



Full wwPDB EM Validation Report ⓘ

Feb 20, 2025 – 02:12 PM EST

PDB ID : 7SW4
EMDB ID : EMD-25462
Title : MicroED structure of proteinase K from a 540 nm thick lamella measured at 200 kV
Authors : Martynowycz, M.W.; Clabbers, M.T.B.; Unge, J.; Hattne, J.; Gonen, T.
Deposited on : 2021-11-19
Resolution : 2.40 Å(reported)
Based on initial model : 6CL7

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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

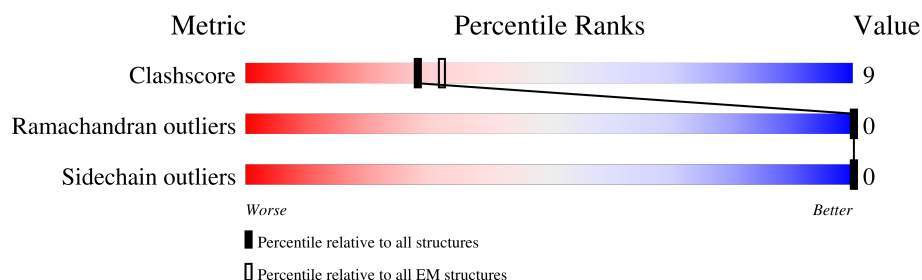
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY


The reported resolution of this entry is 2.40 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 279 |  |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2073 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 Proteinase K.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2029 | 1247 | 357 | 415 | 10 | | |

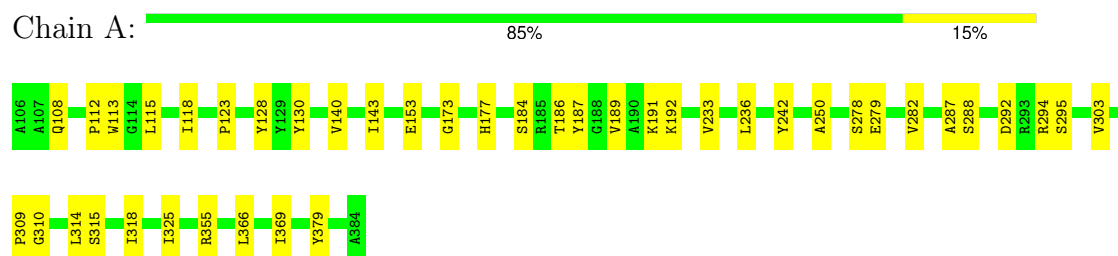
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 2 | A | 44 | Total | O | 0 |
| | | | 44 | 44 | |

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. 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. 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: Proteinase K



4 Experimental information

| Property | Value | Source |
|--------------------------------------|--|-----------|
| EM reconstruction method | CRYSTALLOGRAPHY | Depositor |
| Imposed symmetry | 3D CRYSTAL, $a=67.72$ Å, $b=67.72$ Å, $c=102.85$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, $\gamma=90^\circ$, space group=P 43 21 2 | Depositor |
| Number of images used | Not provided | |
| Resolution determination method | DIFFRACTION PATTERN/LAYERLINES | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 0.01 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI CETA (4k x 4k) | 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 | 0.37 | 0/2068 | 0.60 | 2/2810 (0.1%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 355 | ARG | NE-CZ-NH1 | -6.49 | 117.05 | 120.30 |
| 1 | A | 355 | ARG | N-CA-CB | -5.14 | 101.35 | 110.60 |

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 | 2029 | 0 | 1932 | 37 | 0 |
| 2 | A | 44 | 0 | 0 | 3 | 0 |
| All | All | 2073 | 0 | 1932 | 37 | 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 9.

All (37) 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:186:THR:HB | 1:A:187:TYR:HD2 | 1.42 | 0.85 |
| 1:A:115:LEU:HB3 | 1:A:128:TYR:HD1 | 1.42 | 0.84 |
| 1:A:187:TYR:CE1 | 1:A:314:LEU:HG | 2.12 | 0.84 |
| 1:A:279:GLU:OE1 | 2:A:401:HOH:O | 1.97 | 0.83 |
| 1:A:187:TYR:HD1 | 1:A:315:SER:HA | 1.44 | 0.83 |
| 1:A:128:TYR:CE2 | 1:A:130:TYR:HB3 | 2.17 | 0.80 |
| 1:A:115:LEU:HB3 | 1:A:128:TYR:CD1 | 2.17 | 0.80 |
| 1:A:186:THR:HB | 1:A:187:TYR:CD2 | 2.19 | 0.78 |
| 1:A:187:TYR:HE1 | 1:A:314:LEU:HG | 1.47 | 0.77 |
| 1:A:128:TYR:HE2 | 1:A:130:TYR:HB3 | 1.49 | 0.75 |
| 1:A:128:TYR:CD2 | 1:A:130:TYR:HD1 | 2.05 | 0.74 |
| 1:A:123:PRO:O | 2:A:403:HOH:O | 2.08 | 0.70 |
| 1:A:187:TYR:CD1 | 1:A:315:SER:HA | 2.26 | 0.70 |
| 1:A:184:SER:OG | 1:A:187:TYR:HB2 | 1.93 | 0.69 |
| 1:A:287:ALA:HB1 | 1:A:310:GLY:HA3 | 1.81 | 0.62 |
| 1:A:288:SER:HA | 1:A:295:SER:H | 1.67 | 0.58 |
| 1:A:140:VAL:HG22 | 1:A:233:VAL:HB | 1.88 | 0.56 |
| 1:A:108:GLN:NE2 | 1:A:186:THR:O | 2.24 | 0.55 |
| 1:A:173:GLY:HA2 | 1:A:318:ILE:HG23 | 1.88 | 0.54 |
| 1:A:115:LEU:HD22 | 1:A:128:TYR:HE1 | 1.75 | 0.52 |
| 1:A:177:HIS:CD2 | 1:A:315:SER:HB3 | 2.45 | 0.52 |
| 1:A:118:ILE:HD11 | 1:A:128:TYR:OH | 2.12 | 0.50 |
| 1:A:191:LYS:O | 1:A:192:LYS:HE2 | 2.14 | 0.48 |
| 1:A:177:HIS:CE1 | 1:A:325:ILE:HG12 | 2.49 | 0.48 |
| 1:A:112:PRO:HD2 | 1:A:115:LEU:HD12 | 1.96 | 0.47 |
| 1:A:113:TRP:CH2 | 1:A:309:PRO:HB3 | 2.51 | 0.45 |
| 1:A:250:ALA:HB1 | 1:A:282:VAL:HG11 | 1.99 | 0.45 |
| 1:A:177:HIS:CG | 1:A:315:SER:HB3 | 2.52 | 0.44 |
| 1:A:278:SER:HA | 1:A:303:VAL:HG21 | 2.00 | 0.43 |
| 1:A:118:ILE:HD11 | 1:A:128:TYR:CZ | 2.53 | 0.43 |
| 1:A:128:TYR:OH | 1:A:189:VAL:HG13 | 2.20 | 0.41 |
| 1:A:153:GLU:HB3 | 1:A:184:SER:HB2 | 2.01 | 0.41 |
| 1:A:242:TYR:OH | 2:A:406:HOH:O | 2.18 | 0.41 |
| 1:A:118:ILE:O | 1:A:379:TYR:HA | 2.22 | 0.40 |
| 1:A:143:ILE:HD12 | 1:A:236:LEU:HD11 | 2.02 | 0.40 |
| 1:A:292:ASP:O | 1:A:366:LEU:HA | 2.21 | 0.40 |
| 1:A:294:ARG:HB2 | 1:A:369:ILE:HD13 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 | 277/279 (99%) | 263 (95%) | 14 (5%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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 | 213/213 (100%) | 213 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 174 | HIS |
| 1 | A | 177 | HIS |
| 1 | A | 381 | ASN |

5.3.3 RNA

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](#)

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

This section contains visualisations of the EMDB entry EMD-25462. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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 ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.