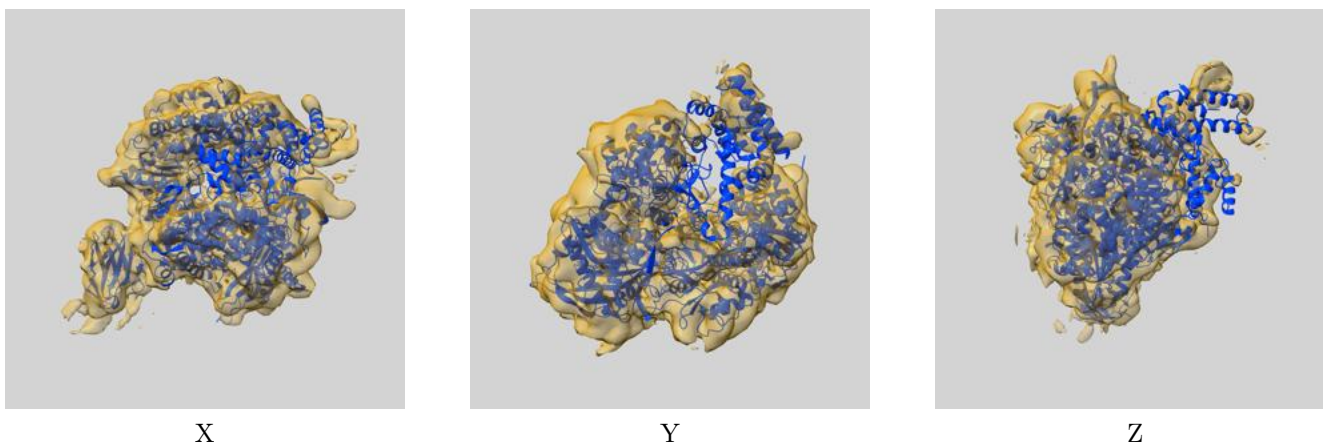
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

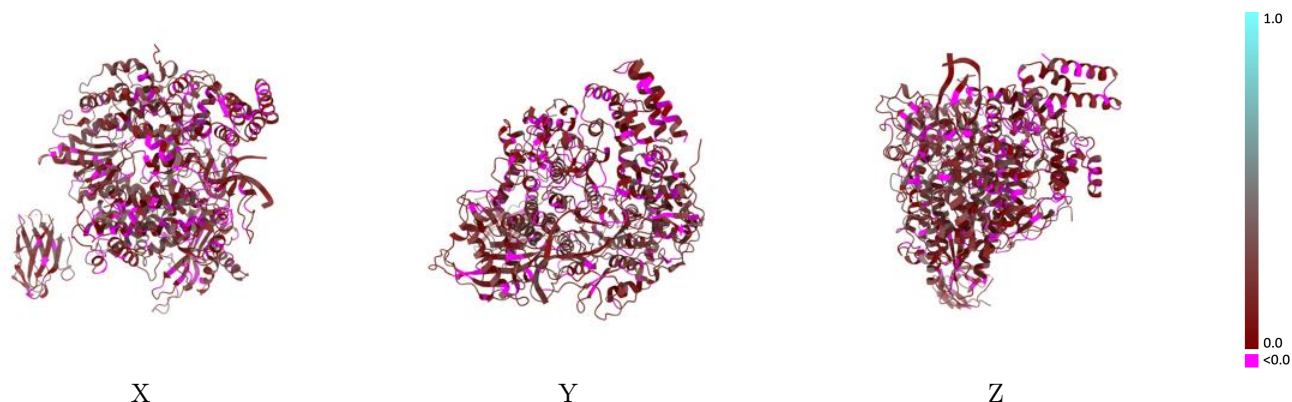
This section contains information regarding the fit between EMDB map EMD-12362 and PDB model 7NIL. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



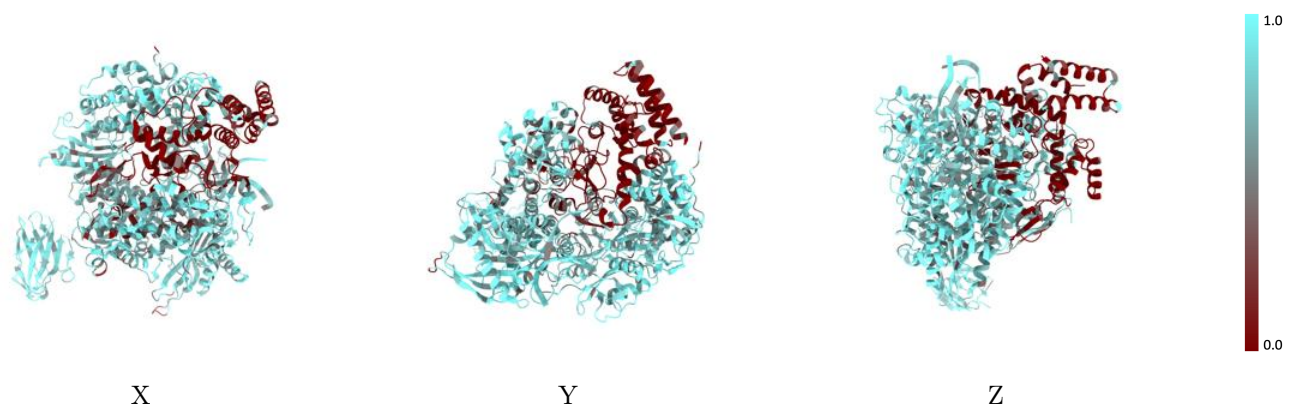
The images above show the 3D surface view of the map at the recommended contour level 1.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



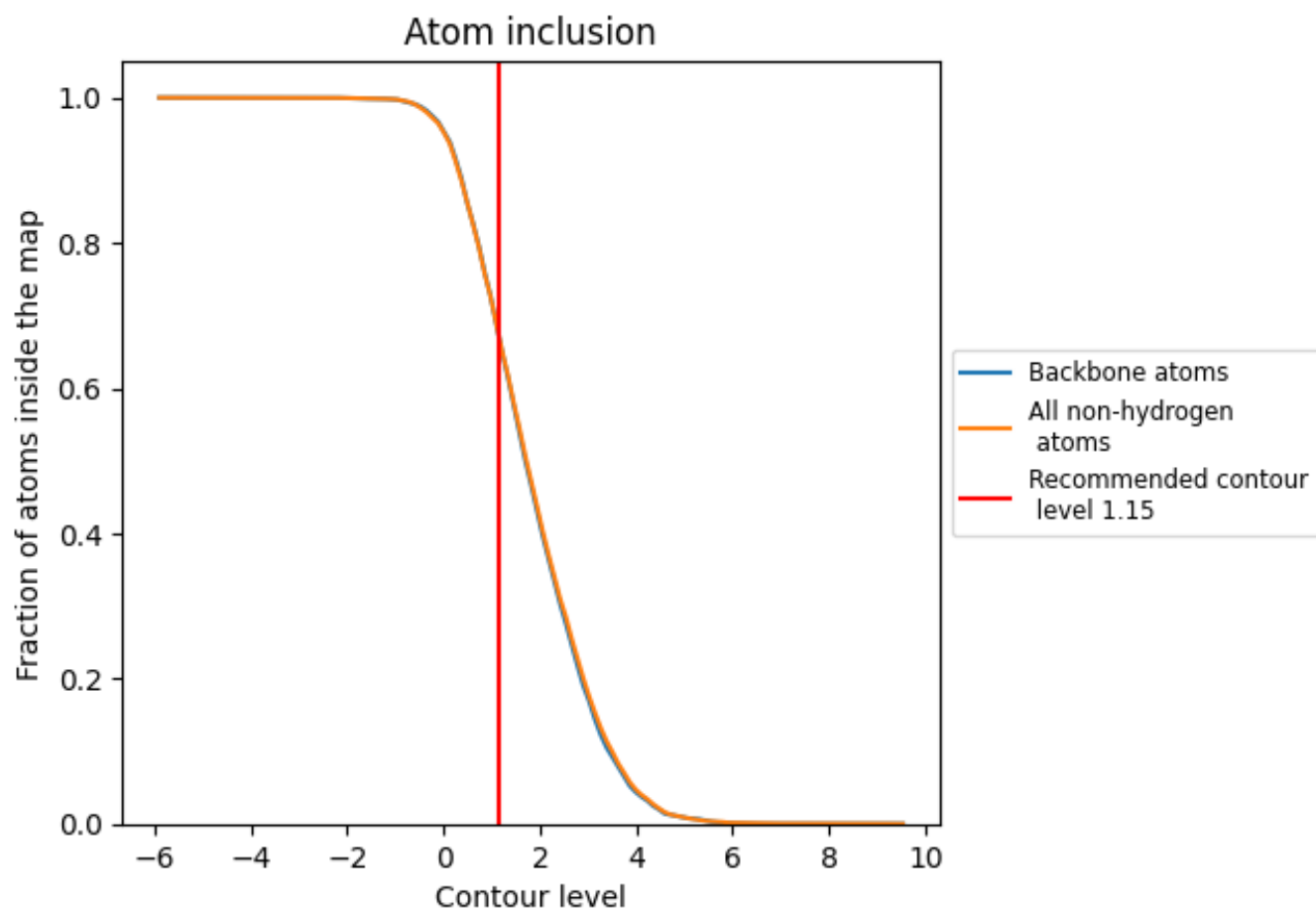
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.15).















9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 67% 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 (1.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6713	 0.1370
A	 0.8065	 0.1630
B	 0.6667	 0.1360
C	 0.3449	 0.0720
D	 0.9110	 0.1820
E	 0.5740	 0.1230
F	 0.8725	 0.1610

