



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:20 PM EDT

PDB ID : 1KLI / pdb\_00001kli  
Title : Cofactor-and substrate-assisted activation of factor VIIa  
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Kresse, G.B.; Kopetzki, E.; Brandstetter, H.  
Deposited on : 2001-12-12  
Resolution : 1.69 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                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | <b>FAILED</b>                                                    |
| 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                                                             |

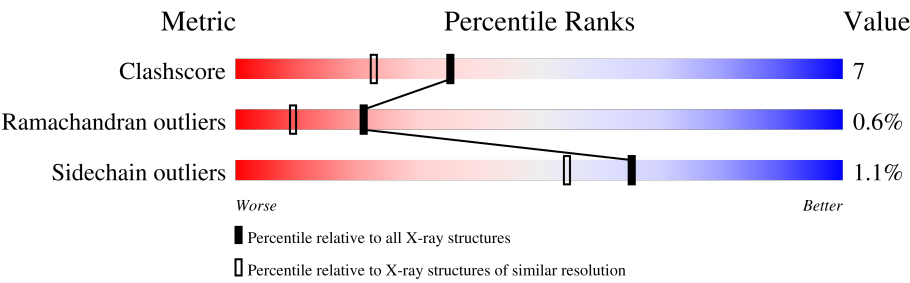
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 5924 (1.70-1.70)                                      |
| Ramachandran outliers | 187476                      | 5846 (1.70-1.70)                                      |
| Sidechain outliers    | 187428                      | 5846 (1.70-1.70)                                      |

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 41 21 2                                                   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 94.44Å 94.44Å 114.31Å<br>90.00° 90.00° 90.00°               | Depositor |
| Resolution (Å)                                           | 20.00 – 1.69                                                | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (20.00-1.69)                                | Depositor |
| $R_{merge}$                                              | 0.06                                                        | Depositor |
| $R_{sym}$                                                | (Not available)                                             | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 1.13 (at 1.66Å)                                             | Xtriage   |
| Refinement program                                       | CNS                                                         | Depositor |
| R, $R_{free}$                                            | 0.209 , 0.225                                               | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 18.0                                                        | Xtriage   |
| Anisotropy                                               | 0.278                                                       | Xtriage   |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage   |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 2796                                                        | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 26.0                                                        | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

### 3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEN, CA, SO4, GOL

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   | L     | 0.34         | 0/482       | 0.75        | 0/651         |
| 2   | H     | 0.35         | 0/2062      | 0.84        | 3/2807 (0.1%) |
| All | All   | 0.35         | 0/2544      | 0.83        | 3/3458 (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 |
|-----|-------|---------------------|---------------------|
| 2   | H     | 0                   | 1                   |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 2   | H     | 199 | HIS  | N-CA-C | -6.12 | 95.39                  | 107.69              |
| 2   | H     | 28  | PRO  | N-CA-C | 5.62  | 121.24                 | 113.98              |
| 2   | H     | 190 | SER  | N-CA-C | -5.31 | 102.89                 | 110.59              |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | H     | 107 | ARG  | Sidechain |

### 3.2 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   | L     | 469   | 0        | 439      | 9       | 0            |
| 2   | H     | 1992  | 0        | 1977     | 30      | 4            |
| 3   | H     | 20    | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 9     | 0        | 8        | 0       | 0            |
| 6   | H     | 6     | 0        | 7        | 0       | 0            |
| 7   | H     | 237   | 0        | 0        | 5       | 4            |
| 7   | L     | 62    | 0        | 0        | 0       | 3            |
| All | All   | 2796  | 0        | 2431     | 36      | 8            |

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 7.

All (36) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:50[B]:ILE:HG22 | 2:H:111:PRO:HB3    | 1.50                     | 0.94              |
| 1:L:88:GLN:HE22    | 1:L:94:GLU:HB2     | 1.47                     | 0.79              |
| 2:H:127:THR:O      | 2:H:129(B):ARG:HG2 | 1.84                     | 0.76              |
| 2:H:50[B]:ILE:CG2  | 2:H:111:PRO:HB3    | 2.18                     | 0.73              |
| 2:H:45:THR:OG1     | 2:H:198:PRO:HB3    | 1.97                     | 0.64              |
| 2:H:35[A]:VAL:HG22 | 2:H:64[A]:LEU:HD23 | 1.81                     | 0.62              |
| 2:H:62:ARG:NH2     | 2:H:250:VAL:HG23   | 2.14                     | 0.62              |
| 2:H:50[B]:ILE:HG22 | 2:H:111:PRO:CB     | 2.28                     | 0.62              |
| 2:H:60(B):ILE:HD12 | 2:H:64[A]:LEU:HD21 | 1.81                     | 0.61              |
| 2:H:64[B]:LEU:HG   | 2:H:85:VAL:HG21    | 1.84                     | 0.60              |
| 1:L:140:ILE:HD11   | 2:H:26:GLU:HG3     | 1.86                     | 0.57              |
| 2:H:48:ASN:HD21    | 2:H:51:TRP:HB2     | 1.69                     | 0.55              |
| 1:L:115:HIS:HE1    | 7:H:516:HOH:O      | 1.89                     | 0.55              |
| 1:L:110:ARG:HD2    | 1:L:110:ARG:C      | 2.34                     | 0.52              |
| 2:H:48:ASN:ND2     | 2:H:51:TRP:HB2     | 2.24                     | 0.52              |
| 2:H:256:PHE:HA     | 2:H:257:PRO:C      | 2.35                     | 0.52              |
| 2:H:144:LEU:HD21   | 2:H:152:ALA:HB2    | 1.92                     | 0.51              |
| 2:H:27:CYS:HB3     | 7:H:568:HOH:O      | 2.10                     | 0.50              |
| 1:L:140:ILE:HD11   | 2:H:26:GLU:CG      | 2.42                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:48:ASN:HB2     | 7:H:627:HOH:O      | 2.13                     | 0.48              |
| 2:H:235:ILE:O      | 2:H:239[A]:GLN:HG3 | 2.13                     | 0.48              |
| 1:L:89:LEU:HG      | 1:L:108:THR:HG23   | 1.95                     | 0.48              |
| 2:H:51:TRP:CZ3     | 2:H:107:ARG:HB2    | 2.51                     | 0.45              |
| 1:L:99:GLU:HA      | 2:H:204:ARG:HD2    | 1.99                     | 0.45              |
| 2:H:98:THR:HB      | 7:H:710:HOH:O      | 2.16                     | 0.44              |
| 2:H:35[A]:VAL:CG2  | 2:H:41:LEU:HD22    | 2.48                     | 0.44              |
| 1:L:101:TYR:OH     | 1:L:115:HIS:HD2    | 2.01                     | 0.44              |
| 2:H:90:ILE:HG23    | 2:H:91:PRO:HD2     | 2.01                     | 0.43              |
| 1:L:105:HIS:HB2    | 1:L:109:LYS:HB2    | 2.01                     | 0.43              |
| 2:H:162:ARG:C      | 2:H:163:LEU:HD12   | 2.44                     | 0.42              |
| 2:H:176:ILE:HD13   | 2:H:182:CYS:SG     | 2.59                     | 0.42              |
| 2:H:100:ASN:HD22   | 2:H:100:ASN:HA     | 1.66                     | 0.41              |
| 2:H:60(D):ASN:HD22 | 2:H:63:ASN:CG      | 2.28                     | 0.41              |
| 2:H:135:PHE:HB3    | 2:H:159:ASN:ND2    | 2.36                     | 0.41              |
| 2:H:135:PHE:HB3    | 2:H:159:ASN:HD21   | 1.86                     | 0.40              |
| 2:H:37:ASN:HB2     | 7:H:740:HOH:O      | 2.21                     | 0.40              |

All (8) 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               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 2:H:77:ASP:O  | 7:L:748:HOH:O[5_555] | 2.03                     | 0.17              |
| 7:H:677:HOH:O | 7:H:774:HOH:O[4_454] | 2.05                     | 0.15              |
| 7:H:673:HOH:O | 7:H:769:HOH:O[4_454] | 2.06                     | 0.14              |
| 2:H:40:GLN:N  | 7:L:530:HOH:O[5_555] | 2.09                     | 0.11              |
| 2:H:74:SER:O  | 7:L:604:HOH:O[5_555] | 2.09                     | 0.11              |
| 2:H:147:ARG:O | 2:H:253:ARG:N[3_555] | 2.10                     | 0.10              |
| 7:H:779:HOH:O | 7:H:788:HOH:O[4_454] | 2.14                     | 0.06              |
| 7:H:598:HOH:O | 7:H:657:HOH:O[4_454] | 2.16                     | 0.04              |

### 3.3 Torsion angles ⓘ

#### 3.3.1 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   | L     | 60/69 (87%)    | 54 (90%)  | 4 (7%)  | 2 (3%)   | 3           | 0   |
| 2   | H     | 257/254 (101%) | 246 (96%) | 11 (4%) | 0        | 100         | 100 |
| All | All   | 317/323 (98%)  | 300 (95%) | 15 (5%) | 2 (1%)   | 21          | 9   |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 86  | ASP  |
| 1   | L     | 88  | GLN  |

### 3.3.2 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   | L     | 55/60 (92%)    | 55 (100%) | 0        | 100         | 100 |
| 2   | H     | 221/216 (102%) | 218 (99%) | 3 (1%)   | 59          | 46  |
| All | All   | 276/276 (100%) | 273 (99%) | 3 (1%)   | 65          | 54  |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 100 | ASN  |
| 2   | H     | 159 | ASN  |
| 2   | H     | 217 | GLN  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 88  | GLN  |
| 1   | L     | 93  | ASN  |
| 1   | L     | 115 | HIS  |
| 2   | H     | 37  | ASN  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 2   | H     | 60(D) | ASN  |
| 2   | H     | 63    | ASN  |
| 2   | H     | 100   | ASN  |
| 2   | H     | 109   | HIS  |
| 2   | H     | 159   | ASN  |
| 2   | H     | 217   | GLN  |

### 3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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 7 ligands modelled in this entry, 7 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 [i](#)

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.