



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:22 PM UTC

PDB ID : 9G7G / pdb\_00009g7g  
Title : Structure of the clippase PaJOS from Pigmentiphaga aceris  
Authors : Baumann, U.; Uthoff, M.; Hermanns, T.; Hofmann, K.  
Deposited on : 2024-07-21  
Resolution : 1.89 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                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

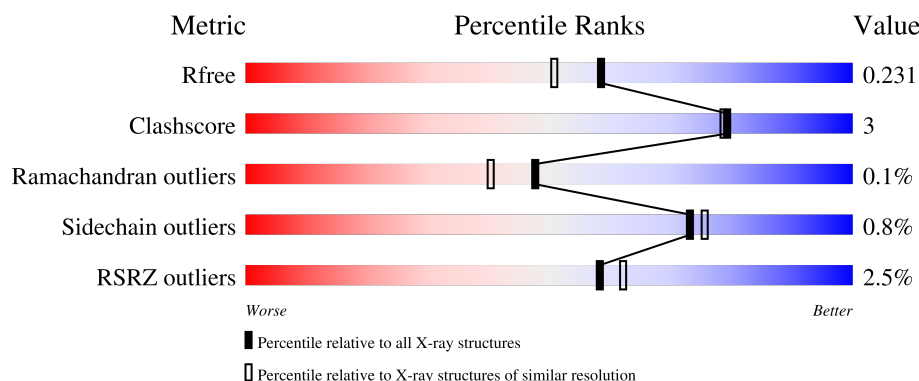
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 7789 (1.90-1.90)                                      |
| Clashscore            | 190562                      | 8410 (1.90-1.90)                                      |
| Ramachandran outliers | 187476                      | 8333 (1.90-1.90)                                      |
| Sidechain outliers    | 187428                      | 8333 (1.90-1.90)                                      |
| RSRZ outliers         | 180081                      | 7790 (1.90-1.90)                                      |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 264    |                  |
| 1   | C     | 264    |                  |
| 1   | E     | 264    |                  |
| 1   | G     | 264    |                  |
| 1   | I     | 264    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K     | 264    |                  |
| 1   | M     | 264    |                  |
| 1   | O     | 264    |                  |
| 1   | Q     | 264    |                  |
| 1   | S     | 264    |                  |
| 1   | U     | 264    |                  |
| 1   | W     | 264    |                  |
| 2   | B     | 75     |                  |
| 2   | D     | 75     |                  |
| 2   | F     | 75     |                  |
| 2   | H     | 75     |                  |
| 2   | J     | 75     |                  |
| 2   | L     | 75     |                  |
| 2   | N     | 75     |                  |
| 2   | P     | 75     |                  |
| 2   | R     | 75     |                  |
| 2   | T     | 75     |                  |
| 2   | V     | 75     |                  |
| 2   | X     | 75     |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28965 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 PaJOS.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 234      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1762  | 1106 | 311 | 343 | 2 |         |         |       |
| 1   | C     | 233      | Total | C    | N   | O   | S | 0       | 5       | 0     |
|     |       |          | 1765  | 1110 | 309 | 344 | 2 |         |         |       |
| 1   | E     | 233      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1750  | 1099 | 310 | 339 | 2 |         |         |       |
| 1   | G     | 236      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1768  | 1109 | 314 | 343 | 2 |         |         |       |
| 1   | I     | 233      | Total | C    | N   | O   | S | 0       | 5       | 0     |
|     |       |          | 1764  | 1110 | 307 | 344 | 3 |         |         |       |
| 1   | K     | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1753  | 1100 | 311 | 340 | 2 |         |         |       |
| 1   | M     | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1759  | 1105 | 310 | 342 | 2 |         |         |       |
| 1   | O     | 235      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1764  | 1107 | 313 | 342 | 2 |         |         |       |
| 1   | Q     | 236      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1770  | 1110 | 316 | 342 | 2 |         |         |       |
| 1   | S     | 231      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1742  | 1095 | 308 | 337 | 2 |         |         |       |
| 1   | U     | 237      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1786  | 1121 | 320 | 343 | 2 |         |         |       |
| 1   | W     | 236      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1767  | 1110 | 313 | 342 | 2 |         |         |       |

- Molecule 2 is a protein called Polyubiquitin-B.

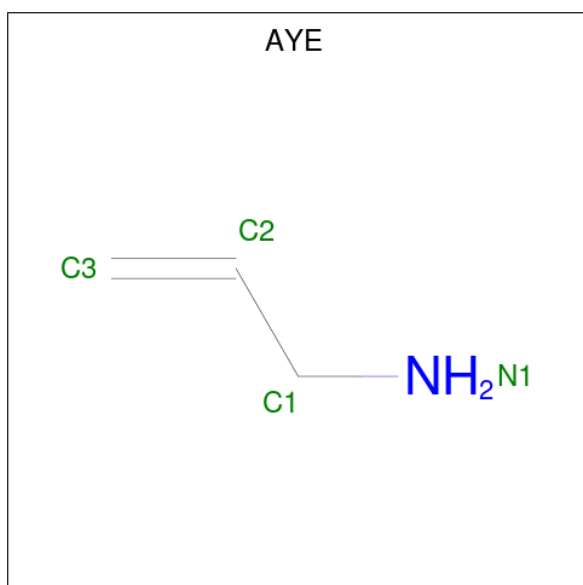
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | D     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | F     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | H     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | J     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | L     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | N     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | P     | 75       | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 602   | 379 | 105 | 117 | 1 |         |         |       |
| 2   | R     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | T     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | V     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |
| 2   | X     | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 597   | 376 | 104 | 116 | 1 |         |         |       |

- Molecule 3 is prop-2-en-1-amine (CCD ID: AYE) (formula: C<sub>3</sub>H<sub>7</sub>N) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | C     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | E     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | G     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | I     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | K     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | M     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | O     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | Q     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | S     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | U     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |
| 3   | W     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 4     | 3 | 1 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 60       | Total | O  | 0       | 0       |
|     |       |          | 60    | 60 |         |         |
| 4   | B     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 4   | C     | 47       | Total | O  | 0       | 0       |
|     |       |          | 47    | 47 |         |         |
| 4   | D     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 4   | E     | 45       | Total | O  | 0       | 0       |
|     |       |          | 45    | 45 |         |         |
| 4   | F     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 4   | G     | 49       | Total | O  | 0       | 0       |
|     |       |          | 49    | 49 |         |         |
| 4   | H     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |

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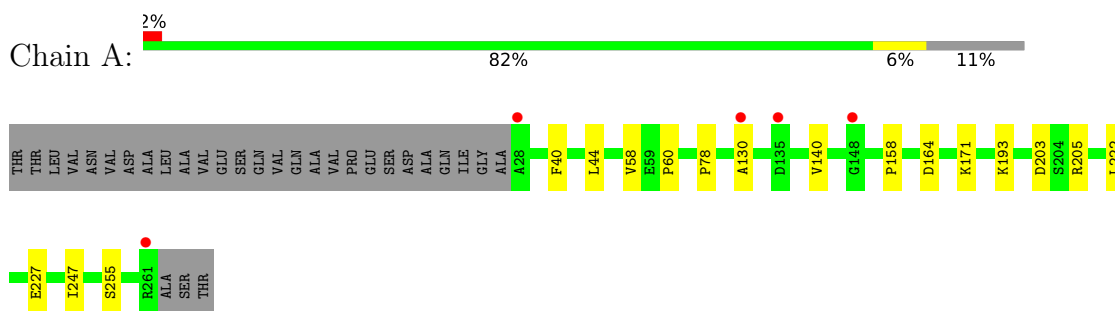
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | I     | 54       | Total<br>54 | O<br>54 | 0       | 0       |
| 4   | J     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 4   | K     | 41       | Total<br>41 | O<br>41 | 0       | 0       |
| 4   | L     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | M     | 48       | Total<br>48 | O<br>48 | 0       | 0       |
| 4   | N     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | O     | 32       | Total<br>32 | O<br>32 | 0       | 0       |
| 4   | P     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | Q     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | R     | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 4   | S     | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 4   | T     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 4   | U     | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 4   | V     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 4   | W     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | X     | 6        | Total<br>6  | O<br>6  | 0       | 0       |

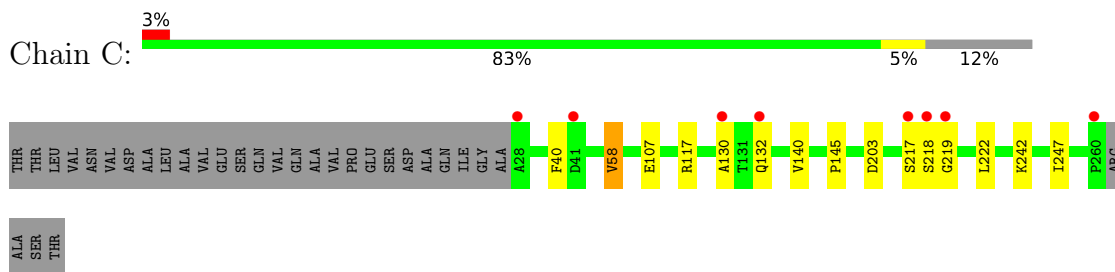
### 3 Residue-property plots [i](#)

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 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 ( $RSRZ > 2$ ). 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.

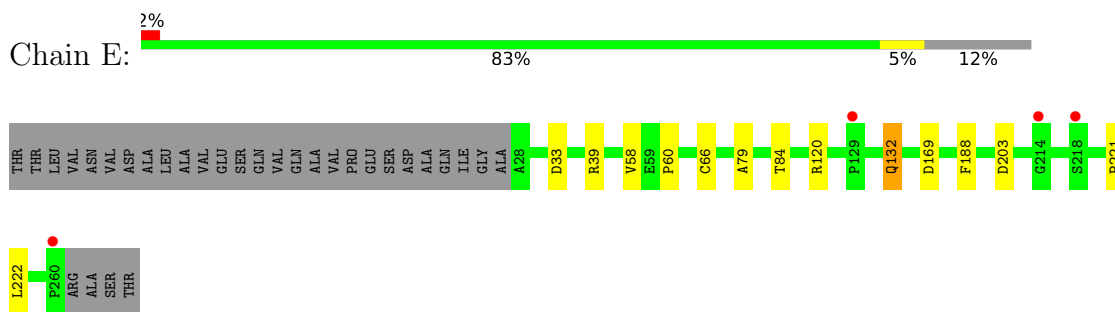
- Molecule 1: PaJOS



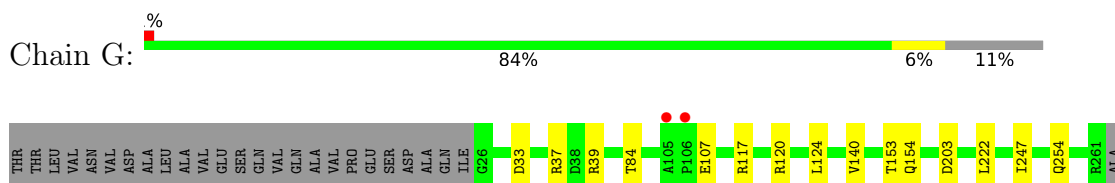
- Molecule 1: PaJOS



- Molecule 1: PaJOS



- Molecule 1: PaJOS



SER  
THR

## ● Molecule 1: PaJOS

Chain I:  85% 12% 3%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA GLN ILE GLY ALA A28 P60 R120 P129 Q132 D135 D164 K193 D203 E216 L222 E227 P260 ARG ALA SER THR

## ● Molecule 1: PaJOS

Chain K:  79% 9% 11% 3%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA GLN ILE GLY ALA A28 F40 L45 L48 V58 C66 V75 A130 T131 Q132 G133 K134 G139 V140 V155 P158 A159 D169 V170 K171 D183

F188 D203 S217 S218 G219 L222 E234 T238 I247 I251 S255 P260 R261 ALA SER THR

## ● Molecule 1: PaJOS

Chain M:  84% 5% 11% 2%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA GLN ILE GLY ALA I25 V58 E59 P60 C66 F74 D81 I82 P83 T87 D135 Q154 R165 D169 F188 E216 S217 S218 P221 P260 ARG ALA SER

THR

## ● Molecule 1: PaJOS

Chain O:  81% 8% 11% 2%

THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA GLN ILE GLY ALA A28 R39 V58 E59 P60 C66 I71 V75 T84 V140 D169 G173 S174 T178 A179 D183 F188 S206 H210

S217 S218 P221 I235 A239 I247 V259 A262 THR

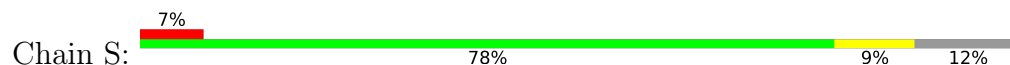
## ● Molecule 1: PaJOS

Chain Q:  83% 6% 11% 3%

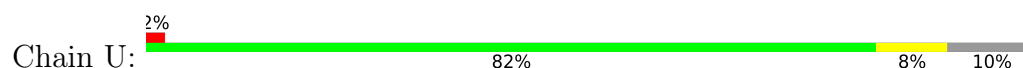
THR THR LEU VAL ASN VAL ASP ALA LEU LEU VAL GLU SER GLN VAL GLN ALA VAL PRO GLU SER ASP ALA GLN ILE G26 R39 L44 C66 T86 T87 T90 D99 A149 A150 M151 P158 A159 D169 F188 L201 A211 P212 E216 L222



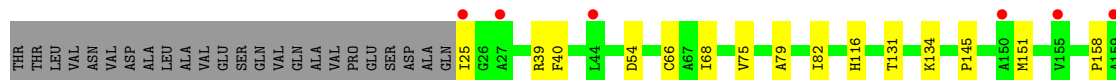
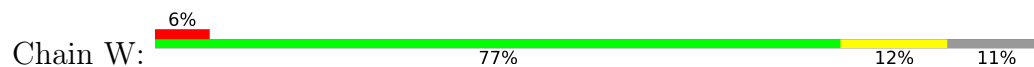
• Molecule 1: PaJOS



• Molecule 1: PaJOS



• Molecule 1: PaJOS



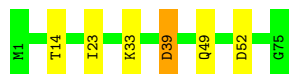
• Molecule 2: Polyubiquitin-B



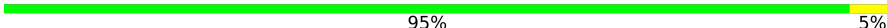
• Molecule 2: Polyubiquitin-B



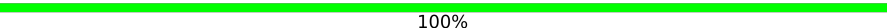
## ● Molecule 2: Polyubiquitin-B

Chain F:  92% 7%

## ● Molecule 2: Polyubiquitin-B

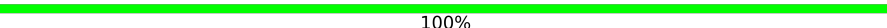
Chain H:  95% 5%

## ● Molecule 2: Polyubiquitin-B

Chain J:  100%

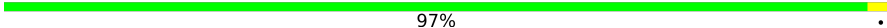
There are no outlier residues recorded for this chain.

## ● Molecule 2: Polyubiquitin-B

Chain L:  100%

There are no outlier residues recorded for this chain.

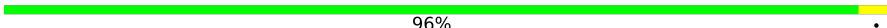
## ● Molecule 2: Polyubiquitin-B

Chain N:  97%

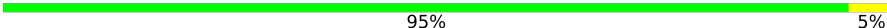
## ● Molecule 2: Polyubiquitin-B

Chain P:  97%

## ● Molecule 2: Polyubiquitin-B

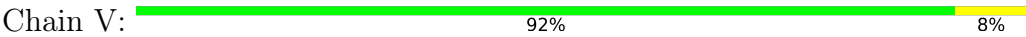
Chain R:  96%

## ● Molecule 2: Polyubiquitin-B

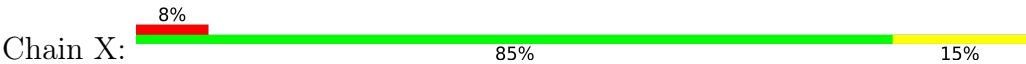
Chain T:  95% 5%



● Molecule 2: Polyubiquitin-B



● Molecule 2: Polyubiquitin-B



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 131.95Å 81.32Å 167.39Å<br>90.00° 90.23° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 49.03 – 1.89<br>49.03 – 1.89                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.6 (49.03-1.89)<br>95.7 (49.03-1.89)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.06 (at 1.90Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (dev_5407: ???)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.204 , 0.231<br>0.204 , 0.231                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2124 reflections (0.77%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.241                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 30.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 28965                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 50.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0274e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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.

## 5 Model quality

### 5.1 Standard geometry

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

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         | 0/1814  | 0.53        | 0/2484  |
| 1   | C     | 0.39         | 0/1826  | 0.53        | 0/2502  |
| 1   | E     | 0.38         | 0/1799  | 0.55        | 0/2464  |
| 1   | G     | 0.36         | 0/1817  | 0.55        | 0/2488  |
| 1   | I     | 0.38         | 0/1825  | 0.55        | 0/2500  |
| 1   | K     | 0.38         | 0/1799  | 0.54        | 0/2464  |
| 1   | M     | 0.38         | 0/1805  | 0.57        | 0/2473  |
| 1   | O     | 0.36         | 0/1813  | 0.53        | 0/2483  |
| 1   | Q     | 0.32         | 0/1819  | 0.48        | 0/2490  |
| 1   | S     | 0.33         | 0/1793  | 0.50        | 0/2454  |
| 1   | U     | 0.31         | 0/1838  | 0.49        | 0/2515  |
| 1   | W     | 0.30         | 0/1816  | 0.48        | 0/2487  |
| 2   | B     | 0.36         | 0/603   | 0.52        | 0/811   |
| 2   | D     | 0.37         | 0/603   | 0.54        | 0/811   |
| 2   | F     | 0.41         | 0/603   | 0.56        | 0/811   |
| 2   | H     | 0.37         | 0/603   | 0.58        | 0/811   |
| 2   | J     | 0.38         | 0/603   | 0.55        | 0/811   |
| 2   | L     | 0.41         | 0/603   | 0.54        | 0/811   |
| 2   | N     | 0.37         | 0/603   | 0.55        | 0/811   |
| 2   | P     | 0.36         | 0/611   | 0.55        | 0/822   |
| 2   | R     | 0.33         | 0/603   | 0.53        | 0/811   |
| 2   | T     | 0.35         | 0/603   | 0.56        | 0/811   |
| 2   | V     | 0.33         | 0/603   | 0.50        | 0/811   |
| 2   | X     | 0.32         | 0/603   | 0.51        | 0/811   |
| All | All   | 0.36         | 0/29008 | 0.53        | 0/39547 |

There are no bond length outliers.

There are no bond angle outliers.

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     | 1762  | 0        | 1701     | 9       | 0            |
| 1   | C     | 1765  | 0        | 1709     | 8       | 0            |
| 1   | E     | 1750  | 0        | 1690     | 11      | 0            |
| 1   | G     | 1768  | 0        | 1706     | 7       | 0            |
| 1   | I     | 1764  | 0        | 1708     | 7       | 0            |
| 1   | K     | 1753  | 0        | 1690     | 16      | 0            |
| 1   | M     | 1759  | 0        | 1696     | 8       | 0            |
| 1   | O     | 1764  | 0        | 1703     | 14      | 0            |
| 1   | Q     | 1770  | 0        | 1711     | 9       | 0            |
| 1   | S     | 1742  | 0        | 1684     | 12      | 0            |
| 1   | U     | 1786  | 0        | 1735     | 10      | 0            |
| 1   | W     | 1767  | 0        | 1709     | 23      | 0            |
| 2   | B     | 597   | 0        | 626      | 1       | 0            |
| 2   | D     | 597   | 0        | 626      | 1       | 0            |
| 2   | F     | 597   | 0        | 626      | 4       | 0            |
| 2   | H     | 597   | 0        | 626      | 2       | 0            |
| 2   | J     | 597   | 0        | 626      | 0       | 0            |
| 2   | L     | 597   | 0        | 626      | 0       | 0            |
| 2   | N     | 597   | 0        | 626      | 1       | 0            |
| 2   | P     | 602   | 0        | 632      | 1       | 0            |
| 2   | R     | 597   | 0        | 626      | 3       | 0            |
| 2   | T     | 597   | 0        | 626      | 3       | 0            |
| 2   | V     | 597   | 0        | 626      | 2       | 0            |
| 2   | X     | 597   | 0        | 626      | 7       | 0            |
| 3   | A     | 4     | 0        | 4        | 0       | 0            |
| 3   | C     | 4     | 0        | 4        | 0       | 0            |
| 3   | E     | 4     | 0        | 4        | 1       | 0            |
| 3   | G     | 4     | 0        | 4        | 0       | 0            |
| 3   | I     | 4     | 0        | 4        | 0       | 0            |
| 3   | K     | 4     | 0        | 4        | 1       | 0            |
| 3   | M     | 4     | 0        | 4        | 1       | 0            |
| 3   | O     | 4     | 0        | 4        | 1       | 0            |
| 3   | Q     | 4     | 0        | 4        | 1       | 0            |
| 3   | S     | 4     | 0        | 4        | 1       | 0            |
| 3   | U     | 4     | 0        | 4        | 1       | 0            |
| 3   | W     | 4     | 0        | 4        | 1       | 0            |
| 4   | A     | 60    | 0        | 0        | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 10    | 0        | 0        | 0       | 0            |
| 4   | C     | 47    | 0        | 0        | 0       | 0            |
| 4   | D     | 14    | 0        | 0        | 1       | 0            |
| 4   | E     | 45    | 0        | 0        | 0       | 0            |
| 4   | F     | 20    | 0        | 0        | 1       | 0            |
| 4   | G     | 49    | 0        | 0        | 0       | 0            |
| 4   | H     | 15    | 0        | 0        | 0       | 0            |
| 4   | I     | 54    | 0        | 0        | 2       | 0            |
| 4   | J     | 14    | 0        | 0        | 0       | 0            |
| 4   | K     | 41    | 0        | 0        | 0       | 0            |
| 4   | L     | 20    | 0        | 0        | 0       | 0            |
| 4   | M     | 48    | 0        | 0        | 0       | 0            |
| 4   | N     | 12    | 0        | 0        | 0       | 0            |
| 4   | O     | 32    | 0        | 0        | 1       | 0            |
| 4   | P     | 12    | 0        | 0        | 0       | 0            |
| 4   | Q     | 12    | 0        | 0        | 0       | 0            |
| 4   | R     | 8     | 0        | 0        | 0       | 0            |
| 4   | S     | 23    | 0        | 0        | 0       | 0            |
| 4   | T     | 9     | 0        | 0        | 1       | 0            |
| 4   | U     | 22    | 0        | 0        | 0       | 0            |
| 4   | V     | 13    | 0        | 0        | 0       | 0            |
| 4   | W     | 12    | 0        | 0        | 1       | 0            |
| 4   | X     | 6     | 0        | 0        | 1       | 0            |
| All | All   | 28965 | 0        | 28008    | 151     | 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 3.

All (151) 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:T:49:GLN:N       | 1:W:216:GLU:OE2  | 2.09                     | 0.82              |
| 1:A:227:GLU:OE2    | 4:A:401:HOH:O    | 2.00                     | 0.78              |
| 1:U:171:LYS:HE2    | 1:U:184:ASP:HB2  | 1.66                     | 0.77              |
| 1:I:227:GLU:OE2    | 4:I:401:HOH:O    | 2.07                     | 0.72              |
| 2:T:11:LYS:NZ      | 4:T:201:HOH:O    | 2.23                     | 0.70              |
| 1:O:140:VAL:HG22   | 1:O:247:ILE:HG12 | 1.73                     | 0.70              |
| 1:W:205[B]:ARG:NH2 | 1:W:207:SER:O    | 2.25                     | 0.69              |
| 2:T:39:ASP:O       | 2:T:72:ARG:NE    | 2.19                     | 0.67              |
| 1:U:151:MET:HE3    | 1:U:240:HIS:HA   | 1.76                     | 0.66              |
| 1:E:132:GLN:OE1    | 1:E:132:GLN:N    | 2.31                     | 0.64              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:X:54:ARG:HH21  | 2:X:58:ASP:HB3     | 1.63                     | 0.63              |
| 1:A:203:ASP:HB3  | 1:A:222:LEU:HB2    | 1.79                     | 0.63              |
| 1:K:159:ALA:HB2  | 1:K:261:ARG:HH22   | 1.64                     | 0.62              |
| 1:C:140:VAL:HG22 | 1:C:247:ILE:HG12   | 1.80                     | 0.62              |
| 2:V:63:LYS:HG3   | 2:V:64:GLU:HG2     | 1.82                     | 0.62              |
| 1:O:174:SER:O    | 1:O:178:THR:HG23   | 2.00                     | 0.61              |
| 1:G:153:THR:OG1  | 1:G:154:GLN:OE1    | 2.08                     | 0.61              |
| 1:K:40:PHE:HE1   | 1:K:75:VAL:HG11    | 1.66                     | 0.60              |
| 2:D:32:ASP:OD2   | 4:D:201:HOH:O      | 2.17                     | 0.58              |
| 1:I:203:ASP:HB3  | 1:I:222:LEU:HB2    | 1.84                     | 0.58              |
| 1:G:140:VAL:HG22 | 1:G:247:ILE:HG12   | 1.83                     | 0.58              |
| 1:K:132:GLN:N    | 1:K:132:GLN:OE1    | 2.36                     | 0.58              |
| 1:E:60:PRO:HD3   | 1:O:60:PRO:HD3     | 1.86                     | 0.57              |
| 1:I:132:GLN:OE1  | 1:I:132:GLN:N      | 2.29                     | 0.57              |
| 1:K:48:LEU:HG    | 1:K:134:LYS:HE3    | 1.86                     | 0.57              |
| 1:Q:151:MET:HE3  | 1:Q:240:HIS:HA     | 1.87                     | 0.57              |
| 1:E:33:ASP:OD2   | 1:E:120[B]:ARG:NH2 | 2.38                     | 0.56              |
| 1:W:131:THR:HA   | 1:W:134:LYS:HD2    | 1.88                     | 0.56              |
| 1:W:177:ARG:NH2  | 1:W:183:ASP:O      | 2.27                     | 0.56              |
| 1:W:187:HIS:CE1  | 1:W:205[B]:ARG:HD3 | 2.42                     | 0.55              |
| 2:X:63:LYS:HG3   | 2:X:64:GLU:HG3     | 1.89                     | 0.55              |
| 2:V:13:ILE:HD13  | 2:V:34:GLU:HG3     | 1.89                     | 0.55              |
| 2:X:1:MET:HA     | 2:X:63:LYS:HZ2     | 1.72                     | 0.54              |
| 1:E:58:VAL:O     | 1:O:60:PRO:HG2     | 2.06                     | 0.54              |
| 1:K:234:GLU:O    | 1:K:238:THR:HB     | 2.07                     | 0.54              |
| 1:W:54:ASP:N     | 1:W:54:ASP:OD1     | 2.40                     | 0.53              |
| 1:Q:158:PRO:HA   | 1:Q:261:ARG:HH22   | 1.74                     | 0.53              |
| 1:S:140:VAL:HG22 | 1:S:247:ILE:HG12   | 1.91                     | 0.53              |
| 1:A:60:PRO:HG2   | 1:C:58:VAL:O       | 2.09                     | 0.52              |
| 1:S:171:LYS:NZ   | 1:W:183:ASP:OD1    | 2.22                     | 0.52              |
| 1:Q:234:GLU:O    | 1:Q:238:THR:OG1    | 2.27                     | 0.52              |
| 2:R:63:LYS:HG3   | 2:R:64:GLU:HG3     | 1.92                     | 0.52              |
| 1:Q:228:PRO:O    | 1:Q:232:LEU:HD23   | 2.09                     | 0.51              |
| 1:K:140:VAL:HG22 | 1:K:247:ILE:HG12   | 1.92                     | 0.51              |
| 1:U:86:THR:O     | 1:U:90:THR:HG23    | 2.10                     | 0.51              |
| 1:K:40:PHE:CE2   | 1:K:130:ALA:HB3    | 2.46                     | 0.51              |
| 1:A:140:VAL:HG22 | 1:A:247:ILE:HG12   | 1.93                     | 0.50              |
| 1:S:164:ASP:HB2  | 1:S:193:LYS:HB2    | 1.94                     | 0.50              |
| 1:W:169:ASP:HB2  | 1:W:188:PHE:CE1    | 2.47                     | 0.50              |
| 1:O:206:SER:OG   | 1:O:217:SER:HB3    | 2.12                     | 0.49              |
| 1:M:81:ASP:CG    | 1:M:83:PRO:HD2     | 2.36                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:X:1:MET:N        | 2:X:17:VAL:O       | 2.32                     | 0.49              |
| 1:W:205[B]:ARG:CZ  | 1:W:205[B]:ARG:HB2 | 2.40                     | 0.49              |
| 1:W:116:HIS:HD2    | 4:X:205:HOH:O      | 1.96                     | 0.49              |
| 2:R:1:MET:HA       | 2:R:63:LYS:HZ3     | 1.76                     | 0.49              |
| 1:C:132:GLN:N      | 1:C:132:GLN:OE1    | 2.46                     | 0.49              |
| 2:F:49:GLN:NE2     | 4:F:201:HOH:O      | 2.26                     | 0.49              |
| 1:W:40:PHE:HE1     | 1:W:75:VAL:HG11    | 1.78                     | 0.49              |
| 1:C:40:PHE:CE2     | 1:C:130:ALA:HB3    | 2.48                     | 0.48              |
| 1:E:203:ASP:HB3    | 1:E:222:LEU:HB3    | 1.94                     | 0.48              |
| 1:G:37:ARG:NH1     | 1:G:124:LEU:O      | 2.45                     | 0.48              |
| 1:W:205[B]:ARG:HB3 | 1:W:217:SER:HB3    | 1.95                     | 0.48              |
| 1:U:71:ILE:O       | 1:U:75:VAL:HG22    | 2.14                     | 0.48              |
| 1:S:177:ARG:NH2    | 1:S:183:ASP:O      | 2.36                     | 0.48              |
| 1:W:158:PRO:HG3    | 1:W:255:SER:HB3    | 1.94                     | 0.48              |
| 1:E:39:ARG:HG2     | 1:E:84:THR:HG21    | 1.96                     | 0.47              |
| 1:O:66:CYS:HB3     | 3:O:301:AYE:H3A    | 1.69                     | 0.47              |
| 1:S:166:LEU:HD22   | 1:S:246:LEU:HD11   | 1.97                     | 0.47              |
| 1:W:203:ASP:HB3    | 1:W:222:LEU:HB3    | 1.96                     | 0.47              |
| 1:A:158:PRO:HG3    | 1:A:255:SER:HB3    | 1.95                     | 0.47              |
| 1:G:203:ASP:HB3    | 1:G:222:LEU:HB3    | 1.95                     | 0.47              |
| 2:F:39:ASP:OD1     | 2:F:39:ASP:N       | 2.47                     | 0.47              |
| 1:G:33:ASP:OD2     | 1:G:120:ARG:NH2    | 2.48                     | 0.47              |
| 1:K:139:GLY:HA3    | 1:K:251:ILE:O      | 2.15                     | 0.47              |
| 2:R:1:MET:HB2      | 2:R:63:LYS:HD3     | 1.97                     | 0.47              |
| 1:I:216:GLU:HG3    | 1:M:154:GLN:OE1    | 2.15                     | 0.46              |
| 1:O:71:ILE:O       | 1:O:75:VAL:HG22    | 2.16                     | 0.46              |
| 1:K:66:CYS:HB3     | 3:K:301:AYE:H3A    | 1.78                     | 0.46              |
| 1:W:168:PHE:CE1    | 1:W:246:LEU:HD13   | 2.50                     | 0.46              |
| 2:X:1:MET:HB2      | 2:X:63:LYS:HD3     | 1.97                     | 0.46              |
| 1:I:60:PRO:HG3     | 1:K:58:VAL:O       | 2.16                     | 0.46              |
| 1:S:203:ASP:HB3    | 1:S:222:LEU:HB3    | 1.98                     | 0.46              |
| 2:X:2:GLN:HA       | 2:X:15:LEU:O       | 2.17                     | 0.45              |
| 1:E:39:ARG:NH1     | 1:E:79:ALA:O       | 2.49                     | 0.45              |
| 1:Q:86:THR:O       | 1:Q:90:THR:HG23    | 2.17                     | 0.45              |
| 1:S:169:ASP:HB2    | 1:S:188:PHE:CE1    | 2.51                     | 0.44              |
| 1:Q:169:ASP:HB2    | 1:Q:188:PHE:CE1    | 2.53                     | 0.44              |
| 1:W:145:PRO:HD3    | 1:W:242:LYS:O      | 2.17                     | 0.44              |
| 1:W:151:MET:HE2    | 1:W:151:MET:HB3    | 1.82                     | 0.44              |
| 1:C:107:GLU:CD     | 1:C:117:ARG:HE     | 2.24                     | 0.44              |
| 1:M:216:GLU:OE2    | 1:M:218:SER:OG     | 2.32                     | 0.44              |
| 1:U:164:ASP:HB2    | 1:U:193:LYS:HB2    | 2.00                     | 0.44              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:W:66:CYS:HB3      | 3:W:301:AYE:H3A  | 1.79                     | 0.44              |
| 1:M:66:CYS:HB3      | 3:M:301:AYE:H3A  | 1.76                     | 0.44              |
| 2:B:22:THR:HA       | 2:B:55:THR:HA    | 2.01                     | 0.43              |
| 1:K:169:ASP:HB2     | 1:K:188:PHE:CE1  | 2.53                     | 0.43              |
| 1:S:184:ASP:OD2     | 1:S:242:LYS:HE2  | 2.18                     | 0.43              |
| 1:C:217:SER:O       | 1:C:219:GLY:N    | 2.47                     | 0.43              |
| 1:W:164:ASP:HB2     | 1:W:193:LYS:HB2  | 2.01                     | 0.43              |
| 1:K:158:PRO:HG3     | 1:K:255:SER:HB3  | 1.99                     | 0.43              |
| 1:Q:66:CYS:HB3      | 3:Q:301:AYE:H3A  | 1.72                     | 0.43              |
| 1:Q:216:GLU:OE1     | 1:Q:216:GLU:N    | 2.42                     | 0.43              |
| 1:E:66:CYS:HB3      | 3:E:301:AYE:H3A  | 1.80                     | 0.43              |
| 1:I:164:ASP:HB2     | 1:I:193:LYS:HB2  | 2.01                     | 0.43              |
| 2:N:22:THR:HA       | 2:N:55:THR:HA    | 2.01                     | 0.43              |
| 1:O:210:HIS:HD2     | 1:O:235:ILE:HG12 | 1.84                     | 0.43              |
| 1:U:145:PRO:HD3     | 1:U:242:LYS:O    | 2.19                     | 0.43              |
| 1:O:239:ALA:HA      | 4:O:404:HOH:O    | 2.18                     | 0.43              |
| 1:E:169:ASP:HB2     | 1:E:188:PHE:CE1  | 2.54                     | 0.42              |
| 1:O:169:ASP:HB2     | 1:O:188:PHE:CE1  | 2.54                     | 0.42              |
| 1:O:173:GLY:O       | 1:O:239:ALA:HB1  | 2.19                     | 0.42              |
| 1:K:45:LEU:HD22     | 1:K:75:VAL:HG12  | 2.02                     | 0.42              |
| 1:U:66:CYS:HB3      | 3:U:301:AYE:H3A  | 1.80                     | 0.42              |
| 1:K:203:ASP:HB3     | 1:K:222:LEU:HB3  | 2.01                     | 0.42              |
| 1:U:139:GLY:HA3     | 1:U:251:ILE:O    | 2.19                     | 0.42              |
| 1:W:68:ILE:HD13     | 1:W:82:ILE:HA    | 2.01                     | 0.42              |
| 1:E:60:PRO:HA       | 1:E:221:PRO:HG3  | 2.01                     | 0.42              |
| 2:F:23:ILE:HB       | 2:F:52:ASP:HA    | 2.01                     | 0.42              |
| 1:K:159:ALA:HB2     | 1:K:261:ARG:HH12 | 1.85                     | 0.42              |
| 1:W:39:ARG:NH1      | 1:W:79:ALA:O     | 2.52                     | 0.42              |
| 1:A:164:ASP:HB2     | 1:A:193:LYS:HB2  | 2.02                     | 0.42              |
| 2:H:13:ILE:HD13     | 2:H:34:GLU:HG3   | 2.01                     | 0.42              |
| 1:W:209:VAL:HG13    | 4:W:404:HOH:O    | 2.19                     | 0.42              |
| 1:A:205:ARG:HD3     | 4:A:404:HOH:O    | 2.19                     | 0.41              |
| 1:K:171:LYS:HB3     | 1:K:171:LYS:HE2  | 1.97                     | 0.41              |
| 1:U:59:GLU:CD       | 1:U:72:ASN:HD22  | 2.28                     | 0.41              |
| 1:W:205[B]:ARG:HH22 | 1:W:208:GLU:C    | 2.28                     | 0.41              |
| 1:I:120:ARG:HD2     | 4:I:404:HOH:O    | 2.21                     | 0.41              |
| 1:S:66:CYS:HB3      | 3:S:301:AYE:H3A  | 1.86                     | 0.41              |
| 1:S:107:GLU:CD      | 1:S:117:ARG:HE   | 2.29                     | 0.41              |
| 2:X:22:THR:HA       | 2:X:55:THR:HA    | 2.03                     | 0.41              |
| 1:A:40:PHE:CE2      | 1:A:130:ALA:HB3  | 2.54                     | 0.41              |
| 1:A:44:LEU:O        | 1:A:78:PRO:HD2   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:107:GLU:CD   | 1:U:117:ARG:HE   | 2.28                     | 0.41              |
| 1:M:81:ASP:OD2   | 1:M:83:PRO:HD2   | 2.20                     | 0.41              |
| 1:C:203:ASP:HB3  | 1:C:222:LEU:HB3  | 2.03                     | 0.41              |
| 1:G:39:ARG:HG2   | 1:G:84:THR:HG21  | 2.02                     | 0.41              |
| 2:H:23:ILE:HB    | 2:H:52:ASP:HA    | 2.02                     | 0.41              |
| 1:O:60:PRO:HG3   | 1:O:221:PRO:HD3  | 2.02                     | 0.41              |
| 2:P:22:THR:HA    | 2:P:55:THR:HA    | 2.03                     | 0.41              |
| 1:E:60:PRO:HG3   | 1:O:58:VAL:O     | 2.20                     | 0.41              |
| 1:Q:201:LEU:HD22 | 1:Q:222:LEU:HD22 | 2.03                     | 0.41              |
| 2:F:14:THR:O     | 2:F:33:LYS:NZ    | 2.42                     | 0.41              |
| 1:S:141:SER:HB2  | 1:S:252:THR:O    | 2.21                     | 0.40              |
| 1:M:169:ASP:HB2  | 1:M:188:PHE:CE1  | 2.56                     | 0.40              |
| 1:M:74:PHE:CZ    | 1:M:165:ARG:HG3  | 2.57                     | 0.40              |
| 1:O:39:ARG:HG2   | 1:O:84:THR:HG21  | 2.04                     | 0.40              |
| 1:S:177:ARG:HG2  | 1:S:213:PRO:HB3  | 2.04                     | 0.40              |
| 1:C:145:PRO:HD3  | 1:C:242:LYS:O    | 2.22                     | 0.40              |
| 1:G:107:GLU:CD   | 1:G:117:ARG:HE   | 2.29                     | 0.40              |
| 1:M:60:PRO:HA    | 1:M:221:PRO:HG3  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 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     | 234/264 (89%) | 231 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | C     | 236/264 (89%) | 232 (98%) | 3 (1%)  | 1 (0%)   | 30          | 22  |
| 1   | E     | 232/264 (88%) | 229 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | G     | 235/264 (89%) | 229 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | I     | 236/264 (89%) | 233 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | K     | 232/264 (88%) | 228 (98%) | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | M     | 234/264 (89%)   | 229 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | O     | 234/264 (89%)   | 232 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | Q     | 235/264 (89%)   | 230 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | S     | 229/264 (87%)   | 226 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | U     | 237/264 (90%)   | 231 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 1   | W     | 235/264 (89%)   | 229 (97%)  | 5 (2%)  | 1 (0%)   | 30          | 22  |
| 2   | B     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | D     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | F     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | H     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | J     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | L     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | N     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | P     | 74/75 (99%)     | 73 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | R     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | T     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | V     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | X     | 73/75 (97%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| All | All   | 3686/4068 (91%) | 3624 (98%) | 60 (2%) | 2 (0%)   | 48          | 40  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 216 | GLU  |
| 1   | C     | 218 | SER  |

### 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     | 185/206 (90%)   | 183 (99%)  | 2 (1%)   | 65          | 67  |
| 1   | C     | 187/206 (91%)   | 186 (100%) | 1 (0%)   | 81          | 84  |
| 1   | E     | 183/206 (89%)   | 182 (100%) | 1 (0%)   | 81          | 84  |
| 1   | G     | 184/206 (89%)   | 183 (100%) | 1 (0%)   | 81          | 84  |
| 1   | I     | 187/206 (91%)   | 187 (100%) | 0        | 100         | 100 |
| 1   | K     | 183/206 (89%)   | 180 (98%)  | 3 (2%)   | 55          | 54  |
| 1   | M     | 183/206 (89%)   | 181 (99%)  | 2 (1%)   | 65          | 67  |
| 1   | O     | 184/206 (89%)   | 183 (100%) | 1 (0%)   | 81          | 84  |
| 1   | Q     | 184/206 (89%)   | 182 (99%)  | 2 (1%)   | 65          | 67  |
| 1   | S     | 183/206 (89%)   | 178 (97%)  | 5 (3%)   | 39          | 34  |
| 1   | U     | 186/206 (90%)   | 184 (99%)  | 2 (1%)   | 65          | 67  |
| 1   | W     | 184/206 (89%)   | 183 (100%) | 1 (0%)   | 81          | 84  |
| 2   | B     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | D     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | F     | 68/68 (100%)    | 67 (98%)   | 1 (2%)   | 57          | 56  |
| 2   | H     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | J     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | L     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | N     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | P     | 69/68 (102%)    | 69 (100%)  | 0        | 100         | 100 |
| 2   | R     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | T     | 68/68 (100%)    | 68 (100%)  | 0        | 100         | 100 |
| 2   | V     | 68/68 (100%)    | 66 (97%)   | 2 (3%)   | 37          | 31  |
| 2   | X     | 68/68 (100%)    | 67 (98%)   | 1 (2%)   | 57          | 56  |
| All | All   | 3030/3288 (92%) | 3005 (99%) | 25 (1%)  | 73          | 75  |

All (25) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 58  | VAL  |
| 1   | A     | 171 | LYS  |
| 1   | C     | 58  | VAL  |
| 1   | E     | 132 | GLN  |
| 2   | F     | 39  | ASP  |
| 1   | G     | 254 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 155 | VAL  |
| 1   | K     | 183 | ASP  |
| 1   | K     | 238 | THR  |
| 1   | M     | 58  | VAL  |
| 1   | M     | 87  | THR  |
| 1   | O     | 183 | ASP  |
| 1   | Q     | 87  | THR  |
| 1   | Q     | 201 | LEU  |
| 1   | S     | 58  | VAL  |
| 1   | S     | 87  | THR  |
| 1   | S     | 151 | MET  |
| 1   | S     | 178 | THR  |
| 1   | S     | 242 | LYS  |
| 1   | U     | 54  | ASP  |
| 1   | U     | 58  | VAL  |
| 2   | V     | 33  | LYS  |
| 2   | V     | 74  | ARG  |
| 1   | W     | 25  | ILE  |
| 2   | X     | 74  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 68  | HIS  |
| 1   | I     | 240 | HIS  |
| 1   | Q     | 34  | GLN  |
| 1   | S     | 154 | GLN  |
| 1   | U     | 225 | GLN  |
| 1   | W     | 116 | HIS  |
| 2   | X     | 68  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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 | $\# Z  > 2$ |
| 3   | AYE  | W     | 301 | 2,1  | 3,3,3        | 0.40 | 0           | 2,2,2       | 0.32 | 0           |
| 3   | AYE  | G     | 301 | 2,1  | 3,3,3        | 0.14 | 0           | 2,2,2       | 0.79 | 0           |
| 3   | AYE  | E     | 301 | 2,1  | 3,3,3        | 0.28 | 0           | 2,2,2       | 0.57 | 0           |
| 3   | AYE  | I     | 301 | 2,1  | 3,3,3        | 0.33 | 0           | 2,2,2       | 0.96 | 0           |
| 3   | AYE  | S     | 301 | 2,1  | 3,3,3        | 0.21 | 0           | 2,2,2       | 0.66 | 0           |
| 3   | AYE  | A     | 301 | 2,1  | 3,3,3        | 0.30 | 0           | 2,2,2       | 0.58 | 0           |
| 3   | AYE  | O     | 301 | 2,1  | 3,3,3        | 0.24 | 0           | 2,2,2       | 0.66 | 0           |
| 3   | AYE  | U     | 301 | 2,1  | 3,3,3        | 0.13 | 0           | 2,2,2       | 0.67 | 0           |
| 3   | AYE  | K     | 301 | 2,1  | 3,3,3        | 0.31 | 0           | 2,2,2       | 0.84 | 0           |
| 3   | AYE  | M     | 301 | 2,1  | 3,3,3        | 0.29 | 0           | 2,2,2       | 0.71 | 0           |
| 3   | AYE  | Q     | 301 | 2,1  | 3,3,3        | 0.19 | 0           | 2,2,2       | 0.64 | 0           |
| 3   | AYE  | C     | 301 | 2,1  | 3,3,3        | 0.23 | 0           | 2,2,2       | 1.32 | 0           |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 3   | AYE  | W     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | G     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | E     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | I     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | S     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | A     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | O     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | U     | 301 | 2,1  | -       | 0/1/1/1  | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 3   | AYE  | K     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | M     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | Q     | 301 | 2,1  | -       | 0/1/1/1  | -     |
| 3   | AYE  | C     | 301 | 2,1  | -       | 0/1/1/1  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

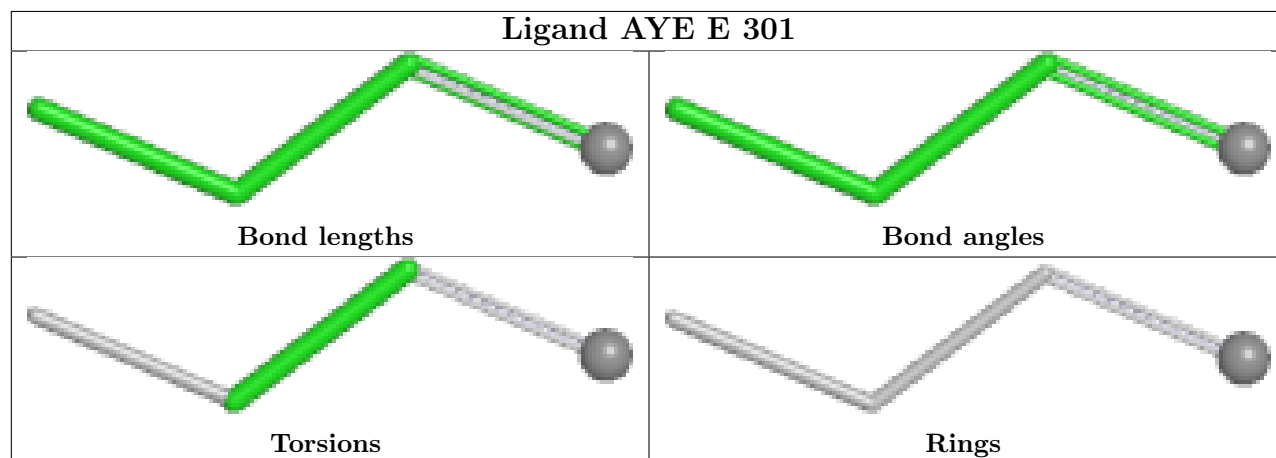
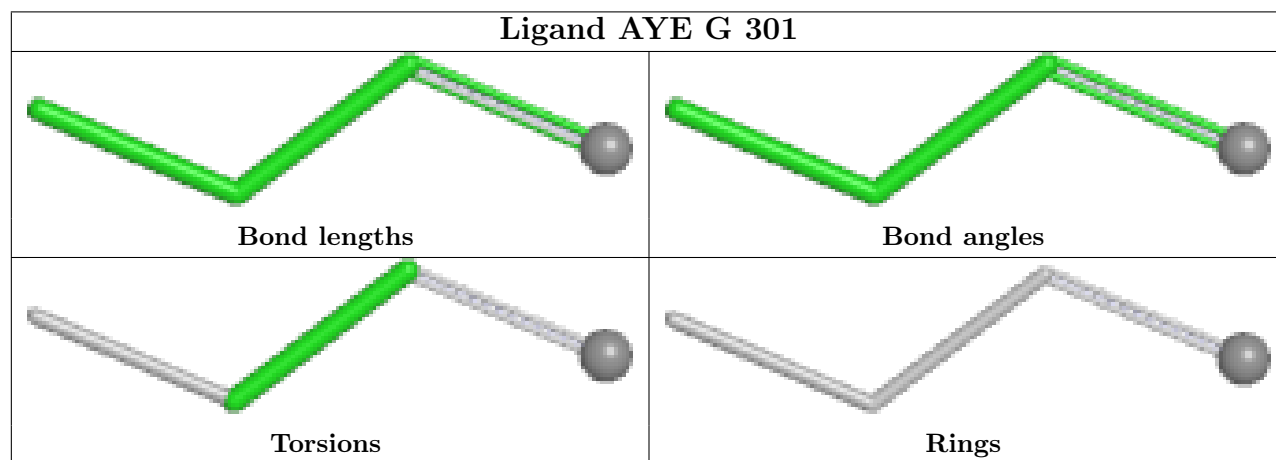
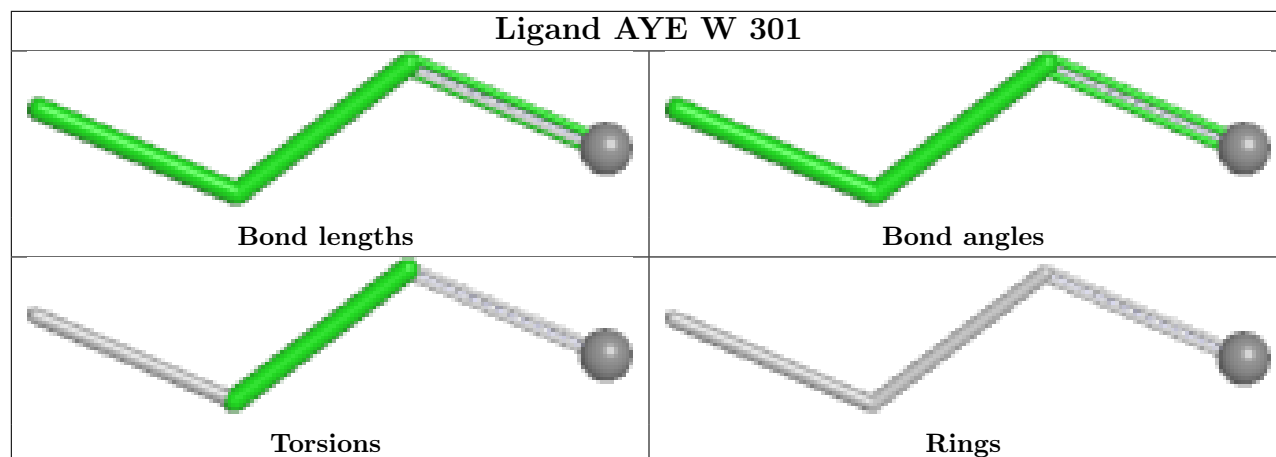
There are no torsion outliers.

There are no ring outliers.

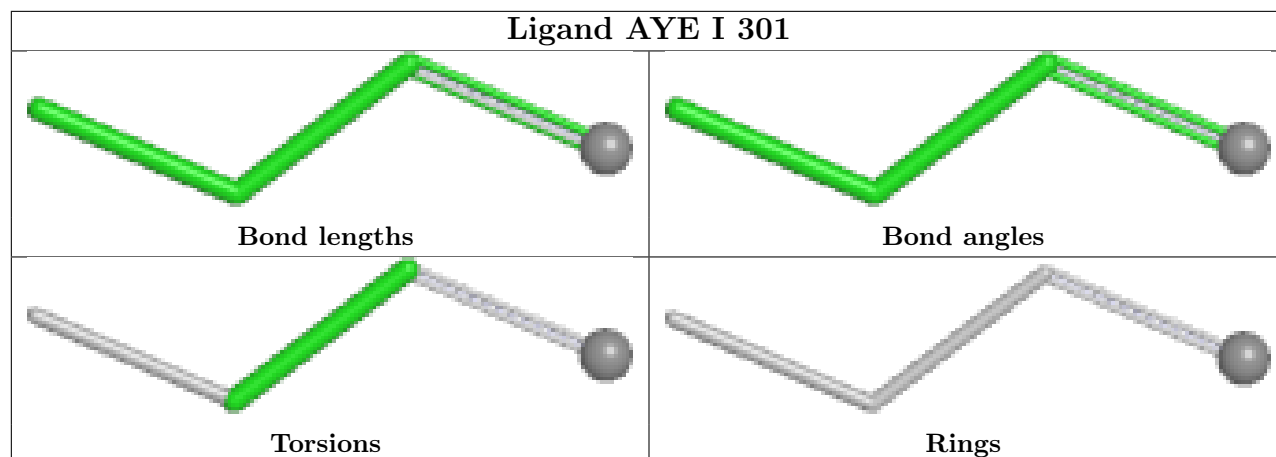
8 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | W     | 301 | AYE  | 1       | 0            |
| 3   | E     | 301 | AYE  | 1       | 0            |
| 3   | S     | 301 | AYE  | 1       | 0            |
| 3   | O     | 301 | AYE  | 1       | 0            |
| 3   | U     | 301 | AYE  | 1       | 0            |
| 3   | K     | 301 | AYE  | 1       | 0            |
| 3   | M     | 301 | AYE  | 1       | 0            |
| 3   | Q     | 301 | AYE  | 1       | 0            |

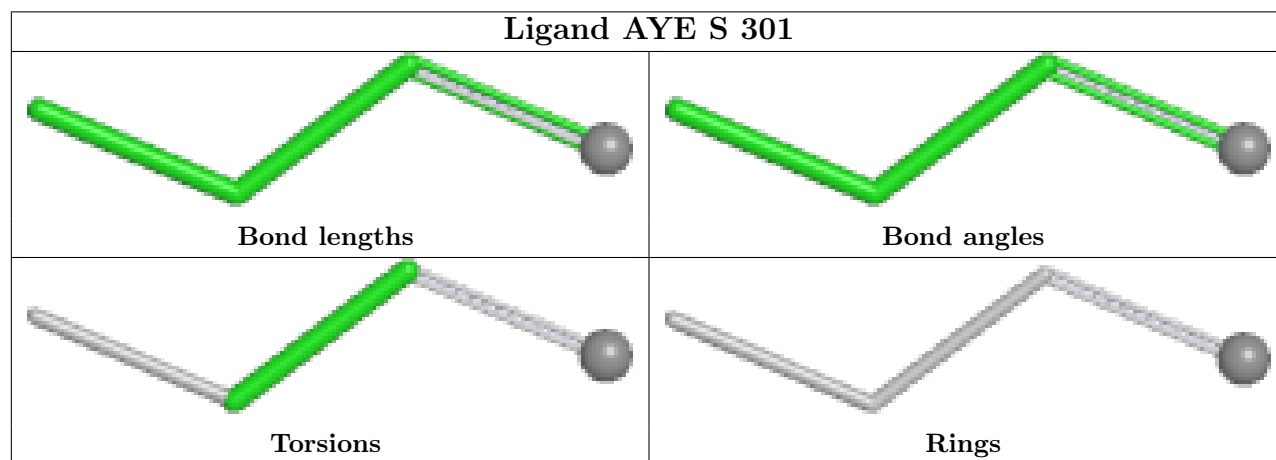
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



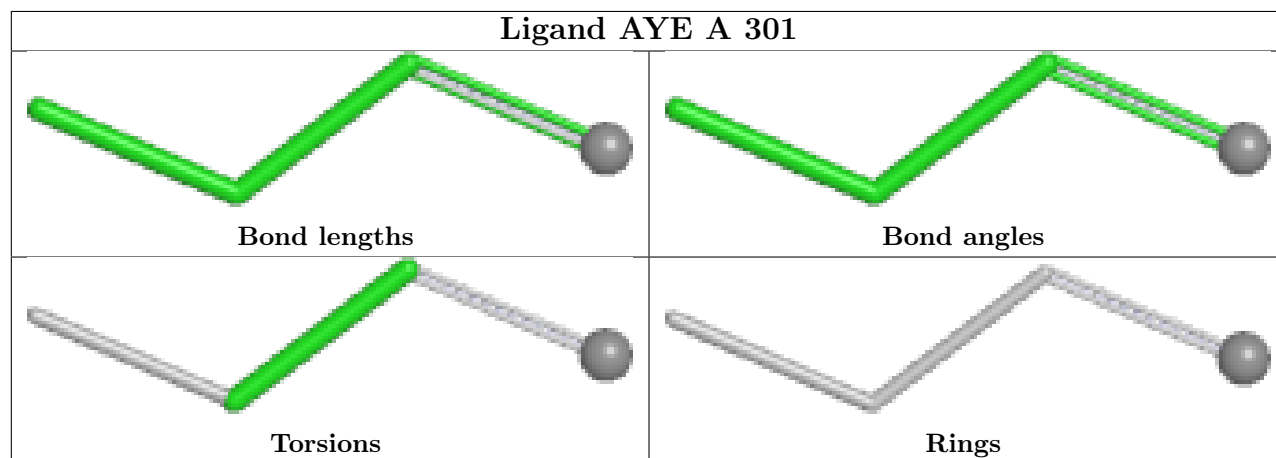
## Ligand AYE I 301



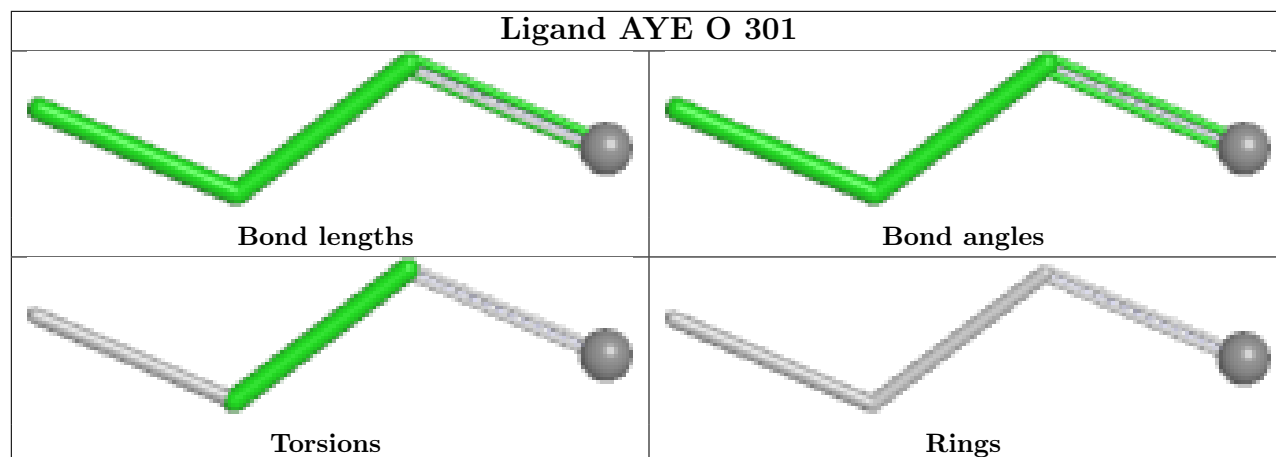
## Ligand AYE S 301



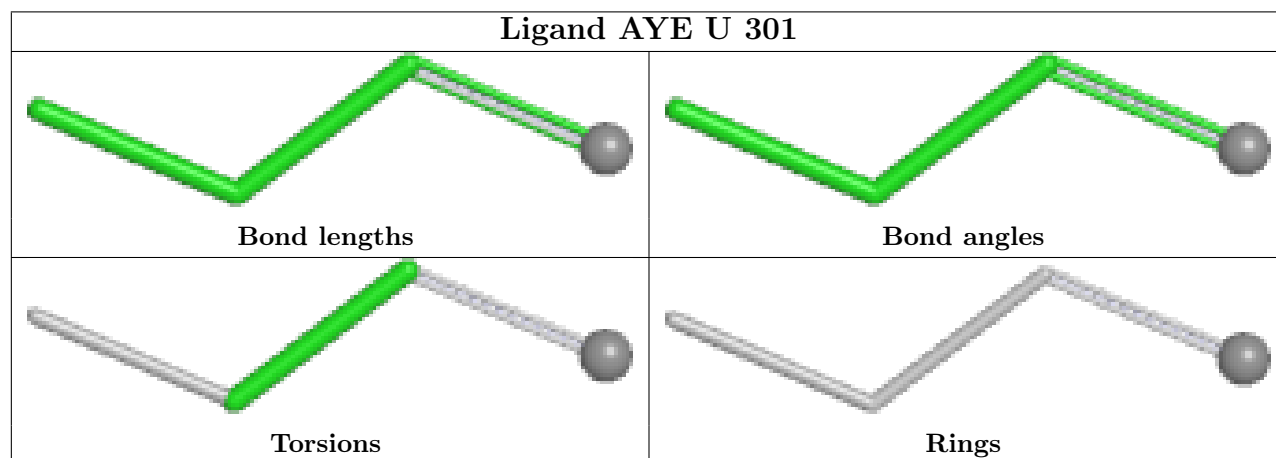
## Ligand AYE A 301



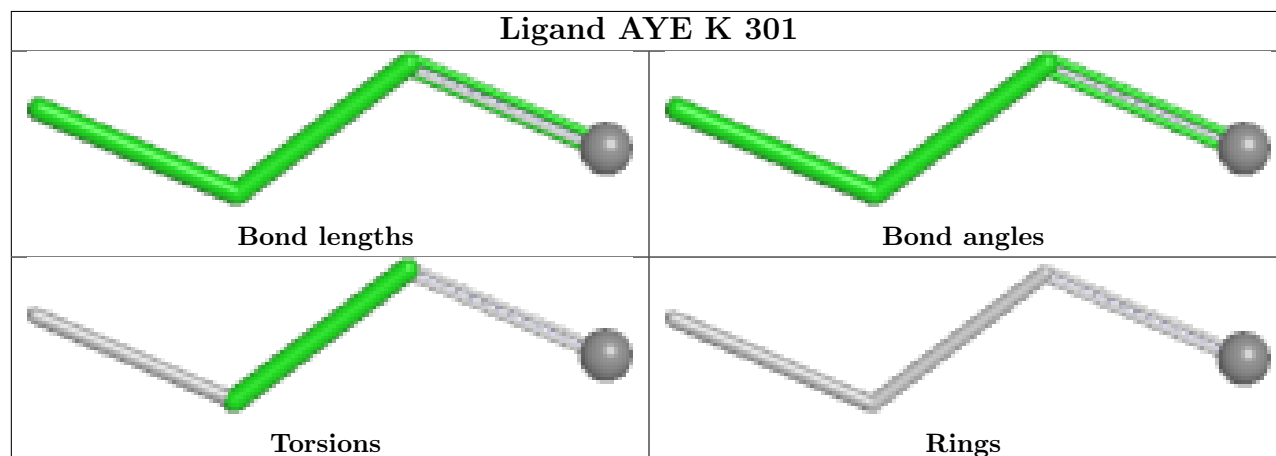
## Ligand AYE O 301

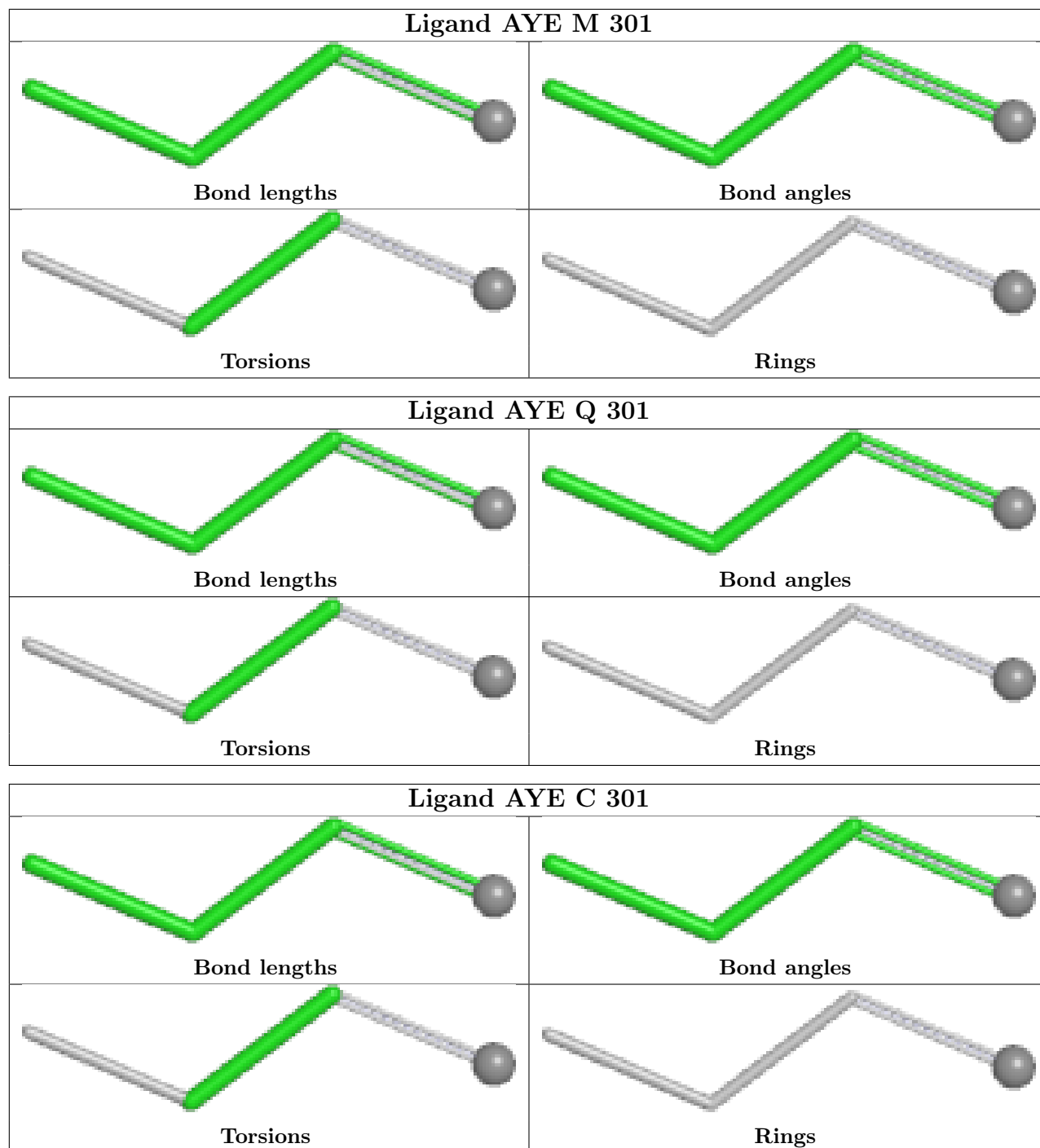


## Ligand AYE U 301



## Ligand AYE K 301





## 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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|---------------|--------|---------------|-----------------------|--------|
| 1   | A     | 234/264 (88%) | 0.02   | 5 (2%) 63 67  | 25, 42, 64, 96        | 2 (0%) |
| 1   | C     | 233/264 (88%) | 0.06   | 8 (3%) 48 51  | 22, 41, 71, 122       | 5 (2%) |
| 1   | E     | 233/264 (88%) | 0.06   | 4 (1%) 69 72  | 25, 42, 72, 90        | 1 (0%) |
| 1   | G     | 236/264 (89%) | -0.00  | 2 (0%) 82 85  | 31, 42, 61, 91        | 1 (0%) |
| 1   | I     | 233/264 (88%) | 0.02   | 3 (1%) 75 78  | 25, 40, 61, 85        | 5 (2%) |
| 1   | K     | 234/264 (88%) | 0.07   | 7 (2%) 52 56  | 30, 42, 68, 99        | 0      |
| 1   | M     | 236/264 (89%) | 0.13   | 3 (1%) 75 78  | 29, 44, 66, 105       | 0      |
| 1   | O     | 235/264 (89%) | 0.27   | 4 (1%) 69 72  | 30, 47, 81, 107       | 1 (0%) |
| 1   | Q     | 236/264 (89%) | 0.60   | 9 (3%) 44 47  | 23, 65, 94, 110       | 1 (0%) |
| 1   | S     | 231/264 (87%) | 0.54   | 18 (7%) 19 20 | 22, 55, 101, 131      | 2 (0%) |
| 1   | U     | 237/264 (89%) | 0.54   | 6 (2%) 58 62  | 22, 57, 82, 111       | 1 (0%) |
| 1   | W     | 236/264 (89%) | 0.72   | 17 (7%) 21 23 | 34, 62, 92, 125       | 1 (0%) |
| 2   | B     | 75/75 (100%)  | 0.08   | 0 100 100     | 33, 50, 65, 68        | 0      |
| 2   | D     | 75/75 (100%)  | 0.01   | 0 100 100     | 33, 47, 62, 72        | 0      |
| 2   | F     | 75/75 (100%)  | -0.14  | 0 100 100     | 32, 41, 56, 57        | 0      |
| 2   | H     | 75/75 (100%)  | 0.24   | 0 100 100     | 33, 48, 65, 68        | 0      |
| 2   | J     | 75/75 (100%)  | 0.14   | 0 100 100     | 31, 47, 63, 72        | 0      |
| 2   | L     | 75/75 (100%)  | -0.02  | 0 100 100     | 34, 43, 57, 63        | 0      |
| 2   | N     | 75/75 (100%)  | 0.12   | 0 100 100     | 31, 49, 68, 69        | 0      |
| 2   | P     | 75/75 (100%)  | 0.12   | 0 100 100     | 33, 48, 65, 70        | 1 (1%) |
| 2   | R     | 75/75 (100%)  | 0.23   | 0 100 100     | 35, 53, 69, 77        | 0      |
| 2   | T     | 75/75 (100%)  | 0.39   | 0 100 100     | 35, 57, 78, 81        | 0      |
| 2   | V     | 75/75 (100%)  | 0.37   | 0 100 100     | 38, 54, 70, 78        | 0      |
| 2   | X     | 75/75 (100%)  | 1.04   | 6 (8%) 18 19  | 42, 78, 101, 111      | 0      |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| All | All   | 3714/4068 (91%) | 0.24   | 92 (2%) 58 62 | 22, 47, 82, 131       | 21 (0%) |

All (92) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | W     | 25  | ILE  | 6.4  |
| 1   | M     | 25  | ILE  | 4.4  |
| 1   | A     | 148 | GLY  | 3.9  |
| 1   | I     | 260 | PRO  | 3.8  |
| 1   | A     | 135 | ASP  | 3.7  |
| 1   | W     | 260 | PRO  | 3.6  |
| 1   | C     | 218 | SER  | 3.5  |
| 1   | A     | 261 | ARG  | 3.5  |
| 1   | E     | 260 | PRO  | 3.4  |
| 1   | S     | 179 | ALA  | 3.4  |
| 1   | C     | 260 | PRO  | 3.3  |
| 1   | W     | 44  | LEU  | 3.3  |
| 1   | C     | 219 | GLY  | 3.2  |
| 1   | S     | 182 | ALA  | 3.2  |
| 2   | X     | 53  | GLY  | 3.2  |
| 1   | S     | 259 | VAL  | 3.1  |
| 1   | K     | 261 | ARG  | 3.1  |
| 1   | S     | 181 | GLY  | 3.0  |
| 1   | S     | 180 | ALA  | 2.9  |
| 1   | W     | 27  | ALA  | 2.9  |
| 1   | W     | 180 | ALA  | 2.9  |
| 1   | K     | 28  | ALA  | 2.9  |
| 1   | A     | 130 | ALA  | 2.8  |
| 1   | O     | 262 | ALA  | 2.8  |
| 1   | K     | 260 | PRO  | 2.7  |
| 1   | S     | 152 | ILE  | 2.7  |
| 1   | A     | 28  | ALA  | 2.6  |
| 1   | W     | 150 | ALA  | 2.6  |
| 1   | W     | 259 | VAL  | 2.6  |
| 1   | Q     | 44  | LEU  | 2.6  |
| 1   | W     | 159 | ALA  | 2.6  |
| 1   | C     | 217 | SER  | 2.6  |
| 1   | G     | 106 | PRO  | 2.5  |
| 1   | C     | 28  | ALA  | 2.5  |
| 1   | Q     | 211 | ALA  | 2.5  |
| 1   | W     | 176 | ALA  | 2.5  |
| 1   | W     | 162 | ASP  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | S     | 260 | PRO  | 2.5  |
| 1   | W     | 219 | GLY  | 2.4  |
| 1   | W     | 179 | ALA  | 2.4  |
| 1   | U     | 177 | ARG  | 2.4  |
| 1   | Q     | 99  | ASP  | 2.4  |
| 1   | U     | 150 | ALA  | 2.4  |
| 1   | U     | 211 | ALA  | 2.4  |
| 2   | X     | 28  | ALA  | 2.4  |
| 1   | C     | 132 | GLN  | 2.4  |
| 1   | K     | 218 | SER  | 2.4  |
| 1   | U     | 25  | ILE  | 2.3  |
| 1   | W     | 181 | GLY  | 2.3  |
| 1   | Q     | 261 | ARG  | 2.3  |
| 1   | S     | 146 | ARG  | 2.3  |
| 2   | X     | 59  | TYR  | 2.3  |
| 1   | G     | 105 | ALA  | 2.3  |
| 1   | W     | 182 | ALA  | 2.3  |
| 1   | E     | 129 | PRO  | 2.3  |
| 1   | S     | 44  | LEU  | 2.3  |
| 1   | E     | 218 | SER  | 2.3  |
| 1   | O     | 179 | ALA  | 2.2  |
| 1   | K     | 132 | GLN  | 2.2  |
| 1   | Q     | 39  | ARG  | 2.2  |
| 1   | W     | 216 | GLU  | 2.2  |
| 2   | X     | 50  | LEU  | 2.2  |
| 1   | U     | 176 | ALA  | 2.2  |
| 1   | S     | 178 | THR  | 2.2  |
| 1   | C     | 41  | ASP  | 2.2  |
| 1   | K     | 219 | GLY  | 2.2  |
| 1   | I     | 129 | PRO  | 2.2  |
| 1   | Q     | 260 | PRO  | 2.2  |
| 1   | Q     | 149 | ALA  | 2.2  |
| 1   | Q     | 159 | ALA  | 2.2  |
| 1   | S     | 162 | ASP  | 2.2  |
| 1   | S     | 213 | PRO  | 2.2  |
| 2   | X     | 4   | PHE  | 2.1  |
| 1   | K     | 217 | SER  | 2.1  |
| 1   | O     | 218 | SER  | 2.1  |
| 1   | E     | 214 | GLY  | 2.1  |
| 1   | S     | 219 | GLY  | 2.1  |
| 1   | M     | 135 | ASP  | 2.1  |
| 1   | O     | 259 | VAL  | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | Q     | 212    | PRO  | 2.1  |
| 2   | X     | 3      | ILE  | 2.1  |
| 1   | S     | 151    | MET  | 2.1  |
| 1   | S     | 136    | TRP  | 2.1  |
| 1   | M     | 260    | PRO  | 2.1  |
| 1   | C     | 130    | ALA  | 2.1  |
| 1   | I     | 135[A] | ASP  | 2.1  |
| 1   | S     | 155    | VAL  | 2.0  |
| 1   | W     | 155    | VAL  | 2.0  |
| 1   | W     | 212    | PRO  | 2.0  |
| 1   | S     | 105    | ALA  | 2.0  |
| 1   | S     | 214    | GLY  | 2.0  |
| 1   | U     | 259    | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

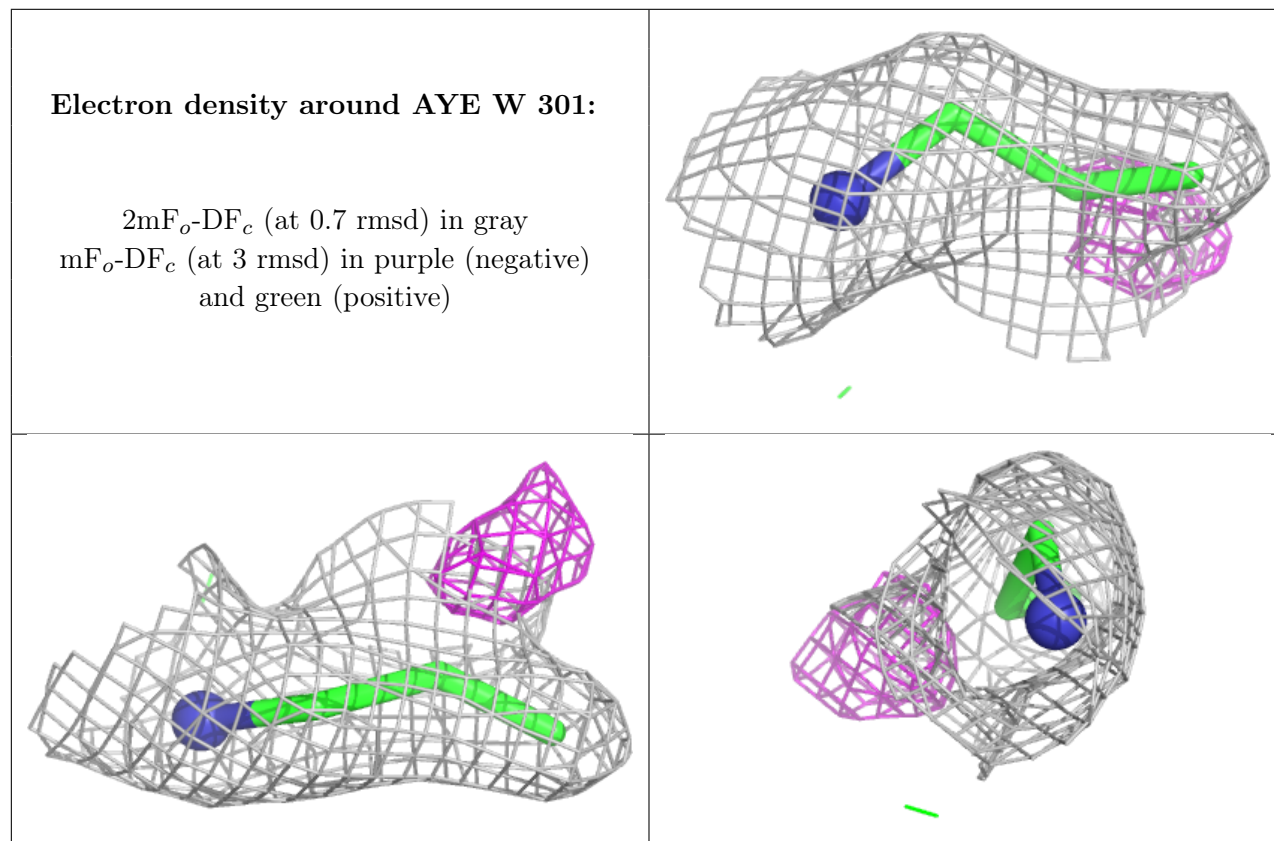
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | AYE  | W     | 301 | 4/4   | 0.90 | 0.13 | 41,42,43,45                 | 0     |
| 3   | AYE  | U     | 301 | 4/4   | 0.93 | 0.12 | 44,45,46,49                 | 0     |
| 3   | AYE  | Q     | 301 | 4/4   | 0.94 | 0.10 | 44,44,50,51                 | 0     |
| 3   | AYE  | A     | 301 | 4/4   | 0.94 | 0.08 | 33,33,34,35                 | 0     |
| 3   | AYE  | I     | 301 | 4/4   | 0.94 | 0.08 | 29,30,33,33                 | 0     |
| 3   | AYE  | O     | 301 | 4/4   | 0.95 | 0.08 | 37,38,40,40                 | 0     |
| 3   | AYE  | E     | 301 | 4/4   | 0.96 | 0.06 | 34,35,35,36                 | 0     |
| 3   | AYE  | S     | 301 | 4/4   | 0.96 | 0.08 | 38,39,40,41                 | 0     |
| 3   | AYE  | K     | 301 | 4/4   | 0.97 | 0.05 | 31,33,34,34                 | 0     |
| 3   | AYE  | G     | 301 | 4/4   | 0.97 | 0.06 | 35,35,36,36                 | 0     |

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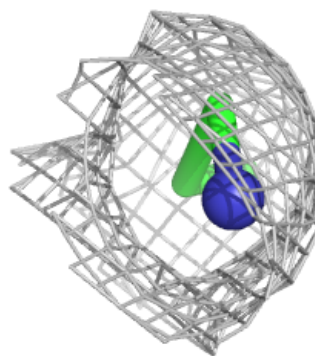
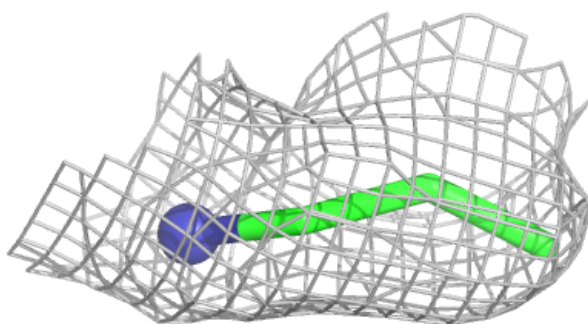
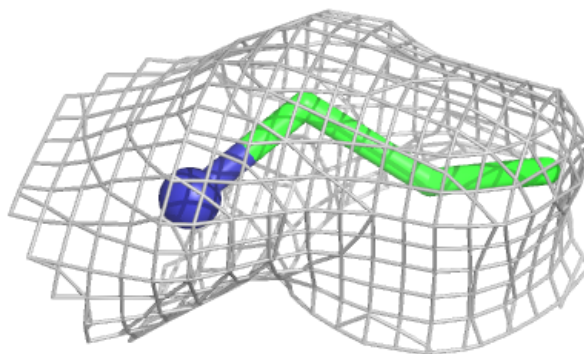
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | AYE  | M     | 301 | 4/4   | 0.98 | 0.06 | 34,36,37,38                 | 0     |
| 3   | AYE  | C     | 301 | 4/4   | 0.98 | 0.06 | 33,33,33,34                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

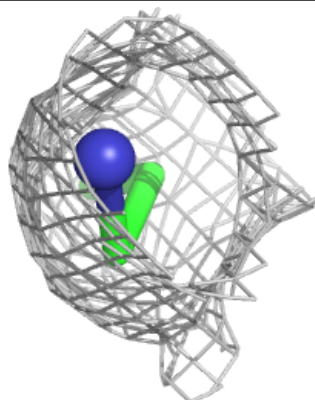
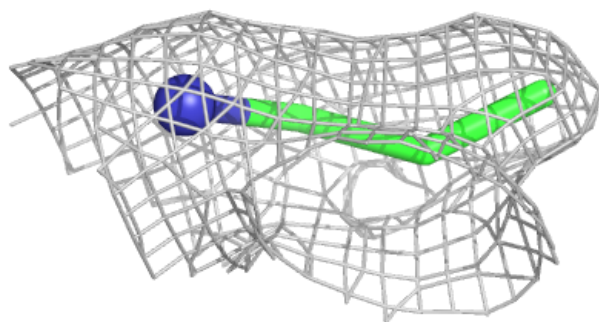
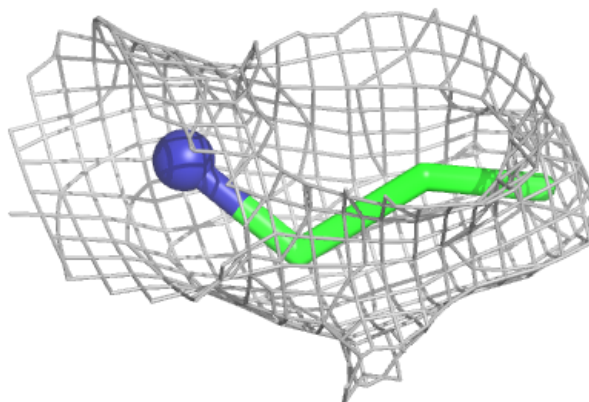


**Electron density around AYE U 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

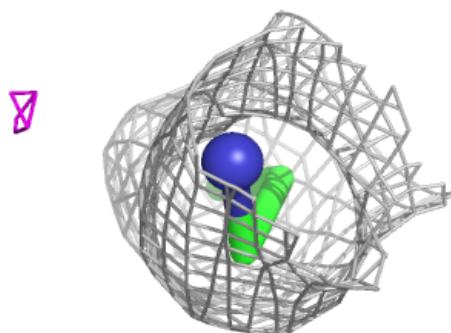
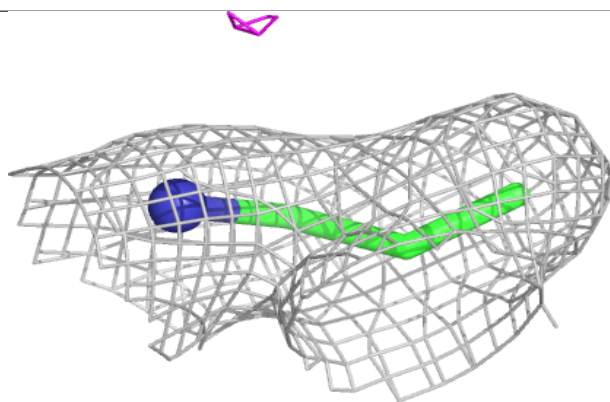
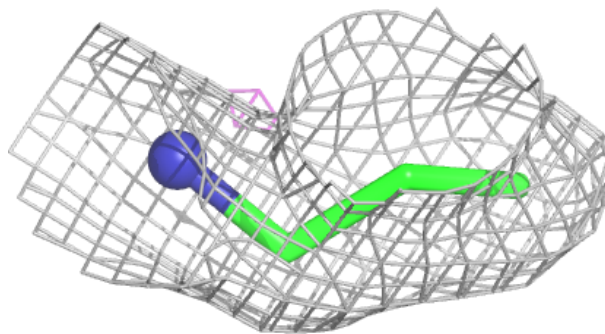
**Electron density around AYE Q 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

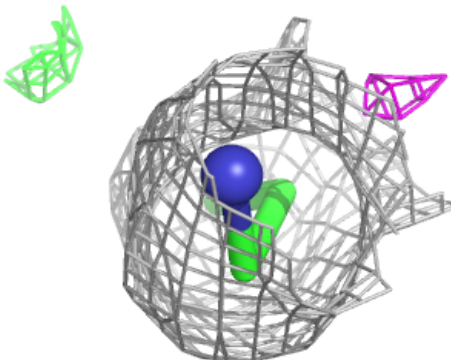
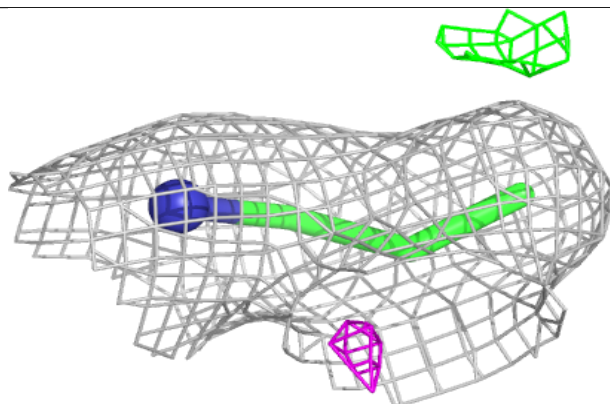
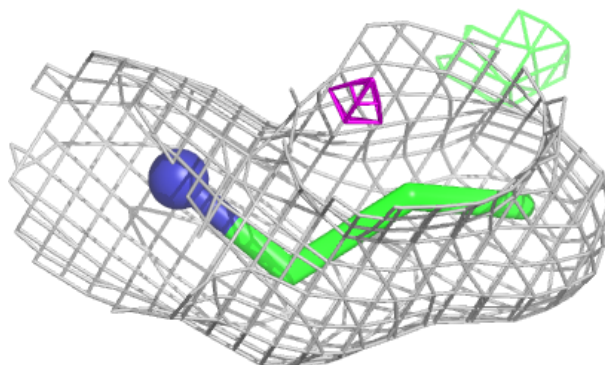


**Electron density around AYE A 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

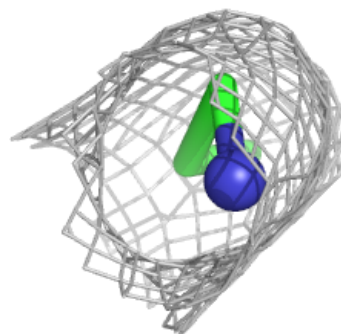
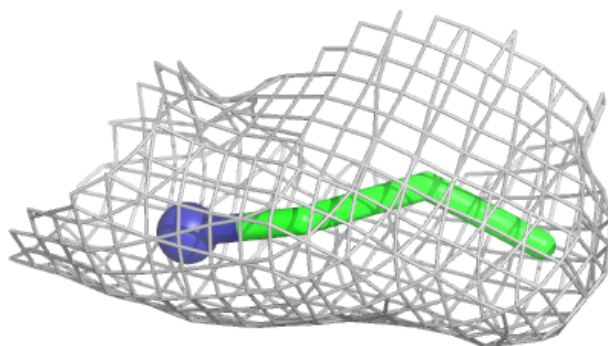
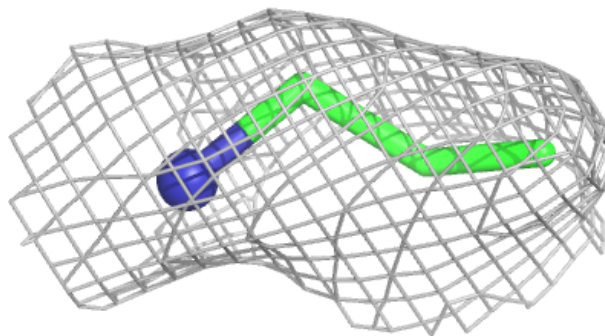
**Electron density around AYE I 301:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

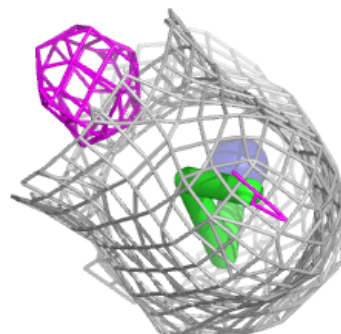
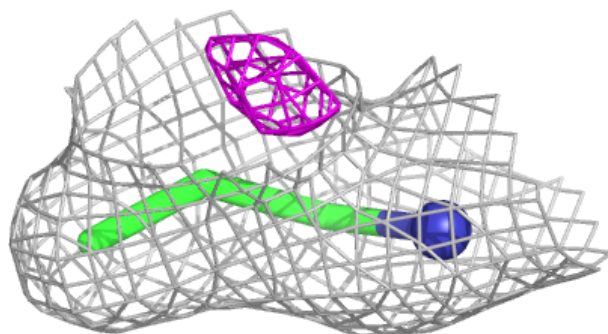
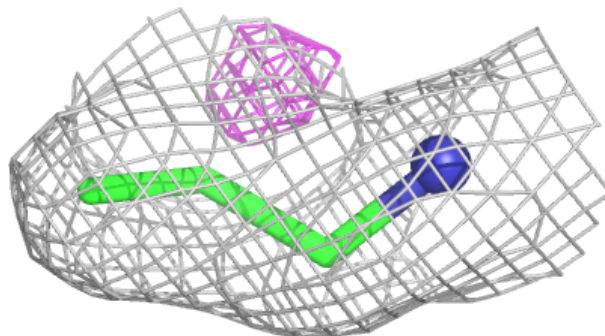


**Electron density around AYE O 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

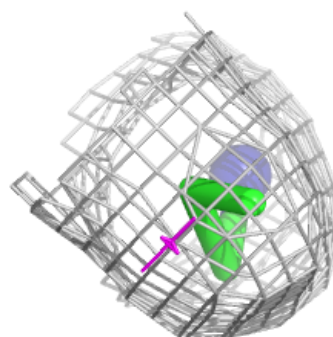
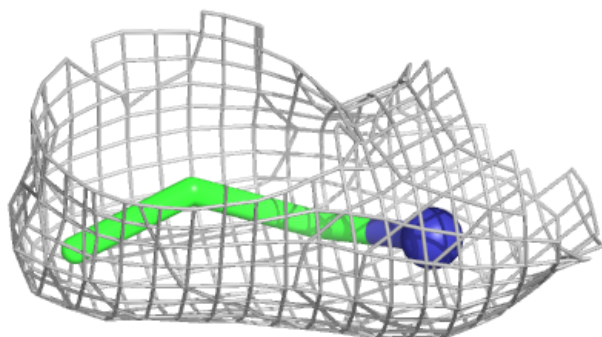
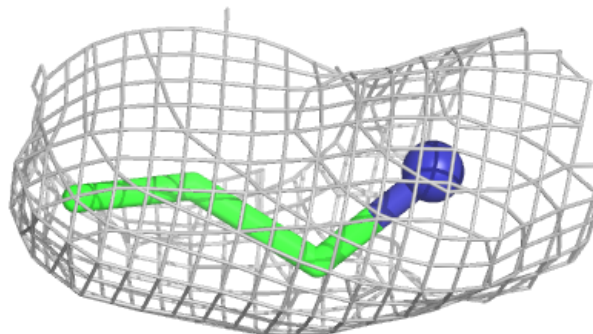
**Electron density around AYE E 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

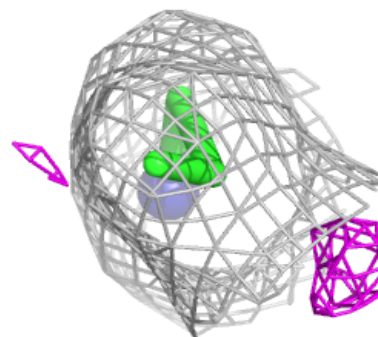
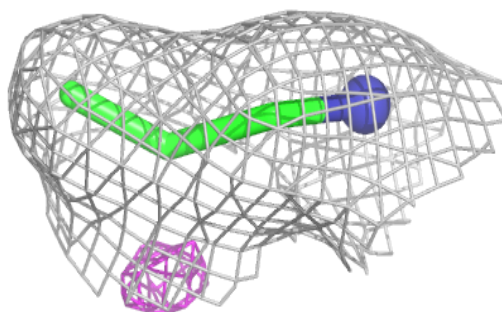
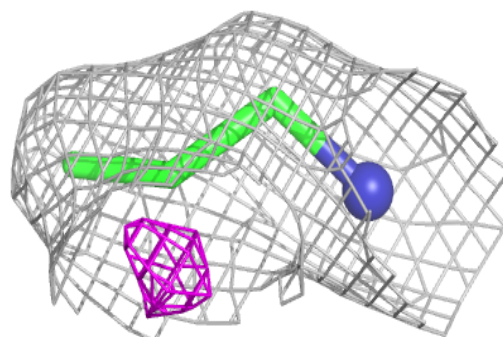


**Electron density around AYE S 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

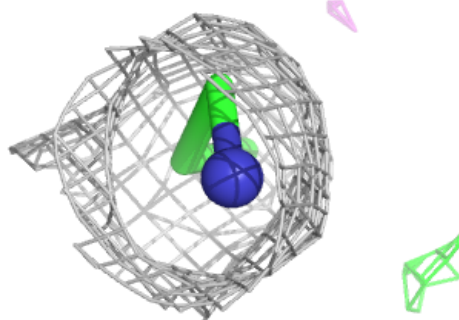
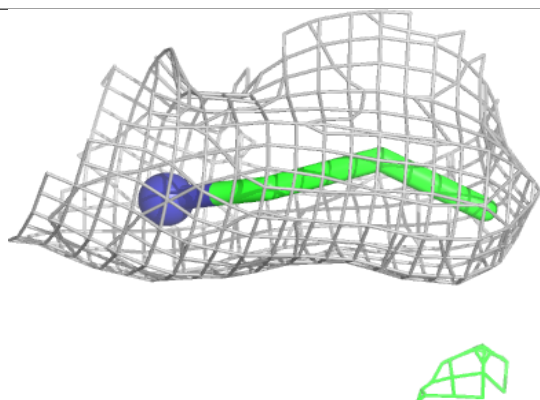
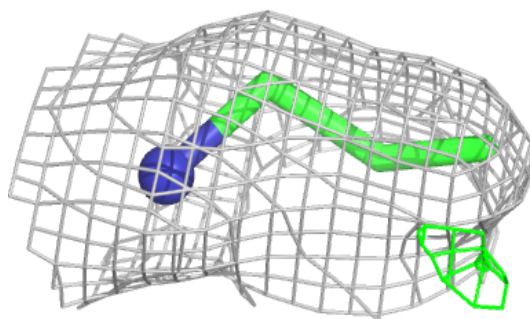
**Electron density around AYE K 301:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

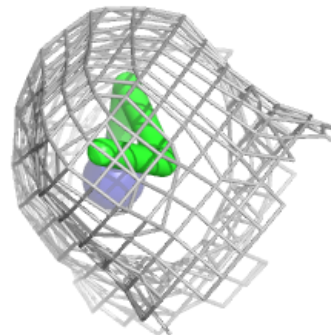
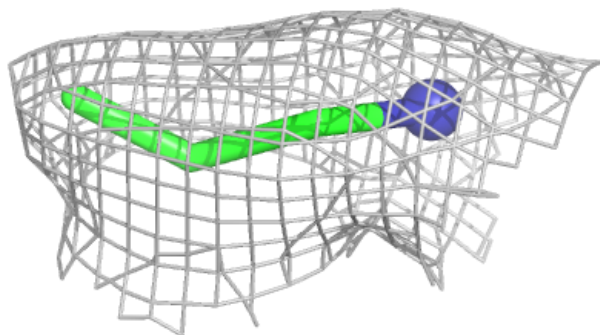
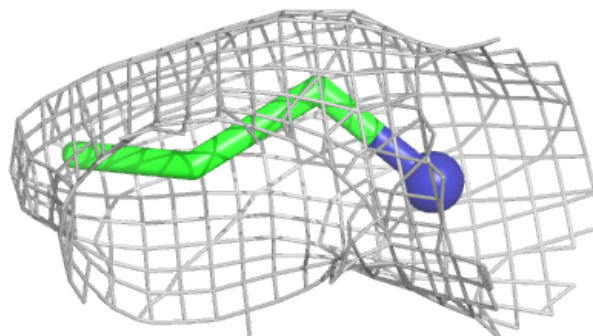


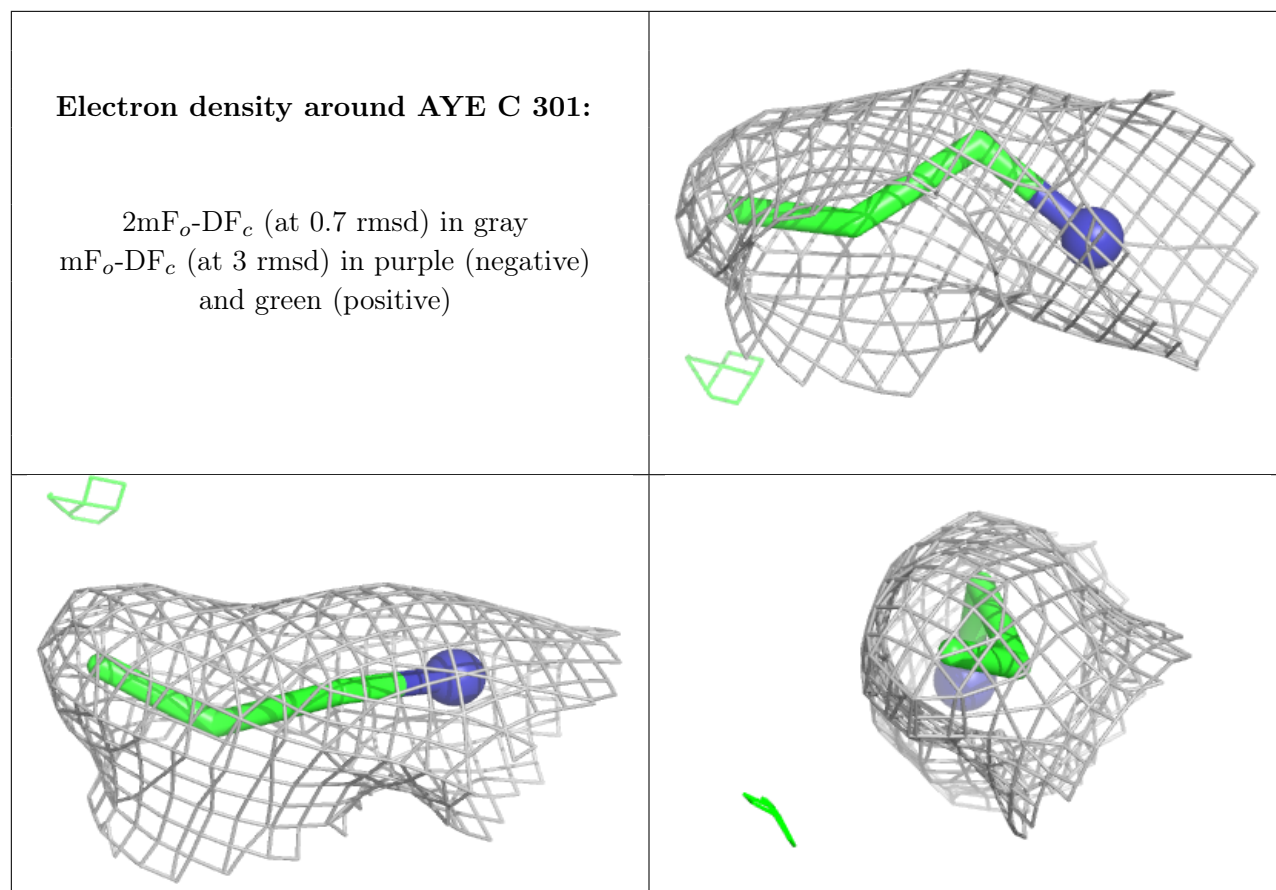
**Electron density around AYE G 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around AYE M 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.