



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:59 PM EDT

PDB ID : 2PCU / pdb\_00002pcu  
Title : Human carboxypeptidase A4 in complex with a cleaved hexapeptide.  
Authors : Bayes, A.; Fernandez, D.; Sola, M.; Marrero, A.; Garcia-Pique, S.; Aviles, F.X.; Vendrell, J.; Gomis-Ruth, F.X.  
Deposited on : 2007-03-30  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity : **FAILED**  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : **FAILED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

There are no overall percentile quality scores available for this entry.

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 21 21 21  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 50.30Å 72.49Å 81.58Å<br>90.00° 90.00° 90.00°                | Depositor |
| Resolution (Å)   | 50.00 – 1.60  | Depositor |
| % Data completeness<br>(in resolution range)             | 98.5 (50.00-1.60)   | Depositor |
| $R_{merge}$  | 0.09  | Depositor |
| $R_{sym}$  | 0.09  | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 3.48 (at 1.60Å)   | Xtrriage  |
| Refinement program                                       | REFMAC  | Depositor |
| R, $R_{free}$  | 0.159 , 0.176   | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 19.5  | Xtrriage  |
| Anisotropy   | 0.533   | Xtrriage  |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$ | Xtrriage  |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtrriage  |
| Total number of atoms                                    | 2792  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 25.0  | wwPDB-VP  |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

### 3 Model quality [i](#)

#### 3.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 3.2 Too-close contacts [i](#)

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#### 3.3 Torsion angles [i](#)

##### 3.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

##### 3.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

##### 3.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

#### 3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

#### 3.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

No monomer is involved in short contacts.

### 3.7 Other polymers

There are no such residues in this entry.

### 3.8 Polymer linkage issues

There are no chain breaks in this entry.

## 4 Fit of model and data

### 4.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 4.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 4.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 4.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 4.5 Other polymers

EDS failed to run properly - this section is therefore empty.