



wwPDB EM Validation Summary Report ⓘ

Jun 2, 2024 – 04:08 AM EDT

PDB ID : 7UT4
EMDB ID : EMD-26754
Title : Gea2 closed/closed conformation (composite structure)
Authors : Muccini, A.; Fromme, J.C.
Deposited on : 2022-04-26
Resolution : 3.90 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 ⓘ 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.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

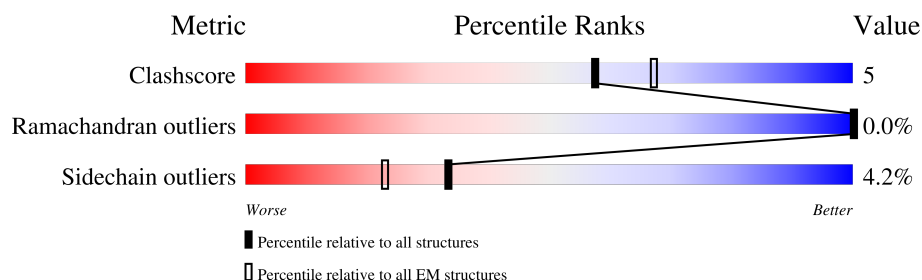
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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 | 1459 | |
| 1 | B | 1459 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39740 atoms, of which 20092 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 GEA2 isoform 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-------|------|------|----|---------|-------|
| 1 | A | 1224 | Total | C | H | N | O | S | 0 | 0 |
| | | | 19870 | 6306 | 10046 | 1603 | 1878 | 37 | | |
| 1 | B | 1224 | Total | C | H | N | O | S | 0 | 0 |
| | | | 19870 | 6306 | 10046 | 1603 | 1878 | 37 | | |

GLN THR ASP
THR SER ASP
PRO ARG
GLU SER
ASN ASP
VAL ASP
GLU THR
ILE ASP
GLU THR
ALA THR
ALA PRO
ILE THR
ASP ASP
ASN ASP
THR ASP

● Molecule 1: GEA2 isoform 1

Chain B:  69% 14% 16%

MET SER ASP
THR ARG
PHE SER
VAL ASP
THR THR
VAL THR
D90 ASP
P11 GLU
V12 THR
I15 THR
T20 PRO
T24 ILE
K28 ASP
TYR THR
SER LYS
PHE ASP
THR LYS
SER THR
GLN PRO
SER LYS
SER SER
GLY ASP
VAL VAL
ALA VAL
LEU GLU
LEU LYS
GLY GLY
GLY SER
SER GLU
ILE THR
PHE THR
SER ASN
ASN ASP
ASP ASP
TYR LEU
LEU ALA
HIS THR
PHE THR
ASN ASN
ASN LEU
ASN THR
ASN THR
LYS LYS
HIS HIS

ASN ASP
P71 THR
L83 THR
L86 THR
L89 THR
N91 GLU
I92 THR
K124 THR
T130 THR
Q136 THR
N137 THR
L149 THR
Q159 THR
S161 THR
D162 THR
D163 THR
V185 THR
L166 THR
L167 THR
V170 THR
F171 THR
L172 THR
L173 THR
R174 THR
S175 THR
D183 THR
L184 THR
L185 THR
I189 THR
L194 THR
S199 THR
L198 THR
L200 THR
N203 THR
R206 THR
S207 THR
E208 THR
R211 THR
T217 THR

T222 THR
S246 THR
D250 THR
D255 THR
N260 THR
VAL THR
GLU THR
SER THR
LYS THR
GLU THR
GLY THR
SER THR
GLN THR
GLU THR
ASP THR
PRO THR
ILE THR
GLY THR
MET THR
LYS THR
VAL THR
ASN THR
ASN THR
GLU THR
GLU THR
ALA THR
ILE THR
SER THR
GLU THR
ASP THR
ASP THR
GLY THR
ILE THR
GLU THR
GLU THR
GLU THR
HIS THR
HIS THR
SER THR
LYS THR
SER THR
THR THR
ASN THR
GLY THR
THR THR
ALA THR
ASN THR
ALA THR
GLN THR
LEU THR
ASP THR
ILE THR
VAL THR
GLN THR

LYS THR
THR THR
ARG THR
ASN THR
SER THR
ARG THR
ILE THR
ALA THR
Y322 THR
Y327 THR
Y335 THR
L342 THR
D348 THR
S352 THR
Y353 THR
L367 THR
F381 THR
I388 THR
F389 THR
I395 THR
T399 THR
I418 THR
L419 THR
Q426 THR
R433 THR
L438 THR
L439 THR
D440 THR
ASP THR
GLY THR
THR THR
ALA THR
ASN THR
ASN THR
SER THR
SER THR
SER THR
SER THR
ASN THR
LYS THR

ASN LYS
P455 THR
I463 THR
T471 THR
R472 THR
F476 THR
T480 THR
D485 THR
C486 THR
N487 THR
L488 THR
D489 THR
R490 THR
S494 THR
F497 THR
T502 THR
L506 THR
P507 THR
E508 THR
S509 THR
S516 THR
S527 THR
D531 THR
D534 THR
D538 THR
I539 THR
D540 THR
E542 THR
M551 THR
E552 THR
N571 THR
D592 THR
M602 THR
R605 THR
M606 THR
N607 THR
L630 THR

S634 THR
D639 THR
S640 THR
L645 THR
L646 THR
F665 THR
D686 THR
D694 THR
A695 THR
D696 THR
S697 THR
S702 THR
Q716 THR
H720 THR
F723 THR
E724 THR
N729 THR
Y743 THR
D753 THR
Q791 THR
L802 THR
F805 THR
D806 THR
S816 THR
T820 THR
L821 THR
F822 THR
R823 THR
L824 THR
L841 THR
D842 THR
F843 THR
C844 THR
L856 THR
L860 THR
R872 THR
SER THR
SER THR
HIS THR

ASP ASP
GLU LEU
SER THR
THR LEU
ALA THR
PHE THR
GLU THR
TYR THR
PRO THR
PHE THR
ALA THR
SER THR
TYR THR
L891 THR
V892 THR
G1004 THR
T1009 THR
E1010 THR
E1011 THR
E1012 THR
I1013 THR
C1022 THR
I1023 THR
N1027 THR
I1028 THR
V1032 THR
N1038 THR
I1039 THR
D1042 THR
L1043 THR
I1044 THR
S1050 THR
R1061 THR
E1064 THR
I1070 THR
L1073 THR
T1074 THR
L1077 THR
L1087 THR
L1088 THR
R1107 THR
T1108 THR
V1109 THR
R1110 THR
N986 THR

L1113 THR
S1121 THR
L1122 THR
C1123 THR
A1124 THR
L1139 THR
T1144 THR
F1145 THR
F1149 THR
F1150 THR
A1151 THR
T1152 THR
L1162 THR
N1178 THR
F1181 THR
Q1191 THR
I1206 THR
V1221 THR
L1224 THR
L1225 THR
I1228 THR
S1229 THR
A1233 THR
GLY THR
ASN THR
HIS THR
TRP THR
GLU THR
ILE THR
GLU THR
TYR THR
LYS THR
LYS THR
LEU THR
THR THR
GLU THR
SER THR
GLY THR
HIS THR
LYS THR
ASP THR
LYS THR
GLU THR
ASN THR
PRO THR
TYR THR
K1259 THR

E1263 THR
L1266 THR
L1271 THR
D1281 THR
E1286 THR
A1289 THR
I1290 THR
Q1297 THR
C1302 THR
K1303 THR
T1312 THR
L1313 THR
E1314 THR
Q1315 THR
T1316 THR
T1325 THR
M1328 THR
E1333 THR
S1357 THR
S1358 THR
T1359 THR
L1360 THR
T1361 THR
Y1367 THR
L1368 THR
H1369 THR
Y1370 THR
G1374 THR
K1375 THR
T1376 THR
S1377 THR
F1381 THR
F1388 THR
I1405 THR
K1408 THR
I1411 THR
S1417 THR
SER THR
SER THR

HIS GLY
SER SER
ALA THR
HIS THR
GLU THR
GLN THR
PRO THR
GLU THR
SER THR
SER THR
ASN THR
ASP THR
VAL THR
ILE THR
ILE THR
GLU THR
ALA THR
THR THR
ALA THR
PRO THR
ILE THR
ASP THR
ASP THR
ASN THR
LYS THR
THR THR
ASP THR
ASP THR
ASN THR
LYS THR
PRO THR
LYS THR
LEU THR
SER THR
ASP THR
VAL THR
GLU THR
LYS THR
ASP THR

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 83665 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.0 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 125.253 | Depositor |
| Minimum map value | -109.998 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 1.500 | Depositor |
| Recommended contour level | 5.85 | Depositor |
| Map size (\AA) | 499.2, 499.2, 499.2 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.664, 1.664, 1.664 | 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 | 0.31 | 0/9981 | 0.61 | 1/13478 (0.0%) |
| 1 | B | 0.31 | 0/9981 | 0.62 | 1/13478 (0.0%) |
| All | All | 0.31 | 0/19962 | 0.61 | 2/26956 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | A | 842 | ASP | CB-CG-OD1 | 9.60 | 126.94 | 118.30 |
| 1 | B | 842 | ASP | CB-CG-OD2 | 8.67 | 126.11 | 118.30 |

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 | 9824 | 10046 | 10046 | 96 | 0 |
| 1 | B | 9824 | 10046 | 10046 | 105 | 0 |
| All | All | 19648 | 20092 | 20092 | 200 | 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 5.

The worst 5 of 200 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:953:LEU:HD11 | 1:A:1023:ILE:HD13 | 1.64 | 0.79 |
| 1:A:1032:VAL:O | 1:A:1038:ASN:ND2 | 2.24 | 0.71 |
| 1:A:498:LEU:O | 1:A:502:THR:OG1 | 2.09 | 0.71 |
| 1:A:705:ILE:HD12 | 1:A:747:ILE:HD11 | 1.74 | 0.70 |
| 1:B:1032:VAL:O | 1:B:1038:ASN:ND2 | 2.23 | 0.70 |

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 | 1208/1459 (83%) | 1150 (95%) | 58 (5%) | 0 | 100 | 100 |
| 1 | B | 1208/1459 (83%) | 1143 (95%) | 64 (5%) | 1 (0%) | 51 | 84 |
| All | All | 2416/2918 (83%) | 2293 (95%) | 122 (5%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1233 | ALA |

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 | 1137/1346 (84%) | 1093 (96%) | 44 (4%) | 32 | 59 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 1 | B | 1137/1346 (84%) | 1085 (95%) | 52 (5%) | 27 55 |
| All | All | 2274/2692 (84%) | 2178 (96%) | 96 (4%) | 33 57 |

5 of 96 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 488 | LEU |
| 1 | B | 724 | GLU |
| 1 | B | 508 | GLU |
| 1 | B | 630 | LEU |
| 1 | B | 802 | 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 [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26754. 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](#)

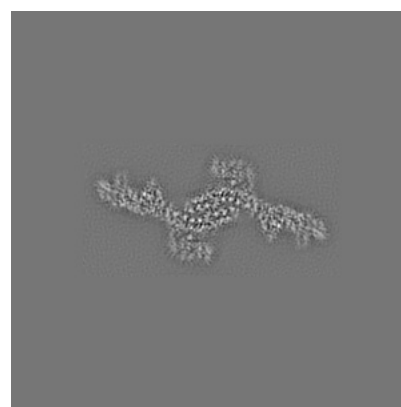
6.1.1 Primary map



X



Y

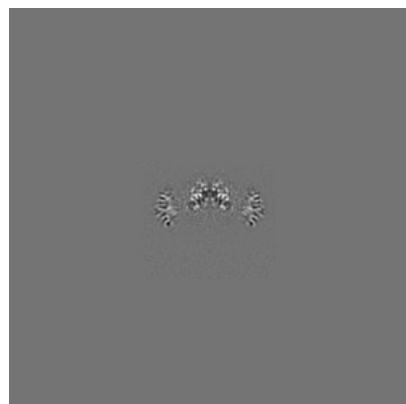


Z

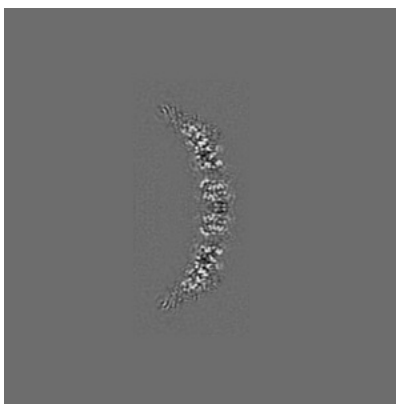
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

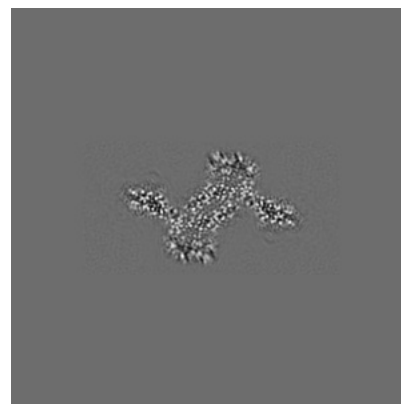
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

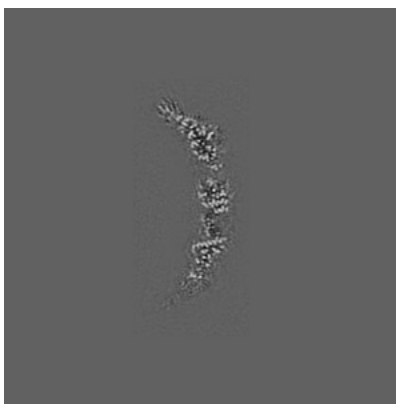
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

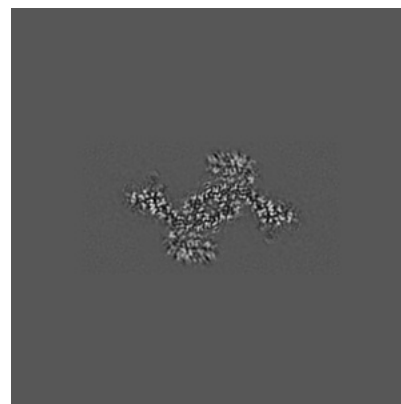
6.3.1 Primary map



X Index: 147



Y Index: 147

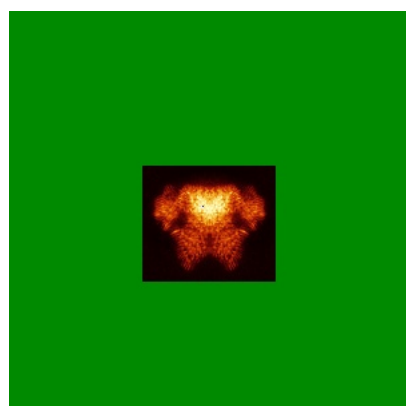


Z Index: 152

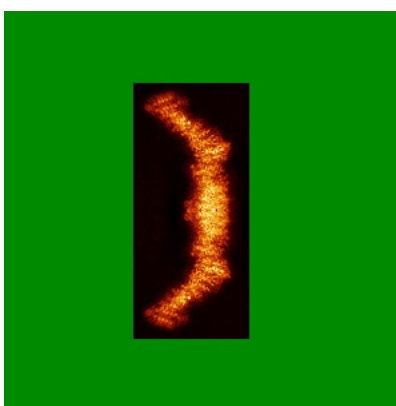
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

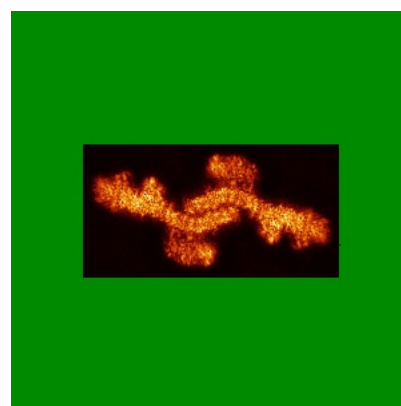
6.4.1 Primary map



X



Y

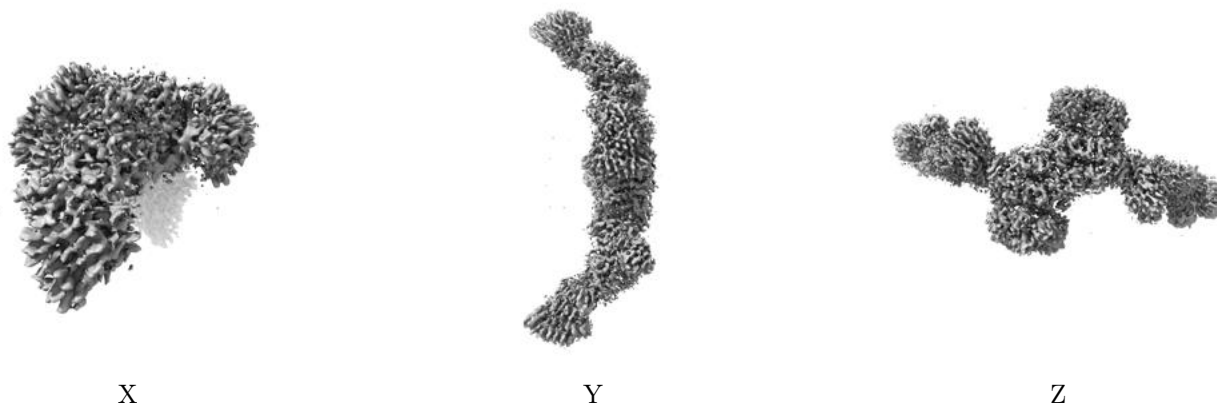


Z

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



The images above show the 3D surface view of the map at the recommended contour level 5.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

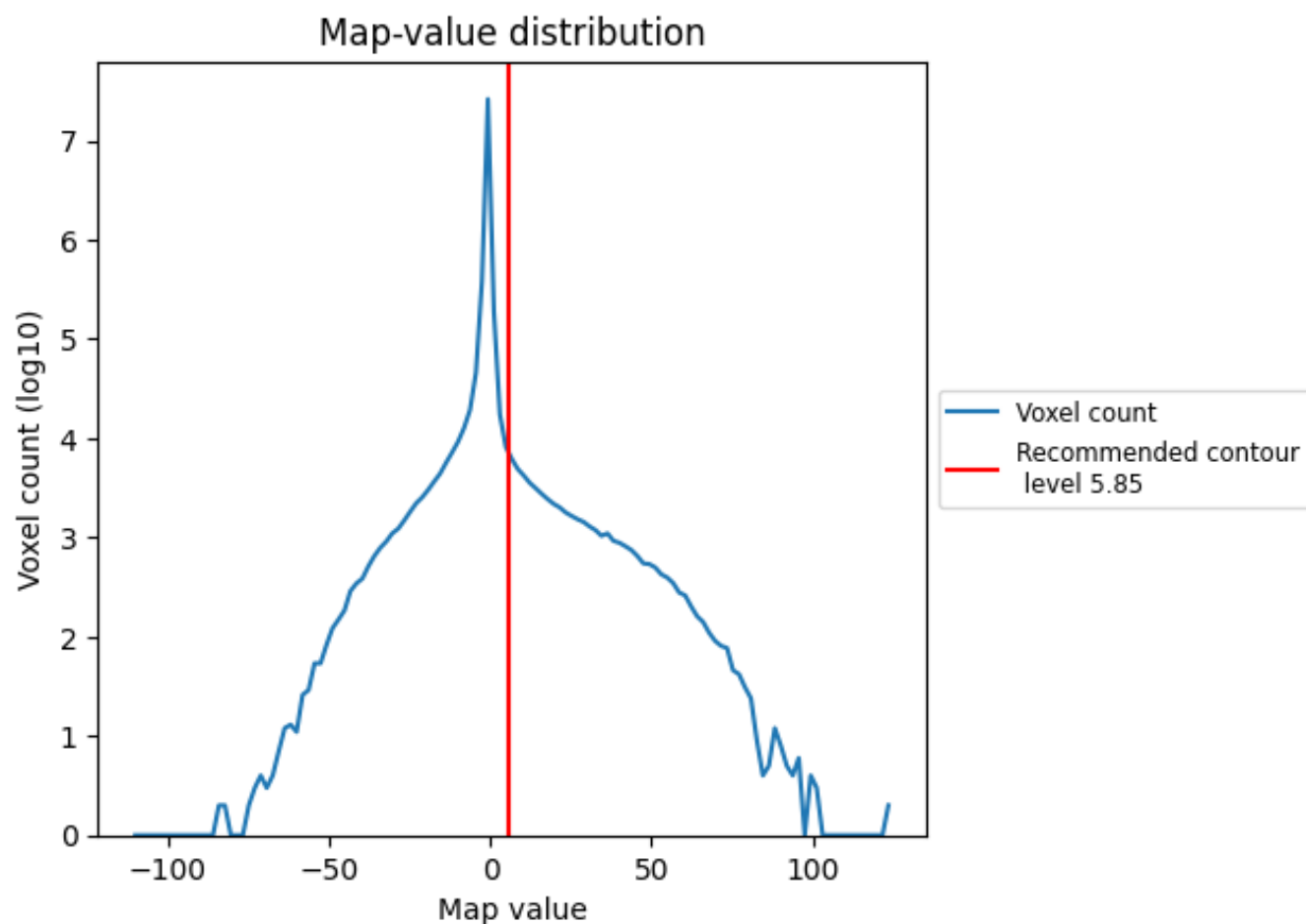
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

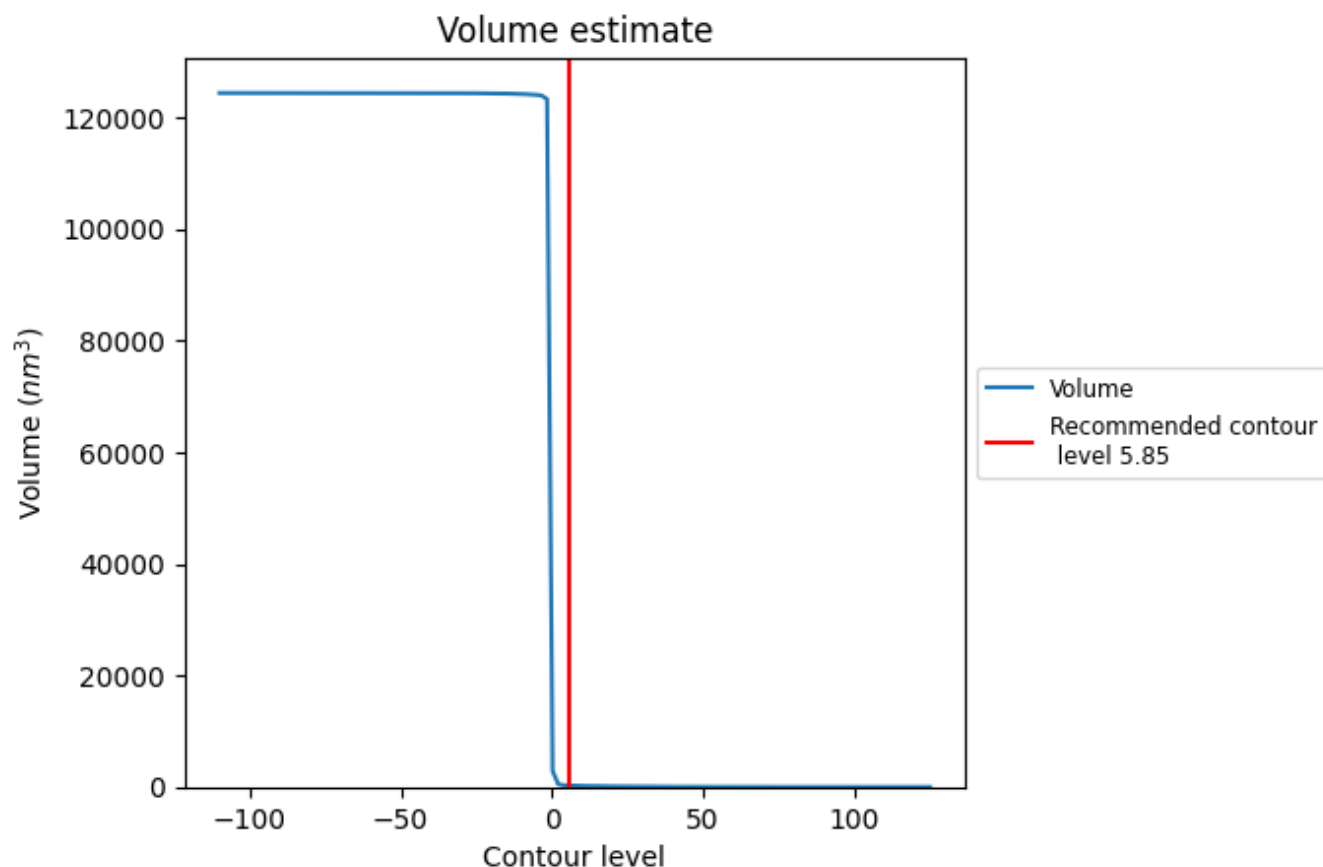
This section contains the results of statistical analysis of the map.

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.

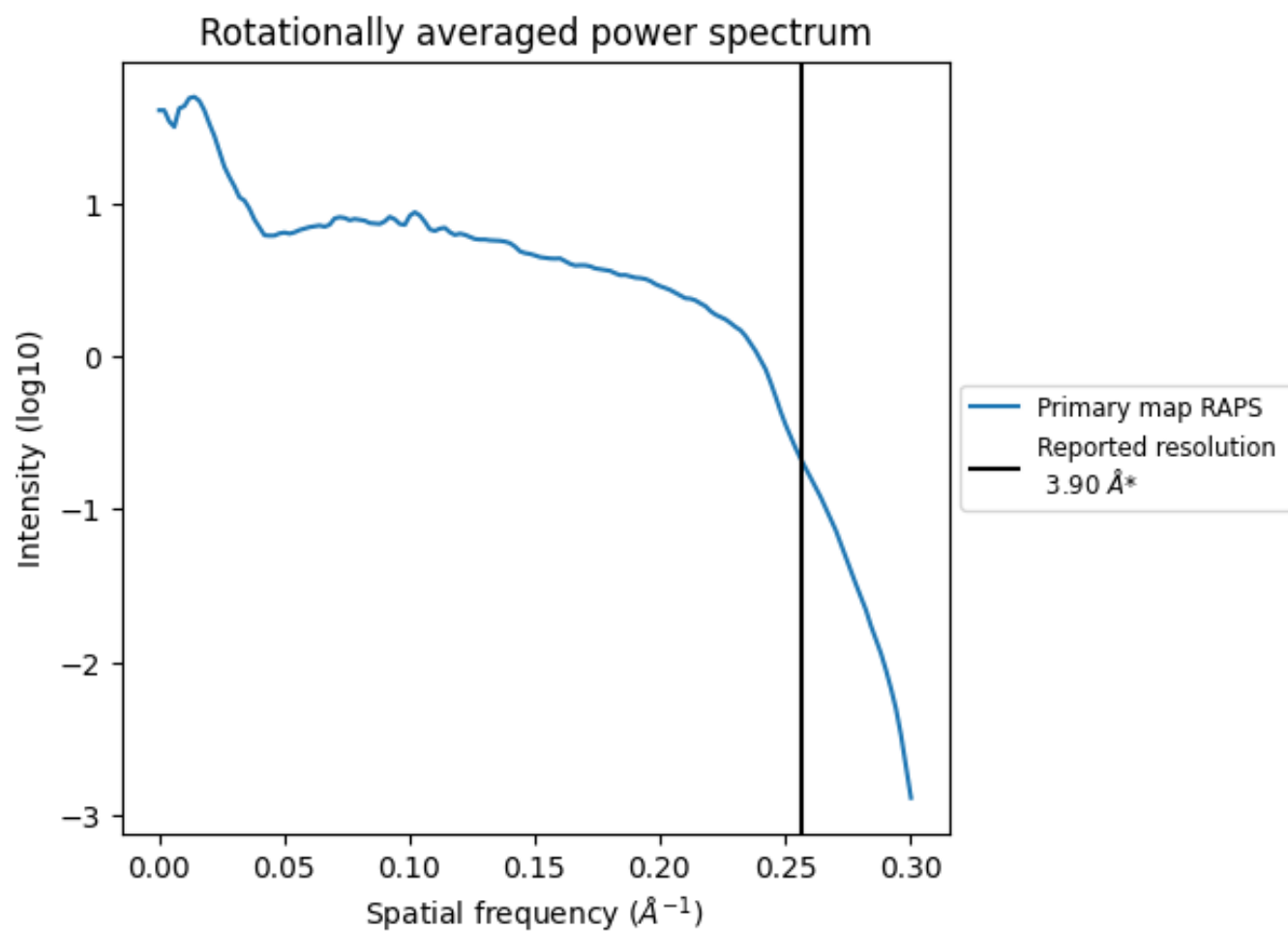
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm³; this corresponds to an approximate mass of 226 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 0.256 Å⁻¹

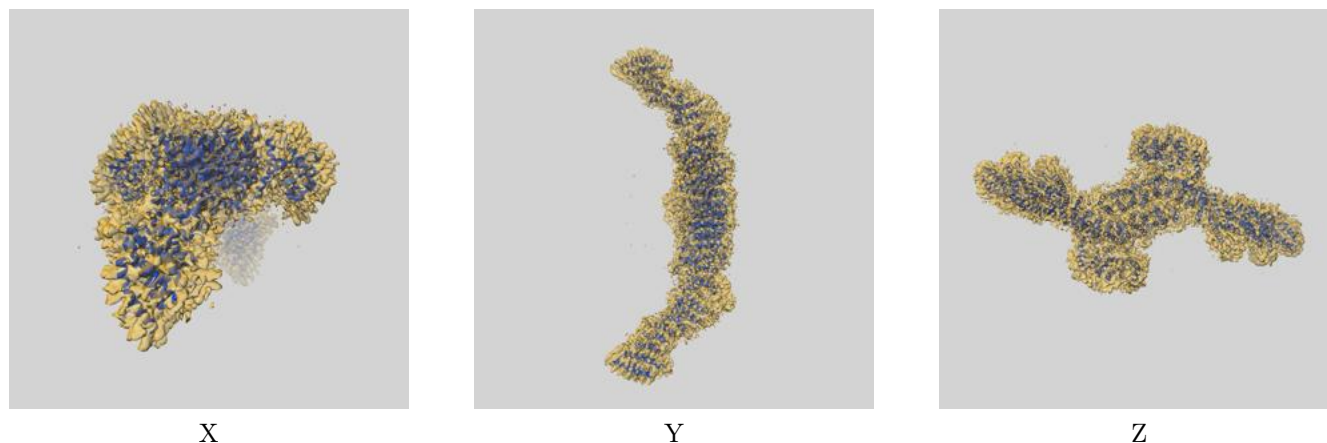
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

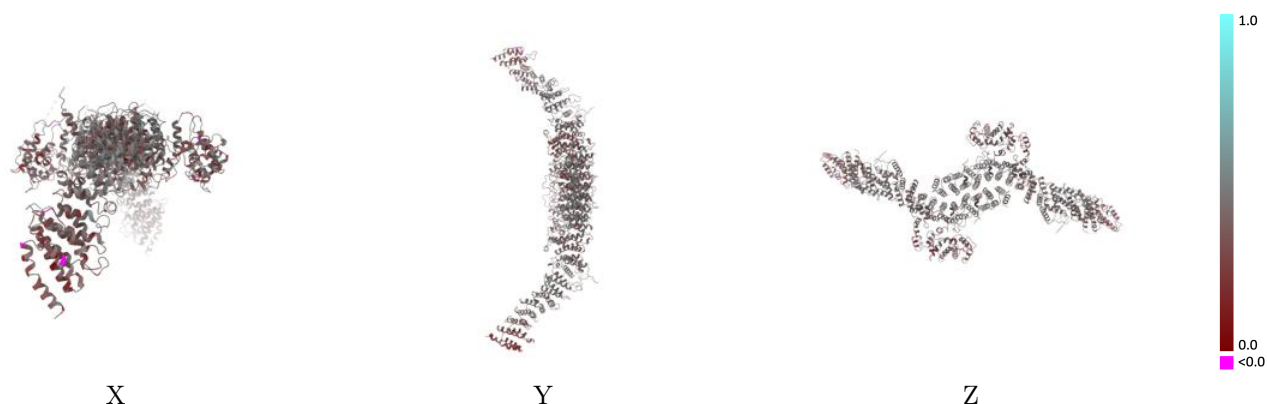
This section contains information regarding the fit between EMDB map EMD-26754 and PDB model 7UT4. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



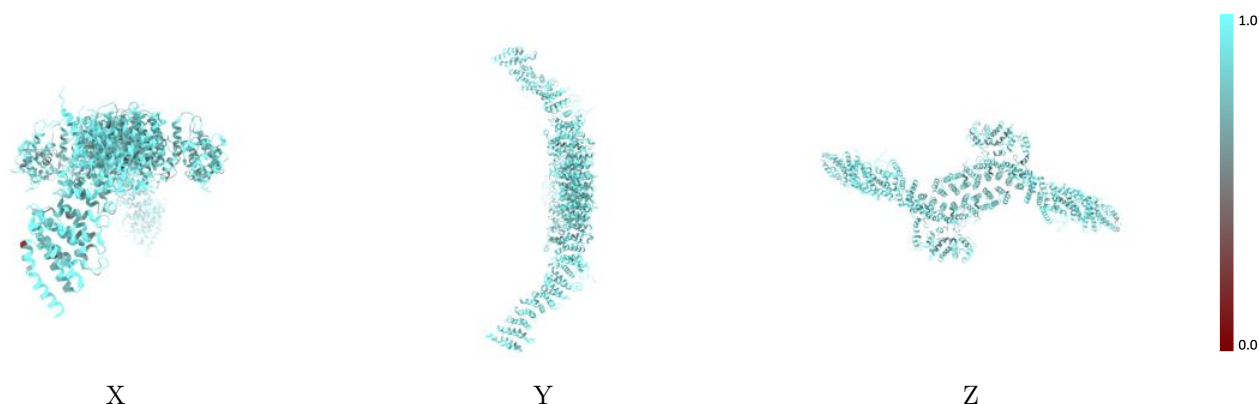
The images above show the 3D surface view of the map at the recommended contour level 5.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



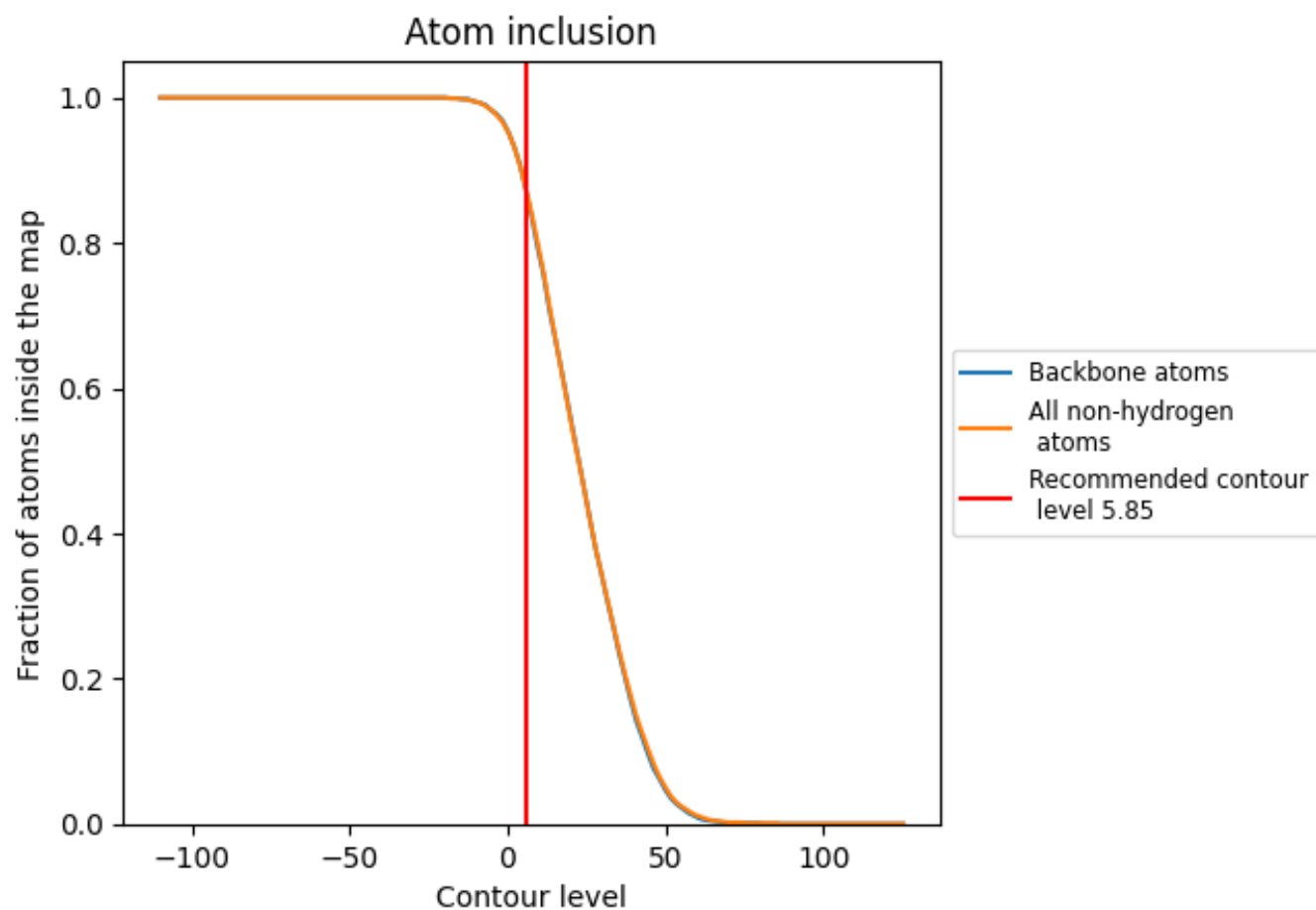
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.85).

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 (5.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|--------------------|
| All | <div></div> 0.8730 | <div></div> 0.4120 |
| A | <div></div> 0.8730 | <div></div> 0.4120 |
| B | <div></div> 0.8760 | <div></div> 0.4120 |

