



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:20 AM GMT

PDB ID : 1HT3
Title : MERCURY INDUCED MODIFICATIONS IN THE STEREOCHEMISTRY OF THE ACTIVE SITE THROUGH CYS-73 IN A SERINE PROTEASE: CRYSTAL STRUCTURE OF THE COMPLEX OF A PARTIALLY MODIFIED PROTEINASE K WITH MERCURY AT 1.8 Å RESOLUTION
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Deposited on : 2000-12-27
Resolution : 1.80 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

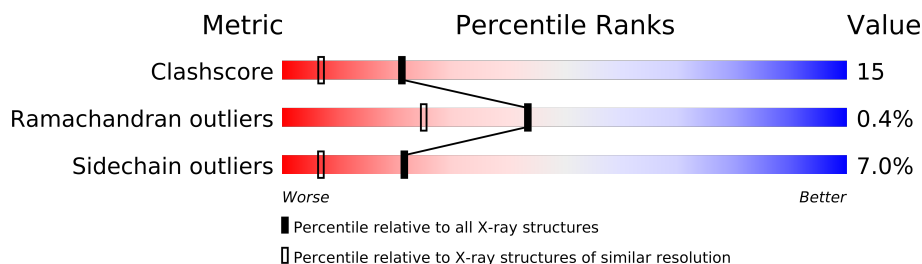
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 79885 | 4461 (1.80-1.80) |
| Ramachandran outliers | 78287 | 4404 (1.80-1.80) |
| Sidechain outliers | 78261 | 4403 (1.80-1.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2278 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 279 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2031 | 1249 | 357 | 415 | 10 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 85 | VAL | ALA | CONFLICT | UNP P06873 |

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | A | 2 | Total | Hg | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | A | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | A | 244 | Total | O | 0 | 0 |
| | | | 244 | 244 | | |

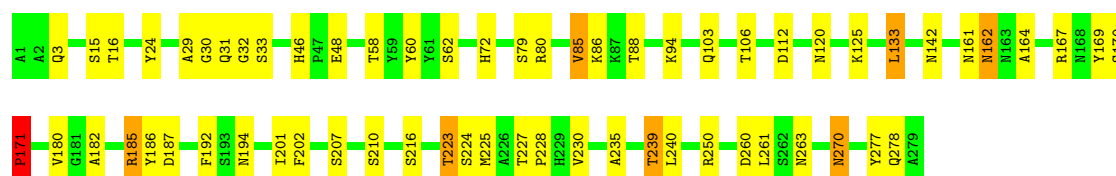
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

• Molecule 1: PROTEINASE K

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 43 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 68.36Å 68.36Å 108.70Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 10.00 – 1.80 | Depositor |
| % Data completeness (in resolution range) | 98.3 (10.00-1.80) | Depositor |
| R_{merge} | 0.05 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | REFMAC | Depositor |
| R, R_{free} | 0.164 , 0.221 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 2278 | wwPDB-VP |
| Average B, all atoms (Å ²) | 16.0 | wwPDB-VP |

5 Model quality

5.1 Standard geometry

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

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 | 0.36 | 0/2070 | 0.65 | 2/2813 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 2 | 5 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|---------|-------|------------------------|---------------------|
| 1 | A | 171 | PRO | CA-N-CD | -5.41 | 103.92 | 111.50 |
| 1 | A | 171 | PRO | O-C-N | -5.10 | 114.54 | 122.70 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 58 | THR | CB |
| 1 | A | 171 | PRO | CA |

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 169 | TYR | Sidechain |
| 1 | A | 170 | SER | Peptide |
| 1 | A | 171 | PRO | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 185 | ARG | Mainchain |
| 1 | A | 260 | ASP | Mainchain |

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2031 | 0 | 1938 | 61 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 244 | 0 | 0 | 8 | 2 |
| All | All | 2278 | 0 | 1938 | 61 | 2 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (61) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:180:VAL:HG21 | 1:A:230:VAL:HG21 | 1.44 | 0.97 |
| 1:A:58:THR:HG21 | 1:A:62:SER:O | 1.72 | 0.89 |
| 1:A:207:SER:HB3 | 4:A:571:HOH:O | 1.74 | 0.87 |
| 1:A:261:LEU:H | 1:A:270:ASN:HD21 | 1.22 | 0.84 |
| 1:A:30:GLY:HA3 | 1:A:85:VAL:CG2 | 2.10 | 0.81 |
| 1:A:30:GLY:HA3 | 1:A:85:VAL:HG23 | 1.62 | 0.81 |
| 1:A:112:ASP:OD2 | 4:A:726:HOH:O | 1.98 | 0.81 |
| 1:A:58:THR:HG22 | 1:A:60:TYR:H | 1.45 | 0.80 |
| 1:A:85:VAL:HG22 | 1:A:88:THR:HB | 1.68 | 0.76 |
| 1:A:29:ALA:O | 1:A:85:VAL:HG23 | 1.88 | 0.74 |
| 1:A:46:HIS:HD2 | 1:A:48:GLU:H | 1.36 | 0.73 |
| 1:A:263:ASN:HB3 | 4:A:641:HOH:O | 1.90 | 0.72 |
| 1:A:180:VAL:CG2 | 1:A:230:VAL:HG21 | 2.19 | 0.69 |
| 1:A:85:VAL:CG2 | 1:A:88:THR:HB | 2.25 | 0.66 |
| 1:A:31:GLN:HE21 | 1:A:32:GLY:H | 1.45 | 0.64 |
| 1:A:223:THR:O | 4:A:555:HOH:O | 2.16 | 0.62 |
| 1:A:171:PRO:O | 1:A:171:PRO:CG | 2.48 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:180:VAL:HG21 | 1:A:230:VAL:CG2 | 2.27 | 0.60 |
| 1:A:171:PRO:O | 1:A:171:PRO:CD | 2.50 | 0.58 |
| 1:A:58:THR:HG23 | 1:A:94:LYS:HD3 | 1.86 | 0.58 |
| 1:A:30:GLY:HA3 | 1:A:85:VAL:HG21 | 1.84 | 0.58 |
| 1:A:171:PRO:O | 1:A:171:PRO:HD3 | 2.03 | 0.58 |
| 1:A:224:SER:HB3 | 1:A:225:MET:HE2 | 1.86 | 0.58 |
| 1:A:227:THR:O | 1:A:230:VAL:HG22 | 2.03 | 0.57 |
| 1:A:224:SER:HB3 | 1:A:225:MET:CE | 2.34 | 0.57 |
| 1:A:182:ALA:HB2 | 1:A:223:THR:HA | 1.87 | 0.57 |
| 1:A:58:THR:HG23 | 1:A:94:LYS:HB3 | 1.86 | 0.56 |
| 1:A:142:ASN:OD1 | 1:A:171:PRO:HD2 | 2.06 | 0.55 |
| 1:A:72:HIS:CD2 | 1:A:210:SER:HB3 | 2.42 | 0.54 |
| 1:A:171:PRO:O | 1:A:171:PRO:HG3 | 2.08 | 0.53 |
| 1:A:164:ALA:H | 1:A:194:ASN:ND2 | 2.08 | 0.51 |
| 1:A:235:ALA:O | 1:A:239:THR:HG23 | 2.12 | 0.50 |
| 1:A:162:ASN:H | 1:A:194:ASN:ND2 | 2.10 | 0.49 |
| 1:A:30:GLY:CA | 1:A:85:VAL:HG23 | 2.40 | 0.48 |
| 1:A:125:LYS:HG3 | 1:A:239:THR:HB | 1.95 | 0.48 |
| 1:A:142:ASN:OD1 | 1:A:171:PRO:CD | 2.61 | 0.48 |
| 1:A:224:SER:HB2 | 4:A:676:HOH:O | 2.14 | 0.47 |
| 1:A:133:LEU:HD23 | 1:A:133:LEU:C | 2.33 | 0.47 |
| 1:A:30:GLY:HA2 | 1:A:239:THR:CG2 | 2.45 | 0.46 |
| 1:A:227:THR:N | 1:A:228:PRO:HD2 | 2.30 | 0.46 |
| 1:A:30:GLY:C | 1:A:239:THR:HG21 | 2.36 | 0.45 |
| 1:A:227:THR:O | 1:A:230:VAL:CG2 | 2.65 | 0.44 |
| 1:A:278:GLN:HG3 | 4:A:658:HOH:O | 2.17 | 0.44 |
| 1:A:31:GLN:HE21 | 1:A:32:GLY:N | 2.13 | 0.44 |
| 1:A:58:THR:CG2 | 1:A:94:LYS:HD3 | 2.48 | 0.44 |
| 1:A:161:ASN:OD1 | 1:A:192:PHE:CD1 | 2.72 | 0.43 |
| 1:A:24:TYR:HB3 | 1:A:277:TYR:CD1 | 2.54 | 0.43 |
| 1:A:201:ILE:HG13 | 1:A:202:PHE:N | 2.33 | 0.43 |
| 1:A:227:THR:HB | 1:A:228:PRO:HD3 | 2.01 | 0.43 |
| 1:A:3:GLN:HE22 | 1:A:86:LYS:NZ | 2.17 | 0.43 |
| 1:A:224:SER:HB2 | 1:A:225:MET:HE3 | 2.00 | 0.43 |
| 1:A:46:HIS:HE1 | 1:A:216:SER:O | 2.02 | 0.42 |
| 1:A:48:GLU:HB3 | 1:A:79:SER:HB2 | 2.00 | 0.42 |
| 1:A:164:ALA:H | 1:A:194:ASN:HD22 | 1.66 | 0.42 |
| 1:A:224:SER:CB | 1:A:225:MET:CE | 2.97 | 0.42 |
| 1:A:80:ARG:HH21 | 1:A:80:ARG:HD2 | 1.66 | 0.42 |
| 1:A:15:SER:HB2 | 4:A:600:HOH:O | 2.20 | 0.41 |
| 1:A:33:SER:HB3 | 1:A:239:THR:HG22 | 2.03 | 0.41 |
| 1:A:186:TYR:O | 1:A:187:ASP:HB2 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:133:LEU:C | 1:A:133:LEU:CD2 | 2.90 | 0.40 |
| 1:A:161:ASN:ND2 | 4:A:676:HOH:O | 2.54 | 0.40 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------|----------------------|-------------|----------|
| 4:A:647:HOH:O | 4:A:647:HOH:O[7_465] | 1.83 | 0.37 |
| 4:A:708:HOH:O | 4:A:708:HOH:O[7_465] | 2.13 | 0.07 |

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 X-ray entries followed by that with respect to entries of similar resolution. 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%) | 267 (96%) | 9 (3%) | 1 (0%) | 43 25 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 171 | PRO |

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 X-ray entries followed by that with respect to entries of similar resolution. 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 | 214/214 (100%) | 199 (93%) | 15 (7%) | 21 7 |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | THR |
| 1 | A | 85 | VAL |
| 1 | A | 103 | GLN |
| 1 | A | 106 | THR |
| 1 | A | 120 | ASN |
| 1 | A | 133 | LEU |
| 1 | A | 162 | ASN |
| 1 | A | 167 | ARG |
| 1 | A | 171 | PRO |
| 1 | A | 185 | ARG |
| 1 | A | 223 | THR |
| 1 | A | 239 | THR |
| 1 | A | 240 | LEU |
| 1 | A | 250 | ARG |
| 1 | A | 270 | ASN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | GLN |
| 1 | A | 31 | GLN |
| 1 | A | 46 | HIS |
| 1 | A | 119 | ASN |
| 1 | A | 162 | ASN |
| 1 | A | 168 | ASN |
| 1 | A | 194 | ASN |
| 1 | A | 229 | HIS |
| 1 | A | 270 | ASN |
| 1 | A | 276 | ASN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.