# wwPDB EM Validation Summary Report

Oct 15, 2024 – 06:54 AM JST

| | | |
|---|---|---|
| PDB ID | : | 7WTE |
| EMDB ID | : | EMD-32780 |
| Title | : | Cryo-EM structure of human pyruvate carboxylase with acetyl-CoA in the intermediate state 2 |
| Authors | : | Chai, P.; Lan, P.; Wu, J.; Lei, M. |
| Deposited on | : | 2022-02-04 |
| Resolution | : | 3.30 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.

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The following versions of software and data (see references ⓘ) were used in the production of this report:

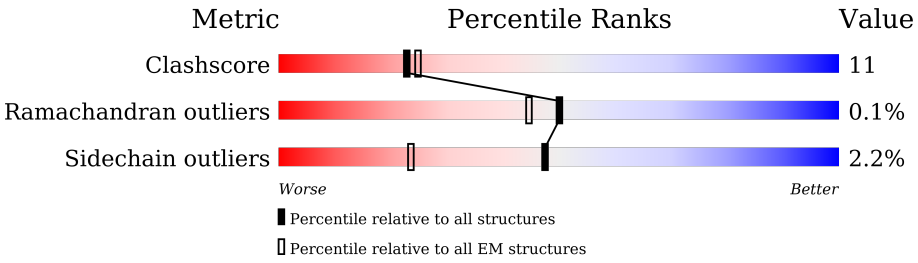
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 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 3.30 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 | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | 1178 | 40% 11% 49% |
| 1 | B | 1178 | 37% 14% 49% |
| 1 | C | 1178 | 7% 72% 24% |
| 1 | D | 1178 | 5% 73% 24% |

## 2 Entry composition (i)

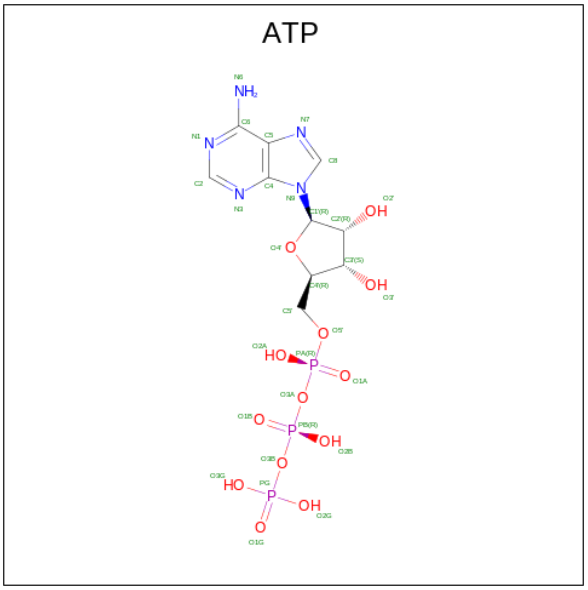
There are 3 unique types of molecules in this entry. The entry contains 27160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase, mitochondrial.

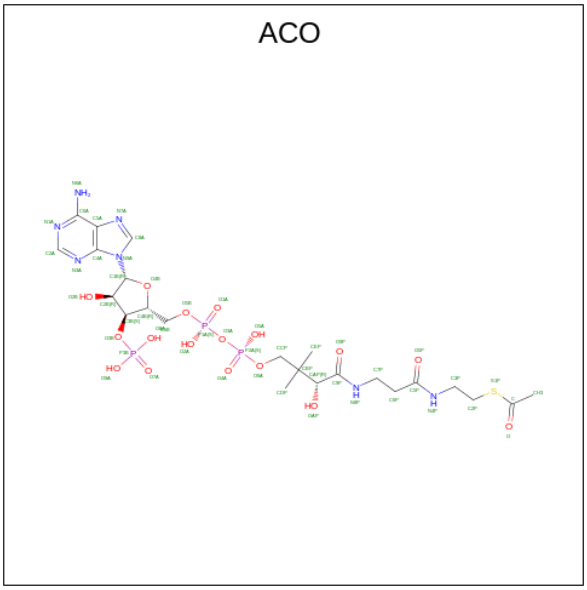
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 600 | Total | C | N | O | S | 0 | 0 |
| | | | 4625 | 2938 | 796 | 863 | 28 | | |
| 1 | B | 600 | Total | C | N | O | S | 0 | 0 |
| | | | 4625 | 2938 | 796 | 863 | 28 | | |
| 1 | C | 1146 | Total | C | N | O | S | 0 | 0 |
| | | | 8869 | 5612 | 1559 | 1651 | 47 | | |
| 1 | D | 1147 | Total | C | N | O | S | 0 | 0 |
| | | | 8877 | 5618 | 1560 | 1652 | 47 | | |

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



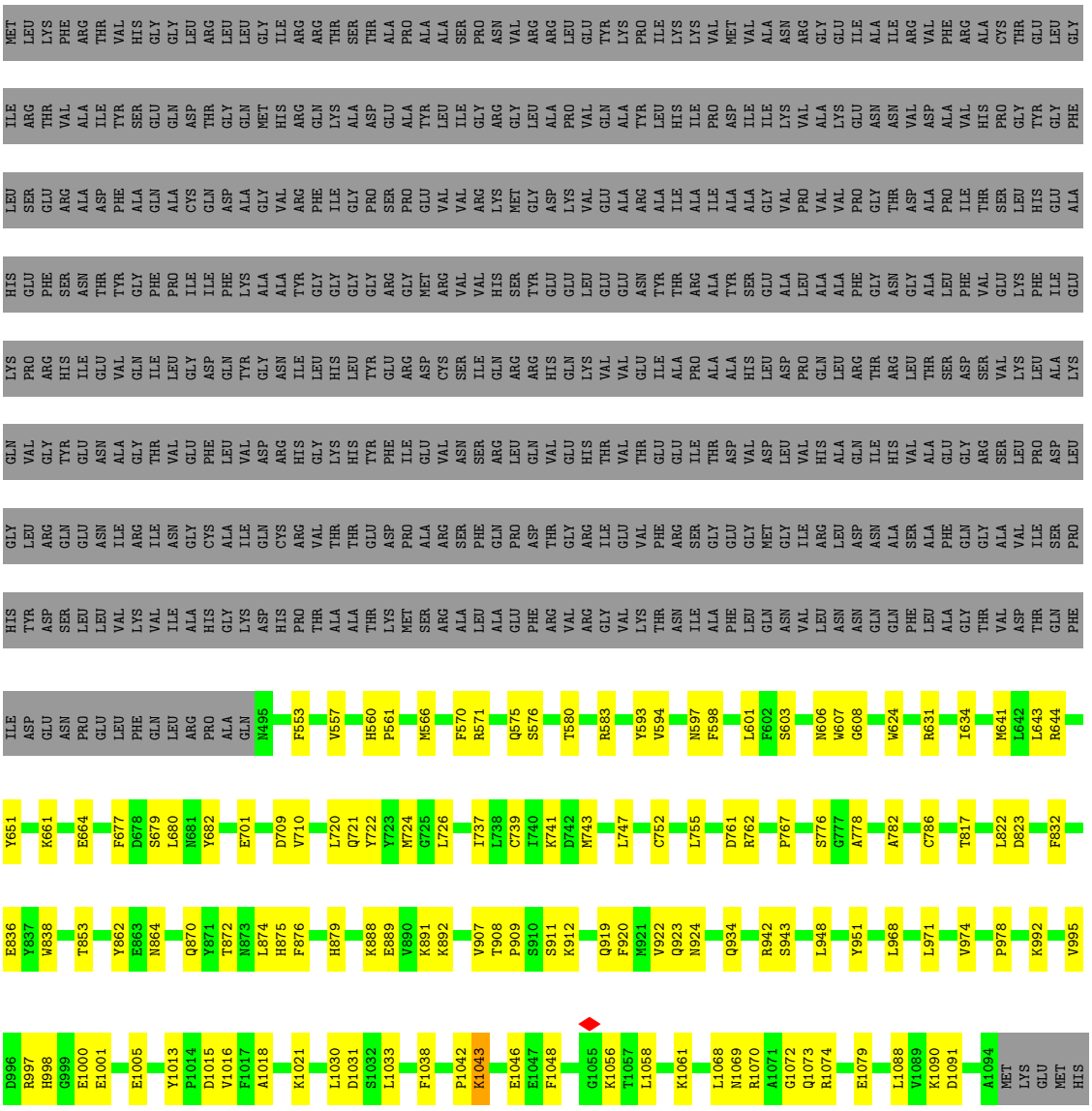

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 1 | Total | C | N | O | P | S | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | |
| 3 | D | 1 | Total | C | N | O | P | S | 0 |
| | | | 51 | 23 | 7 | 17 | 3 | 1 | |

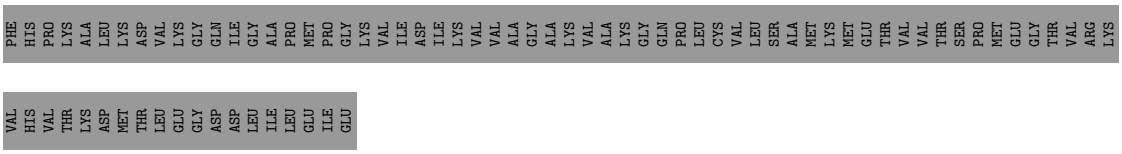
# 3 Residue-property plots (i)

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: Pyruvate carboxylase, mitochondrial

Chain A:

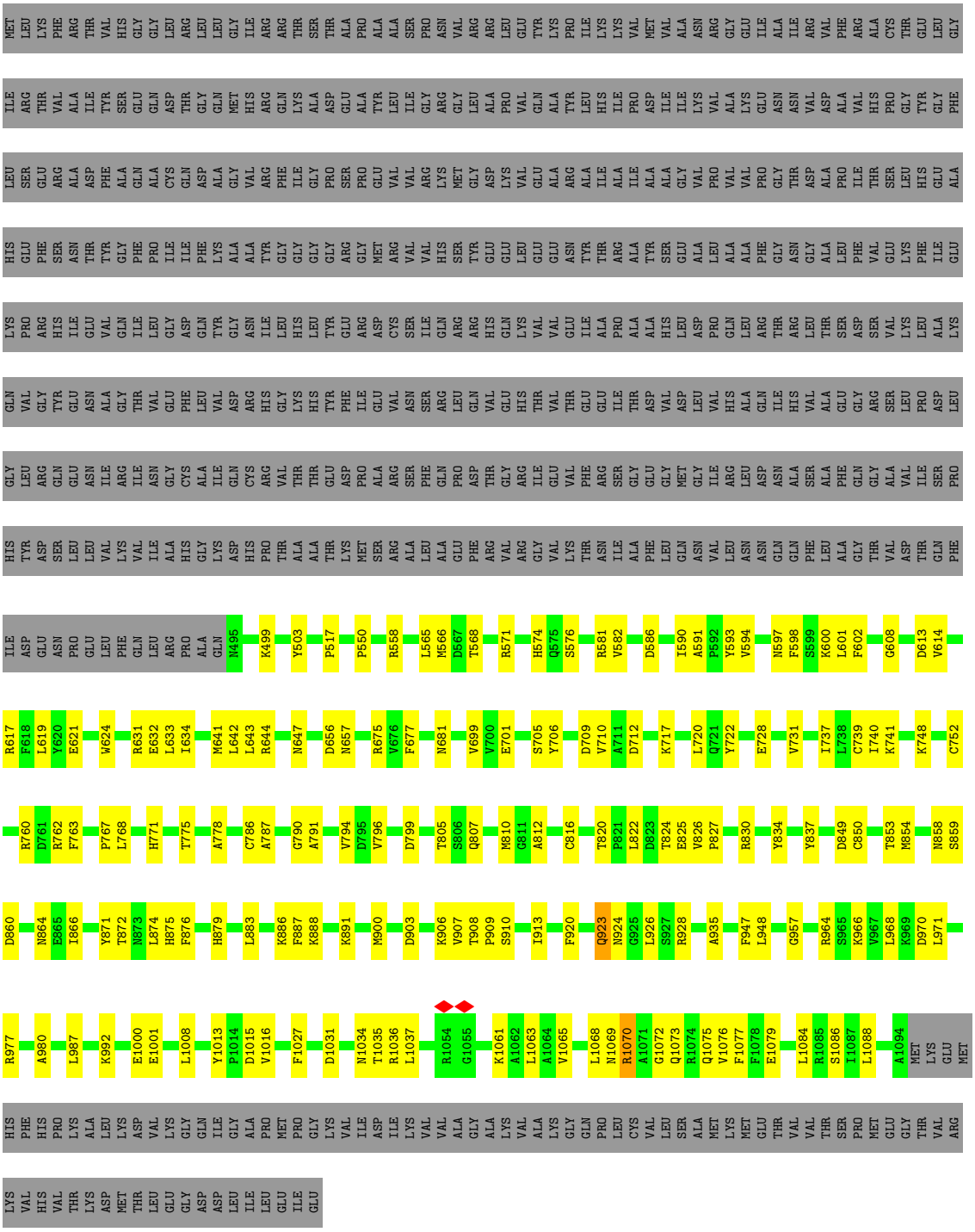







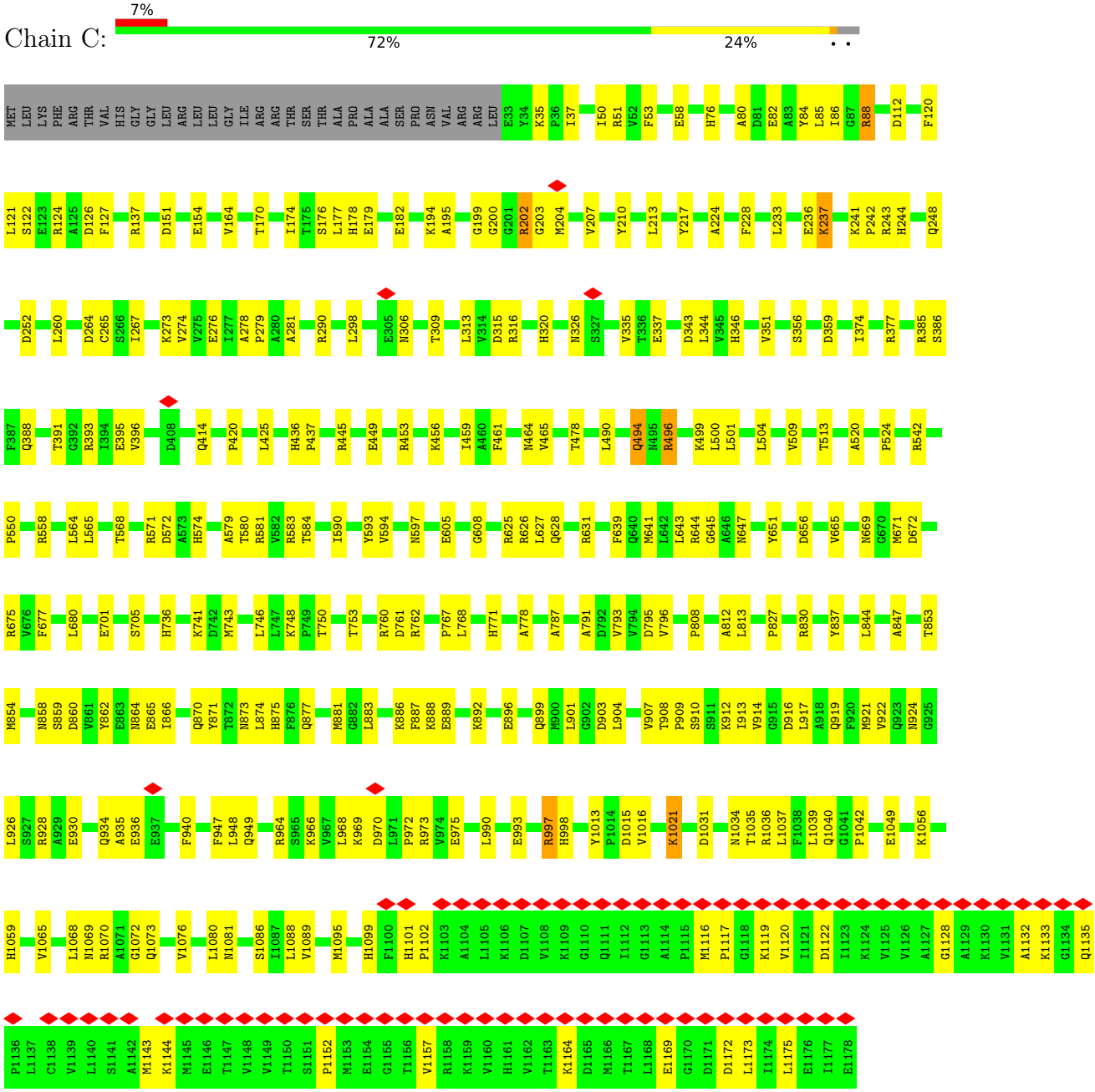
• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain B:

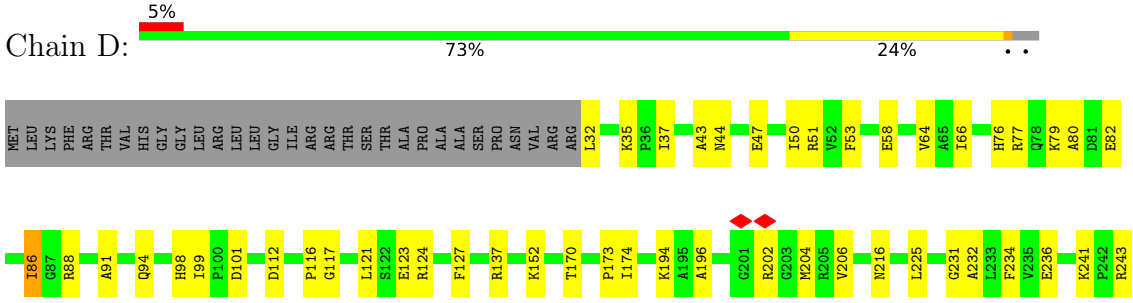
• Molecule 1: Pyruvate carboxylase, mitochondrial

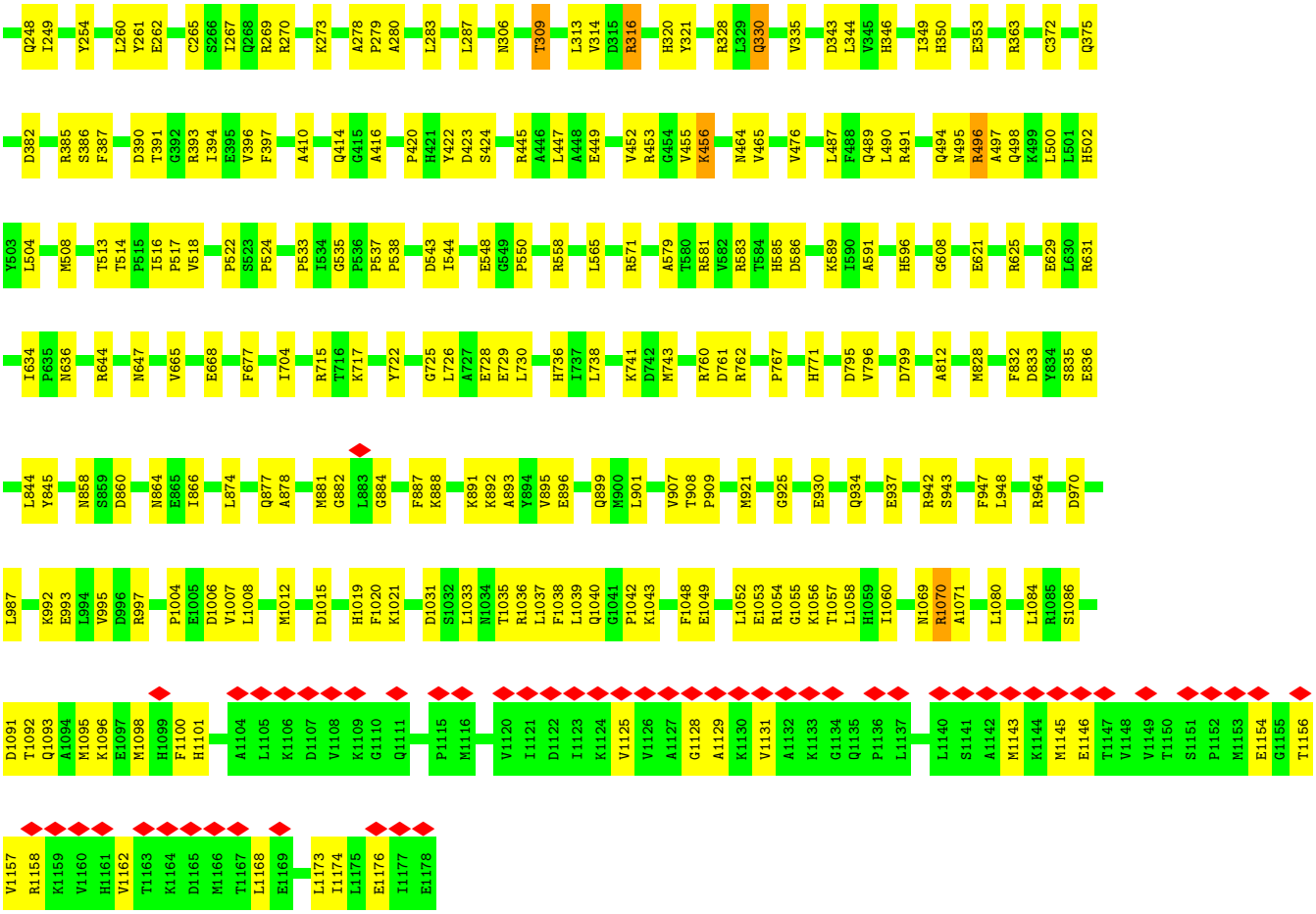
Chain C:




• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain D:




Q248 I249 Y254 L260 Y261 E262 C265 S266 I267 Q268 R269 R270 K273 A278 P279 A280 L283 L287 N306 T309 L313 V314 D315 R316 H320 Y321 R328 L329 Q330 V335 D343 L344 V345 H346 I349 H350 E353 R363 C372 Q375
D382 R385 S386 F387 D390 T391 G392 R393 I394 E395 V396 F397 A410 Q414 G415 A416 P420 H421 Y422 D423 S424 R445 A446 L447 A448 E449 V452 R453 G454 V455 K456 M464 V465 V476 L487 F488 Q489 L490 R491 Q494 N495 R496 A497 Q498 K499 L500 L501 H502
Y503 L504 M508 T513 T514 P515 I516 P517 V518 P522 S523 P524 P533 I534 G535 P536 P537 P538 D543 I544 E548 G549 P550 R558 L565 R571 A579 T580 R581 V582 R583 T584 H585 D586 K589 I590 A591 H596 G608 E621 R625 E629 L630 R631
I634 P635 N636 R644 N647 V665 E668 F677 I704 R715 T716 K717 Y722 G725 L726 A727 E728 E729 L730 H736 I737 L738 K741 D742 M743 R760 D761 R762 P767 H771 D795 V796 D799 A812 M828 F832 D833 Y834 S835 E836
L844 Y845 N858 S859 D860 N864 E865 I866 L874 Q877 A878 M881 G882 L883 G884 F887 K888 K891 K892 A893 Y894 V895 E896 Q899 M900 L901 V907 T908 P909 M921 G925 E930 Q934 E937 R942 S943 F947 L948 R964 D970
L987 K992 E993 L994 V995 D996 R997 P1004 E1005 D1006 V1007 L1008 M1012 D1015 H1019 F1020 K1021 D1031 S1032 L1033 N1034 T1035 R1036 L1037 F1038 L1039 Q1040 G1041 P1042 K1043 F1048 E1049 L1052 E1053 R1054 G1055 K1056 T1057 L1058 H1059 I1060 N1069 R1070 A1071 L1080 L1084 R1085 S1086
D1091 T1092 Q1093 A1094 M1095 K1096 E1097 M1098 H1099 F1100 H1101 A1104 L1105 K1106 D1107 V1108 K1109 G1110 Q1111 P1115 M1116 V1120 I1121 D1122 I1123 K1124 V1125 V1126 A1127 G1128 A1129 K1130 V1131 A1132 K1133 G1134 Q1135 P1136 L1137 L1140 S1141 A1142 M1143 K1144 M1145 E1146 T1147 V1148 V1149 T1150 S1151 P1152 M1153 E1154 G1155 T1156
V1157 R1158 K1159 V1160 H1161 V1162 T1163 K1164 D1165 M1166 T1167 L1168 E1169 L1173 I1174 L1175 E1176 I1177 E1178

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 139123 | 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 ($e^-/Å^2$) | 40 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.043 | Depositor |
| Minimum map value | -0.023 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.006 | Depositor |
| Map size (Å) | 343.2, 343.2, 343.2 | wwPDB |
| Map dimensions | 312, 312, 312 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1, 1.1, 1.1 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, ATP

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 | 0.28 | 0/4734 | 0.52 | 1/6425 (0.0%) |
| 1 | B | 0.27 | 0/4734 | 0.49 | 1/6425 (0.0%) |
| 1 | C | 0.30 | 0/9060 | 0.52 | 1/12277 (0.0%) |
| 1 | D | 0.31 | 0/9068 | 0.52 | 0/12288 |
| All | All | 0.30 | 0/27596 | 0.52 | 3/37415 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1031 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | C | 970 | ASP | CB-CG-OD2 | 5.25 | 123.03 | 118.30 |
| 1 | B | 970 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |

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 | 4625 | 0 | 4573 | 80 | 0 |
| 1 | B | 4625 | 0 | 4573 | 118 | 0 |
| 1 | C | 8869 | 0 | 8831 | 202 | 0 |
| 1 | D | 8877 | 0 | 8842 | 203 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | C | 31 | 0 | 12 | 8 | 0 |
| 2 | D | 31 | 0 | 12 | 0 | 0 |
| 3 | C | 51 | 0 | 34 | 14 | 0 |
| 3 | D | 51 | 0 | 34 | 5 | 0 |
| All | All | 27160 | 0 | 26911 | 596 | 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 11.

The worst 5 of 596 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:C:524:PRO:CA | 1:C:1036:ARG:HH22 | 1.10 | 1.64 |
| 1:C:583:ARG:NH2 | 1:C:1031:ASP:HA | 1.39 | 1.33 |
| 1:B:1079:GLU:HG3 | 1:B:1084:LEU:CD2 | 1.71 | 1.21 |
| 1:C:524:PRO:HA | 1:C:1036:ARG:NH2 | 0.88 | 1.19 |
| 1:D:514:THR:HG21 | 1:D:1038:PHE:CZ | 1.81 | 1.16 |

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 | 598/1178 (51%) | 563 (94%) | 35 (6%) | 0 | 100 | 100 |
| 1 | B | 598/1178 (51%) | 547 (92%) | 51 (8%) | 0 | 100 | 100 |
| 1 | C | 1144/1178 (97%) | 1064 (93%) | 79 (7%) | 1 (0%) | 48 | 76 |
| 1 | D | 1145/1178 (97%) | 1081 (94%) | 63 (6%) | 1 (0%) | 48 | 76 |
| All | All | 3485/4712 (74%) | 3255 (93%) | 228 (6%) | 2 (0%) | 50 | 76 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 517 | PRO |
| 1 | C | 972 | PRO |

### 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 | 493/968 (51%) | 487 (99%) | 6 (1%) | 67 80 |
| 1 | B | 493/968 (51%) | 490 (99%) | 3 (1%) | 84 90 |
| 1 | C | 942/968 (97%) | 919 (98%) | 23 (2%) | 44 68 |
| 1 | D | 943/968 (97%) | 911 (97%) | 32 (3%) | 32 59 |
| All | All | 2871/3872 (74%) | 2807 (98%) | 64 (2%) | 47 69 |

5 of 64 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 1021 | LYS |
| 1 | D | 1080 | LEU |
| 1 | C | 496 | ARG |
| 1 | C | 494 | GLN |
| 1 | D | 1084 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 44 | ASN |
| 1 | D | 248 | GLN |
| 1 | D | 864 | ASN |
| 1 | D | 640 | GLN |
| 1 | C | 773 | HIS |

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | ATP | C | 2000 | - | 26,33,33 | 0.65 | 0 | 31,52,52 | 0.72 | 1 (3%) |
| 3 | ACO | D | 2001 | - | 45,53,53 | 0.55 | 0 | 56,79,79 | 0.60 | 1 (1%) |
| 3 | ACO | C | 2001 | - | 45,53,53 | 0.55 | 0 | 56,79,79 | 0.61 | 1 (1%) |
| 2 | ATP | D | 2002 | - | 26,33,33 | 0.60 | 0 | 31,52,52 | 0.74 | 2 (6%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | ATP | C | 2000 | - | - | 7/18/38/38 | 0/3/3/3 |
| 3 | ACO | D | 2001 | - | - | 22/47/67/67 | 0/3/3/3 |
| 3 | ACO | C | 2001 | - | - | 22/47/67/67 | 0/3/3/3 |
| 2 | ATP | D | 2002 | - | - | 5/18/38/38 | 0/3/3/3 |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 2001 | ACO | C5A-C6A-N6A | 2.33 | 123.89 | 120.35 |
| 3 | D | 2001 | ACO | C5A-C6A-N6A | 2.29 | 123.83 | 120.35 |
| 2 | C | 2000 | ATP | C5-C6-N6 | 2.28 | 123.81 | 120.35 |
| 2 | D | 2002 | ATP | C5-C6-N6 | 2.27 | 123.80 | 120.35 |
| 2 | D | 2002 | ATP | PB-O3B-PG | 2.04 | 139.84 | 132.83 |

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | C | 2000 | ATP | PB-O3B-PG-O3G |
| 2 | C | 2000 | ATP | C5'-O5'-PA-O1A |
| 2 | C | 2000 | ATP | C5'-O5'-PA-O2A |
| 2 | D | 2002 | ATP | C5'-O5'-PA-O1A |
| 2 | D | 2002 | ATP | C5'-O5'-PA-O2A |

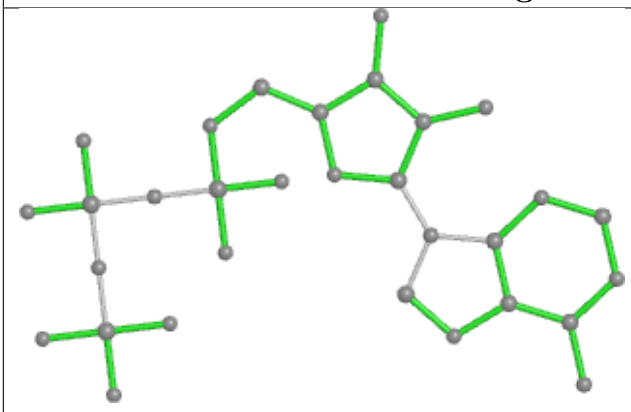
There are no ring outliers.

3 monomers are involved in 27 short contacts:

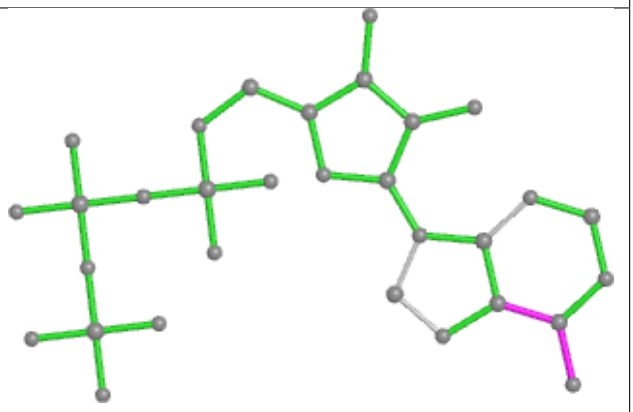
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | C | 2000 | ATP | 8 | 0 |
| 3 | D | 2001 | ACO | 5 | 0 |
| 3 | C | 2001 | ACO | 14 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

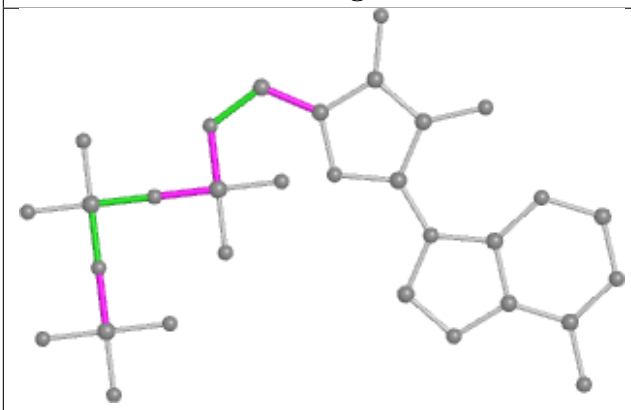
## Ligand ATP C 2000



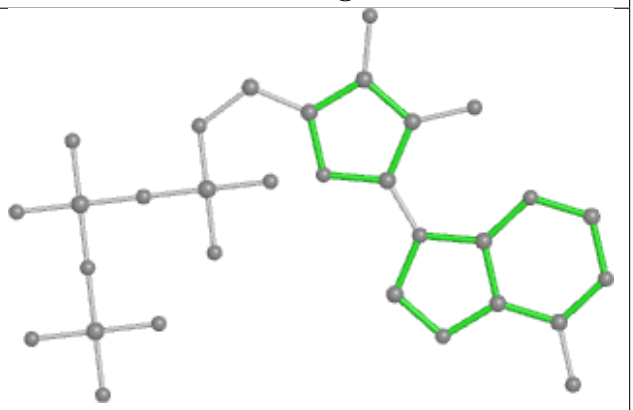
Bond lengths



Bond angles

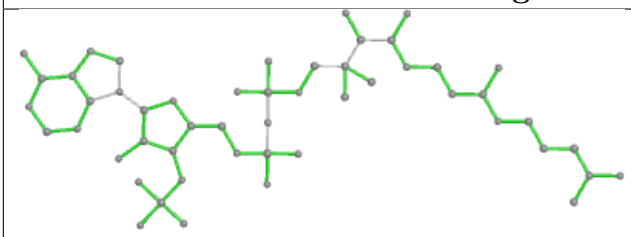


Torsions

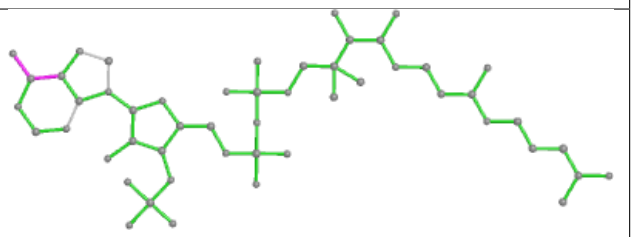


Rings

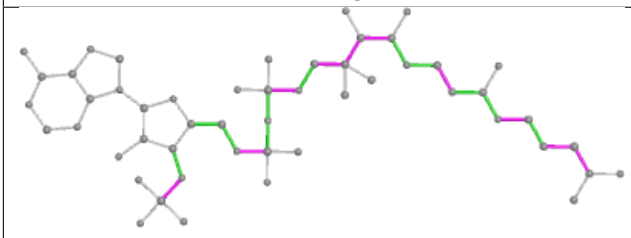
## Ligand ACO D 2001



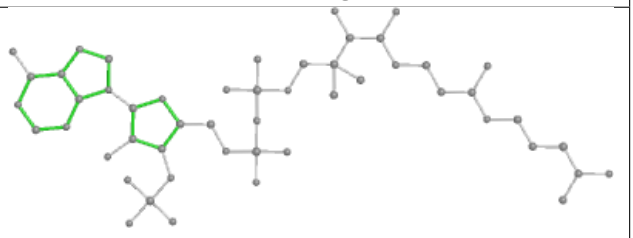
Bond lengths



Bond angles

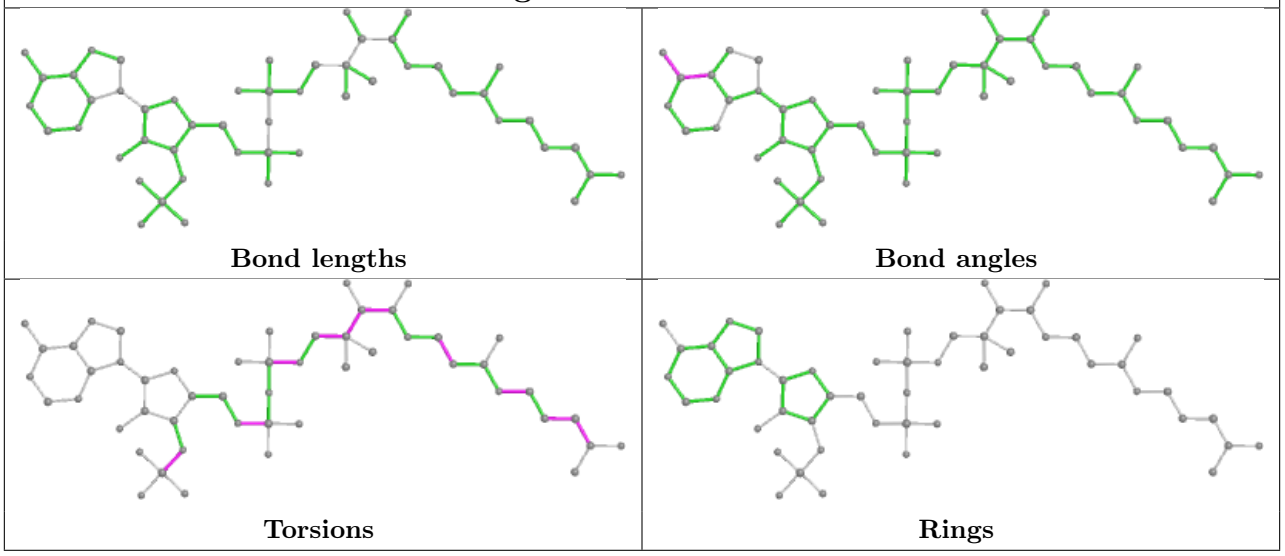


Torsions

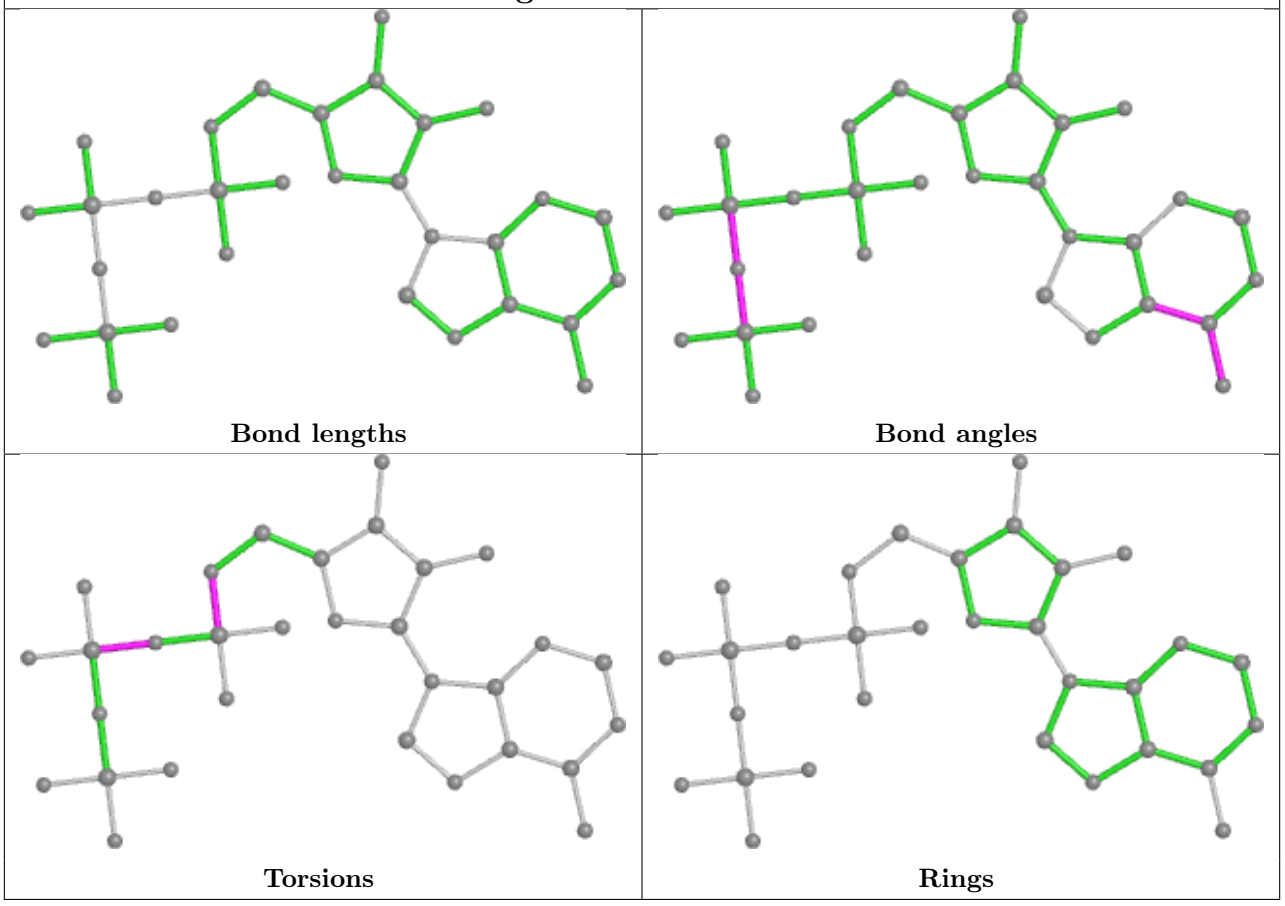


Rings

**Ligand ACO C 2001**




**Ligand ATP D 2002**




## 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.

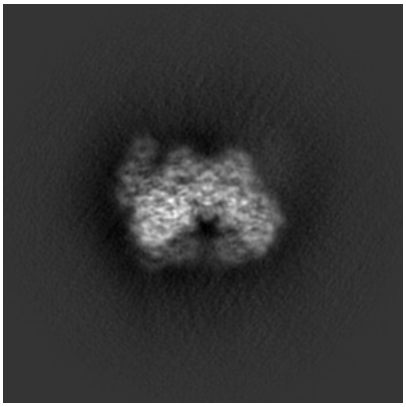
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32780. These allow visual inspection of the internal detail of the map and identification of artifacts.

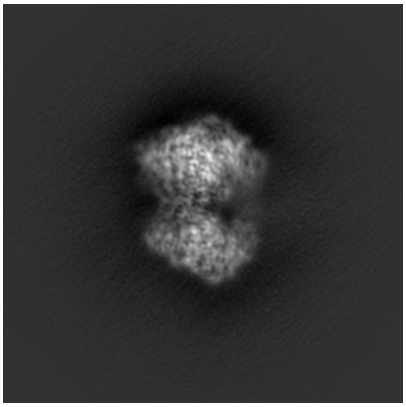
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

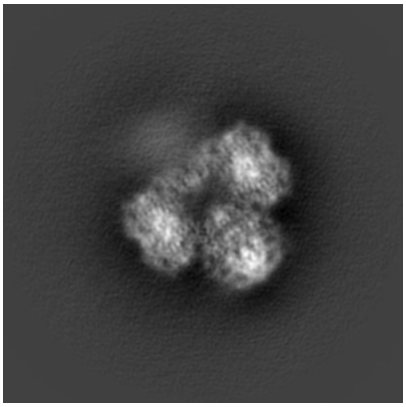
### 6.1.1 Primary map



X



Y

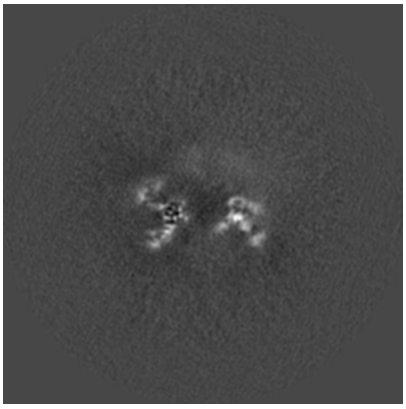


Z

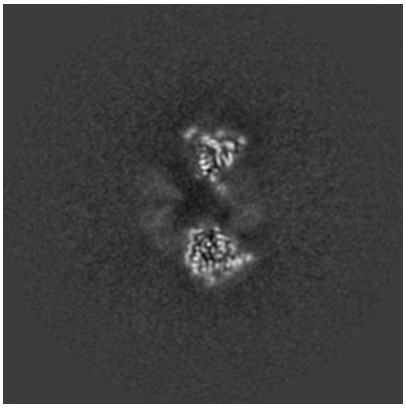
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

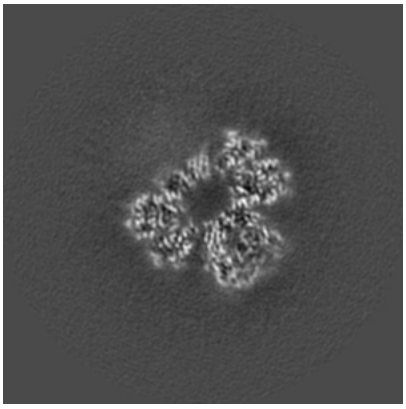
### 6.2.1 Primary map



X Index: 156



Y Index: 156

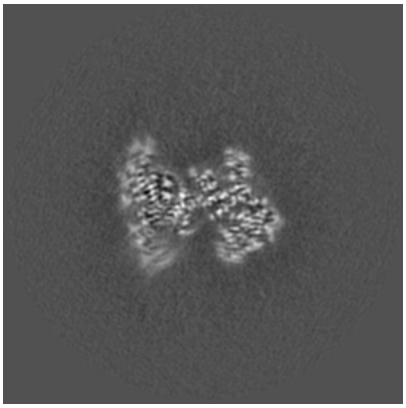


Z Index: 156

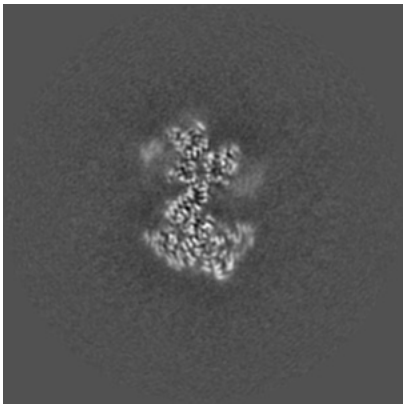
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

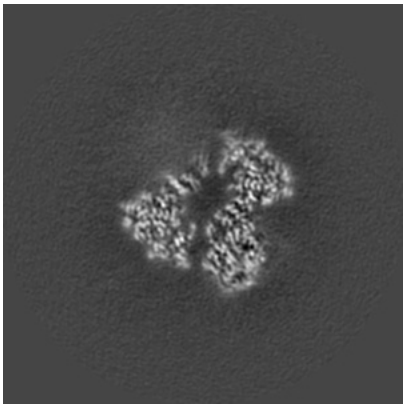
### 6.3.1 Primary map



X Index: 193



Y Index: 129

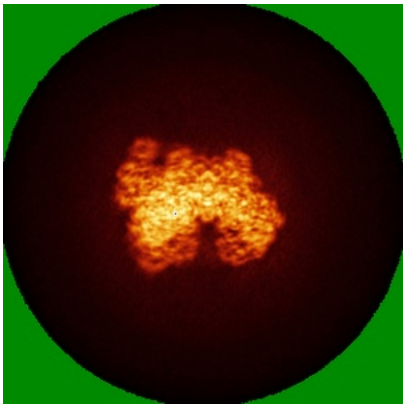


Z Index: 160

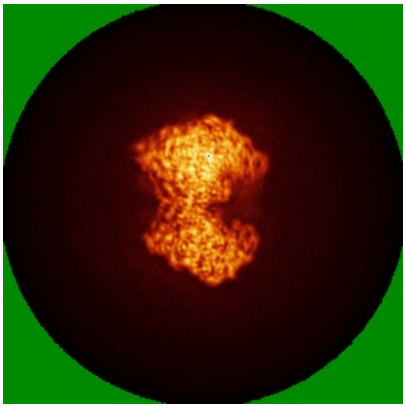
The images above show the largest variance slices of the map in three orthogonal directions.

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

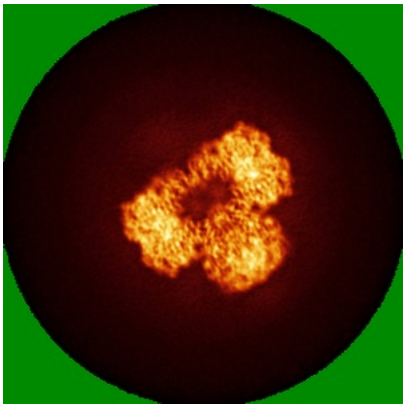
### 6.4.1 Primary map



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

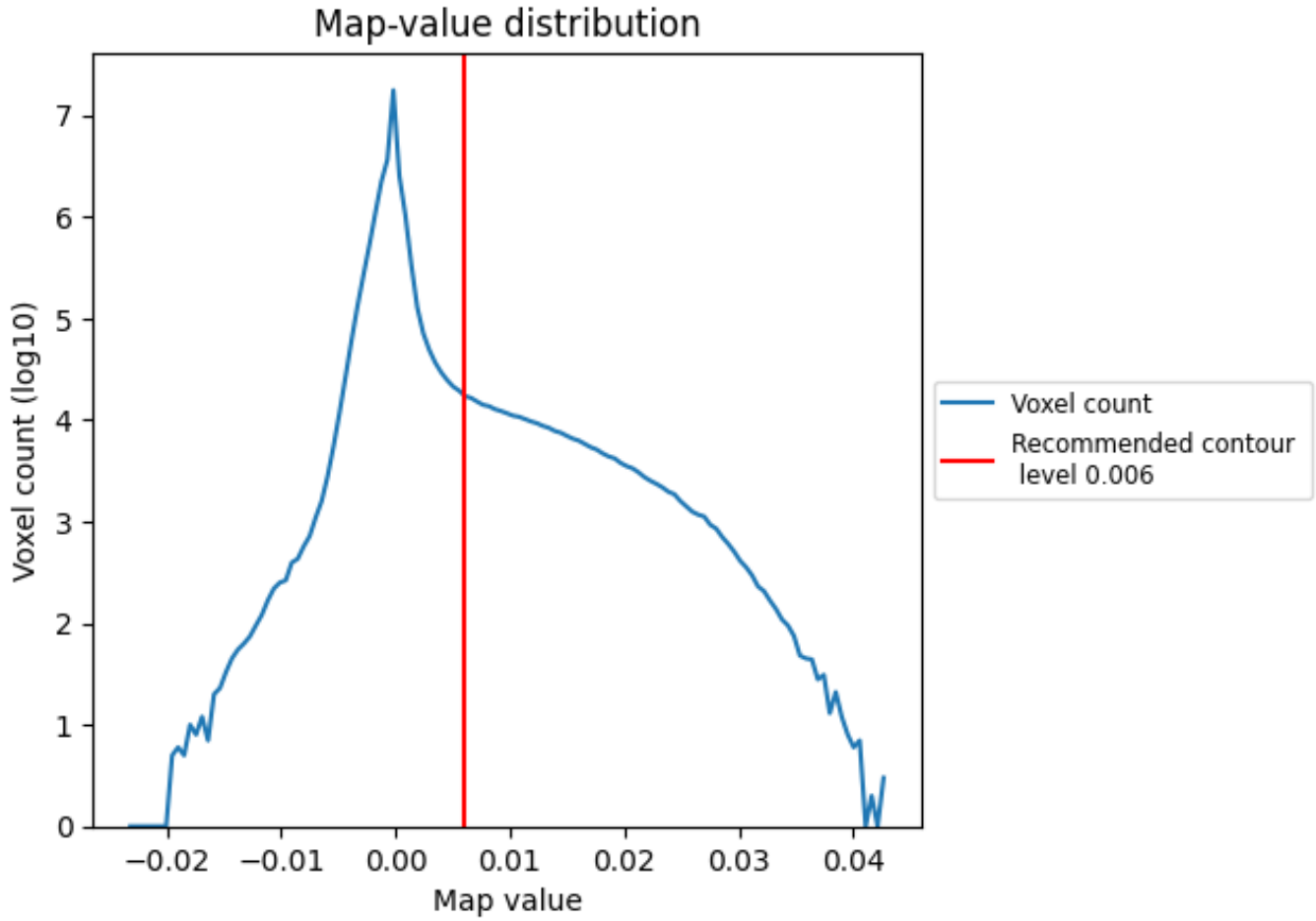
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

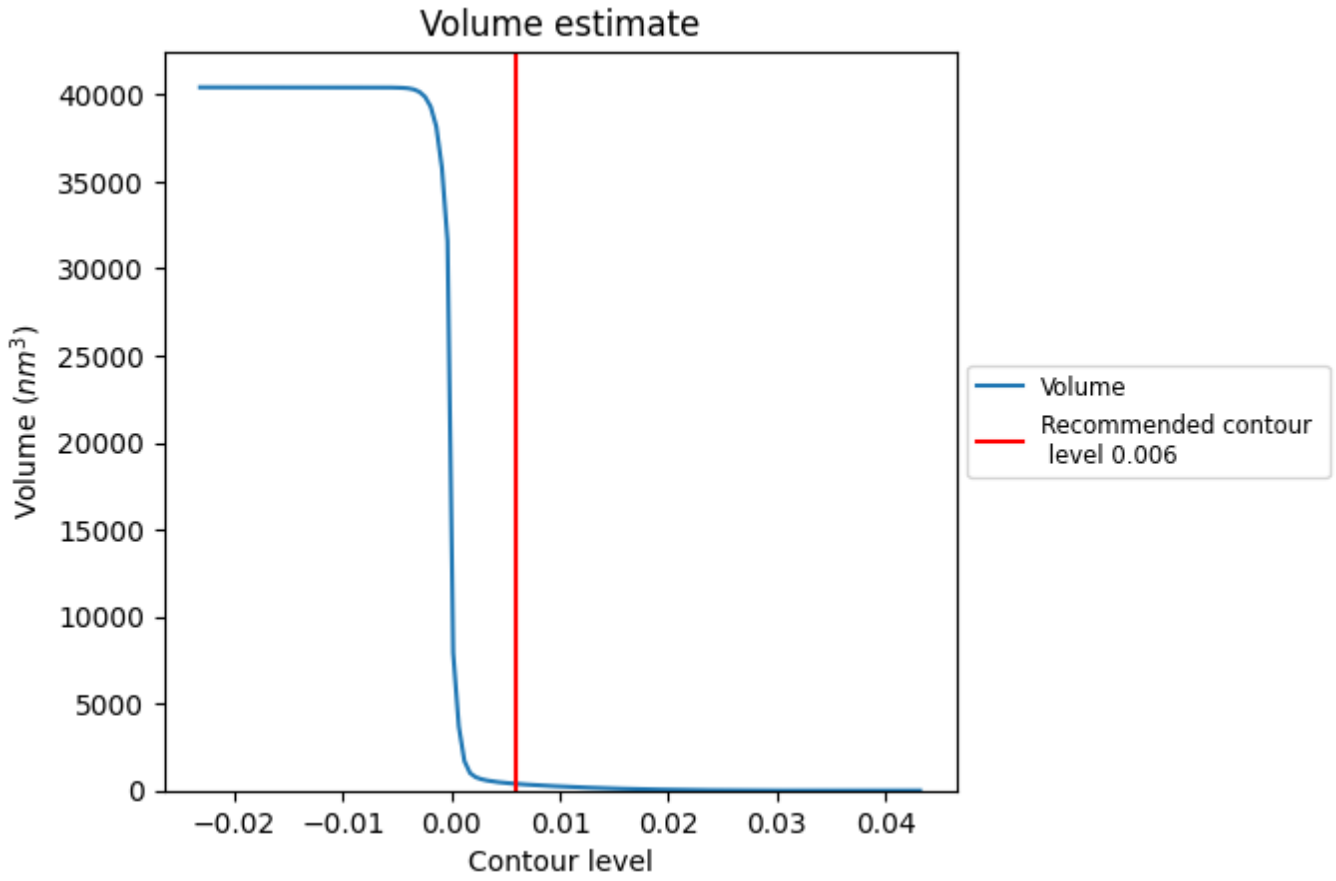
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

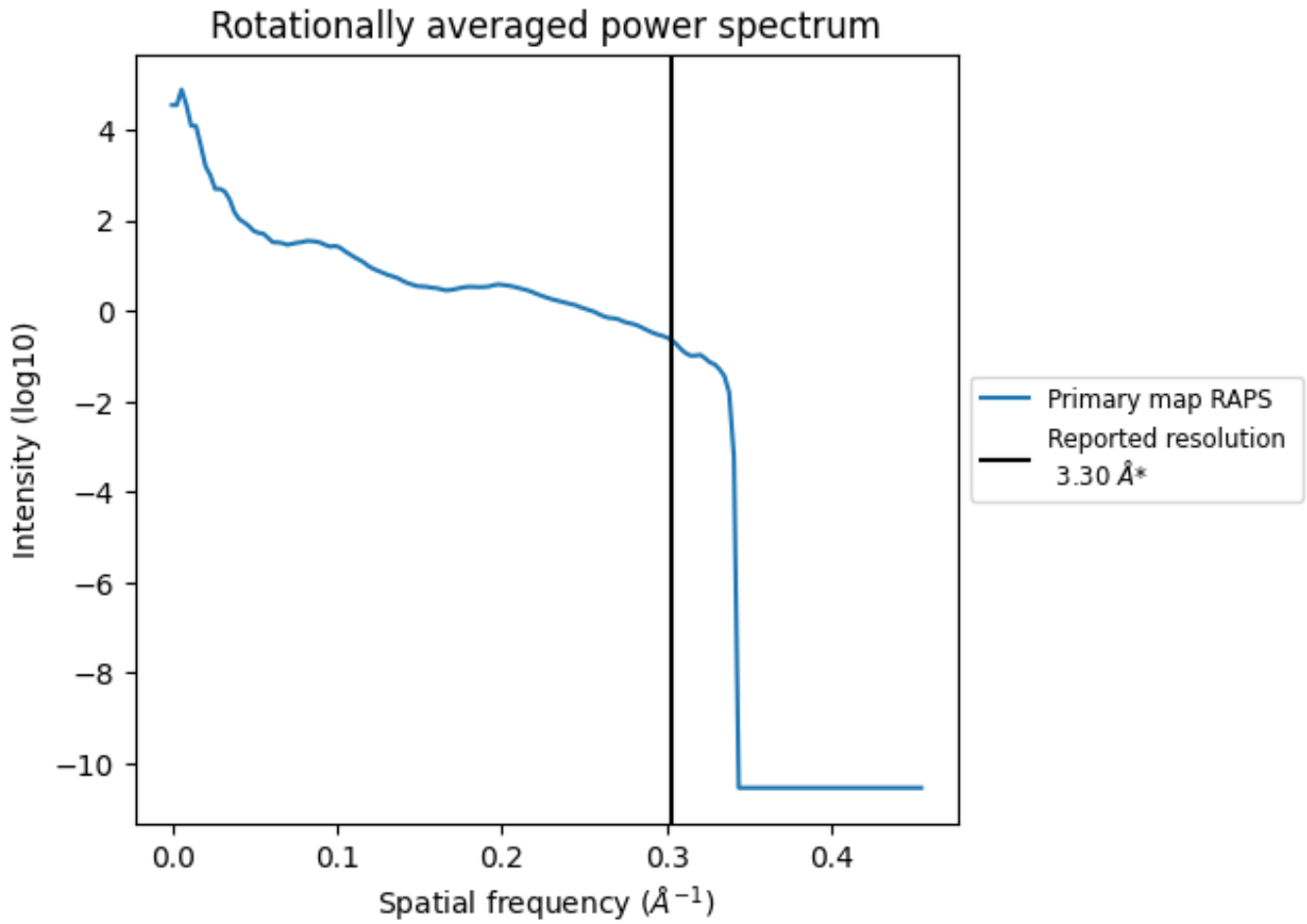
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 386 $nm^3$; this corresponds to an approximate mass of 348 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 0.303 Å$^{-1}$

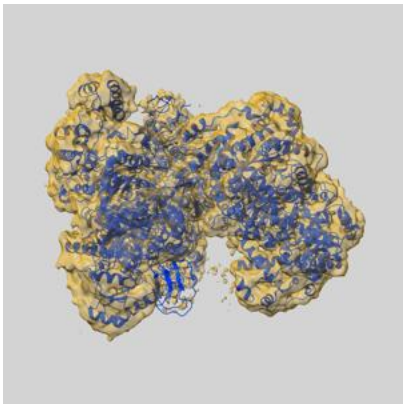
# 8 Fourier-Shell correlation (i)

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

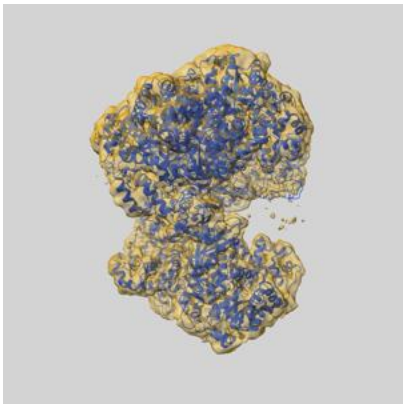
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32780 and PDB model 7WTE. Per-residue inclusion information can be found in section 3 on page 5.

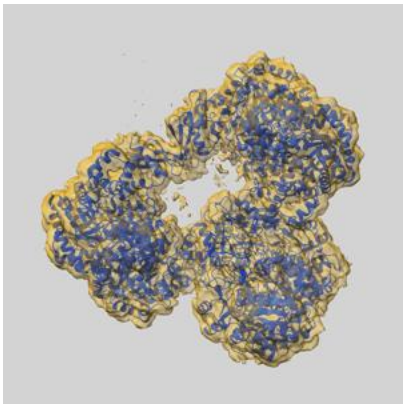
## 9.1 Map-model overlay



X



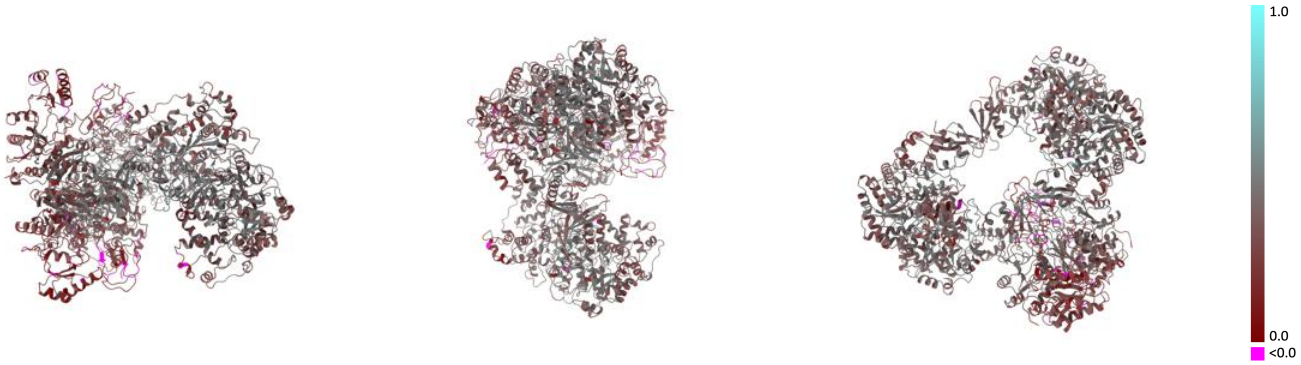
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

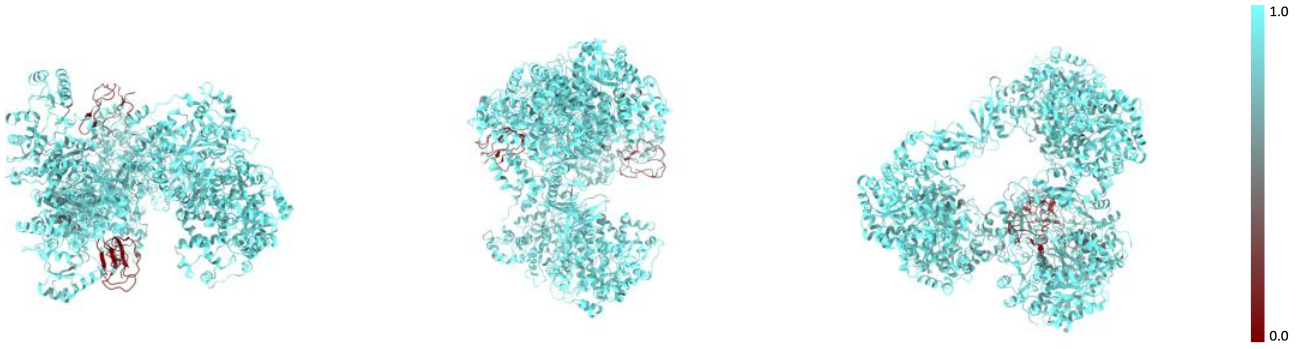
## 9.2 Q-score mapped to coordinate model




X Y Z

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.

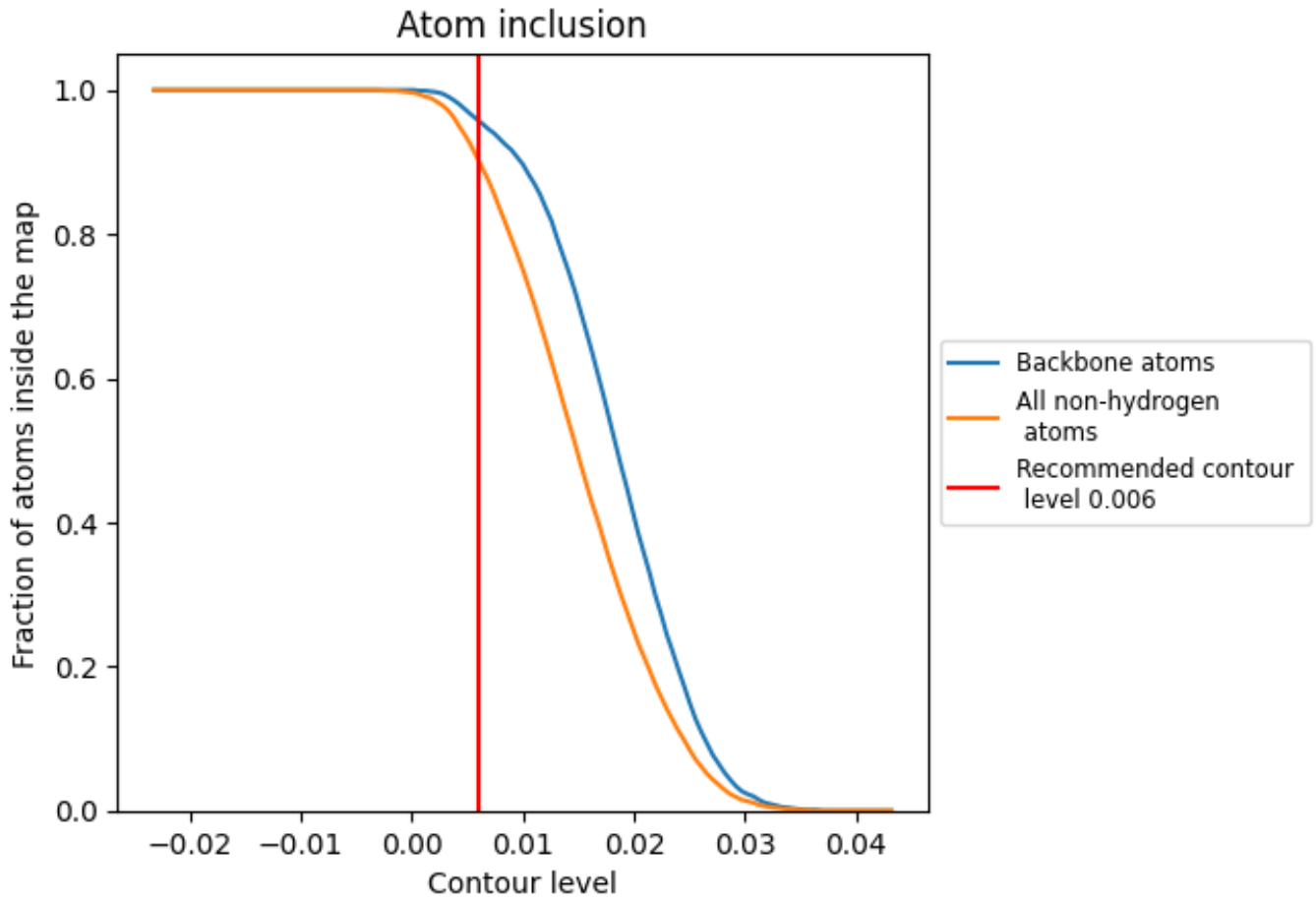
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

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 (0.006).

## 9.4 Atom inclusion (i)




At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.006) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9030 | 0.3600 |
| A | 0.9530 | 0.3810 |
| B | 0.9540 | 0.3920 |
| C | 0.8670 | 0.3370 |
| D | 0.8880 | 0.3550 |