



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:40 PM UTC

PDB ID : 1NL6 / pdb\_00001nl6  
Title : Crystal Structure Of The Cysteine Protease Human Cathepsin K In Complex  
With A Covalent Azepanone Inhibitor  
Authors : Smith, W.W.; Janson, C.A.; Zhao, B.  
Deposited on : 2003-01-06  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

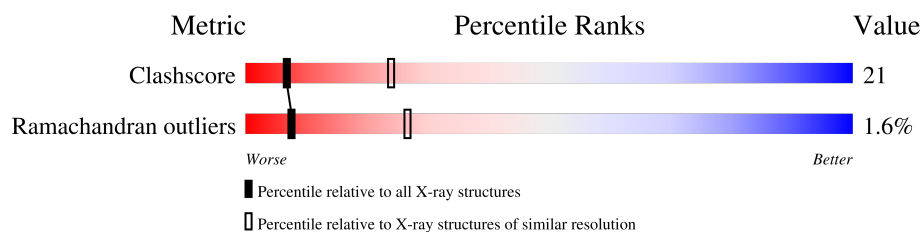
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                                                                                                                                                                                                                                                                                                           |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 215    | <div> <div style="width: 62%; background-color: green;"></div> <div style="width: 36%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>62% 36% .</div> |
| 1   | B     | 215    | <div> <div style="width: 62%; background-color: green;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>62% 35% .</div> |

## 2 Entry composition [i](#)

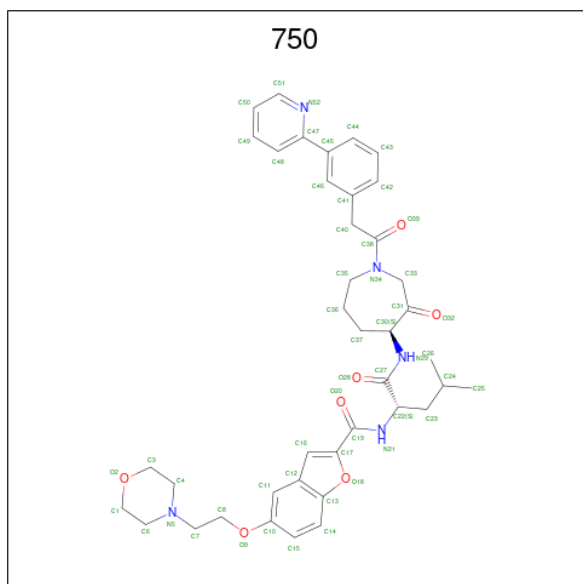
There are 2 unique types of molecules in this entry. The entry contains 3402 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cathepsin K.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1649  | 1030 | 291 | 316 | 12 |         |         |       |
| 1   | B     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1649  | 1030 | 291 | 316 | 12 |         |         |       |

- Molecule 2 is 5-(2-MORPHOLIN-4-YLETHOXY)BENZOFURAN-2-CARBOXYLIC ACID ((S)-3-METHYL-1-{(S)-3-OXO-1-[2-(3-PYRIDIN-2-YLPHENYL)ACETYL]AZEPAN-4-YLCARBAMOYL}BUTYL)AMIDE (CCD ID: 750) (formula: C<sub>40</sub>H<sub>47</sub>N<sub>5</sub>O<sub>7</sub>).





Note EDS was not executed.

- Chain A:
- 
- 62% 36%
- A1 S4 R8 V13 T14 G20 V31 E35 G36 Q37 K41 T42 G43 K44 N47 L48 S49 N52 L53 V57 S58 E59 G62 C63 G66 V67 M68 T69 N70 A71 R79 G80 E84 Y87 P88 G91 Q92 E93 N99 P100 T101 G102 K103
- K106 C107 R108 R111 E112 I113 P114 E115 G116 R123 A124 V125 V131 L139 Q143 Y151 D152 E153 S154 N161 H162 A163 V164 L165 A166 V167 Q172 H177 I180 K181 N182 S183 G184 E185 M186 N187 L188 G189 Y193 I194 L195 M196 A197 R198 N199 N202
- G205 I206 A207 A210 K214 M215

- Chain B:

## 4 Data and refinement statistics

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

| Property                                                 | Value                                         | Source    |
|----------------------------------------------------------|-----------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                    | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 71.82Å 75.89Å 114.84Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 6.00 – 2.80                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 97.0 (6.00-2.80)                              | Depositor |
| $R_{merge}$                                              | 0.58                                          | Depositor |
| $R_{sym}$                                                | 0.58                                          | Depositor |
| Refinement program                                       | CNS                                           | Depositor |
| R, $R_{free}$                                            | 0.246 , 0.298                                 | Depositor |
| Estimated twinning fraction                              | No twinning to report.                        | Xtriage   |
| Total number of atoms                                    | 3402                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 17.0                                          | 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: 750

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     | 0.55         | 0/1684      | 1.00        | 7/2270 (0.3%)  |
| 1   | B     | 0.54         | 0/1684      | 0.99        | 6/2270 (0.3%)  |
| All | All   | 0.55         | 0/3368      | 0.99        | 13/4540 (0.3%) |

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 59  | GLU  | N-CA-C | -6.38 | 105.46      | 113.18   |
| 1   | A     | 165 | LEU  | N-CA-C | 5.99  | 118.17      | 108.34   |
| 1   | B     | 87  | TYR  | CA-C-N | 5.91  | 125.86      | 119.78   |
| 1   | B     | 87  | TYR  | C-N-CA | 5.91  | 125.86      | 119.78   |
| 1   | A     | 59  | GLU  | N-CA-C | -5.73 | 106.25      | 113.18   |

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     | 1649  | 0        | 1595     | 72      | 1            |
| 1   | B     | 1649  | 0        | 1595     | 71      | 1            |
| 2   | A     | 52    | 0        | 47       | 7       | 0            |
| 2   | B     | 52    | 0        | 47       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 3402  | 0        | 3284     | 143     | 1            |

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 21.

The worst 5 of 143 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:B:8:ARG:HG2    | 1:B:13:VAL:HG21 | 1.51                     | 0.93              |
| 1:A:8:ARG:HG2    | 1:A:13:VAL:HG21 | 1.50                     | 0.92              |
| 1:B:80:GLY:HA3   | 1:B:103:LYS:HD3 | 1.58                     | 0.84              |
| 1:A:80:GLY:HA3   | 1:A:103:LYS:HD3 | 1.58                     | 0.84              |
| 1:A:172:GLN:HE21 | 1:A:172:GLN:HA  | 1.44                     | 0.82              |

All (1) 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) |
|-----------------|----------------------|--------------------------|-------------------|
| 1:A:186:GLU:OE2 | 1:B:101:THR:N[2_454] | 2.14                     | 0.06              |

## 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 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     | 213/215 (99%) | 180 (84%) | 29 (14%) | 4 (2%)   | 6           | 22 |
| 1   | B     | 213/215 (99%) | 177 (83%) | 33 (16%) | 3 (1%)   | 9           | 30 |
| All | All   | 426/430 (99%) | 357 (84%) | 62 (15%) | 7 (2%)   | 7           | 27 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 151 | TYR  |
| 1   | B     | 151 | TYR  |
| 1   | B     | 153 | GLU  |
| 1   | A     | 153 | GLU  |
| 1   | A     | 124 | ALA  |

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

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

### 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](#)

2 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   | 750  | B     | 501 | 1    | 54,57,57     | 2.88 | 26 (48%)    | 71,78,78    | 1.97 | 18 (25%)    |
| 2   | 750  | A     | 501 | 1    | 54,57,57     | 2.83 | 28 (51%)    | 71,78,78    | 1.95 | 24 (33%)    |

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   | 750  | B     | 501 | 1    | -       | 5/36/60/60 | 0/5/6/6 |
| 2   | 750  | A     | 501 | 1    | -       | 5/36/60/60 | 0/5/6/6 |

The worst 5 of 54 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 501 | 750  | O32-C31 | 13.91 | 1.44        | 1.21     |
| 2   | A     | 501 | 750  | O32-C31 | 12.51 | 1.42        | 1.21     |
| 2   | A     | 501 | 750  | C40-C38 | 4.46  | 1.57        | 1.52     |
| 2   | A     | 501 | 750  | C46-C45 | 4.46  | 1.47        | 1.39     |
| 2   | A     | 501 | 750  | C48-C47 | 4.13  | 1.48        | 1.39     |

The worst 5 of 42 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2   | B     | 501 | 750  | C51-N52-C47 | 5.56 | 125.03      | 117.24   |
| 2   | A     | 501 | 750  | C51-N52-C47 | 5.35 | 124.73      | 117.24   |
| 2   | B     | 501 | 750  | C8-O9-C10   | 5.18 | 131.40      | 117.93   |
| 2   | A     | 501 | 750  | C40-C38-N34 | 5.13 | 125.98      | 117.52   |
| 2   | A     | 501 | 750  | C8-O9-C10   | 4.85 | 130.53      | 117.93   |

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 501 | 750  | O39-C38-N34-C33 |
| 2   | A     | 501 | 750  | C8-C7-N5-C4     |
| 2   | B     | 501 | 750  | C8-C7-N5-C4     |
| 2   | B     | 501 | 750  | C11-C10-O9-C8   |
| 2   | B     | 501 | 750  | C15-C10-O9-C8   |

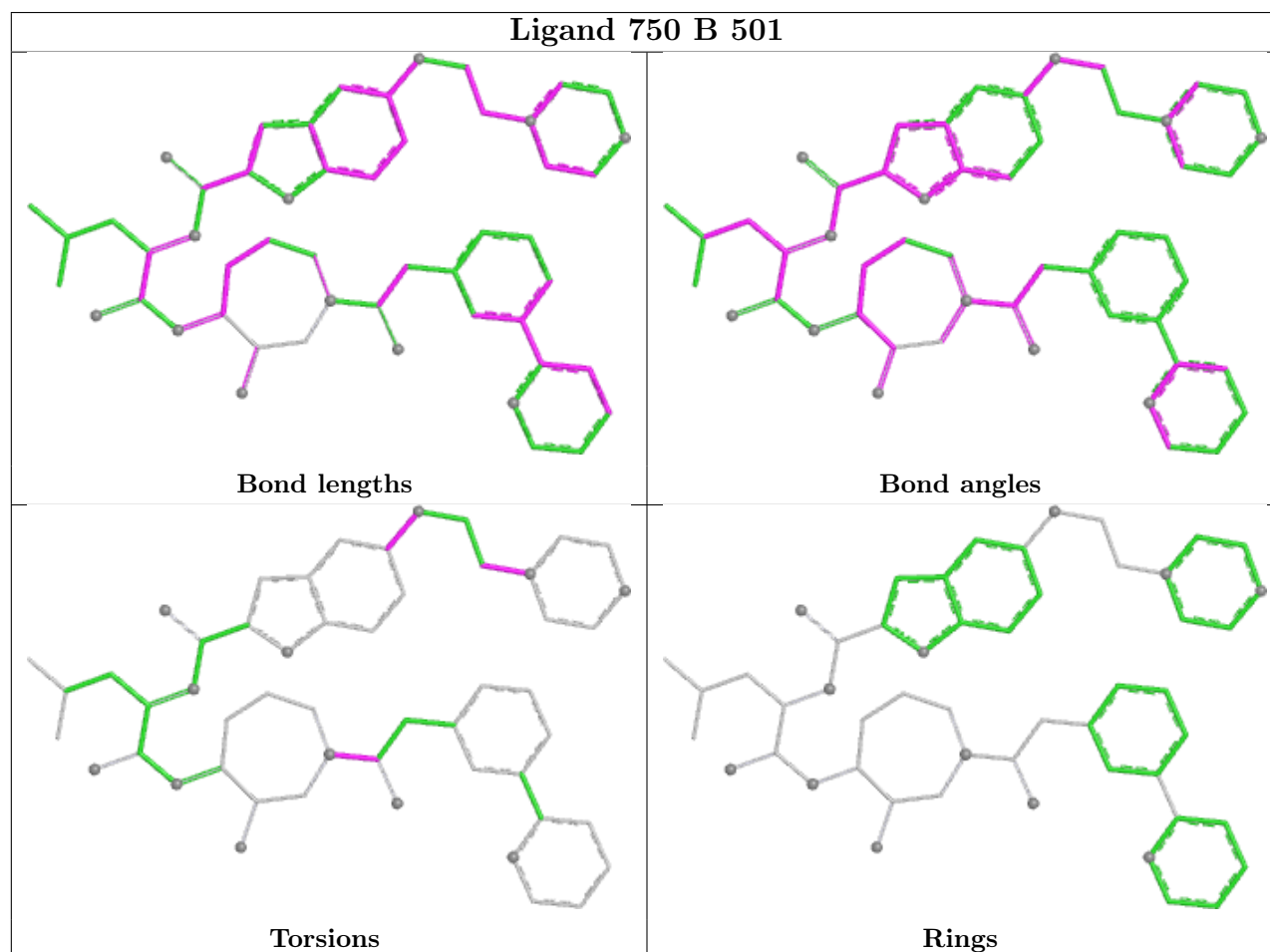
There are no ring outliers.

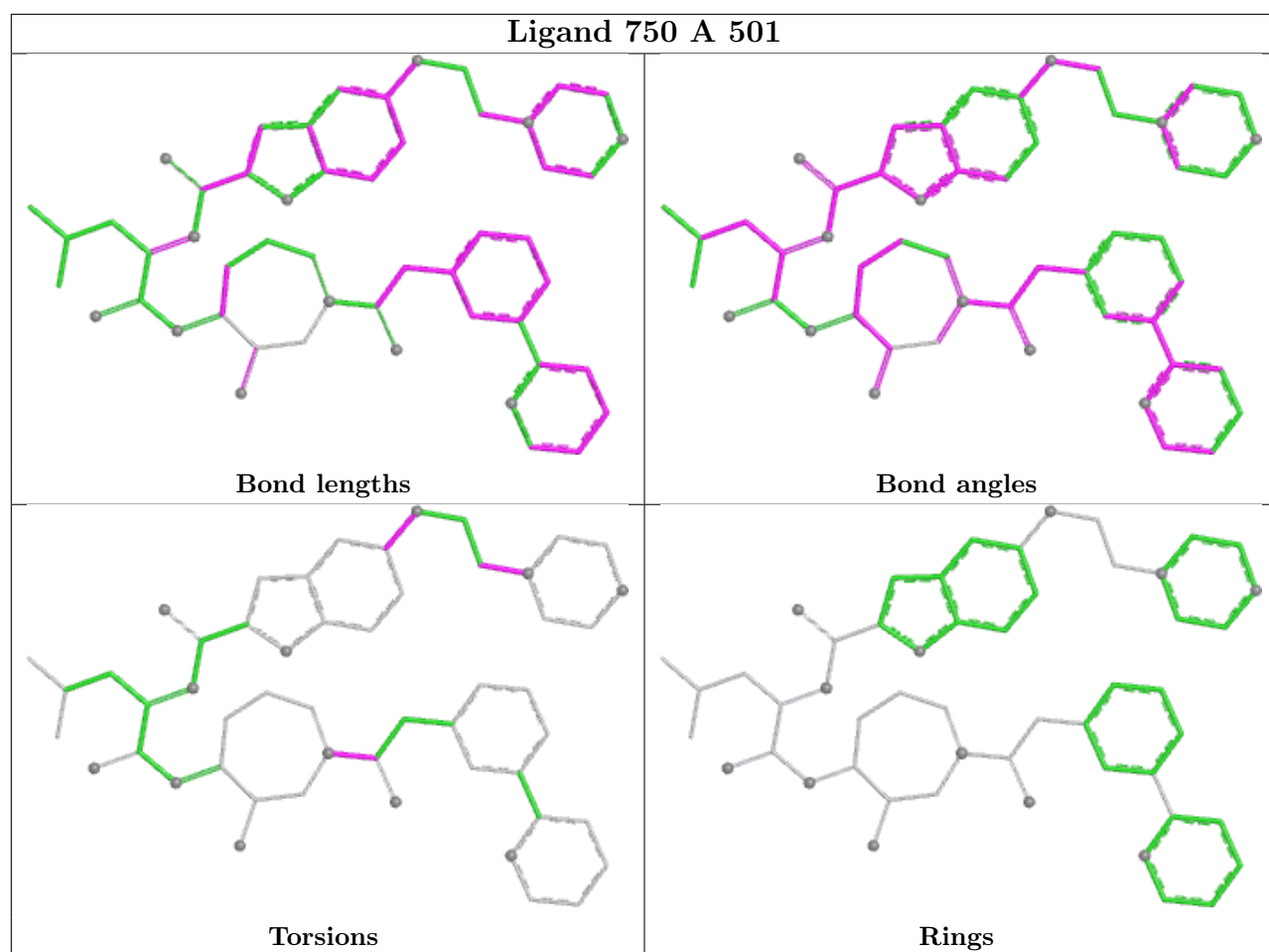
2 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 501 | 750  | 3       | 0            |
| 2   | A     | 501 | 750  | 7       | 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 than 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.





## 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.