Full wwPDB EM Validation Report (i)

Apr 28, 2024 – 10:42 pm BST

PDB ID	:	2C8I
EMDB ID	:	EMD-1183
Title	:	Complex Of Echovirus Type 12 With Domains 1, 2, 3 and 4 Of Its Receptor Decay Accelerating Factor (Cd55) By Cryo Electron Microscopy At 16 A
Authors	:	Pettigrew, D.M.; Williams, D.T.; Kerrigan, D.; Evans, D.J.; Lea, S.M.; Bhella, D.
Deposited on	:	2005-12-05
Resolution	:	14.00 Å(reported)
Based on initial model	:	1H8T

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 (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 (i)) were used in the production of this report:

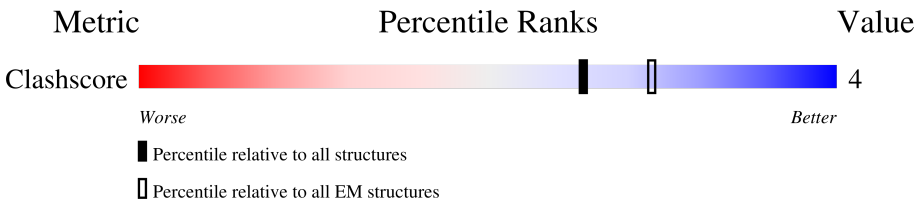
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 14.00 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

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	289	16% / 100%
2	B	252	12% / 100%
3	C	238	10% / 100%
4	D	60	• / 100%
5	E	316	80% / 78% • 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1161 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 ECHOVIRUS 11 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
1	A	289	289	289	0	289

- Molecule 2 is a protein called ECHOVIRUS 11 COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
2	B	252	252	252	0	252

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	226	PHE	SER	conflict	UNP P29813

- Molecule 3 is a protein called ECHOVIRUS 11 COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	C	238	238	238	0	238

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	63	GLU	GLN	conflict	UNP P29813

- Molecule 4 is a protein called ECHOVIRUS 11 COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
4	D	60	60	60	0	60

- Molecule 5 is a protein called COMPLEMENT DECAY-ACCELERATING FACTOR.

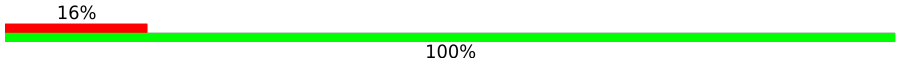
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
5	E	252	322	322	70	252

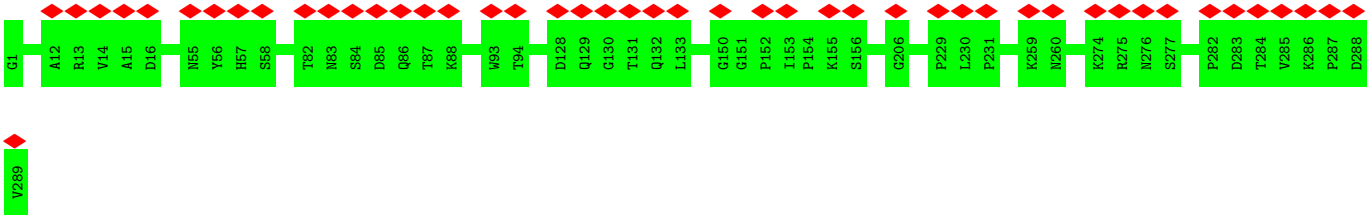
3 Residue-property plots (i)

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: ECHOVIRUS 11 COAT PROTEIN VP1

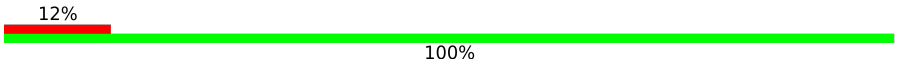
Chain A:

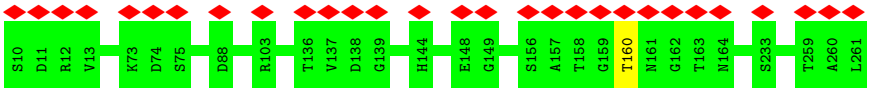




• Molecule 2: ECHOVIRUS 11 COAT PROTEIN VP2

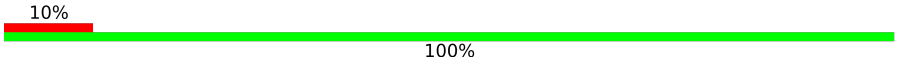
Chain B:

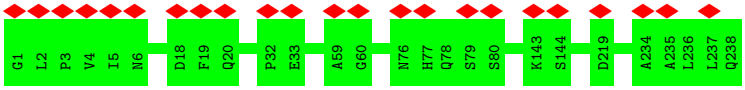




• Molecule 3: ECHOVIRUS 11 COAT PROTEIN VP3

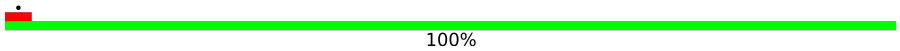
Chain C:

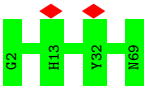




• Molecule 4: ECHOVIRUS 11 COAT PROTEIN VP4

Chain D:





• Molecule 5: COMPLEMENT DECAY-ACCELERATING FACTOR

Chain E:

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

CYS ASN ARG SER Q2 D3 C4 G5 L6 P7 P8 D9 V10 P11 N12 A13 Q14 P15 A16 L17 E18 G19 R20 T21 S22 F23 P24 E25 D26 T27 V28 I29 T30 Y31 K32 C33 E34 E35 S36 F37 V38 K39 I40 P41 G42 E43 K44 D45 S46 V47 I48 C49 L50 K51 G52 S53 Q54 W55 S56 D57

I58 E59 E60 F61 C62 N63 R64 S65 C66 E67 V68 P69 T70 R71 L72 N73 S74 A75 S76 L77 K78 Q79 P80 Y81 I82 T83 Q84 N85 Y86 F87 P88 V89 G90 T91 V92 V93 E94 Y95 E96 C97 R98 P99 G100 Y101 R102 R103 E104 P105 S106 L107 S108 P109 K110 L111 T112 C113 L114 Q115 N116 L117

K118 W119 S120 T121 A122 V123 E124 F125 C126 K127 K128 K129 S130 C131 P132 N133 P134 G135 E136 I137 R138 N139 G140 Q141 I142 D143 V144 P145 G146 G147 I148 L149 F150 G151 A152 T153 I154 S155 F156 S157 C158 N159 T160 G161 Y162 K163 L164 F165 G166 S167 T168 S169 S170 F171 C172 L173 I174 S175 G176 S177

S178 V179 Q180 W181 S182 D183 P184 L185 P186 E187 C188 R189 E190 I191 Y192 C193 P194 A195 P196 P197 Q198 I199 D200 N201 G202 I203 I204 Q205 G206 E207 R208 D209 H210 Y211 G212 Y213 R214 Q215 S216 V217 T218 Y219 A220 C221 N222 K223 G224 F225 T226 M227 I228 G229 E230 H231 S232 I233 Y234 C235 T236 V237

N238 N239 D240 E241 G242 E243 W244 S245 G246 P247 P248 P249 E250 C251 R252 G253

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1501	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS PAIR IMAGES OF INDIVIDUAL PARTICLES	Depositor
Microscope	JEOL 1200	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	29100	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	445.578	Depositor
Minimum map value	-239.684	Depositor
Average map value	6.396	Depositor
Map value standard deviation	58.957	Depositor
Recommended contour level	148.0	Depositor
Map size (Å)	555.9, 555.9, 555.9	wwPDB
Map dimensions	255, 255, 255	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.18, 2.18, 2.18	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).

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 (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	289	0	0	0	0
2	B	252	0	0	1	0
3	C	238	0	0	0	0
4	D	60	0	0	0	0
5	E	322	0	0	5	0
All	All	1161	0	0	5	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 4.

All (5) 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:160:THR:CA	5:E:159:ASN:CA	2.47	0.92
5:E:18[A]:GLU:CA	5:E:19[A]:GLY:CA	2.84	0.56
5:E:18[B]:GLU:CA	5:E:19[B]:GLY:CA	2.84	0.55
5:E:79:GLN:CA	5:E:80:PRO:CA	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:PRO:CA	5:E:100:GLY:CA	2.88	0.52

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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.

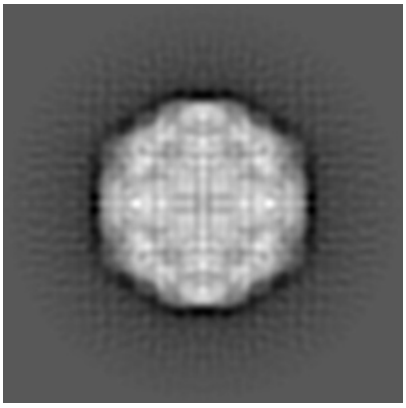
6 Map visualisation (i)

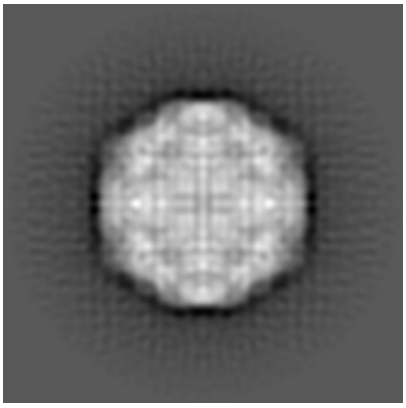
This section contains visualisations of the EMDB entry EMD-1183. These allow visual inspection of the internal detail of the map and identification of artifacts.

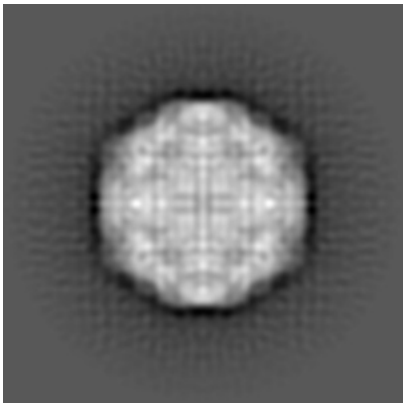
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

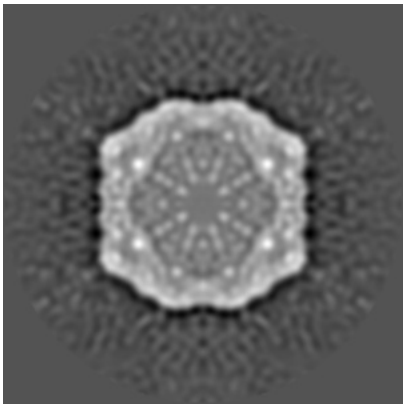

Y

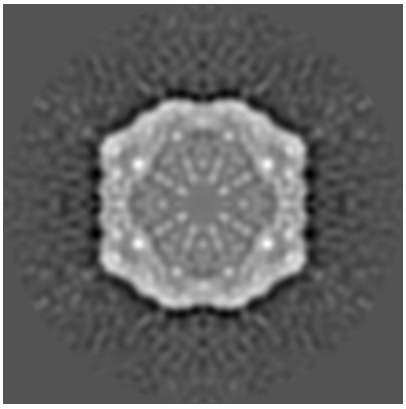

Z

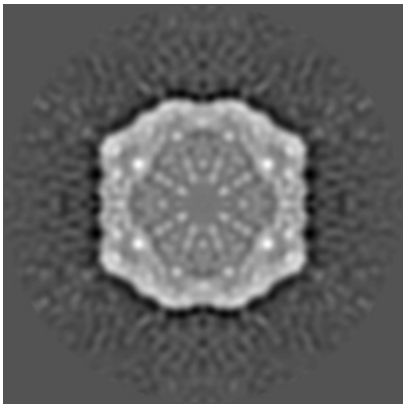
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 127

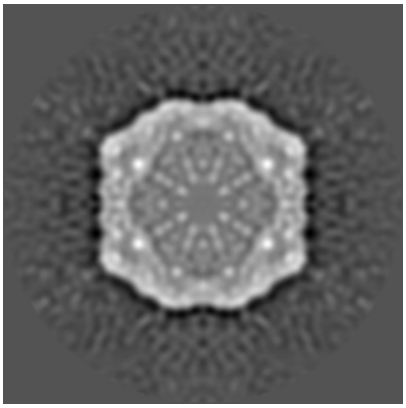

Y Index: 127

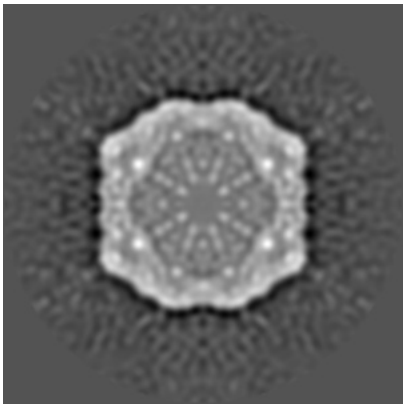

Z Index: 127

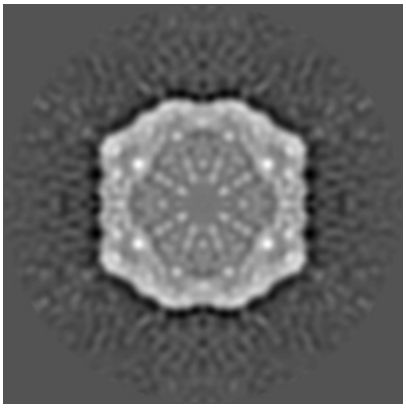
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 127

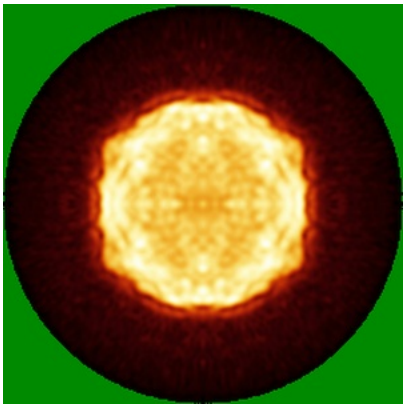

Y Index: 127

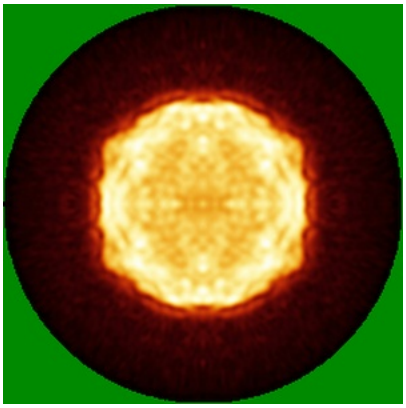

Z Index: 127

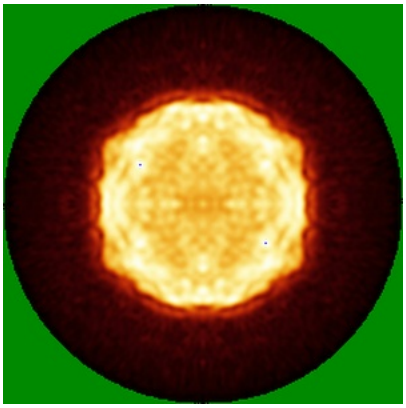
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

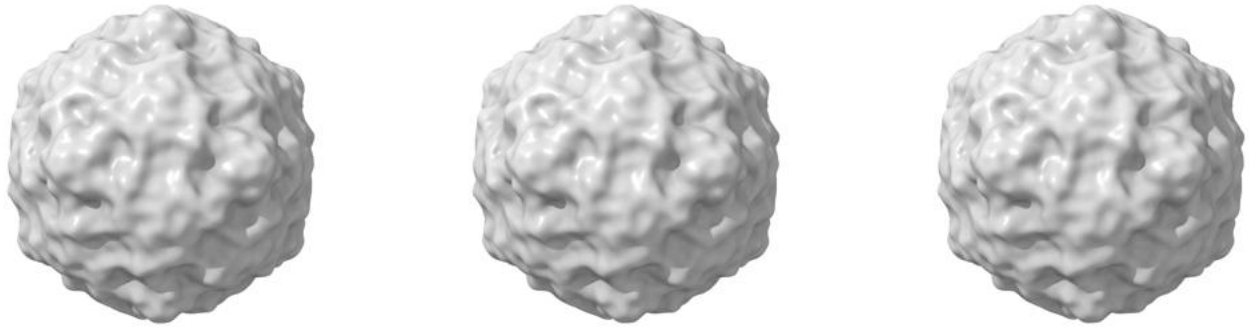

Y


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

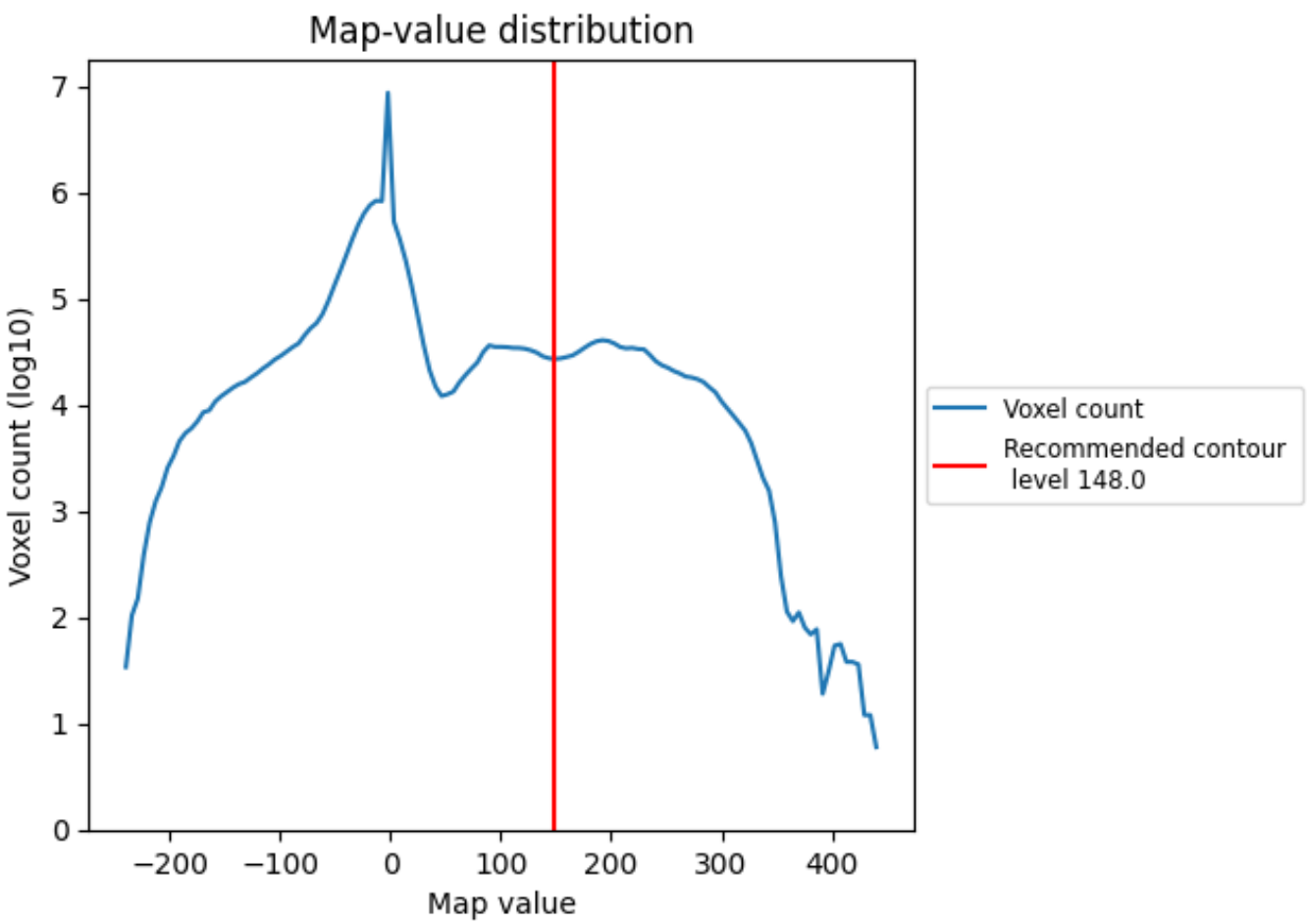
6.6 Mask visualisation (i)

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

7 Map analysis (i)

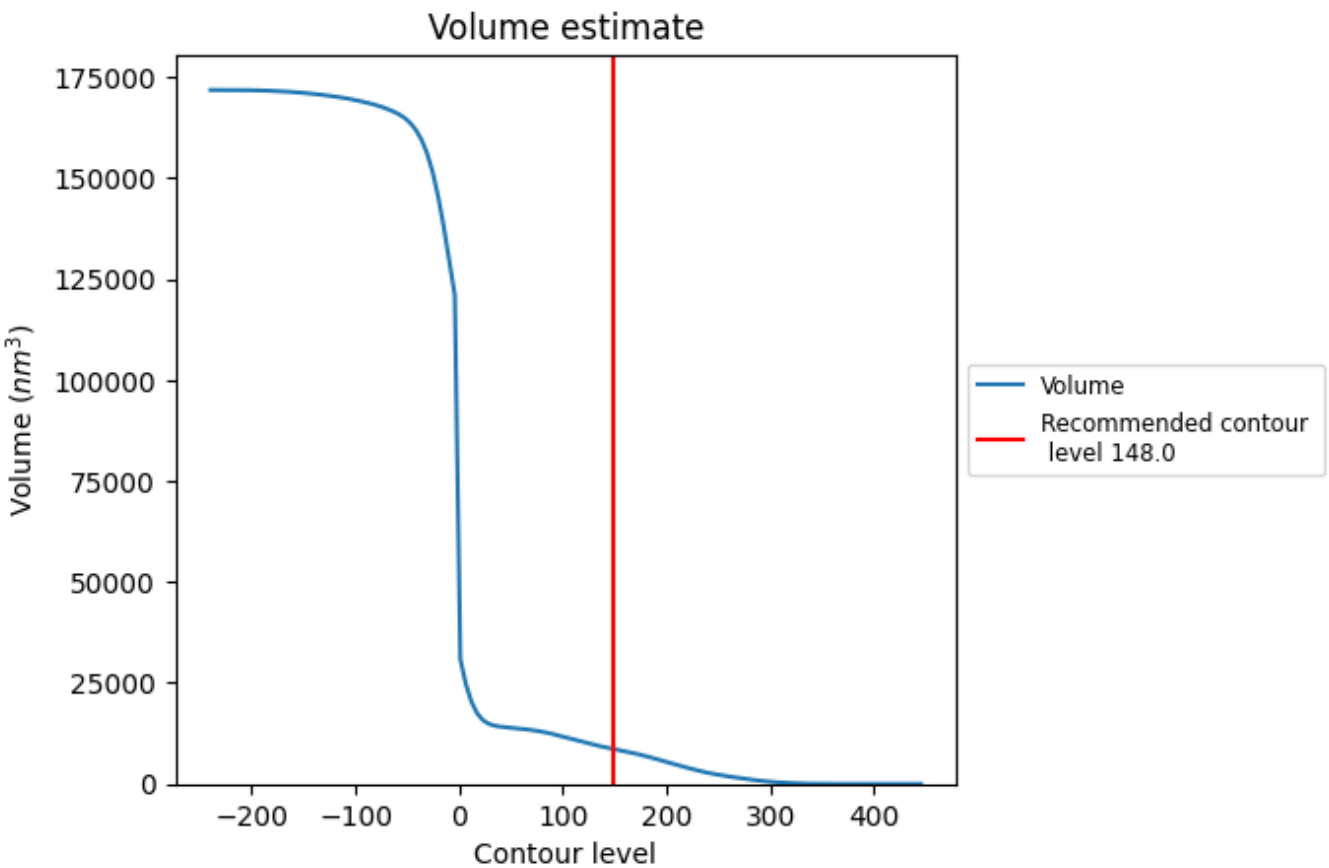
This section contains the results of statistical analysis of the map.

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.

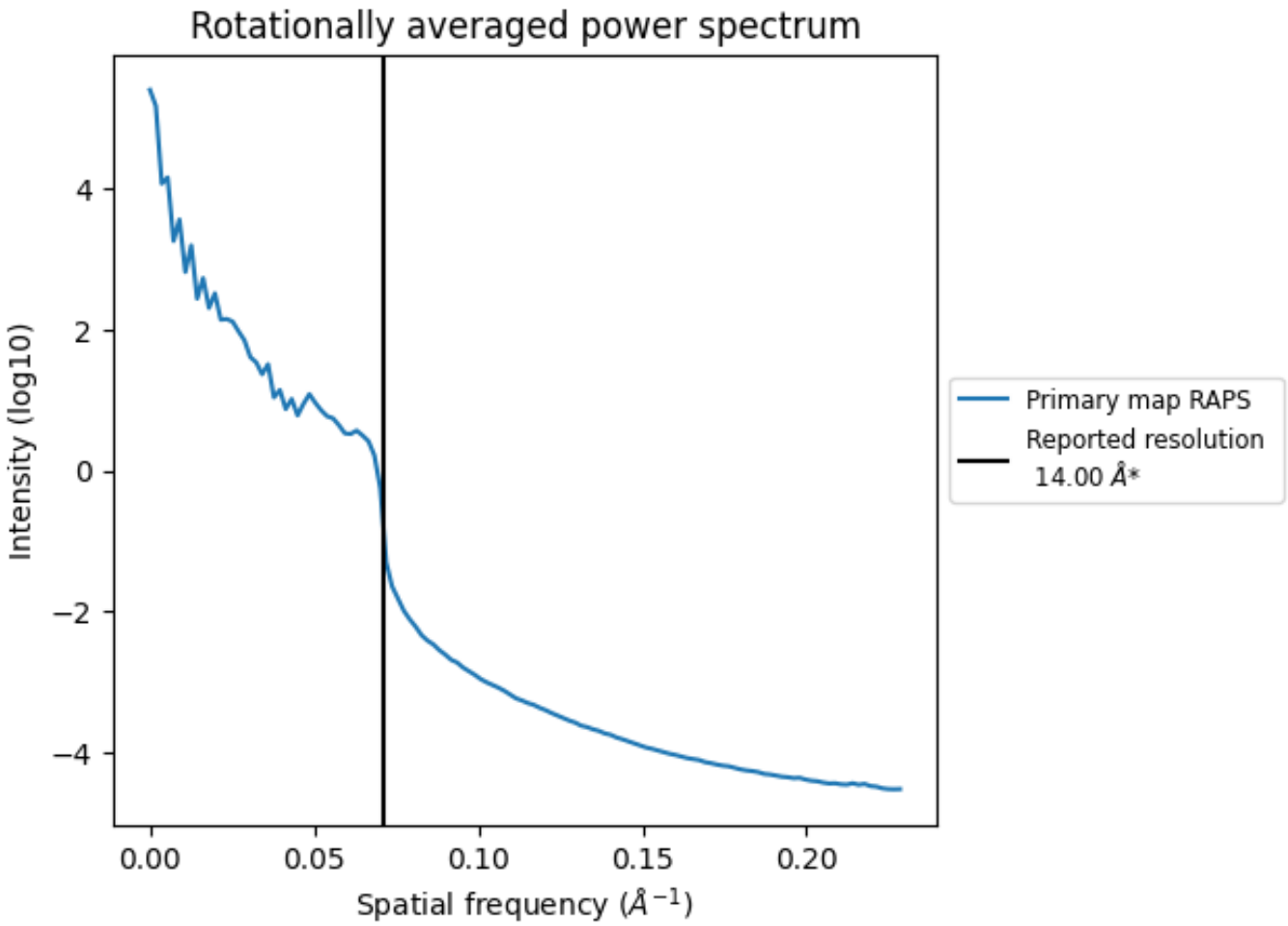
7.2 Volume estimate (i)



The volume at the recommended contour level is 8698 nm^3; this corresponds to an approximate mass of 7857 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 0.071 Å^{-1}

8 Fourier-Shell correlation (i)

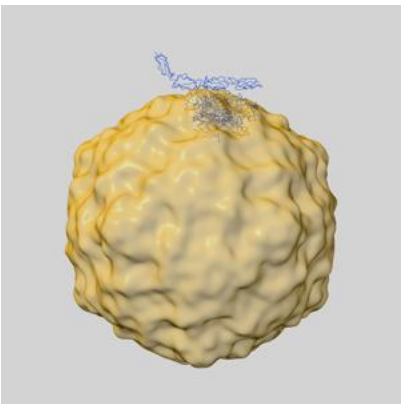
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

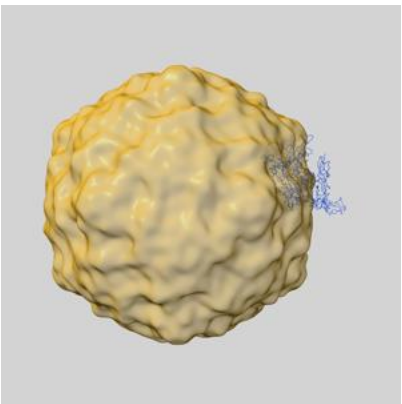
This section contains information regarding the fit between EMDB map EMD-1183 and PDB model 2C8I. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

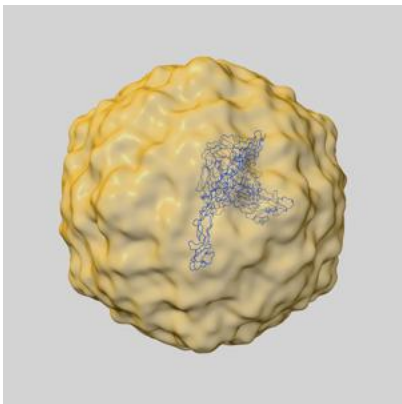
9.1.1 Map-model overlay (i)



X

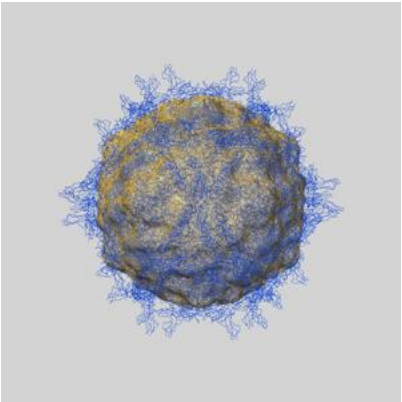


Y

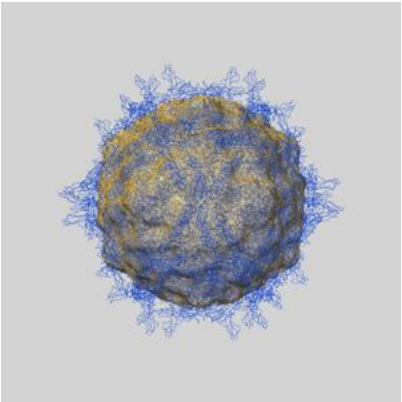


Z

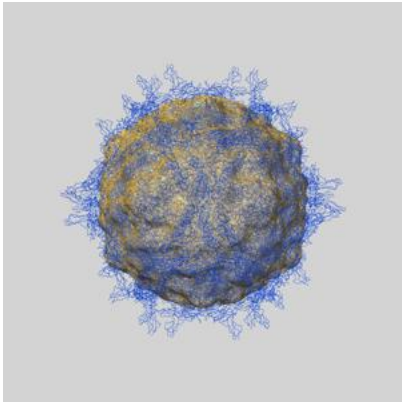
9.1.2 Map-model assembly overlay (i)



X



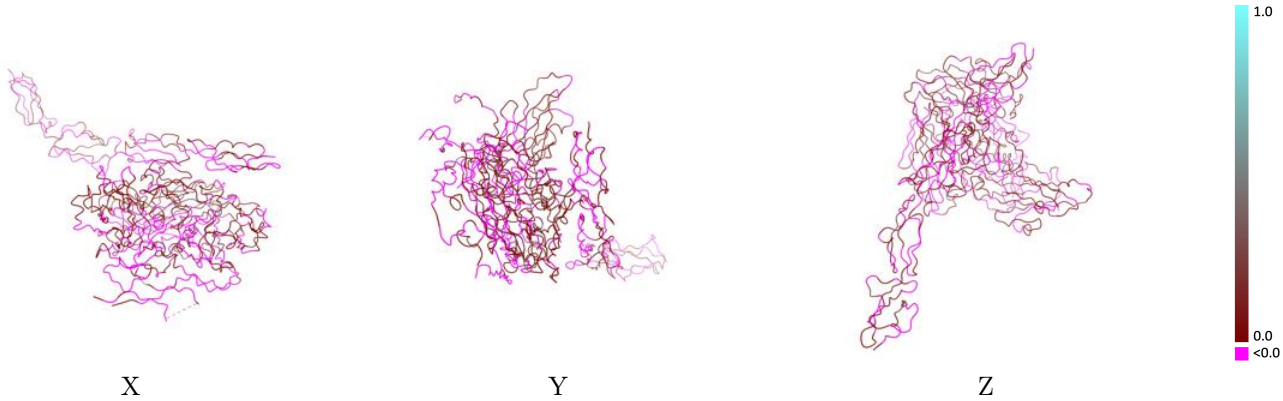
Y



Z

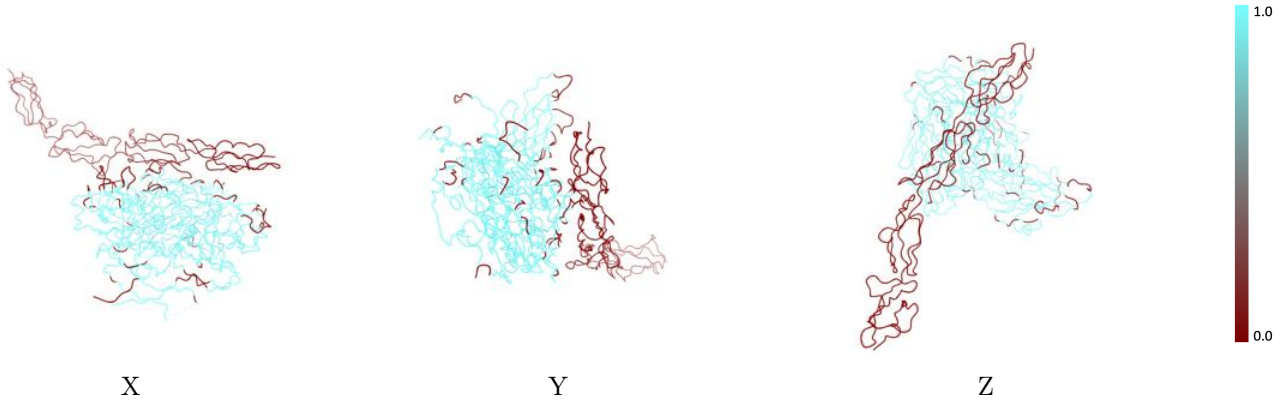
The images above show the 3D surface view of the map at the recommended contour level 148.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



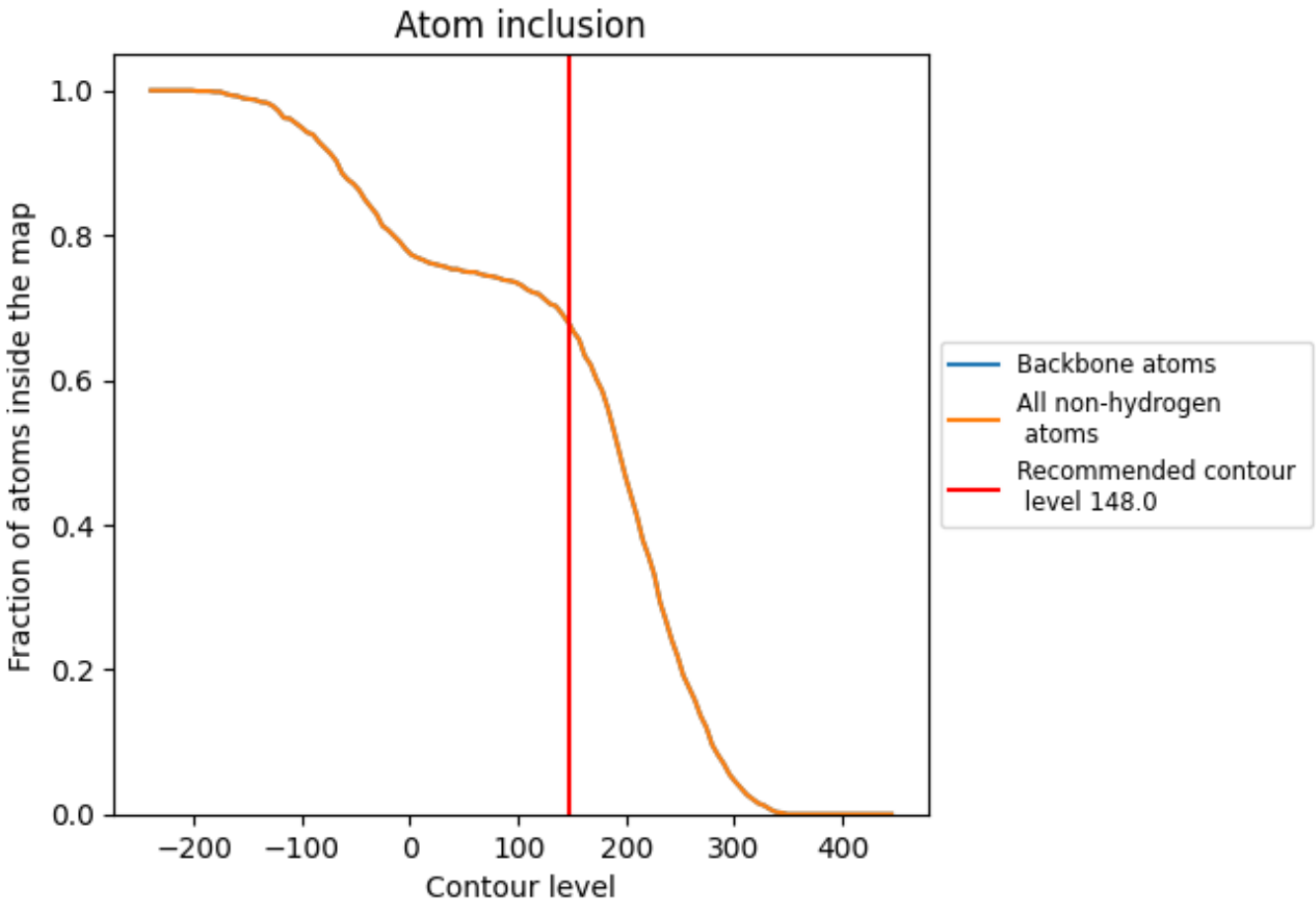
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (148.0).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (148.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6760	0.0110
A	0.8370	0.0170
B	0.8850	0.0220
C	0.9030	0.0280
D	0.9670	-0.0400
E	0.0000	-0.0090