



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2020 – 05:45 am BST

PDB ID : 6ODE  
Title : Crystal Structure of Mycobacterium tuberculosis Proteasome in Complex with Phenylimidazole-based Inhibitor B6  
Authors : Hsu, H.C.; Li, H.  
Deposited on : 2019-03-26  
Resolution : 2.90 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.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

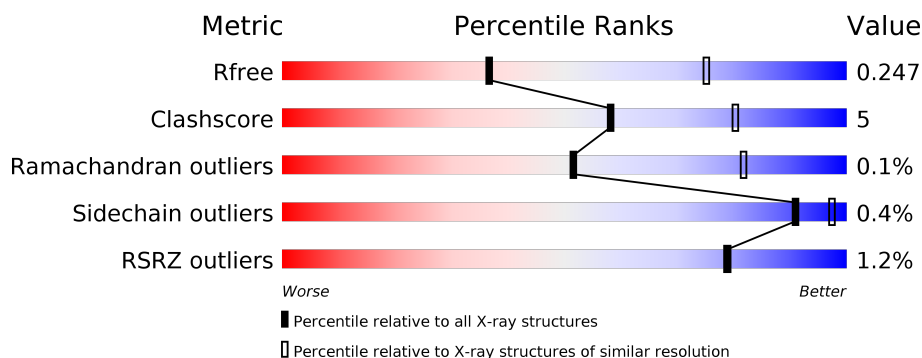
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1957 (2.90-2.90)                                      |
| Clashscore            | 141614                      | 2172 (2.90-2.90)                                      |
| Ramachandran outliers | 138981                      | 2115 (2.90-2.90)                                      |
| Sidechain outliers    | 138945                      | 2117 (2.90-2.90)                                      |
| RSRZ outliers         | 127900                      | 1906 (2.90-2.90)                                      |

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 on 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     | 240    | <div> <div></div> <div>73%18%9%</div> </div>    |
| 1   | B     | 240    | <div> <div>4%</div> <div>76%14%10%</div> </div> |
| 1   | C     | 240    | <div> <div>5%</div> <div>66%23%10%</div> </div> |
| 1   | D     | 240    | <div> <div>2%</div> <div>72%17%11%</div> </div> |
| 1   | E     | 240    | <div> <div>%</div> <div>73%17%10%</div> </div>  |
| 1   | F     | 240    | <div> <div>%</div> <div>73%16%11%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 240    |                  |
| 1   | O     | 240    |                  |
| 1   | P     | 240    |                  |
| 1   | Q     | 240    |                  |
| 1   | R     | 240    |                  |
| 1   | S     | 240    |                  |
| 1   | T     | 240    |                  |
| 1   | U     | 240    |                  |
| 2   | H     | 234    |                  |
| 2   | I     | 234    |                  |
| 2   | J     | 234    |                  |
| 2   | K     | 234    |                  |
| 2   | L     | 234    |                  |
| 2   | M     | 234    |                  |
| 2   | N     | 234    |                  |
| 2   | V     | 234    |                  |
| 2   | W     | 234    |                  |
| 2   | X     | 234    |                  |
| 2   | Y     | 234    |                  |
| 2   | Z     | 234    |                  |
| 2   | a     | 234    |                  |
| 2   | b     | 234    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47311 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 Proteasome subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1677  | 1050 | 306 | 317 | 4 |         |         |       |
| 1   | B     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1660  | 1041 | 303 | 312 | 4 |         |         |       |
| 1   | C     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1664  | 1043 | 304 | 313 | 4 |         |         |       |
| 1   | D     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1649  | 1032 | 302 | 311 | 4 |         |         |       |
| 1   | E     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1671  | 1047 | 305 | 315 | 4 |         |         |       |
| 1   | F     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1653  | 1036 | 302 | 311 | 4 |         |         |       |
| 1   | G     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1662  | 1040 | 304 | 314 | 4 |         |         |       |
| 1   | O     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1664  | 1042 | 304 | 314 | 4 |         |         |       |
| 1   | P     | 219      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1685  | 1054 | 307 | 320 | 4 |         |         |       |
| 1   | Q     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1660  | 1041 | 303 | 312 | 4 |         |         |       |
| 1   | R     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1038 | 303 | 312 | 4 |         |         |       |
| 1   | S     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1678  | 1050 | 306 | 318 | 4 |         |         |       |
| 1   | T     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1671  | 1047 | 305 | 315 | 4 |         |         |       |
| 1   | U     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1664  | 1043 | 304 | 313 | 4 |         |         |       |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| C     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| D     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| E     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| F     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| G     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| O     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| P     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| Q     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| R     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| S     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| T     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |
| U     | 9       | MET      | -      | initiating methionine | UNP P9WHU1 |

- Molecule 2 is a protein called Proteasome subunit beta.

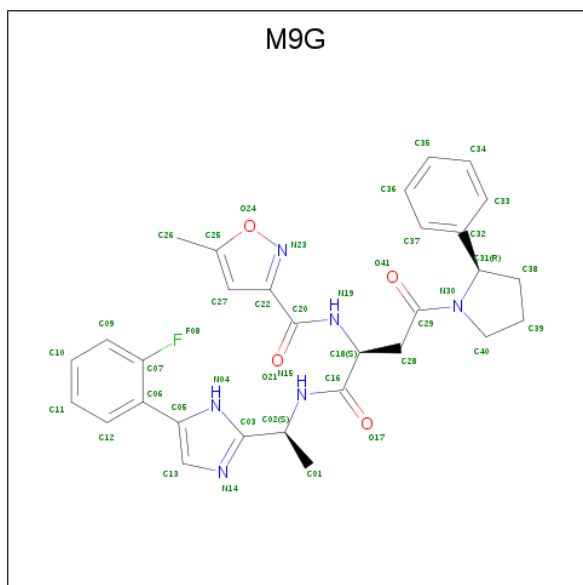
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | H     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | I     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | J     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | K     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | L     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | M     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | N     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | V     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | W     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | X     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1638  | 1027 | 282 | 324 | 5 |         |         |       |
| 2   | Y     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | Z     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |
| 2   | a     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | b     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1642  | 1029 | 283 | 325 | 5 |         |         |       |

- Molecule 3 is N-{(2S)-1-((1S)-1-[5-(2-fluorophenyl)-1H-imidazol-2-yl]ethyl)amino)-1,4-dioxo-4-[(2R)-2-phenylpyrrolidin-1-yl]butan-2-yl}-5-methyl-1,2-oxazole-3-carboxamide (three-letter code: M9G) (formula: C<sub>30</sub>H<sub>31</sub>FN<sub>6</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 3   | H     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | I     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | J     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | L     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | L     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | M     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | N     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | V     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |
| 3   | W     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 41    | 30 | 1 | 6 | 4 |         |         |

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| Mol | Chain | Residues | Atoms       |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 3   | X     | 1        | Total<br>41 | C<br>30 | F<br>1 | N<br>6 | O<br>4 | 0       | 0       |
| 3   | Y     | 1        | Total<br>41 | C<br>30 | F<br>1 | N<br>6 | O<br>4 | 0       | 0       |
| 3   | Z     | 1        | Total<br>41 | C<br>30 | F<br>1 | N<br>6 | O<br>4 | 0       | 0       |
| 3   | a     | 1        | Total<br>41 | C<br>30 | F<br>1 | N<br>6 | O<br>4 | 0       | 0       |
| 3   | b     | 1        | Total<br>41 | C<br>30 | F<br>1 | N<br>6 | O<br>4 | 0       | 0       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | A     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 4   | B     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 4   | C     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 4   | D     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 4   | E     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 4   | F     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 4   | G     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 4   | H     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 4   | I     | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 4   | J     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 4   | K     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | L     | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 4   | M     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | N     | 22       | Total<br>22 | O<br>22 | 0       | 0       |

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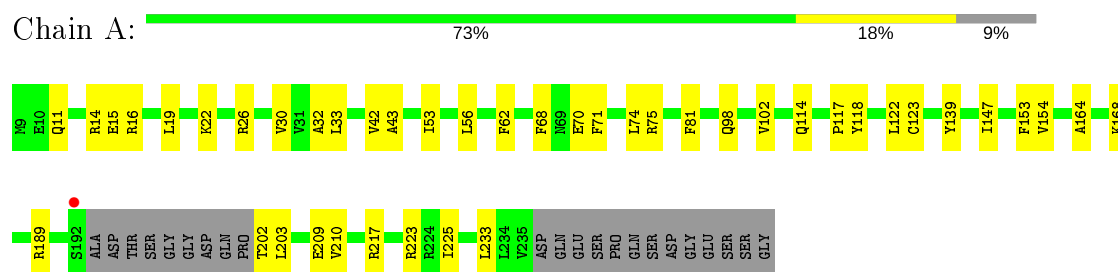
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | O     | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 4   | P     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 4   | Q     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 4   | R     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 4   | S     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 4   | T     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | U     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 4   | V     | 27       | Total<br>27 | O<br>27 | 0       | 0       |
| 4   | W     | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 4   | X     | 27       | Total<br>27 | O<br>27 | 0       | 0       |
| 4   | Y     | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 4   | Z     | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 4   | a     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 4   | b     | 19       | Total<br>19 | O<br>19 | 0       | 0       |



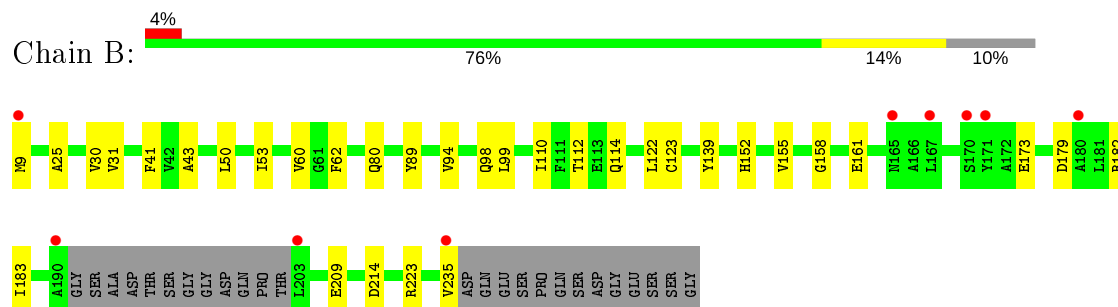
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

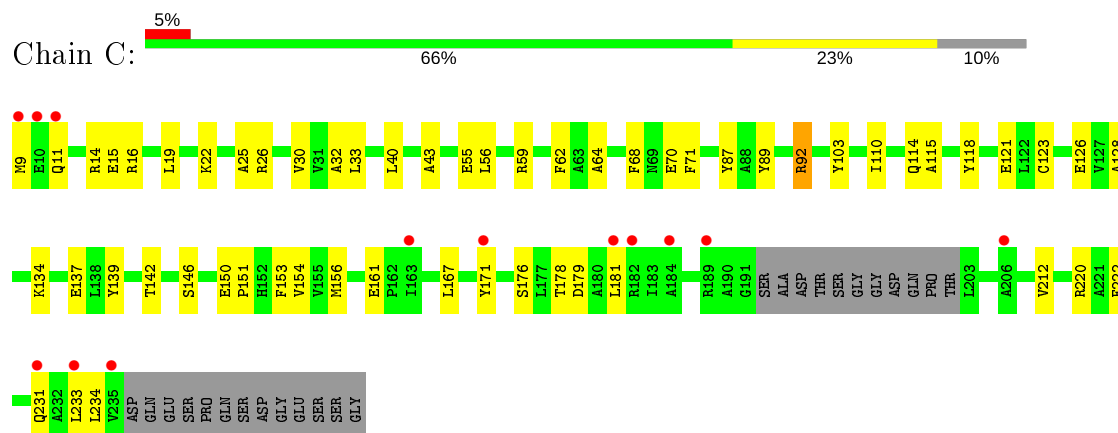
- Molecule 1: Proteasome subunit alpha



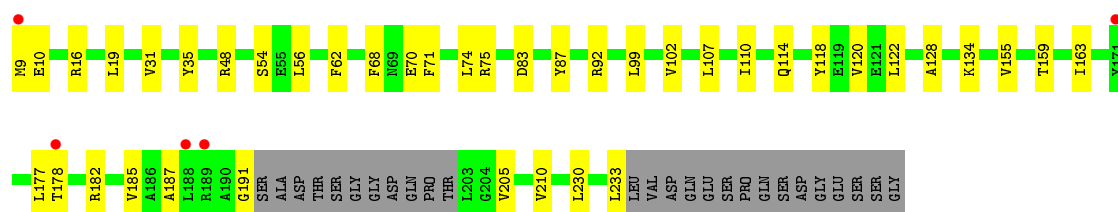
- Molecule 1: Proteasome subunit alpha



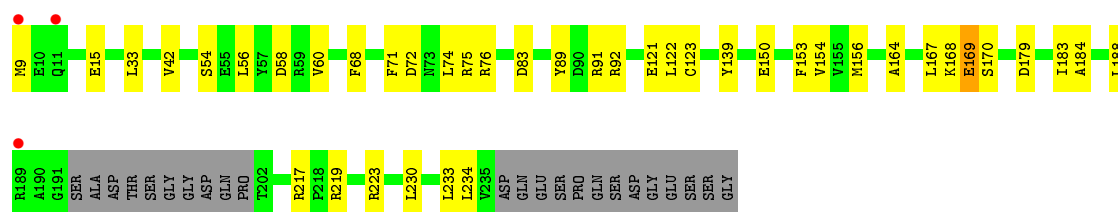
- Molecule 1: Proteasome subunit alpha



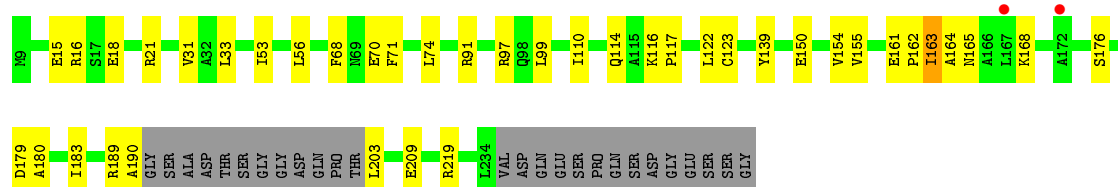
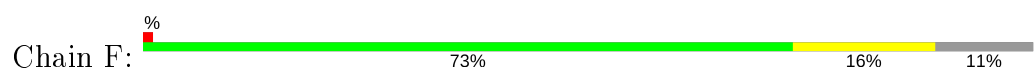
- Molecule 1: Proteasome subunit alpha



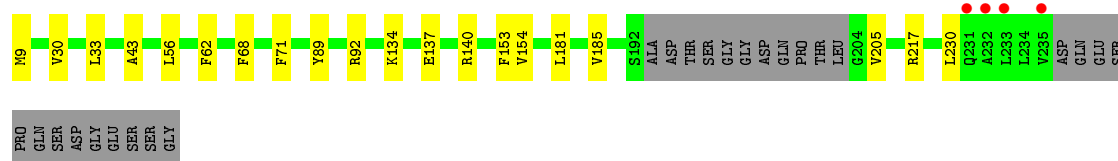
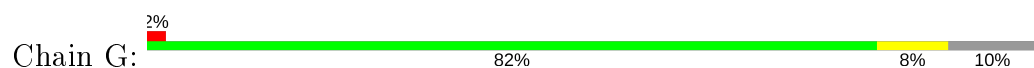
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

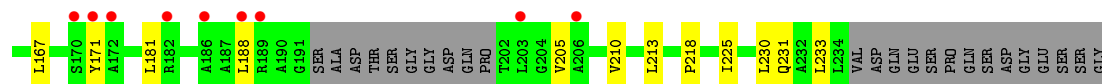


- Molecule 1: Proteasome subunit alpha

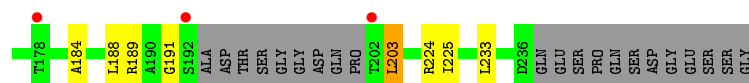
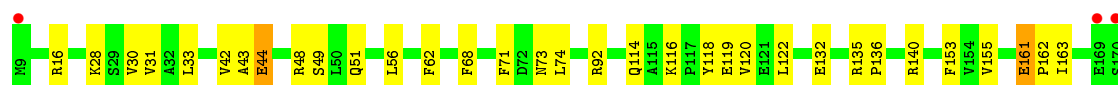


- Molecule 1: Proteasome subunit alpha

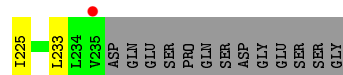
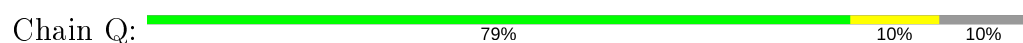




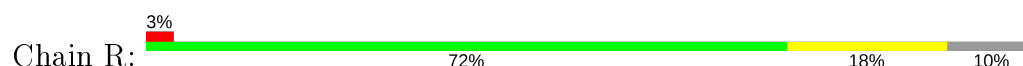
- Molecule 1: Proteasome subunit alpha



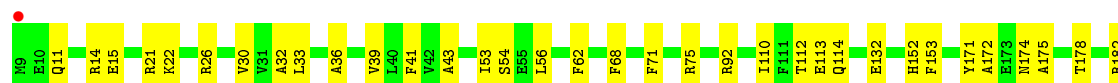
- Molecule 1: Proteasome subunit alpha



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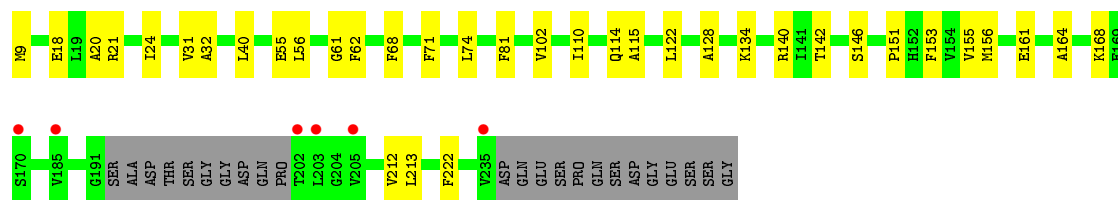


- Molecule 1: Proteasome subunit alpha

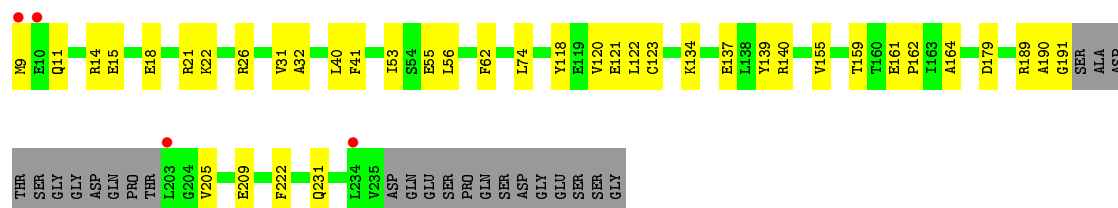
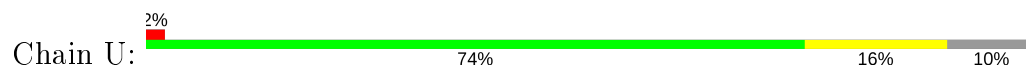


- Molecule 1: Proteasome subunit alpha

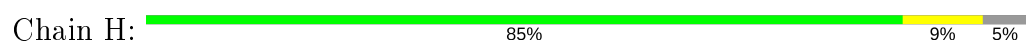




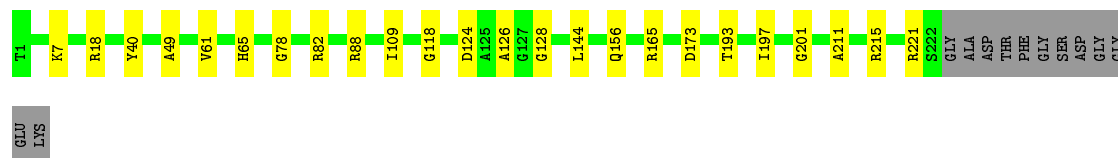
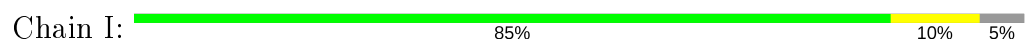
- Molecule 1: Proteasome subunit alpha



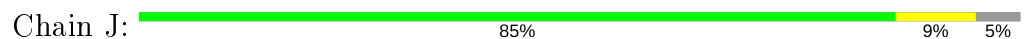
- Molecule 2: Proteasome subunit beta



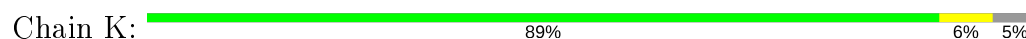
- Molecule 2: Proteasome subunit beta




- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta




- Molecule 2: Proteasome subunit beta

Chain L:  89% 6% 5%



- Molecule 2: Proteasome subunit beta

Chain M:  88% 7% 5%




- Molecule 2: Proteasome subunit beta

Chain N:  89% 6% 5%



- Molecule 2: Proteasome subunit beta

Chain V:  90% 6% 5%




- Molecule 2: Proteasome subunit beta

Chain W:  92% 5% 5%




- Molecule 2: Proteasome subunit beta

Chain X:  86% 9% 5%




- Molecule 2: Proteasome subunit beta

Chain Y:  88% 8% 5%



- Molecule 2: Proteasome subunit beta

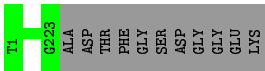
Chain Z:  90% 5% 5%



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 120.60Å 198.38Å 166.51Å<br>90.00° 103.10° 90.00°            | Depositor        |
| Resolution (Å)  | 53.97 – 2.90<br>53.97 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (53.97-2.90)<br>99.9 (53.97-2.90)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.18  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.05 (at 2.91Å)   | Xtriage          |
| Refinement program  | PHENIX  | Depositor        |
| R, $R_{free}$   | 0.197 , 0.247<br>0.197 , 0.247                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8403 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.9  | Xtriage          |
| Anisotropy  | 0.376   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 45.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 47311   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 34.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M9G

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     | 0.26         | 0/1701  | 0.45        | 0/2297  |
| 1   | B     | 0.25         | 0/1684  | 0.44        | 0/2274  |
| 1   | C     | 0.26         | 0/1688  | 0.46        | 0/2279  |
| 1   | D     | 0.25         | 0/1673  | 0.46        | 0/2258  |
| 1   | E     | 0.25         | 0/1695  | 0.45        | 0/2289  |
| 1   | F     | 0.33         | 0/1677  | 0.49        | 0/2264  |
| 1   | G     | 0.25         | 0/1686  | 0.44        | 0/2276  |
| 1   | O     | 0.27         | 0/1688  | 0.45        | 0/2279  |
| 1   | P     | 0.28         | 0/1709  | 0.46        | 0/2308  |
| 1   | Q     | 0.26         | 0/1684  | 0.44        | 0/2274  |
| 1   | R     | 0.36         | 0/1681  | 0.47        | 0/2269  |
| 1   | S     | 0.25         | 0/1702  | 0.45        | 0/2298  |
| 1   | T     | 0.25         | 0/1695  | 0.45        | 0/2289  |
| 1   | U     | 0.25         | 0/1688  | 0.44        | 0/2279  |
| 2   | H     | 0.26         | 0/1662  | 0.47        | 0/2254  |
| 2   | I     | 0.26         | 0/1662  | 0.47        | 0/2254  |
| 2   | J     | 0.25         | 0/1662  | 0.45        | 0/2254  |
| 2   | K     | 0.26         | 0/1666  | 0.46        | 0/2259  |
| 2   | L     | 0.26         | 0/1666  | 0.46        | 0/2259  |
| 2   | M     | 0.25         | 0/1662  | 0.45        | 0/2254  |
| 2   | N     | 0.26         | 0/1666  | 0.46        | 0/2259  |
| 2   | V     | 0.26         | 0/1666  | 0.46        | 0/2259  |
| 2   | W     | 0.25         | 0/1666  | 0.47        | 0/2259  |
| 2   | X     | 0.25         | 0/1662  | 0.46        | 0/2254  |
| 2   | Y     | 0.26         | 0/1666  | 0.46        | 0/2259  |
| 2   | Z     | 0.25         | 0/1666  | 0.46        | 0/2259  |
| 2   | a     | 0.26         | 0/1666  | 0.47        | 0/2259  |
| 2   | b     | 0.26         | 0/1666  | 0.46        | 0/2259  |
| All | All   | 0.26         | 0/46955 | 0.46        | 0/63534 |

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     | 1677  | 0        | 1680     | 26      | 0            |
| 1   | B     | 1660  | 0        | 1665     | 23      | 0            |
| 1   | C     | 1664  | 0        | 1668     | 41      | 0            |
| 1   | D     | 1649  | 0        | 1648     | 30      | 0            |
| 1   | E     | 1671  | 0        | 1675     | 28      | 0            |
| 1   | F     | 1653  | 0        | 1656     | 23      | 0            |
| 1   | G     | 1662  | 0        | 1662     | 12      | 0            |
| 1   | O     | 1664  | 0        | 1666     | 31      | 0            |
| 1   | P     | 1685  | 0        | 1684     | 27      | 0            |
| 1   | Q     | 1660  | 0        | 1665     | 16      | 0            |
| 1   | R     | 1657  | 0        | 1659     | 25      | 0            |
| 1   | S     | 1678  | 0        | 1677     | 23      | 0            |
| 1   | T     | 1671  | 0        | 1675     | 20      | 0            |
| 1   | U     | 1664  | 0        | 1668     | 19      | 0            |
| 2   | H     | 1638  | 0        | 1633     | 13      | 0            |
| 2   | I     | 1638  | 0        | 1633     | 13      | 0            |
| 2   | J     | 1638  | 0        | 1633     | 16      | 0            |
| 2   | K     | 1642  | 0        | 1636     | 10      | 0            |
| 2   | L     | 1642  | 0        | 1636     | 10      | 0            |
| 2   | M     | 1638  | 0        | 1633     | 12      | 0            |
| 2   | N     | 1642  | 0        | 1636     | 8       | 0            |
| 2   | V     | 1642  | 0        | 1636     | 8       | 0            |
| 2   | W     | 1642  | 0        | 1636     | 4       | 0            |
| 2   | X     | 1638  | 0        | 1633     | 12      | 0            |
| 2   | Y     | 1642  | 0        | 1636     | 11      | 0            |
| 2   | Z     | 1642  | 0        | 1636     | 6       | 0            |
| 2   | a     | 1642  | 0        | 1636     | 0       | 0            |
| 2   | b     | 1642  | 0        | 1636     | 0       | 0            |
| 3   | H     | 41    | 0        | 0        | 0       | 0            |
| 3   | I     | 41    | 0        | 0        | 1       | 0            |
| 3   | J     | 41    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | L     | 82    | 0        | 0        | 0       | 0            |
| 3   | M     | 41    | 0        | 0        | 1       | 0            |
| 3   | N     | 41    | 0        | 0        | 1       | 0            |
| 3   | V     | 41    | 0        | 0        | 0       | 0            |
| 3   | W     | 41    | 0        | 0        | 0       | 0            |
| 3   | X     | 41    | 0        | 0        | 0       | 0            |
| 3   | Y     | 41    | 0        | 0        | 0       | 0            |
| 3   | Z     | 41    | 0        | 0        | 0       | 0            |
| 3   | a     | 41    | 0        | 0        | 0       | 0            |
| 3   | b     | 41    | 0        | 0        | 0       | 0            |
| 4   | A     | 15    | 0        | 0        | 0       | 0            |
| 4   | B     | 11    | 0        | 0        | 1       | 0            |
| 4   | C     | 10    | 0        | 0        | 0       | 0            |
| 4   | D     | 6     | 0        | 0        | 0       | 0            |
| 4   | E     | 6     | 0        | 0        | 0       | 0            |
| 4   | F     | 9     | 0        | 0        | 0       | 0            |
| 4   | G     | 11    | 0        | 0        | 0       | 0            |
| 4   | H     | 14    | 0        | 0        | 0       | 0            |
| 4   | I     | 21    | 0        | 0        | 0       | 0            |
| 4   | J     | 28    | 0        | 0        | 1       | 0            |
| 4   | K     | 20    | 0        | 0        | 0       | 0            |
| 4   | L     | 24    | 0        | 0        | 0       | 0            |
| 4   | M     | 20    | 0        | 0        | 0       | 0            |
| 4   | N     | 22    | 0        | 0        | 0       | 0            |
| 4   | O     | 7     | 0        | 0        | 0       | 0            |
| 4   | P     | 11    | 0        | 0        | 1       | 0            |
| 4   | Q     | 15    | 0        | 0        | 0       | 0            |
| 4   | R     | 15    | 0        | 0        | 1       | 0            |
| 4   | S     | 10    | 0        | 0        | 1       | 0            |
| 4   | T     | 12    | 0        | 0        | 0       | 0            |
| 4   | U     | 11    | 0        | 0        | 0       | 0            |
| 4   | V     | 27    | 0        | 0        | 0       | 0            |
| 4   | W     | 21    | 0        | 0        | 0       | 0            |
| 4   | X     | 27    | 0        | 0        | 0       | 0            |
| 4   | Y     | 23    | 0        | 0        | 0       | 0            |
| 4   | Z     | 23    | 0        | 0        | 0       | 0            |
| 4   | a     | 16    | 0        | 0        | 0       | 0            |
| 4   | b     | 19    | 0        | 0        | 0       | 0            |
| All | All   | 47311 | 0        | 46237    | 424     | 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 5.

All (424) 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:O:31:VAL:HG12  | 1:O:155:VAL:HG22 | 1.64                     | 0.78              |
| 1:P:161:GLU:HG2  | 1:P:162:PRO:HD3  | 1.65                     | 0.78              |
| 1:F:161:GLU:O    | 1:F:165:ASN:ND2  | 2.19                     | 0.76              |
| 1:C:231:GLN:HA   | 1:C:234:LEU:HD12 | 1.68                     | 0.75              |
| 1:S:110:ILE:HG23 | 1:S:114:GLN:HG3  | 1.69                     | 0.73              |
| 1:S:112:THR:HG22 | 1:S:113:GLU:HG3  | 1.69                     | 0.73              |
| 1:A:16:ARG:NH1   | 1:A:114:GLN:O    | 2.23                     | 0.72              |
| 1:P:189:ARG:NH1  | 1:P:203:LEU:HD11 | 2.05                     | 0.72              |
| 1:A:33:LEU:HD23  | 1:A:153:PHE:HB3  | 1.73                     | 0.70              |
| 1:B:182:ARG:NH1  | 1:B:235:VAL:O    | 2.25                     | 0.70              |
| 1:S:92:ARG:NH2   | 1:S:132:GLU:OE1  | 2.25                     | 0.69              |
| 1:C:33:LEU:HD23  | 1:C:153:PHE:HB3  | 1.75                     | 0.69              |
| 1:A:189:ARG:HE   | 1:A:202:THR:HG22 | 1.57                     | 0.69              |
| 1:O:181:LEU:HD23 | 1:O:233:LEU:HD12 | 1.74                     | 0.69              |
| 1:E:217:ARG:HH21 | 1:E:223:ARG:HD3  | 1.57                     | 0.68              |
| 1:T:56:LEU:HG    | 1:T:62:PHE:HB2   | 1.75                     | 0.66              |
| 1:U:74:LEU:HD13  | 1:U:122:LEU:HD11 | 1.77                     | 0.66              |
| 1:C:30:VAL:HG13  | 1:C:43:ALA:HB2   | 1.78                     | 0.66              |
| 1:P:135:ARG:HD2  | 1:P:136:PRO:HD2  | 1.77                     | 0.66              |
| 1:C:9:MET:HG3    | 1:D:19:LEU:HD13  | 1.79                     | 0.65              |
| 1:D:210:VAL:HG11 | 1:D:230:LEU:HD13 | 1.78                     | 0.65              |
| 1:A:189:ARG:HH21 | 1:A:203:LEU:H    | 1.45                     | 0.65              |
| 1:P:16:ARG:NH1   | 1:P:114:GLN:O    | 2.28                     | 0.64              |
| 1:E:42:VAL:HG11  | 1:E:184:ALA:HB1  | 1.78                     | 0.64              |
| 2:I:173:ASP:OD1  | 2:I:221:ARG:NH2  | 2.31                     | 0.64              |
| 2:L:165:ARG:NH2  | 2:L:169:GLU:OE2  | 2.31                     | 0.64              |
| 1:F:219:ARG:NH2  | 2:M:64:GLU:OE2   | 2.26                     | 0.64              |
| 1:U:31:VAL:HG12  | 1:U:155:VAL:HG12 | 1.77                     | 0.64              |
| 1:U:41:PHE:HB3   | 1:U:53:ILE:HD13  | 1.79                     | 0.64              |
| 1:A:74:LEU:HD13  | 1:A:122:LEU:HD11 | 1.80                     | 0.63              |
| 1:P:116:LYS:NZ   | 1:P:119:GLU:OE1  | 2.30                     | 0.63              |
| 1:F:56:LEU:HD13  | 1:F:99:LEU:HD23  | 1.80                     | 0.63              |
| 1:B:110:ILE:HA   | 1:B:114:GLN:HG3  | 1.79                     | 0.63              |
| 1:A:56:LEU:HG    | 1:A:62:PHE:HB2   | 1.81                     | 0.62              |
| 1:Q:225:ILE:HG21 | 1:Q:233:LEU:HD12 | 1.82                     | 0.62              |
| 1:T:31:VAL:HG22  | 1:T:155:VAL:HG22 | 1.80                     | 0.62              |
| 1:A:11:GLN:HA    | 1:A:14:ARG:HD2   | 1.81                     | 0.62              |
| 1:R:42:VAL:HG11  | 1:R:184:ALA:HB1  | 1.82                     | 0.61              |
| 2:L:165:ARG:HG2  | 2:L:213:LEU:HD22 | 1.80                     | 0.61              |
| 1:F:53:ILE:HD12  | 1:F:209:GLU:HG2  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:18:ARG:NH2   | 4:J:401:HOH:O    | 2.33                     | 0.61              |
| 1:D:128:ALA:HB2  | 1:D:134:LYS:HB3  | 1.81                     | 0.61              |
| 1:D:9:MET:N      | 1:E:15:GLU:OE1   | 2.34                     | 0.61              |
| 1:D:35:TYR:CZ    | 1:D:177:LEU:HD23 | 2.35                     | 0.60              |
| 1:P:189:ARG:NH1  | 1:P:203:LEU:CD1  | 2.63                     | 0.60              |
| 1:R:205:VAL:HG13 | 1:R:230:LEU:HD23 | 1.84                     | 0.60              |
| 1:O:74:LEU:HD13  | 1:O:122:LEU:HD11 | 1.84                     | 0.60              |
| 2:Y:161:ASP:OD1  | 2:Y:209:ARG:NH2  | 2.34                     | 0.60              |
| 2:J:20:SER:HB3   | 2:J:28:GLY:HA3   | 1.83                     | 0.59              |
| 1:Q:31:VAL:HG12  | 1:Q:155:VAL:HG22 | 1.84                     | 0.59              |
| 1:T:110:ILE:HA   | 1:T:114:GLN:HG3  | 1.84                     | 0.59              |
| 1:E:74:LEU:HD13  | 1:E:122:LEU:HD11 | 1.85                     | 0.59              |
| 1:P:33:LEU:HD23  | 1:P:153:PHE:HB3  | 1.84                     | 0.59              |
| 1:E:164:ALA:O    | 1:E:168:LYS:HB2  | 2.03                     | 0.59              |
| 1:C:92:ARG:HB3   | 2:K:75:THR:HG21  | 1.84                     | 0.58              |
| 2:J:38:ASP:HB3   | 2:J:41:THR:OG1   | 2.03                     | 0.58              |
| 1:D:163:ILE:HG13 | 1:D:187:ALA:O    | 2.02                     | 0.58              |
| 1:O:205:VAL:HG21 | 1:O:231:GLN:HG3  | 1.84                     | 0.58              |
| 1:U:11:GLN:HA    | 1:U:14:ARG:HB2   | 1.84                     | 0.58              |
| 1:E:33:LEU:HD23  | 1:E:153:PHE:HB3  | 1.85                     | 0.58              |
| 1:O:205:VAL:HG13 | 1:O:230:LEU:HD23 | 1.85                     | 0.58              |
| 1:C:33:LEU:HD21  | 1:C:167:LEU:HD22 | 1.85                     | 0.58              |
| 1:D:87:TYR:O     | 2:K:57:ARG:NH2   | 2.36                     | 0.58              |
| 1:U:123:CYS:HA   | 1:U:139:TYR:O    | 2.05                     | 0.57              |
| 1:B:152:HIS:NE2  | 1:B:173:GLU:OE2  | 2.37                     | 0.57              |
| 1:B:53:ILE:HD12  | 1:B:209:GLU:HG2  | 1.85                     | 0.57              |
| 1:Q:97:ARG:NH2   | 1:R:49:SER:O     | 2.37                     | 0.57              |
| 1:P:225:ILE:HG21 | 1:P:233:LEU:HD12 | 1.87                     | 0.57              |
| 1:S:41:PHE:HB3   | 1:S:53:ILE:HD13  | 1.86                     | 0.57              |
| 1:U:53:ILE:HD12  | 1:U:209:GLU:HG2  | 1.87                     | 0.57              |
| 1:A:225:ILE:HG21 | 1:A:233:LEU:HD12 | 1.86                     | 0.56              |
| 1:D:92:ARG:HB3   | 2:L:75:THR:HG21  | 1.86                     | 0.56              |
| 1:R:89:TYR:CD1   | 2:Z:82:ARG:HD3   | 2.40                     | 0.56              |
| 1:G:30:VAL:HG13  | 1:G:43:ALA:HB2   | 1.86                     | 0.56              |
| 1:R:33:LEU:HD21  | 1:R:167:LEU:HD22 | 1.87                     | 0.56              |
| 2:X:64:GLU:HG2   | 2:X:68:LYS:HE2   | 1.88                     | 0.56              |
| 1:Q:60:VAL:HG11  | 1:Q:99:LEU:HD12  | 1.87                     | 0.56              |
| 1:R:30:VAL:HG13  | 1:R:43:ALA:HB2   | 1.88                     | 0.56              |
| 1:Q:110:ILE:HG23 | 1:Q:114:GLN:HG3  | 1.87                     | 0.56              |
| 1:Q:28:LYS:HD2   | 1:Q:44:GLU:HG2   | 1.88                     | 0.56              |
| 1:D:182:ARG:HA   | 1:D:185:VAL:HG22 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:31:VAL:HG12  | 1:F:155:VAL:HG12 | 1.86                     | 0.55              |
| 2:H:156:GLN:OE1  | 2:H:165:ARG:NH2  | 2.39                     | 0.55              |
| 1:O:41:PHE:HB3   | 1:O:53:ILE:HD13  | 1.88                     | 0.55              |
| 1:G:56:LEU:HG    | 1:G:62:PHE:HB2   | 1.89                     | 0.55              |
| 2:H:3:ILE:O      | 2:H:138:ALA:HA   | 2.07                     | 0.55              |
| 1:F:74:LEU:HD13  | 1:F:122:LEU:HD11 | 1.88                     | 0.55              |
| 2:H:38:ASP:OD2   | 2:H:39:ASP:N     | 2.39                     | 0.55              |
| 1:E:150:GLU:HG3  | 1:E:154:VAL:HG22 | 1.89                     | 0.55              |
| 1:P:30:VAL:HG13  | 1:P:43:ALA:HB2   | 1.89                     | 0.55              |
| 1:Q:56:LEU:HG    | 1:Q:62:PHE:HB2   | 1.89                     | 0.55              |
| 2:Y:48:THR:HG21  | 2:Y:98:LEU:HD22  | 1.88                     | 0.55              |
| 1:O:163:ILE:HD13 | 1:O:188:LEU:HA   | 1.89                     | 0.55              |
| 1:E:68:PHE:HA    | 1:E:71:PHE:CE2   | 2.42                     | 0.55              |
| 1:S:152:HIS:HB3  | 1:S:171:TYR:CZ   | 2.42                     | 0.54              |
| 2:J:38:ASP:OD2   | 2:J:79:LYS:NZ    | 2.40                     | 0.54              |
| 1:P:56:LEU:HG    | 1:P:62:PHE:HB2   | 1.89                     | 0.54              |
| 1:D:74:LEU:HD13  | 1:D:122:LEU:HD11 | 1.90                     | 0.54              |
| 1:F:162:PRO:HB2  | 1:F:190:ALA:O    | 2.07                     | 0.54              |
| 2:J:64:GLU:HG2   | 2:J:68:LYS:HE2   | 1.87                     | 0.54              |
| 1:O:153:PHE:CZ   | 1:O:167:LEU:HB3  | 2.42                     | 0.54              |
| 1:O:205:VAL:HG22 | 1:O:230:LEU:HG   | 1.89                     | 0.53              |
| 1:Q:140:ARG:NH1  | 1:Q:155:VAL:O    | 2.36                     | 0.53              |
| 1:D:99:LEU:HA    | 1:D:102:VAL:HG12 | 1.90                     | 0.53              |
| 1:F:18:GLU:OE1   | 1:F:21:ARG:NH1   | 2.41                     | 0.53              |
| 1:T:18:GLU:OE1   | 1:T:21:ARG:NH2   | 2.41                     | 0.53              |
| 1:F:164:ALA:O    | 1:F:168:LYS:HG3  | 2.09                     | 0.53              |
| 2:M:3:ILE:HB     | 2:M:139:VAL:HG12 | 1.91                     | 0.53              |
| 2:Z:20:SER:HB3   | 2:Z:28:GLY:HA3   | 1.90                     | 0.53              |
| 1:P:74:LEU:HD13  | 1:P:122:LEU:HD11 | 1.89                     | 0.52              |
| 1:O:68:PHE:HA    | 1:O:71:PHE:CE2   | 2.44                     | 0.52              |
| 1:T:9:MET:N      | 1:U:15:GLU:OE1   | 2.42                     | 0.52              |
| 1:U:32:ALA:HA    | 1:U:40:LEU:O     | 2.09                     | 0.52              |
| 1:C:16:ARG:NH1   | 1:C:114:GLN:O    | 2.38                     | 0.52              |
| 1:C:176:SER:OG   | 1:C:179:ASP:OD1  | 2.28                     | 0.52              |
| 1:O:38:GLY:HA3   | 1:O:213:LEU:O    | 2.10                     | 0.52              |
| 2:K:150:MET:O    | 2:K:154:TYR:HB2  | 2.10                     | 0.52              |
| 1:R:203:LEU:N    | 4:R:301:HOH:O    | 2.43                     | 0.52              |
| 1:C:161:GLU:OE1  | 1:C:161:GLU:N    | 2.43                     | 0.52              |
| 1:E:230:LEU:O    | 1:E:234:LEU:HD12 | 2.09                     | 0.52              |
| 1:G:33:LEU:HD23  | 1:G:153:PHE:HB3  | 1.91                     | 0.52              |
| 1:P:92:ARG:NH1   | 1:P:132:GLU:OE1  | 2.37                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:16:ARG:HB3   | 1:A:117:PRO:HG3  | 1.91                     | 0.52              |
| 1:B:9:MET:N      | 1:C:15:GLU:OE1   | 2.43                     | 0.52              |
| 1:C:87:TYR:O     | 2:J:57:ARG:NH2   | 2.42                     | 0.52              |
| 1:G:134:LYS:NZ   | 1:G:137:GLU:OE2  | 2.42                     | 0.52              |
| 2:L:88:ARG:HD3   | 2:L:126:ALA:O    | 2.10                     | 0.52              |
| 1:P:224:ARG:NH2  | 4:P:302:HOH:O    | 2.43                     | 0.52              |
| 1:S:22:LYS:O     | 1:S:26:ARG:HG3   | 2.10                     | 0.51              |
| 2:V:81:ASN:O     | 2:V:85:ILE:HG12  | 2.11                     | 0.51              |
| 1:D:205:VAL:HG13 | 1:D:230:LEU:HD23 | 1.93                     | 0.51              |
| 1:R:51:GLN:OE1   | 1:R:224:ARG:NH2  | 2.43                     | 0.51              |
| 1:O:87:TYR:OH    | 2:V:54:GLU:OE1   | 2.24                     | 0.51              |
| 1:C:150:GLU:HG3  | 1:C:154:VAL:HG22 | 1.92                     | 0.51              |
| 1:R:128:ALA:HB2  | 1:R:134:LYS:HB3  | 1.92                     | 0.51              |
| 2:H:5:ALA:HA     | 2:H:13:VAL:O     | 2.11                     | 0.51              |
| 2:X:3:ILE:HG21   | 2:X:44:GLY:HA3   | 1.91                     | 0.51              |
| 1:S:30:VAL:HG13  | 1:S:43:ALA:HB2   | 1.93                     | 0.51              |
| 1:U:56:LEU:HG    | 1:U:62:PHE:HB2   | 1.93                     | 0.51              |
| 1:P:28:LYS:HD3   | 1:P:44:GLU:HG2   | 1.92                     | 0.51              |
| 1:S:36:ALA:HB2   | 1:S:174:ASN:HA   | 1.92                     | 0.51              |
| 1:U:118:TYR:HB3  | 1:U:120:VAL:HG22 | 1.91                     | 0.51              |
| 1:C:128:ALA:HB2  | 1:C:134:LYS:HB3  | 1.93                     | 0.51              |
| 1:Q:87:TYR:O     | 2:X:57:ARG:NH1   | 2.44                     | 0.51              |
| 1:O:41:PHE:O     | 1:O:210:VAL:HA   | 2.12                     | 0.50              |
| 1:T:74:LEU:HD13  | 1:T:122:LEU:HD11 | 1.94                     | 0.50              |
| 1:R:18:GLU:OE1   | 1:R:21:ARG:NH1   | 2.35                     | 0.50              |
| 1:B:214:ASP:OD2  | 1:B:223:ARG:NH2  | 2.44                     | 0.50              |
| 2:M:1:THR:HG23   | 2:M:33:LYS:HD3   | 1.94                     | 0.50              |
| 1:C:121:GLU:HG2  | 1:C:156:MET:HG2  | 1.93                     | 0.49              |
| 1:P:118:TYR:HB3  | 1:P:120:VAL:HG22 | 1.94                     | 0.49              |
| 1:P:51:GLN:OE1   | 1:P:224:ARG:NH2  | 2.45                     | 0.49              |
| 1:S:68:PHE:HA    | 1:S:71:PHE:CE2   | 2.46                     | 0.49              |
| 1:C:167:LEU:O    | 1:C:171:TYR:N    | 2.45                     | 0.49              |
| 1:D:163:ILE:HG23 | 1:D:187:ALA:HB1  | 1.94                     | 0.49              |
| 1:O:72:ASP:O     | 1:O:76:ARG:HG3   | 2.12                     | 0.49              |
| 1:P:68:PHE:HA    | 1:P:71:PHE:CE2   | 2.48                     | 0.49              |
| 1:S:56:LEU:HG    | 1:S:62:PHE:HB2   | 1.93                     | 0.49              |
| 1:D:83:ASP:OD2   | 2:K:65:HIS:ND1   | 2.39                     | 0.49              |
| 1:O:33:LEU:HA    | 1:O:153:PHE:HB3  | 1.95                     | 0.49              |
| 1:B:9:MET:HB3    | 1:C:15:GLU:HB3   | 1.94                     | 0.49              |
| 1:C:32:ALA:HA    | 1:C:40:LEU:O     | 2.13                     | 0.49              |
| 1:E:56:LEU:HB2   | 1:E:60:VAL:HG12  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:20:SER:HB3   | 2:M:28:GLY:HA3   | 1.94                     | 0.48              |
| 1:E:58:ASP:OD1   | 1:E:91:ARG:NH1   | 2.46                     | 0.48              |
| 2:J:18:ARG:HD3   | 2:J:193:THR:HG23 | 1.96                     | 0.48              |
| 2:K:64:GLU:HG2   | 2:K:68:LYS:HE2   | 1.95                     | 0.48              |
| 1:O:97:ARG:NH1   | 1:P:49:SER:O     | 2.47                     | 0.48              |
| 1:F:164:ALA:HB1  | 1:F:168:LYS:HE2  | 1.94                     | 0.48              |
| 2:J:62:GLU:OE2   | 2:J:82:ARG:HD3   | 2.14                     | 0.48              |
| 1:O:121:GLU:HG2  | 1:O:142:THR:HA   | 1.94                     | 0.48              |
| 1:A:30:VAL:HG13  | 1:A:43:ALA:HB2   | 1.95                     | 0.48              |
| 1:R:58:ASP:OD1   | 1:R:91:ARG:NH1   | 2.46                     | 0.48              |
| 1:U:134:LYS:NZ   | 1:U:137:GLU:OE2  | 2.40                     | 0.48              |
| 1:E:72:ASP:O     | 1:E:76:ARG:HG3   | 2.13                     | 0.48              |
| 1:P:31:VAL:HG22  | 1:P:42:VAL:HG22  | 1.96                     | 0.48              |
| 1:Q:42:VAL:HG22  | 1:Q:210:VAL:HG22 | 1.95                     | 0.48              |
| 2:H:78:GLY:O     | 2:H:82:ARG:HG2   | 2.14                     | 0.48              |
| 2:I:78:GLY:O     | 2:I:82:ARG:HG2   | 2.13                     | 0.48              |
| 2:J:132:GLU:HG3  | 2:J:137:GLN:HB2  | 1.96                     | 0.48              |
| 2:X:1:THR:HG23   | 2:X:33:LYS:NZ    | 2.28                     | 0.48              |
| 1:C:178:THR:HA   | 1:C:233:LEU:HD11 | 1.95                     | 0.48              |
| 2:N:38:ASP:OD2   | 2:N:79:LYS:NZ    | 2.30                     | 0.48              |
| 1:U:121:GLU:OE2  | 1:U:140:ARG:NH2  | 2.47                     | 0.48              |
| 1:A:42:VAL:HG13  | 1:A:210:VAL:HG22 | 1.95                     | 0.48              |
| 1:B:94:VAL:HA    | 1:B:98:GLN:NE2   | 2.29                     | 0.48              |
| 1:S:54:SER:OG    | 1:S:75:ARG:HD2   | 2.13                     | 0.48              |
| 1:C:123:CYS:HA   | 1:C:139:TYR:O    | 2.14                     | 0.47              |
| 1:D:110:ILE:HA   | 1:D:114:GLN:HG3  | 1.96                     | 0.47              |
| 1:T:140:ARG:NH1  | 1:T:155:VAL:O    | 2.32                     | 0.47              |
| 1:A:98:GLN:O     | 1:A:102:VAL:HG23 | 2.14                     | 0.47              |
| 1:F:176:SER:HB3  | 1:F:179:ASP:OD1  | 2.14                     | 0.47              |
| 2:J:109:ILE:HG13 | 2:J:110:HIS:ND1  | 2.29                     | 0.47              |
| 2:M:6:LEU:HD21   | 2:M:163:GLY:O    | 2.14                     | 0.47              |
| 2:Y:18:ARG:HB3   | 2:Y:30:ASP:HA    | 1.96                     | 0.47              |
| 1:E:219:ARG:NH2  | 2:L:64:GLU:OE1   | 2.47                     | 0.47              |
| 2:X:173:ASP:OD1  | 2:X:221:ARG:NH1  | 2.36                     | 0.47              |
| 1:C:137:GLU:OE2  | 1:D:48:ARG:NH1   | 2.48                     | 0.47              |
| 1:E:83:ASP:OD2   | 2:L:65:HIS:ND1   | 2.45                     | 0.47              |
| 1:T:81:PHE:CZ    | 1:T:102:VAL:HG21 | 2.50                     | 0.47              |
| 1:A:147:ILE:HG23 | 1:B:50:LEU:HD21  | 1.97                     | 0.47              |
| 2:Y:88:ARG:HD3   | 2:Y:126:ALA:O    | 2.15                     | 0.47              |
| 1:B:31:VAL:HG23  | 1:B:155:VAL:HG22 | 1.97                     | 0.47              |
| 1:F:97:ARG:NH1   | 1:F:97:ARG:HG2   | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:56:LEU:HG    | 1:D:62:PHE:HB2   | 1.97                     | 0.47              |
| 1:F:68:PHE:HA    | 1:F:71:PHE:CE2   | 2.50                     | 0.47              |
| 1:O:130:TYR:HB2  | 1:O:218:PRO:HA   | 1.96                     | 0.47              |
| 1:Q:53:ILE:O     | 1:Q:224:ARG:NH2  | 2.46                     | 0.47              |
| 2:V:198:ASP:N    | 2:V:198:ASP:OD1  | 2.48                     | 0.47              |
| 1:A:217:ARG:HD2  | 1:A:223:ARG:HD3  | 1.96                     | 0.46              |
| 1:D:118:TYR:HB3  | 1:D:120:VAL:HG22 | 1.96                     | 0.46              |
| 1:D:10:GLU:N     | 1:E:15:GLU:OE1   | 2.34                     | 0.46              |
| 1:S:225:ILE:HG22 | 1:S:230:LEU:HB2  | 1.97                     | 0.46              |
| 1:O:24:ILE:HD13  | 1:O:121:GLU:HG3  | 1.97                     | 0.46              |
| 1:C:181:LEU:HD13 | 1:C:233:LEU:HD12 | 1.98                     | 0.46              |
| 1:D:16:ARG:NH2   | 1:D:114:GLN:O    | 2.27                     | 0.46              |
| 1:D:68:PHE:HA    | 1:D:71:PHE:CE2   | 2.50                     | 0.46              |
| 1:O:210:VAL:HG21 | 1:O:230:LEU:HD13 | 1.98                     | 0.46              |
| 1:T:68:PHE:HA    | 1:T:71:PHE:CE2   | 2.51                     | 0.46              |
| 1:E:123:CYS:HA   | 1:E:139:TYR:O    | 2.16                     | 0.46              |
| 1:D:178:THR:HG22 | 1:D:233:LEU:HG   | 1.97                     | 0.46              |
| 1:F:70:GLU:OE2   | 1:F:116:LYS:NZ   | 2.49                     | 0.46              |
| 1:P:33:LEU:HD12  | 1:P:184:ALA:HB2  | 1.98                     | 0.46              |
| 1:S:21:ARG:HD3   | 4:S:307:HOH:O    | 2.16                     | 0.46              |
| 2:Z:150:MET:O    | 2:Z:154:TYR:HB2  | 2.14                     | 0.46              |
| 1:G:68:PHE:HA    | 1:G:71:PHE:CZ    | 2.51                     | 0.46              |
| 1:B:41:PHE:HB3   | 1:B:53:ILE:HD13  | 1.96                     | 0.46              |
| 1:T:164:ALA:O    | 1:T:168:LYS:HB2  | 2.15                     | 0.46              |
| 1:F:123:CYS:HA   | 1:F:139:TYR:O    | 2.15                     | 0.46              |
| 2:K:132:GLU:HG3  | 2:K:137:GLN:HB2  | 1.97                     | 0.46              |
| 1:R:87:TYR:O     | 2:Y:57:ARG:NH2   | 2.48                     | 0.46              |
| 1:S:11:GLN:HG3   | 1:S:14:ARG:NH1   | 2.31                     | 0.46              |
| 1:U:155:VAL:HG21 | 1:U:164:ALA:HB2  | 1.98                     | 0.46              |
| 1:S:219:ARG:NH2  | 2:Z:64:GLU:OE1   | 2.40                     | 0.46              |
| 1:T:161:GLU:OE1  | 1:T:161:GLU:N    | 2.32                     | 0.46              |
| 1:G:181:LEU:O    | 1:G:185:VAL:HG23 | 2.16                     | 0.45              |
| 1:C:40:LEU:HA    | 1:C:212:VAL:HG12 | 1.97                     | 0.45              |
| 1:E:72:ASP:OD2   | 1:E:76:ARG:NH1   | 2.46                     | 0.45              |
| 1:P:163:ILE:HG12 | 1:P:191:GLY:HA3  | 1.97                     | 0.45              |
| 1:U:18:GLU:OE1   | 1:U:21:ARG:NH2   | 2.36                     | 0.45              |
| 2:Y:18:ARG:HD3   | 2:Y:193:THR:HG23 | 1.98                     | 0.45              |
| 1:G:205:VAL:HG13 | 1:G:230:LEU:HD23 | 1.97                     | 0.45              |
| 1:B:112:THR:HG22 | 1:C:115:ALA:HB3  | 1.98                     | 0.45              |
| 1:E:89:TYR:CD1   | 2:M:82:ARG:HD3   | 2.52                     | 0.45              |
| 2:W:20:SER:HB3   | 2:W:28:GLY:HA3   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:25:ALA:O     | 1:B:158:GLY:HA2  | 2.17                     | 0.45              |
| 2:H:15:ALA:HA    | 2:H:193:THR:O    | 2.17                     | 0.45              |
| 1:O:81:PHE:CZ    | 1:O:102:VAL:HG21 | 2.51                     | 0.45              |
| 1:A:123:CYS:HA   | 1:A:139:TYR:O    | 2.16                     | 0.45              |
| 1:G:92:ARG:HB3   | 2:H:75:THR:HG21  | 1.99                     | 0.45              |
| 1:U:189:ARG:O    | 1:U:191:GLY:N    | 2.48                     | 0.45              |
| 2:I:40:TYR:CZ    | 2:I:109:ILE:HD11 | 2.52                     | 0.45              |
| 1:E:92:ARG:HB3   | 2:M:75:THR:HG21  | 1.97                     | 0.45              |
| 2:N:109:ILE:HD12 | 2:N:110:HIS:CD2  | 2.52                     | 0.45              |
| 1:O:151:PRO:HB3  | 1:P:48:ARG:HH12  | 1.82                     | 0.45              |
| 1:Q:203:LEU:HD23 | 1:Q:203:LEU:HA   | 1.81                     | 0.45              |
| 1:S:178:THR:O    | 1:S:182:ARG:HD3  | 2.17                     | 0.45              |
| 2:Y:143:SER:O    | 2:Y:147:LYS:HB2  | 2.17                     | 0.45              |
| 1:F:163:ILE:HG12 | 1:F:163:ILE:H    | 1.51                     | 0.45              |
| 2:L:159:ASP:N    | 2:L:159:ASP:OD1  | 2.49                     | 0.45              |
| 2:M:37:THR:OG1   | 2:M:41:THR:HG23  | 2.16                     | 0.45              |
| 1:B:60:VAL:HG11  | 1:B:99:LEU:HD12  | 1.99                     | 0.45              |
| 1:U:205:VAL:HG21 | 1:U:231:GLN:HB2  | 1.98                     | 0.45              |
| 1:B:89:TYR:CE1   | 2:J:82:ARG:HD2   | 2.52                     | 0.44              |
| 1:F:110:ILE:HA   | 1:F:114:GLN:HG3  | 1.98                     | 0.44              |
| 1:R:68:PHE:HA    | 1:R:71:PHE:CZ    | 2.52                     | 0.44              |
| 2:H:132:GLU:HG3  | 2:H:137:GLN:HB2  | 1.99                     | 0.44              |
| 1:U:161:GLU:N    | 1:U:162:PRO:HD2  | 2.32                     | 0.44              |
| 1:E:179:ASP:O    | 1:E:183:ILE:HG22 | 2.17                     | 0.44              |
| 2:H:150:MET:O    | 2:H:154:TYR:HB2  | 2.18                     | 0.44              |
| 1:T:128:ALA:HB2  | 1:T:134:LYS:HB3  | 1.99                     | 0.44              |
| 1:C:70:GLU:HB3   | 1:C:118:TYR:CD2  | 2.52                     | 0.44              |
| 1:U:22:LYS:O     | 1:U:26:ARG:HG3   | 2.18                     | 0.44              |
| 2:V:61:VAL:O     | 2:V:65:HIS:HB2   | 2.17                     | 0.44              |
| 1:C:11:GLN:HA    | 1:C:14:ARG:CD    | 2.47                     | 0.44              |
| 2:K:13:VAL:HB    | 2:K:196:ILE:HD12 | 2.00                     | 0.44              |
| 2:N:20:SER:HB3   | 2:N:28:GLY:HA3   | 1.99                     | 0.44              |
| 1:O:97:ARG:HD3   | 1:P:49:SER:HB3   | 1.99                     | 0.44              |
| 1:S:33:LEU:HD12  | 1:S:153:PHE:HB3  | 2.00                     | 0.44              |
| 1:E:230:LEU:HG   | 1:E:234:LEU:HD11 | 2.00                     | 0.44              |
| 2:V:20:SER:HB3   | 2:V:28:GLY:HA3   | 2.00                     | 0.44              |
| 2:I:144:LEU:HA   | 2:I:144:LEU:HD23 | 1.83                     | 0.44              |
| 1:P:140:ARG:NH2  | 1:P:155:VAL:O    | 2.49                     | 0.44              |
| 1:S:172:ALA:HB3  | 1:S:175:ALA:HB2  | 2.00                     | 0.44              |
| 2:Y:162:SER:O    | 2:Y:166:VAL:HG13 | 2.17                     | 0.44              |
| 1:A:68:PHE:HA    | 1:A:71:PHE:CZ    | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:124:ASP:OD1  | 2:I:128:GLY:N    | 2.50                     | 0.43              |
| 2:M:116:SER:OG   | 2:M:116:SER:O    | 2.28                     | 0.43              |
| 2:N:88:ARG:HD3   | 2:N:126:ALA:O    | 2.18                     | 0.43              |
| 1:R:161:GLU:HB2  | 1:R:162:PRO:HD3  | 2.00                     | 0.43              |
| 1:R:56:LEU:HB2   | 1:R:60:VAL:HG12  | 2.01                     | 0.43              |
| 2:Y:164:LEU:O    | 2:Y:168:VAL:HG23 | 2.17                     | 0.43              |
| 1:R:12:ALA:O     | 1:R:16:ARG:HG3   | 2.17                     | 0.43              |
| 1:R:55:GLU:HB2   | 1:R:222:PHE:CG   | 2.53                     | 0.43              |
| 2:X:1:THR:HG23   | 2:X:33:LYS:HZ3   | 1.83                     | 0.43              |
| 2:Z:88:ARG:HD3   | 2:Z:126:ALA:O    | 2.18                     | 0.43              |
| 1:R:56:LEU:HG    | 1:R:62:PHE:HB2   | 2.01                     | 0.43              |
| 1:C:22:LYS:HD3   | 1:C:25:ALA:HB3   | 2.00                     | 0.43              |
| 1:C:220:ARG:NH2  | 2:J:67:GLU:OE1   | 2.39                     | 0.43              |
| 1:B:123:CYS:HA   | 1:B:139:TYR:O    | 2.18                     | 0.43              |
| 1:B:179:ASP:O    | 1:B:183:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:220:ARG:HH22 | 2:J:67:GLU:CD    | 2.19                     | 0.43              |
| 1:E:169:GLU:OE1  | 1:E:170:SER:OG   | 2.36                     | 0.43              |
| 1:E:33:LEU:HD21  | 1:E:167:LEU:HD22 | 1.99                     | 0.43              |
| 1:A:62:PHE:CE1   | 1:A:75:ARG:HB2   | 2.53                     | 0.43              |
| 2:I:49:ALA:HB2   | 3:I:301:M9G:C13  | 2.48                     | 0.43              |
| 1:O:210:VAL:HG23 | 1:O:225:ILE:HB   | 2.00                     | 0.43              |
| 1:C:22:LYS:HG3   | 1:C:26:ARG:NE    | 2.34                     | 0.43              |
| 1:D:35:TYR:CE2   | 1:D:177:LEU:HD23 | 2.53                     | 0.43              |
| 2:M:113:ASP:OD2  | 2:M:116:SER:N    | 2.50                     | 0.43              |
| 1:O:105:GLN:NE2  | 1:P:73:ASN:OD1   | 2.52                     | 0.43              |
| 1:A:32:ALA:HB3   | 1:A:154:VAL:HG22 | 2.00                     | 0.43              |
| 2:N:49:ALA:HB2   | 3:N:301:M9G:C13  | 2.49                     | 0.43              |
| 1:A:22:LYS:O     | 1:A:26:ARG:HG3   | 2.18                     | 0.43              |
| 1:E:9:MET:HB3    | 1:F:15:GLU:OE1   | 2.19                     | 0.43              |
| 2:J:176:ASP:OD1  | 2:W:188:ARG:NH1  | 2.52                     | 0.43              |
| 1:C:55:GLU:HB2   | 1:C:222:PHE:CG   | 2.54                     | 0.42              |
| 2:L:18:ARG:HH11  | 2:L:193:THR:CG2  | 2.32                     | 0.42              |
| 1:O:54:SER:CB    | 1:O:75:ARG:HD2   | 2.49                     | 0.42              |
| 1:Q:68:PHE:HA    | 1:Q:71:PHE:CE2   | 2.54                     | 0.42              |
| 2:V:37:THR:HG21  | 2:V:59:TYR:HD2   | 1.84                     | 0.42              |
| 2:X:20:SER:HB3   | 2:X:28:GLY:HA3   | 2.01                     | 0.42              |
| 2:J:211:ALA:O    | 2:J:215:ARG:HG3  | 2.19                     | 0.42              |
| 2:W:104:LEU:HB3  | 2:W:121:VAL:HB   | 2.01                     | 0.42              |
| 1:E:230:LEU:O    | 1:E:233:LEU:N    | 2.50                     | 0.42              |
| 2:I:156:GLN:OE1  | 2:I:165:ARG:NH2  | 2.52                     | 0.42              |
| 2:I:88:ARG:HD3   | 2:I:126:ALA:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:8:TYR:CE2    | 2:K:196:ILE:HD11 | 2.55                     | 0.42              |
| 2:X:29:ARG:NH1   | 2:Y:134:GLU:OE2  | 2.52                     | 0.42              |
| 1:A:70:GLU:HB3   | 1:A:118:TYR:CD2  | 2.54                     | 0.42              |
| 2:H:88:ARG:HD3   | 2:H:126:ALA:O    | 2.19                     | 0.42              |
| 1:B:80:GLN:HG3   | 4:B:311:HOH:O    | 2.20                     | 0.42              |
| 1:E:54:SER:CB    | 1:E:75:ARG:HD2   | 2.50                     | 0.42              |
| 2:M:47:GLY:O     | 3:M:301:M9G:N04  | 2.52                     | 0.42              |
| 1:T:32:ALA:O     | 1:T:153:PHE:HA   | 2.20                     | 0.42              |
| 2:X:83:LEU:O     | 2:X:87:VAL:HG23  | 2.20                     | 0.42              |
| 1:B:94:VAL:HA    | 1:B:98:GLN:HE21  | 1.85                     | 0.42              |
| 2:H:20:SER:HB2   | 2:H:31:VAL:HG21  | 2.01                     | 0.42              |
| 2:I:61:VAL:O     | 2:I:65:HIS:HB2   | 2.19                     | 0.42              |
| 1:C:64:ALA:HA    | 1:C:121:GLU:O    | 2.20                     | 0.42              |
| 1:G:217:ARG:HD3  | 1:G:217:ARG:HA   | 1.95                     | 0.42              |
| 1:G:89:TYR:CD1   | 2:H:82:ARG:HD3   | 2.55                     | 0.42              |
| 1:A:189:ARG:HH21 | 1:A:202:THR:N    | 2.18                     | 0.42              |
| 2:N:3:ILE:O      | 2:N:138:ALA:HA   | 2.19                     | 0.42              |
| 1:S:11:GLN:NE2   | 1:S:15:GLU:OE2   | 2.51                     | 0.42              |
| 1:U:55:GLU:HB2   | 1:U:222:PHE:CG   | 2.55                     | 0.42              |
| 1:C:150:GLU:HA   | 1:C:151:PRO:HD3  | 1.90                     | 0.42              |
| 1:F:150:GLU:HG3  | 1:F:154:VAL:HG22 | 2.02                     | 0.42              |
| 2:I:7:LYS:NZ     | 2:I:118:GLY:O    | 2.52                     | 0.42              |
| 1:O:92:ARG:HB3   | 1:O:92:ARG:HE    | 1.66                     | 0.42              |
| 1:A:164:ALA:O    | 1:A:168:LYS:HB2  | 2.20                     | 0.41              |
| 1:C:68:PHE:HA    | 1:C:71:PHE:CE2   | 2.54                     | 0.41              |
| 1:D:68:PHE:HA    | 1:D:71:PHE:CZ    | 2.55                     | 0.41              |
| 2:I:18:ARG:HD3   | 2:I:193:THR:HG23 | 2.02                     | 0.41              |
| 1:Q:180:ALA:HA   | 1:Q:183:ILE:HG22 | 2.02                     | 0.41              |
| 1:R:10:GLU:HG3   | 1:R:11:GLN:N     | 2.34                     | 0.41              |
| 1:C:181:LEU:HD21 | 1:C:234:LEU:HD23 | 2.03                     | 0.41              |
| 2:L:150:MET:O    | 2:L:154:TYR:HB2  | 2.19                     | 0.41              |
| 1:T:55:GLU:HB2   | 1:T:222:PHE:CG   | 2.55                     | 0.41              |
| 1:A:11:GLN:O     | 1:A:15:GLU:HG3   | 2.20                     | 0.41              |
| 1:A:19:LEU:HD13  | 1:G:9:MET:HG3    | 2.02                     | 0.41              |
| 1:R:67:LYS:HG2   | 1:R:69:ASN:OD1   | 2.20                     | 0.41              |
| 1:S:112:THR:HG23 | 1:T:115:ALA:HB3  | 2.02                     | 0.41              |
| 1:B:62:PHE:CE1   | 1:B:122:LEU:HD22 | 2.56                     | 0.41              |
| 1:B:30:VAL:HG13  | 1:B:43:ALA:HB2   | 2.02                     | 0.41              |
| 1:B:9:MET:HG3    | 1:C:19:LEU:HD13  | 2.01                     | 0.41              |
| 1:F:33:LEU:HD22  | 1:F:180:ALA:HB1  | 2.01                     | 0.41              |
| 2:N:165:ARG:HA   | 2:N:213:LEU:HD13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:140:ARG:HD2  | 1:G:154:VAL:HG13 | 2.01                     | 0.41              |
| 1:Q:44:GLU:OE1   | 1:Q:203:LEU:HD21 | 2.20                     | 0.41              |
| 1:T:156:MET:HE2  | 1:T:156:MET:HB2  | 1.97                     | 0.41              |
| 2:X:197:ILE:HA   | 2:X:201:GLY:O    | 2.21                     | 0.41              |
| 1:F:16:ARG:HB3   | 1:F:117:PRO:HG3  | 2.03                     | 0.41              |
| 2:N:150:MET:O    | 2:N:154:TYR:HB2  | 2.20                     | 0.41              |
| 1:O:18:GLU:O     | 1:O:22:LYS:HG3   | 2.20                     | 0.41              |
| 1:S:68:PHE:HA    | 1:S:71:PHE:CZ    | 2.56                     | 0.41              |
| 1:C:110:ILE:HG23 | 1:C:114:GLN:HG3  | 2.01                     | 0.41              |
| 1:T:142:THR:OG1  | 1:T:146:SER:HB2  | 2.20                     | 0.41              |
| 1:D:70:GLU:HB3   | 1:D:118:TYR:CD2  | 2.56                     | 0.41              |
| 1:D:159:THR:O    | 1:D:163:ILE:HD13 | 2.21                     | 0.41              |
| 2:I:211:ALA:O    | 2:I:215:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:81:PHE:CZ    | 1:A:102:VAL:HG21 | 2.56                     | 0.41              |
| 1:B:161:GLU:N    | 1:B:161:GLU:OE1  | 2.53                     | 0.41              |
| 1:D:31:VAL:HG12  | 1:D:155:VAL:HG22 | 2.02                     | 0.41              |
| 1:F:189:ARG:HG3  | 1:F:203:LEU:HD12 | 2.03                     | 0.41              |
| 1:O:62:PHE:CZ    | 1:O:64:ALA:HB2   | 2.56                     | 0.41              |
| 2:K:29:ARG:NH2   | 2:V:176:ASP:O    | 2.48                     | 0.41              |
| 2:W:83:LEU:HD21  | 2:W:102:PRO:HG3  | 2.03                     | 0.41              |
| 1:Q:89:TYR:CD1   | 2:Y:82:ARG:HD3   | 2.56                     | 0.41              |
| 2:Z:211:ALA:O    | 2:Z:215:ARG:HG2  | 2.20                     | 0.41              |
| 1:D:74:LEU:HD11  | 1:D:107:LEU:HD21 | 2.03                     | 0.41              |
| 1:O:153:PHE:HE2  | 1:O:171:TYR:HB2  | 1.86                     | 0.41              |
| 1:A:53:ILE:HD12  | 1:A:209:GLU:HG2  | 2.03                     | 0.41              |
| 1:C:56:LEU:HG    | 1:C:62:PHE:HB2   | 2.03                     | 0.41              |
| 1:E:121:GLU:HG2  | 1:E:156:MET:HG2  | 2.02                     | 0.41              |
| 2:I:197:ILE:HA   | 2:I:201:GLY:O    | 2.21                     | 0.41              |
| 2:J:61:VAL:O     | 2:J:65:HIS:HB2   | 2.21                     | 0.41              |
| 1:R:68:PHE:HA    | 1:R:71:PHE:CE2   | 2.56                     | 0.41              |
| 1:T:61:GLY:N     | 1:T:213:LEU:HD11 | 2.36                     | 0.41              |
| 1:T:20:ALA:O     | 1:T:24:ILE:HG13  | 2.21                     | 0.41              |
| 2:X:150:MET:O    | 2:X:154:TYR:HB2  | 2.21                     | 0.41              |
| 1:C:68:PHE:HA    | 1:C:71:PHE:CZ    | 2.57                     | 0.40              |
| 1:P:42:VAL:HG23  | 1:P:188:LEU:HD11 | 2.02                     | 0.40              |
| 1:D:163:ILE:HD11 | 1:D:191:GLY:HA3  | 2.03                     | 0.40              |
| 1:F:180:ALA:HA   | 1:F:183:ILE:HG22 | 2.04                     | 0.40              |
| 1:P:56:LEU:HA    | 1:P:56:LEU:HD23  | 1.88                     | 0.40              |
| 1:T:32:ALA:HA    | 1:T:40:LEU:O     | 2.21                     | 0.40              |
| 2:V:112:SER:O    | 2:V:114:PRO:HD3  | 2.22                     | 0.40              |
| 1:C:59:ARG:O     | 1:C:126:GLU:HA   | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:142:THR:OG1  | 1:C:146:SER:HB2  | 2.21                     | 0.40              |
| 2:L:157:VAL:HG22 | 2:L:163:GLY:HA2  | 2.03                     | 0.40              |
| 1:R:219:ARG:HB2  | 1:R:220:ARG:H    | 1.70                     | 0.40              |
| 1:R:61:GLY:N     | 1:R:213:LEU:HD11 | 2.36                     | 0.40              |
| 1:S:32:ALA:O     | 1:S:153:PHE:HA   | 2.21                     | 0.40              |
| 1:S:39:VAL:HB    | 1:S:213:LEU:HB2  | 2.03                     | 0.40              |
| 2:X:105:ALA:HA   | 2:X:119:ARG:O    | 2.20                     | 0.40              |
| 1:C:89:TYR:CE1   | 2:K:82:ARG:HD3   | 2.57                     | 0.40              |
| 2:H:7:LYS:HE3    | 2:H:7:LYS:HB3    | 1.88                     | 0.40              |
| 2:M:1:THR:HG21   | 2:M:46:ALA:HA    | 2.02                     | 0.40              |
| 1:O:18:GLU:OE1   | 1:O:21:ARG:NE    | 2.55                     | 0.40              |
| 1:R:180:ALA:O    | 1:R:183:ILE:HG13 | 2.21                     | 0.40              |
| 1:D:54:SER:CB    | 1:D:75:ARG:HD2   | 2.52                     | 0.40              |
| 1:E:188:LEU:HA   | 1:E:188:LEU:HD23 | 1.95                     | 0.40              |
| 1:R:44:GLU:HA    | 1:R:208:LEU:HD23 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 214/240 (89%) | 207 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | B     | 211/240 (88%) | 202 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 1   | C     | 212/240 (88%) | 202 (95%) | 10 (5%) | 0        | 100         | 100 |
| 1   | D     | 210/240 (88%) | 199 (95%) | 11 (5%) | 0        | 100         | 100 |
| 1   | E     | 213/240 (89%) | 207 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | F     | 210/240 (88%) | 207 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | G     | 212/240 (88%) | 206 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | O     | 212/240 (88%) | 206 (97%) | 6 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | P     | 215/240 (90%)   | 207 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | Q     | 211/240 (88%)   | 203 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | R     | 211/240 (88%)   | 205 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 1   | S     | 214/240 (89%)   | 206 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | T     | 213/240 (89%)   | 205 (96%)  | 7 (3%)   | 1 (0%)   | 29          | 61  |
| 1   | U     | 212/240 (88%)   | 202 (95%)  | 9 (4%)   | 1 (0%)   | 29          | 61  |
| 2   | H     | 220/234 (94%)   | 213 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 2   | I     | 220/234 (94%)   | 215 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | J     | 220/234 (94%)   | 212 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | K     | 221/234 (94%)   | 216 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | L     | 221/234 (94%)   | 215 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 2   | M     | 220/234 (94%)   | 214 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 2   | N     | 221/234 (94%)   | 215 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 2   | V     | 221/234 (94%)   | 219 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 2   | W     | 221/234 (94%)   | 217 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | X     | 220/234 (94%)   | 215 (98%)  | 4 (2%)   | 1 (0%)   | 29          | 61  |
| 2   | Y     | 221/234 (94%)   | 214 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 2   | Z     | 221/234 (94%)   | 215 (97%)  | 5 (2%)   | 1 (0%)   | 29          | 61  |
| 2   | a     | 221/234 (94%)   | 217 (98%)  | 3 (1%)   | 1 (0%)   | 29          | 61  |
| 2   | b     | 221/234 (94%)   | 215 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| All | All   | 6059/6636 (91%) | 5876 (97%) | 178 (3%) | 5 (0%)   | 51          | 82  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | U     | 190 | ALA  |
| 1   | T     | 151 | PRO  |
| 2   | a     | 9   | PRO  |
| 2   | Z     | 9   | PRO  |
| 2   | X     | 9   | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 167/184 (91%)   | 167 (100%)  | 0        | 100         | 100 |
| 1   | B     | 165/184 (90%)   | 165 (100%)  | 0        | 100         | 100 |
| 1   | C     | 165/184 (90%)   | 163 (99%)   | 2 (1%)   | 71          | 91  |
| 1   | D     | 163/184 (89%)   | 163 (100%)  | 0        | 100         | 100 |
| 1   | E     | 166/184 (90%)   | 165 (99%)   | 1 (1%)   | 86          | 96  |
| 1   | F     | 164/184 (89%)   | 162 (99%)   | 2 (1%)   | 71          | 91  |
| 1   | G     | 165/184 (90%)   | 165 (100%)  | 0        | 100         | 100 |
| 1   | O     | 165/184 (90%)   | 164 (99%)   | 1 (1%)   | 86          | 96  |
| 1   | P     | 168/184 (91%)   | 165 (98%)   | 3 (2%)   | 59          | 85  |
| 1   | Q     | 165/184 (90%)   | 164 (99%)   | 1 (1%)   | 86          | 96  |
| 1   | R     | 164/184 (89%)   | 164 (100%)  | 0        | 100         | 100 |
| 1   | S     | 167/184 (91%)   | 167 (100%)  | 0        | 100         | 100 |
| 1   | T     | 166/184 (90%)   | 165 (99%)   | 1 (1%)   | 86          | 96  |
| 1   | U     | 165/184 (90%)   | 162 (98%)   | 3 (2%)   | 59          | 85  |
| 2   | H     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | I     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | J     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | K     | 165/172 (96%)   | 163 (99%)   | 2 (1%)   | 71          | 91  |
| 2   | L     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | M     | 165/172 (96%)   | 164 (99%)   | 1 (1%)   | 86          | 96  |
| 2   | N     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | V     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | W     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | X     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | Y     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| 2   | Z     | 165/172 (96%)   | 164 (99%)   | 1 (1%)   | 86          | 96  |
| 2   | a     | 165/172 (96%)   | 163 (99%)   | 2 (1%)   | 71          | 91  |
| 2   | b     | 165/172 (96%)   | 165 (100%)  | 0        | 100         | 100 |
| All | All   | 4625/4984 (93%) | 4605 (100%) | 20 (0%)  | 91          | 97  |

All (20) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 92  | ARG  |
| 1   | C     | 103 | TYR  |
| 1   | E     | 169 | GLU  |
| 1   | F     | 91  | ARG  |
| 1   | F     | 163 | ILE  |
| 2   | K     | 122 | SER  |
| 2   | K     | 196 | ILE  |
| 2   | M     | 37  | THR  |
| 1   | O     | 163 | ILE  |
| 1   | P     | 44  | GLU  |
| 1   | P     | 161 | GLU  |
| 1   | P     | 203 | LEU  |
| 1   | Q     | 44  | GLU  |
| 1   | T     | 212 | VAL  |
| 1   | U     | 9   | MET  |
| 1   | U     | 159 | THR  |
| 1   | U     | 179 | ASP  |
| 2   | Z     | 38  | ASP  |
| 2   | a     | 196 | ILE  |
| 2   | a     | 220 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 129 | HIS  |
| 2   | b     | 22  | GLN  |

### 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 carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

14 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   | M9G  | J     | 301 | -    | 41,45,45     | 3.28 | 16 (39%) | 49,63,63    | 1.78 | 10 (20%) |
| 3   | M9G  | M     | 301 | -    | 41,45,45     | 3.30 | 16 (39%) | 49,63,63    | 1.50 | 8 (16%)  |
| 3   | M9G  | H     | 301 | -    | 41,45,45     | 3.30 | 16 (39%) | 49,63,63    | 1.56 | 7 (14%)  |
| 3   | M9G  | V     | 301 | -    | 41,45,45     | 3.29 | 16 (39%) | 49,63,63    | 1.67 | 11 (22%) |
| 3   | M9G  | I     | 301 | -    | 41,45,45     | 3.28 | 17 (41%) | 49,63,63    | 1.61 | 10 (20%) |
| 3   | M9G  | W     | 301 | -    | 41,45,45     | 3.27 | 16 (39%) | 49,63,63    | 1.63 | 9 (18%)  |
| 3   | M9G  | Z     | 301 | -    | 41,45,45     | 3.30 | 16 (39%) | 49,63,63    | 1.45 | 7 (14%)  |
| 3   | M9G  | X     | 301 | -    | 41,45,45     | 3.27 | 16 (39%) | 49,63,63    | 1.83 | 11 (22%) |
| 3   | M9G  | Y     | 301 | -    | 41,45,45     | 3.28 | 16 (39%) | 49,63,63    | 1.48 | 7 (14%)  |
| 3   | M9G  | L     | 302 | -    | 41,45,45     | 3.33 | 15 (36%) | 49,63,63    | 1.60 | 8 (16%)  |
| 3   | M9G  | b     | 301 | -    | 41,45,45     | 3.31 | 16 (39%) | 49,63,63    | 1.57 | 10 (20%) |
| 3   | M9G  | N     | 301 | -    | 41,45,45     | 3.25 | 16 (39%) | 49,63,63    | 1.57 | 6 (12%)  |
| 3   | M9G  | a     | 301 | -    | 41,45,45     | 3.29 | 16 (39%) | 49,63,63    | 1.55 | 8 (16%)  |
| 3   | M9G  | L     | 301 | -    | 41,45,45     | 3.30 | 16 (39%) | 49,63,63    | 1.56 | 9 (18%)  |

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   | M9G  | J     | 301 | -    | -       | 0/30/46/46 | 0/5/5/5 |
| 3   | M9G  | M     | 301 | -    | -       | 2/30/46/46 | 0/5/5/5 |
| 3   | M9G  | H     | 301 | -    | -       | 1/30/46/46 | 0/5/5/5 |
| 3   | M9G  | V     | 301 | -    | -       | 3/30/46/46 | 0/5/5/5 |
| 3   | M9G  | I     | 301 | -    | -       | 4/30/46/46 | 0/5/5/5 |
| 3   | M9G  | W     | 301 | -    | -       | 1/30/46/46 | 0/5/5/5 |
| 3   | M9G  | Z     | 301 | -    | -       | 0/30/46/46 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | M9G  | X     | 301 | -    | -       | 2/30/46/46 | 0/5/5/5 |
| 3   | M9G  | Y     | 301 | -    | -       | 1/30/46/46 | 0/5/5/5 |
| 3   | M9G  | L     | 302 | -    | -       | 3/30/46/46 | 0/5/5/5 |
| 3   | M9G  | b     | 301 | -    | -       | 1/30/46/46 | 0/5/5/5 |
| 3   | M9G  | N     | 301 | -    | -       | 1/30/46/46 | 0/5/5/5 |
| 3   | M9G  | a     | 301 | -    | -       | 0/30/46/46 | 0/5/5/5 |
| 3   | M9G  | L     | 301 | -    | -       | 2/30/46/46 | 0/5/5/5 |

All (224) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | L     | 302 | M9G  | C38-C31 | -9.21 | 1.30        | 1.54     |
| 3   | I     | 301 | M9G  | C38-C31 | -9.12 | 1.30        | 1.54     |
| 3   | a     | 301 | M9G  | C38-C31 | -9.12 | 1.30        | 1.54     |
| 3   | N     | 301 | M9G  | C38-C31 | -9.10 | 1.30        | 1.54     |
| 3   | L     | 301 | M9G  | C38-C31 | -9.06 | 1.30        | 1.54     |
| 3   | b     | 301 | M9G  | C38-C31 | -9.05 | 1.30        | 1.54     |
| 3   | Y     | 301 | M9G  | C38-C31 | -9.02 | 1.30        | 1.54     |
| 3   | V     | 301 | M9G  | C38-C31 | -9.02 | 1.30        | 1.54     |
| 3   | X     | 301 | M9G  | C38-C31 | -9.01 | 1.30        | 1.54     |
| 3   | M     | 301 | M9G  | C38-C31 | -9.00 | 1.30        | 1.54     |
| 3   | J     | 301 | M9G  | C38-C31 | -8.99 | 1.30        | 1.54     |
| 3   | W     | 301 | M9G  | C38-C31 | -8.99 | 1.30        | 1.54     |
| 3   | H     | 301 | M9G  | C38-C31 | -8.99 | 1.30        | 1.54     |
| 3   | Z     | 301 | M9G  | C38-C31 | -8.94 | 1.30        | 1.54     |
| 3   | L     | 301 | M9G  | C16-N15 | 8.25  | 1.52        | 1.34     |
| 3   | Y     | 301 | M9G  | C16-N15 | 8.24  | 1.52        | 1.34     |
| 3   | H     | 301 | M9G  | C16-N15 | 8.14  | 1.52        | 1.34     |
| 3   | V     | 301 | M9G  | C16-N15 | 8.11  | 1.51        | 1.34     |
| 3   | W     | 301 | M9G  | C16-N15 | 8.10  | 1.51        | 1.34     |
| 3   | L     | 302 | M9G  | C16-N15 | 8.09  | 1.51        | 1.34     |
| 3   | b     | 301 | M9G  | C16-N15 | 8.07  | 1.51        | 1.34     |
| 3   | a     | 301 | M9G  | C16-N15 | 8.06  | 1.51        | 1.34     |
| 3   | N     | 301 | M9G  | C16-N15 | 8.05  | 1.51        | 1.34     |
| 3   | M     | 301 | M9G  | C16-N15 | 8.05  | 1.51        | 1.34     |
| 3   | X     | 301 | M9G  | C16-N15 | 8.02  | 1.51        | 1.34     |
| 3   | Z     | 301 | M9G  | C16-N15 | 7.97  | 1.51        | 1.34     |
| 3   | J     | 301 | M9G  | C16-N15 | 7.95  | 1.51        | 1.34     |
| 3   | I     | 301 | M9G  | C16-N15 | 7.94  | 1.51        | 1.34     |
| 3   | Z     | 301 | M9G  | C31-N30 | 7.91  | 1.60        | 1.47     |
| 3   | L     | 302 | M9G  | C20-N19 | 7.88  | 1.51        | 1.34     |
| 3   | M     | 301 | M9G  | C31-N30 | 7.79  | 1.60        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | a     | 301 | M9G  | C20-N19 | 7.74 | 1.51        | 1.34     |
| 3   | L     | 301 | M9G  | C20-N19 | 7.73 | 1.51        | 1.34     |
| 3   | b     | 301 | M9G  | C31-N30 | 7.71 | 1.60        | 1.47     |
| 3   | b     | 301 | M9G  | C20-N19 | 7.70 | 1.50        | 1.34     |
| 3   | H     | 301 | M9G  | C20-N19 | 7.70 | 1.50        | 1.34     |
| 3   | M     | 301 | M9G  | C20-N19 | 7.68 | 1.50        | 1.34     |
| 3   | Z     | 301 | M9G  | C20-N19 | 7.63 | 1.50        | 1.34     |
| 3   | L     | 302 | M9G  | C31-N30 | 7.63 | 1.60        | 1.47     |
| 3   | V     | 301 | M9G  | C31-N30 | 7.63 | 1.60        | 1.47     |
| 3   | J     | 301 | M9G  | C31-N30 | 7.62 | 1.60        | 1.47     |
| 3   | Y     | 301 | M9G  | C20-N19 | 7.55 | 1.50        | 1.34     |
| 3   | H     | 301 | M9G  | C31-N30 | 7.54 | 1.60        | 1.47     |
| 3   | J     | 301 | M9G  | C20-N19 | 7.53 | 1.50        | 1.34     |
| 3   | X     | 301 | M9G  | C31-N30 | 7.52 | 1.60        | 1.47     |
| 3   | Y     | 301 | M9G  | C31-N30 | 7.51 | 1.59        | 1.47     |
| 3   | I     | 301 | M9G  | C31-N30 | 7.50 | 1.59        | 1.47     |
| 3   | W     | 301 | M9G  | C20-N19 | 7.50 | 1.50        | 1.34     |
| 3   | I     | 301 | M9G  | C20-N19 | 7.49 | 1.50        | 1.34     |
| 3   | N     | 301 | M9G  | C20-N19 | 7.48 | 1.50        | 1.34     |
| 3   | L     | 301 | M9G  | C31-N30 | 7.48 | 1.59        | 1.47     |
| 3   | W     | 301 | M9G  | C31-N30 | 7.46 | 1.59        | 1.47     |
| 3   | a     | 301 | M9G  | C31-N30 | 7.45 | 1.59        | 1.47     |
| 3   | V     | 301 | M9G  | C20-N19 | 7.44 | 1.50        | 1.34     |
| 3   | X     | 301 | M9G  | C20-N19 | 7.43 | 1.50        | 1.34     |
| 3   | N     | 301 | M9G  | C31-N30 | 7.28 | 1.59        | 1.47     |
| 3   | L     | 302 | M9G  | C29-N30 | 5.73 | 1.52        | 1.35     |
| 3   | Z     | 301 | M9G  | C29-N30 | 5.73 | 1.52        | 1.35     |
| 3   | W     | 301 | M9G  | C29-N30 | 5.73 | 1.52        | 1.35     |
| 3   | L     | 301 | M9G  | C29-N30 | 5.70 | 1.52        | 1.35     |
| 3   | X     | 301 | M9G  | C29-N30 | 5.68 | 1.52        | 1.35     |
| 3   | b     | 301 | M9G  | C29-N30 | 5.66 | 1.52        | 1.35     |
| 3   | M     | 301 | M9G  | C29-N30 | 5.65 | 1.52        | 1.35     |
| 3   | I     | 301 | M9G  | C29-N30 | 5.64 | 1.52        | 1.35     |
| 3   | H     | 301 | M9G  | C29-N30 | 5.63 | 1.52        | 1.35     |
| 3   | V     | 301 | M9G  | C29-N30 | 5.60 | 1.52        | 1.35     |
| 3   | J     | 301 | M9G  | C29-N30 | 5.58 | 1.52        | 1.35     |
| 3   | N     | 301 | M9G  | C29-N30 | 5.57 | 1.52        | 1.35     |
| 3   | a     | 301 | M9G  | C29-N30 | 5.52 | 1.52        | 1.35     |
| 3   | Y     | 301 | M9G  | C29-N30 | 5.47 | 1.51        | 1.35     |
| 3   | L     | 302 | M9G  | C03-C02 | 5.19 | 1.61        | 1.50     |
| 3   | H     | 301 | M9G  | C03-C02 | 5.05 | 1.60        | 1.50     |
| 3   | J     | 301 | M9G  | C03-C02 | 5.05 | 1.60        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | L     | 301 | M9G  | C03-C02 | 4.96  | 1.60        | 1.50     |
| 3   | Z     | 301 | M9G  | C32-C31 | 4.95  | 1.59        | 1.51     |
| 3   | I     | 301 | M9G  | C03-C02 | 4.94  | 1.60        | 1.50     |
| 3   | a     | 301 | M9G  | C03-C02 | 4.94  | 1.60        | 1.50     |
| 3   | J     | 301 | M9G  | C32-C31 | 4.92  | 1.59        | 1.51     |
| 3   | b     | 301 | M9G  | C03-C02 | 4.90  | 1.60        | 1.50     |
| 3   | M     | 301 | M9G  | C03-C02 | 4.88  | 1.60        | 1.50     |
| 3   | L     | 301 | M9G  | C39-C40 | -4.84 | 1.34        | 1.51     |
| 3   | V     | 301 | M9G  | C32-C31 | 4.83  | 1.59        | 1.51     |
| 3   | Y     | 301 | M9G  | C03-C02 | 4.83  | 1.60        | 1.50     |
| 3   | V     | 301 | M9G  | C03-C02 | 4.83  | 1.60        | 1.50     |
| 3   | a     | 301 | M9G  | C32-C31 | 4.81  | 1.59        | 1.51     |
| 3   | X     | 301 | M9G  | C03-C02 | 4.80  | 1.60        | 1.50     |
| 3   | M     | 301 | M9G  | C39-C40 | -4.80 | 1.35        | 1.51     |
| 3   | Z     | 301 | M9G  | C39-C40 | -4.80 | 1.35        | 1.51     |
| 3   | b     | 301 | M9G  | C39-C40 | -4.80 | 1.35        | 1.51     |
| 3   | Y     | 301 | M9G  | C39-C40 | -4.79 | 1.35        | 1.51     |
| 3   | V     | 301 | M9G  | C39-C40 | -4.74 | 1.35        | 1.51     |
| 3   | W     | 301 | M9G  | C39-C40 | -4.73 | 1.35        | 1.51     |
| 3   | I     | 301 | M9G  | C32-C31 | 4.73  | 1.59        | 1.51     |
| 3   | J     | 301 | M9G  | C39-C40 | -4.72 | 1.35        | 1.51     |
| 3   | H     | 301 | M9G  | C39-C40 | -4.72 | 1.35        | 1.51     |
| 3   | Z     | 301 | M9G  | C03-C02 | 4.72  | 1.60        | 1.50     |
| 3   | N     | 301 | M9G  | C39-C40 | -4.71 | 1.35        | 1.51     |
| 3   | L     | 302 | M9G  | C32-C31 | 4.70  | 1.59        | 1.51     |
| 3   | X     | 301 | M9G  | C39-C40 | -4.70 | 1.35        | 1.51     |
| 3   | H     | 301 | M9G  | C32-C31 | 4.69  | 1.59        | 1.51     |
| 3   | L     | 302 | M9G  | C39-C40 | -4.69 | 1.35        | 1.51     |
| 3   | W     | 301 | M9G  | C03-C02 | 4.69  | 1.60        | 1.50     |
| 3   | a     | 301 | M9G  | C39-C40 | -4.67 | 1.35        | 1.51     |
| 3   | I     | 301 | M9G  | C39-C40 | -4.66 | 1.35        | 1.51     |
| 3   | N     | 301 | M9G  | C03-C02 | 4.65  | 1.60        | 1.50     |
| 3   | W     | 301 | M9G  | C32-C31 | 4.65  | 1.58        | 1.51     |
| 3   | N     | 301 | M9G  | C32-C31 | 4.58  | 1.58        | 1.51     |
| 3   | b     | 301 | M9G  | C32-C31 | 4.57  | 1.58        | 1.51     |
| 3   | M     | 301 | M9G  | C32-C31 | 4.54  | 1.58        | 1.51     |
| 3   | Y     | 301 | M9G  | C32-C31 | 4.53  | 1.58        | 1.51     |
| 3   | X     | 301 | M9G  | C32-C31 | 4.51  | 1.58        | 1.51     |
| 3   | L     | 301 | M9G  | C32-C31 | 4.43  | 1.58        | 1.51     |
| 3   | Y     | 301 | M9G  | O41-C29 | -3.15 | 1.16        | 1.23     |
| 3   | a     | 301 | M9G  | O41-C29 | -3.11 | 1.16        | 1.23     |
| 3   | a     | 301 | M9G  | C39-C38 | 3.11  | 1.64        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | I     | 301 | M9G  | C39-C38 | 3.07  | 1.64        | 1.51     |
| 3   | N     | 301 | M9G  | C39-C38 | 3.06  | 1.64        | 1.51     |
| 3   | J     | 301 | M9G  | C39-C38 | 3.06  | 1.64        | 1.51     |
| 3   | M     | 301 | M9G  | C39-C38 | 3.05  | 1.64        | 1.51     |
| 3   | V     | 301 | M9G  | O41-C29 | -3.05 | 1.16        | 1.23     |
| 3   | Y     | 301 | M9G  | C39-C38 | 3.05  | 1.64        | 1.51     |
| 3   | V     | 301 | M9G  | C39-C38 | 3.05  | 1.64        | 1.51     |
| 3   | W     | 301 | M9G  | C39-C38 | 3.04  | 1.64        | 1.51     |
| 3   | X     | 301 | M9G  | C39-C38 | 3.04  | 1.64        | 1.51     |
| 3   | H     | 301 | M9G  | C39-C38 | 3.04  | 1.64        | 1.51     |
| 3   | L     | 302 | M9G  | C39-C38 | 3.03  | 1.64        | 1.51     |
| 3   | b     | 301 | M9G  | O41-C29 | -3.03 | 1.16        | 1.23     |
| 3   | L     | 301 | M9G  | C39-C38 | 3.03  | 1.64        | 1.51     |
| 3   | b     | 301 | M9G  | C39-C38 | 3.02  | 1.64        | 1.51     |
| 3   | I     | 301 | M9G  | O41-C29 | -3.02 | 1.16        | 1.23     |
| 3   | H     | 301 | M9G  | O41-C29 | -3.01 | 1.16        | 1.23     |
| 3   | M     | 301 | M9G  | O41-C29 | -3.01 | 1.16        | 1.23     |
| 3   | Z     | 301 | M9G  | C39-C38 | 3.01  | 1.64        | 1.51     |
| 3   | N     | 301 | M9G  | C06-C05 | -2.99 | 1.41        | 1.48     |
| 3   | N     | 301 | M9G  | O41-C29 | -2.98 | 1.16        | 1.23     |
| 3   | b     | 301 | M9G  | C06-C05 | -2.97 | 1.41        | 1.48     |
| 3   | W     | 301 | M9G  | O41-C29 | -2.96 | 1.16        | 1.23     |
| 3   | L     | 301 | M9G  | O41-C29 | -2.95 | 1.16        | 1.23     |
| 3   | X     | 301 | M9G  | O41-C29 | -2.95 | 1.16        | 1.23     |
| 3   | V     | 301 | M9G  | C06-C05 | -2.95 | 1.41        | 1.48     |
| 3   | J     | 301 | M9G  | O41-C29 | -2.92 | 1.16        | 1.23     |
| 3   | L     | 302 | M9G  | O41-C29 | -2.91 | 1.16        | 1.23     |
| 3   | Y     | 301 | M9G  | C26-C25 | 2.89  | 1.52        | 1.48     |
| 3   | W     | 301 | M9G  | C06-C05 | -2.89 | 1.41        | 1.48     |
| 3   | Z     | 301 | M9G  | O41-C29 | -2.88 | 1.16        | 1.23     |
| 3   | Z     | 301 | M9G  | C06-C05 | -2.87 | 1.41        | 1.48     |
| 3   | a     | 301 | M9G  | C06-C05 | -2.87 | 1.41        | 1.48     |
| 3   | L     | 302 | M9G  | C40-N30 | 2.86  | 1.53        | 1.47     |
| 3   | H     | 301 | M9G  | C28-C29 | 2.84  | 1.56        | 1.51     |
| 3   | J     | 301 | M9G  | C06-C05 | -2.84 | 1.41        | 1.48     |
| 3   | N     | 301 | M9G  | C40-N30 | 2.84  | 1.53        | 1.47     |
| 3   | X     | 301 | M9G  | C06-C05 | -2.83 | 1.41        | 1.48     |
| 3   | I     | 301 | M9G  | C06-C05 | -2.83 | 1.41        | 1.48     |
| 3   | Y     | 301 | M9G  | C06-C05 | -2.83 | 1.41        | 1.48     |
| 3   | H     | 301 | M9G  | C40-N30 | 2.82  | 1.53        | 1.47     |
| 3   | M     | 301 | M9G  | C26-C25 | 2.82  | 1.51        | 1.48     |
| 3   | L     | 301 | M9G  | C26-C25 | 2.82  | 1.51        | 1.48     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | a     | 301 | M9G  | C26-C25 | 2.81  | 1.51        | 1.48     |
| 3   | L     | 302 | M9G  | C06-C05 | -2.80 | 1.41        | 1.48     |
| 3   | W     | 301 | M9G  | C40-N30 | 2.80  | 1.53        | 1.47     |
| 3   | H     | 301 | M9G  | C06-C05 | -2.80 | 1.41        | 1.48     |
| 3   | L     | 302 | M9G  | C28-C29 | 2.79  | 1.56        | 1.51     |
| 3   | X     | 301 | M9G  | C40-N30 | 2.79  | 1.53        | 1.47     |
| 3   | M     | 301 | M9G  | C06-C05 | -2.79 | 1.41        | 1.48     |
| 3   | Z     | 301 | M9G  | C40-N30 | 2.78  | 1.53        | 1.47     |
| 3   | J     | 301 | M9G  | C40-N30 | 2.78  | 1.53        | 1.47     |
| 3   | L     | 301 | M9G  | C40-N30 | 2.78  | 1.53        | 1.47     |
| 3   | J     | 301 | M9G  | C26-C25 | 2.78  | 1.51        | 1.48     |
| 3   | L     | 302 | M9G  | C26-C25 | 2.77  | 1.51        | 1.48     |
| 3   | I     | 301 | M9G  | C26-C25 | 2.76  | 1.51        | 1.48     |
| 3   | a     | 301 | M9G  | C40-N30 | 2.75  | 1.52        | 1.47     |
| 3   | X     | 301 | M9G  | C26-C25 | 2.75  | 1.51        | 1.48     |
| 3   | X     | 301 | M9G  | C28-C29 | 2.75  | 1.56        | 1.51     |
| 3   | W     | 301 | M9G  | C26-C25 | 2.74  | 1.51        | 1.48     |
| 3   | I     | 301 | M9G  | C40-N30 | 2.74  | 1.52        | 1.47     |
| 3   | H     | 301 | M9G  | C26-C25 | 2.74  | 1.51        | 1.48     |
| 3   | V     | 301 | M9G  | C40-N30 | 2.73  | 1.52        | 1.47     |
| 3   | L     | 301 | M9G  | C28-C29 | 2.73  | 1.56        | 1.51     |
| 3   | V     | 301 | M9G  | C26-C25 | 2.72  | 1.51        | 1.48     |
| 3   | b     | 301 | M9G  | C26-C25 | 2.71  | 1.51        | 1.48     |
| 3   | W     | 301 | M9G  | C28-C29 | 2.71  | 1.56        | 1.51     |
| 3   | Z     | 301 | M9G  | C26-C25 | 2.70  | 1.51        | 1.48     |
| 3   | I     | 301 | M9G  | C28-C29 | 2.70  | 1.56        | 1.51     |
| 3   | b     | 301 | M9G  | C28-C29 | 2.70  | 1.56        | 1.51     |
| 3   | L     | 301 | M9G  | C06-C05 | -2.69 | 1.41        | 1.48     |
| 3   | b     | 301 | M9G  | C40-N30 | 2.69  | 1.52        | 1.47     |
| 3   | Y     | 301 | M9G  | C40-N30 | 2.67  | 1.52        | 1.47     |
| 3   | N     | 301 | M9G  | C26-C25 | 2.66  | 1.51        | 1.48     |
| 3   | M     | 301 | M9G  | C40-N30 | 2.65  | 1.52        | 1.47     |
| 3   | Z     | 301 | M9G  | C28-C29 | 2.64  | 1.56        | 1.51     |
| 3   | H     | 301 | M9G  | C13-C05 | 2.61  | 1.42        | 1.37     |
| 3   | J     | 301 | M9G  | C13-C05 | 2.59  | 1.42        | 1.37     |
| 3   | L     | 302 | M9G  | C13-C05 | 2.58  | 1.42        | 1.37     |
| 3   | Y     | 301 | M9G  | C28-C29 | 2.57  | 1.56        | 1.51     |
| 3   | V     | 301 | M9G  | C28-C29 | 2.56  | 1.56        | 1.51     |
| 3   | I     | 301 | M9G  | C13-C05 | 2.55  | 1.42        | 1.37     |
| 3   | a     | 301 | M9G  | C13-C05 | 2.53  | 1.42        | 1.37     |
| 3   | W     | 301 | M9G  | C13-C05 | 2.53  | 1.42        | 1.37     |
| 3   | b     | 301 | M9G  | C13-C05 | 2.53  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | L     | 301 | M9G  | C13-C05 | 2.51  | 1.42        | 1.37     |
| 3   | X     | 301 | M9G  | C13-C05 | 2.50  | 1.42        | 1.37     |
| 3   | M     | 301 | M9G  | C28-C29 | 2.50  | 1.56        | 1.51     |
| 3   | Y     | 301 | M9G  | C13-C05 | 2.50  | 1.42        | 1.37     |
| 3   | Z     | 301 | M9G  | C13-C05 | 2.50  | 1.42        | 1.37     |
| 3   | a     | 301 | M9G  | C28-C29 | 2.50  | 1.56        | 1.51     |
| 3   | N     | 301 | M9G  | C13-C05 | 2.48  | 1.42        | 1.37     |
| 3   | N     | 301 | M9G  | C28-C29 | 2.48  | 1.56        | 1.51     |
| 3   | M     | 301 | M9G  | C13-C05 | 2.47  | 1.42        | 1.37     |
| 3   | J     | 301 | M9G  | C28-C29 | 2.44  | 1.56        | 1.51     |
| 3   | M     | 301 | M9G  | C13-N14 | -2.39 | 1.32        | 1.36     |
| 3   | L     | 301 | M9G  | C13-N14 | -2.39 | 1.32        | 1.36     |
| 3   | Y     | 301 | M9G  | C13-N14 | -2.39 | 1.32        | 1.36     |
| 3   | V     | 301 | M9G  | C13-C05 | 2.38  | 1.41        | 1.37     |
| 3   | Z     | 301 | M9G  | C13-N14 | -2.36 | 1.32        | 1.36     |
| 3   | X     | 301 | M9G  | C13-N14 | -2.32 | 1.32        | 1.36     |
| 3   | W     | 301 | M9G  | C13-N14 | -2.29 | 1.32        | 1.36     |
| 3   | H     | 301 | M9G  | C13-N14 | -2.26 | 1.32        | 1.36     |
| 3   | I     | 301 | M9G  | C13-N14 | -2.24 | 1.32        | 1.36     |
| 3   | V     | 301 | M9G  | C13-N14 | -2.24 | 1.32        | 1.36     |
| 3   | b     | 301 | M9G  | C13-N14 | -2.20 | 1.33        | 1.36     |
| 3   | a     | 301 | M9G  | C13-N14 | -2.17 | 1.33        | 1.36     |
| 3   | J     | 301 | M9G  | C13-N14 | -2.17 | 1.33        | 1.36     |
| 3   | N     | 301 | M9G  | C13-N14 | -2.12 | 1.33        | 1.36     |
| 3   | I     | 301 | M9G  | C18-N19 | -2.04 | 1.41        | 1.45     |

All (121) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | Z     | 301 | M9G  | C40-N30-C31 | -5.39 | 105.57      | 111.83   |
| 3   | X     | 301 | M9G  | C40-N30-C31 | -5.23 | 105.76      | 111.83   |
| 3   | M     | 301 | M9G  | C40-N30-C31 | -5.15 | 105.85      | 111.83   |
| 3   | J     | 301 | M9G  | C40-N30-C31 | -5.12 | 105.88      | 111.83   |
| 3   | L     | 301 | M9G  | C40-N30-C31 | -5.09 | 105.92      | 111.83   |
| 3   | V     | 301 | M9G  | C40-N30-C31 | -5.05 | 105.97      | 111.83   |
| 3   | W     | 301 | M9G  | C40-N30-C31 | -5.02 | 106.00      | 111.83   |
| 3   | b     | 301 | M9G  | C40-N30-C31 | -5.00 | 106.03      | 111.83   |
| 3   | L     | 302 | M9G  | C40-N30-C31 | -4.77 | 106.28      | 111.83   |
| 3   | J     | 301 | M9G  | C22-C20-N19 | 4.74  | 124.00      | 115.20   |
| 3   | W     | 301 | M9G  | C38-C31-N30 | 4.59  | 107.21      | 101.94   |
| 3   | I     | 301 | M9G  | C40-N30-C31 | -4.59 | 106.50      | 111.83   |
| 3   | H     | 301 | M9G  | C40-N30-C31 | -4.54 | 106.56      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | X     | 301 | M9G  | C38-C31-N30 | 4.53  | 107.14      | 101.94   |
| 3   | N     | 301 | M9G  | C38-C31-N30 | 4.51  | 107.11      | 101.94   |
| 3   | L     | 302 | M9G  | C18-C28-C29 | 4.42  | 120.98      | 112.25   |
| 3   | L     | 301 | M9G  | C38-C31-N30 | 4.38  | 106.96      | 101.94   |
| 3   | Y     | 301 | M9G  | C40-N30-C31 | -4.36 | 106.77      | 111.83   |
| 3   | I     | 301 | M9G  | C38-C31-N30 | 4.32  | 106.90      | 101.94   |
| 3   | N     | 301 | M9G  | C40-N30-C31 | -4.28 | 106.86      | 111.83   |
| 3   | V     | 301 | M9G  | C38-C31-N30 | 4.25  | 106.81      | 101.94   |
| 3   | Y     | 301 | M9G  | C38-C31-N30 | 4.21  | 106.77      | 101.94   |
| 3   | H     | 301 | M9G  | C38-C31-N30 | 4.19  | 106.75      | 101.94   |
| 3   | M     | 301 | M9G  | C38-C31-N30 | 4.15  | 106.71      | 101.94   |
| 3   | L     | 302 | M9G  | C38-C31-N30 | 4.14  | 106.69      | 101.94   |
| 3   | a     | 301 | M9G  | C40-N30-C31 | -4.14 | 107.02      | 111.83   |
| 3   | b     | 301 | M9G  | C38-C31-N30 | 3.98  | 106.50      | 101.94   |
| 3   | I     | 301 | M9G  | C18-C28-C29 | 3.86  | 119.89      | 112.25   |
| 3   | J     | 301 | M9G  | C38-C31-N30 | 3.81  | 106.32      | 101.94   |
| 3   | X     | 301 | M9G  | C22-C20-N19 | 3.79  | 122.24      | 115.20   |
| 3   | a     | 301 | M9G  | C38-C31-N30 | 3.75  | 106.24      | 101.94   |
| 3   | J     | 301 | M9G  | C18-N19-C20 | -3.72 | 112.50      | 121.60   |
| 3   | Z     | 301 | M9G  | C38-C31-N30 | 3.63  | 106.11      | 101.94   |
| 3   | N     | 301 | M9G  | C09-C07-C06 | -3.58 | 118.92      | 123.30   |
| 3   | X     | 301 | M9G  | C02-N15-C16 | -3.54 | 117.95      | 122.93   |
| 3   | b     | 301 | M9G  | C09-C07-C06 | -3.52 | 119.00      | 123.30   |
| 3   | V     | 301 | M9G  | C09-C07-C06 | -3.51 | 119.01      | 123.30   |
| 3   | H     | 301 | M9G  | C18-C28-C29 | 3.42  | 119.00      | 112.25   |
| 3   | J     | 301 | M9G  | C09-C07-C06 | -3.41 | 119.14      | 123.30   |
| 3   | a     | 301 | M9G  | C18-C28-C29 | 3.36  | 118.89      | 112.25   |
| 3   | X     | 301 | M9G  | C18-C28-C29 | 3.36  | 118.89      | 112.25   |
| 3   | X     | 301 | M9G  | C09-C07-C06 | -3.35 | 119.21      | 123.30   |
| 3   | W     | 301 | M9G  | C09-C07-C06 | -3.33 | 119.23      | 123.30   |
| 3   | H     | 301 | M9G  | C09-C07-C06 | -3.25 | 119.33      | 123.30   |
| 3   | Z     | 301 | M9G  | C09-C07-C06 | -3.22 | 119.36      | 123.30   |
| 3   | a     | 301 | M9G  | C09-C07-C06 | -3.22 | 119.37      | 123.30   |
| 3   | J     | 301 | M9G  | C18-C28-C29 | 3.20  | 118.58      | 112.25   |
| 3   | V     | 301 | M9G  | C12-C06-C07 | 3.18  | 120.69      | 116.10   |
| 3   | I     | 301 | M9G  | C09-C07-C06 | -3.12 | 119.48      | 123.30   |
| 3   | I     | 301 | M9G  | C02-N15-C16 | -3.11 | 118.56      | 122.93   |
| 3   | N     | 301 | M9G  | C12-C06-C07 | 3.09  | 120.56      | 116.10   |
| 3   | a     | 301 | M9G  | C22-C20-N19 | 3.09  | 120.93      | 115.20   |
| 3   | V     | 301 | M9G  | C22-C20-N19 | 3.07  | 120.90      | 115.20   |
| 3   | X     | 301 | M9G  | C18-N19-C20 | -3.01 | 114.23      | 121.60   |
| 3   | b     | 301 | M9G  | C12-C06-C07 | 3.01  | 120.44      | 116.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | L     | 302 | M9G  | C09-C07-C06 | -2.98 | 119.66      | 123.30   |
| 3   | Y     | 301 | M9G  | C09-C07-C06 | -2.98 | 119.66      | 123.30   |
| 3   | N     | 301 | M9G  | C32-C31-N30 | -2.97 | 107.66      | 112.99   |
| 3   | M     | 301 | M9G  | C09-C07-C06 | -2.93 | 119.71      | 123.30   |
| 3   | X     | 301 | M9G  | C12-C06-C07 | 2.92  | 120.31      | 116.10   |
| 3   | L     | 301 | M9G  | C18-C28-C29 | 2.90  | 117.99      | 112.25   |
| 3   | W     | 301 | M9G  | C12-C06-C07 | 2.88  | 120.25      | 116.10   |
| 3   | Z     | 301 | M9G  | C12-C06-C07 | 2.87  | 120.24      | 116.10   |
| 3   | a     | 301 | M9G  | C12-C06-C07 | 2.83  | 120.18      | 116.10   |
| 3   | J     | 301 | M9G  | C12-C06-C07 | 2.80  | 120.14      | 116.10   |
| 3   | W     | 301 | M9G  | C02-N15-C16 | -2.79 | 119.01      | 122.93   |
| 3   | H     | 301 | M9G  | C12-C06-C07 | 2.78  | 120.11      | 116.10   |
| 3   | L     | 302 | M9G  | C12-C06-C07 | 2.78  | 120.10      | 116.10   |
| 3   | W     | 301 | M9G  | C32-C31-N30 | -2.74 | 108.06      | 112.99   |
| 3   | I     | 301 | M9G  | C12-C06-C07 | 2.72  | 120.02      | 116.10   |
| 3   | L     | 301 | M9G  | C22-C20-N19 | 2.67  | 120.16      | 115.20   |
| 3   | Y     | 301 | M9G  | C12-C06-C07 | 2.66  | 119.94      | 116.10   |
| 3   | L     | 301 | M9G  | C12-C06-C07 | 2.65  | 119.93      | 116.10   |
| 3   | L     | 301 | M9G  | C09-C07-C06 | -2.64 | 120.07      | 123.30   |
| 3   | L     | 302 | M9G  | C22-C20-N19 | 2.63  | 120.08      | 115.20   |
| 3   | J     | 301 | M9G  | O21-C20-N19 | -2.62 | 117.62      | 122.45   |
| 3   | H     | 301 | M9G  | C02-N15-C16 | -2.62 | 119.25      | 122.93   |
| 3   | M     | 301 | M9G  | C02-N15-C16 | -2.62 | 119.25      | 122.93   |
| 3   | V     | 301 | M9G  | C18-N19-C20 | -2.57 | 115.31      | 121.60   |
| 3   | X     | 301 | M9G  | C38-C31-C32 | -2.56 | 108.66      | 113.61   |
| 3   | X     | 301 | M9G  | C32-C31-N30 | -2.54 | 108.42      | 112.99   |
| 3   | M     | 301 | M9G  | C38-C31-C32 | -2.54 | 108.69      | 113.61   |
| 3   | L     | 301 | M9G  | C38-C31-C32 | -2.53 | 108.71      | 113.61   |
| 3   | J     | 301 | M9G  | C02-N15-C16 | -2.50 | 119.41      | 122.93   |
| 3   | M     | 301 | M9G  | C12-C06-C07 | 2.50  | 119.71      | 116.10   |
| 3   | X     | 301 | M9G  | O21-C20-N19 | -2.47 | 117.90      | 122.45   |
| 3   | H     | 301 | M9G  | C38-C31-C32 | -2.45 | 108.87      | 113.61   |
| 3   | V     | 301 | M9G  | C18-C28-C29 | 2.43  | 117.06      | 112.25   |
| 3   | b     | 301 | M9G  | C18-C28-C29 | 2.42  | 117.03      | 112.25   |
| 3   | M     | 301 | M9G  | C18-C28-C29 | 2.40  | 117.00      | 112.25   |
| 3   | Y     | 301 | M9G  | C38-C31-C32 | -2.39 | 108.98      | 113.61   |
| 3   | b     | 301 | M9G  | C02-N15-C16 | -2.39 | 119.58      | 122.93   |
| 3   | a     | 301 | M9G  | C28-C18-C16 | -2.37 | 104.83      | 110.42   |
| 3   | M     | 301 | M9G  | C31-N30-C29 | 2.36  | 127.93      | 120.83   |
| 3   | a     | 301 | M9G  | C38-C31-C32 | -2.36 | 109.04      | 113.61   |
| 3   | V     | 301 | M9G  | O21-C20-N19 | -2.35 | 118.13      | 122.45   |
| 3   | Z     | 301 | M9G  | C18-C28-C29 | 2.34  | 116.87      | 112.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | N     | 301 | M9G  | C38-C31-C32 | -2.33 | 109.09      | 113.61   |
| 3   | L     | 302 | M9G  | C02-N15-C16 | -2.32 | 119.67      | 122.93   |
| 3   | W     | 301 | M9G  | C22-C20-N19 | 2.31  | 119.50      | 115.20   |
| 3   | J     | 301 | M9G  | C38-C31-C32 | -2.29 | 109.17      | 113.61   |
| 3   | b     | 301 | M9G  | C38-C31-C32 | -2.28 | 109.20      | 113.61   |
| 3   | Y     | 301 | M9G  | C18-C28-C29 | 2.28  | 116.75      | 112.25   |
| 3   | Z     | 301 | M9G  | C38-C31-C32 | -2.27 | 109.20      | 113.61   |
| 3   | W     | 301 | M9G  | C18-C28-C29 | 2.26  | 116.72      | 112.25   |
| 3   | V     | 301 | M9G  | C32-C31-N30 | -2.26 | 108.94      | 112.99   |
| 3   | L     | 302 | M9G  | C32-C31-N30 | -2.24 | 108.97      | 112.99   |
| 3   | b     | 301 | M9G  | C31-N30-C29 | 2.22  | 127.50      | 120.83   |
| 3   | Z     | 301 | M9G  | C31-N30-C29 | 2.22  | 127.50      | 120.83   |
| 3   | I     | 301 | M9G  | C38-C31-C32 | -2.17 | 109.40      | 113.61   |
| 3   | I     | 301 | M9G  | C39-C40-N30 | 2.15  | 107.03      | 103.25   |
| 3   | V     | 301 | M9G  | C38-C31-C32 | -2.15 | 109.44      | 113.61   |
| 3   | I     | 301 | M9G  | C28-C18-C16 | -2.11 | 105.46      | 110.42   |
| 3   | L     | 301 | M9G  | C32-C31-N30 | -2.09 | 109.23      | 112.99   |
| 3   | L     | 301 | M9G  | C31-N30-C29 | 2.07  | 127.05      | 120.83   |
| 3   | W     | 301 | M9G  | C38-C31-C32 | -2.06 | 109.62      | 113.61   |
| 3   | b     | 301 | M9G  | C22-C20-N19 | 2.05  | 119.02      | 115.20   |
| 3   | V     | 301 | M9G  | C02-N15-C16 | -2.05 | 120.05      | 122.93   |
| 3   | Y     | 301 | M9G  | C01-C02-C03 | -2.03 | 108.61      | 110.95   |
| 3   | b     | 301 | M9G  | C32-C31-N30 | -2.03 | 109.34      | 112.99   |
| 3   | I     | 301 | M9G  | C32-C31-N30 | -2.02 | 109.36      | 112.99   |

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | V     | 301 | M9G  | O21-C20-C22-C27 |
| 3   | X     | 301 | M9G  | O21-C20-C22-C27 |
| 3   | I     | 301 | M9G  | C13-C05-C06-C07 |
| 3   | L     | 302 | M9G  | C13-C05-C06-C12 |
| 3   | L     | 302 | M9G  | N04-C05-C06-C12 |
| 3   | b     | 301 | M9G  | C13-C05-C06-C07 |
| 3   | N     | 301 | M9G  | C13-C05-C06-C07 |
| 3   | V     | 301 | M9G  | C18-C28-C29-O41 |
| 3   | V     | 301 | M9G  | C18-C28-C29-N30 |
| 3   | I     | 301 | M9G  | O17-C16-C18-N19 |
| 3   | W     | 301 | M9G  | O17-C16-C18-N19 |
| 3   | M     | 301 | M9G  | O21-C20-C22-C27 |
| 3   | H     | 301 | M9G  | O21-C20-C22-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | I     | 301 | M9G  | O21-C20-C22-C27 |
| 3   | Y     | 301 | M9G  | O21-C20-C22-C27 |
| 3   | L     | 302 | M9G  | O21-C20-C22-C27 |
| 3   | L     | 301 | M9G  | O21-C20-C22-C27 |
| 3   | M     | 301 | M9G  | O17-C16-C18-N19 |
| 3   | X     | 301 | M9G  | O17-C16-C18-N19 |
| 3   | L     | 301 | M9G  | O17-C16-C18-N19 |
| 3   | I     | 301 | M9G  | N15-C16-C18-N19 |

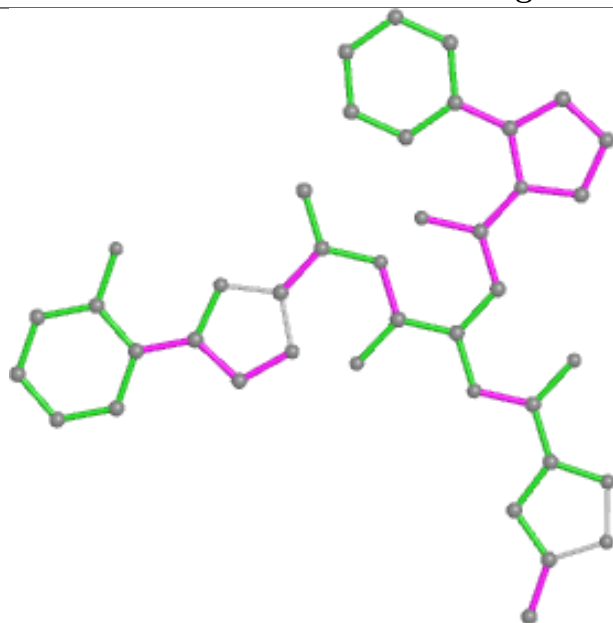
There are no ring outliers.

3 monomers are involved in 3 short contacts:

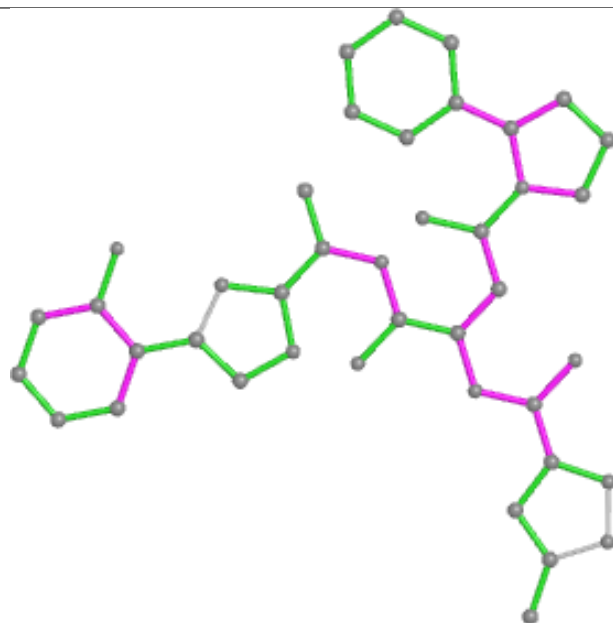
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | M     | 301 | M9G  | 1       | 0            |
| 3   | I     | 301 | M9G  | 1       | 0            |
| 3   | N     | 301 | M9G  | 1       | 0            |

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.

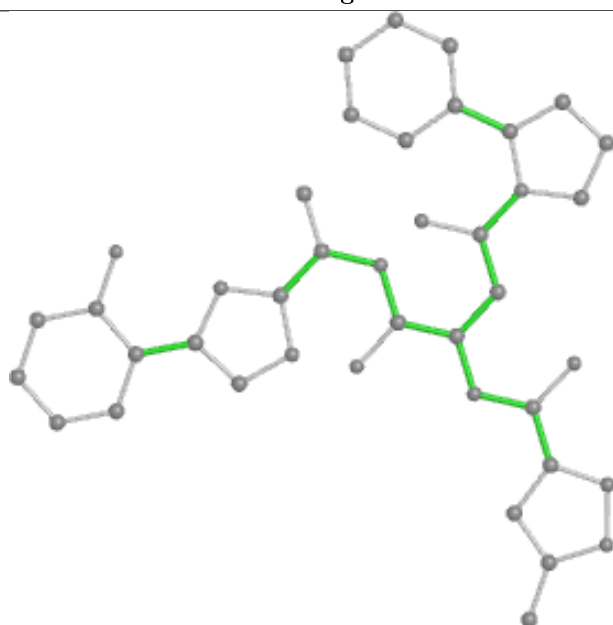
## Ligand M9G J 301



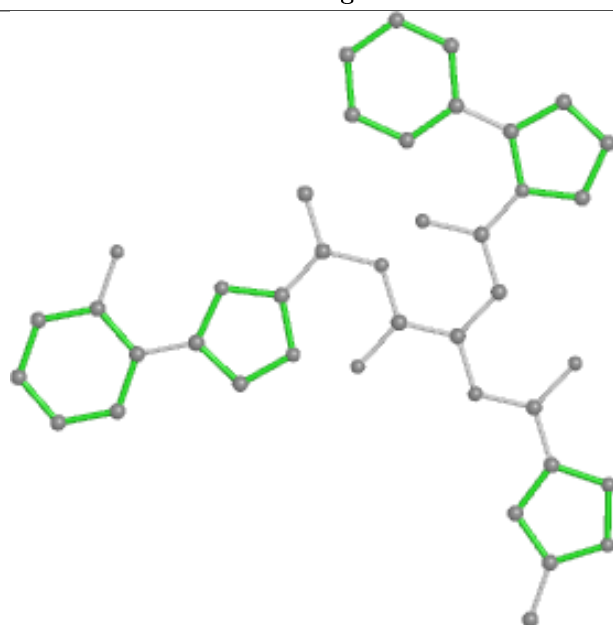
Bond lengths



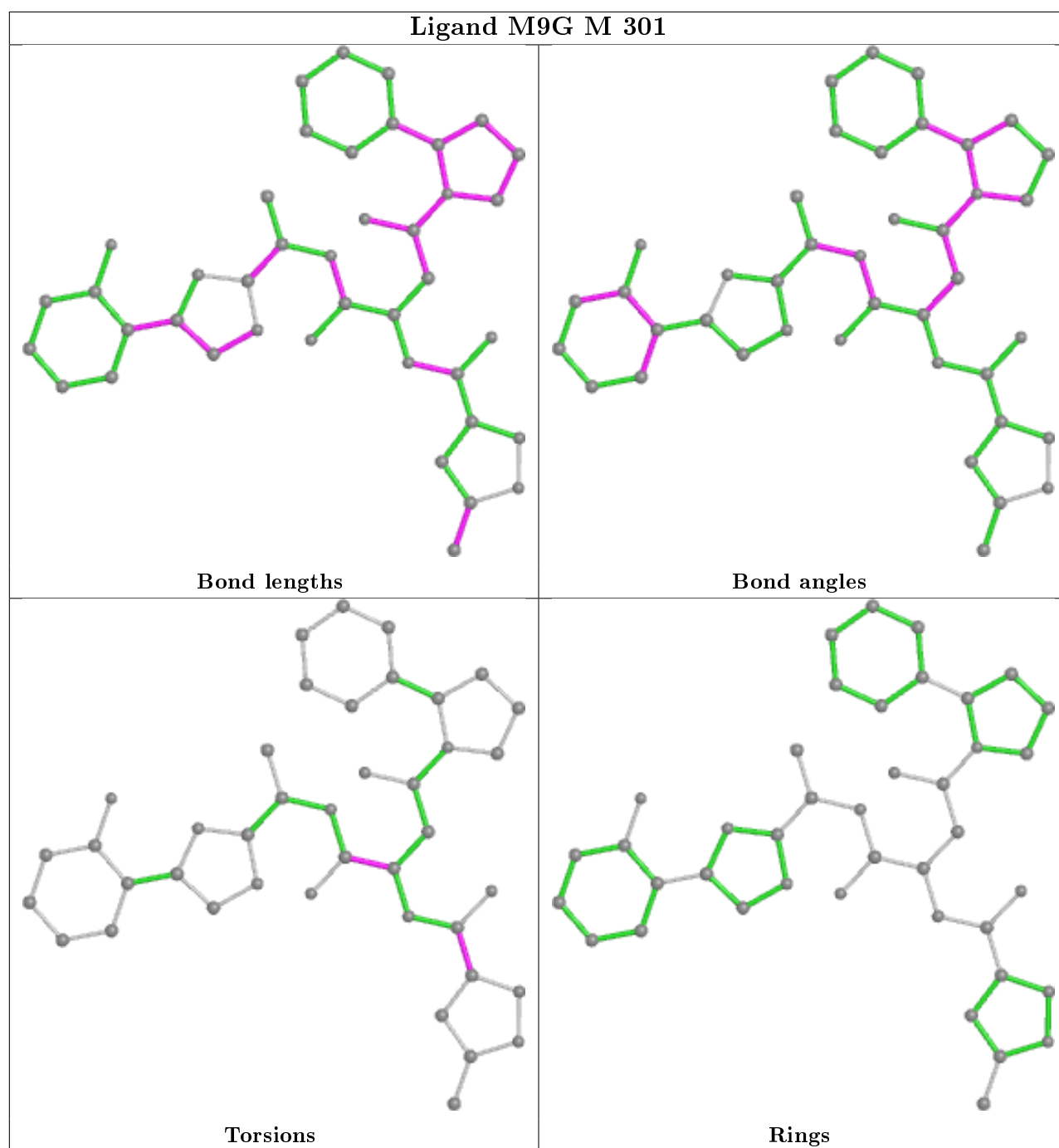
Bond angles

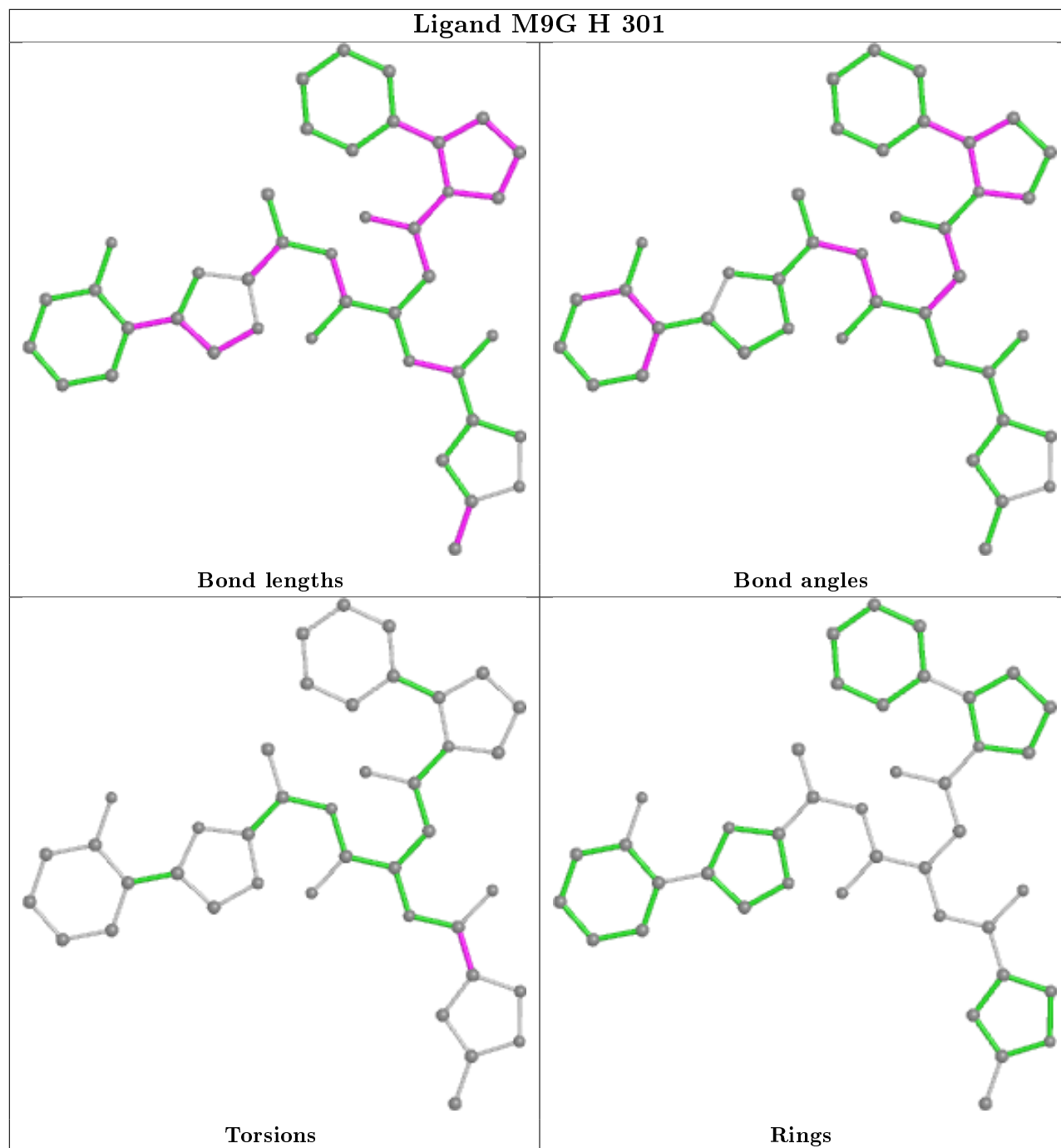


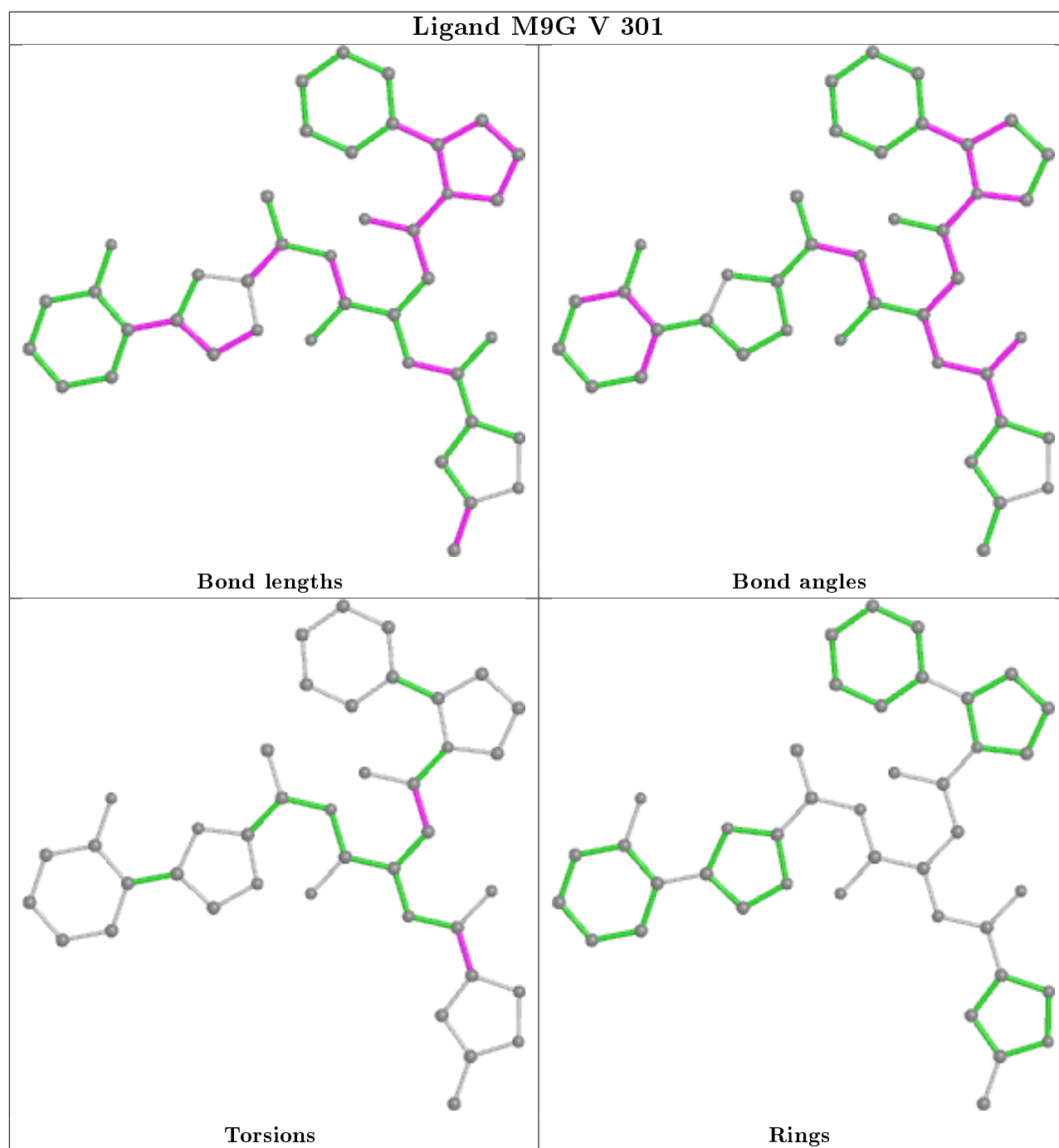
Torsions



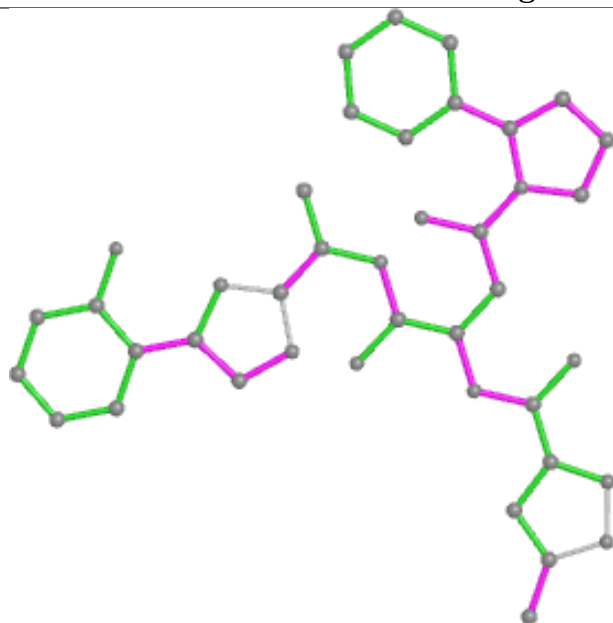
Rings



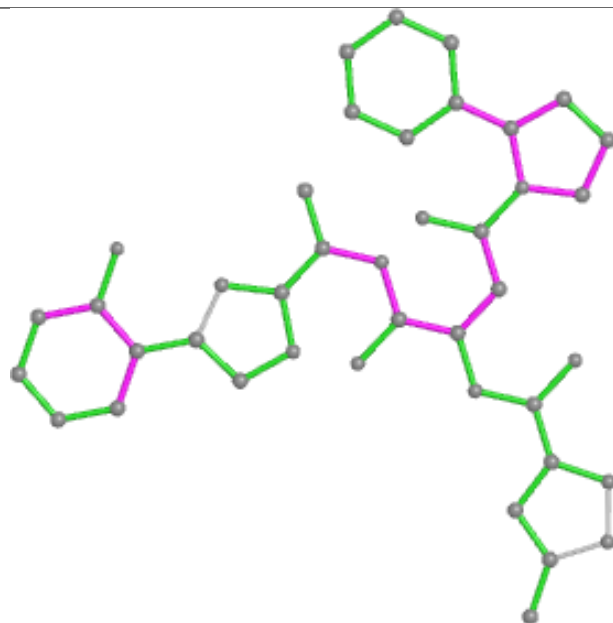




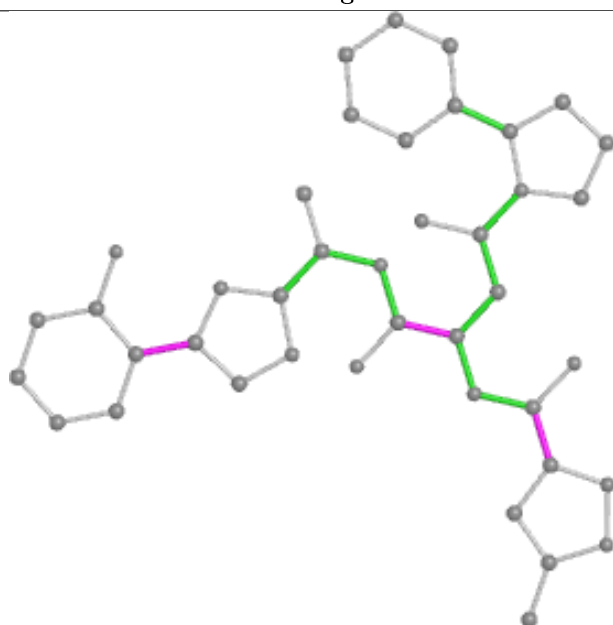
## Ligand M9G I 301



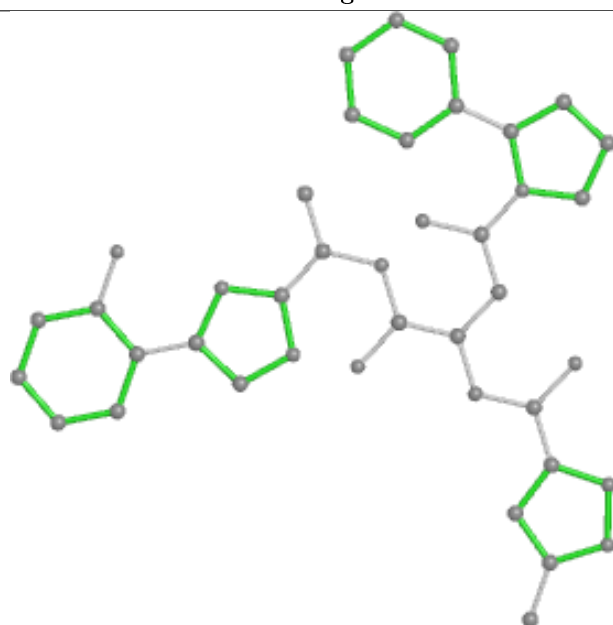
Bond lengths



Bond angles

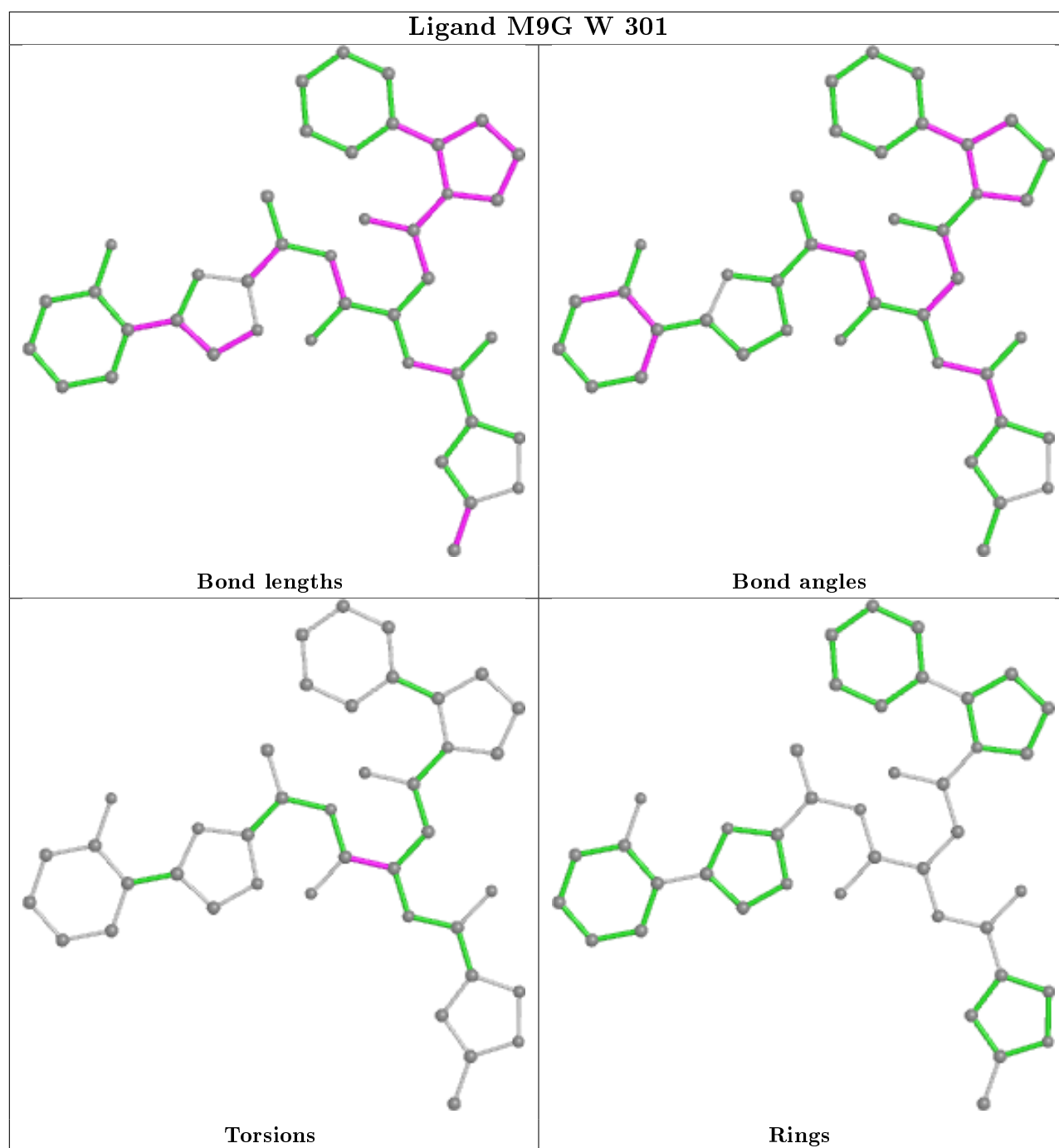


Torsions

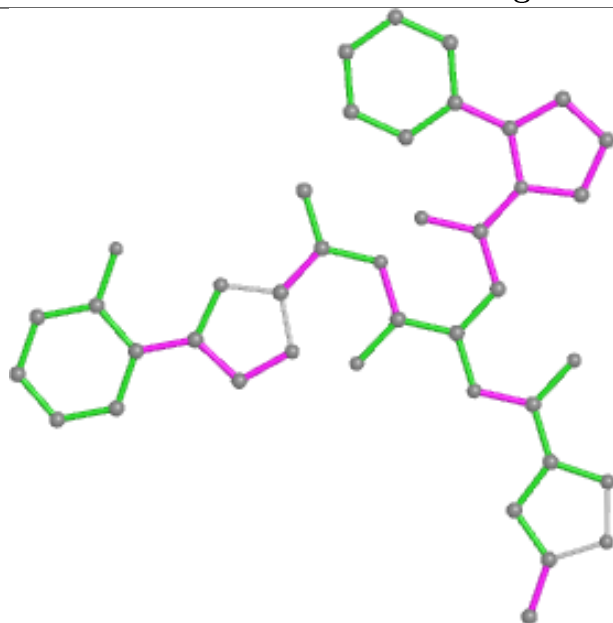


Rings

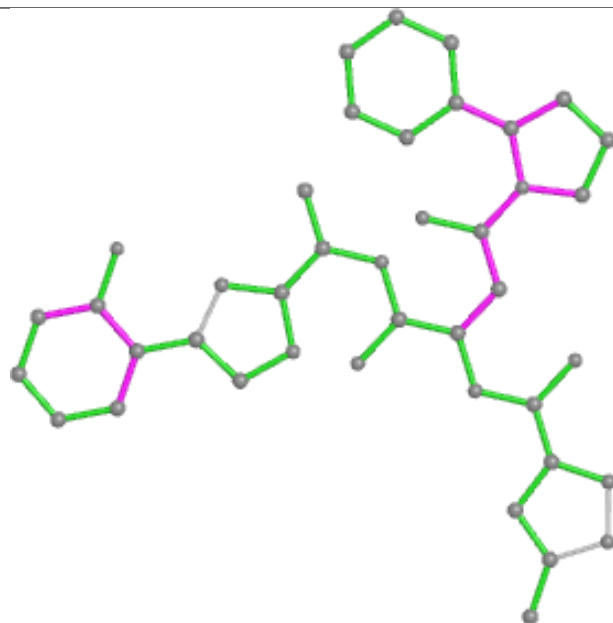




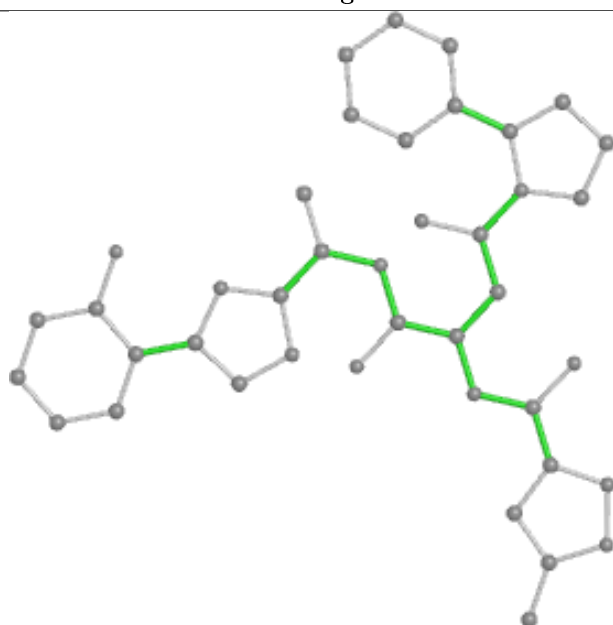
## Ligand M9G Z 301



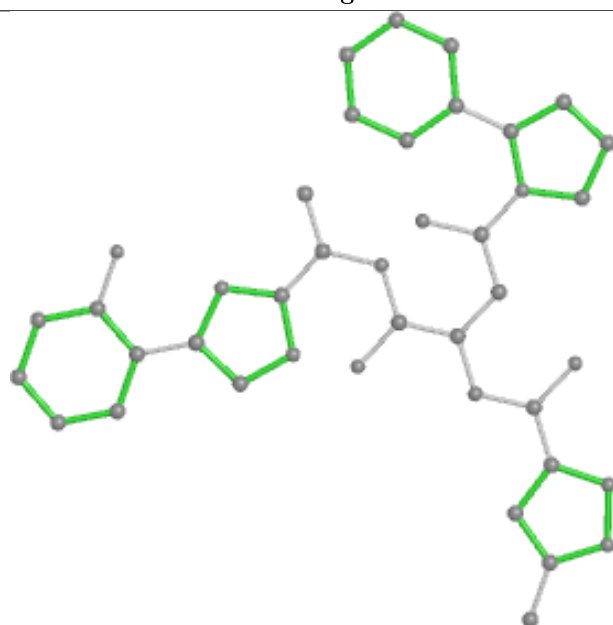
Bond lengths



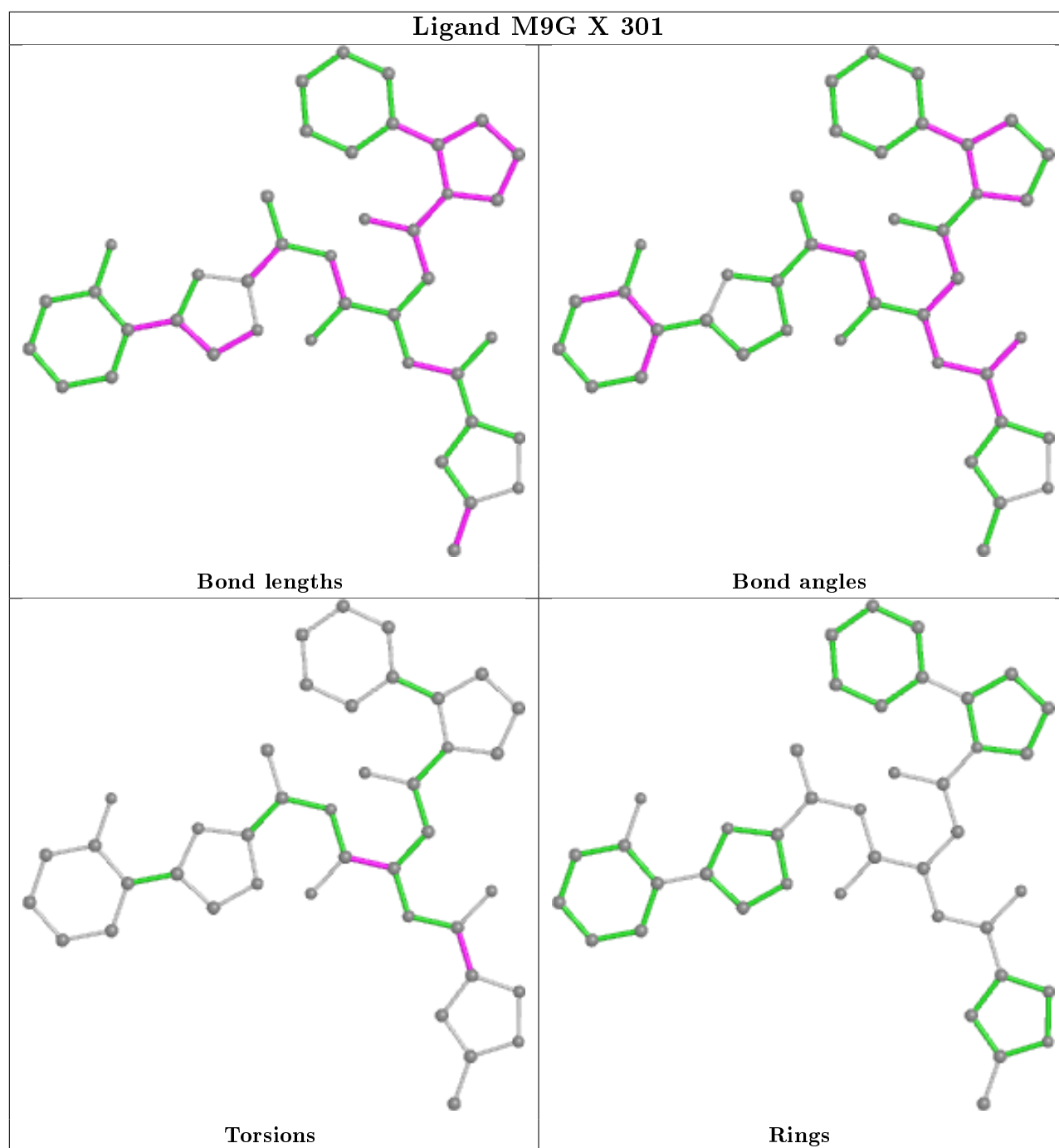
Bond angles

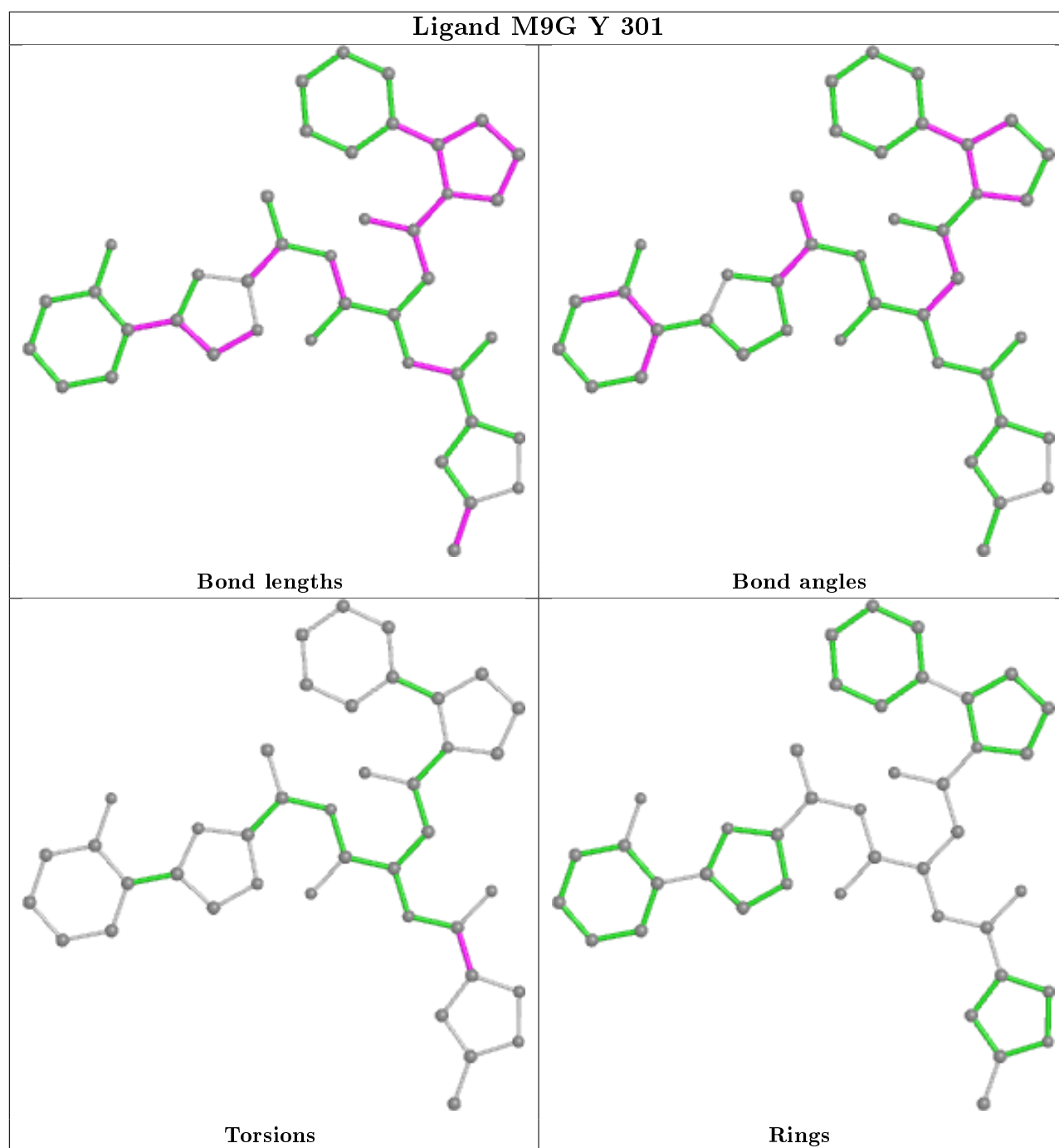


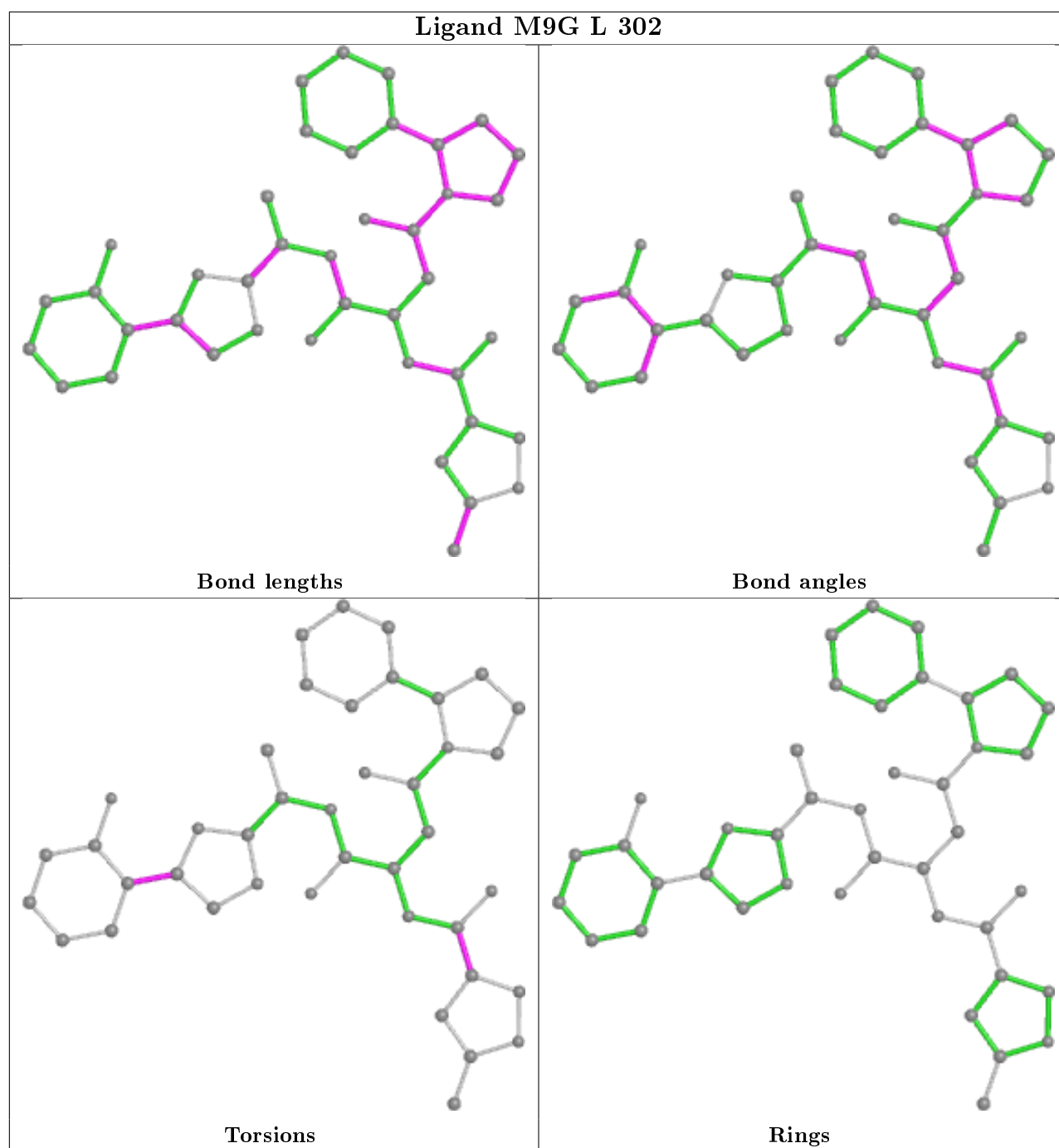
Torsions



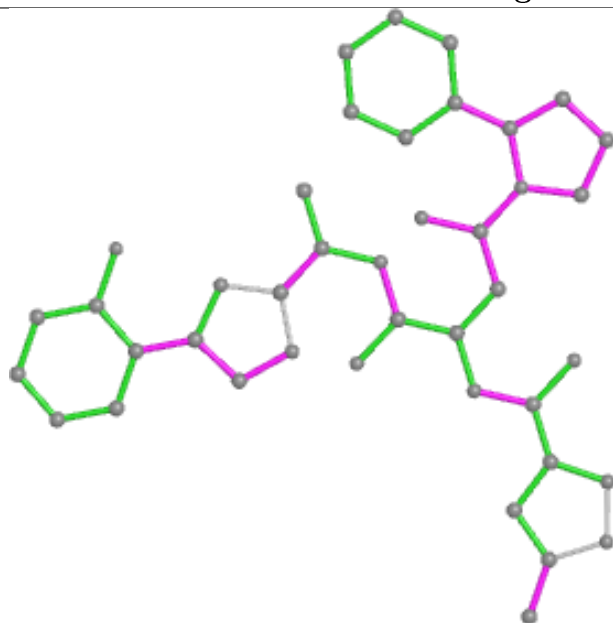
Rings



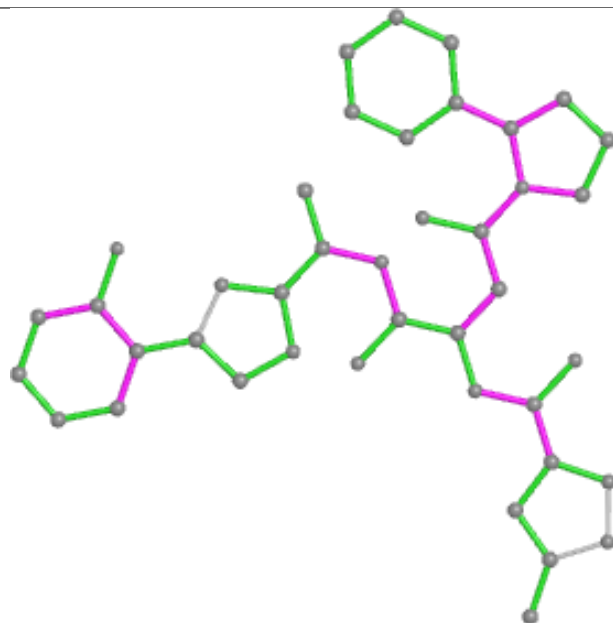




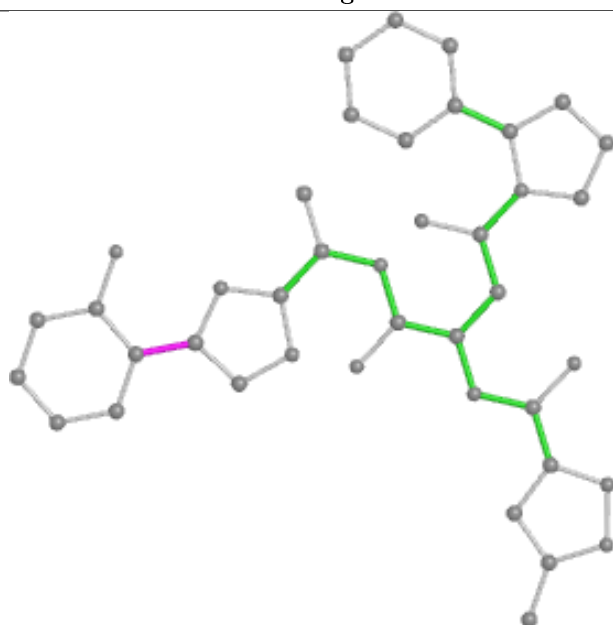
## Ligand M9G b 301



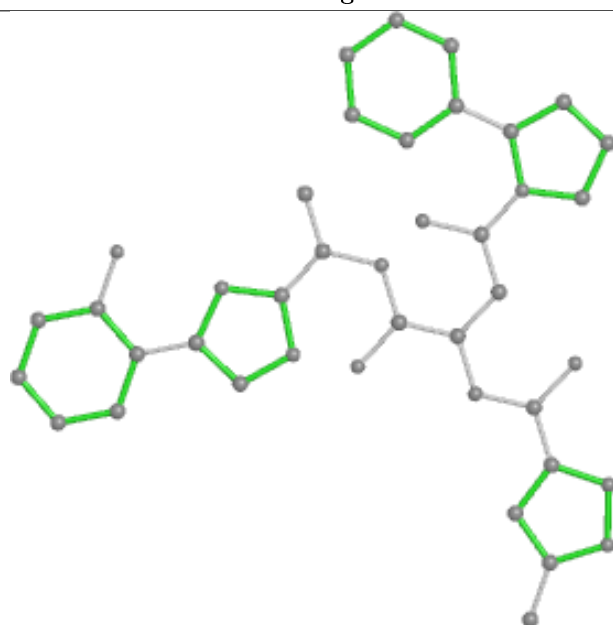
Bond lengths



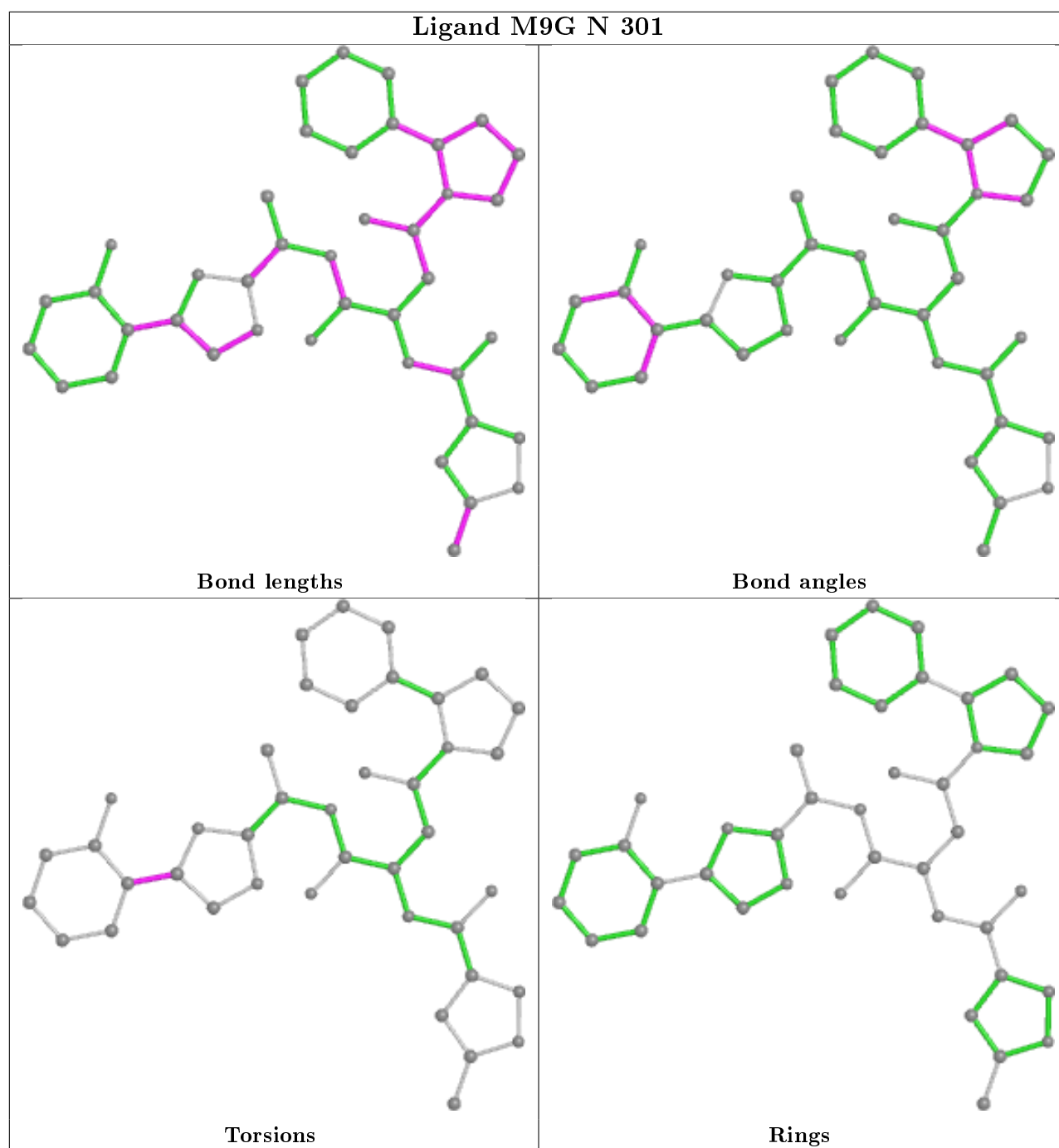
Bond angles



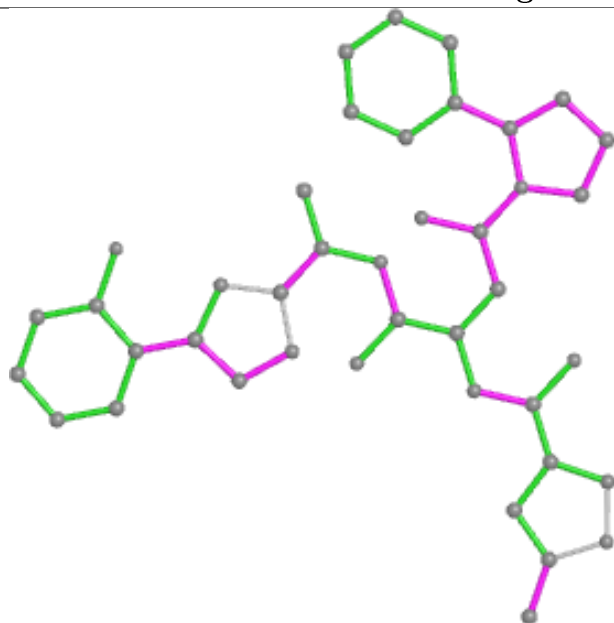
Torsions



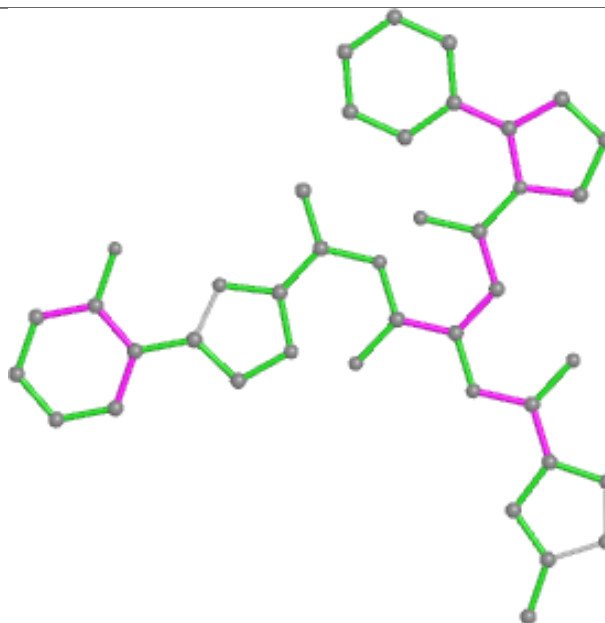
Rings



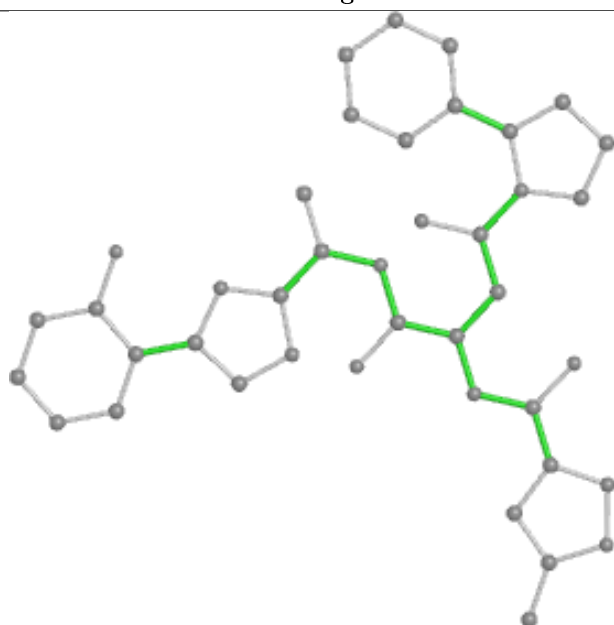
## Ligand M9G a 301



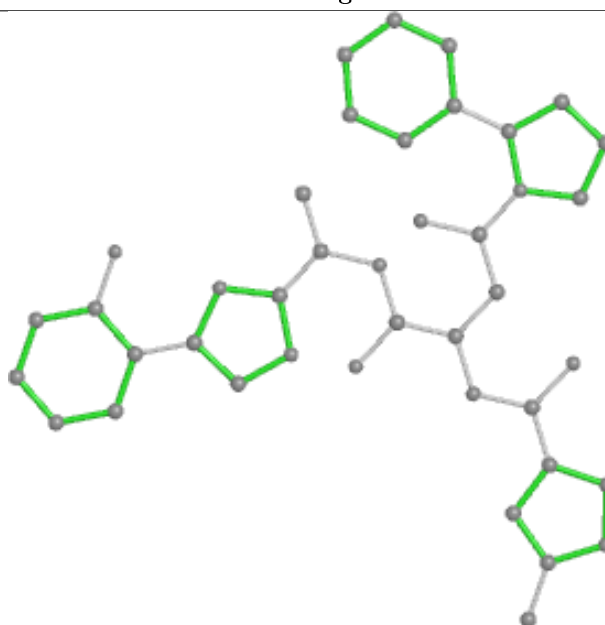
Bond lengths



Bond angles

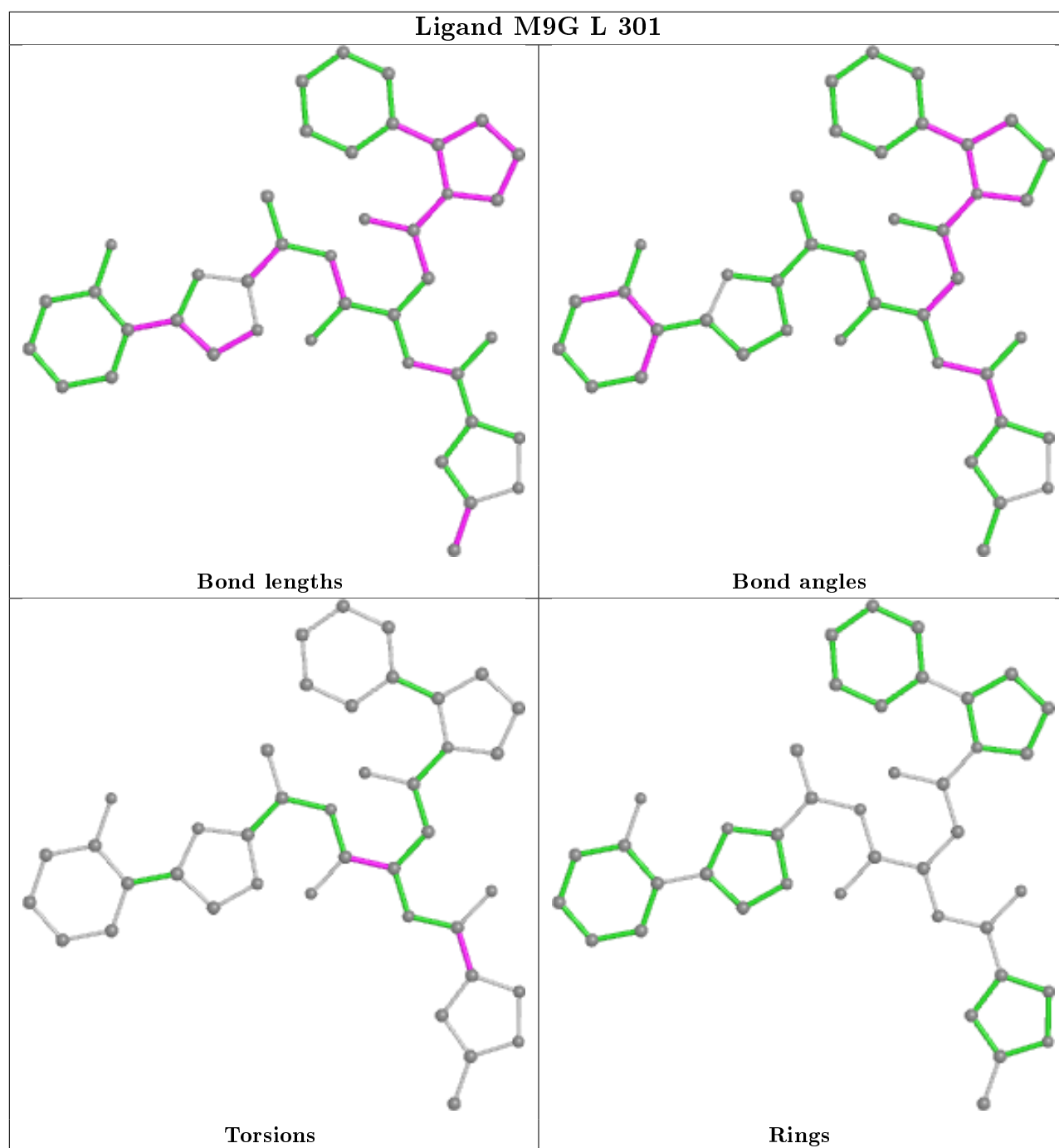


Torsions



Rings





## 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     | 218/240 (90%) | -0.16  | 1 (0%) 91 91  | 18, 33, 55, 81        | 0     |
| 1   | B     | 215/240 (89%) | 0.08   | 9 (4%) 36 32  | 20, 42, 71, 90        | 0     |
| 1   | C     | 216/240 (90%) | 0.31   | 13 (6%) 21 18 | 21, 46, 75, 89        | 0     |
| 1   | D     | 214/240 (89%) | 0.11   | 5 (2%) 60 58  | 23, 44, 68, 84        | 0     |
| 1   | E     | 217/240 (90%) | -0.02  | 3 (1%) 75 75  | 21, 42, 68, 83        | 0     |
| 1   | F     | 214/240 (89%) | 0.07   | 2 (0%) 84 84  | 18, 44, 71, 81        | 0     |
| 1   | G     | 216/240 (90%) | -0.22  | 4 (1%) 66 65  | 17, 36, 64, 78        | 0     |
| 1   | O     | 216/240 (90%) | 0.21   | 10 (4%) 32 29 | 22, 46, 74, 87        | 0     |
| 1   | P     | 219/240 (91%) | -0.05  | 6 (2%) 54 50  | 19, 40, 67, 86        | 0     |
| 1   | Q     | 215/240 (89%) | -0.12  | 1 (0%) 91 91  | 20, 39, 61, 75        | 0     |
| 1   | R     | 215/240 (89%) | 0.13   | 8 (3%) 41 37  | 17, 38, 58, 66        | 0     |
| 1   | S     | 218/240 (90%) | -0.23  | 2 (0%) 84 84  | 18, 34, 59, 76        | 0     |
| 1   | T     | 217/240 (90%) | 0.21   | 6 (2%) 53 49  | 22, 45, 69, 100       | 0     |
| 1   | U     | 216/240 (90%) | -0.07  | 4 (1%) 66 65  | 19, 38, 66, 84        | 0     |
| 2   | H     | 222/234 (94%) | -0.39  | 0 100 100     | 15, 24, 42, 67        | 0     |
| 2   | I     | 222/234 (94%) | -0.53  | 0 100 100     | 15, 23, 41, 61        | 0     |
| 2   | J     | 222/234 (94%) | -0.45  | 0 100 100     | 15, 25, 42, 59        | 0     |
| 2   | K     | 223/234 (95%) | -0.48  | 0 100 100     | 11, 23, 40, 54        | 0     |
| 2   | L     | 223/234 (95%) | -0.45  | 0 100 100     | 16, 24, 41, 58        | 0     |
| 2   | M     | 222/234 (94%) | -0.38  | 0 100 100     | 17, 27, 47, 63        | 0     |
| 2   | N     | 223/234 (95%) | -0.38  | 0 100 100     | 16, 28, 49, 64        | 0     |
| 2   | V     | 223/234 (95%) | -0.47  | 0 100 100     | 14, 24, 40, 54        | 0     |
| 2   | W     | 223/234 (95%) | -0.46  | 0 100 100     | 16, 25, 42, 56        | 0     |
| 2   | X     | 222/234 (94%) | -0.45  | 0 100 100     | 16, 25, 43, 65        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 2   | Y     | 223/234 (95%)   | -0.43  | 1 (0%) 92 93  | 14, 24, 41, 66        | 0     |
| 2   | Z     | 223/234 (95%)   | -0.42  | 0 100 100     | 15, 26, 46, 60        | 0     |
| 2   | a     | 223/234 (95%)   | -0.37  | 0 100 100     | 19, 28, 48, 66        | 0     |
| 2   | b     | 223/234 (95%)   | -0.43  | 0 100 100     | 17, 27, 45, 64        | 0     |
| All | All   | 6143/6636 (92%) | -0.21  | 75 (1%) 79 79 | 11, 31, 64, 100       | 0     |

All (75) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | T     | 202 | THR  | 5.0  |
| 1   | C     | 9   | MET  | 3.8  |
| 1   | P     | 170 | SER  | 3.7  |
| 1   | T     | 203 | LEU  | 3.6  |
| 1   | O     | 188 | LEU  | 3.6  |
| 1   | R     | 171 | TYR  | 3.5  |
| 1   | B     | 171 | TYR  | 3.4  |
| 1   | C     | 11  | GLN  | 3.4  |
| 1   | E     | 11  | GLN  | 3.4  |
| 1   | S     | 9   | MET  | 3.3  |
| 1   | O     | 171 | TYR  | 3.2  |
| 1   | O     | 206 | ALA  | 3.1  |
| 1   | F     | 172 | ALA  | 3.1  |
| 1   | T     | 235 | VAL  | 3.0  |
| 1   | O     | 172 | ALA  | 3.0  |
| 1   | R     | 165 | ASN  | 3.0  |
| 1   | U     | 9   | MET  | 3.0  |
| 1   | C     | 235 | VAL  | 3.0  |
| 1   | F     | 167 | LEU  | 3.0  |
| 1   | R     | 172 | ALA  | 2.9  |
| 1   | C     | 171 | TYR  | 2.9  |
| 1   | D     | 171 | TYR  | 2.9  |
| 1   | B     | 165 | ASN  | 2.9  |
| 1   | G     | 233 | LEU  | 2.8  |
| 1   | C     | 189 | ARG  | 2.7  |
| 1   | B     | 167 | LEU  | 2.7  |
| 1   | C     | 10  | GLU  | 2.7  |
| 1   | O     | 170 | SER  | 2.6  |
| 1   | O     | 203 | LEU  | 2.6  |
| 1   | C     | 231 | GLN  | 2.5  |
| 1   | R     | 180 | ALA  | 2.5  |
| 1   | U     | 10  | GLU  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | P     | 9   | MET  | 2.5  |
| 1   | C     | 233 | LEU  | 2.5  |
| 1   | C     | 182 | ARG  | 2.5  |
| 1   | O     | 186 | ALA  | 2.5  |
| 1   | E     | 189 | ARG  | 2.5  |
| 1   | D     | 178 | THR  | 2.5  |
| 1   | B     | 235 | VAL  | 2.5  |
| 1   | G     | 235 | VAL  | 2.4  |
| 1   | R     | 160 | THR  | 2.4  |
| 1   | T     | 205 | VAL  | 2.4  |
| 1   | T     | 185 | VAL  | 2.4  |
| 1   | T     | 170 | SER  | 2.4  |
| 1   | P     | 169 | GLU  | 2.3  |
| 1   | D     | 9   | MET  | 2.3  |
| 1   | O     | 189 | ARG  | 2.3  |
| 1   | U     | 203 | LEU  | 2.3  |
| 1   | E     | 9   | MET  | 2.3  |
| 1   | O     | 162 | PRO  | 2.3  |
| 1   | C     | 163 | ILE  | 2.3  |
| 1   | S     | 192 | SER  | 2.3  |
| 1   | C     | 206 | ALA  | 2.3  |
| 1   | B     | 190 | ALA  | 2.2  |
| 1   | R     | 186 | ALA  | 2.2  |
| 1   | R     | 159 | THR  | 2.2  |
| 1   | O     | 182 | ARG  | 2.2  |
| 1   | R     | 163 | ILE  | 2.2  |
| 1   | G     | 231 | GLN  | 2.2  |
| 1   | D     | 189 | ARG  | 2.2  |
| 1   | C     | 181 | LEU  | 2.1  |
| 1   | B     | 180 | ALA  | 2.1  |
| 1   | P     | 192 | SER  | 2.1  |
| 1   | C     | 184 | ALA  | 2.1  |
| 1   | P     | 178 | THR  | 2.1  |
| 1   | B     | 203 | LEU  | 2.1  |
| 1   | A     | 192 | SER  | 2.1  |
| 1   | B     | 9   | MET  | 2.1  |
| 1   | U     | 234 | LEU  | 2.0  |
| 1   | G     | 232 | ALA  | 2.0  |
| 1   | Q     | 235 | VAL  | 2.0  |
| 1   | B     | 170 | SER  | 2.0  |
| 2   | Y     | 115 | GLN  | 2.0  |
| 1   | P     | 202 | THR  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 188 | LEU  | 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

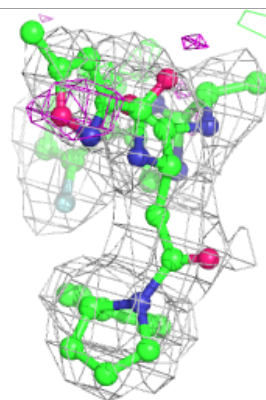
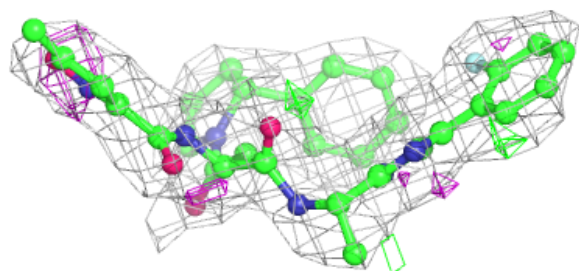
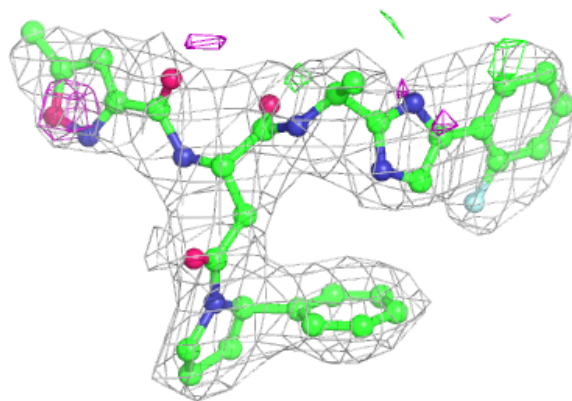
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | M9G  | N     | 301 | 41/41 | 0.94 | 0.19 | 13,24,36,49                | 0     |
| 3   | M9G  | M     | 301 | 41/41 | 0.95 | 0.21 | 18,26,40,51                | 0     |
| 3   | M9G  | H     | 301 | 41/41 | 0.95 | 0.20 | 17,24,36,50                | 0     |
| 3   | M9G  | V     | 301 | 41/41 | 0.95 | 0.20 | 19,24,41,53                | 0     |
| 3   | M9G  | W     | 301 | 41/41 | 0.95 | 0.20 | 19,28,38,48                | 0     |
| 3   | M9G  | J     | 301 | 41/41 | 0.95 | 0.21 | 18,27,38,42                | 0     |
| 3   | M9G  | X     | 301 | 41/41 | 0.96 | 0.16 | 18,26,39,45                | 0     |
| 3   | M9G  | Y     | 301 | 41/41 | 0.96 | 0.20 | 13,24,35,45                | 0     |
| 3   | M9G  | L     | 302 | 41/41 | 0.96 | 0.20 | 17,26,36,48                | 0     |
| 3   | M9G  | b     | 301 | 41/41 | 0.96 | 0.18 | 15,24,35,40                | 0     |
| 3   | M9G  | Z     | 301 | 41/41 | 0.96 | 0.20 | 17,26,37,49                | 0     |
| 3   | M9G  | L     | 301 | 41/41 | 0.96 | 0.20 | 15,25,43,51                | 0     |
| 3   | M9G  | a     | 301 | 41/41 | 0.97 | 0.18 | 19,27,36,45                | 0     |
| 3   | M9G  | I     | 301 | 41/41 | 0.97 | 0.16 | 15,24,40,45                | 0     |

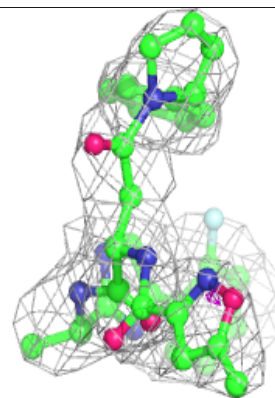
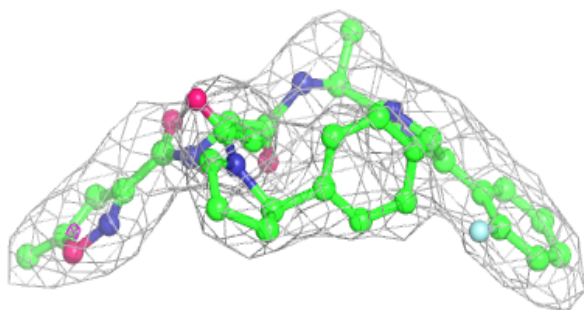
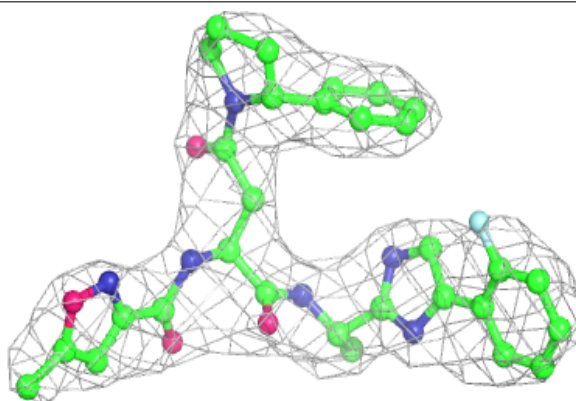
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around M9G N 301:**

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

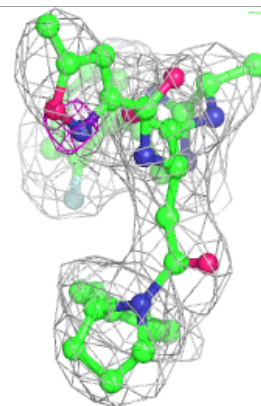
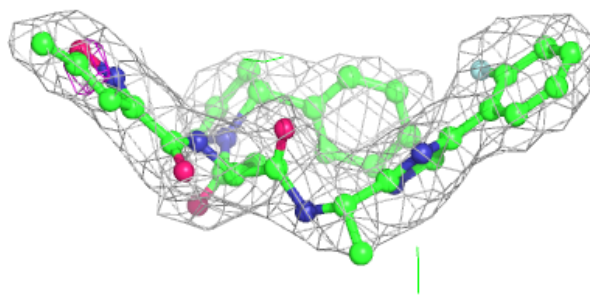
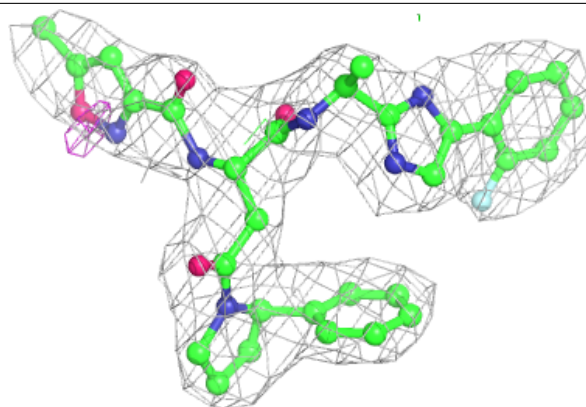
**Electron density around M9G M 301:**

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

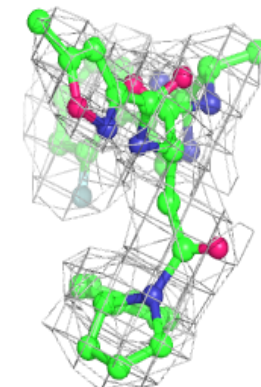
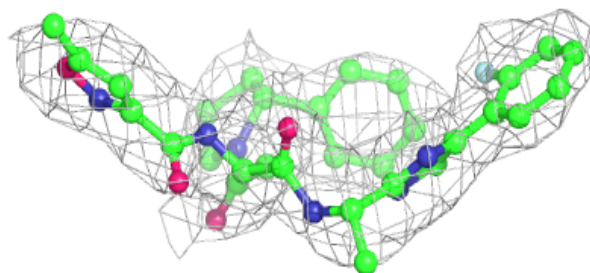
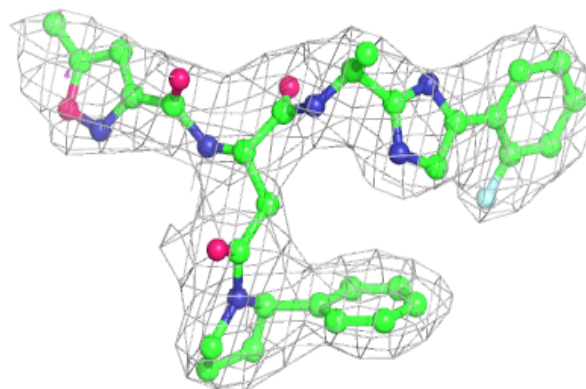


**Electron density around M9G H 301:**

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

**Electron density around M9G V 301:**

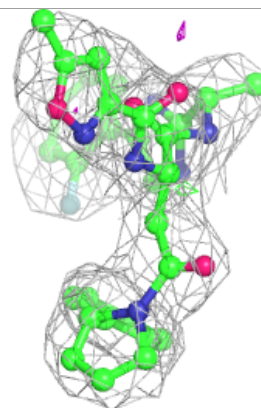
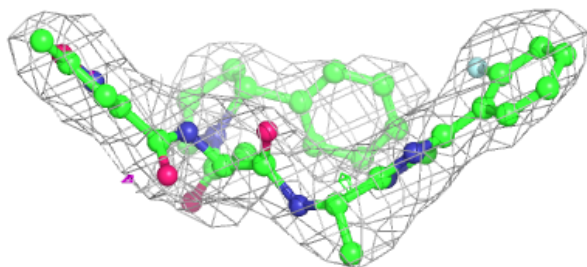
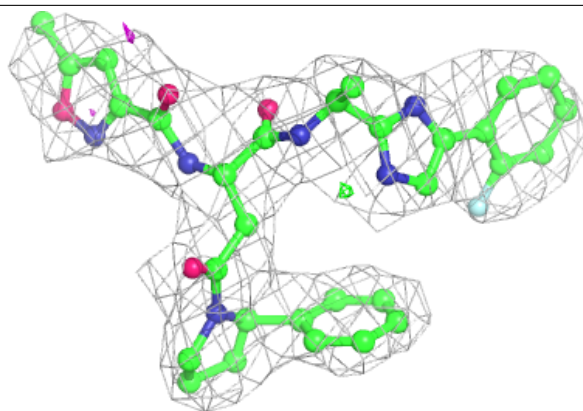
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



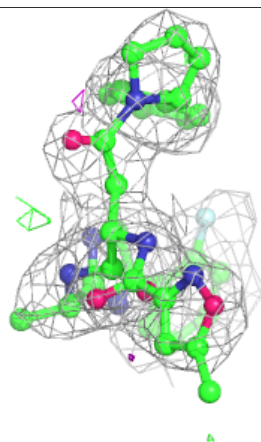
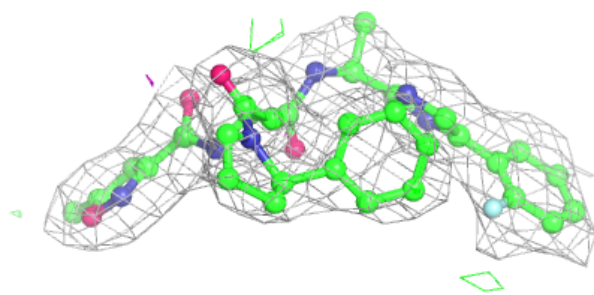
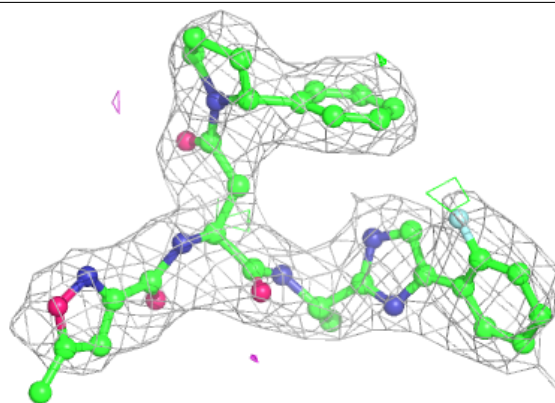


**Electron density around M9G W 301:**

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

**Electron density around M9G J 301:**

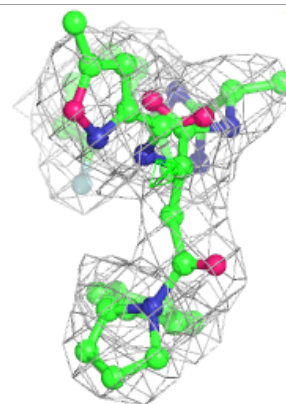
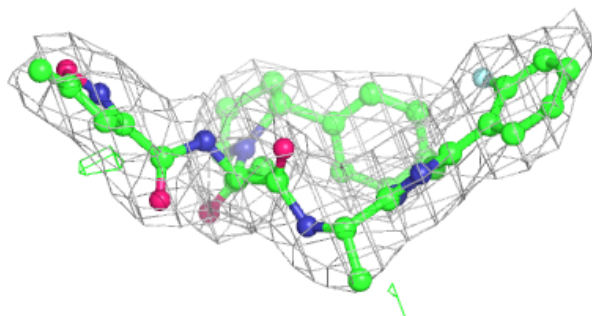
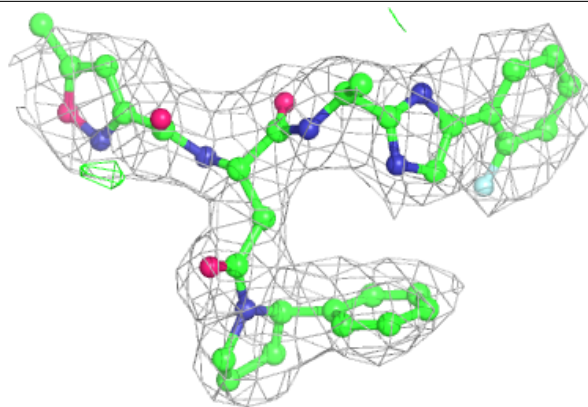
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



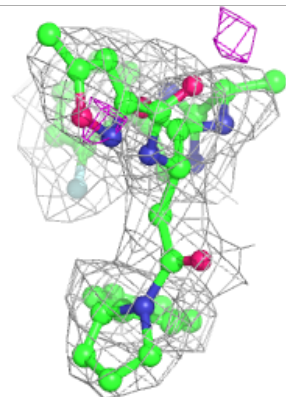
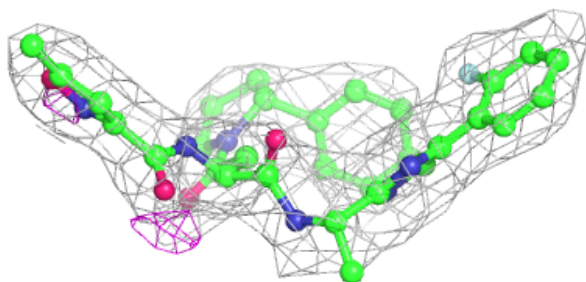
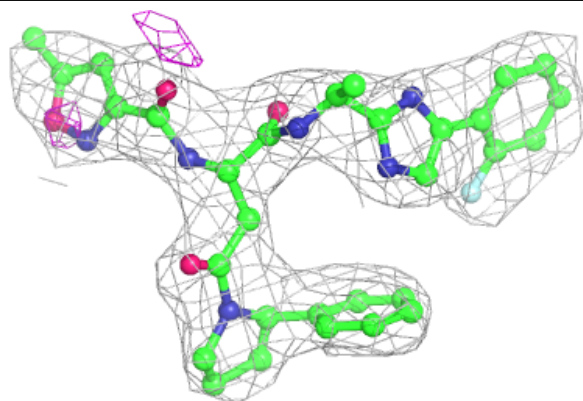


**Electron density around M9G X 301:**

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

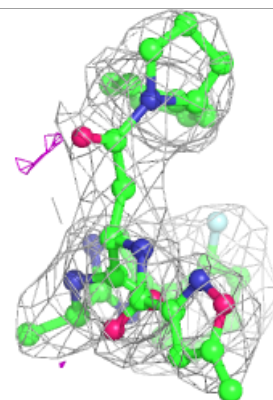
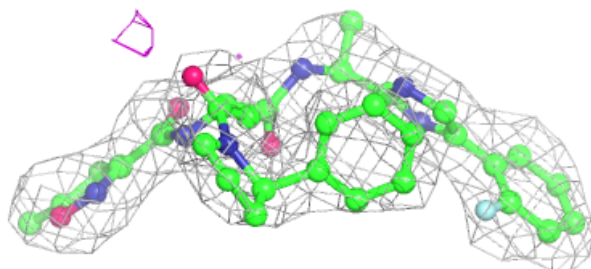
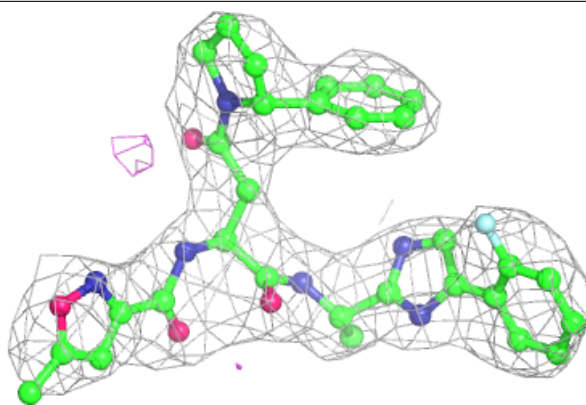
**Electron density around M9G Y 301:**

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

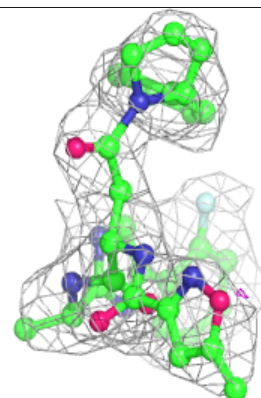
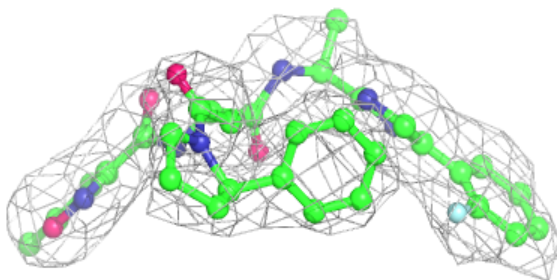
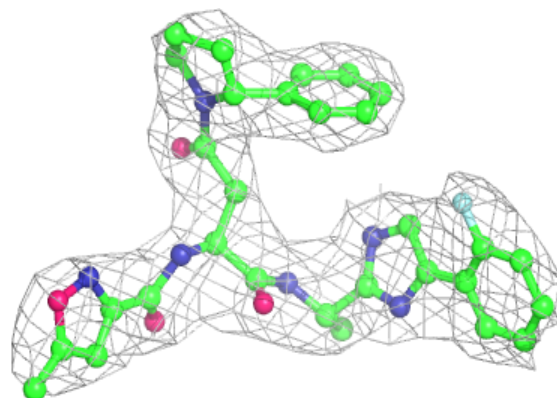


**Electron density around M9G L 302:**

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

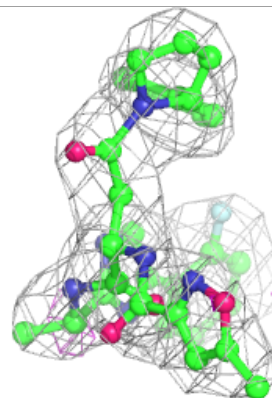
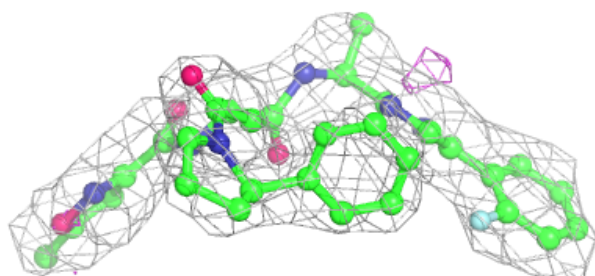
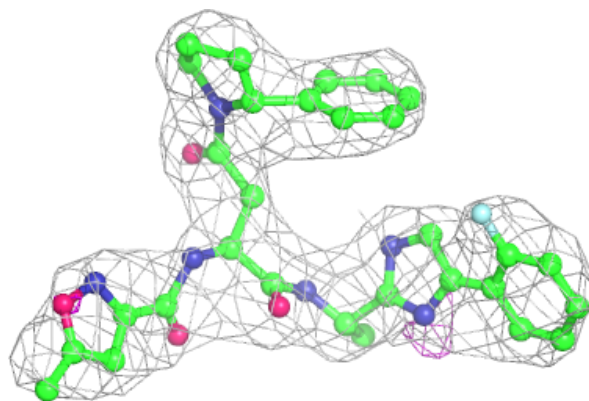
**Electron density around M9G b 301:**

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

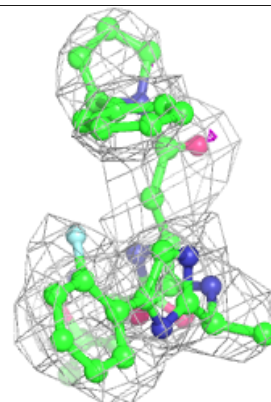
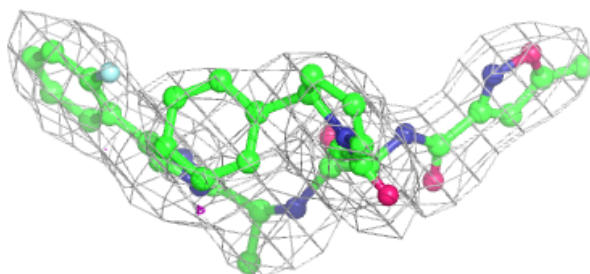
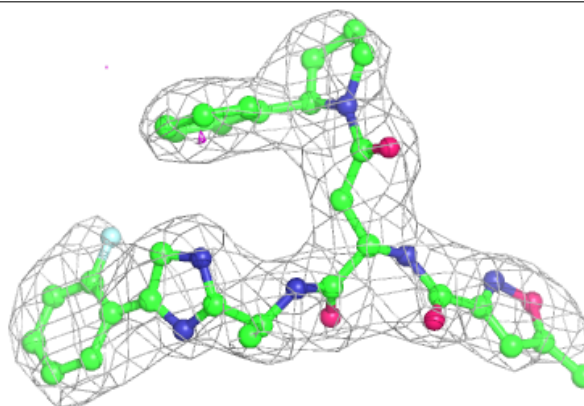


**Electron density around M9G Z 301:**

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

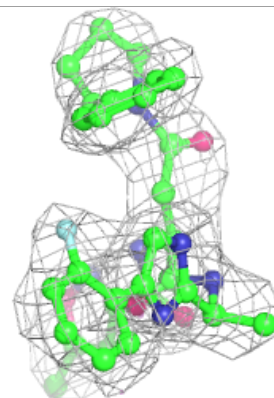
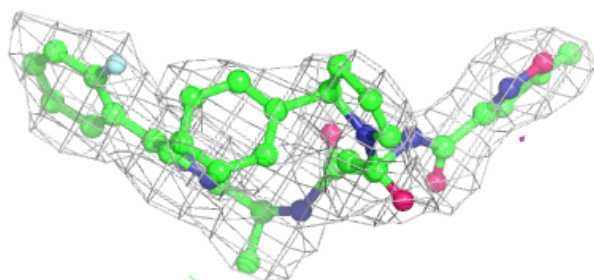
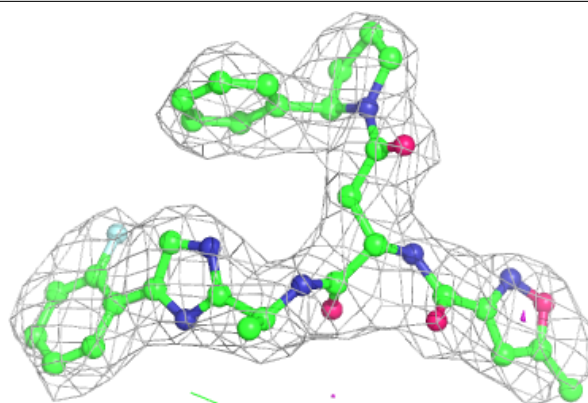
**Electron density around M9G L 301:**

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

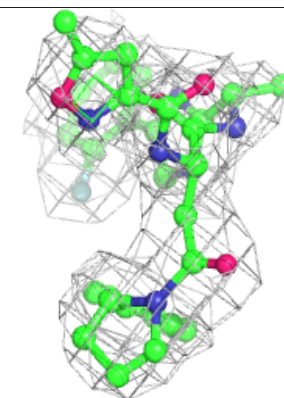
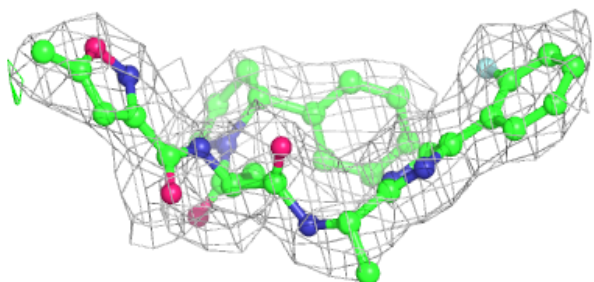
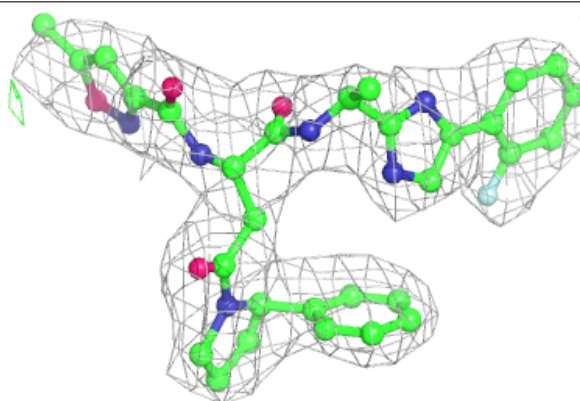


**Electron density around M9G a 301:**

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

**Electron density around M9G I 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 [i](#)

There are no such residues in this entry.