



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:21 PM EST

PDB ID : 3IYO
EMDB ID : EMD-5173
Title : Cryo-EM model of virion-sized HEV virion-sized capsid
Authors : Xing, L.; Mayazaki, N.; Li, T.C.; Simons, M.N.; Wall, J.S.; Moore, M.; Wang, C.Y.; Takeda, N.; Wakita, T.; Miyamura, T.; Cheng, R.H.
Deposited on : 2010-03-19
Resolution : 10.50 Å(reported)
Based on initial model : 2ZZQ

This is a Full wwPDB EM Validation 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


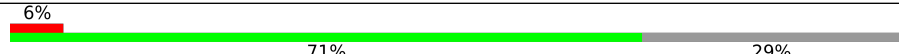
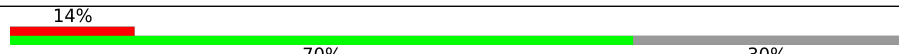
The reported resolution of this entry is 10.50 Å.

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

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	660	
1	B	660	
1	D	660	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1397 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.

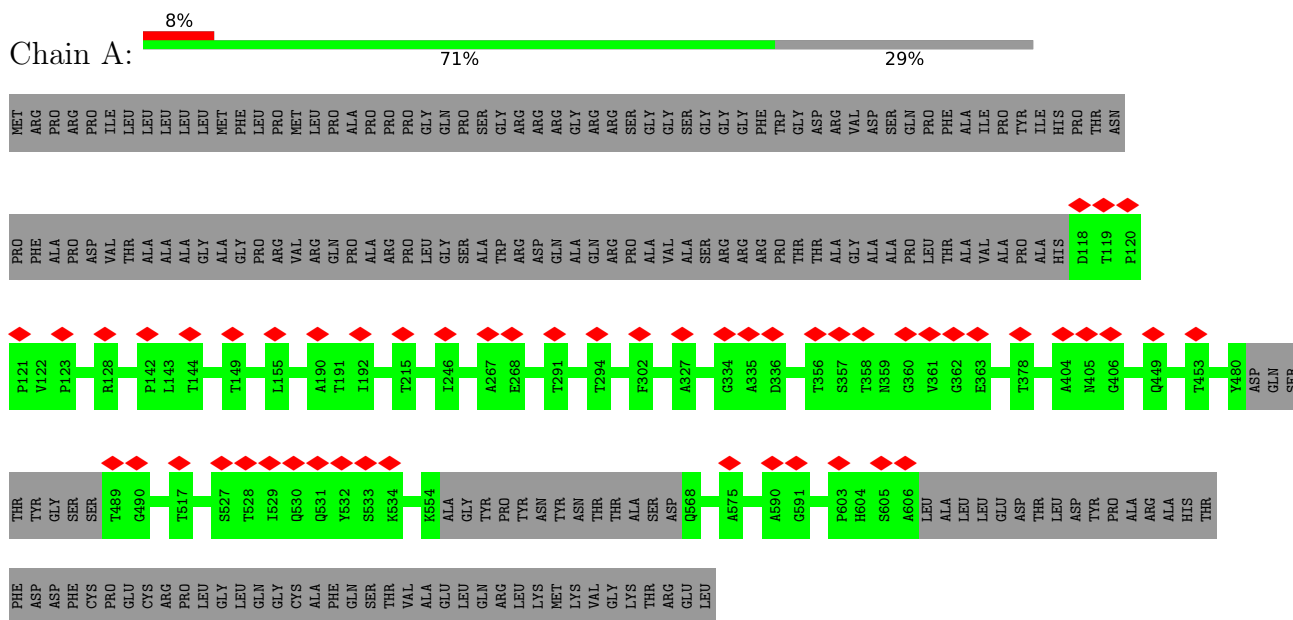
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	468	Total 468	C 468	0	468
1	B	468	Total 468	C 468	0	468
1	D	461	Total 461	C 461	0	461

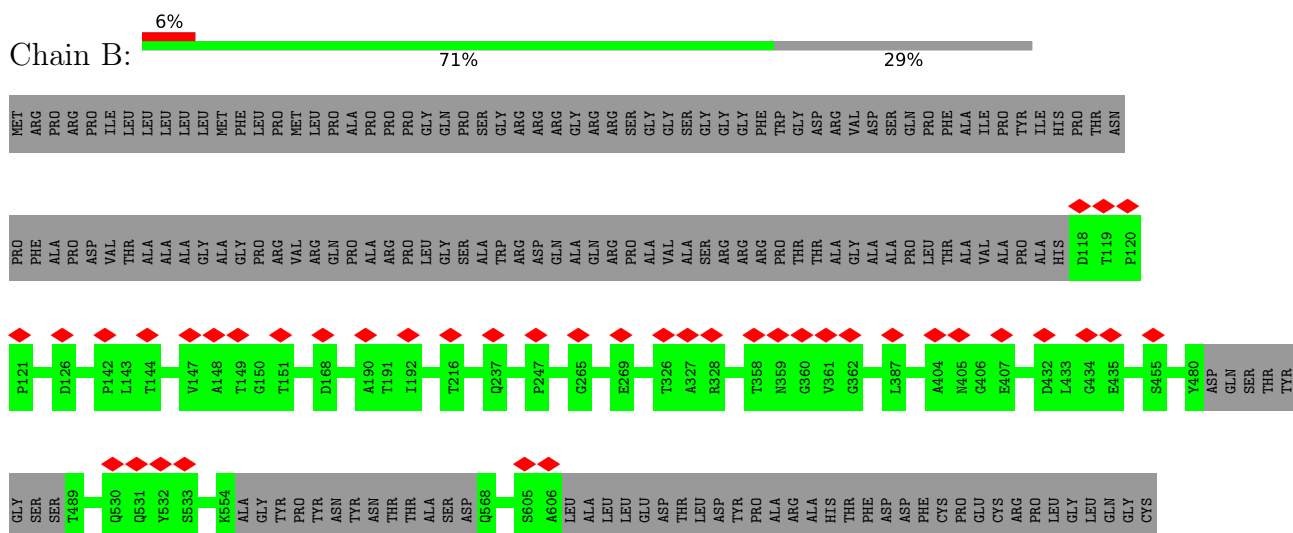
3 Residue-property plots

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: Capsid protein



• Molecule 1: Capsid protein



ALA
PHE
GLN
SER
THR
VAL
ALA
GLU
LEU
LEU
GLN
ARG
LEU
LYS
MET
LYS
VAL
VAL
GLY
LYS
THR
ARG
GLU
LEU

● Molecule 1: Capsid protein



MET
ARG
PRO
ARG
PRO
ILE
LEU
LEU
LEU
LEU
LEU
MET
PHE
LEU
PRO
MET
LEU
PRO
ALA
PRO
PRO
GLY
GLN
PRO
SER
GLY
ARG
ARG
GLN
GLY
ARG
ARG
SER
GLY
ASP
ARG
VAL
ASP
SER
GLN
PRO
PHE
ALA
ILE
PRO
TYR
ILE
HIS
PRO
THR
ASN

PRO
PHE
ALA
PRO
ASP
VAL
THR
ALA
ALA
ALA
GLY
GLY
GLY
GLY
GLY
GLY
PHE
TRP
GLY
ASP
ARG
VAL
ASP
SER
GLN
PRO
PHE
ALA
ALA
VAL
VAL
ALA
ALA
HIS
D118
T119
P120

P121
V122
P123
D124
V125
D126
S127
R128
G129
S146
V147
A148
T149
A158
I246
S264
G265
V266
T291
P292
A303
R319
T326
A327
R328
R351
T356
S357
T358
N359
D377
T378
A404
N405
G406
E407
E448
GLN
ASP
ARG
PRO
THR
PRO
SER
P456
A457
P458

S459
S463
V464
L465
R466
A477
A478
E479
Y490
ASP
GLN
SER
THR
TYR
GLY
SER
SER
T489
G490
P491
V494
S495
D496
S497
T505
G506
A507
Q508
A509
V510
A511
R512
S513
L514
D515
W516
T517
K518
V519
T520
L521
D522
G523
R524
S527
T528
I529
Q530
Q531
Y532
S533
K534
T535
F536

A550
G551
A584
ALA
TYR
PRO
TYR
TYR
ASN
ASN
THR
THR
ALA
SER
ASP
Q568
A574
A575
G576
H577
S582
T583
Y584
T585
T586
S587
L588
G589
A590
G591
P592
V593
S605
A606
LEU
ALA
LEU
LEU
GLU
ASP
THR
LEU
ASP
TYR
PRO
ALA
ALA
ALA
HIS
THR
PHE
ASP
PHE
CYS

PRO
GLU
CYS
ARG
PRO
LEU
GLY
LEU
GLN
GLY
CYS
PHE
GLN
SER
THR
VAL
ALA
GLU
LEU
GLN
ARG
LEU
LYS
MET
LYS
VAL
GLY
LYS
THR
ARG
GLU
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4348	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEOL 2100F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	50000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	30.429	Depositor
Minimum map value	-22.953	Depositor
Average map value	-0.064	Depositor
Map value standard deviation	3.546	Depositor
Recommended contour level	5.2	Depositor
Map size (\AA)	634, 634, 634	wwPDB
Map dimensions	317, 317, 317	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2, 2, 2	Depositor

5 Model quality

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	468	0	0	0	0
1	B	468	0	0	0	0
1	D	461	0	0	0	0
All	All	1397	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 [i](#)

There are no chain breaks in this entry.

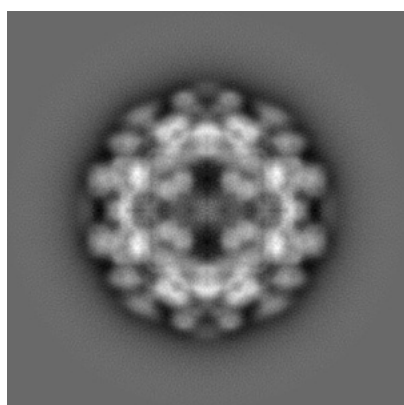
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5173. These allow visual inspection of the internal detail of the map and identification of artifacts.

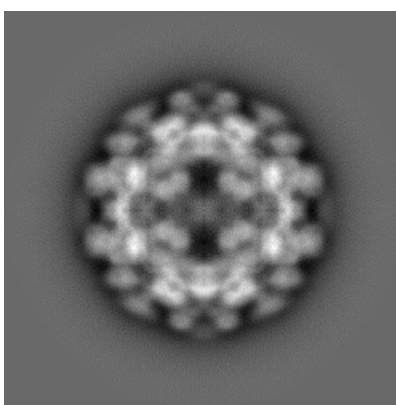
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

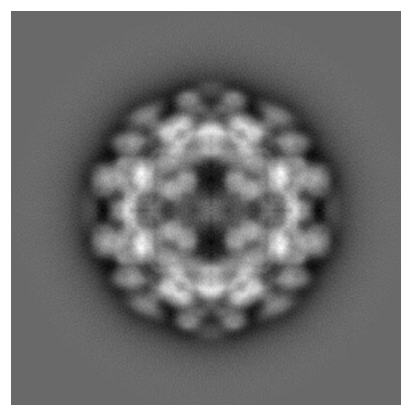
6.1.1 Primary map



X



Y

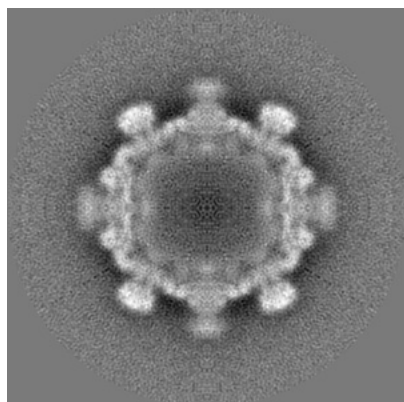


Z

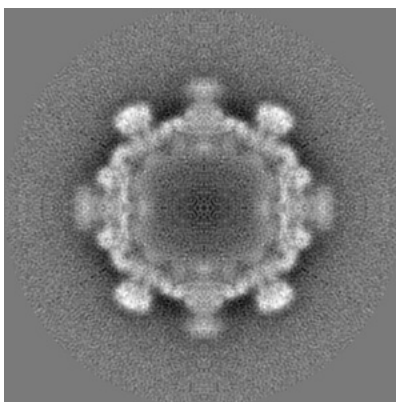
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

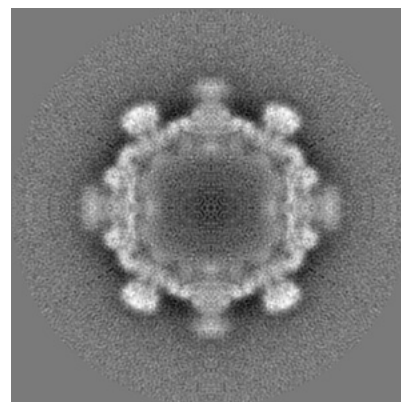
6.2.1 Primary map



X Index: 158



Y Index: 158

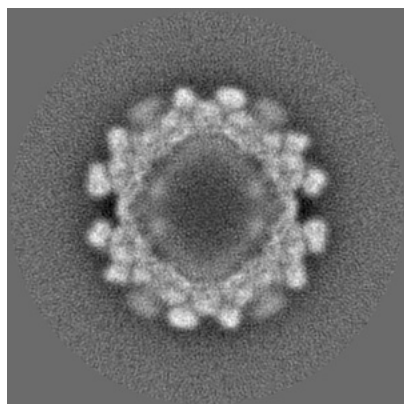


Z Index: 158

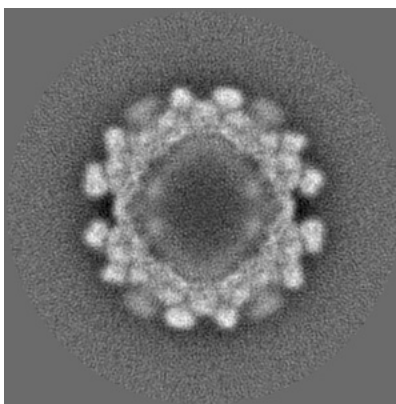
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

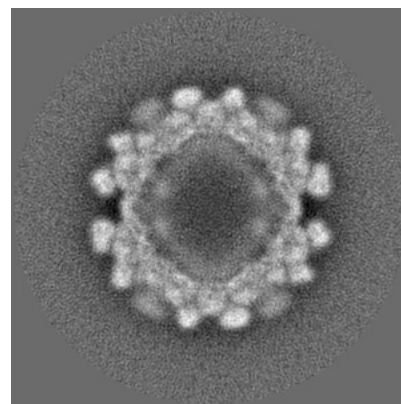
6.3.1 Primary map



X Index: 181



Y Index: 181

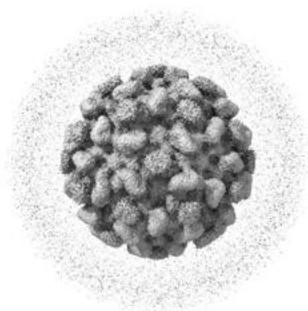


Z Index: 135

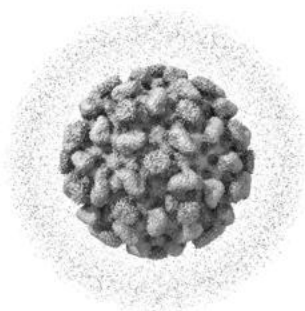
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

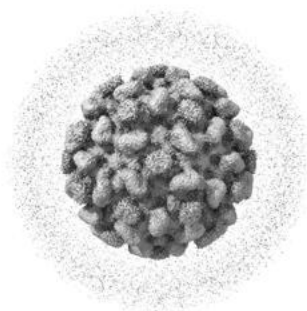
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

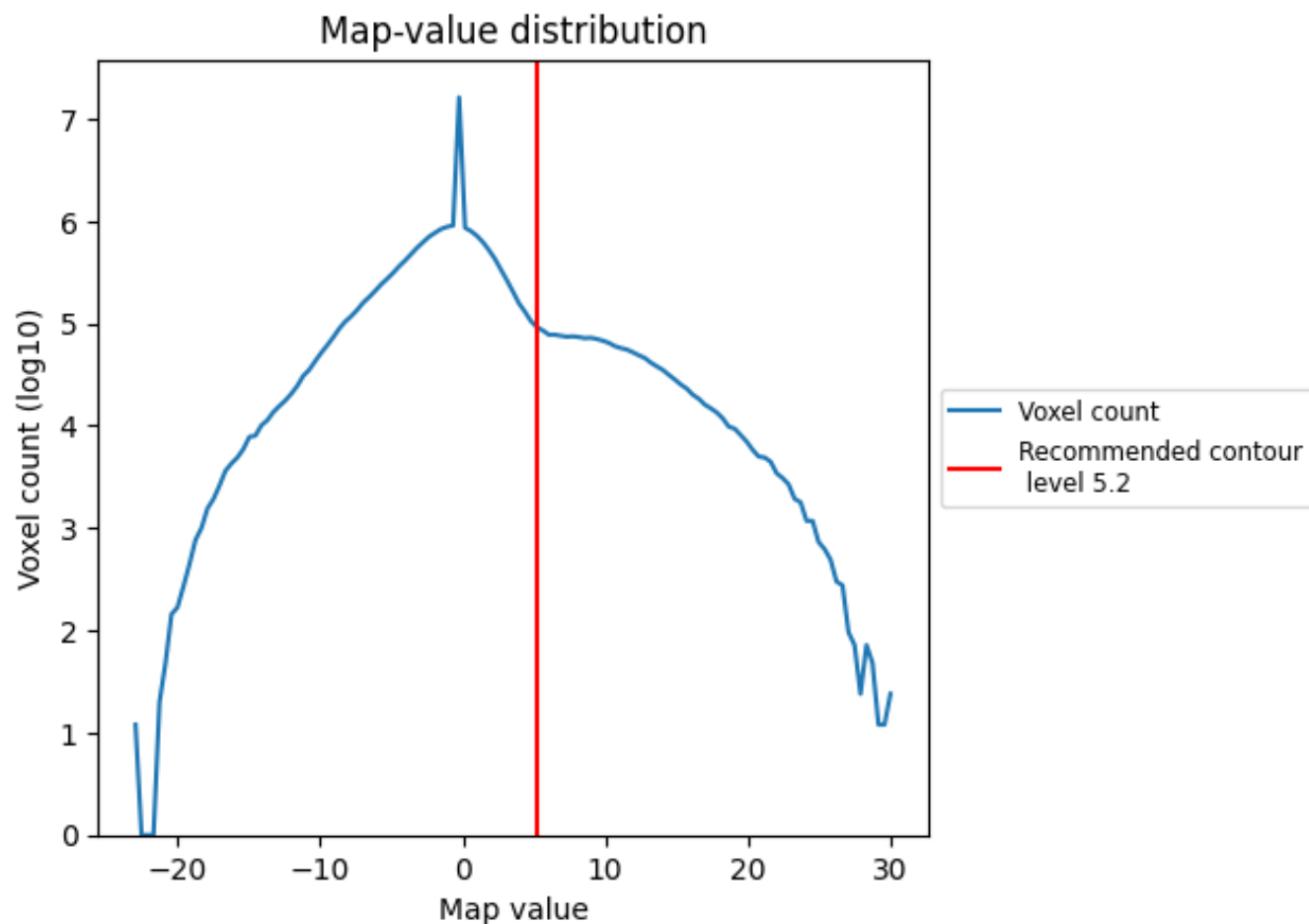
6.5 Mask visualisation

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

7 Map analysis [i](#)

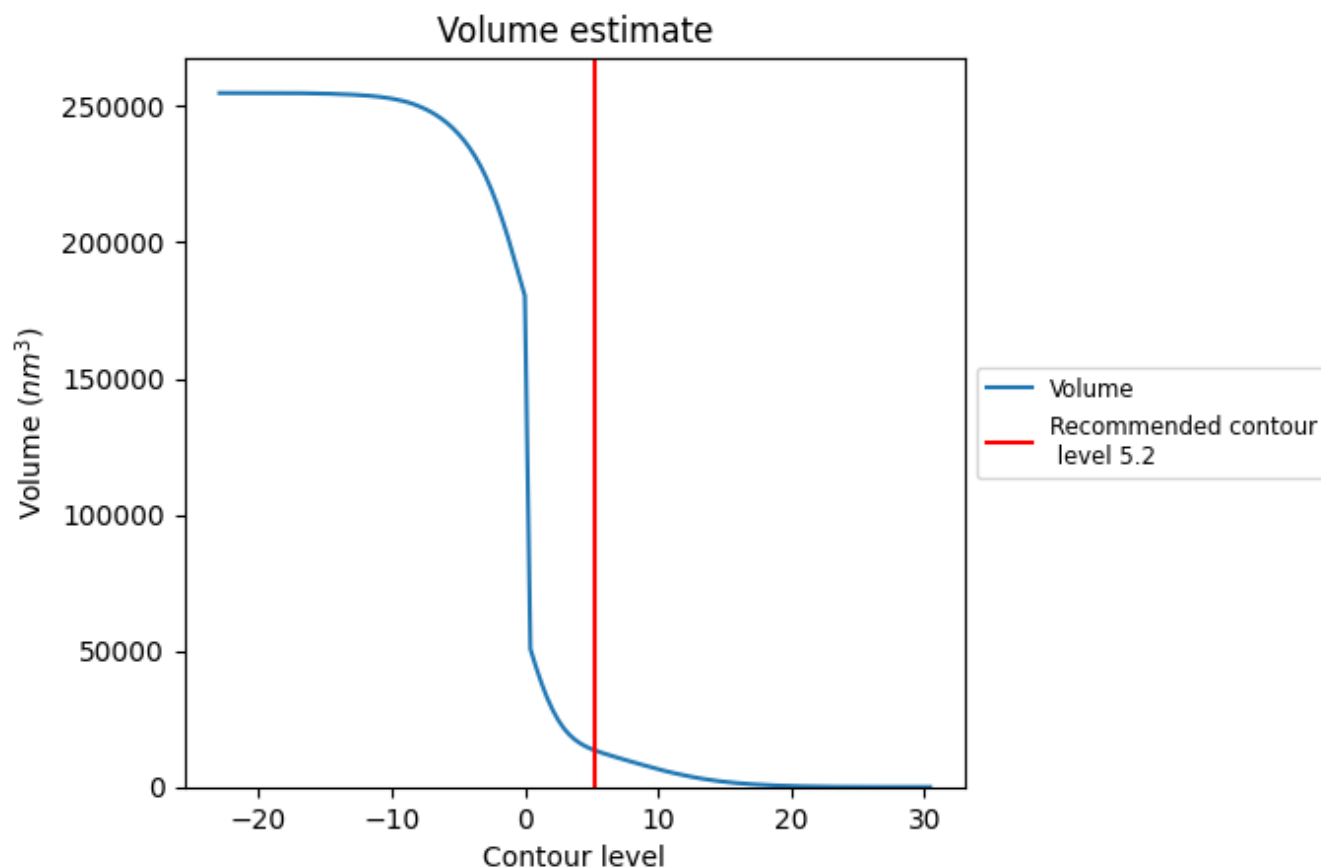
This section contains the results of statistical analysis of the map.

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.

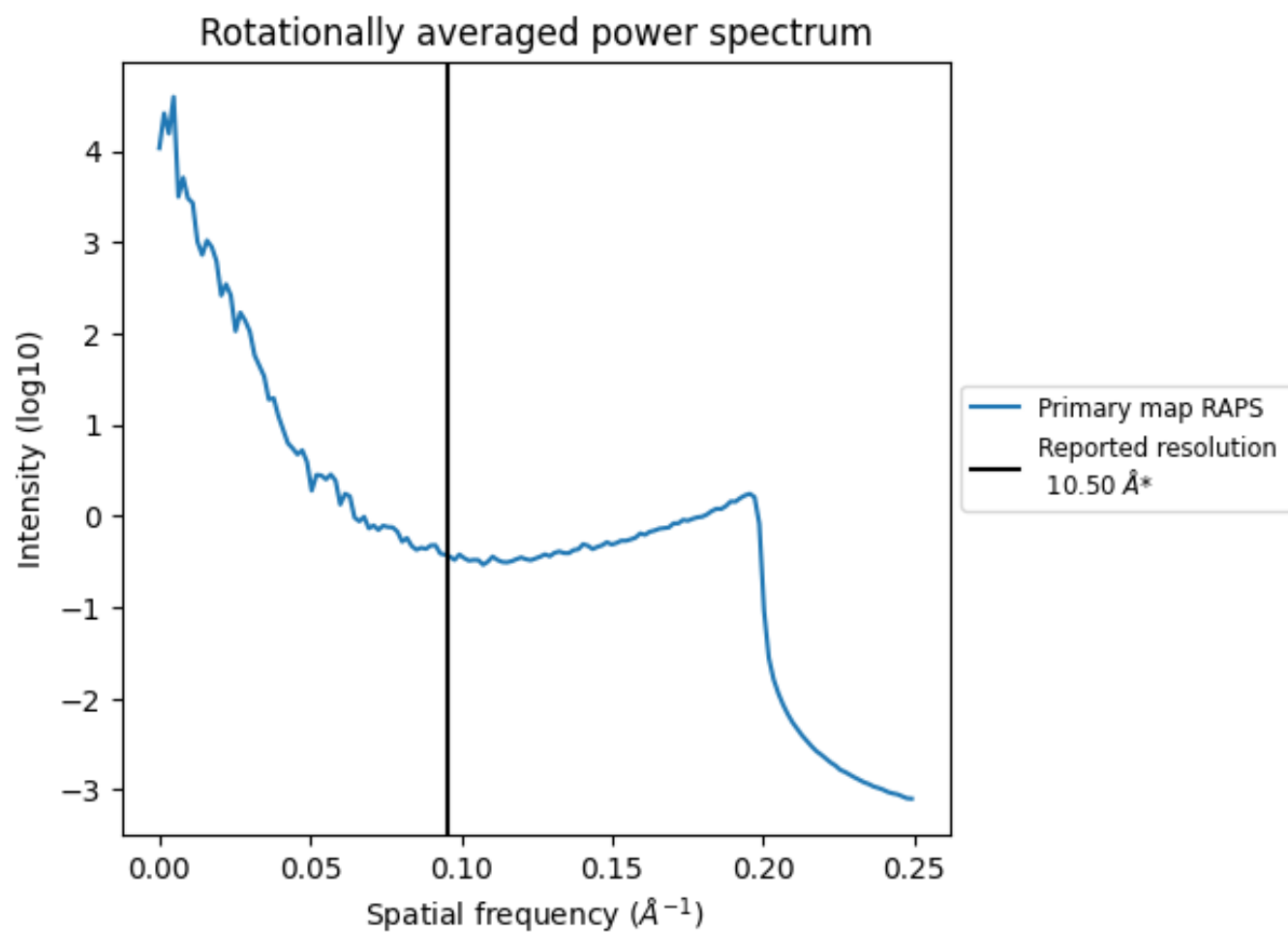
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13531 nm^3 ; this corresponds to an approximate mass of 12223 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.095 Å⁻¹

8 Fourier-Shell correlation

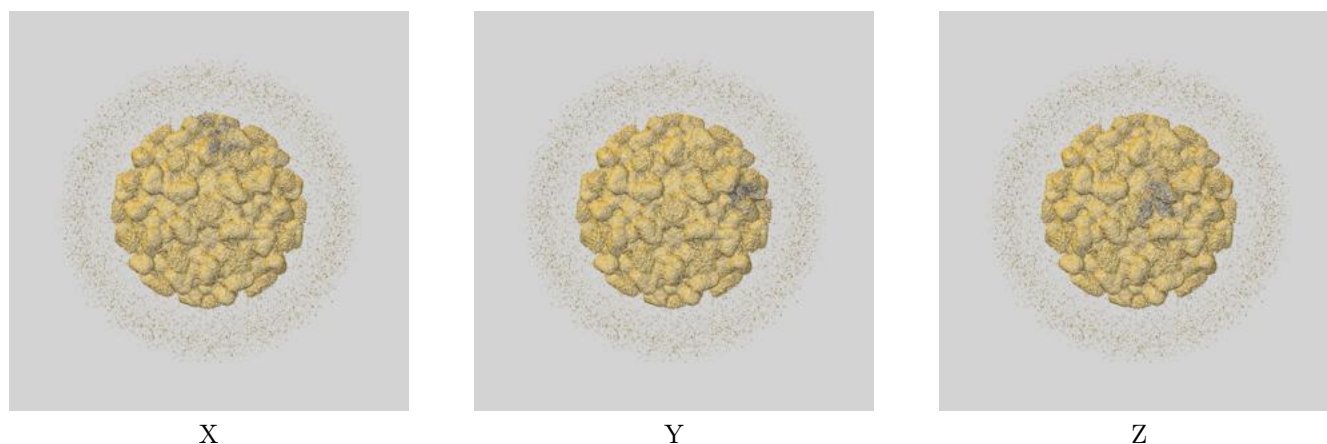
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

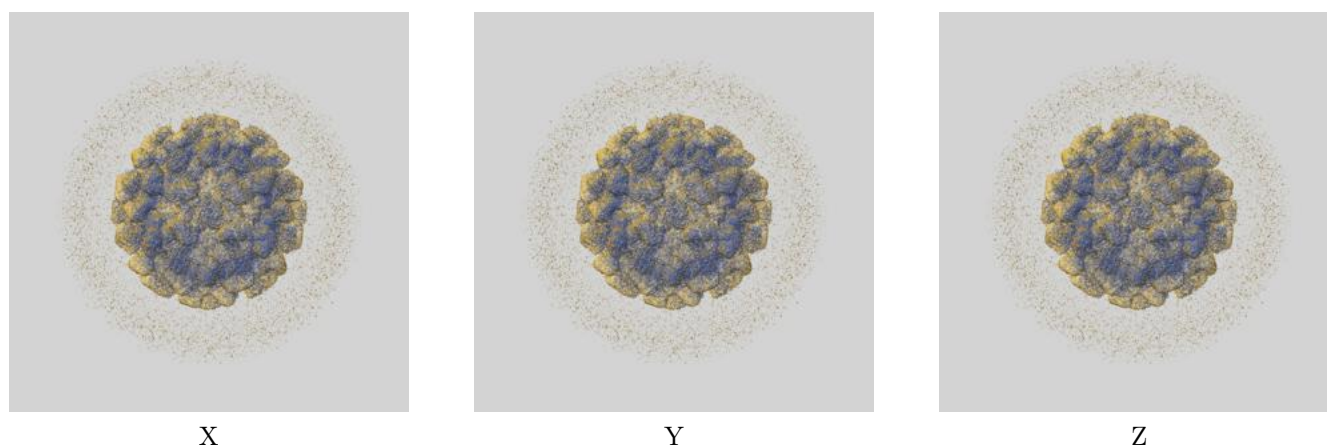
This section contains information regarding the fit between EMDB map EMD-5173 and PDB model 3IYO. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

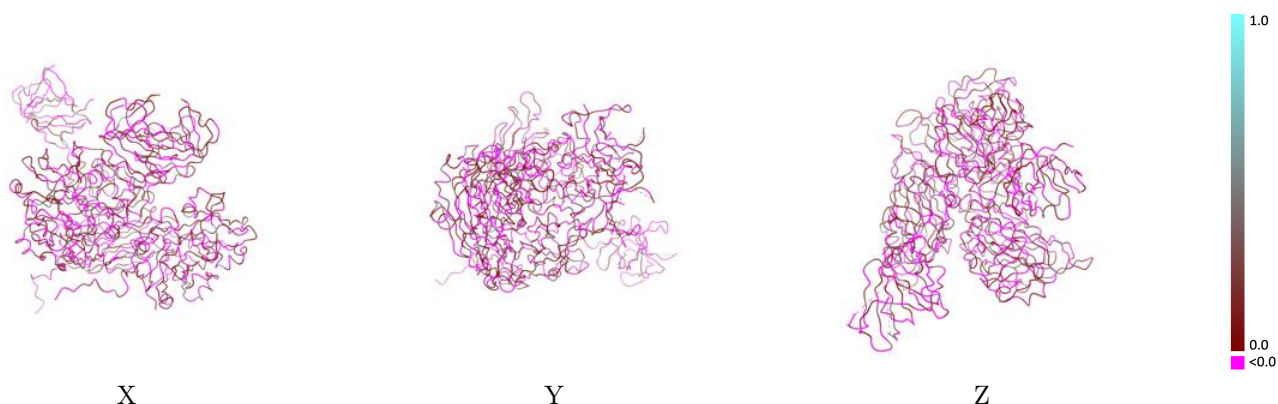


9.1.2 Map-model assembly overlay [i](#)



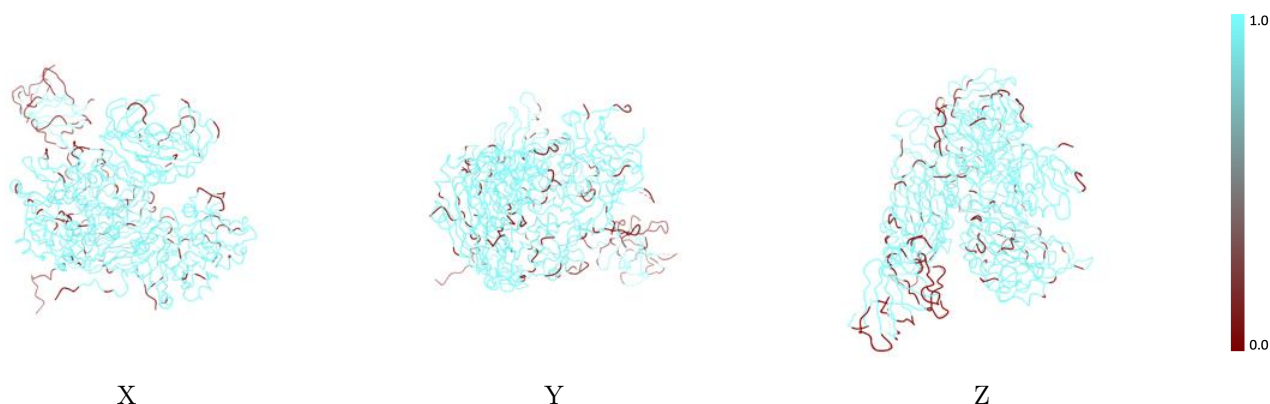
The images above show the 3D surface view of the map at the recommended contour level 5.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



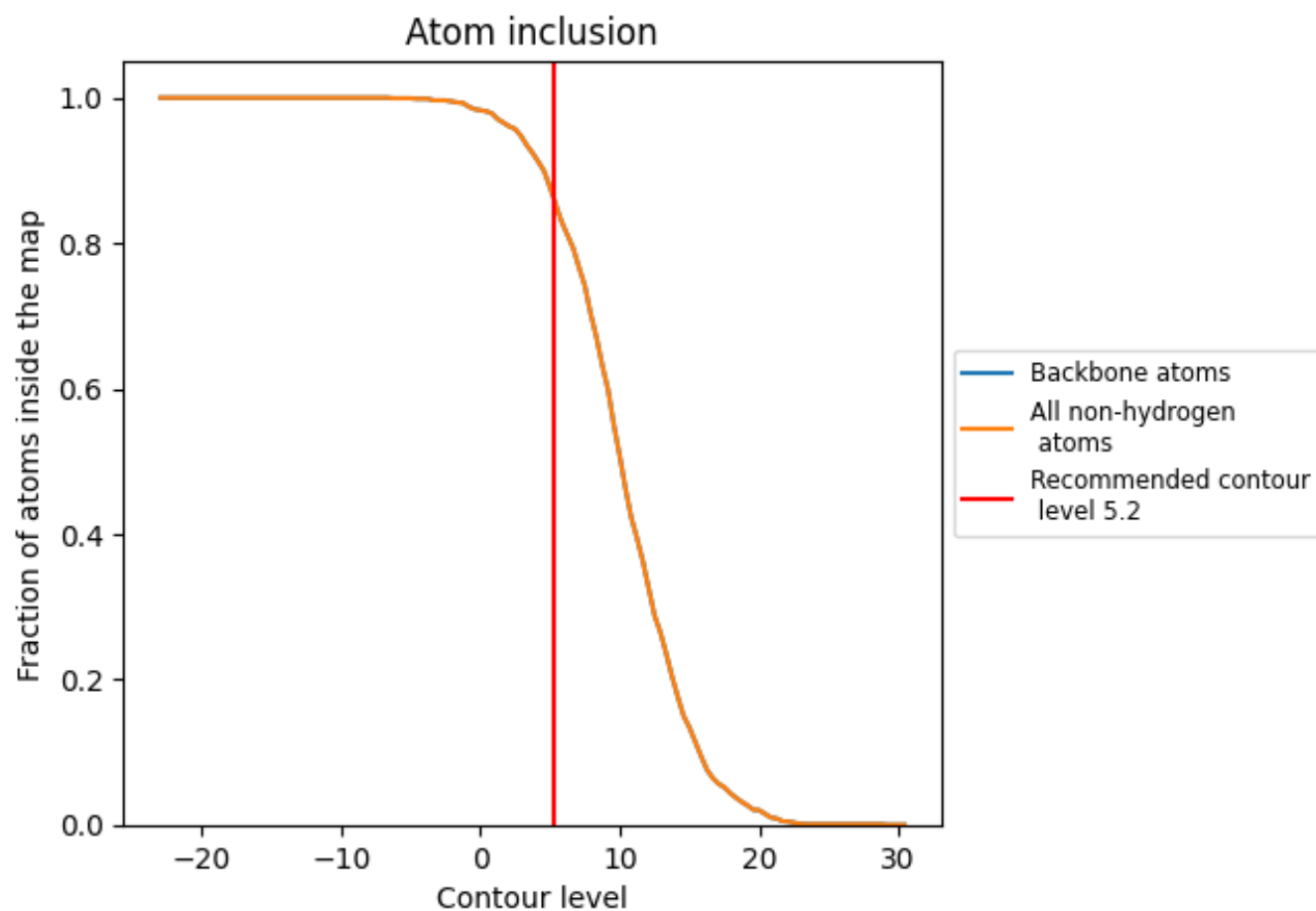
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (5.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8654	<div><div></div></div> 0.0350
A	<div><div></div></div> 0.8868	<div><div></div></div> 0.0290
B	<div><div></div></div> 0.9124	<div><div></div></div> 0.0370
D	<div><div></div></div> 0.7961	<div><div></div></div> 0.0400

