



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:05 AM UTC

PDB ID : 3KO0 / pdb\_00003ko0  
Title : Structure of the tfp-ca<sup>2+</sup>-bound activated form of the s100a4 Metastasis factor  
Authors : Malashkevich, V.N.; Dulyaninova, N.G.; Knight, D.; Almo, S.C.; Bresnick, A.R.  
Deposited on : 2009-11-12  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

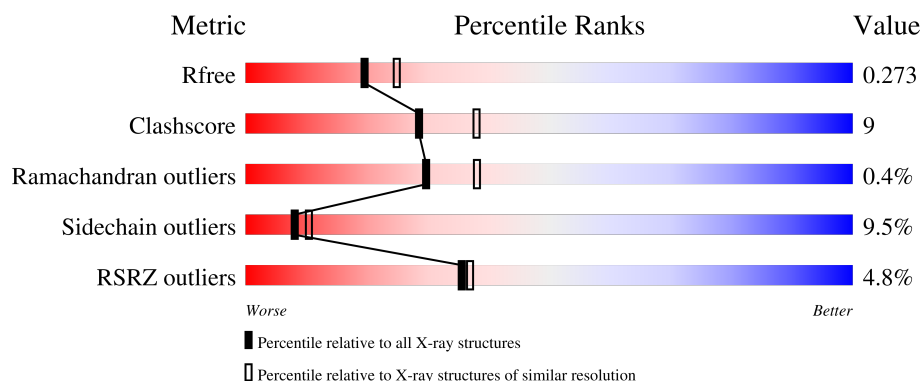
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6319 (2.30-2.30)                                      |
| Clashscore            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |
| RSRZ outliers         | 180081                      | 6325 (2.30-2.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                              |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------|
| 1   | A     | 101    | <div> <div>5%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>8%</div> </div> </div>  |
| 1   | B     | 101    | <div> <div>5%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>•</div> <div>8%</div> </div> </div>  |
| 1   | C     | 101    | <div> <div>2%</div> <div> <div></div> <div>66%</div> <div>24%</div> <div>•</div> <div>8%</div> </div> </div>  |
| 1   | D     | 101    | <div> <div>5%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>7%</div> <div>8%</div> </div> </div> |
| 1   | E     | 101    | <div> <div>•</div> <div> <div></div> <div>65%</div> <div>19%</div> <div>7%</div> <div>9%</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 101    |                  |
| 1   | G     | 101    |                  |
| 1   | H     | 101    |                  |
| 1   | I     | 101    |                  |
| 1   | J     | 101    |                  |
| 1   | K     | 101    |                  |
| 1   | L     | 101    |                  |
| 1   | M     | 101    |                  |
| 1   | N     | 101    |                  |
| 1   | O     | 101    |                  |
| 1   | P     | 101    |                  |
| 1   | Q     | 101    |                  |
| 1   | R     | 101    |                  |
| 1   | S     | 101    |                  |
| 1   | T     | 101    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16855 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 Protein S100-A4.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 93       | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 754   | 481 | 121 | 144 | 8  |         |         |       |
| 1   | B     | 93       | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 740   | 471 | 118 | 142 | 9  |         |         |       |
| 1   | C     | 93       | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 746   | 475 | 118 | 144 | 9  |         |         |       |
| 1   | D     | 93       | Total | C   | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 752   | 479 | 119 | 144 | 10 |         |         |       |
| 1   | E     | 92       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 741   | 471 | 119 | 143 | 8  |         |         |       |
| 1   | F     | 90       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 709   | 451 | 110 | 140 | 8  |         |         |       |
| 1   | G     | 90       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 718   | 459 | 113 | 138 | 8  |         |         |       |
| 1   | H     | 94       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 752   | 477 | 120 | 147 | 8  |         |         |       |
| 1   | I     | 93       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 744   | 473 | 119 | 144 | 8  |         |         |       |
| 1   | J     | 93       | Total | C   | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 756   | 482 | 120 | 144 | 10 |         |         |       |
| 1   | K     | 93       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 738   | 470 | 116 | 144 | 8  |         |         |       |
| 1   | L     | 93       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 744   | 473 | 119 | 144 | 8  |         |         |       |
| 1   | M     | 92       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 731   | 465 | 115 | 143 | 8  |         |         |       |
| 1   | N     | 92       | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 743   | 473 | 118 | 143 | 9  |         |         |       |
| 1   | O     | 93       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 745   | 474 | 119 | 144 | 8  |         |         |       |
| 1   | P     | 92       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 733   | 465 | 117 | 143 | 8  |         |         |       |

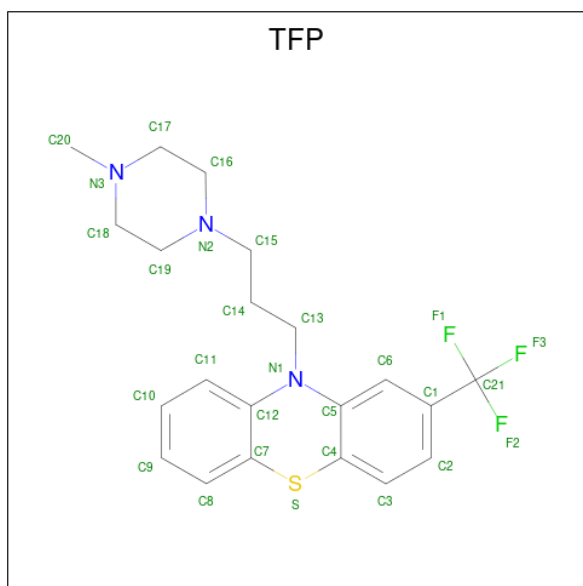
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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | Q     | 88       | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 702   | 450 | 107 | 136 | 9 |         |         |       |
| 1   | R     | 93       | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 745   | 474 | 118 | 144 | 9 |         |         |       |
| 1   | S     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 748   | 476 | 120 | 144 | 8 |         |         |       |
| 1   | T     | 93       | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 744   | 475 | 116 | 144 | 9 |         |         |       |

- Molecule 2 is 10-[3-(4-METHYL-PIPERAZIN-1-YL)-PROPYL]-2-TRIFLUOROMETHYL-10H-PHENOTHIAZINE (CCD ID: TFP) (formula:  $C_{21}H_{24}F_3N_3S$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 28    | 21 | 3 | 3 | 1 |         |         |
| 2   | A     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 28    | 21 | 3 | 3 | 1 |         |         |
| 2   | B     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 28    | 21 | 3 | 3 | 1 |         |         |
| 2   | B     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 28    | 21 | 3 | 3 | 1 |         |         |
| 2   | C     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 28    | 21 | 3 | 3 | 1 |         |         |
| 2   | C     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 28    | 21 | 3 | 3 | 1 |         |         |
| 2   | D     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 28    | 21 | 3 | 3 | 1 |         |         |

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| Mol | Chain | Residues | Atoms       |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 2   | D     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | E     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | E     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | F     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | F     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | G     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | G     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | H     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | H     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | I     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | I     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | J     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | J     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | K     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | K     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | L     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | L     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | M     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | M     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | N     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | N     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 2   | O     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | O     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | P     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | P     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | Q     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | Q     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | R     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | R     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | S     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | S     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | T     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |
| 2   | T     | 1        | Total<br>28 | C<br>21 | F<br>3 | N<br>3 | S<br>1 | 0       | 0       |

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | A     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | B     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | C     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | D     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | E     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | F     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | G     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | H     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | I     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | J     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | K     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | L     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | M     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | N     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | O     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | P     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | Q     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | R     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | S     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 3   | T     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | A     | 57       | Total<br>57 | O<br>57 | 0       | 0       |
| 4   | B     | 75       | Total<br>75 | O<br>75 | 0       | 0       |
| 4   | C     | 56       | Total<br>56 | O<br>56 | 0       | 0       |
| 4   | D     | 48       | Total<br>48 | O<br>48 | 0       | 0       |
| 4   | E     | 47       | Total<br>47 | O<br>47 | 0       | 0       |
| 4   | F     | 41       | Total<br>41 | O<br>41 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | G     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 4   | H     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 4   | I     | 51       | Total<br>51 | O<br>51 | 0       | 0       |
| 4   | J     | 65       | Total<br>65 | O<br>65 | 0       | 0       |
| 4   | K     | 52       | Total<br>52 | O<br>52 | 0       | 0       |
| 4   | L     | 53       | Total<br>53 | O<br>53 | 0       | 0       |
| 4   | M     | 35       | Total<br>35 | O<br>35 | 0       | 0       |
| 4   | N     | 49       | Total<br>49 | O<br>49 | 0       | 0       |
| 4   | O     | 33       | Total<br>33 | O<br>33 | 0       | 0       |
| 4   | P     | 42       | Total<br>42 | O<br>42 | 0       | 0       |
| 4   | Q     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 4   | R     | 32       | Total<br>32 | O<br>32 | 0       | 0       |
| 4   | S     | 60       | Total<br>60 | O<br>60 | 0       | 0       |
| 4   | T     | 32       | Total<br>32 | O<br>32 | 0       | 0       |

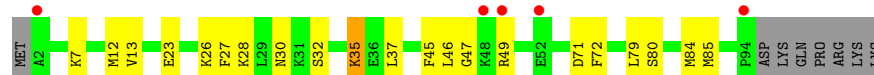
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

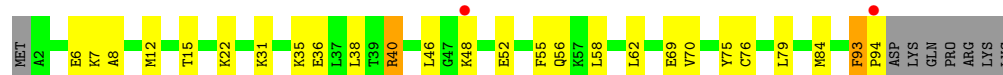
- Molecule 1: Protein S100-A4



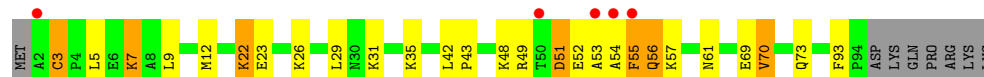
- Molecule 1: Protein S100-A4



- Molecule 1: Protein S100-A4



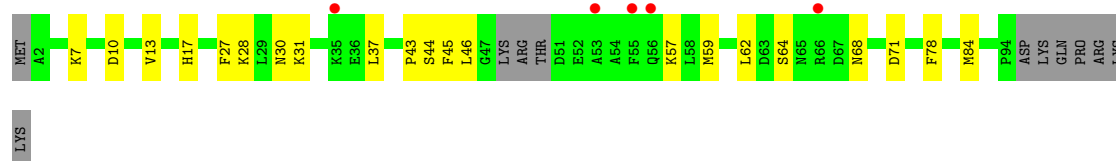
- Molecule 1: Protein S100-A4



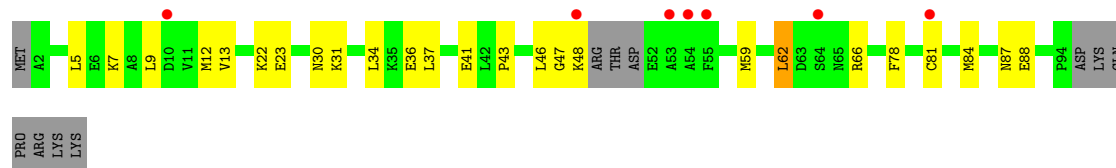
- Molecule 1: Protein S100-A4



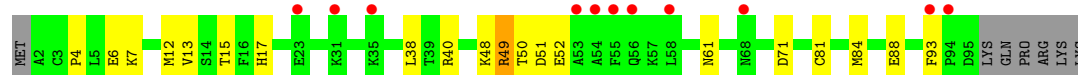
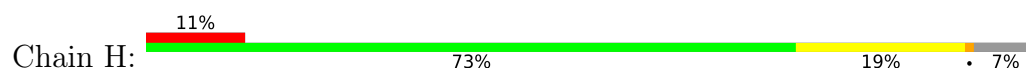
- Molecule 1: Protein S100-A4



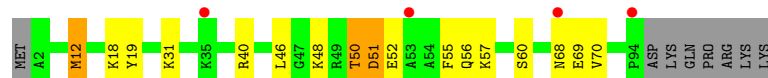
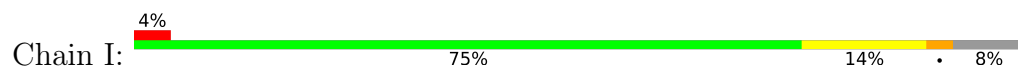
• Molecule 1: Protein S100-A4



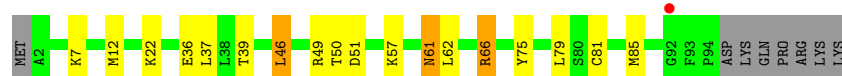
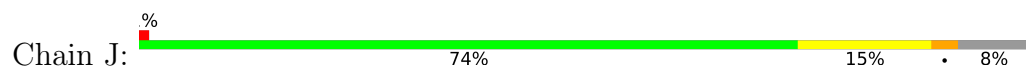
• Molecule 1: Protein S100-A4



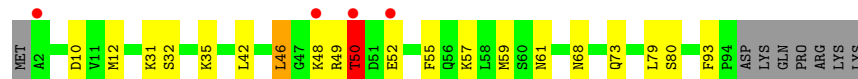
• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4

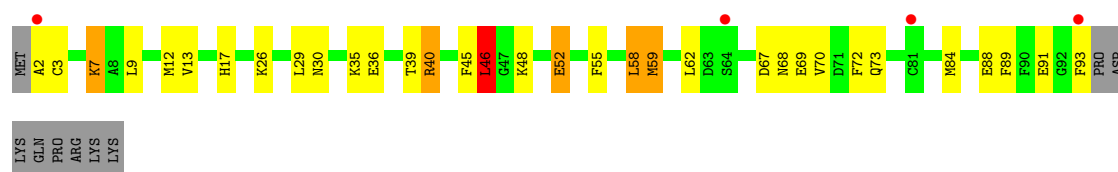


• Molecule 1: Protein S100-A4

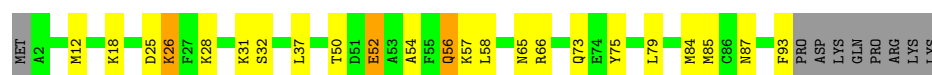




• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4



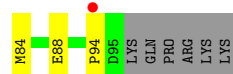
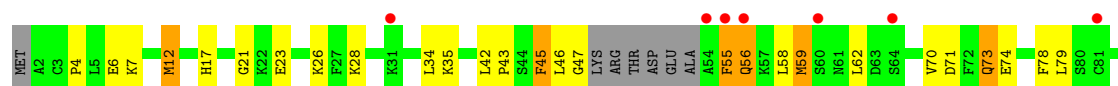
• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4



• Molecule 1: Protein S100-A4



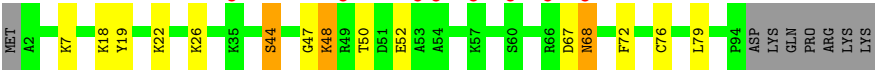
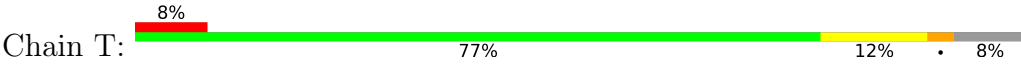




● Molecule 1: Protein S100-A4



● Molecule 1: Protein S100-A4



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 108.79Å 102.49Å 116.63Å<br>90.00° 92.59° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.94 – 2.30<br>19.94 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.7 (19.94-2.30)<br>97.5 (19.94-2.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.48 (at 2.30Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.206 , 0.259<br>0.226 , 0.273                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5579 reflections (5.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.039                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 39.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | 0.002 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 16855                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7495e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 1.15         | 1/771 (0.1%)    | 1.06        | 2/1030 (0.2%)   |
| 1   | B     | 1.06         | 0/757           | 1.01        | 0/1015          |
| 1   | C     | 0.98         | 2/763 (0.3%)    | 1.03        | 1/1022 (0.1%)   |
| 1   | D     | 1.13         | 2/772 (0.3%)    | 1.20        | 6/1033 (0.6%)   |
| 1   | E     | 1.11         | 2/754 (0.3%)    | 1.04        | 2/1007 (0.2%)   |
| 1   | F     | 0.80         | 0/722           | 1.07        | 2/969 (0.2%)    |
| 1   | G     | 0.84         | 0/731           | 1.01        | 0/977           |
| 1   | H     | 0.78         | 0/766           | 1.00        | 3/1026 (0.3%)   |
| 1   | I     | 0.96         | 2/758 (0.3%)    | 1.04        | 1/1015 (0.1%)   |
| 1   | J     | 0.92         | 0/776           | 1.01        | 0/1037          |
| 1   | K     | 1.09         | 1/752 (0.1%)    | 1.09        | 5/1008 (0.5%)   |
| 1   | L     | 1.17         | 4/758 (0.5%)    | 1.11        | 1/1015 (0.1%)   |
| 1   | M     | 0.85         | 0/744           | 1.04        | 2/996 (0.2%)    |
| 1   | N     | 0.95         | 1/759 (0.1%)    | 1.02        | 0/1014          |
| 1   | O     | 0.92         | 1/759 (0.1%)    | 1.05        | 1/1016 (0.1%)   |
| 1   | P     | 0.88         | 0/746           | 1.03        | 1/999 (0.1%)    |
| 1   | Q     | 1.03         | 2/718 (0.3%)    | 1.07        | 3/961 (0.3%)    |
| 1   | R     | 0.88         | 0/762           | 1.03        | 2/1021 (0.2%)   |
| 1   | S     | 0.95         | 1/762 (0.1%)    | 0.99        | 0/1019          |
| 1   | T     | 0.87         | 0/761           | 1.04        | 0/1019          |
| All | All   | 0.97         | 19/15091 (0.1%) | 1.05        | 32/20199 (0.2%) |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | L     | 69  | GLU  | C-O   | -7.51 | 1.14        | 1.23     |
| 1   | K     | 32  | SER  | C-O   | -6.69 | 1.16        | 1.24     |
| 1   | D     | 69  | GLU  | C-O   | -6.19 | 1.16        | 1.23     |
| 1   | L     | 70  | VAL  | C-O   | -6.17 | 1.17        | 1.24     |
| 1   | O     | 39  | THR  | C-O   | -6.15 | 1.16        | 1.24     |
| 1   | L     | 16  | PHE  | C-O   | -6.15 | 1.17        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | I     | 12  | MET  | SD-CE | -6.07 | 1.64        | 1.79     |
| 1   | Q     | 6   | GLU  | C-O   | -5.90 | 1.17        | 1.24     |
| 1   | I     | 70  | VAL  | C-O   | -5.71 | 1.17        | 1.24     |
| 1   | D     | 70  | VAL  | C-O   | -5.64 | 1.18        | 1.24     |
| 1   | Q     | 4   | PRO  | C-O   | -5.54 | 1.17        | 1.24     |
| 1   | S     | 63  | ASP  | C-O   | -5.41 | 1.17        | 1.23     |
| 1   | E     | 35  | LYS  | C-O   | -5.32 | 1.18        | 1.24     |
| 1   | N     | 31  | LYS  | C-O   | -5.30 | 1.17        | 1.24     |
| 1   | A     | 40  | ARG  | C-O   | -5.28 | 1.17        | 1.24     |
| 1   | C     | 69  | GLU  | C-O   | -5.25 | 1.17        | 1.23     |
| 1   | E     | 31  | LYS  | C-O   | -5.12 | 1.18        | 1.24     |
| 1   | C     | 70  | VAL  | C-O   | -5.08 | 1.18        | 1.24     |
| 1   | L     | 11  | VAL  | C-O   | -5.03 | 1.18        | 1.24     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | D     | 53  | ALA  | N-CA-C   | -12.97 | 97.14       | 111.28   |
| 1   | Q     | 56  | GLN  | N-CA-C   | 9.81   | 121.98      | 111.28   |
| 1   | K     | 48  | LYS  | N-CA-C   | 9.49   | 123.48      | 111.24   |
| 1   | F     | 46  | LEU  | N-CA-C   | 9.24   | 121.12      | 111.14   |
| 1   | R     | 48  | LYS  | N-CA-C   | 8.27   | 120.07      | 111.14   |
| 1   | M     | 46  | LEU  | N-CA-C   | 8.12   | 120.21      | 111.36   |
| 1   | K     | 50  | THR  | N-CA-C   | 7.25   | 121.40      | 111.39   |
| 1   | Q     | 17  | HIS  | N-CA-C   | 7.04   | 119.03      | 111.36   |
| 1   | M     | 52  | GLU  | N-CA-C   | 6.77   | 118.66      | 111.28   |
| 1   | D     | 53  | ALA  | CA-C-N   | 6.26   | 128.66      | 120.28   |
| 1   | D     | 53  | ALA  | C-N-CA   | 6.26   | 128.66      | 120.28   |
| 1   | D     | 22  | LYS  | N-CA-C   | 6.23   | 118.07      | 111.28   |
| 1   | Q     | 45  | PHE  | N-CA-C   | 6.13   | 117.96      | 111.28   |
| 1   | K     | 46  | LEU  | N-CA-C   | 6.00   | 117.82      | 111.28   |
| 1   | A     | 93  | PHE  | C-N-CD   | -5.78  | 101.30      | 125.00   |
| 1   | H     | 93  | PHE  | CA-C-N   | 5.69   | 124.89      | 118.97   |
| 1   | H     | 93  | PHE  | C-N-CA   | 5.69   | 124.89      | 118.97   |
| 1   | E     | 31  | LYS  | N-CA-C   | 5.58   | 117.80      | 111.11   |
| 1   | E     | 92  | GLY  | N-CA-C   | 5.57   | 122.16      | 114.92   |
| 1   | P     | 77  | VAL  | N-CA-C   | -5.56  | 105.10      | 110.72   |
| 1   | I     | 12  | MET  | CG-SD-CE | 5.41   | 112.81      | 100.90   |
| 1   | R     | 46  | LEU  | N-CA-C   | 5.38   | 117.23      | 111.36   |
| 1   | F     | 37  | LEU  | N-CA-C   | -5.35  | 105.35      | 111.07   |
| 1   | L     | 46  | LEU  | N-CA-C   | 5.29   | 116.86      | 111.14   |
| 1   | K     | 52  | GLU  | N-CA-C   | 5.28   | 117.04      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 61  | ASN  | N-CA-C | 5.22  | 117.06      | 111.36   |
| 1   | A     | 93  | PHE  | N-CA-C | -5.18 | 98.37       | 109.81   |
| 1   | C     | 76  | CYS  | N-CA-C | 5.12  | 116.55      | 111.07   |
| 1   | O     | 53  | ALA  | N-CA-C | 5.07  | 116.66      | 111.03   |
| 1   | H     | 13  | VAL  | N-CA-C | 5.07  | 115.29      | 110.53   |
| 1   | D     | 42  | LEU  | CA-C-N | 5.05  | 124.35      | 118.85   |
| 1   | D     | 42  | LEU  | C-N-CA | 5.05  | 124.35      | 118.85   |

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     | 754   | 0        | 742      | 14      | 0            |
| 1   | B     | 740   | 0        | 710      | 18      | 0            |
| 1   | C     | 746   | 0        | 718      | 19      | 0            |
| 1   | D     | 752   | 0        | 732      | 22      | 0            |
| 1   | E     | 741   | 0        | 722      | 20      | 0            |
| 1   | F     | 709   | 0        | 662      | 18      | 0            |
| 1   | G     | 718   | 0        | 693      | 19      | 0            |
| 1   | H     | 752   | 0        | 722      | 10      | 0            |
| 1   | I     | 744   | 0        | 718      | 5       | 0            |
| 1   | J     | 756   | 0        | 743      | 12      | 0            |
| 1   | K     | 738   | 0        | 707      | 13      | 0            |
| 1   | L     | 744   | 0        | 718      | 15      | 0            |
| 1   | M     | 731   | 0        | 700      | 34      | 0            |
| 1   | N     | 743   | 0        | 722      | 18      | 0            |
| 1   | O     | 745   | 0        | 720      | 14      | 0            |
| 1   | P     | 733   | 0        | 700      | 13      | 0            |
| 1   | Q     | 702   | 0        | 671      | 19      | 0            |
| 1   | R     | 745   | 0        | 716      | 10      | 0            |
| 1   | S     | 748   | 0        | 729      | 15      | 0            |
| 1   | T     | 744   | 0        | 718      | 10      | 0            |
| 2   | A     | 56    | 0        | 48       | 0       | 0            |
| 2   | B     | 56    | 0        | 48       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 56    | 0        | 48       | 0       | 0            |
| 2   | D     | 56    | 0        | 48       | 0       | 0            |
| 2   | E     | 56    | 0        | 48       | 2       | 0            |
| 2   | F     | 56    | 0        | 48       | 2       | 0            |
| 2   | G     | 56    | 0        | 48       | 2       | 0            |
| 2   | H     | 56    | 0        | 48       | 0       | 0            |
| 2   | I     | 56    | 0        | 48       | 0       | 0            |
| 2   | J     | 56    | 0        | 48       | 0       | 0            |
| 2   | K     | 56    | 0        | 48       | 0       | 0            |
| 2   | L     | 56    | 0        | 48       | 1       | 0            |
| 2   | M     | 56    | 0        | 48       | 3       | 0            |
| 2   | N     | 56    | 0        | 48       | 2       | 0            |
| 2   | O     | 56    | 0        | 48       | 1       | 0            |
| 2   | P     | 56    | 0        | 48       | 2       | 0            |
| 2   | Q     | 56    | 0        | 48       | 1       | 0            |
| 2   | R     | 56    | 0        | 48       | 1       | 0            |
| 2   | S     | 56    | 0        | 48       | 2       | 0            |
| 2   | T     | 56    | 0        | 48       | 0       | 0            |
| 3   | A     | 2     | 0        | 0        | 0       | 0            |
| 3   | B     | 2     | 0        | 0        | 0       | 0            |
| 3   | C     | 2     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 2     | 0        | 0        | 0       | 0            |
| 3   | F     | 2     | 0        | 0        | 0       | 0            |
| 3   | G     | 2     | 0        | 0        | 0       | 0            |
| 3   | H     | 2     | 0        | 0        | 0       | 0            |
| 3   | I     | 2     | 0        | 0        | 0       | 0            |
| 3   | J     | 2     | 0        | 0        | 0       | 0            |
| 3   | K     | 2     | 0        | 0        | 0       | 0            |
| 3   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | M     | 2     | 0        | 0        | 0       | 0            |
| 3   | N     | 2     | 0        | 0        | 0       | 0            |
| 3   | O     | 2     | 0        | 0        | 0       | 0            |
| 3   | P     | 2     | 0        | 0        | 0       | 0            |
| 3   | Q     | 2     | 0        | 0        | 0       | 0            |
| 3   | R     | 2     | 0        | 0        | 0       | 0            |
| 3   | S     | 2     | 0        | 0        | 0       | 0            |
| 3   | T     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 57    | 0        | 0        | 0       | 0            |
| 4   | B     | 75    | 0        | 0        | 2       | 0            |
| 4   | C     | 56    | 0        | 0        | 3       | 0            |
| 4   | D     | 48    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | E     | 47    | 0        | 0        | 3       | 0            |
| 4   | F     | 41    | 0        | 0        | 1       | 0            |
| 4   | G     | 28    | 0        | 0        | 0       | 0            |
| 4   | H     | 26    | 0        | 0        | 3       | 0            |
| 4   | I     | 51    | 0        | 0        | 0       | 0            |
| 4   | J     | 65    | 0        | 0        | 1       | 0            |
| 4   | K     | 52    | 0        | 0        | 0       | 0            |
| 4   | L     | 53    | 0        | 0        | 1       | 0            |
| 4   | M     | 35    | 0        | 0        | 0       | 0            |
| 4   | N     | 49    | 0        | 0        | 3       | 0            |
| 4   | O     | 33    | 0        | 0        | 0       | 0            |
| 4   | P     | 42    | 0        | 0        | 0       | 0            |
| 4   | Q     | 28    | 0        | 0        | 0       | 0            |
| 4   | R     | 32    | 0        | 0        | 4       | 0            |
| 4   | S     | 60    | 0        | 0        | 1       | 0            |
| 4   | T     | 32    | 0        | 0        | 1       | 0            |
| All | All   | 16855 | 0        | 15223    | 273     | 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 9.

All (273) 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:12:MET:SD     | 1:P:12:MET:HE1   | 1.91                     | 1.09              |
| 1:Q:12[A]:MET:HE1 | 4:R:1326:HOH:O   | 1.52                     | 1.08              |
| 1:A:93:PHE:N      | 1:A:94:PRO:CD    | 2.16                     | 1.04              |
| 1:A:92:GLY:O      | 1:A:93:PHE:HB2   | 1.59                     | 1.00              |
| 1:M:12:MET:SD     | 1:N:12[A]:MET:SD | 2.59                     | 0.99              |
| 1:A:93:PHE:N      | 1:A:94:PRO:HD2   | 1.82                     | 0.94              |
| 1:G:12:MET:HE1    | 4:H:1515:HOH:O   | 1.68                     | 0.93              |
| 1:O:85:MET:HE3    | 1:O:85:MET:HA    | 1.51                     | 0.93              |
| 1:I:12:MET:SD     | 1:J:12[A]:MET:SD | 2.69                     | 0.91              |
| 1:M:29:LEU:HB2    | 1:M:70:VAL:CG2   | 2.03                     | 0.89              |
| 1:E:87:ASN:HD22   | 1:F:17:HIS:HE1   | 1.18                     | 0.87              |
| 1:O:12:MET:SD     | 1:P:12:MET:CE    | 2.64                     | 0.86              |
| 1:B:49:ARG:HB3    | 1:B:49:ARG:NH1   | 1.92                     | 0.85              |
| 1:A:93:PHE:H      | 1:A:94:PRO:HD2   | 1.37                     | 0.84              |
| 1:N:52:GLU:HA     | 1:N:52:GLU:OE1   | 1.77                     | 0.83              |
| 1:O:35:LYS:O      | 1:O:39:THR:HG23  | 1.78                     | 0.83              |
| 1:E:6:GLU:OE1     | 1:F:44:SER:HB2   | 1.80                     | 0.81              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:G:34:LEU:HD23 | 1:G:59:MET:HG2    | 1.64                     | 0.80              |
| 1:C:8:ALA:O     | 1:C:12[A]:MET:HG3 | 1.81                     | 0.80              |
| 1:Q:46:LEU:O    | 1:Q:47:GLY:C      | 2.23                     | 0.79              |
| 1:G:12:MET:SD   | 1:H:12:MET:HE1    | 2.23                     | 0.79              |
| 1:O:12:MET:SD   | 1:P:12:MET:SD     | 2.81                     | 0.79              |
| 1:M:2:ALA:HB3   | 1:M:7:LYS:NZ      | 1.99                     | 0.77              |
| 1:D:52:GLU:O    | 1:D:52:GLU:HG2    | 1.83                     | 0.76              |
| 1:C:6:GLU:OE2   | 1:D:43:PRO:HD2    | 1.86                     | 0.76              |
| 1:N:52:GLU:O    | 1:N:56:GLN:HB2    | 1.87                     | 0.75              |
| 1:T:67:ASP:O    | 1:T:68:ASN:CB     | 2.30                     | 0.75              |
| 1:Q:71:ASP:OD1  | 1:Q:73:GLN:HG2    | 1.87                     | 0.74              |
| 1:A:93:PHE:H    | 1:A:94:PRO:CD     | 1.88                     | 0.73              |
| 1:E:87:ASN:ND2  | 1:F:17:HIS:HE1    | 1.87                     | 0.73              |
| 1:H:4:PRO:HA    | 1:H:7:LYS:HE2     | 1.69                     | 0.73              |
| 1:E:87:ASN:HD22 | 1:F:17:HIS:CE1    | 2.06                     | 0.72              |
| 1:M:30:ASN:HA   | 1:M:69:GLU:HG2    | 1.72                     | 0.72              |
| 1:M:29:LEU:HB2  | 1:M:70:VAL:HG22   | 1.72                     | 0.71              |
| 1:M:12:MET:HE3  | 4:N:1099:HOH:O    | 1.89                     | 0.70              |
| 1:E:87:ASN:ND2  | 1:F:17:HIS:CE1    | 2.60                     | 0.69              |
| 1:K:12:MET:SD   | 1:L:12:MET:HE1    | 2.32                     | 0.69              |
| 1:J:66:ARG:HH11 | 1:J:66:ARG:CG     | 2.05                     | 0.69              |
| 1:B:47:GLY:HA3  | 2:B:201:TFP:H201  | 1.73                     | 0.69              |
| 1:M:67:ASP:O    | 1:M:68:ASN:HB2    | 1.93                     | 0.69              |
| 1:T:67:ASP:O    | 1:T:68:ASN:HB2    | 1.93                     | 0.69              |
| 1:E:12:MET:HE3  | 1:E:79:LEU:HD12   | 1.74                     | 0.69              |
| 1:M:39:THR:HG22 | 1:M:46:LEU:HD12   | 1.75                     | 0.68              |
| 1:Q:55:PHE:CD1  | 1:Q:55:PHE:C      | 2.70                     | 0.68              |
| 1:M:2:ALA:HB3   | 1:M:7:LYS:HZ1     | 1.58                     | 0.68              |
| 1:K:49:ARG:CB   | 1:T:26:LYS:HE2    | 2.24                     | 0.67              |
| 1:L:40:ARG:NH1  | 4:L:2343:HOH:O    | 2.24                     | 0.67              |
| 1:C:84:MET:HE1  | 1:D:73:GLN:HG3    | 1.77                     | 0.67              |
| 4:C:1146:HOH:O  | 1:D:3:CYS:HB2     | 1.93                     | 0.66              |
| 1:O:35:LYS:HA   | 1:O:55:PHE:CZ     | 2.31                     | 0.66              |
| 1:C:93:PHE:CB   | 1:C:94:PRO:HD3    | 2.26                     | 0.66              |
| 1:D:51:ASP:OD1  | 1:D:51:ASP:N      | 2.29                     | 0.66              |
| 1:O:85:MET:HA   | 1:O:85:MET:CE     | 2.24                     | 0.65              |
| 1:N:25:ASP:OD2  | 1:N:28:LYS:HE2    | 1.95                     | 0.65              |
| 1:B:49:ARG:HB3  | 1:B:49:ARG:HH11   | 1.60                     | 0.65              |
| 1:G:9:LEU:HD23  | 1:H:12:MET:HE2    | 1.79                     | 0.65              |
| 1:H:49:ARG:HH11 | 1:H:49:ARG:HB2    | 1.62                     | 0.65              |
| 1:A:26:LYS:HG2  | 1:J:49:ARG:NH1    | 2.13                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:28:LYS:HD3    | 1:B:71:ASP:HB3    | 1.79                     | 0.63              |
| 1:M:12:MET:CE     | 1:N:12[A]:MET:SD  | 2.87                     | 0.63              |
| 1:E:6:GLU:OE1     | 1:F:44:SER:CB     | 2.47                     | 0.62              |
| 1:E:36:GLU:OE1    | 1:E:40:ARG:NH1    | 2.32                     | 0.62              |
| 1:G:34:LEU:CD2    | 1:G:59:MET:HG2    | 2.30                     | 0.62              |
| 1:M:73:GLN:HG3    | 1:N:84:MET:HE1    | 1.82                     | 0.62              |
| 1:K:46:LEU:HD13   | 1:K:50:THR:HG21   | 1.82                     | 0.61              |
| 1:O:35:LYS:HA     | 1:O:55:PHE:HZ     | 1.65                     | 0.61              |
| 1:R:68:ASN:ND2    | 4:R:1832:HOH:O    | 2.33                     | 0.61              |
| 1:A:92:GLY:O      | 1:A:93:PHE:CB     | 2.40                     | 0.60              |
| 1:Q:43:PRO:O      | 1:Q:47:GLY:N      | 2.33                     | 0.60              |
| 4:C:1838:HOH:O    | 1:D:12[A]:MET:HE1 | 2.02                     | 0.60              |
| 1:J:66:ARG:HH11   | 1:J:66:ARG:HG2    | 1.67                     | 0.59              |
| 1:N:52:GLU:OE1    | 1:N:52:GLU:CA     | 2.50                     | 0.59              |
| 1:S:12:MET:HG3    | 1:S:79:LEU:CD1    | 2.32                     | 0.59              |
| 1:L:36:GLU:O      | 1:L:40:ARG:HG2    | 2.03                     | 0.58              |
| 1:K:49:ARG:CB     | 1:T:26:LYS:CE     | 2.81                     | 0.58              |
| 1:C:84:MET:CE     | 1:D:73:GLN:HG3    | 2.34                     | 0.58              |
| 1:D:7:LYS:NZ      | 4:D:709:HOH:O     | 2.37                     | 0.57              |
| 1:C:93:PHE:HB2    | 1:C:94:PRO:HD3    | 1.86                     | 0.57              |
| 1:A:50:THR:HG23   | 1:A:55:PHE:CE2    | 2.40                     | 0.57              |
| 1:Q:62:LEU:HD22   | 1:Q:78:PHE:HB2    | 1.86                     | 0.57              |
| 1:M:45:PHE:HE1    | 2:M:201:TFP:C8    | 2.19                     | 0.56              |
| 1:G:87:ASN:OD1    | 1:H:17:HIS:HE1    | 1.88                     | 0.56              |
| 1:K:73:GLN:HG3    | 1:L:84:MET:HE1    | 1.86                     | 0.56              |
| 1:R:12[B]:MET:HE3 | 4:R:1847:HOH:O    | 2.05                     | 0.56              |
| 1:L:21:GLY:HA3    | 1:S:48:LYS:HG2    | 1.87                     | 0.56              |
| 1:M:17:HIS:HE1    | 1:N:87:ASN:OD1    | 1.89                     | 0.56              |
| 1:Q:28:LYS:HE2    | 1:Q:71:ASP:HB3    | 1.89                     | 0.55              |
| 1:G:87:ASN:OD1    | 1:H:17:HIS:CE1    | 2.59                     | 0.54              |
| 1:A:91:GLU:HG3    | 1:B:27:PHE:CD1    | 2.42                     | 0.54              |
| 1:J:61:ASN:C      | 1:J:61:ASN:ND2    | 2.64                     | 0.54              |
| 1:S:6:GLU:OE1     | 1:T:44:SER:OG     | 2.24                     | 0.54              |
| 1:E:9:LEU:O       | 1:E:13:VAL:HG12   | 2.07                     | 0.54              |
| 1:Q:26:LYS:HE3    | 4:T:1968:HOH:O    | 2.08                     | 0.54              |
| 1:M:2:ALA:HB3     | 1:M:7:LYS:HZ2     | 1.72                     | 0.54              |
| 1:M:58:LEU:O      | 1:M:62:LEU:HG     | 2.08                     | 0.54              |
| 1:M:3:CYS:H       | 1:M:7:LYS:NZ      | 2.06                     | 0.54              |
| 1:N:93:PHE:C      | 4:N:1615:HOH:O    | 2.50                     | 0.54              |
| 1:G:22:LYS:NZ     | 1:G:36:GLU:OE2    | 2.36                     | 0.54              |
| 1:D:9:LEU:HD23    | 1:D:12[B]:MET:CE  | 2.37                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:45:PHE:HE1    | 2:F:201:TFP:C8   | 2.21                     | 0.53              |
| 1:G:62:LEU:HD11   | 1:G:78:PHE:CG    | 2.43                     | 0.53              |
| 1:M:46:LEU:HD11   | 1:M:55:PHE:CE1   | 2.44                     | 0.53              |
| 1:C:22:LYS:NZ     | 1:C:36:GLU:OE1   | 2.42                     | 0.53              |
| 1:E:90:PHE:CE1    | 1:F:13:VAL:HG12  | 2.43                     | 0.53              |
| 1:K:12:MET:HG3    | 1:K:79:LEU:HD12  | 1.91                     | 0.53              |
| 1:F:31:LYS:HA     | 1:F:59:MET:CE    | 2.38                     | 0.53              |
| 1:G:47:GLY:HA3    | 2:G:201:TFP:H201 | 1.91                     | 0.53              |
| 1:I:18:LYS:HD3    | 1:I:19:TYR:CE2   | 2.44                     | 0.52              |
| 1:E:50:THR:HB     | 1:E:55:PHE:CE1   | 2.45                     | 0.52              |
| 1:G:62:LEU:CD1    | 1:G:78:PHE:HB2   | 2.40                     | 0.52              |
| 1:J:39:THR:HA     | 1:J:46:LEU:HD12  | 1.91                     | 0.52              |
| 1:R:25:ASP:OD2    | 1:R:28:LYS:HD2   | 2.09                     | 0.52              |
| 1:G:62:LEU:HD11   | 1:G:78:PHE:HB2   | 1.92                     | 0.52              |
| 1:A:75:TYR:CZ     | 1:A:79:LEU:HD11  | 2.46                     | 0.51              |
| 1:B:26:LYS:HE2    | 1:C:48:LYS:O     | 2.10                     | 0.51              |
| 1:M:70:VAL:HG23   | 1:M:70:VAL:O     | 2.09                     | 0.51              |
| 1:R:12[B]:MET:HE2 | 1:R:79:LEU:HD12  | 1.92                     | 0.51              |
| 1:E:45:PHE:O      | 2:E:201:TFP:H171 | 2.11                     | 0.51              |
| 1:C:93:PHE:CB     | 1:C:94:PRO:CD    | 2.88                     | 0.51              |
| 1:D:52:GLU:O      | 1:D:52:GLU:CG    | 2.55                     | 0.51              |
| 1:M:3:CYS:H       | 1:M:7:LYS:HZ2    | 1.59                     | 0.51              |
| 1:T:18:LYS:HD3    | 1:T:19:TYR:CE2   | 2.45                     | 0.51              |
| 1:B:49:ARG:HB3    | 1:B:49:ARG:CZ    | 2.40                     | 0.51              |
| 1:R:46:LEU:HD13   | 1:R:50:THR:HG21  | 1.92                     | 0.50              |
| 1:H:71:ASP:HB2    | 4:H:1259:HOH:O   | 2.10                     | 0.50              |
| 1:B:37:LEU:HD23   | 1:B:37:LEU:C     | 2.37                     | 0.50              |
| 1:E:91:GLU:HG2    | 1:F:27:PHE:CD1   | 2.47                     | 0.50              |
| 1:N:75:TYR:CZ     | 1:N:79:LEU:HD11  | 2.47                     | 0.50              |
| 1:G:62:LEU:HD11   | 1:G:78:PHE:CB    | 2.42                     | 0.50              |
| 1:S:35:LYS:HG3    | 1:S:55:PHE:CZ    | 2.47                     | 0.49              |
| 1:R:49:ARG:NH2    | 1:S:24:GLY:O     | 2.41                     | 0.49              |
| 1:D:51:ASP:OD1    | 1:D:54:ALA:HB3   | 2.12                     | 0.49              |
| 1:H:84:MET:O      | 1:H:88:GLU:HG2   | 2.13                     | 0.49              |
| 1:G:43:PRO:HD2    | 1:H:6:GLU:OE2    | 2.13                     | 0.49              |
| 1:I:68:ASN:O      | 1:I:69:GLU:HG3   | 2.12                     | 0.49              |
| 1:F:30:ASN:OD1    | 1:F:30:ASN:C     | 2.56                     | 0.48              |
| 1:K:12:MET:HG3    | 1:K:79:LEU:CD1   | 2.44                     | 0.48              |
| 1:O:29:LEU:HD13   | 1:O:34:LEU:HD12  | 1.94                     | 0.48              |
| 1:E:58:LEU:HD23   | 4:E:932:HOH:O    | 2.13                     | 0.48              |
| 1:Q:34:LEU:CD2    | 1:Q:59:MET:HG2   | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Q:59:MET:SD     | 1:Q:59:MET:C      | 2.97                     | 0.48              |
| 1:A:80:SER:O      | 1:A:84:MET:HG3    | 2.14                     | 0.48              |
| 1:M:12:MET:HE1    | 1:N:12[A]:MET:SD  | 2.54                     | 0.48              |
| 1:Q:21:GLY:HA2    | 1:Q:26:LYS:HG3    | 1.96                     | 0.48              |
| 1:Q:59:MET:SD     | 1:Q:59:MET:O      | 2.72                     | 0.48              |
| 1:B:85:MET:HG3    | 2:B:201:TFP:C11   | 2.44                     | 0.47              |
| 1:R:62:LEU:HD21   | 1:R:78:PHE:CD1    | 2.49                     | 0.47              |
| 1:J:61:ASN:C      | 1:J:61:ASN:HD22   | 2.23                     | 0.47              |
| 1:B:35:LYS:HD3    | 4:B:439:HOH:O     | 2.13                     | 0.47              |
| 1:M:17:HIS:CE1    | 1:N:87:ASN:OD1    | 2.67                     | 0.47              |
| 1:I:51:ASP:OD1    | 1:I:51:ASP:N      | 2.31                     | 0.47              |
| 1:C:93:PHE:HB3    | 1:C:94:PRO:HD3    | 1.95                     | 0.47              |
| 1:E:2:ALA:HB3     | 4:E:2123:HOH:O    | 2.14                     | 0.47              |
| 1:M:84:MET:HE1    | 1:N:73:GLN:HG2    | 1.96                     | 0.47              |
| 1:L:18:LYS:HD3    | 1:L:19:TYR:CE2    | 2.50                     | 0.46              |
| 2:M:201:TFP:H6    | 1:P:93:PHE:HE2    | 1.81                     | 0.46              |
| 1:O:17:HIS:HE1    | 1:P:87:ASN:OD1    | 1.98                     | 0.46              |
| 1:P:9:LEU:O       | 1:P:13:VAL:HG23   | 2.16                     | 0.46              |
| 1:D:51:ASP:O      | 1:D:52:GLU:HB3    | 2.16                     | 0.46              |
| 1:M:35:LYS:HB2    | 1:M:35:LYS:HE3    | 1.63                     | 0.46              |
| 1:J:22:LYS:HE2    | 1:J:36:GLU:OE1    | 2.15                     | 0.46              |
| 1:L:45:PHE:HE1    | 2:L:201:TFP:C8    | 2.29                     | 0.46              |
| 1:M:29:LEU:HD12   | 1:M:70:VAL:CG2    | 2.46                     | 0.46              |
| 1:C:12[A]:MET:HE1 | 1:D:12[A]:MET:HB2 | 1.98                     | 0.45              |
| 1:J:66:ARG:CG     | 1:J:66:ARG:NH1    | 2.70                     | 0.45              |
| 2:S:202:TFP:H6    | 2:S:202:TFP:H131  | 1.73                     | 0.45              |
| 1:A:36:GLU:O      | 1:A:40:ARG:HG3    | 2.16                     | 0.45              |
| 1:R:92:GLY:O      | 1:R:93:PHE:O      | 2.33                     | 0.45              |
| 1:B:30:ASN:OD1    | 1:B:30:ASN:C      | 2.59                     | 0.45              |
| 1:F:7:LYS:NZ      | 4:F:1050:HOH:O    | 2.34                     | 0.45              |
| 1:K:59:MET:CE     | 1:K:68:ASN:C      | 2.90                     | 0.45              |
| 1:Q:45:PHE:HE1    | 2:Q:201:TFP:C8    | 2.30                     | 0.45              |
| 1:Q:12[A]:MET:CE  | 4:R:1326:HOH:O    | 2.34                     | 0.45              |
| 1:D:93:PHE:HE2    | 2:E:201:TFP:H6    | 1.82                     | 0.45              |
| 1:J:37:LEU:C      | 1:J:37:LEU:HD23   | 2.42                     | 0.45              |
| 1:D:57:LYS:O      | 1:D:61:ASN:HB2    | 2.17                     | 0.45              |
| 1:E:86:CYS:HB2    | 1:F:13:VAL:HG21   | 1.98                     | 0.45              |
| 1:F:28:LYS:HG2    | 1:F:71:ASP:HB3    | 1.98                     | 0.45              |
| 4:C:1838:HOH:O    | 1:D:12[A]:MET:CE  | 2.63                     | 0.45              |
| 1:E:37:LEU:HD23   | 1:E:37:LEU:C      | 2.42                     | 0.44              |
| 1:I:50:THR:HB     | 1:I:55:PHE:CE2    | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:12:MET:HE3   | 1:O:79:LEU:HD12  | 1.99                     | 0.44              |
| 1:S:12:MET:HG3   | 1:S:79:LEU:HD12  | 1.98                     | 0.44              |
| 1:M:36:GLU:O     | 1:M:40:ARG:HG3   | 2.17                     | 0.44              |
| 1:M:39:THR:HG22  | 1:M:46:LEU:CD1   | 2.44                     | 0.44              |
| 1:R:63:ASP:OD2   | 1:R:66:ARG:HA    | 2.17                     | 0.44              |
| 1:S:37:LEU:HD23  | 1:S:37:LEU:C     | 2.41                     | 0.44              |
| 1:B:46:LEU:HA    | 1:B:46:LEU:HD12  | 1.69                     | 0.44              |
| 1:S:85:MET:HG3   | 2:S:201:TFP:C12  | 2.48                     | 0.44              |
| 1:T:79:LEU:HD23  | 1:T:79:LEU:HA    | 1.85                     | 0.44              |
| 1:S:23:GLU:N     | 1:S:33:GLU:OE2   | 2.50                     | 0.44              |
| 1:B:12:MET:HG3   | 1:B:79:LEU:HD12  | 1.98                     | 0.44              |
| 1:L:9:LEU:O      | 1:L:13:VAL:HG23  | 2.18                     | 0.44              |
| 1:K:10:ASP:OD1   | 2:N:202:TFP:N3   | 2.51                     | 0.44              |
| 1:G:12:MET:CE    | 4:H:1515:HOH:O   | 2.45                     | 0.44              |
| 1:P:12:MET:HG2   | 1:P:79:LEU:HD13  | 2.00                     | 0.44              |
| 1:T:67:ASP:O     | 1:T:68:ASN:HB3   | 2.14                     | 0.44              |
| 1:R:48:LYS:HG2   | 1:S:21:GLY:HA3   | 1.99                     | 0.44              |
| 1:O:58:LEU:O     | 1:O:62:LEU:HG    | 2.18                     | 0.43              |
| 1:B:84:MET:HE3   | 4:B:1840:HOH:O   | 2.19                     | 0.43              |
| 1:G:9:LEU:O      | 1:G:13:VAL:HG23  | 2.19                     | 0.43              |
| 1:L:80:SER:O     | 1:L:84:MET:HG2   | 2.19                     | 0.43              |
| 1:J:75:TYR:CZ    | 1:J:79:LEU:HD11  | 2.53                     | 0.43              |
| 1:P:86:CYS:O     | 1:P:89:PHE:HB3   | 2.17                     | 0.43              |
| 1:F:45:PHE:HE1   | 2:F:201:TFP:H8   | 1.83                     | 0.43              |
| 2:G:201:TFP:H142 | 2:G:201:TFP:H162 | 1.63                     | 0.43              |
| 1:L:26:LYS:HE2   | 1:S:49:ARG:HB2   | 2.01                     | 0.43              |
| 1:C:36:GLU:O     | 1:C:40:ARG:CG    | 2.67                     | 0.43              |
| 1:K:46:LEU:HD22  | 1:K:50:THR:CG2   | 2.48                     | 0.43              |
| 1:A:92:GLY:C     | 1:A:94:PRO:N     | 2.72                     | 0.43              |
| 1:D:56:GLN:HE21  | 1:D:56:GLN:HA    | 1.84                     | 0.43              |
| 1:B:13:VAL:HG22  | 1:B:72:PHE:HZ    | 1.84                     | 0.43              |
| 1:E:40:ARG:NH2   | 4:E:1729:HOH:O   | 2.50                     | 0.43              |
| 1:S:73:GLN:HG3   | 4:S:265:HOH:O    | 2.17                     | 0.43              |
| 1:M:93:PHE:HD1   | 2:P:201:TFP:H131 | 1.84                     | 0.42              |
| 2:O:202:TFP:H6   | 2:O:202:TFP:H131 | 1.79                     | 0.42              |
| 1:C:58:LEU:O     | 1:C:62:LEU:HG    | 2.19                     | 0.42              |
| 1:D:29:LEU:HB2   | 1:D:70:VAL:HB    | 2.01                     | 0.42              |
| 1:P:84:MET:HE2   | 1:P:84:MET:HB2   | 1.93                     | 0.42              |
| 1:Q:70:VAL:HA    | 1:Q:74:GLU:OE1   | 2.18                     | 0.42              |
| 2:P:202:TFP:H6   | 2:P:202:TFP:H131 | 1.81                     | 0.42              |
| 1:D:35:LYS:HG2   | 1:D:55:PHE:CZ    | 2.54                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:92:GLY:O    | 1:E:93:PHE:C     | 2.62                     | 0.42              |
| 1:G:5:LEU:HD22  | 1:H:15:THR:HG21  | 2.00                     | 0.42              |
| 1:K:35:LYS:HG3  | 1:K:55:PHE:CZ    | 2.55                     | 0.42              |
| 1:L:93:PHE:HA   | 1:L:94:PRO:HD2   | 1.87                     | 0.42              |
| 1:B:45:PHE:HE1  | 2:B:201:TFP:C8   | 2.32                     | 0.42              |
| 1:Q:26:LYS:HD3  | 1:T:48:LYS:HG2   | 2.01                     | 0.42              |
| 1:G:23:GLU:HG3  | 1:G:30:ASN:HD21  | 1.84                     | 0.42              |
| 1:M:46:LEU:HD23 | 1:M:46:LEU:HA    | 1.74                     | 0.42              |
| 1:M:59:MET:HE1  | 1:M:69:GLU:HA    | 2.02                     | 0.42              |
| 1:Q:84:MET:O    | 1:Q:88:GLU:HG2   | 2.19                     | 0.42              |
| 1:C:35:LYS:HG3  | 1:C:55:PHE:CZ    | 2.55                     | 0.42              |
| 1:E:6:GLU:OE2   | 1:F:43:PRO:HD2   | 2.20                     | 0.42              |
| 1:C:31:LYS:HE2  | 1:C:35:LYS:NZ    | 2.35                     | 0.42              |
| 1:Q:79:LEU:HD23 | 1:Q:79:LEU:HA    | 1.85                     | 0.42              |
| 1:S:12:MET:CG   | 1:S:79:LEU:HD12  | 2.49                     | 0.41              |
| 1:C:35:LYS:HE3  | 1:C:35:LYS:HB2   | 1.89                     | 0.41              |
| 1:L:26:LYS:HG3  | 1:S:49:ARG:NH2   | 2.36                     | 0.41              |
| 1:T:72:PHE:CE2  | 1:T:76:CYS:SG    | 3.14                     | 0.41              |
| 1:D:51:ASP:OD1  | 1:D:54:ALA:CB    | 2.69                     | 0.41              |
| 1:O:17:HIS:CE1  | 1:P:87:ASN:OD1   | 2.74                     | 0.41              |
| 1:C:46:LEU:HD21 | 1:C:55:PHE:CZ    | 2.56                     | 0.41              |
| 2:M:202:TFP:C6  | 2:M:202:TFP:H141 | 2.51                     | 0.41              |
| 1:B:85:MET:HG3  | 2:B:201:TFP:C12  | 2.51                     | 0.41              |
| 1:F:62:LEU:HD22 | 1:F:78:PHE:HB2   | 2.03                     | 0.41              |
| 1:G:37:LEU:O    | 1:G:41:GLU:HB2   | 2.20                     | 0.41              |
| 1:O:82:ILE:HG21 | 1:P:9:LEU:HD13   | 2.01                     | 0.41              |
| 1:P:59:MET:HE1  | 1:P:69:GLU:HA    | 2.03                     | 0.41              |
| 1:N:85:MET:HG3  | 2:N:201:TFP:C12  | 2.51                     | 0.41              |
| 1:Q:42:LEU:N    | 1:Q:43:PRO:CD    | 2.83                     | 0.41              |
| 1:B:12:MET:HG3  | 1:B:79:LEU:CD1   | 2.51                     | 0.41              |
| 1:F:7:LYS:O     | 1:F:10:ASP:HB3   | 2.21                     | 0.41              |
| 1:K:46:LEU:HD23 | 1:K:46:LEU:HA    | 1.60                     | 0.41              |
| 1:N:50:THR:CG2  | 1:N:54:ALA:HB3   | 2.51                     | 0.41              |
| 1:P:67:ASP:O    | 1:P:68:ASN:HB2   | 2.20                     | 0.41              |
| 1:C:15:THR:HG21 | 1:D:5:LEU:HD22   | 2.03                     | 0.40              |
| 1:D:35:LYS:C    | 1:D:35:LYS:HD3   | 2.46                     | 0.40              |
| 1:J:85:MET:HE3  | 4:J:1161:HOH:O   | 2.20                     | 0.40              |
| 1:L:49:ARG:NH1  | 1:M:26:LYS:HG2   | 2.36                     | 0.40              |
| 1:M:89:PHE:CD2  | 1:M:89:PHE:C     | 2.99                     | 0.40              |
| 1:N:26:LYS:NZ   | 1:N:26:LYS:H     | 2.19                     | 0.40              |
| 1:N:37:LEU:HD23 | 1:N:37:LEU:C     | 2.46                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:R:202:TFP:H141 | 2:R:202:TFP:C6  | 2.51                     | 0.40              |
| 1:K:42:LEU:HD23  | 1:L:6:GLU:HG2   | 2.02                     | 0.40              |
| 1:M:13:VAL:HG22  | 1:M:72:PHE:HZ   | 1.86                     | 0.40              |
| 1:S:42:LEU:N     | 1:S:43:PRO:CD   | 2.84                     | 0.40              |
| 1:C:75:TYR:CZ    | 1:C:79:LEU:HD11 | 2.56                     | 0.40              |
| 1:M:9:LEU:HD23   | 1:M:12:MET:HE2  | 2.04                     | 0.40              |
| 1:M:29:LEU:HD12  | 1:M:70:VAL:HG23 | 2.03                     | 0.40              |
| 1:N:18:LYS:HE3   | 4:N:2273:HOH:O  | 2.22                     | 0.40              |
| 1:L:85:MET:HA    | 1:L:85:MET:HE2  | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed     | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 92/101 (91%) | 91 (99%)  | 0       | 1 (1%)   | 11          | 13  |
| 1   | B     | 92/101 (91%) | 91 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | C     | 92/101 (91%) | 90 (98%)  | 1 (1%)  | 1 (1%)   | 11          | 13  |
| 1   | D     | 93/101 (92%) | 92 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | E     | 90/101 (89%) | 88 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | F     | 86/101 (85%) | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 1   | G     | 86/101 (85%) | 85 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | H     | 92/101 (91%) | 87 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 1   | I     | 91/101 (90%) | 90 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | J     | 93/101 (92%) | 92 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | K     | 91/101 (90%) | 90 (99%)  | 0       | 1 (1%)   | 11          | 13  |
| 1   | L     | 91/101 (90%) | 88 (97%)  | 2 (2%)  | 1 (1%)   | 11          | 13  |
| 1   | M     | 90/101 (89%) | 90 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | N     | 91/101 (90%)    | 91 (100%)  | 0       | 0        | 100         | 100 |
| 1   | O     | 91/101 (90%)    | 87 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 1   | P     | 90/101 (89%)    | 89 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | Q     | 85/101 (84%)    | 82 (96%)   | 2 (2%)  | 1 (1%)   | 10          | 12  |
| 1   | R     | 92/101 (91%)    | 89 (97%)   | 2 (2%)  | 1 (1%)   | 11          | 13  |
| 1   | S     | 91/101 (90%)    | 88 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 1   | T     | 92/101 (91%)    | 87 (95%)   | 4 (4%)  | 1 (1%)   | 11          | 13  |
| All | All   | 1811/2020 (90%) | 1770 (98%) | 34 (2%) | 7 (0%)   | 30          | 38  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 93  | PHE  |
| 1   | C     | 93  | PHE  |
| 1   | T     | 47  | GLY  |
| 1   | R     | 93  | PHE  |
| 1   | Q     | 94  | PRO  |
| 1   | K     | 93  | PHE  |
| 1   | L     | 93  | PHE  |

### 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     | 85/92 (92%) | 75 (88%)  | 10 (12%) | 5           | 6  |
| 1   | B     | 82/92 (89%) | 77 (94%)  | 5 (6%)   | 17          | 24 |
| 1   | C     | 83/92 (90%) | 78 (94%)  | 5 (6%)   | 17          | 25 |
| 1   | D     | 85/92 (92%) | 74 (87%)  | 11 (13%) | 4           | 4  |
| 1   | E     | 83/92 (90%) | 72 (87%)  | 11 (13%) | 4           | 4  |
| 1   | F     | 78/92 (85%) | 74 (95%)  | 4 (5%)   | 21          | 32 |
| 1   | G     | 80/92 (87%) | 71 (89%)  | 9 (11%)  | 5           | 7  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | H     | 84/92 (91%)     | 75 (89%)   | 9 (11%)   | 6           | 8  |
| 1   | I     | 83/92 (90%)     | 73 (88%)   | 10 (12%)  | 5           | 5  |
| 1   | J     | 86/92 (94%)     | 76 (88%)   | 10 (12%)  | 5           | 6  |
| 1   | K     | 82/92 (89%)     | 78 (95%)   | 4 (5%)    | 22          | 34 |
| 1   | L     | 83/92 (90%)     | 77 (93%)   | 6 (7%)    | 13          | 18 |
| 1   | M     | 81/92 (88%)     | 72 (89%)   | 9 (11%)   | 6           | 7  |
| 1   | N     | 83/92 (90%)     | 75 (90%)   | 8 (10%)   | 8           | 10 |
| 1   | O     | 83/92 (90%)     | 75 (90%)   | 8 (10%)   | 8           | 10 |
| 1   | P     | 81/92 (88%)     | 75 (93%)   | 6 (7%)    | 13          | 17 |
| 1   | Q     | 79/92 (86%)     | 69 (87%)   | 10 (13%)  | 4           | 5  |
| 1   | R     | 83/92 (90%)     | 74 (89%)   | 9 (11%)   | 6           | 7  |
| 1   | S     | 84/92 (91%)     | 77 (92%)   | 7 (8%)    | 10          | 14 |
| 1   | T     | 83/92 (90%)     | 76 (92%)   | 7 (8%)    | 10          | 14 |
| All | All   | 1651/1840 (90%) | 1493 (90%) | 158 (10%) | 8           | 10 |

All (158) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 35[A] | LYS  |
| 1   | A     | 35[B] | LYS  |
| 1   | A     | 40    | ARG  |
| 1   | A     | 52    | GLU  |
| 1   | A     | 58    | LEU  |
| 1   | A     | 61    | ASN  |
| 1   | A     | 69    | GLU  |
| 1   | A     | 81    | CYS  |
| 1   | A     | 91    | GLU  |
| 1   | A     | 93    | PHE  |
| 1   | B     | 7     | LYS  |
| 1   | B     | 23    | GLU  |
| 1   | B     | 32    | SER  |
| 1   | B     | 35    | LYS  |
| 1   | B     | 80    | SER  |
| 1   | C     | 7     | LYS  |
| 1   | C     | 38    | LEU  |
| 1   | C     | 40    | ARG  |
| 1   | C     | 52    | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 56  | GLN  |
| 1   | D     | 3   | CYS  |
| 1   | D     | 7   | LYS  |
| 1   | D     | 22  | LYS  |
| 1   | D     | 23  | GLU  |
| 1   | D     | 26  | LYS  |
| 1   | D     | 31  | LYS  |
| 1   | D     | 48  | LYS  |
| 1   | D     | 49  | ARG  |
| 1   | D     | 51  | ASP  |
| 1   | D     | 55  | PHE  |
| 1   | D     | 56  | GLN  |
| 1   | E     | 6   | GLU  |
| 1   | E     | 12  | MET  |
| 1   | E     | 13  | VAL  |
| 1   | E     | 32  | SER  |
| 1   | E     | 35  | LYS  |
| 1   | E     | 38  | LEU  |
| 1   | E     | 48  | LYS  |
| 1   | E     | 52  | GLU  |
| 1   | E     | 57  | LYS  |
| 1   | E     | 58  | LEU  |
| 1   | E     | 93  | PHE  |
| 1   | F     | 57  | LYS  |
| 1   | F     | 64  | SER  |
| 1   | F     | 68  | ASN  |
| 1   | F     | 84  | MET  |
| 1   | G     | 7   | LYS  |
| 1   | G     | 31  | LYS  |
| 1   | G     | 46  | LEU  |
| 1   | G     | 48  | LYS  |
| 1   | G     | 62  | LEU  |
| 1   | G     | 66  | ARG  |
| 1   | G     | 81  | CYS  |
| 1   | G     | 84  | MET  |
| 1   | G     | 88  | GLU  |
| 1   | H     | 38  | LEU  |
| 1   | H     | 40  | ARG  |
| 1   | H     | 48  | LYS  |
| 1   | H     | 49  | ARG  |
| 1   | H     | 50  | THR  |
| 1   | H     | 51  | ASP  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | H     | 52    | GLU  |
| 1   | H     | 61    | ASN  |
| 1   | H     | 81    | CYS  |
| 1   | I     | 31    | LYS  |
| 1   | I     | 40    | ARG  |
| 1   | I     | 46    | LEU  |
| 1   | I     | 48    | LYS  |
| 1   | I     | 50    | THR  |
| 1   | I     | 51    | ASP  |
| 1   | I     | 52    | GLU  |
| 1   | I     | 56    | GLN  |
| 1   | I     | 57    | LYS  |
| 1   | I     | 60    | SER  |
| 1   | J     | 7     | LYS  |
| 1   | J     | 46    | LEU  |
| 1   | J     | 50    | THR  |
| 1   | J     | 51    | ASP  |
| 1   | J     | 57    | LYS  |
| 1   | J     | 61    | ASN  |
| 1   | J     | 62    | LEU  |
| 1   | J     | 66    | ARG  |
| 1   | J     | 81[A] | CYS  |
| 1   | J     | 81[B] | CYS  |
| 1   | K     | 31    | LYS  |
| 1   | K     | 50    | THR  |
| 1   | K     | 57    | LYS  |
| 1   | K     | 80    | SER  |
| 1   | L     | 7     | LYS  |
| 1   | L     | 58    | LEU  |
| 1   | L     | 60    | SER  |
| 1   | L     | 66    | ARG  |
| 1   | L     | 88    | GLU  |
| 1   | L     | 91    | GLU  |
| 1   | M     | 7     | LYS  |
| 1   | M     | 40    | ARG  |
| 1   | M     | 46    | LEU  |
| 1   | M     | 48    | LYS  |
| 1   | M     | 52    | GLU  |
| 1   | M     | 58    | LEU  |
| 1   | M     | 59    | MET  |
| 1   | M     | 88    | GLU  |
| 1   | M     | 91    | GLU  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | N     | 26    | LYS  |
| 1   | N     | 32    | SER  |
| 1   | N     | 52    | GLU  |
| 1   | N     | 56    | GLN  |
| 1   | N     | 57    | LYS  |
| 1   | N     | 58    | LEU  |
| 1   | N     | 65    | ASN  |
| 1   | N     | 66    | ARG  |
| 1   | O     | 7     | LYS  |
| 1   | O     | 22    | LYS  |
| 1   | O     | 39    | THR  |
| 1   | O     | 56    | GLN  |
| 1   | O     | 61    | ASN  |
| 1   | O     | 81    | CYS  |
| 1   | O     | 85    | MET  |
| 1   | O     | 91    | GLU  |
| 1   | P     | 12    | MET  |
| 1   | P     | 31    | LYS  |
| 1   | P     | 40    | ARG  |
| 1   | P     | 52    | GLU  |
| 1   | P     | 59    | MET  |
| 1   | P     | 73    | GLN  |
| 1   | Q     | 7     | LYS  |
| 1   | Q     | 12[A] | MET  |
| 1   | Q     | 12[B] | MET  |
| 1   | Q     | 23    | GLU  |
| 1   | Q     | 35    | LYS  |
| 1   | Q     | 55    | PHE  |
| 1   | Q     | 56    | GLN  |
| 1   | Q     | 58    | LEU  |
| 1   | Q     | 59    | MET  |
| 1   | Q     | 73    | GLN  |
| 1   | R     | 26    | LYS  |
| 1   | R     | 40    | ARG  |
| 1   | R     | 46    | LEU  |
| 1   | R     | 48    | LYS  |
| 1   | R     | 50    | THR  |
| 1   | R     | 64    | SER  |
| 1   | R     | 73    | GLN  |
| 1   | R     | 77    | VAL  |
| 1   | R     | 91    | GLU  |
| 1   | S     | 7     | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 31  | LYS  |
| 1   | S     | 38  | LEU  |
| 1   | S     | 48  | LYS  |
| 1   | S     | 50  | THR  |
| 1   | S     | 62  | LEU  |
| 1   | S     | 80  | SER  |
| 1   | T     | 7   | LYS  |
| 1   | T     | 22  | LYS  |
| 1   | T     | 44  | SER  |
| 1   | T     | 48  | LYS  |
| 1   | T     | 50  | THR  |
| 1   | T     | 52  | GLU  |
| 1   | T     | 68  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 56  | GLN  |
| 1   | B     | 68  | ASN  |
| 1   | C     | 61  | ASN  |
| 1   | C     | 73  | GLN  |
| 1   | D     | 56  | GLN  |
| 1   | E     | 61  | ASN  |
| 1   | E     | 68  | ASN  |
| 1   | E     | 87  | ASN  |
| 1   | F     | 17  | HIS  |
| 1   | F     | 68  | ASN  |
| 1   | H     | 17  | HIS  |
| 1   | H     | 61  | ASN  |
| 1   | H     | 73  | GLN  |
| 1   | J     | 56  | GLN  |
| 1   | K     | 61  | ASN  |
| 1   | M     | 17  | HIS  |
| 1   | M     | 73  | GLN  |
| 1   | O     | 17  | HIS  |
| 1   | O     | 56  | GLN  |
| 1   | P     | 17  | HIS  |
| 1   | P     | 73  | GLN  |
| 1   | Q     | 17  | HIS  |
| 1   | R     | 73  | GLN  |
| 1   | T     | 68  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 40 are monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | TFP  | B     | 201 | -    | 31,31,31     | 2.37 | 6 (19%)     | 45,45,45    | 1.69 | 10 (22%)    |
| 2   | TFP  | I     | 201 | -    | 31,31,31     | 2.14 | 4 (12%)     | 45,45,45    | 1.48 | 7 (15%)     |
| 2   | TFP  | N     | 202 | -    | 31,31,31     | 1.97 | 4 (12%)     | 45,45,45    | 1.45 | 7 (15%)     |
| 2   | TFP  | D     | 202 | -    | 31,31,31     | 2.11 | 4 (12%)     | 45,45,45    | 1.27 | 4 (8%)      |
| 2   | TFP  | H     | 202 | -    | 31,31,31     | 2.02 | 4 (12%)     | 45,45,45    | 1.20 | 4 (8%)      |
| 2   | TFP  | G     | 202 | -    | 31,31,31     | 2.05 | 5 (16%)     | 45,45,45    | 1.58 | 12 (26%)    |
| 2   | TFP  | O     | 202 | -    | 31,31,31     | 1.85 | 4 (12%)     | 45,45,45    | 1.24 | 5 (11%)     |
| 2   | TFP  | S     | 202 | -    | 31,31,31     | 1.91 | 4 (12%)     | 45,45,45    | 1.50 | 10 (22%)    |
| 2   | TFP  | T     | 202 | -    | 31,31,31     | 2.10 | 4 (12%)     | 45,45,45    | 1.86 | 12 (26%)    |
| 2   | TFP  | S     | 201 | -    | 31,31,31     | 2.32 | 4 (12%)     | 45,45,45    | 1.63 | 10 (22%)    |
| 2   | TFP  | L     | 202 | -    | 31,31,31     | 2.01 | 4 (12%)     | 45,45,45    | 1.48 | 7 (15%)     |
| 2   | TFP  | J     | 202 | -    | 31,31,31     | 2.07 | 4 (12%)     | 45,45,45    | 1.33 | 3 (6%)      |
| 2   | TFP  | A     | 202 | -    | 31,31,31     | 1.83 | 5 (16%)     | 45,45,45    | 1.53 | 10 (22%)    |
| 2   | TFP  | D     | 201 | -    | 31,31,31     | 2.39 | 5 (16%)     | 45,45,45    | 1.65 | 13 (28%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | TFP  | C     | 202 | -    | 31,31,31     | 1.77 | 4 (12%)  | 45,45,45    | 1.27 | 7 (15%)  |
| 2   | TFP  | H     | 201 | -    | 31,31,31     | 2.49 | 6 (19%)  | 45,45,45    | 1.28 | 8 (17%)  |
| 2   | TFP  | F     | 201 | -    | 31,31,31     | 2.36 | 4 (12%)  | 45,45,45    | 1.26 | 8 (17%)  |
| 2   | TFP  | M     | 201 | -    | 31,31,31     | 2.38 | 4 (12%)  | 45,45,45    | 1.45 | 9 (20%)  |
| 2   | TFP  | P     | 201 | -    | 31,31,31     | 2.34 | 5 (16%)  | 45,45,45    | 1.65 | 10 (22%) |
| 2   | TFP  | Q     | 202 | -    | 31,31,31     | 2.13 | 5 (16%)  | 45,45,45    | 1.51 | 11 (24%) |
| 2   | TFP  | J     | 201 | -    | 31,31,31     | 2.30 | 5 (16%)  | 45,45,45    | 1.99 | 12 (26%) |
| 2   | TFP  | B     | 202 | -    | 31,31,31     | 1.92 | 4 (12%)  | 45,45,45    | 1.53 | 9 (20%)  |
| 2   | TFP  | I     | 202 | -    | 31,31,31     | 1.77 | 4 (12%)  | 45,45,45    | 1.51 | 6 (13%)  |
| 2   | TFP  | E     | 202 | -    | 31,31,31     | 1.87 | 4 (12%)  | 45,45,45    | 1.38 | 6 (13%)  |
| 2   | TFP  | K     | 202 | -    | 31,31,31     | 1.83 | 4 (12%)  | 45,45,45    | 1.58 | 10 (22%) |
| 2   | TFP  | T     | 201 | -    | 31,31,31     | 2.35 | 5 (16%)  | 45,45,45    | 1.42 | 7 (15%)  |
| 2   | TFP  | F     | 202 | -    | 31,31,31     | 1.70 | 3 (9%)   | 45,45,45    | 1.36 | 7 (15%)  |
| 2   | TFP  | C     | 201 | -    | 31,31,31     | 2.51 | 5 (16%)  | 45,45,45    | 1.73 | 11 (24%) |
| 2   | TFP  | E     | 201 | -    | 31,31,31     | 2.47 | 4 (12%)  | 45,45,45    | 1.67 | 10 (22%) |
| 2   | TFP  | P     | 202 | -    | 31,31,31     | 1.81 | 4 (12%)  | 45,45,45    | 1.49 | 9 (20%)  |
| 2   | TFP  | R     | 202 | -    | 31,31,31     | 2.17 | 4 (12%)  | 45,45,45    | 1.44 | 6 (13%)  |
| 2   | TFP  | M     | 202 | -    | 31,31,31     | 2.22 | 4 (12%)  | 45,45,45    | 1.43 | 7 (15%)  |
| 2   | TFP  | Q     | 201 | -    | 31,31,31     | 2.38 | 4 (12%)  | 45,45,45    | 1.29 | 5 (11%)  |
| 2   | TFP  | K     | 201 | -    | 31,31,31     | 2.23 | 5 (16%)  | 45,45,45    | 1.77 | 12 (26%) |
| 2   | TFP  | N     | 201 | -    | 31,31,31     | 2.36 | 6 (19%)  | 45,45,45    | 1.29 | 6 (13%)  |
| 2   | TFP  | O     | 201 | -    | 31,31,31     | 2.40 | 4 (12%)  | 45,45,45    | 1.98 | 12 (26%) |
| 2   | TFP  | R     | 201 | -    | 31,31,31     | 2.09 | 4 (12%)  | 45,45,45    | 1.54 | 10 (22%) |
| 2   | TFP  | L     | 201 | -    | 31,31,31     | 2.24 | 4 (12%)  | 45,45,45    | 1.86 | 12 (26%) |
| 2   | TFP  | G     | 201 | -    | 31,31,31     | 2.40 | 4 (12%)  | 45,45,45    | 1.31 | 7 (15%)  |
| 2   | TFP  | A     | 201 | -    | 31,31,31     | 2.28 | 4 (12%)  | 45,45,45    | 1.97 | 12 (26%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | TFP  | B     | 201 | -    | -       | 5/12/34/34 | 0/4/4/4 |
| 2   | TFP  | I     | 201 | -    | -       | 1/12/34/34 | 0/4/4/4 |
| 2   | TFP  | N     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | TFP  | D     | 202 | -    | -       | 1/12/34/34 | 0/4/4/4 |
| 2   | TFP  | H     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | G     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | O     | 202 | -    | -       | 2/12/34/34 | 0/4/4/4 |
| 2   | TFP  | S     | 202 | -    | -       | 3/12/34/34 | 0/4/4/4 |
| 2   | TFP  | T     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | S     | 201 | -    | -       | 2/12/34/34 | 0/4/4/4 |
| 2   | TFP  | L     | 202 | -    | -       | 1/12/34/34 | 0/4/4/4 |
| 2   | TFP  | J     | 202 | -    | -       | 1/12/34/34 | 0/4/4/4 |
| 2   | TFP  | A     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | D     | 201 | -    | -       | 1/12/34/34 | 0/4/4/4 |
| 2   | TFP  | C     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | H     | 201 | -    | -       | 2/12/34/34 | 0/4/4/4 |
| 2   | TFP  | F     | 201 | -    | -       | 3/12/34/34 | 0/4/4/4 |
| 2   | TFP  | M     | 201 | -    | -       | 2/12/34/34 | 0/4/4/4 |
| 2   | TFP  | P     | 201 | -    | -       | 3/12/34/34 | 0/4/4/4 |
| 2   | TFP  | Q     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | J     | 201 | -    | -       | 3/12/34/34 | 0/4/4/4 |
| 2   | TFP  | B     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | I     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | E     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | K     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | T     | 201 | -    | -       | 2/12/34/34 | 0/4/4/4 |
| 2   | TFP  | F     | 202 | -    | -       | 1/12/34/34 | 0/4/4/4 |
| 2   | TFP  | C     | 201 | -    | -       | 5/12/34/34 | 0/4/4/4 |
| 2   | TFP  | E     | 201 | -    | -       | 4/12/34/34 | 0/4/4/4 |
| 2   | TFP  | P     | 202 | -    | -       | 1/12/34/34 | 0/4/4/4 |
| 2   | TFP  | R     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | M     | 202 | -    | -       | 0/12/34/34 | 0/4/4/4 |
| 2   | TFP  | Q     | 201 | -    | -       | 2/12/34/34 | 0/4/4/4 |
| 2   | TFP  | K     | 201 | -    | -       | 5/12/34/34 | 0/4/4/4 |
| 2   | TFP  | N     | 201 | -    | -       | 3/12/34/34 | 0/4/4/4 |
| 2   | TFP  | O     | 201 | -    | -       | 5/12/34/34 | 0/4/4/4 |
| 2   | TFP  | R     | 201 | -    | -       | 3/12/34/34 | 0/4/4/4 |
| 2   | TFP  | L     | 201 | -    | -       | 4/12/34/34 | 0/4/4/4 |
| 2   | TFP  | G     | 201 | -    | -       | 5/12/34/34 | 0/4/4/4 |
| 2   | TFP  | A     | 201 | -    | -       | 4/12/34/34 | 0/4/4/4 |

All (174) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | O     | 201 | TFP  | C12-C7 | 9.19 | 1.51        | 1.40     |
| 2   | M     | 202 | TFP  | C12-C7 | 8.85 | 1.50        | 1.40     |
| 2   | D     | 201 | TFP  | C5-C4  | 8.79 | 1.50        | 1.40     |
| 2   | G     | 201 | TFP  | C12-C7 | 8.77 | 1.50        | 1.40     |
| 2   | E     | 201 | TFP  | C12-C7 | 8.52 | 1.50        | 1.40     |
| 2   | C     | 201 | TFP  | C12-C7 | 8.49 | 1.50        | 1.40     |
| 2   | E     | 201 | TFP  | C5-C4  | 8.49 | 1.50        | 1.40     |
| 2   | H     | 201 | TFP  | C12-C7 | 8.35 | 1.50        | 1.40     |
| 2   | S     | 201 | TFP  | C12-C7 | 8.34 | 1.50        | 1.40     |
| 2   | F     | 201 | TFP  | C12-C7 | 8.33 | 1.50        | 1.40     |
| 2   | P     | 201 | TFP  | C12-C7 | 8.32 | 1.50        | 1.40     |
| 2   | R     | 202 | TFP  | C5-C4  | 8.20 | 1.50        | 1.40     |
| 2   | K     | 201 | TFP  | C5-C4  | 8.19 | 1.50        | 1.40     |
| 2   | B     | 201 | TFP  | C12-C7 | 8.10 | 1.49        | 1.40     |
| 2   | Q     | 201 | TFP  | C12-C7 | 8.04 | 1.49        | 1.40     |
| 2   | T     | 201 | TFP  | C12-C7 | 8.03 | 1.49        | 1.40     |
| 2   | C     | 201 | TFP  | C5-C4  | 7.93 | 1.49        | 1.40     |
| 2   | T     | 201 | TFP  | C5-C4  | 7.92 | 1.49        | 1.40     |
| 2   | B     | 201 | TFP  | C5-C4  | 7.92 | 1.49        | 1.40     |
| 2   | D     | 202 | TFP  | C5-C4  | 7.82 | 1.49        | 1.40     |
| 2   | A     | 201 | TFP  | C12-C7 | 7.80 | 1.49        | 1.40     |
| 2   | N     | 201 | TFP  | C12-C7 | 7.77 | 1.49        | 1.40     |
| 2   | O     | 201 | TFP  | C5-C4  | 7.73 | 1.49        | 1.40     |
| 2   | J     | 201 | TFP  | C12-C7 | 7.73 | 1.49        | 1.40     |
| 2   | H     | 201 | TFP  | C5-C4  | 7.65 | 1.49        | 1.40     |
| 2   | A     | 201 | TFP  | C5-C4  | 7.64 | 1.49        | 1.40     |
| 2   | Q     | 202 | TFP  | C12-C7 | 7.64 | 1.49        | 1.40     |
| 2   | M     | 201 | TFP  | C12-C7 | 7.63 | 1.49        | 1.40     |
| 2   | Q     | 201 | TFP  | C5-C4  | 7.62 | 1.49        | 1.40     |
| 2   | M     | 201 | TFP  | C5-C4  | 7.60 | 1.49        | 1.40     |
| 2   | P     | 201 | TFP  | C5-C4  | 7.58 | 1.49        | 1.40     |
| 2   | D     | 201 | TFP  | C12-C7 | 7.57 | 1.49        | 1.40     |
| 2   | J     | 201 | TFP  | C5-C4  | 7.56 | 1.49        | 1.40     |
| 2   | G     | 201 | TFP  | C5-C4  | 7.54 | 1.49        | 1.40     |
| 2   | L     | 201 | TFP  | C12-C7 | 7.52 | 1.49        | 1.40     |
| 2   | S     | 201 | TFP  | C5-C4  | 7.50 | 1.49        | 1.40     |
| 2   | N     | 201 | TFP  | C5-C4  | 7.43 | 1.49        | 1.40     |
| 2   | L     | 201 | TFP  | C5-C4  | 7.38 | 1.49        | 1.40     |
| 2   | N     | 202 | TFP  | C5-C4  | 7.33 | 1.49        | 1.40     |
| 2   | F     | 201 | TFP  | C5-C4  | 7.27 | 1.48        | 1.40     |
| 2   | K     | 201 | TFP  | C12-C7 | 7.20 | 1.48        | 1.40     |
| 2   | R     | 201 | TFP  | C5-C4  | 7.19 | 1.48        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | R     | 202 | TFP  | C12-C7 | 7.12  | 1.48        | 1.40     |
| 2   | L     | 202 | TFP  | C5-C4  | 7.12  | 1.48        | 1.40     |
| 2   | H     | 202 | TFP  | C12-C7 | 7.10  | 1.48        | 1.40     |
| 2   | H     | 202 | TFP  | C5-C4  | 7.09  | 1.48        | 1.40     |
| 2   | T     | 202 | TFP  | C5-C4  | 7.06  | 1.48        | 1.40     |
| 2   | T     | 202 | TFP  | C12-C7 | 7.05  | 1.48        | 1.40     |
| 2   | K     | 202 | TFP  | C5-C4  | 7.00  | 1.48        | 1.40     |
| 2   | E     | 202 | TFP  | C5-C4  | 6.98  | 1.48        | 1.40     |
| 2   | I     | 201 | TFP  | C5-C4  | 6.97  | 1.48        | 1.40     |
| 2   | G     | 202 | TFP  | C5-C4  | 6.88  | 1.48        | 1.40     |
| 2   | I     | 201 | TFP  | C12-C7 | 6.84  | 1.48        | 1.40     |
| 2   | J     | 202 | TFP  | C5-C4  | 6.82  | 1.48        | 1.40     |
| 2   | Q     | 202 | TFP  | C5-C4  | 6.81  | 1.48        | 1.40     |
| 2   | C     | 202 | TFP  | C12-C7 | 6.76  | 1.48        | 1.40     |
| 2   | J     | 202 | TFP  | C12-C7 | 6.66  | 1.48        | 1.40     |
| 2   | M     | 202 | TFP  | C5-C4  | 6.65  | 1.48        | 1.40     |
| 2   | R     | 201 | TFP  | C12-C7 | 6.57  | 1.48        | 1.40     |
| 2   | O     | 202 | TFP  | C12-C7 | 6.54  | 1.48        | 1.40     |
| 2   | D     | 202 | TFP  | C12-C7 | 6.42  | 1.47        | 1.40     |
| 2   | S     | 202 | TFP  | C12-C7 | 6.40  | 1.47        | 1.40     |
| 2   | L     | 202 | TFP  | C12-C7 | 6.26  | 1.47        | 1.40     |
| 2   | E     | 202 | TFP  | C12-C7 | 6.25  | 1.47        | 1.40     |
| 2   | B     | 202 | TFP  | C5-C4  | 6.25  | 1.47        | 1.40     |
| 2   | G     | 202 | TFP  | C12-C7 | 6.24  | 1.47        | 1.40     |
| 2   | I     | 202 | TFP  | C12-C7 | 6.20  | 1.47        | 1.40     |
| 2   | P     | 202 | TFP  | C5-C4  | 6.12  | 1.47        | 1.40     |
| 2   | A     | 202 | TFP  | C12-C7 | 6.08  | 1.47        | 1.40     |
| 2   | N     | 202 | TFP  | C12-C7 | 6.02  | 1.47        | 1.40     |
| 2   | O     | 202 | TFP  | C5-C4  | 5.98  | 1.47        | 1.40     |
| 2   | B     | 202 | TFP  | C12-C7 | 5.77  | 1.47        | 1.40     |
| 2   | F     | 202 | TFP  | C5-C4  | 5.67  | 1.47        | 1.40     |
| 2   | K     | 202 | TFP  | C12-C7 | 5.66  | 1.47        | 1.40     |
| 2   | M     | 201 | TFP  | C4-S   | -5.44 | 1.67        | 1.76     |
| 2   | P     | 202 | TFP  | C12-C7 | 5.34  | 1.46        | 1.40     |
| 2   | I     | 202 | TFP  | C5-C4  | 5.33  | 1.46        | 1.40     |
| 2   | C     | 202 | TFP  | C5-C4  | 5.04  | 1.46        | 1.40     |
| 2   | S     | 202 | TFP  | C5-C4  | 5.02  | 1.46        | 1.40     |
| 2   | F     | 202 | TFP  | C12-C7 | 4.96  | 1.46        | 1.40     |
| 2   | Q     | 201 | TFP  | C7-S   | -4.89 | 1.67        | 1.76     |
| 2   | A     | 202 | TFP  | C5-C4  | 4.68  | 1.45        | 1.40     |
| 2   | D     | 201 | TFP  | C4-S   | -4.67 | 1.68        | 1.76     |
| 2   | S     | 202 | TFP  | C7-S   | -4.67 | 1.68        | 1.76     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | G     | 201 | TFP  | C4-S  | -4.59 | 1.68        | 1.76     |
| 2   | A     | 202 | TFP  | C7-S  | -4.58 | 1.68        | 1.76     |
| 2   | F     | 201 | TFP  | C4-S  | -4.51 | 1.68        | 1.76     |
| 2   | L     | 202 | TFP  | C7-S  | -4.47 | 1.68        | 1.76     |
| 2   | H     | 201 | TFP  | C4-S  | -4.26 | 1.69        | 1.76     |
| 2   | G     | 202 | TFP  | C7-S  | -4.24 | 1.69        | 1.76     |
| 2   | H     | 201 | TFP  | C7-S  | -4.21 | 1.69        | 1.76     |
| 2   | E     | 201 | TFP  | C4-S  | -4.19 | 1.69        | 1.76     |
| 2   | B     | 202 | TFP  | C7-S  | -4.17 | 1.69        | 1.76     |
| 2   | M     | 201 | TFP  | C7-S  | -4.16 | 1.69        | 1.76     |
| 2   | I     | 201 | TFP  | C7-S  | -4.13 | 1.69        | 1.76     |
| 2   | R     | 201 | TFP  | C4-S  | -4.10 | 1.69        | 1.76     |
| 2   | C     | 201 | TFP  | C7-S  | -4.08 | 1.69        | 1.76     |
| 2   | A     | 201 | TFP  | C4-S  | -4.06 | 1.69        | 1.76     |
| 2   | C     | 201 | TFP  | C4-S  | -4.05 | 1.69        | 1.76     |
| 2   | D     | 202 | TFP  | C7-S  | -4.04 | 1.69        | 1.76     |
| 2   | Q     | 201 | TFP  | C4-S  | -4.02 | 1.69        | 1.76     |
| 2   | T     | 202 | TFP  | C7-S  | -4.01 | 1.69        | 1.76     |
| 2   | B     | 201 | TFP  | C4-S  | -3.98 | 1.69        | 1.76     |
| 2   | N     | 201 | TFP  | C4-S  | -3.98 | 1.69        | 1.76     |
| 2   | R     | 201 | TFP  | C7-S  | -3.90 | 1.69        | 1.76     |
| 2   | K     | 201 | TFP  | C4-S  | -3.89 | 1.69        | 1.76     |
| 2   | J     | 202 | TFP  | C4-S  | -3.88 | 1.69        | 1.76     |
| 2   | P     | 201 | TFP  | C7-S  | -3.88 | 1.69        | 1.76     |
| 2   | P     | 201 | TFP  | C4-S  | -3.82 | 1.69        | 1.76     |
| 2   | I     | 201 | TFP  | C4-S  | -3.82 | 1.69        | 1.76     |
| 2   | T     | 201 | TFP  | C4-S  | -3.78 | 1.69        | 1.76     |
| 2   | Q     | 202 | TFP  | C7-S  | -3.73 | 1.69        | 1.76     |
| 2   | F     | 201 | TFP  | C7-S  | -3.71 | 1.70        | 1.76     |
| 2   | L     | 201 | TFP  | C4-S  | -3.69 | 1.70        | 1.76     |
| 2   | E     | 201 | TFP  | C7-S  | -3.65 | 1.70        | 1.76     |
| 2   | J     | 201 | TFP  | C4-S  | -3.58 | 1.70        | 1.76     |
| 2   | P     | 202 | TFP  | C4-S  | -3.57 | 1.70        | 1.76     |
| 2   | J     | 202 | TFP  | C7-S  | -3.54 | 1.70        | 1.76     |
| 2   | S     | 201 | TFP  | C4-S  | -3.46 | 1.70        | 1.76     |
| 2   | L     | 201 | TFP  | C7-S  | -3.43 | 1.70        | 1.76     |
| 2   | N     | 201 | TFP  | C7-S  | -3.35 | 1.70        | 1.76     |
| 2   | J     | 201 | TFP  | C7-S  | -3.33 | 1.70        | 1.76     |
| 2   | M     | 202 | TFP  | C7-S  | -3.33 | 1.70        | 1.76     |
| 2   | T     | 201 | TFP  | C7-S  | -3.32 | 1.70        | 1.76     |
| 2   | G     | 201 | TFP  | C7-S  | -3.27 | 1.70        | 1.76     |
| 2   | S     | 202 | TFP  | C4-S  | -3.20 | 1.70        | 1.76     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | C     | 202 | TFP  | C7-S   | -3.16 | 1.70        | 1.76     |
| 2   | I     | 202 | TFP  | C4-S   | -3.16 | 1.70        | 1.76     |
| 2   | B     | 201 | TFP  | C7-S   | -3.16 | 1.70        | 1.76     |
| 2   | S     | 201 | TFP  | C7-S   | -3.12 | 1.71        | 1.76     |
| 2   | R     | 202 | TFP  | C4-S   | -3.12 | 1.71        | 1.76     |
| 2   | I     | 202 | TFP  | C7-S   | -3.10 | 1.71        | 1.76     |
| 2   | O     | 201 | TFP  | C7-S   | -3.06 | 1.71        | 1.76     |
| 2   | A     | 202 | TFP  | C4-S   | -3.03 | 1.71        | 1.76     |
| 2   | F     | 202 | TFP  | C7-S   | -2.98 | 1.71        | 1.76     |
| 2   | H     | 201 | TFP  | C5-N1  | 2.88  | 1.45        | 1.40     |
| 2   | T     | 202 | TFP  | C3-C2  | 2.84  | 1.43        | 1.38     |
| 2   | N     | 202 | TFP  | C7-S   | -2.84 | 1.71        | 1.76     |
| 2   | K     | 201 | TFP  | C7-S   | -2.83 | 1.71        | 1.76     |
| 2   | O     | 202 | TFP  | C4-S   | -2.83 | 1.71        | 1.76     |
| 2   | G     | 202 | TFP  | C4-S   | -2.81 | 1.71        | 1.76     |
| 2   | C     | 201 | TFP  | C12-N1 | 2.77  | 1.45        | 1.40     |
| 2   | N     | 201 | TFP  | C12-N1 | 2.76  | 1.45        | 1.40     |
| 2   | K     | 202 | TFP  | C7-S   | -2.72 | 1.71        | 1.76     |
| 2   | C     | 202 | TFP  | C4-S   | -2.72 | 1.71        | 1.76     |
| 2   | N     | 202 | TFP  | C4-S   | -2.71 | 1.71        | 1.76     |
| 2   | B     | 201 | TFP  | C5-N1  | 2.70  | 1.45        | 1.40     |
| 2   | H     | 202 | TFP  | C7-S   | -2.69 | 1.71        | 1.76     |
| 2   | O     | 202 | TFP  | C7-S   | -2.68 | 1.71        | 1.76     |
| 2   | D     | 201 | TFP  | C7-S   | -2.59 | 1.71        | 1.76     |
| 2   | P     | 202 | TFP  | C7-S   | -2.58 | 1.71        | 1.76     |
| 2   | O     | 201 | TFP  | C4-S   | -2.57 | 1.71        | 1.76     |
| 2   | L     | 202 | TFP  | C4-S   | -2.57 | 1.71        | 1.76     |
| 2   | J     | 201 | TFP  | C5-N1  | 2.56  | 1.44        | 1.40     |
| 2   | H     | 202 | TFP  | C4-S   | -2.55 | 1.71        | 1.76     |
| 2   | E     | 202 | TFP  | C4-S   | -2.50 | 1.72        | 1.76     |
| 2   | T     | 201 | TFP  | C12-N1 | 2.50  | 1.44        | 1.40     |
| 2   | A     | 201 | TFP  | C7-S   | -2.45 | 1.72        | 1.76     |
| 2   | D     | 201 | TFP  | C5-N1  | 2.43  | 1.44        | 1.40     |
| 2   | N     | 201 | TFP  | C5-N1  | 2.42  | 1.44        | 1.40     |
| 2   | A     | 202 | TFP  | C3-C2  | 2.41  | 1.42        | 1.38     |
| 2   | B     | 202 | TFP  | C4-S   | -2.40 | 1.72        | 1.76     |
| 2   | R     | 202 | TFP  | C7-S   | -2.37 | 1.72        | 1.76     |
| 2   | Q     | 202 | TFP  | C4-S   | -2.26 | 1.72        | 1.76     |
| 2   | K     | 202 | TFP  | C4-S   | -2.25 | 1.72        | 1.76     |
| 2   | G     | 202 | TFP  | C12-N1 | 2.18  | 1.44        | 1.40     |
| 2   | D     | 202 | TFP  | C4-S   | -2.16 | 1.72        | 1.76     |
| 2   | Q     | 202 | TFP  | C12-N1 | 2.15  | 1.44        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | P     | 201 | TFP  | C12-N1 | 2.10  | 1.44        | 1.40     |
| 2   | E     | 202 | TFP  | C7-S   | -2.08 | 1.72        | 1.76     |
| 2   | H     | 201 | TFP  | C12-N1 | 2.05  | 1.43        | 1.40     |
| 2   | M     | 202 | TFP  | C12-N1 | 2.04  | 1.43        | 1.40     |
| 2   | K     | 201 | TFP  | C12-N1 | 2.03  | 1.43        | 1.40     |
| 2   | B     | 201 | TFP  | C12-N1 | 2.01  | 1.43        | 1.40     |

All (343) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | A     | 201 | TFP  | C13-N1-C12 | 6.09  | 127.52      | 119.03   |
| 2   | J     | 201 | TFP  | C13-N1-C12 | -5.74 | 111.03      | 119.03   |
| 2   | O     | 201 | TFP  | C6-C5-N1   | -5.73 | 114.33      | 121.64   |
| 2   | P     | 201 | TFP  | C13-N1-C5  | -5.61 | 111.21      | 119.03   |
| 2   | B     | 201 | TFP  | C13-N1-C5  | 5.59  | 126.82      | 119.03   |
| 2   | T     | 202 | TFP  | C3-C4-C5   | -5.32 | 114.26      | 120.00   |
| 2   | A     | 201 | TFP  | C13-N1-C5  | -5.18 | 111.81      | 119.03   |
| 2   | J     | 201 | TFP  | C13-N1-C5  | 5.08  | 126.10      | 119.03   |
| 2   | E     | 202 | TFP  | C13-N1-C5  | -4.98 | 112.08      | 119.03   |
| 2   | C     | 201 | TFP  | C17-C16-N2 | -4.89 | 100.80      | 110.65   |
| 2   | L     | 201 | TFP  | C13-N1-C5  | -4.81 | 112.32      | 119.03   |
| 2   | J     | 202 | TFP  | C13-N1-C5  | -4.70 | 112.47      | 119.03   |
| 2   | L     | 201 | TFP  | C13-N1-C12 | 4.65  | 125.50      | 119.03   |
| 2   | I     | 202 | TFP  | C13-N1-C5  | -4.41 | 112.88      | 119.03   |
| 2   | E     | 201 | TFP  | C6-C5-N1   | -4.35 | 116.09      | 121.64   |
| 2   | L     | 201 | TFP  | C6-C5-N1   | -4.32 | 116.13      | 121.64   |
| 2   | K     | 201 | TFP  | C6-C5-N1   | -4.31 | 116.14      | 121.64   |
| 2   | P     | 202 | TFP  | C13-N1-C5  | -4.30 | 113.03      | 119.03   |
| 2   | O     | 201 | TFP  | C4-C5-N1   | 4.29  | 126.86      | 119.98   |
| 2   | I     | 201 | TFP  | C16-C17-N3 | -4.18 | 104.13      | 110.86   |
| 2   | S     | 202 | TFP  | C13-N1-C5  | -4.17 | 113.22      | 119.03   |
| 2   | S     | 201 | TFP  | C13-N1-C5  | 4.14  | 124.79      | 119.03   |
| 2   | R     | 202 | TFP  | C16-C17-N3 | -4.04 | 104.37      | 110.86   |
| 2   | M     | 202 | TFP  | C3-C4-C5   | -3.98 | 115.70      | 120.00   |
| 2   | O     | 202 | TFP  | C13-N1-C5  | -3.96 | 113.50      | 119.03   |
| 2   | Q     | 202 | TFP  | C13-N1-C5  | -3.92 | 113.56      | 119.03   |
| 2   | D     | 201 | TFP  | C13-N1-C12 | -3.92 | 113.57      | 119.03   |
| 2   | O     | 201 | TFP  | C6-C1-C21  | -3.85 | 114.47      | 119.57   |
| 2   | O     | 201 | TFP  | C13-N1-C5  | -3.85 | 113.67      | 119.03   |
| 2   | T     | 202 | TFP  | C13-N1-C5  | -3.79 | 113.75      | 119.03   |
| 2   | N     | 202 | TFP  | F1-C21-C1  | -3.77 | 104.82      | 112.90   |
| 2   | T     | 202 | TFP  | C3-C4-S    | 3.75  | 126.45      | 118.36   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | L     | 202 | TFP  | C13-N1-C5  | -3.75 | 113.80      | 119.03   |
| 2   | K     | 201 | TFP  | C13-N1-C5  | -3.74 | 113.82      | 119.03   |
| 2   | B     | 201 | TFP  | C13-N1-C12 | -3.74 | 113.82      | 119.03   |
| 2   | A     | 201 | TFP  | C6-C5-N1   | -3.71 | 116.91      | 121.64   |
| 2   | G     | 202 | TFP  | C11-C12-N1 | 3.70  | 126.80      | 121.76   |
| 2   | E     | 201 | TFP  | C4-C5-N1   | 3.69  | 125.90      | 119.98   |
| 2   | E     | 201 | TFP  | C13-N1-C5  | -3.69 | 113.89      | 119.03   |
| 2   | C     | 201 | TFP  | C18-C19-N2 | -3.67 | 103.25      | 110.65   |
| 2   | L     | 201 | TFP  | C4-C5-N1   | 3.59  | 125.73      | 119.98   |
| 2   | T     | 202 | TFP  | C4-C5-N1   | -3.55 | 114.29      | 119.98   |
| 2   | F     | 202 | TFP  | C4-C5-N1   | -3.55 | 114.30      | 119.98   |
| 2   | T     | 201 | TFP  | C16-C17-N3 | -3.54 | 105.17      | 110.86   |
| 2   | B     | 202 | TFP  | C6-C5-N1   | 3.54  | 126.15      | 121.64   |
| 2   | C     | 201 | TFP  | C18-N3-C17 | 3.51  | 115.13      | 109.54   |
| 2   | J     | 201 | TFP  | C4-C5-N1   | 3.49  | 125.57      | 119.98   |
| 2   | B     | 202 | TFP  | C11-C12-N1 | 3.49  | 126.51      | 121.76   |
| 2   | R     | 201 | TFP  | C13-N1-C12 | -3.48 | 114.17      | 119.03   |
| 2   | T     | 202 | TFP  | C16-C17-N3 | -3.47 | 105.29      | 110.86   |
| 2   | E     | 202 | TFP  | C14-C13-N1 | -3.46 | 102.84      | 112.98   |
| 2   | S     | 201 | TFP  | C4-C5-N1   | 3.42  | 125.47      | 119.98   |
| 2   | T     | 202 | TFP  | C6-C5-C4   | 3.41  | 122.85      | 119.02   |
| 2   | O     | 201 | TFP  | C2-C1-C21  | 3.39  | 125.41      | 119.96   |
| 2   | K     | 201 | TFP  | C13-N1-C12 | 3.39  | 123.75      | 119.03   |
| 2   | H     | 202 | TFP  | F2-C21-C1  | -3.34 | 105.75      | 112.90   |
| 2   | R     | 201 | TFP  | C16-C17-N3 | -3.33 | 105.50      | 110.86   |
| 2   | C     | 201 | TFP  | C13-N1-C5  | -3.30 | 114.42      | 119.03   |
| 2   | I     | 201 | TFP  | C6-C5-N1   | -3.30 | 117.43      | 121.64   |
| 2   | K     | 202 | TFP  | F2-C21-C1  | -3.28 | 105.87      | 112.90   |
| 2   | R     | 201 | TFP  | C11-C12-N1 | -3.28 | 117.29      | 121.76   |
| 2   | J     | 201 | TFP  | C19-N2-C16 | 3.26  | 115.86      | 108.84   |
| 2   | A     | 201 | TFP  | C14-C13-N1 | 3.23  | 122.46      | 112.98   |
| 2   | J     | 201 | TFP  | C12-N1-C5  | -3.22 | 112.70      | 120.18   |
| 2   | D     | 202 | TFP  | C4-C5-N1   | -3.22 | 114.83      | 119.98   |
| 2   | B     | 202 | TFP  | C4-C5-N1   | -3.20 | 114.85      | 119.98   |
| 2   | E     | 201 | TFP  | C12-N1-C5  | -3.20 | 112.77      | 120.18   |
| 2   | I     | 202 | TFP  | C11-C12-N1 | 3.19  | 126.10      | 121.76   |
| 2   | S     | 202 | TFP  | C11-C12-N1 | 3.17  | 126.07      | 121.76   |
| 2   | K     | 201 | TFP  | C12-N1-C5  | -3.15 | 112.86      | 120.18   |
| 2   | R     | 202 | TFP  | C7-C12-N1  | -3.15 | 114.93      | 119.98   |
| 2   | K     | 202 | TFP  | C7-C12-N1  | -3.15 | 114.93      | 119.98   |
| 2   | T     | 201 | TFP  | C18-C19-N2 | -3.15 | 104.30      | 110.65   |
| 2   | A     | 202 | TFP  | C11-C12-N1 | 3.13  | 126.01      | 121.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 202 | TFP  | C11-C12-N1  | 3.10  | 125.98      | 121.76   |
| 2   | G     | 202 | TFP  | F2-C21-C1   | -3.10 | 106.26      | 112.90   |
| 2   | P     | 202 | TFP  | F3-C21-F2   | 3.09  | 116.94      | 105.77   |
| 2   | O     | 201 | TFP  | C13-N1-C12  | 3.09  | 123.33      | 119.03   |
| 2   | A     | 202 | TFP  | C4-C5-N1    | -3.09 | 115.03      | 119.98   |
| 2   | K     | 201 | TFP  | C4-C5-N1    | 3.09  | 124.92      | 119.98   |
| 2   | I     | 201 | TFP  | C19-C18-N3  | -3.08 | 105.90      | 110.86   |
| 2   | A     | 202 | TFP  | C7-C12-N1   | -3.06 | 115.08      | 119.98   |
| 2   | K     | 202 | TFP  | C4-C5-N1    | -3.04 | 115.11      | 119.98   |
| 2   | M     | 202 | TFP  | C4-C5-N1    | -3.04 | 115.11      | 119.98   |
| 2   | M     | 201 | TFP  | C13-N1-C12  | -3.02 | 114.82      | 119.03   |
| 2   | S     | 201 | TFP  | C11-C12-N1  | -2.99 | 117.68      | 121.76   |
| 2   | D     | 201 | TFP  | C4-C5-N1    | 2.98  | 124.75      | 119.98   |
| 2   | A     | 201 | TFP  | C19-C18-N3  | -2.97 | 106.09      | 110.86   |
| 2   | M     | 202 | TFP  | C14-C13-N1  | -2.95 | 104.32      | 112.98   |
| 2   | S     | 201 | TFP  | C19-C18-N3  | -2.95 | 106.11      | 110.86   |
| 2   | P     | 201 | TFP  | F3-C21-C1   | -2.93 | 106.63      | 112.90   |
| 2   | N     | 202 | TFP  | C13-N1-C5   | -2.92 | 114.96      | 119.03   |
| 2   | S     | 201 | TFP  | C14-C13-N1  | 2.90  | 121.48      | 112.98   |
| 2   | R     | 202 | TFP  | F1-C21-C1   | -2.90 | 106.69      | 112.90   |
| 2   | B     | 202 | TFP  | C7-C12-N1   | -2.88 | 115.36      | 119.98   |
| 2   | Q     | 202 | TFP  | C11-C12-N1  | 2.88  | 125.68      | 121.76   |
| 2   | F     | 202 | TFP  | C6-C5-N1    | 2.86  | 125.29      | 121.64   |
| 2   | D     | 201 | TFP  | C6-C5-C4    | -2.86 | 115.81      | 119.02   |
| 2   | Q     | 201 | TFP  | C13-N1-C12  | -2.86 | 115.04      | 119.03   |
| 2   | J     | 201 | TFP  | C11-C12-N1  | -2.85 | 117.88      | 121.76   |
| 2   | O     | 201 | TFP  | C12-N1-C5   | -2.84 | 113.59      | 120.18   |
| 2   | Q     | 201 | TFP  | F3-C21-C1   | -2.83 | 106.83      | 112.90   |
| 2   | D     | 201 | TFP  | F2-C21-C1   | -2.83 | 106.84      | 112.90   |
| 2   | B     | 201 | TFP  | C12-N1-C5   | -2.82 | 113.63      | 120.18   |
| 2   | Q     | 201 | TFP  | C7-C12-N1   | 2.82  | 124.50      | 119.98   |
| 2   | M     | 201 | TFP  | C4-C5-N1    | 2.82  | 124.49      | 119.98   |
| 2   | M     | 201 | TFP  | C12-N1-C5   | -2.81 | 113.65      | 120.18   |
| 2   | A     | 202 | TFP  | F2-C21-C1   | -2.81 | 106.87      | 112.90   |
| 2   | F     | 202 | TFP  | C7-C12-N1   | -2.81 | 115.48      | 119.98   |
| 2   | N     | 202 | TFP  | C7-C12-N1   | -2.81 | 115.48      | 119.98   |
| 2   | K     | 202 | TFP  | C3-C4-S     | 2.81  | 124.41      | 118.36   |
| 2   | A     | 201 | TFP  | C15-C14-C13 | -2.81 | 103.40      | 112.91   |
| 2   | G     | 201 | TFP  | C17-C16-N2  | -2.80 | 105.01      | 110.65   |
| 2   | S     | 201 | TFP  | C12-N1-C5   | -2.79 | 113.70      | 120.18   |
| 2   | C     | 202 | TFP  | C7-C12-N1   | -2.79 | 115.52      | 119.98   |
| 2   | O     | 202 | TFP  | C7-C12-N1   | -2.78 | 115.53      | 119.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 201 | TFP  | C19-C18-N3  | -2.78 | 106.39      | 110.86   |
| 2   | R     | 201 | TFP  | C15-N2-C16  | -2.78 | 103.84      | 111.24   |
| 2   | S     | 201 | TFP  | C6-C5-N1    | -2.77 | 118.10      | 121.64   |
| 2   | K     | 201 | TFP  | C7-C12-N1   | 2.77  | 124.42      | 119.98   |
| 2   | L     | 202 | TFP  | C19-C18-N3  | -2.77 | 106.40      | 110.86   |
| 2   | P     | 201 | TFP  | C12-N1-C5   | -2.77 | 113.75      | 120.18   |
| 2   | L     | 201 | TFP  | C6-C1-C21   | -2.76 | 115.92      | 119.57   |
| 2   | J     | 201 | TFP  | C6-C5-N1    | -2.76 | 118.12      | 121.64   |
| 2   | S     | 202 | TFP  | C4-C5-N1    | -2.74 | 115.59      | 119.98   |
| 2   | O     | 201 | TFP  | F3-C21-C1   | -2.73 | 107.05      | 112.90   |
| 2   | B     | 201 | TFP  | C7-C12-N1   | 2.73  | 124.35      | 119.98   |
| 2   | B     | 202 | TFP  | C19-N2-C16  | 2.73  | 114.72      | 108.84   |
| 2   | N     | 202 | TFP  | C19-N2-C16  | 2.72  | 114.71      | 108.84   |
| 2   | A     | 201 | TFP  | C15-N2-C16  | -2.72 | 103.99      | 111.24   |
| 2   | A     | 202 | TFP  | C13-N1-C5   | -2.72 | 115.23      | 119.03   |
| 2   | K     | 202 | TFP  | C14-C13-N1  | -2.72 | 105.01      | 112.98   |
| 2   | P     | 201 | TFP  | C16-C17-N3  | -2.72 | 106.49      | 110.86   |
| 2   | L     | 202 | TFP  | C4-C5-N1    | -2.69 | 115.68      | 119.98   |
| 2   | S     | 201 | TFP  | C6-C5-C4    | -2.68 | 116.01      | 119.02   |
| 2   | N     | 202 | TFP  | C12-N1-C5   | -2.68 | 113.97      | 120.18   |
| 2   | P     | 202 | TFP  | C7-C12-N1   | -2.67 | 115.69      | 119.98   |
| 2   | M     | 201 | TFP  | F3-C21-C1   | -2.65 | 107.22      | 112.90   |
| 2   | A     | 201 | TFP  | C4-C5-N1    | 2.65  | 124.23      | 119.98   |
| 2   | J     | 201 | TFP  | C6-C5-C4    | -2.65 | 116.04      | 119.02   |
| 2   | A     | 202 | TFP  | C3-C4-S     | 2.64  | 124.05      | 118.36   |
| 2   | H     | 201 | TFP  | C16-C17-N3  | -2.64 | 106.62      | 110.86   |
| 2   | T     | 202 | TFP  | F2-C21-C1   | -2.64 | 107.25      | 112.90   |
| 2   | J     | 201 | TFP  | C8-C7-C12   | -2.63 | 117.17      | 120.00   |
| 2   | I     | 202 | TFP  | C16-C17-N3  | -2.62 | 106.64      | 110.86   |
| 2   | Q     | 202 | TFP  | F2-C21-C1   | -2.62 | 107.28      | 112.90   |
| 2   | P     | 201 | TFP  | C15-C14-C13 | -2.62 | 104.02      | 112.91   |
| 2   | L     | 201 | TFP  | C14-C13-N1  | 2.62  | 120.65      | 112.98   |
| 2   | Q     | 202 | TFP  | C6-C5-N1    | 2.61  | 124.97      | 121.64   |
| 2   | C     | 201 | TFP  | C15-C14-C13 | -2.61 | 104.06      | 112.91   |
| 2   | G     | 202 | TFP  | C7-C12-N1   | -2.61 | 115.80      | 119.98   |
| 2   | M     | 201 | TFP  | C11-C12-N1  | -2.61 | 118.21      | 121.76   |
| 2   | R     | 201 | TFP  | C6-C5-N1    | -2.60 | 118.32      | 121.64   |
| 2   | P     | 201 | TFP  | C14-C13-N1  | 2.59  | 120.58      | 112.98   |
| 2   | M     | 201 | TFP  | C7-C12-N1   | 2.59  | 124.13      | 119.98   |
| 2   | J     | 201 | TFP  | C19-C18-N3  | -2.58 | 106.71      | 110.86   |
| 2   | K     | 202 | TFP  | C3-C4-C5    | -2.58 | 117.22      | 120.00   |
| 2   | M     | 201 | TFP  | C6-C5-N1    | -2.57 | 118.36      | 121.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 202 | TFP  | C3-C4-S     | 2.57  | 123.89      | 118.36   |
| 2   | F     | 201 | TFP  | C6-C5-N1    | -2.56 | 118.37      | 121.64   |
| 2   | C     | 201 | TFP  | C7-C12-N1   | 2.55  | 124.07      | 119.98   |
| 2   | P     | 201 | TFP  | C15-N2-C16  | -2.55 | 104.44      | 111.24   |
| 2   | D     | 201 | TFP  | C11-C12-N1  | -2.55 | 118.28      | 121.76   |
| 2   | B     | 201 | TFP  | C11-C12-N1  | -2.54 | 118.29      | 121.76   |
| 2   | C     | 202 | TFP  | C16-C17-N3  | -2.54 | 106.77      | 110.86   |
| 2   | A     | 202 | TFP  | C3-C4-C5    | -2.53 | 117.27      | 120.00   |
| 2   | F     | 202 | TFP  | C13-N1-C5   | -2.53 | 115.50      | 119.03   |
| 2   | D     | 201 | TFP  | C13-N1-C5   | 2.52  | 122.53      | 119.03   |
| 2   | G     | 202 | TFP  | C4-C5-N1    | -2.51 | 115.96      | 119.98   |
| 2   | B     | 201 | TFP  | F3-C21-C1   | -2.51 | 107.52      | 112.90   |
| 2   | G     | 202 | TFP  | C3-C4-S     | 2.51  | 123.76      | 118.36   |
| 2   | O     | 201 | TFP  | C11-C12-N1  | -2.51 | 118.34      | 121.76   |
| 2   | G     | 202 | TFP  | C16-C17-N3  | -2.50 | 106.84      | 110.86   |
| 2   | P     | 202 | TFP  | F2-C21-C1   | -2.49 | 107.56      | 112.90   |
| 2   | S     | 202 | TFP  | F2-C21-C1   | -2.49 | 107.56      | 112.90   |
| 2   | T     | 202 | TFP  | C7-C12-N1   | -2.49 | 115.99      | 119.98   |
| 2   | A     | 201 | TFP  | C16-C17-N3  | -2.49 | 106.86      | 110.86   |
| 2   | E     | 201 | TFP  | C16-C17-N3  | 2.48  | 114.85      | 110.86   |
| 2   | D     | 201 | TFP  | C14-C13-N1  | 2.48  | 120.24      | 112.98   |
| 2   | Q     | 202 | TFP  | C4-C5-N1    | -2.47 | 116.02      | 119.98   |
| 2   | A     | 201 | TFP  | C12-N1-C5   | -2.47 | 114.44      | 120.18   |
| 2   | H     | 201 | TFP  | C6-C5-C4    | -2.47 | 116.25      | 119.02   |
| 2   | F     | 201 | TFP  | C4-C5-N1    | 2.46  | 123.92      | 119.98   |
| 2   | N     | 201 | TFP  | C15-N2-C19  | -2.45 | 104.72      | 111.24   |
| 2   | K     | 202 | TFP  | C17-C16-N2  | -2.44 | 105.73      | 110.65   |
| 2   | K     | 201 | TFP  | C11-C12-N1  | -2.43 | 118.44      | 121.76   |
| 2   | L     | 202 | TFP  | C18-C19-N2  | -2.43 | 105.75      | 110.65   |
| 2   | H     | 202 | TFP  | C7-C12-N1   | -2.43 | 116.09      | 119.98   |
| 2   | R     | 201 | TFP  | C19-N2-C16  | 2.43  | 114.07      | 108.84   |
| 2   | P     | 201 | TFP  | C4-C5-N1    | 2.42  | 123.85      | 119.98   |
| 2   | T     | 202 | TFP  | F3-C21-C1   | 2.41  | 118.06      | 112.90   |
| 2   | N     | 201 | TFP  | C7-C12-N1   | 2.41  | 123.85      | 119.98   |
| 2   | K     | 201 | TFP  | C10-C11-C12 | 2.41  | 123.15      | 118.28   |
| 2   | K     | 202 | TFP  | C11-C12-N1  | 2.41  | 125.04      | 121.76   |
| 2   | L     | 201 | TFP  | C11-C12-N1  | -2.41 | 118.47      | 121.76   |
| 2   | O     | 202 | TFP  | C11-C12-N1  | 2.41  | 125.03      | 121.76   |
| 2   | S     | 201 | TFP  | C14-C15-N2  | -2.40 | 107.18      | 113.93   |
| 2   | P     | 202 | TFP  | C4-C5-N1    | -2.40 | 116.14      | 119.98   |
| 2   | K     | 202 | TFP  | C13-N1-C5   | -2.40 | 115.69      | 119.03   |
| 2   | D     | 201 | TFP  | C8-C7-C12   | -2.40 | 117.42      | 120.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | R     | 201 | TFP  | C7-C12-N1   | 2.40  | 123.82      | 119.98   |
| 2   | T     | 201 | TFP  | C19-C18-N3  | -2.39 | 107.02      | 110.86   |
| 2   | L     | 202 | TFP  | C3-C4-S     | 2.38  | 123.50      | 118.36   |
| 2   | O     | 202 | TFP  | C14-C13-N1  | -2.38 | 105.99      | 112.98   |
| 2   | L     | 202 | TFP  | C16-C17-N3  | -2.38 | 107.03      | 110.86   |
| 2   | D     | 201 | TFP  | C12-N1-C5   | -2.38 | 114.66      | 120.18   |
| 2   | B     | 202 | TFP  | C3-C4-S     | 2.38  | 123.48      | 118.36   |
| 2   | M     | 202 | TFP  | C11-C12-N1  | 2.37  | 124.99      | 121.76   |
| 2   | C     | 201 | TFP  | F3-C21-C1   | -2.37 | 107.82      | 112.90   |
| 2   | G     | 202 | TFP  | C5-C4-S     | -2.37 | 116.61      | 120.39   |
| 2   | C     | 201 | TFP  | C11-C12-C7  | -2.36 | 115.38      | 118.59   |
| 2   | S     | 202 | TFP  | C12-C7-S    | -2.36 | 116.62      | 120.39   |
| 2   | M     | 202 | TFP  | C7-C12-N1   | -2.35 | 116.21      | 119.98   |
| 2   | G     | 201 | TFP  | C4-C5-N1    | 2.35  | 123.74      | 119.98   |
| 2   | T     | 202 | TFP  | C18-C19-N2  | -2.34 | 105.92      | 110.65   |
| 2   | R     | 201 | TFP  | C4-C5-N1    | 2.34  | 123.73      | 119.98   |
| 2   | S     | 202 | TFP  | F1-C21-C1   | -2.34 | 107.89      | 112.90   |
| 2   | T     | 202 | TFP  | C11-C12-N1  | 2.34  | 124.94      | 121.76   |
| 2   | I     | 202 | TFP  | C7-C12-N1   | -2.33 | 116.25      | 119.98   |
| 2   | M     | 201 | TFP  | C2-C1-C6    | 2.33  | 122.34      | 117.86   |
| 2   | P     | 201 | TFP  | C6-C5-N1    | -2.32 | 118.67      | 121.64   |
| 2   | H     | 201 | TFP  | C4-C5-N1    | 2.32  | 123.70      | 119.98   |
| 2   | A     | 202 | TFP  | C19-C18-N3  | -2.31 | 107.15      | 110.86   |
| 2   | E     | 201 | TFP  | C7-C12-N1   | 2.30  | 123.67      | 119.98   |
| 2   | H     | 202 | TFP  | C16-C17-N3  | -2.30 | 107.16      | 110.86   |
| 2   | F     | 201 | TFP  | C13-N1-C5   | -2.30 | 115.82      | 119.03   |
| 2   | F     | 201 | TFP  | C17-C16-N2  | -2.30 | 106.02      | 110.65   |
| 2   | K     | 202 | TFP  | C18-C19-N2  | -2.29 | 106.02      | 110.65   |
| 2   | D     | 202 | TFP  | C19-C18-N3  | -2.29 | 107.17      | 110.86   |
| 2   | G     | 201 | TFP  | C6-C5-N1    | -2.29 | 118.72      | 121.64   |
| 2   | L     | 201 | TFP  | C15-N2-C19  | -2.29 | 105.14      | 111.24   |
| 2   | F     | 201 | TFP  | C11-C12-N1  | -2.29 | 118.64      | 121.76   |
| 2   | G     | 201 | TFP  | C15-C14-C13 | -2.28 | 105.19      | 112.91   |
| 2   | D     | 202 | TFP  | C6-C5-N1    | 2.28  | 124.54      | 121.64   |
| 2   | B     | 202 | TFP  | C14-C13-N1  | -2.27 | 106.32      | 112.98   |
| 2   | A     | 201 | TFP  | C17-C16-N2  | -2.27 | 106.07      | 110.65   |
| 2   | K     | 201 | TFP  | C18-N3-C17  | 2.27  | 113.15      | 109.54   |
| 2   | H     | 201 | TFP  | C14-C13-N1  | 2.27  | 119.63      | 112.98   |
| 2   | I     | 201 | TFP  | C4-C5-N1    | 2.27  | 123.61      | 119.98   |
| 2   | C     | 201 | TFP  | C4-C5-N1    | 2.26  | 123.60      | 119.98   |
| 2   | G     | 202 | TFP  | C2-C1-C6    | 2.26  | 122.21      | 117.86   |
| 2   | N     | 202 | TFP  | C11-C12-N1  | 2.25  | 124.82      | 121.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 201 | TFP  | C11-C12-N1  | -2.25 | 118.69      | 121.76   |
| 2   | T     | 201 | TFP  | C7-C12-N1   | 2.25  | 123.59      | 119.98   |
| 2   | A     | 202 | TFP  | C14-C15-N2  | -2.25 | 107.61      | 113.93   |
| 2   | S     | 202 | TFP  | C8-C7-C12   | 2.25  | 122.43      | 120.00   |
| 2   | N     | 202 | TFP  | C4-C5-N1    | -2.25 | 116.38      | 119.98   |
| 2   | Q     | 202 | TFP  | C9-C10-C11  | 2.25  | 123.01      | 120.24   |
| 2   | E     | 202 | TFP  | C3-C4-S     | 2.24  | 123.19      | 118.36   |
| 2   | Q     | 201 | TFP  | C11-C12-N1  | -2.24 | 118.71      | 121.76   |
| 2   | L     | 201 | TFP  | C2-C1-C21   | 2.24  | 123.55      | 119.96   |
| 2   | P     | 202 | TFP  | C11-C12-N1  | 2.24  | 124.80      | 121.76   |
| 2   | L     | 202 | TFP  | C7-C12-N1   | -2.24 | 116.40      | 119.98   |
| 2   | T     | 202 | TFP  | F3-C21-F1   | -2.24 | 97.69       | 105.77   |
| 2   | N     | 201 | TFP  | C10-C11-C12 | 2.22  | 122.76      | 118.28   |
| 2   | I     | 201 | TFP  | F2-C21-C1   | -2.22 | 108.15      | 112.90   |
| 2   | M     | 202 | TFP  | C3-C4-S     | 2.22  | 123.14      | 118.36   |
| 2   | G     | 202 | TFP  | F1-C21-C1   | -2.22 | 108.15      | 112.90   |
| 2   | L     | 201 | TFP  | C16-C17-N3  | -2.21 | 107.30      | 110.86   |
| 2   | F     | 201 | TFP  | C7-C12-N1   | 2.21  | 123.52      | 119.98   |
| 2   | E     | 202 | TFP  | C4-C5-N1    | -2.20 | 116.45      | 119.98   |
| 2   | Q     | 202 | TFP  | C14-C13-N1  | -2.20 | 106.53      | 112.98   |
| 2   | O     | 201 | TFP  | C3-C4-C5    | -2.20 | 117.63      | 120.00   |
| 2   | I     | 202 | TFP  | C19-N2-C16  | 2.19  | 113.56      | 108.84   |
| 2   | J     | 202 | TFP  | C7-C12-N1   | -2.19 | 116.47      | 119.98   |
| 2   | C     | 201 | TFP  | C15-N2-C16  | 2.19  | 117.07      | 111.24   |
| 2   | I     | 202 | TFP  | C12-N1-C5   | -2.19 | 115.10      | 120.18   |
| 2   | D     | 201 | TFP  | C7-C12-N1   | 2.18  | 123.48      | 119.98   |
| 2   | O     | 202 | TFP  | C16-C17-N3  | -2.18 | 107.35      | 110.86   |
| 2   | T     | 201 | TFP  | C6-C5-N1    | -2.18 | 118.86      | 121.64   |
| 2   | Q     | 202 | TFP  | C6-C1-C21   | 2.18  | 122.44      | 119.57   |
| 2   | P     | 201 | TFP  | C19-N2-C16  | 2.17  | 113.52      | 108.84   |
| 2   | E     | 201 | TFP  | C11-C12-N1  | -2.17 | 118.80      | 121.76   |
| 2   | A     | 202 | TFP  | C6-C5-C4    | 2.17  | 121.46      | 119.02   |
| 2   | S     | 201 | TFP  | C19-N2-C16  | 2.17  | 113.51      | 108.84   |
| 2   | T     | 201 | TFP  | C4-C5-N1    | 2.16  | 123.44      | 119.98   |
| 2   | H     | 201 | TFP  | C17-C16-N2  | -2.16 | 106.29      | 110.65   |
| 2   | C     | 202 | TFP  | C6-C5-N1    | 2.16  | 124.39      | 121.64   |
| 2   | J     | 201 | TFP  | C6-C1-C21   | -2.16 | 116.72      | 119.57   |
| 2   | Q     | 201 | TFP  | C6-C1-C21   | 2.15  | 122.41      | 119.57   |
| 2   | C     | 202 | TFP  | C11-C12-N1  | 2.15  | 124.68      | 121.76   |
| 2   | N     | 201 | TFP  | C20-N3-C18  | -2.14 | 106.55      | 110.63   |
| 2   | K     | 201 | TFP  | C20-N3-C17  | -2.14 | 106.55      | 110.63   |
| 2   | G     | 202 | TFP  | C14-C15-N2  | -2.14 | 107.91      | 113.93   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | R     | 201 | TFP  | C12-N1-C5   | -2.14 | 115.22      | 120.18   |
| 2   | S     | 202 | TFP  | C7-C12-N1   | -2.14 | 116.56      | 119.98   |
| 2   | N     | 201 | TFP  | C11-C12-N1  | -2.14 | 118.85      | 121.76   |
| 2   | G     | 201 | TFP  | C7-C12-N1   | 2.14  | 123.40      | 119.98   |
| 2   | B     | 201 | TFP  | C4-C5-N1    | 2.13  | 123.40      | 119.98   |
| 2   | C     | 201 | TFP  | C12-N1-C5   | -2.13 | 115.25      | 120.18   |
| 2   | B     | 201 | TFP  | C6-C5-C4    | -2.12 | 116.63      | 119.02   |
| 2   | H     | 201 | TFP  | C12-N1-C5   | -2.12 | 115.25      | 120.18   |
| 2   | D     | 201 | TFP  | C2-C1-C6    | 2.12  | 121.94      | 117.86   |
| 2   | O     | 201 | TFP  | C7-C12-N1   | 2.12  | 123.38      | 119.98   |
| 2   | E     | 202 | TFP  | C3-C4-C5    | -2.11 | 117.72      | 120.00   |
| 2   | C     | 202 | TFP  | F1-C21-C1   | -2.11 | 108.38      | 112.90   |
| 2   | G     | 202 | TFP  | C6-C5-N1    | 2.11  | 124.33      | 121.64   |
| 2   | P     | 202 | TFP  | C14-C13-N1  | -2.10 | 106.81      | 112.98   |
| 2   | Q     | 202 | TFP  | C8-C7-C12   | 2.10  | 122.28      | 120.00   |
| 2   | R     | 202 | TFP  | C8-C7-C12   | -2.10 | 117.73      | 120.00   |
| 2   | N     | 201 | TFP  | C6-C1-C21   | 2.10  | 122.34      | 119.57   |
| 2   | H     | 201 | TFP  | C7-C12-N1   | 2.10  | 123.34      | 119.98   |
| 2   | R     | 202 | TFP  | C18-N3-C17  | 2.10  | 112.88      | 109.54   |
| 2   | D     | 202 | TFP  | C16-C17-N3  | -2.10 | 107.49      | 110.86   |
| 2   | R     | 201 | TFP  | C10-C9-C8   | 2.09  | 122.82      | 120.24   |
| 2   | D     | 201 | TFP  | C14-C15-N2  | -2.09 | 108.06      | 113.93   |
| 2   | M     | 202 | TFP  | C13-N1-C5   | -2.09 | 116.12      | 119.03   |
| 2   | M     | 201 | TFP  | F1-C21-C1   | -2.09 | 108.43      | 112.90   |
| 2   | C     | 202 | TFP  | C4-C5-N1    | -2.08 | 116.64      | 119.98   |
| 2   | R     | 202 | TFP  | C4-C5-N1    | -2.08 | 116.64      | 119.98   |
| 2   | G     | 201 | TFP  | C11-C12-N1  | -2.08 | 118.92      | 121.76   |
| 2   | P     | 202 | TFP  | C5-C6-C1    | -2.08 | 117.48      | 120.69   |
| 2   | K     | 201 | TFP  | C15-N2-C16  | -2.07 | 105.72      | 111.24   |
| 2   | I     | 201 | TFP  | C10-C11-C12 | 2.07  | 122.45      | 118.28   |
| 2   | E     | 201 | TFP  | C19-C18-N3  | -2.07 | 107.54      | 110.86   |
| 2   | F     | 201 | TFP  | C19-C18-N3  | -2.06 | 107.54      | 110.86   |
| 2   | P     | 202 | TFP  | C2-C3-C4    | -2.06 | 116.52      | 119.94   |
| 2   | H     | 202 | TFP  | C2-C1-C6    | 2.06  | 121.83      | 117.86   |
| 2   | S     | 202 | TFP  | C2-C1-C6    | 2.06  | 121.82      | 117.86   |
| 2   | G     | 201 | TFP  | C19-C18-N3  | -2.06 | 107.55      | 110.86   |
| 2   | F     | 201 | TFP  | C12-N1-C5   | -2.06 | 115.41      | 120.18   |
| 2   | E     | 201 | TFP  | C6-C1-C21   | -2.05 | 116.86      | 119.57   |
| 2   | B     | 202 | TFP  | C17-C16-N2  | -2.05 | 106.52      | 110.65   |
| 2   | L     | 201 | TFP  | C12-N1-C5   | -2.04 | 115.44      | 120.18   |
| 2   | J     | 202 | TFP  | C3-C2-C1    | 2.04  | 123.98      | 121.17   |
| 2   | Q     | 202 | TFP  | C12-N1-C5   | -2.04 | 115.45      | 120.18   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | Q     | 202 | TFP  | C3-C4-S     | 2.03  | 122.74      | 118.36   |
| 2   | G     | 202 | TFP  | C12-C7-S    | -2.03 | 117.14      | 120.39   |
| 2   | K     | 201 | TFP  | C8-C7-C12   | -2.03 | 117.81      | 120.00   |
| 2   | O     | 201 | TFP  | C12-C7-S    | 2.03  | 123.64      | 120.39   |
| 2   | B     | 201 | TFP  | C16-C17-N3  | -2.03 | 107.60      | 110.86   |
| 2   | I     | 201 | TFP  | C14-C15-N2  | -2.03 | 108.24      | 113.93   |
| 2   | J     | 201 | TFP  | C20-N3-C18  | -2.02 | 106.78      | 110.63   |
| 2   | B     | 202 | TFP  | C20-N3-C17  | -2.02 | 106.78      | 110.63   |
| 2   | E     | 201 | TFP  | C19-N2-C16  | 2.02  | 113.20      | 108.84   |
| 2   | E     | 202 | TFP  | C7-C12-N1   | -2.02 | 116.74      | 119.98   |
| 2   | S     | 202 | TFP  | C3-C4-S     | 2.02  | 122.71      | 118.36   |
| 2   | C     | 202 | TFP  | C13-N1-C5   | -2.02 | 116.22      | 119.03   |
| 2   | D     | 201 | TFP  | C6-C5-N1    | -2.01 | 119.07      | 121.64   |
| 2   | T     | 201 | TFP  | C17-C16-N2  | -2.01 | 106.60      | 110.65   |
| 2   | L     | 201 | TFP  | C14-C15-N2  | -2.01 | 108.29      | 113.93   |
| 2   | F     | 202 | TFP  | C8-C7-S     | 2.01  | 122.68      | 118.36   |
| 2   | B     | 201 | TFP  | C10-C11-C12 | 2.00  | 122.32      | 118.28   |

There are no chirality outliers.

All (74) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | A     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | E     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | K     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | L     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | O     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | P     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | C     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | T     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | B     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | C     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | F     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | G     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | G     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | K     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | F     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | J     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | N     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | A     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | C     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | P     | 201 | TFP  | C13-C14-C15-N2 |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | G     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | H     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | E     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | S     | 202 | TFP  | N1-C13-C14-C15 |
| 2   | J     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | A     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | A     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | B     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | C     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | L     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | L     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | B     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | R     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | T     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | L     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | O     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | B     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | F     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | O     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | G     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | P     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | O     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | S     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | M     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | J     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | Q     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | S     | 202 | TFP  | C13-C14-C15-N2 |
| 2   | S     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | M     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | O     | 202 | TFP  | N1-C13-C14-C15 |
| 2   | P     | 202 | TFP  | N1-C13-C14-C15 |
| 2   | K     | 201 | TFP  | C14-C15-N2-C16 |
| 2   | E     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | I     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | N     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | D     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | Q     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | R     | 201 | TFP  | N1-C13-C14-C15 |
| 2   | B     | 201 | TFP  | C14-C13-N1-C12 |
| 2   | G     | 201 | TFP  | C13-C14-C15-N2 |
| 2   | N     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | O     | 201 | TFP  | C14-C13-N1-C5  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | O     | 202 | TFP  | C14-C15-N2-C19 |
| 2   | K     | 201 | TFP  | C14-C15-N2-C19 |
| 2   | J     | 202 | TFP  | N1-C13-C14-C15 |
| 2   | S     | 202 | TFP  | C14-C13-N1-C12 |
| 2   | K     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | E     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | R     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | D     | 202 | TFP  | C14-C13-N1-C12 |
| 2   | H     | 201 | TFP  | C14-C13-N1-C5  |
| 2   | F     | 202 | TFP  | C14-C13-N1-C12 |
| 2   | L     | 202 | TFP  | C13-C14-C15-N2 |
| 2   | C     | 201 | TFP  | C14-C13-N1-C5  |

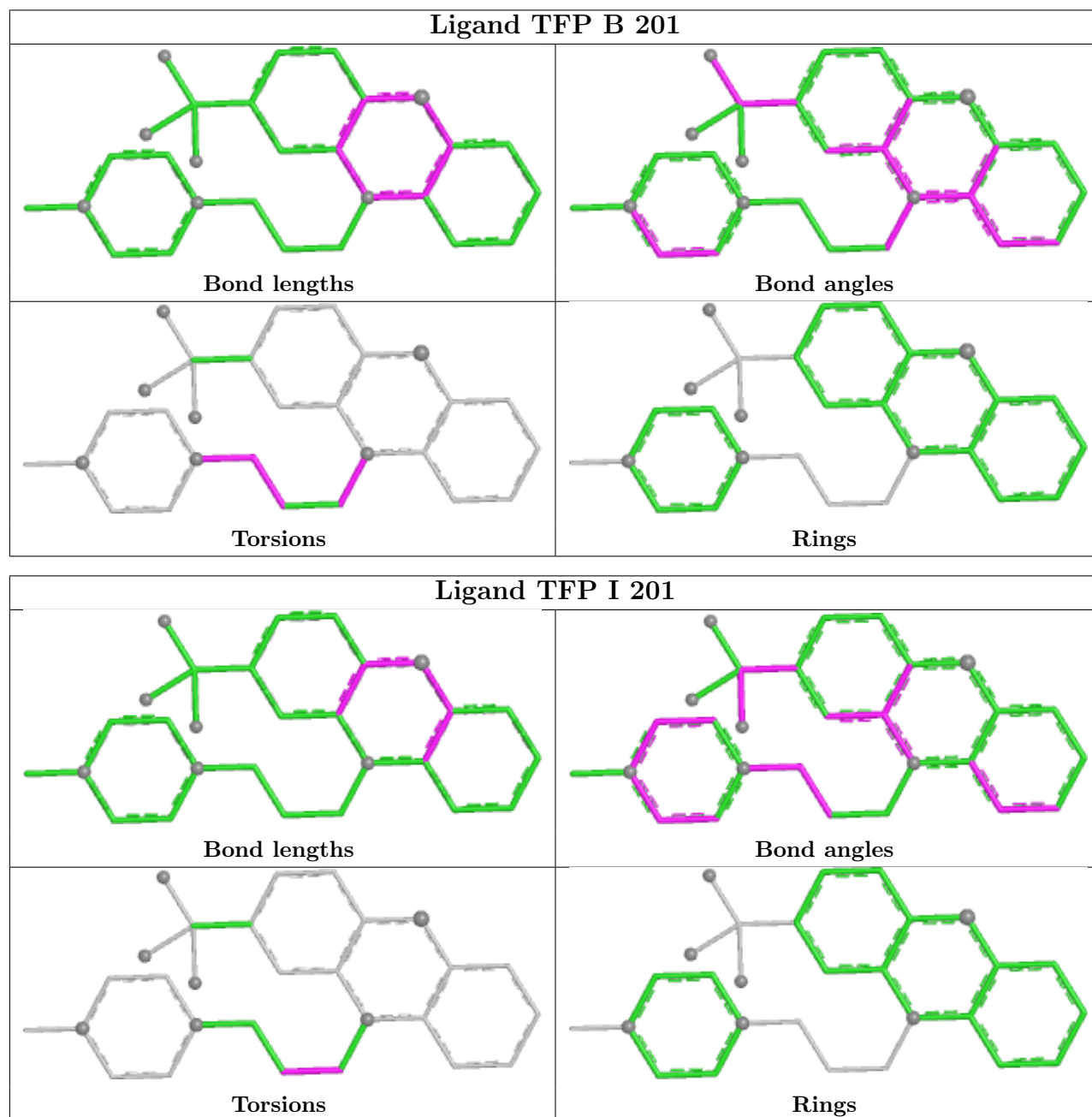
There are no ring outliers.

16 monomers are involved in 23 short contacts:

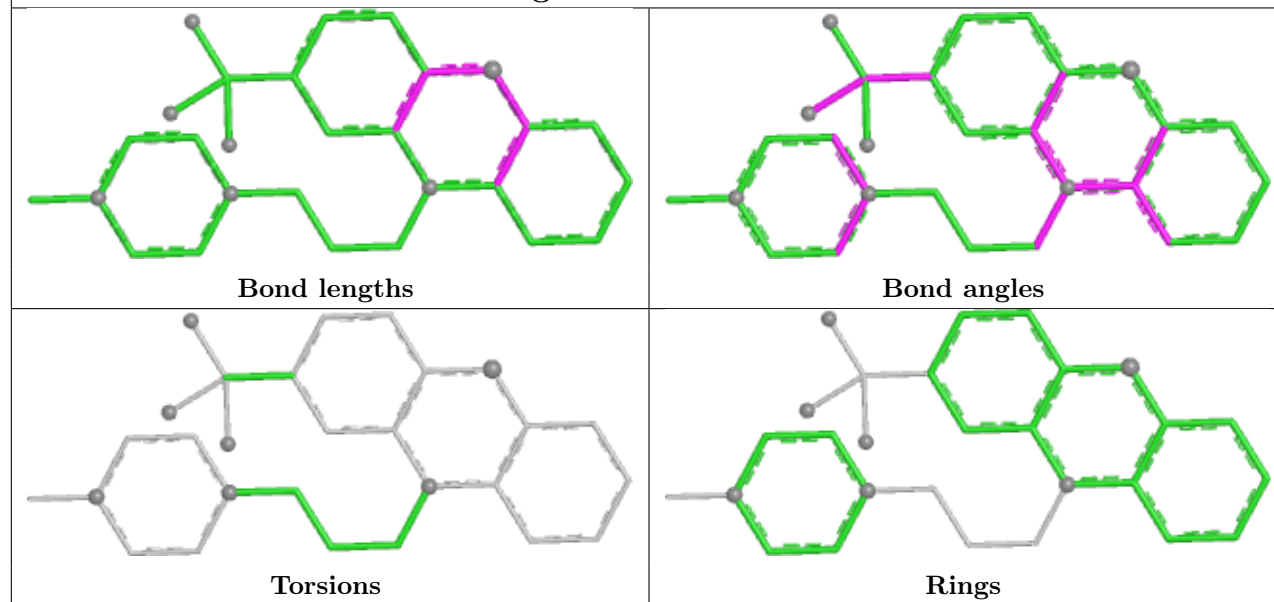
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 201 | TFP  | 4       | 0            |
| 2   | N     | 202 | TFP  | 1       | 0            |
| 2   | O     | 202 | TFP  | 1       | 0            |
| 2   | S     | 202 | TFP  | 1       | 0            |
| 2   | S     | 201 | TFP  | 1       | 0            |
| 2   | F     | 201 | TFP  | 2       | 0            |
| 2   | M     | 201 | TFP  | 2       | 0            |
| 2   | P     | 201 | TFP  | 1       | 0            |
| 2   | E     | 201 | TFP  | 2       | 0            |
| 2   | P     | 202 | TFP  | 1       | 0            |
| 2   | R     | 202 | TFP  | 1       | 0            |
| 2   | M     | 202 | TFP  | 1       | 0            |
| 2   | Q     | 201 | TFP  | 1       | 0            |
| 2   | N     | 201 | TFP  | 1       | 0            |
| 2   | L     | 201 | TFP  | 1       | 0            |
| 2   | G     | 201 | TFP  | 2       | 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

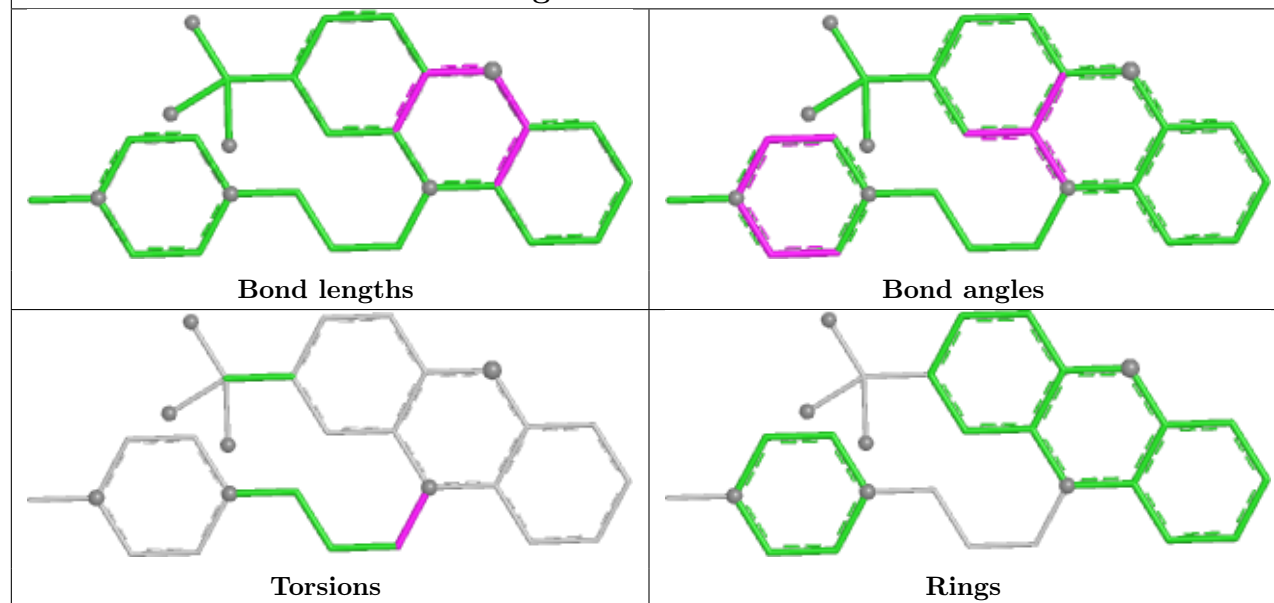
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand TFP N 202

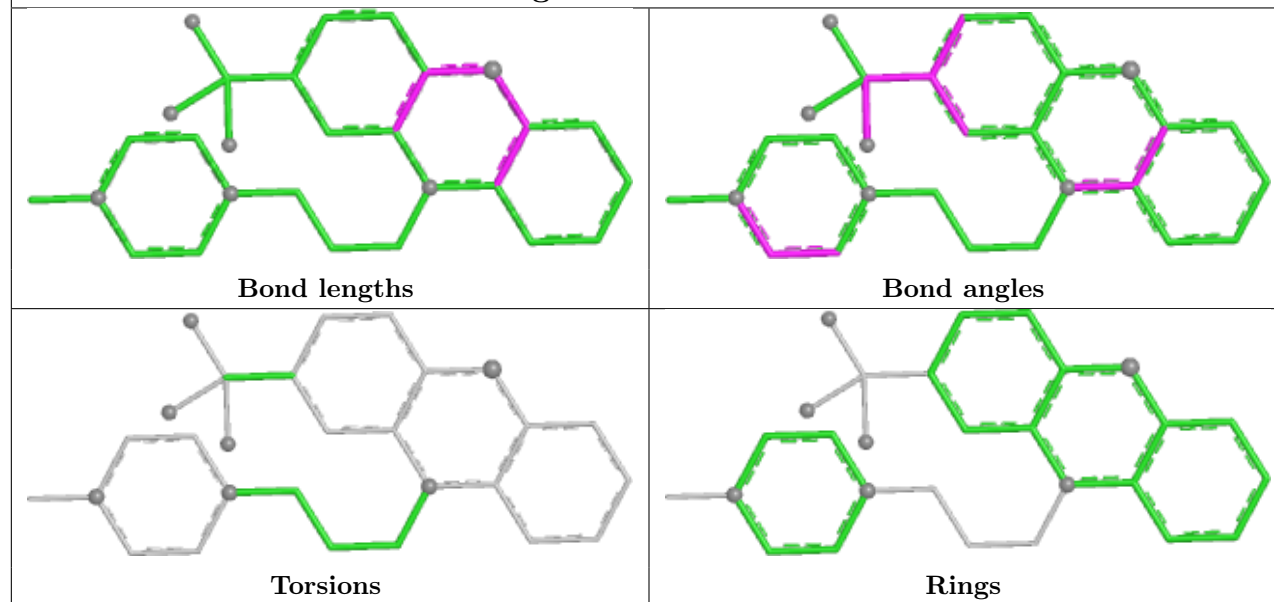


## Ligand TFP D 202

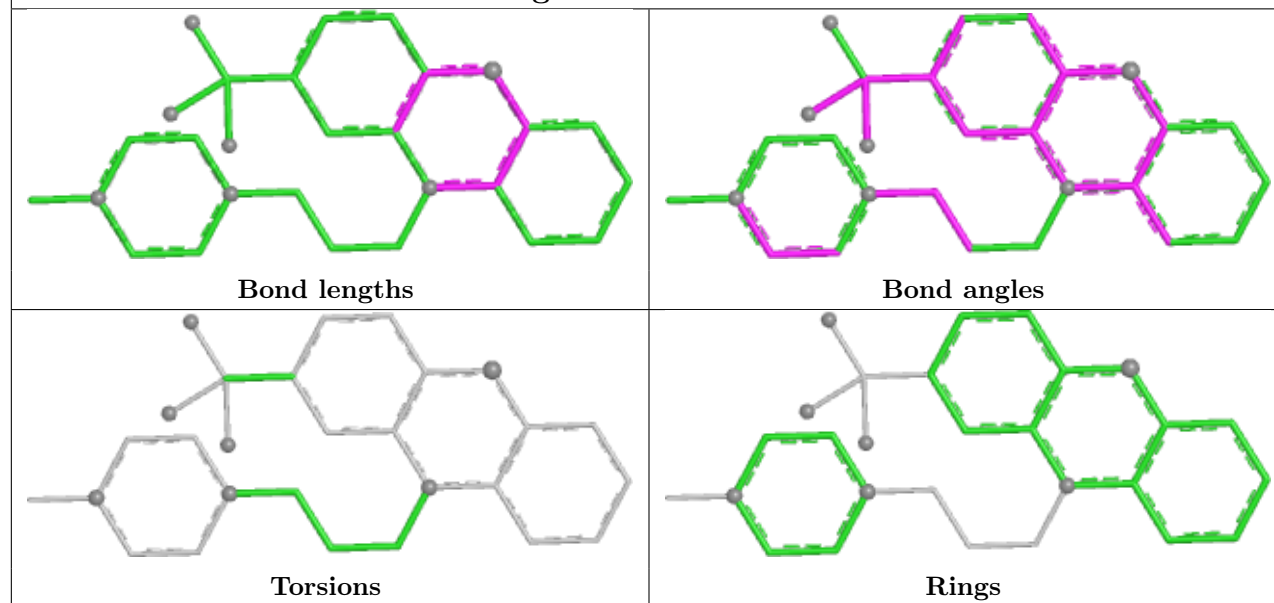




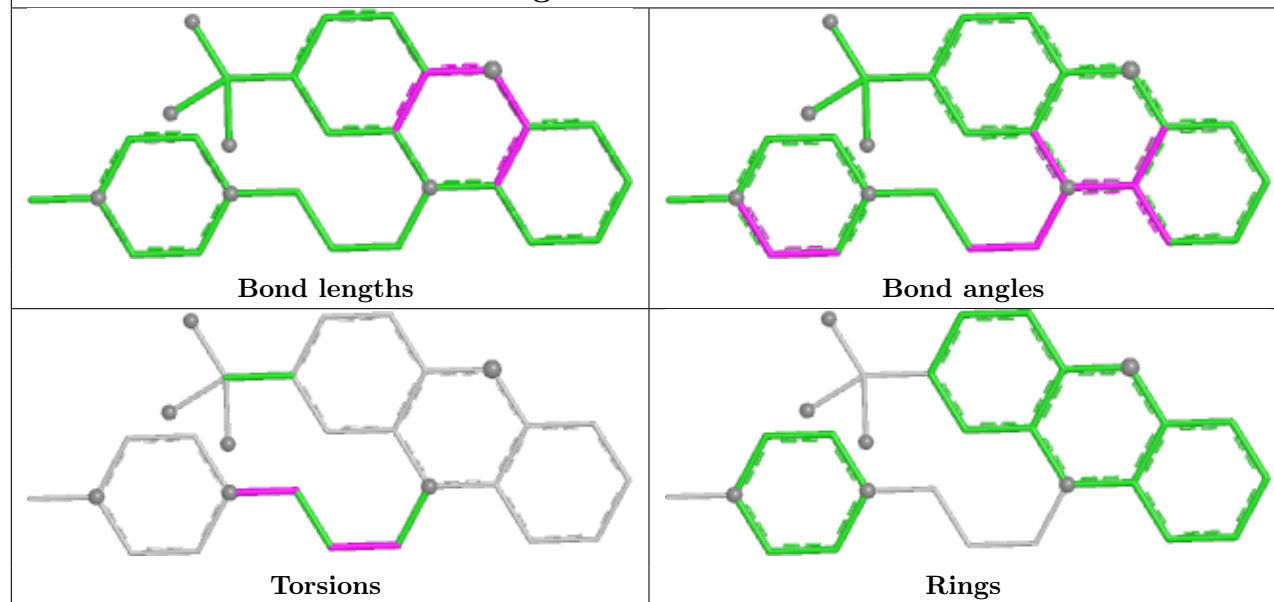
## Ligand TFP H 202



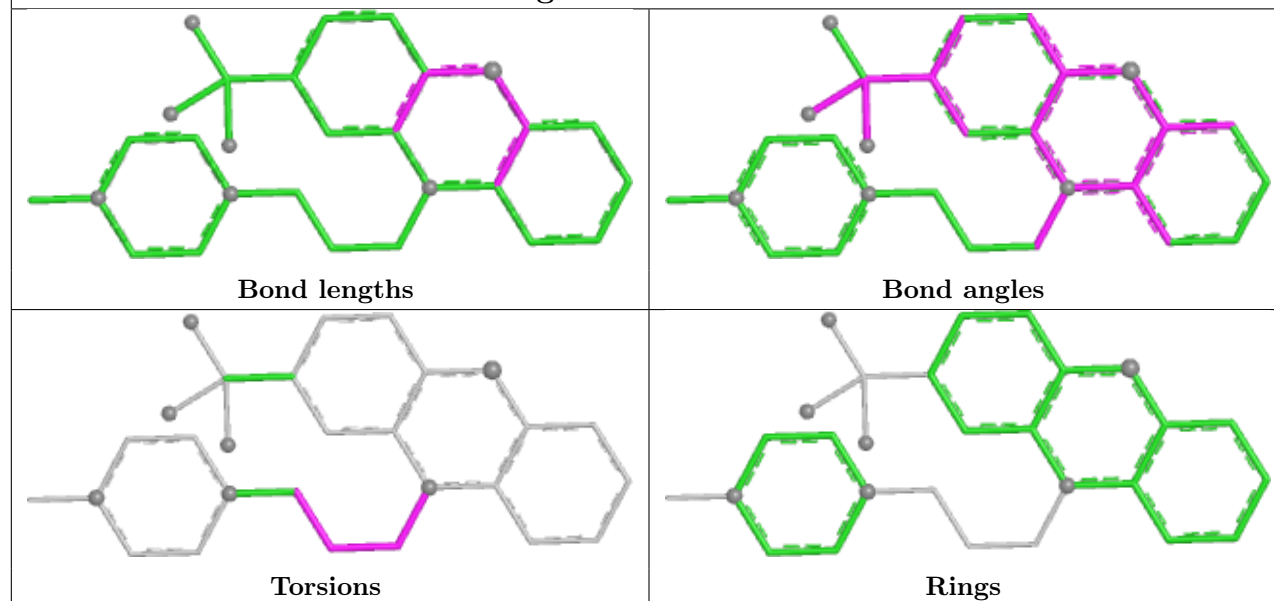
## Ligand TFP G 202



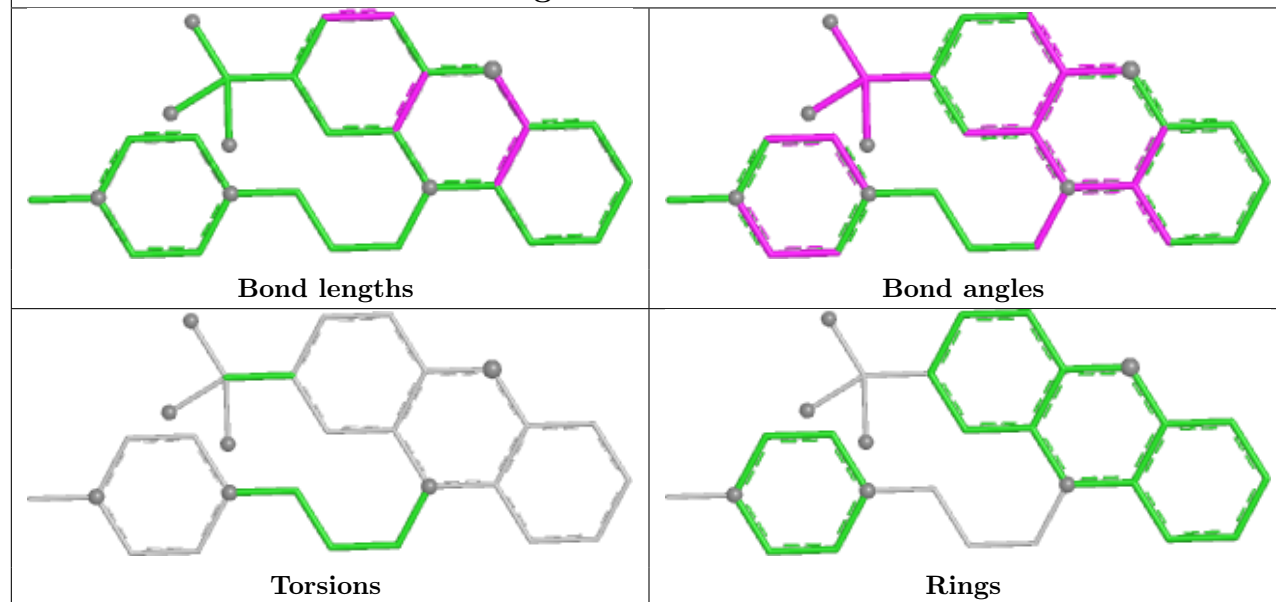
## Ligand TFP O 202



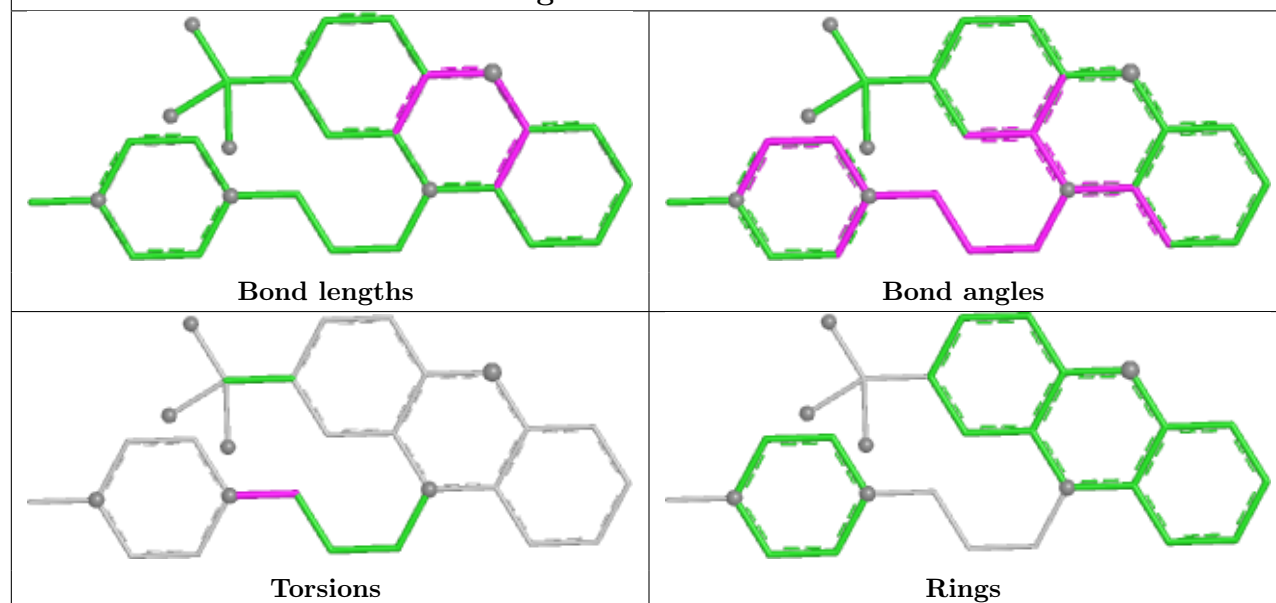
## Ligand TFP S 202

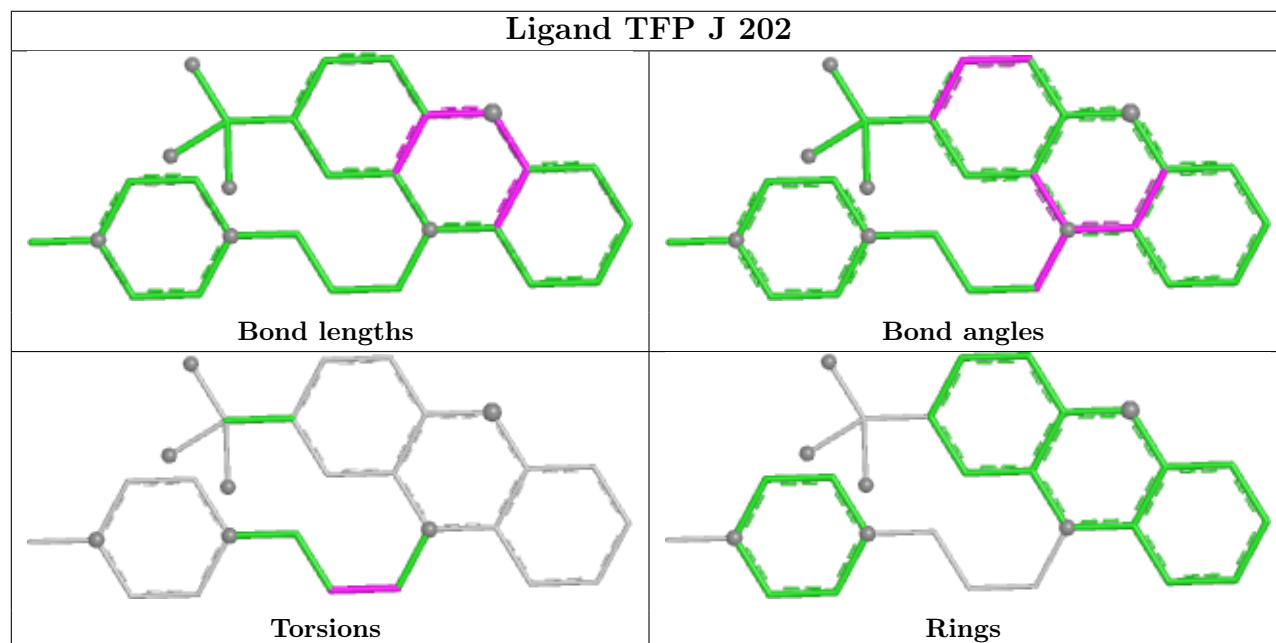
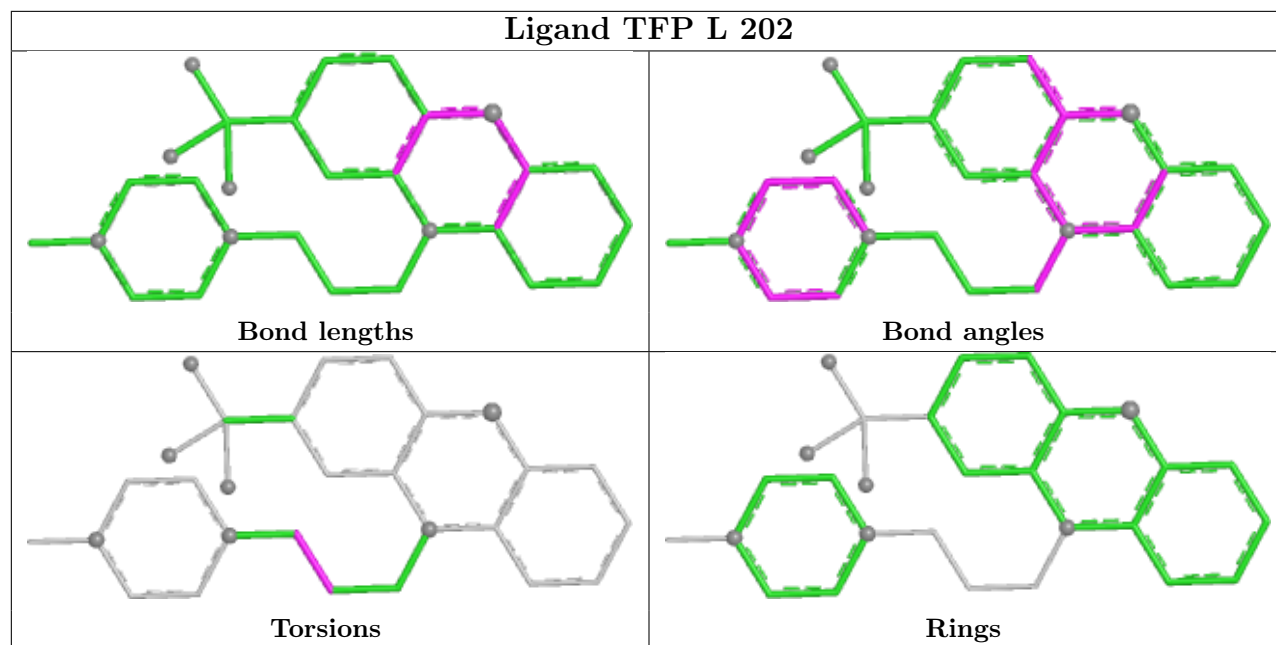


## Ligand TFP T 202

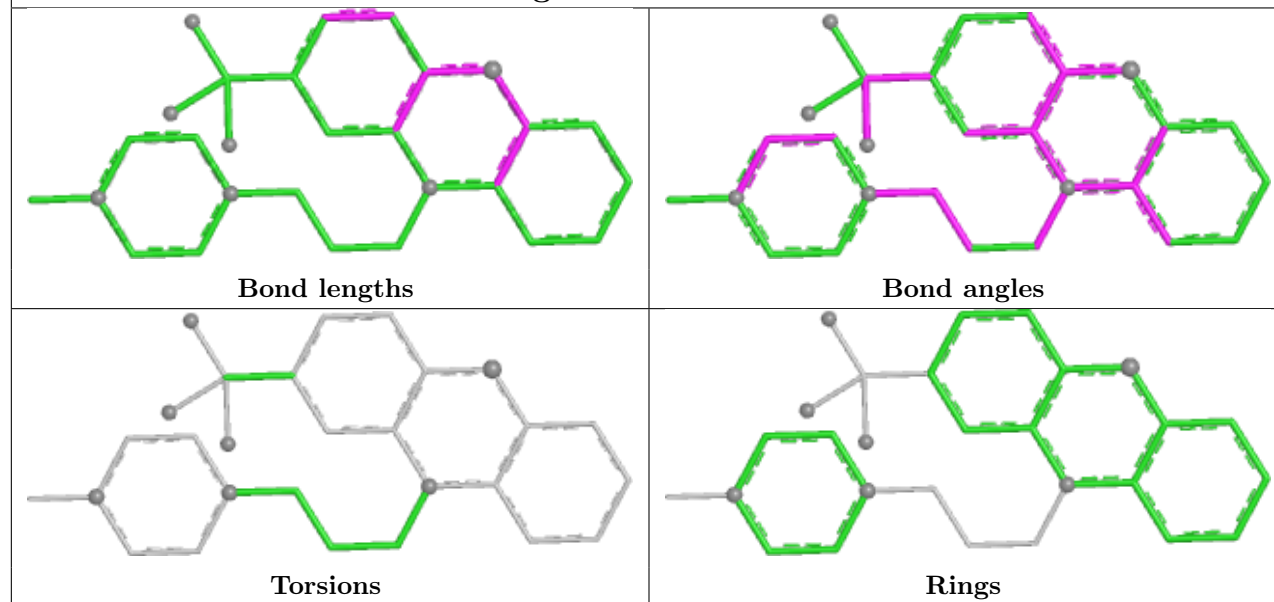


## Ligand TFP S 201

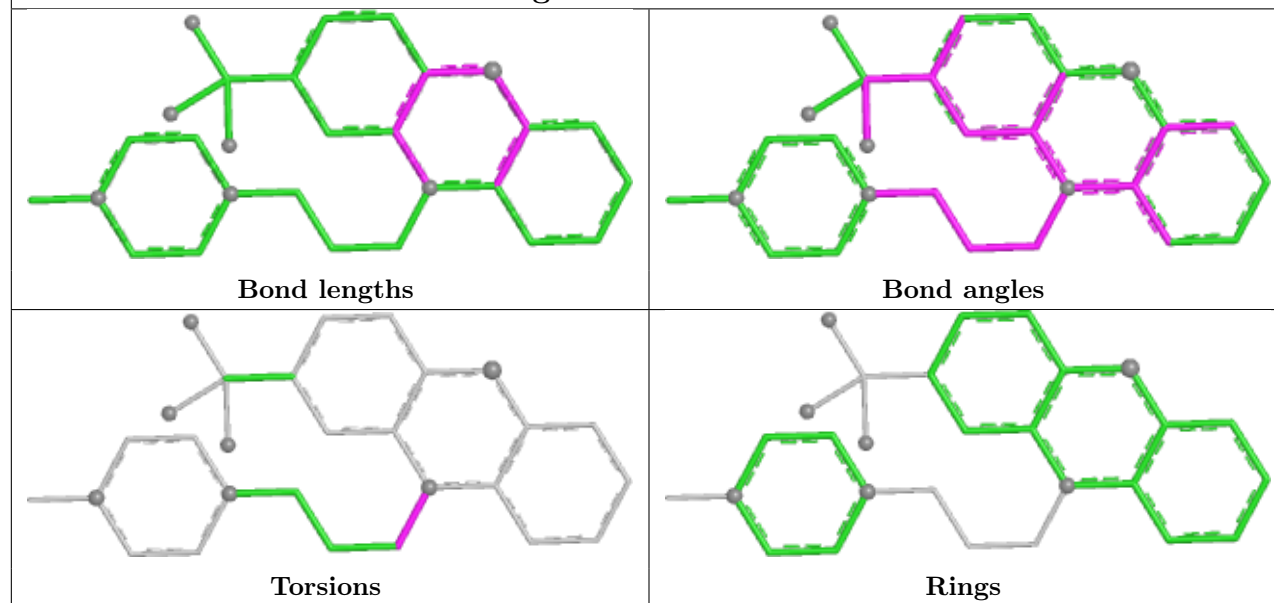




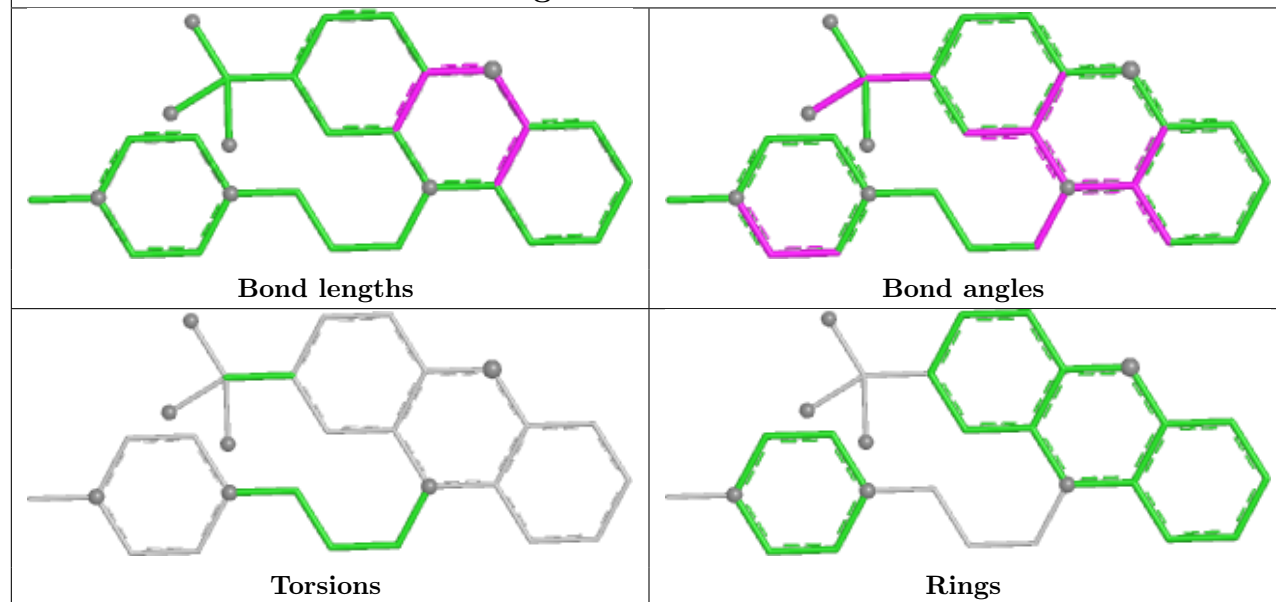
## Ligand TFP A 202



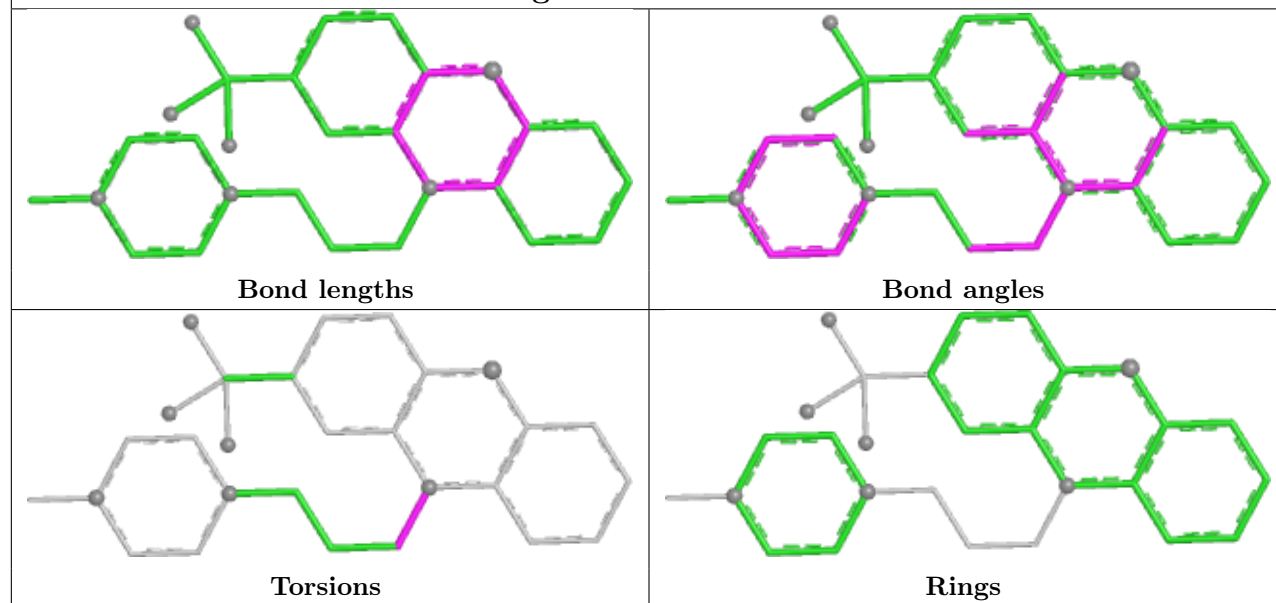
## Ligand TFP D 201



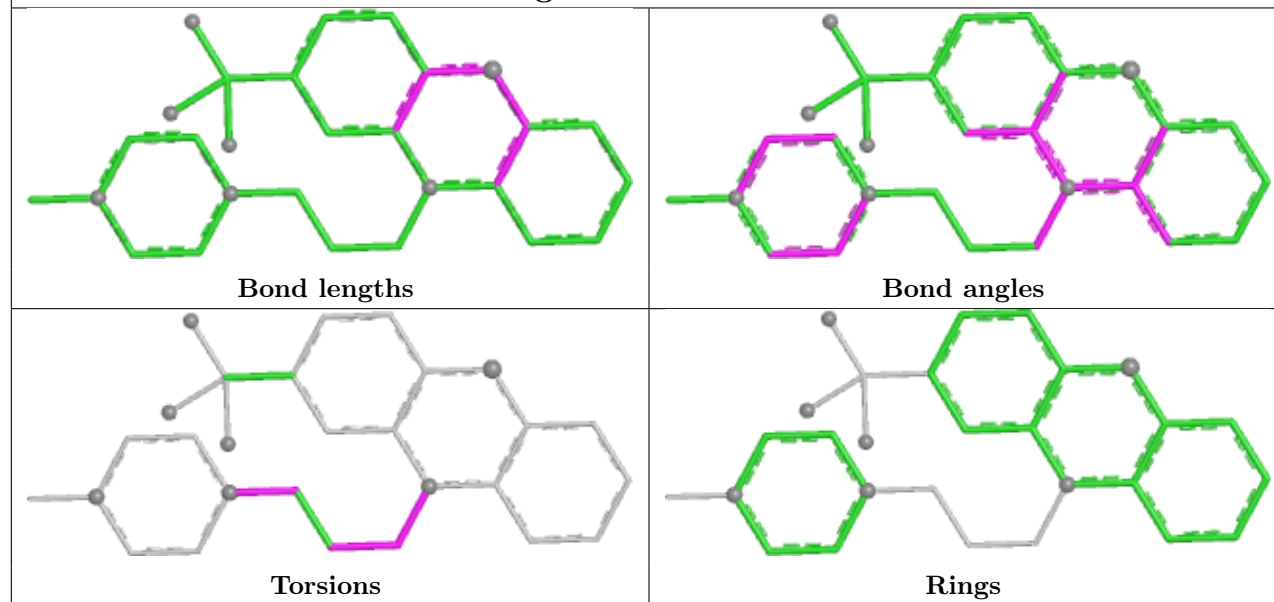
## Ligand TFP C 202



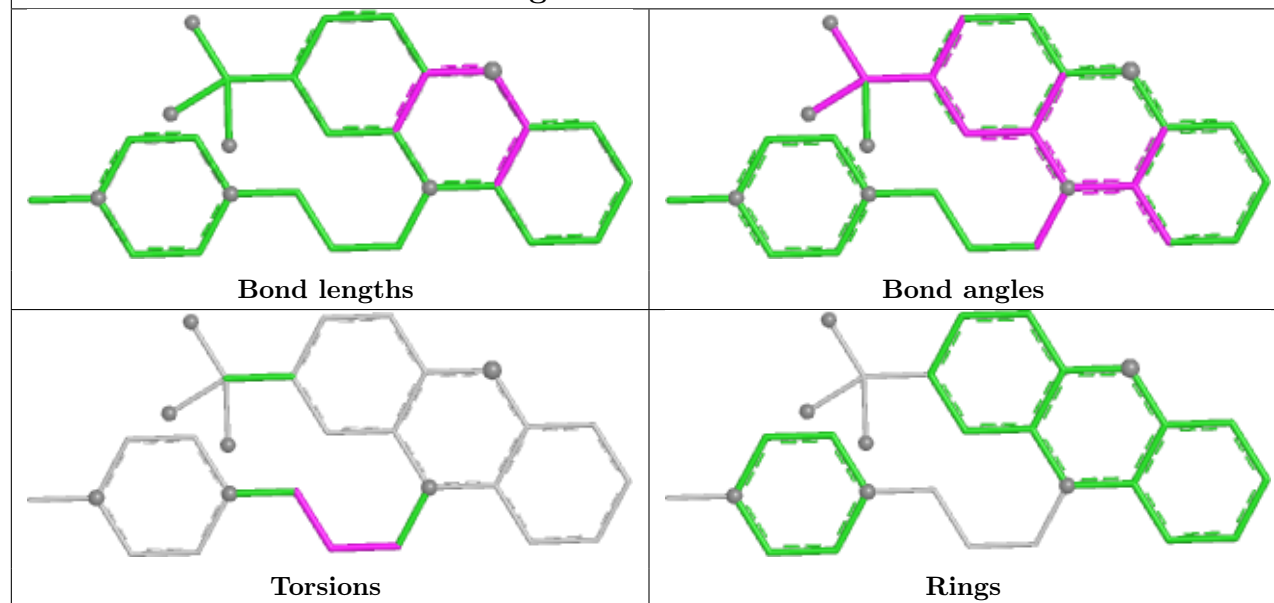
## Ligand TFP H 201



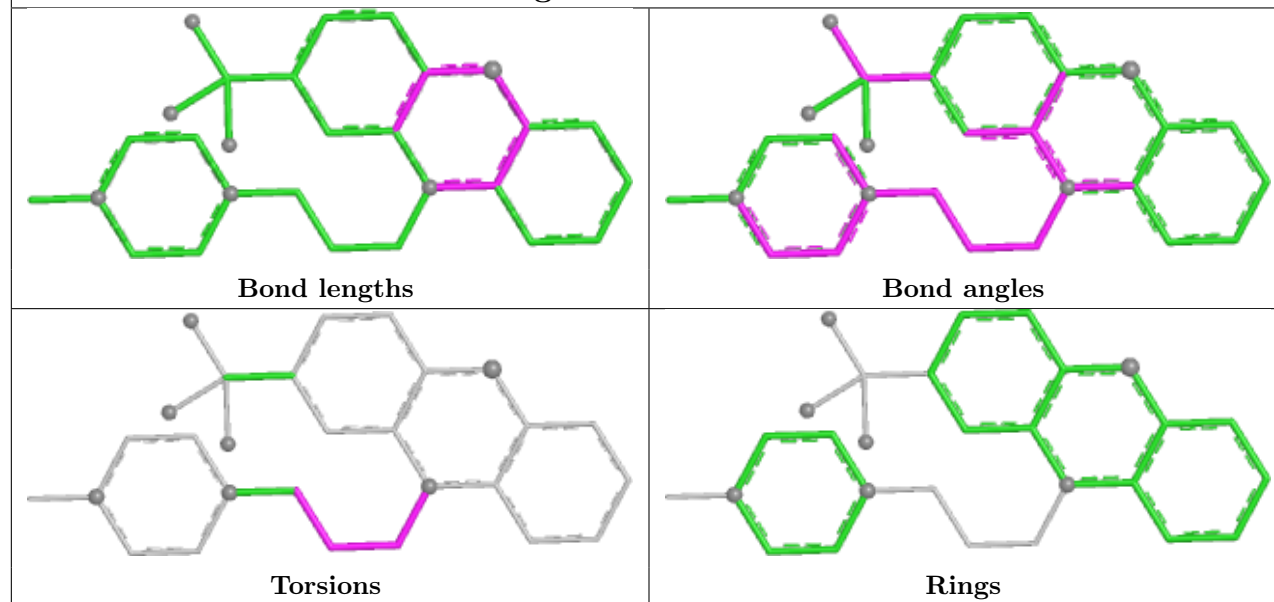
## Ligand TFP F 201



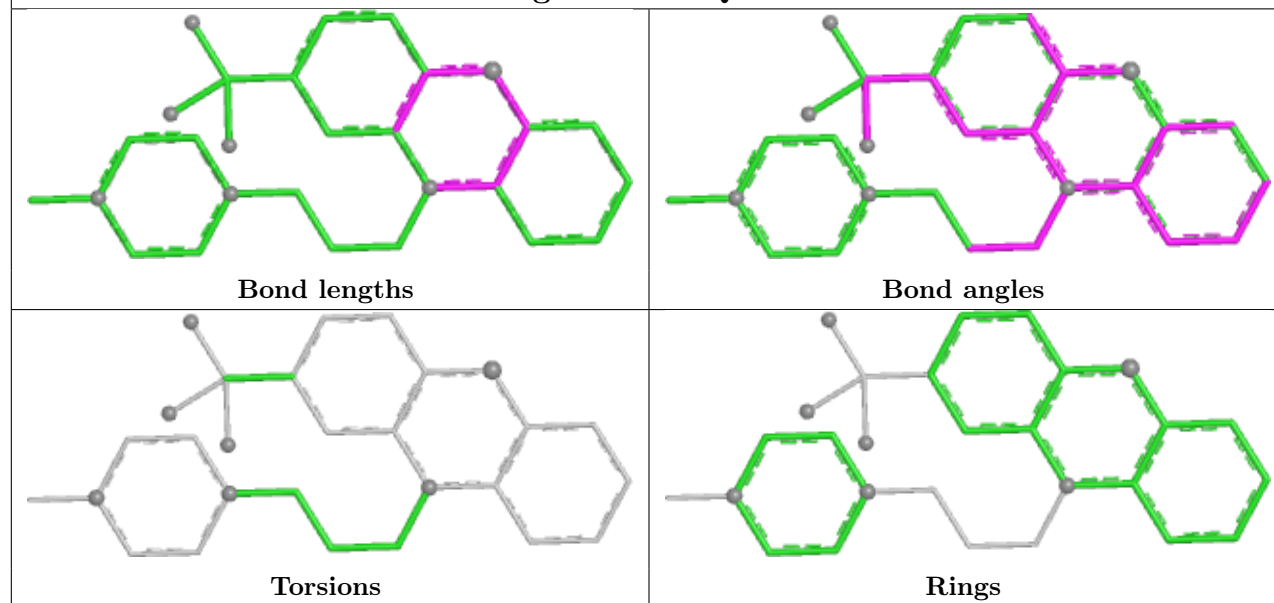
## Ligand TFP M 201



## Ligand TFP P 201

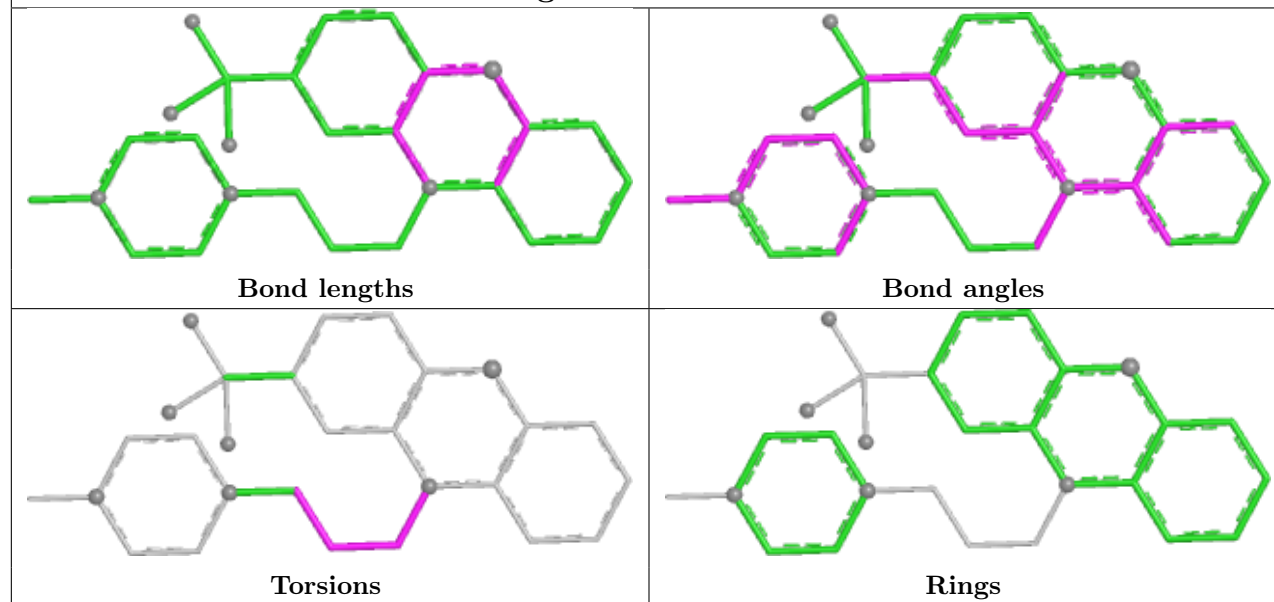


## Ligand TFP Q 202

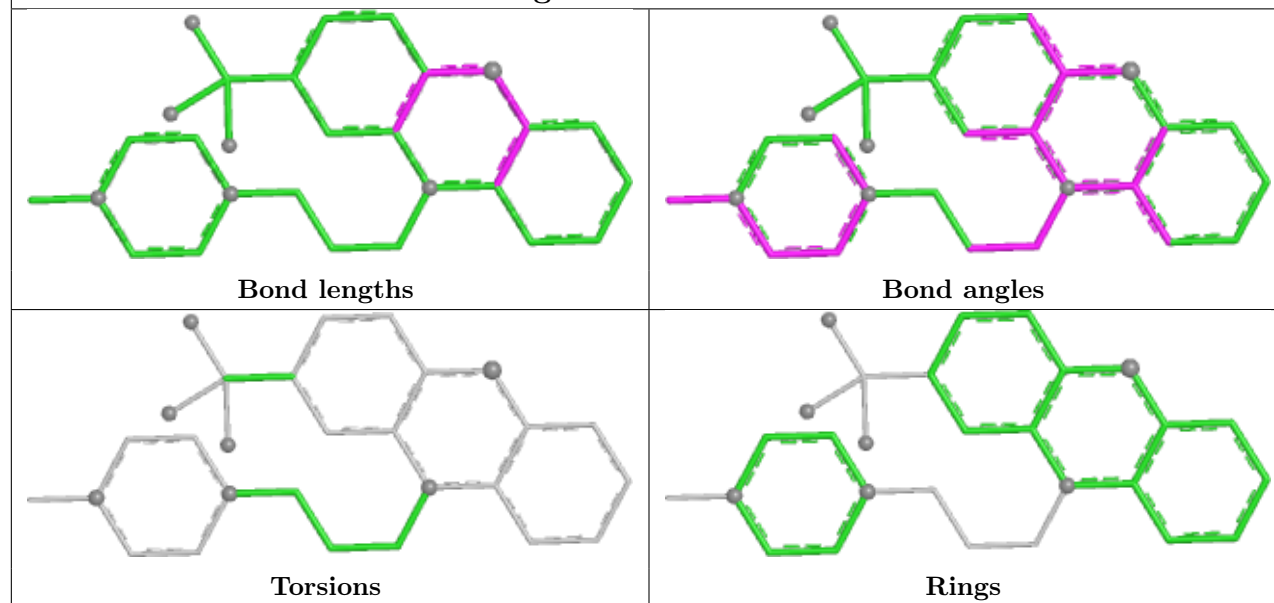


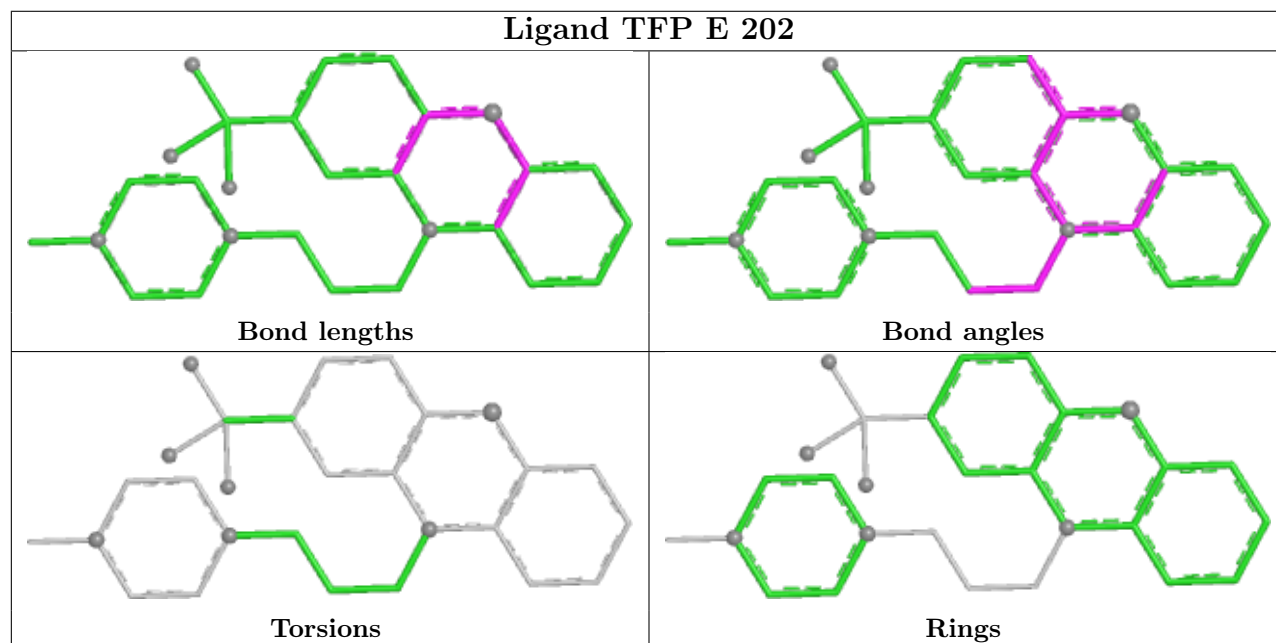
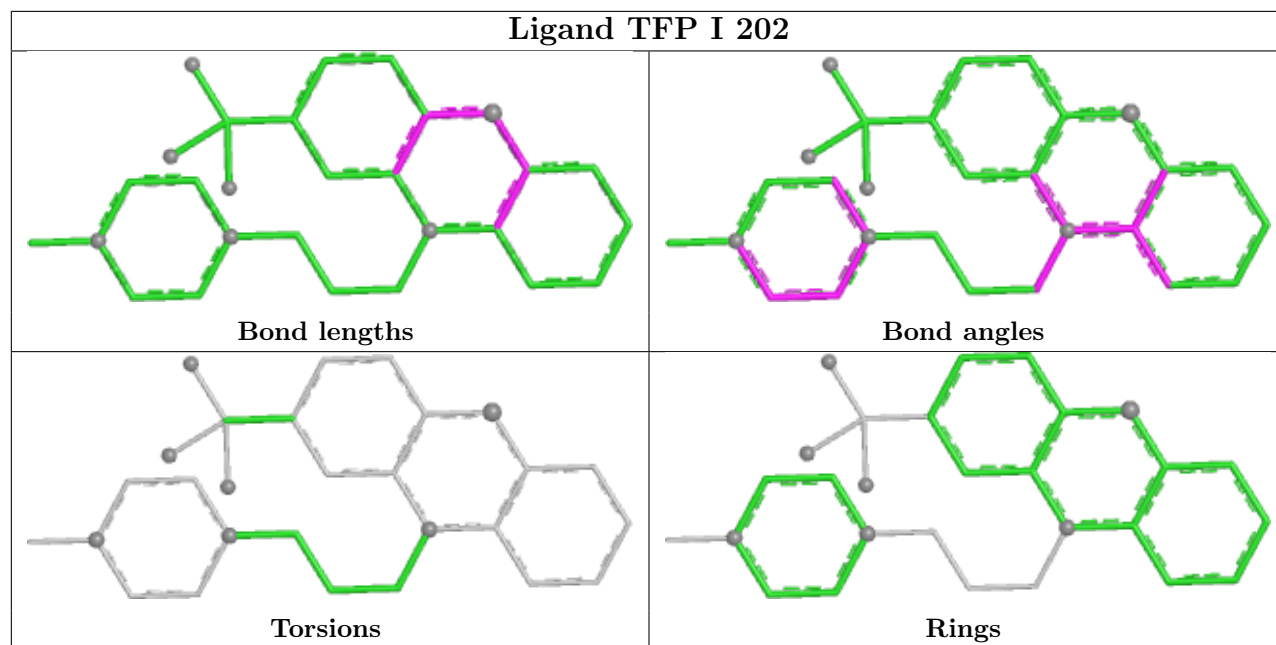


## Ligand TFP J 201

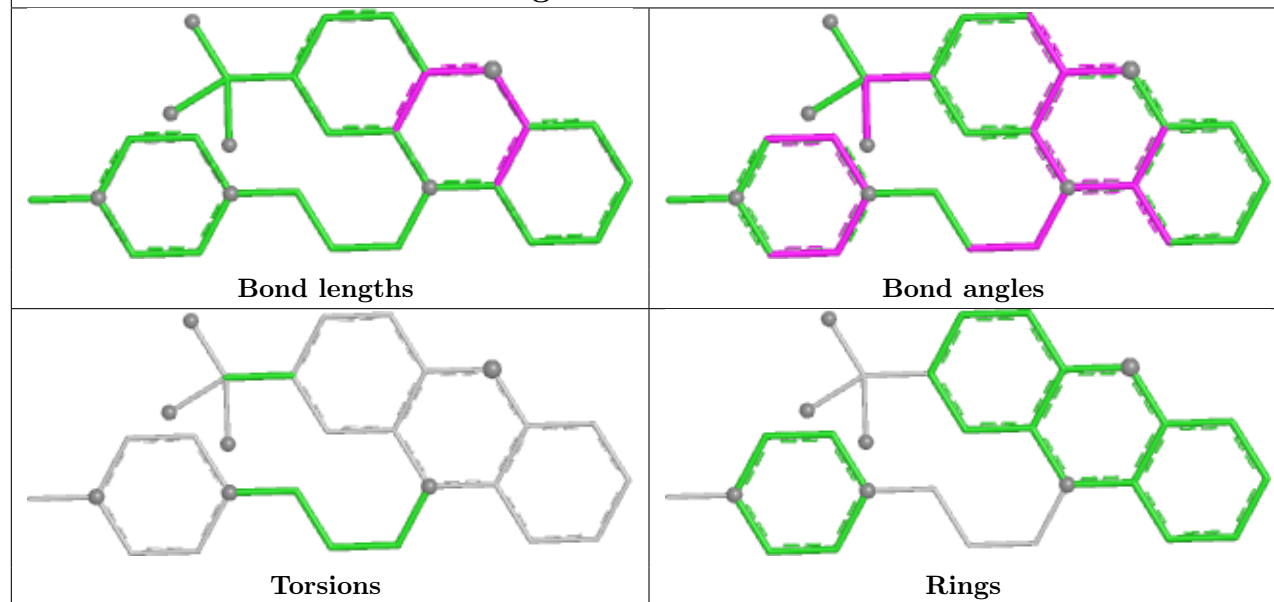


## Ligand TFP B 202

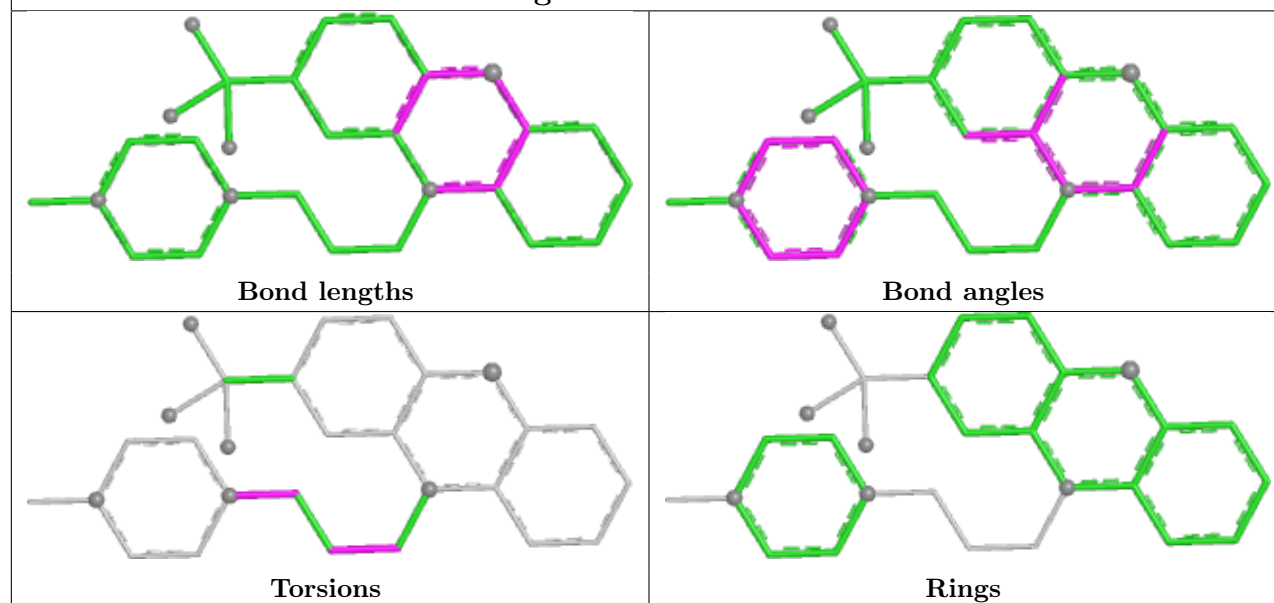




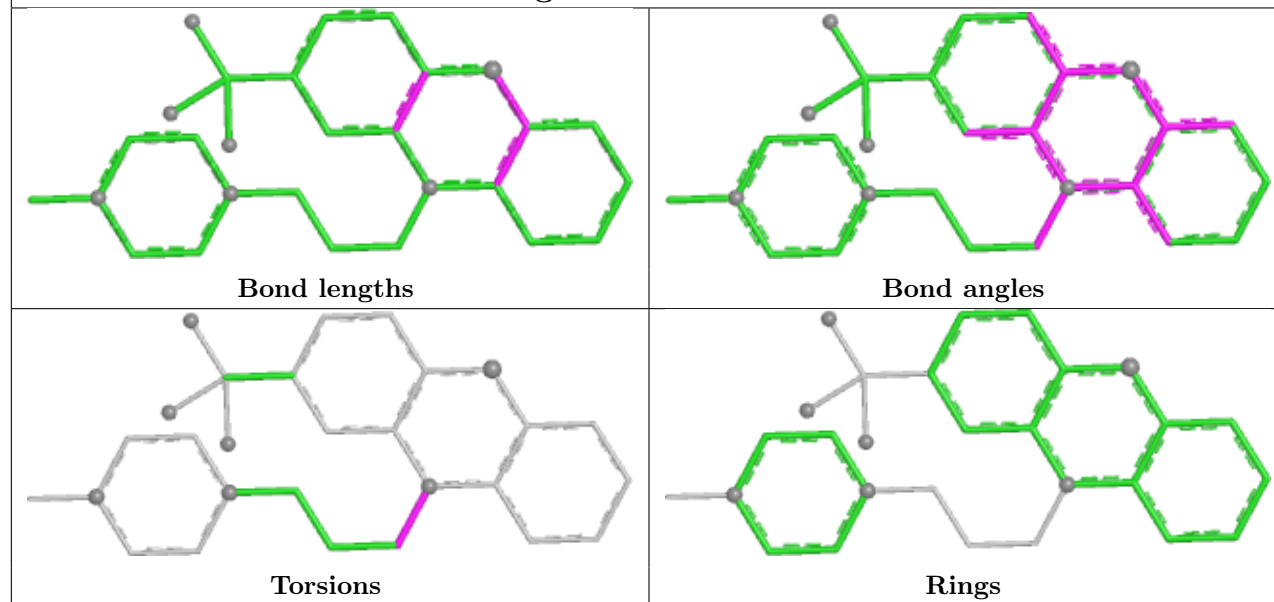
## Ligand TFP K 202



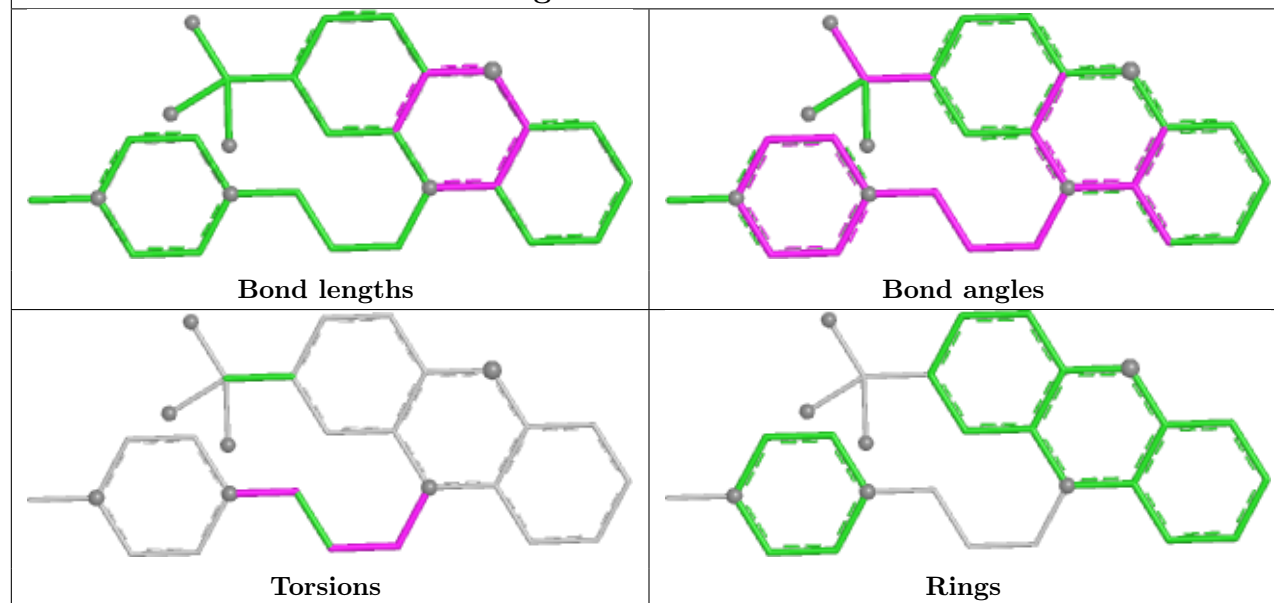
## Ligand TFP T 201



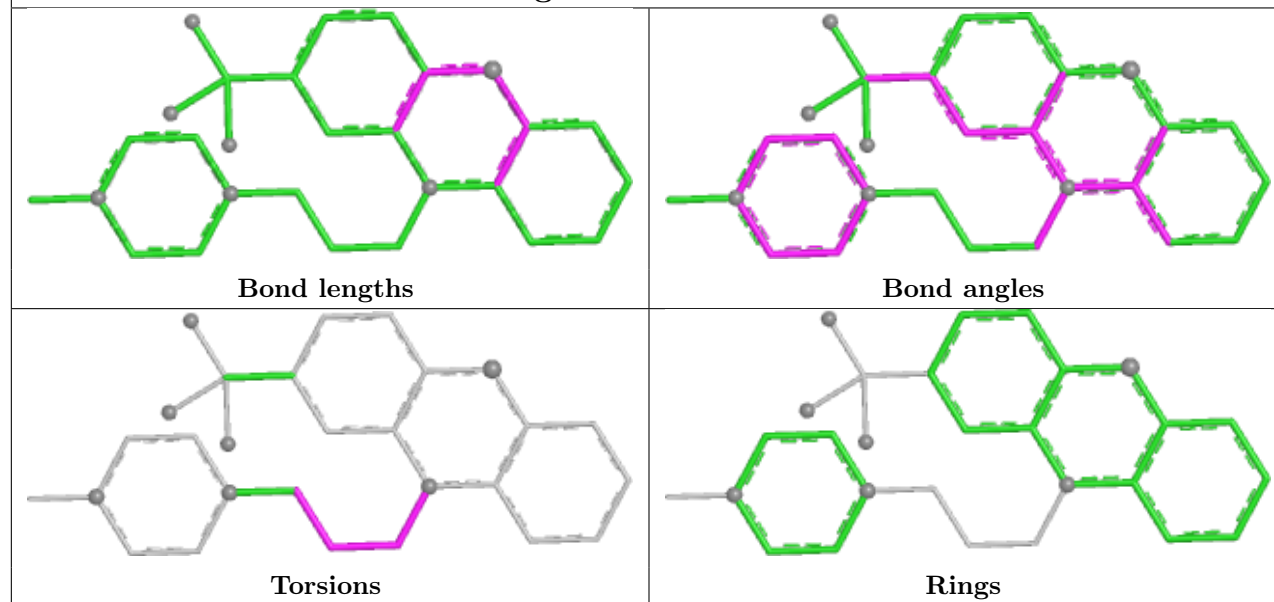
## Ligand TFP F 202



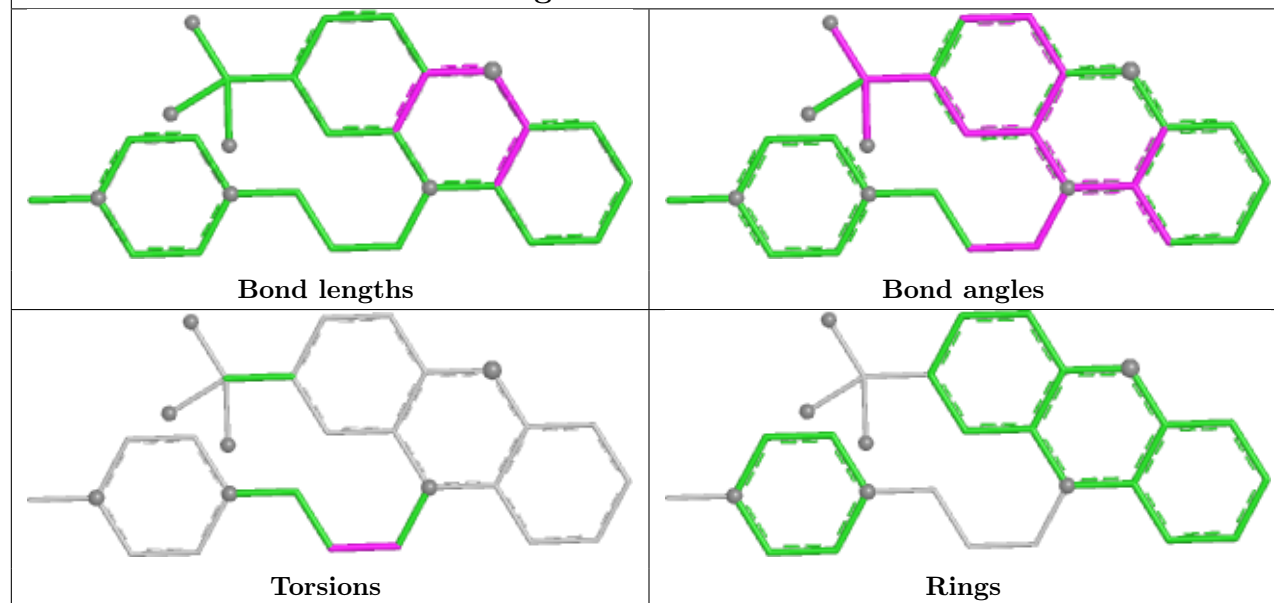
## Ligand TFP C 201



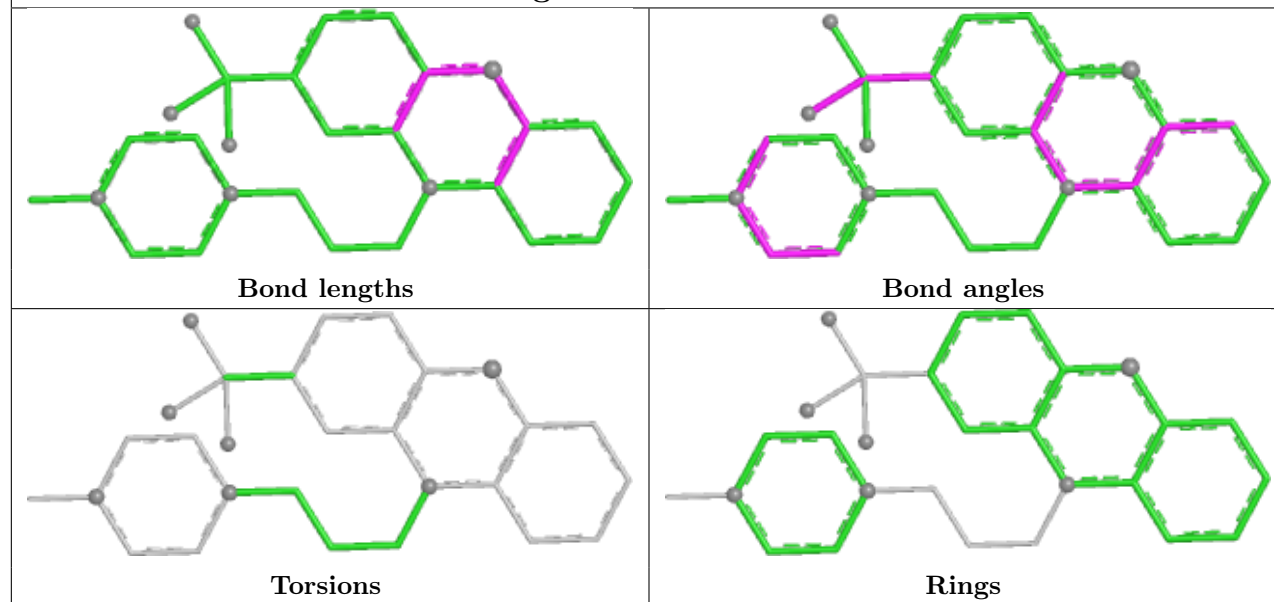
## Ligand TFP E 201



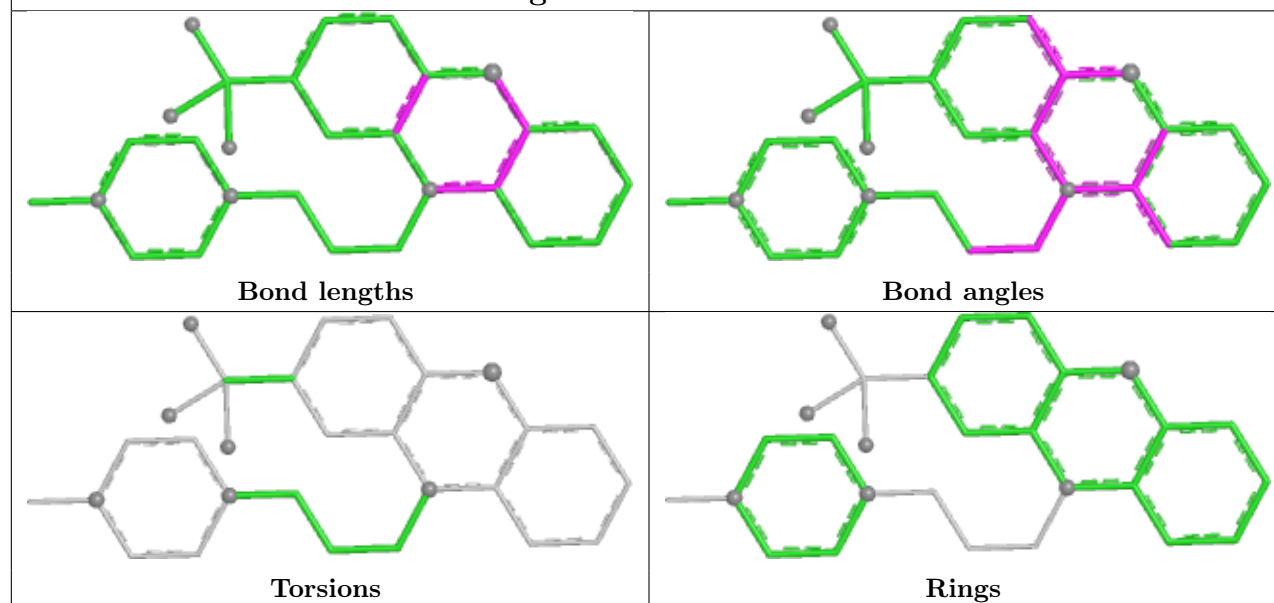
## Ligand TFP P 202



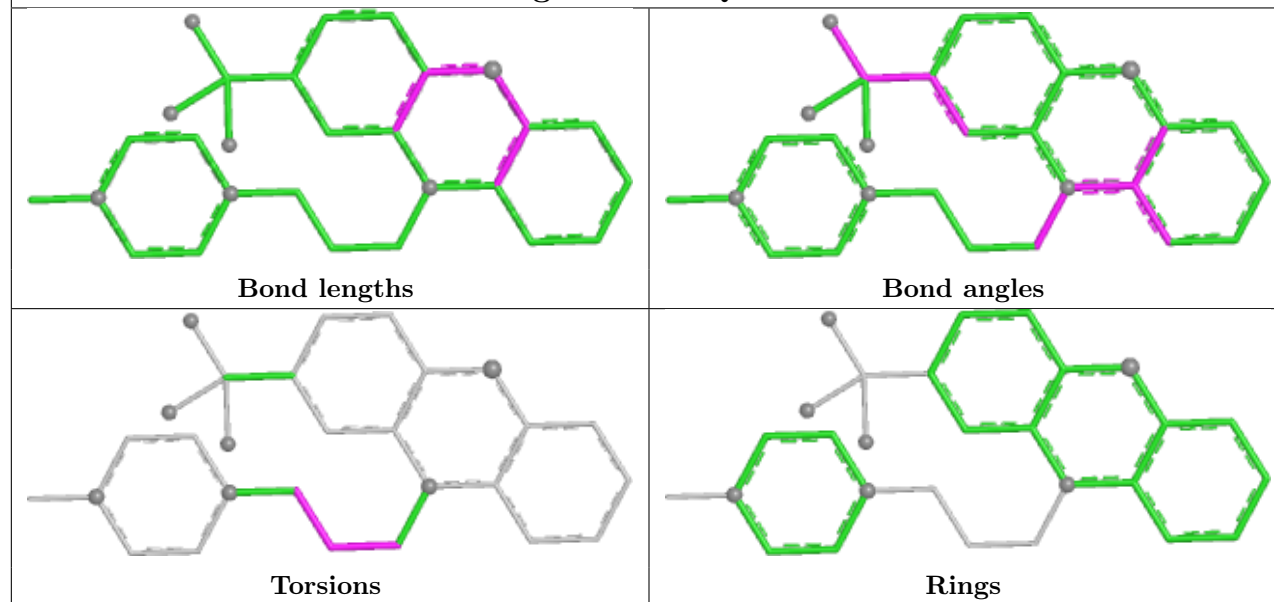
## Ligand TFP R 202



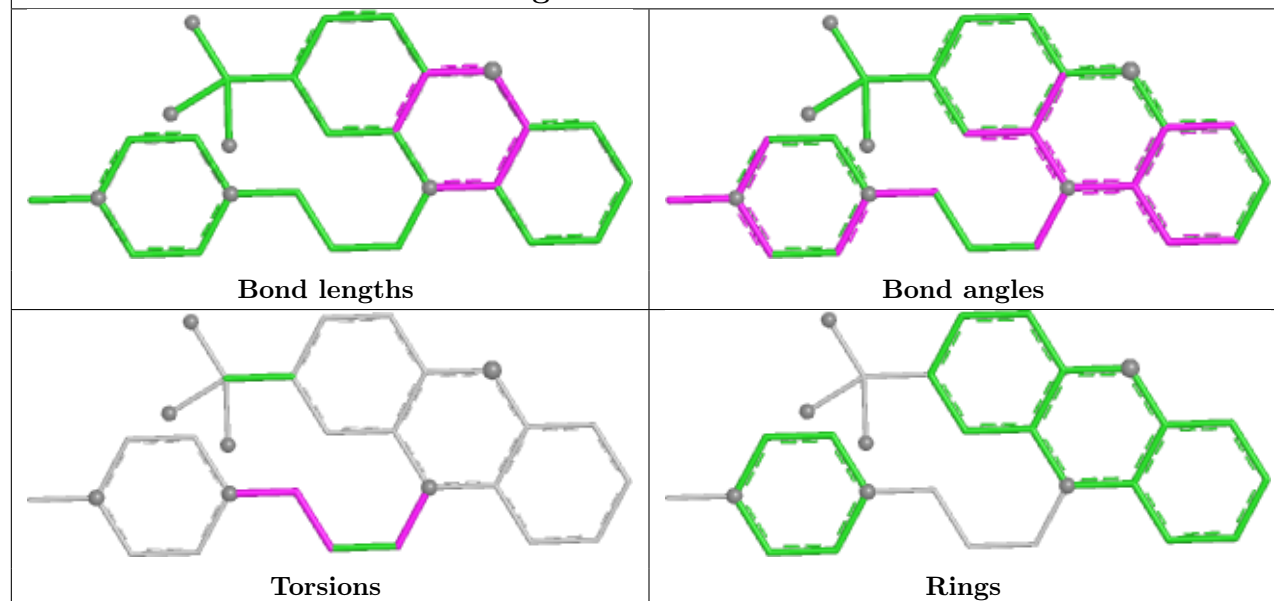
## Ligand TFP M 202



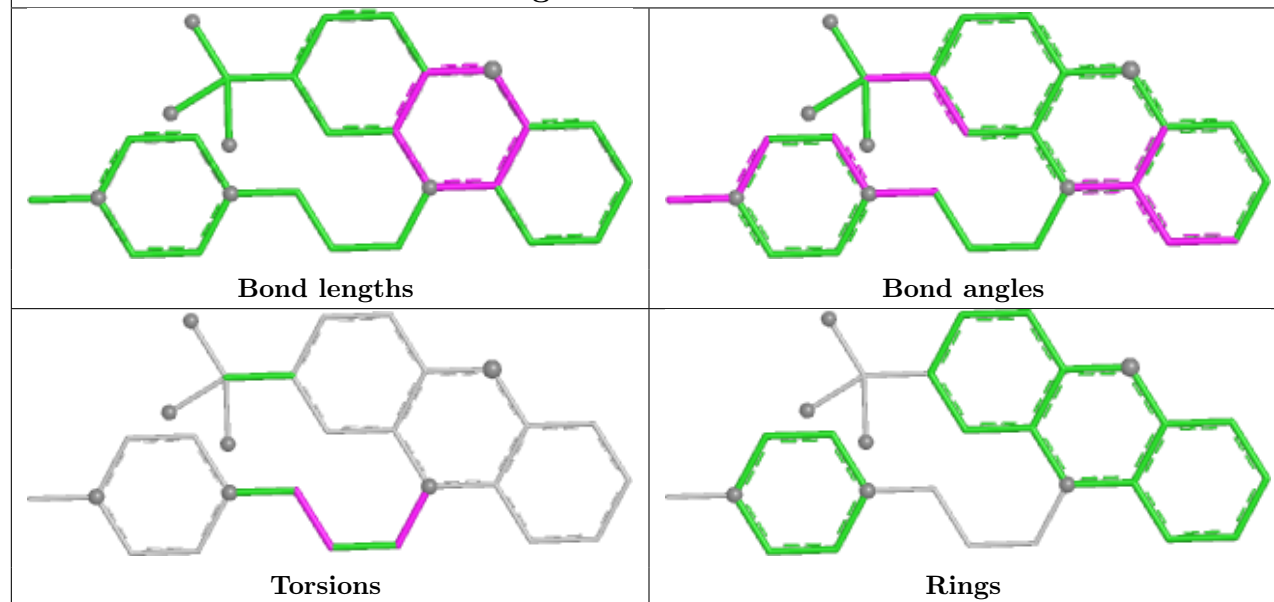
## Ligand TFP Q 201



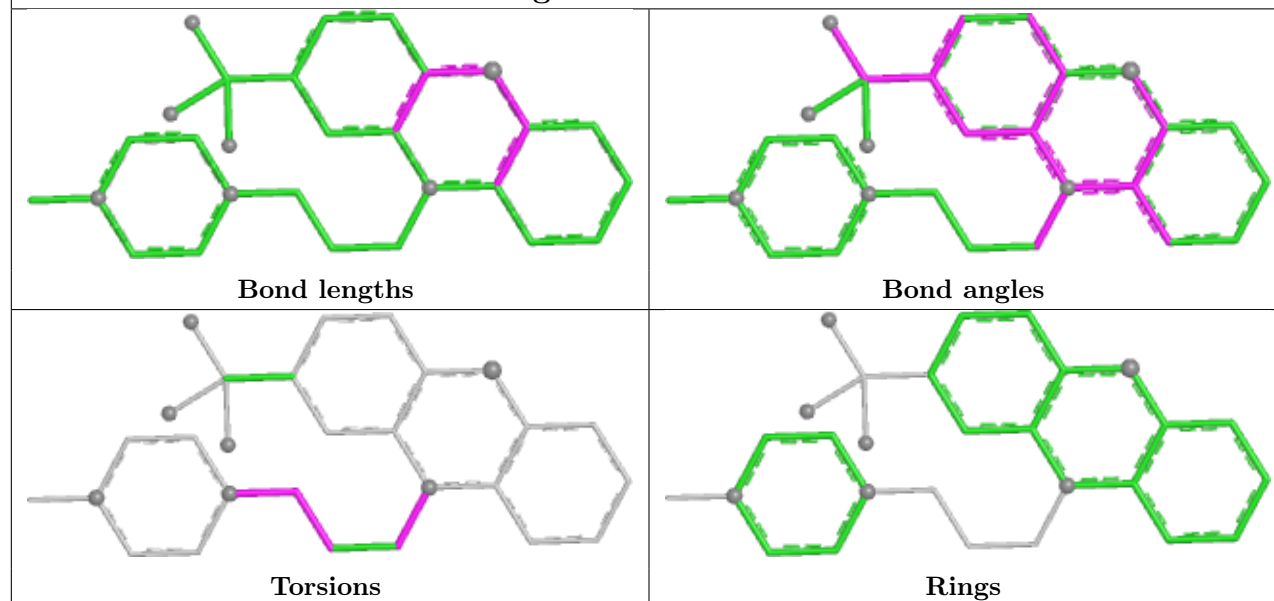
## Ligand TFP K 201



## Ligand TFP N 201

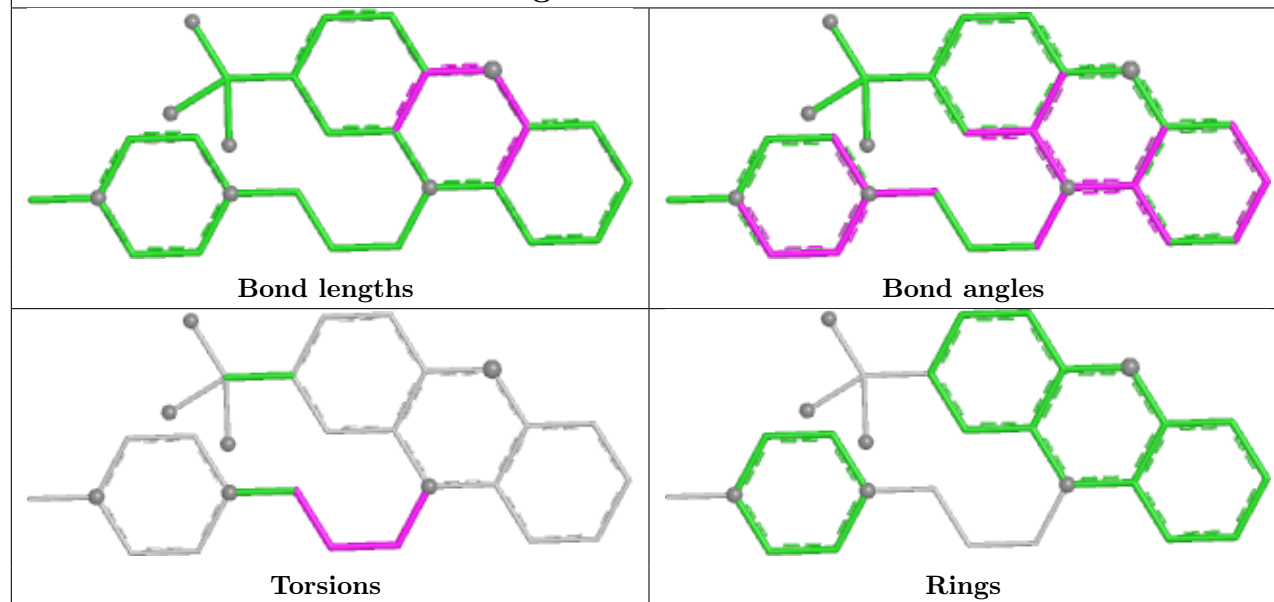


## Ligand TFP O 201

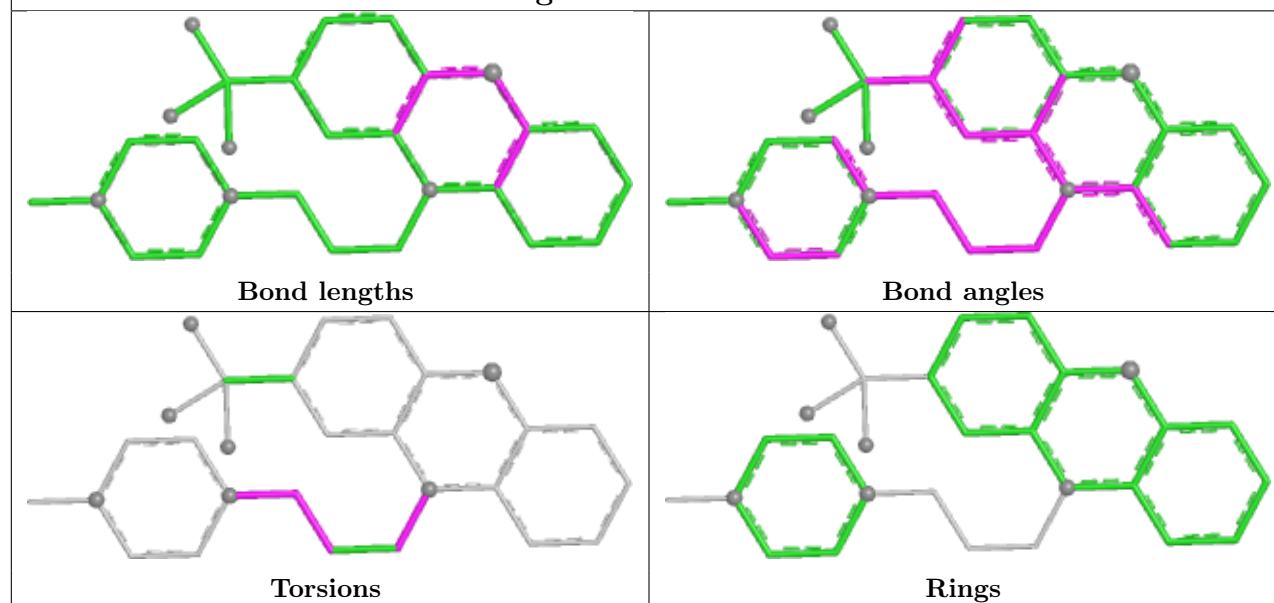


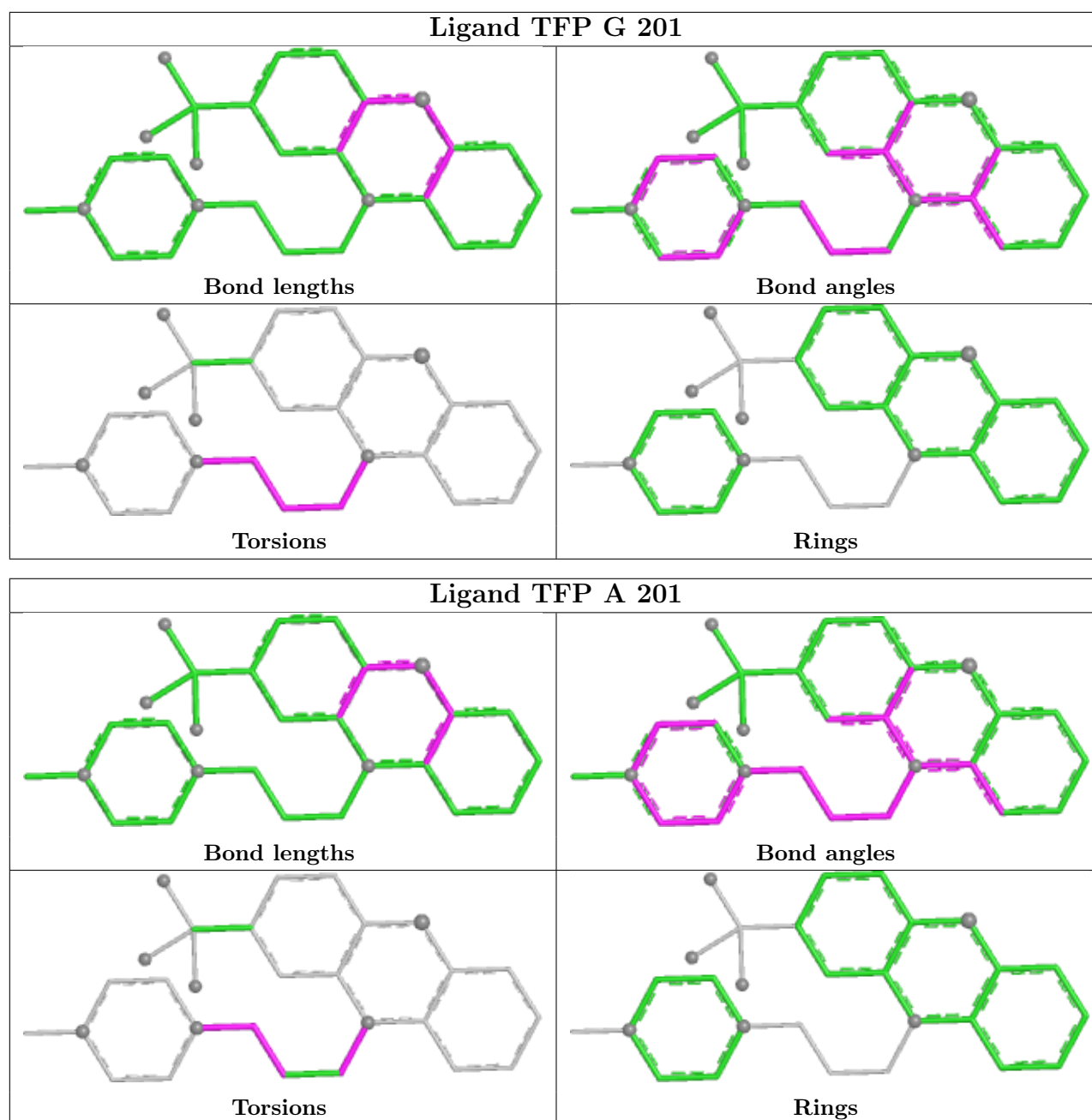


## Ligand TFP R 201



## Ligand TFP L 201





## 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     | 93/101 (92%)    | 0.14   | 5 (5%) 31 33  | 10, 20, 47, 57        | 1 (1%)  |
| 1   | B     | 93/101 (92%)    | 0.08   | 5 (5%) 31 33  | 13, 22, 48, 66        | 1 (1%)  |
| 1   | C     | 93/101 (92%)    | -0.03  | 2 (2%) 62 64  | 11, 21, 37, 48        | 1 (1%)  |
| 1   | D     | 93/101 (92%)    | 0.33   | 5 (5%) 31 33  | 14, 25, 70, 77        | 2 (2%)  |
| 1   | E     | 92/101 (91%)    | 0.10   | 1 (1%) 78 79  | 14, 24, 45, 51        | 0       |
| 1   | F     | 90/101 (89%)    | 0.41   | 5 (5%) 30 32  | 11, 27, 51, 69        | 1 (1%)  |
| 1   | G     | 90/101 (89%)    | 0.47   | 7 (7%) 19 21  | 3, 27, 49, 56         | 3 (3%)  |
| 1   | H     | 94/101 (93%)    | 0.80   | 11 (11%) 9 10 | 16, 33, 63, 67        | 1 (1%)  |
| 1   | I     | 93/101 (92%)    | 0.14   | 4 (4%) 40 41  | 9, 27, 42, 49         | 1 (1%)  |
| 1   | J     | 93/101 (92%)    | -0.07  | 1 (1%) 78 79  | 12, 22, 39, 49        | 2 (2%)  |
| 1   | K     | 93/101 (92%)    | 0.06   | 4 (4%) 40 41  | 13, 23, 48, 54        | 0       |
| 1   | L     | 93/101 (92%)    | -0.01  | 5 (5%) 31 33  | 15, 22, 46, 60        | 0       |
| 1   | M     | 92/101 (91%)    | 0.37   | 4 (4%) 40 41  | 10, 28, 53, 60        | 2 (2%)  |
| 1   | N     | 92/101 (91%)    | 0.02   | 0 100 100     | 9, 21, 45, 52         | 2 (2%)  |
| 1   | O     | 93/101 (92%)    | 0.36   | 7 (7%) 20 22  | 6, 29, 43, 49         | 2 (2%)  |
| 1   | P     | 92/101 (91%)    | 0.12   | 1 (1%) 78 79  | 15, 26, 44, 50        | 0       |
| 1   | Q     | 88/101 (87%)    | 0.61   | 8 (9%) 15 16  | 13, 33, 56, 58        | 3 (3%)  |
| 1   | R     | 93/101 (92%)    | 0.17   | 2 (2%) 62 64  | 17, 30, 49, 56        | 1 (1%)  |
| 1   | S     | 93/101 (92%)    | -0.05  | 3 (3%) 50 52  | 2, 21, 39, 45         | 2 (2%)  |
| 1   | T     | 93/101 (92%)    | 0.40   | 8 (8%) 16 17  | 10, 27, 58, 64        | 2 (2%)  |
| All | All   | 1846/2020 (91%) | 0.22   | 88 (4%) 35 37 | 2, 26, 49, 77         | 27 (1%) |

All (88) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 81  | CYS  | 7.1  |
| 1   | G     | 64  | SER  | 6.1  |
| 1   | O     | 64  | SER  | 6.0  |
| 1   | Q     | 64  | SER  | 5.9  |
| 1   | S     | 64  | SER  | 5.8  |
| 1   | Q     | 81  | CYS  | 5.7  |
| 1   | G     | 10  | ASP  | 5.3  |
| 1   | O     | 10  | ASP  | 5.0  |
| 1   | M     | 64  | SER  | 4.8  |
| 1   | Q     | 54  | ALA  | 4.8  |
| 1   | A     | 92  | GLY  | 4.3  |
| 1   | H     | 54  | ALA  | 4.1  |
| 1   | A     | 93  | PHE  | 3.8  |
| 1   | G     | 48  | LYS  | 3.7  |
| 1   | B     | 48  | LYS  | 3.7  |
| 1   | H     | 53  | ALA  | 3.6  |
| 1   | S     | 10  | ASP  | 3.6  |
| 1   | T     | 57  | LYS  | 3.5  |
| 1   | O     | 54  | ALA  | 3.5  |
| 1   | T     | 35  | LYS  | 3.5  |
| 1   | C     | 94  | PRO  | 3.5  |
| 1   | H     | 94  | PRO  | 3.4  |
| 1   | H     | 93  | PHE  | 3.2  |
| 1   | F     | 55  | PHE  | 3.2  |
| 1   | K     | 50  | THR  | 3.2  |
| 1   | F     | 35  | LYS  | 3.1  |
| 1   | D     | 50  | THR  | 3.1  |
| 1   | T     | 53  | ALA  | 3.0  |
| 1   | R     | 93  | PHE  | 3.0  |
| 1   | G     | 54  | ALA  | 3.0  |
| 1   | K     | 2   | ALA  | 2.9  |
| 1   | G     | 55  | PHE  | 2.9  |
| 1   | B     | 52  | GLU  | 2.9  |
| 1   | K     | 48  | LYS  | 2.8  |
| 1   | L     | 94  | PRO  | 2.8  |
| 1   | G     | 53  | ALA  | 2.8  |
| 1   | I     | 35  | LYS  | 2.8  |
| 1   | D     | 54  | ALA  | 2.8  |
| 1   | E     | 93  | PHE  | 2.7  |
| 1   | H     | 31  | LYS  | 2.7  |
| 1   | S     | 48  | LYS  | 2.7  |
| 1   | H     | 56  | GLN  | 2.6  |
| 1   | J     | 92  | GLY  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | T     | 49  | ARG  | 2.6  |
| 1   | P     | 2   | ALA  | 2.6  |
| 1   | I     | 68  | ASN  | 2.6  |
| 1   | T     | 54  | ALA  | 2.6  |
| 1   | B     | 2   | ALA  | 2.5  |
| 1   | A     | 94  | PRO  | 2.5  |
| 1   | L     | 48  | LYS  | 2.5  |
| 1   | M     | 93  | PHE  | 2.5  |
| 1   | O     | 51  | ASP  | 2.5  |
| 1   | Q     | 31  | LYS  | 2.5  |
| 1   | H     | 58  | LEU  | 2.5  |
| 1   | F     | 66  | ARG  | 2.4  |
| 1   | A     | 50  | THR  | 2.4  |
| 1   | K     | 52  | GLU  | 2.4  |
| 1   | O     | 57  | LYS  | 2.4  |
| 1   | O     | 55  | PHE  | 2.4  |
| 1   | L     | 52  | GLU  | 2.4  |
| 1   | R     | 68  | ASN  | 2.3  |
| 1   | Q     | 55  | PHE  | 2.3  |
| 1   | O     | 68  | ASN  | 2.3  |
| 1   | A     | 52  | GLU  | 2.3  |
| 1   | D     | 53  | ALA  | 2.3  |
| 1   | H     | 55  | PHE  | 2.3  |
| 1   | F     | 53  | ALA  | 2.3  |
| 1   | T     | 66  | ARG  | 2.3  |
| 1   | D     | 55  | PHE  | 2.2  |
| 1   | H     | 68  | ASN  | 2.2  |
| 1   | B     | 49  | ARG  | 2.2  |
| 1   | T     | 68  | ASN  | 2.2  |
| 1   | H     | 35  | LYS  | 2.2  |
| 1   | L     | 2   | ALA  | 2.2  |
| 1   | Q     | 94  | PRO  | 2.2  |
| 1   | Q     | 60  | SER  | 2.2  |
| 1   | M     | 81  | CYS  | 2.2  |
| 1   | M     | 2   | ALA  | 2.2  |
| 1   | I     | 53  | ALA  | 2.1  |
| 1   | L     | 93  | PHE  | 2.1  |
| 1   | Q     | 56  | GLN  | 2.1  |
| 1   | C     | 48  | LYS  | 2.1  |
| 1   | H     | 23  | GLU  | 2.1  |
| 1   | B     | 94  | PRO  | 2.1  |
| 1   | I     | 94  | PRO  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 2   | ALA  | 2.1  |
| 1   | T     | 60  | SER  | 2.0  |
| 1   | F     | 56  | GLN  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | TFP  | F     | 201 | 28/28 | 0.89 | 0.11 | 40,42,49,49                | 0     |
| 2   | TFP  | G     | 201 | 28/28 | 0.90 | 0.10 | 44,45,47,47                | 0     |
| 2   | TFP  | H     | 201 | 28/28 | 0.90 | 0.10 | 27,30,31,31                | 0     |
| 2   | TFP  | O     | 201 | 28/28 | 0.90 | 0.10 | 31,37,39,39                | 0     |
| 2   | TFP  | P     | 201 | 28/28 | 0.90 | 0.10 | 36,40,44,44                | 0     |
| 3   | CA   | G     | 302 | 1/1   | 0.90 | 0.05 | 26,26,26,26                | 0     |
| 3   | CA   | H     | 302 | 1/1   | 0.90 | 0.08 | 32,32,32,32                | 0     |
| 3   | CA   | T     | 301 | 1/1   | 0.90 | 0.05 | 21,21,21,21                | 0     |
| 3   | CA   | T     | 302 | 1/1   | 0.90 | 0.05 | 33,33,33,33                | 0     |
| 2   | TFP  | B     | 201 | 28/28 | 0.91 | 0.10 | 37,39,40,41                | 0     |
| 2   | TFP  | D     | 201 | 28/28 | 0.91 | 0.10 | 37,40,45,46                | 0     |
| 2   | TFP  | E     | 201 | 28/28 | 0.91 | 0.09 | 37,38,40,40                | 0     |
| 2   | TFP  | J     | 201 | 28/28 | 0.92 | 0.09 | 31,34,40,40                | 0     |
| 2   | TFP  | Q     | 201 | 28/28 | 0.92 | 0.09 | 44,47,50,50                | 0     |
| 2   | TFP  | R     | 201 | 28/28 | 0.92 | 0.10 | 30,32,36,37                | 0     |
| 2   | TFP  | L     | 201 | 28/28 | 0.92 | 0.09 | 28,31,34,34                | 0     |
| 2   | TFP  | M     | 201 | 28/28 | 0.92 | 0.09 | 41,45,49,50                | 0     |
| 3   | CA   | N     | 302 | 1/1   | 0.92 | 0.04 | 14,14,14,14                | 0     |
| 2   | TFP  | F     | 202 | 28/28 | 0.92 | 0.08 | 19,26,29,30                | 0     |
| 2   | TFP  | O     | 202 | 28/28 | 0.92 | 0.08 | 14,27,31,33                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | TFP  | T     | 201 | 28/28 | 0.93 | 0.08 | 27,30,33,33                 | 0     |
| 3   | CA   | A     | 302 | 1/1   | 0.93 | 0.04 | 12,12,12,12                 | 0     |
| 3   | CA   | D     | 301 | 1/1   | 0.93 | 0.04 | 23,23,23,23                 | 0     |
| 2   | TFP  | P     | 202 | 28/28 | 0.93 | 0.07 | 11,20,27,29                 | 0     |
| 2   | TFP  | E     | 202 | 28/28 | 0.93 | 0.08 | 13,21,26,27                 | 0     |
| 2   | TFP  | Q     | 202 | 28/28 | 0.93 | 0.08 | 24,31,35,36                 | 0     |
| 3   | CA   | O     | 301 | 1/1   | 0.93 | 0.08 | 31,31,31,31                 | 0     |
| 2   | TFP  | K     | 201 | 28/28 | 0.93 | 0.09 | 32,34,38,39                 | 0     |
| 2   | TFP  | I     | 201 | 28/28 | 0.93 | 0.09 | 25,29,33,34                 | 0     |
| 2   | TFP  | M     | 202 | 28/28 | 0.94 | 0.08 | 15,24,28,29                 | 0     |
| 2   | TFP  | I     | 202 | 28/28 | 0.94 | 0.08 | 16,22,32,32                 | 0     |
| 2   | TFP  | C     | 201 | 28/28 | 0.94 | 0.08 | 24,26,31,32                 | 0     |
| 3   | CA   | Q     | 301 | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 2   | TFP  | H     | 202 | 28/28 | 0.94 | 0.07 | 14,21,29,30                 | 0     |
| 3   | CA   | H     | 301 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 3   | CA   | F     | 301 | 1/1   | 0.95 | 0.05 | 23,23,23,23                 | 0     |
| 2   | TFP  | N     | 202 | 28/28 | 0.95 | 0.07 | 12,14,22,24                 | 0     |
| 2   | TFP  | N     | 201 | 28/28 | 0.95 | 0.07 | 26,27,32,33                 | 0     |
| 2   | TFP  | A     | 202 | 28/28 | 0.95 | 0.08 | 6,14,24,26                  | 0     |
| 3   | CA   | M     | 302 | 1/1   | 0.95 | 0.07 | 28,28,28,28                 | 0     |
| 2   | TFP  | S     | 201 | 28/28 | 0.95 | 0.07 | 22,26,32,33                 | 0     |
| 2   | TFP  | G     | 202 | 28/28 | 0.95 | 0.07 | 14,24,32,33                 | 0     |
| 2   | TFP  | C     | 202 | 28/28 | 0.95 | 0.07 | 12,16,24,25                 | 0     |
| 3   | CA   | B     | 301 | 1/1   | 0.95 | 0.03 | 14,14,14,14                 | 0     |
| 2   | TFP  | D     | 202 | 28/28 | 0.95 | 0.07 | 10,21,29,30                 | 0     |
| 2   | TFP  | T     | 202 | 28/28 | 0.96 | 0.06 | 12,18,26,27                 | 0     |
| 2   | TFP  | J     | 202 | 28/28 | 0.96 | 0.07 | 10,13,24,25                 | 0     |
| 2   | TFP  | K     | 202 | 28/28 | 0.96 | 0.07 | 9,18,27,27                  | 0     |
| 3   | CA   | L     | 302 | 1/1   | 0.96 | 0.04 | 18,18,18,18                 | 0     |
| 3   | CA   | M     | 301 | 1/1   | 0.96 | 0.03 | 32,32,32,32                 | 0     |
| 2   | TFP  | A     | 201 | 28/28 | 0.96 | 0.06 | 20,24,25,26                 | 0     |
| 3   | CA   | N     | 301 | 1/1   | 0.96 | 0.03 | 18,18,18,18                 | 0     |
| 3   | CA   | B     | 302 | 1/1   | 0.96 | 0.04 | 18,18,18,18                 | 0     |
| 3   | CA   | C     | 302 | 1/1   | 0.96 | 0.03 | 17,17,17,17                 | 0     |
| 3   | CA   | O     | 302 | 1/1   | 0.96 | 0.06 | 25,25,25,25                 | 0     |
| 3   | CA   | P     | 302 | 1/1   | 0.96 | 0.05 | 20,20,20,20                 | 0     |
| 2   | TFP  | S     | 202 | 28/28 | 0.96 | 0.06 | 10,14,21,22                 | 0     |
| 3   | CA   | R     | 302 | 1/1   | 0.96 | 0.04 | 37,37,37,37                 | 0     |
| 3   | CA   | S     | 302 | 1/1   | 0.96 | 0.04 | 13,13,13,13                 | 0     |
| 3   | CA   | D     | 302 | 1/1   | 0.96 | 0.03 | 19,19,19,19                 | 0     |
| 2   | TFP  | L     | 202 | 28/28 | 0.96 | 0.07 | 14,17,26,27                 | 0     |
| 3   | CA   | K     | 302 | 1/1   | 0.97 | 0.06 | 20,20,20,20                 | 0     |

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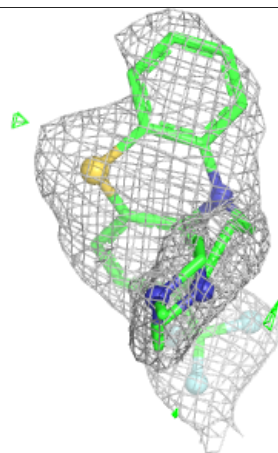
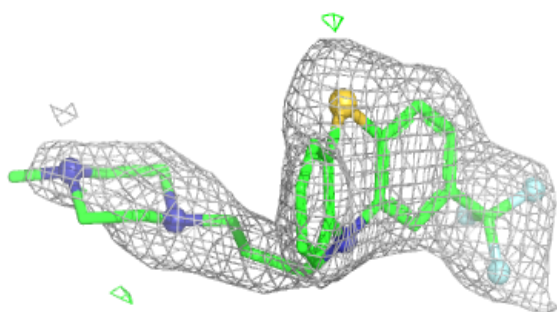
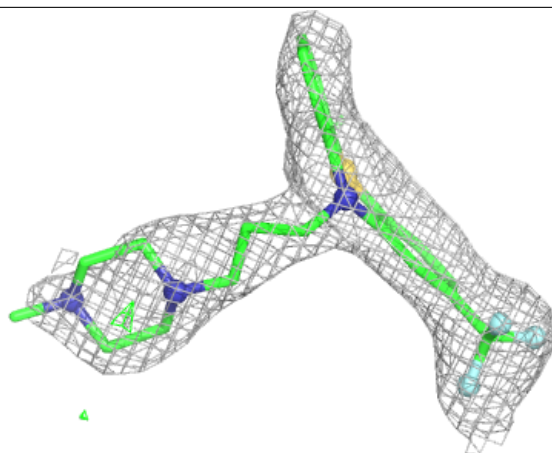
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | CA   | F     | 302 | 1/1   | 0.97 | 0.05 | 28,28,28,28                 | 0     |
| 3   | CA   | G     | 301 | 1/1   | 0.97 | 0.06 | 24,24,24,24                 | 0     |
| 3   | CA   | Q     | 302 | 1/1   | 0.97 | 0.04 | 48,48,48,48                 | 0     |
| 3   | CA   | R     | 301 | 1/1   | 0.97 | 0.03 | 27,27,27,27                 | 0     |
| 2   | TFP  | R     | 202 | 28/28 | 0.97 | 0.06 | 17,28,33,34                 | 0     |
| 3   | CA   | E     | 301 | 1/1   | 0.97 | 0.06 | 19,19,19,19                 | 0     |
| 2   | TFP  | B     | 202 | 28/28 | 0.97 | 0.06 | 13,16,27,27                 | 0     |
| 3   | CA   | K     | 301 | 1/1   | 0.97 | 0.03 | 17,17,17,17                 | 0     |
| 3   | CA   | L     | 301 | 1/1   | 0.98 | 0.04 | 17,17,17,17                 | 0     |
| 3   | CA   | I     | 302 | 1/1   | 0.98 | 0.02 | 27,27,27,27                 | 0     |
| 3   | CA   | C     | 301 | 1/1   | 0.98 | 0.03 | 17,17,17,17                 | 0     |
| 3   | CA   | I     | 301 | 1/1   | 0.98 | 0.02 | 24,24,24,24                 | 0     |
| 3   | CA   | E     | 302 | 1/1   | 0.99 | 0.02 | 23,23,23,23                 | 0     |
| 3   | CA   | P     | 301 | 1/1   | 0.99 | 0.04 | 16,16,16,16                 | 0     |
| 3   | CA   | S     | 301 | 1/1   | 0.99 | 0.02 | 14,14,14,14                 | 0     |
| 3   | CA   | J     | 301 | 1/1   | 0.99 | 0.02 | 13,13,13,13                 | 0     |
| 3   | CA   | J     | 302 | 1/1   | 0.99 | 0.02 | 14,14,14,14                 | 0     |
| 3   | CA   | A     | 301 | 1/1   | 0.99 | 0.04 | 15,15,15,15                 | 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.



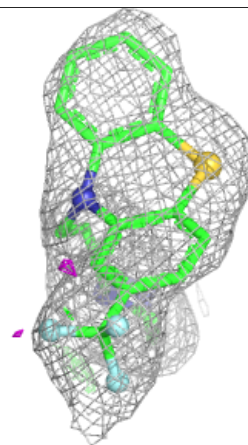
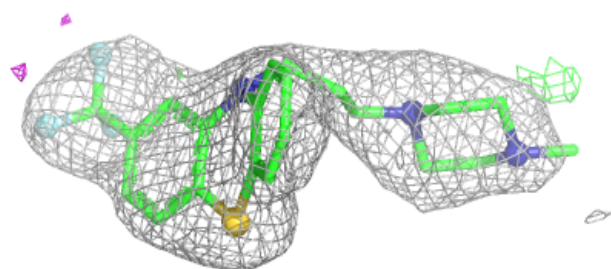
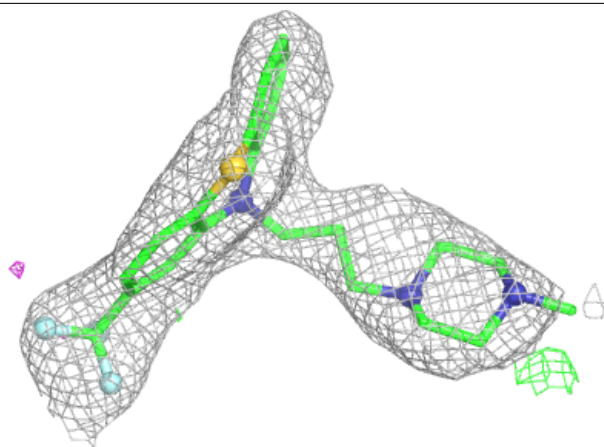
**Electron density around TFP F 201:**

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



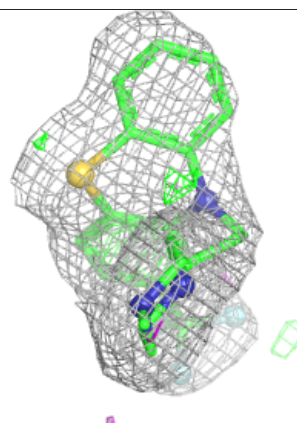
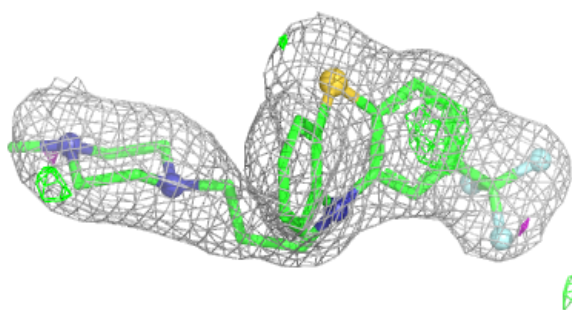
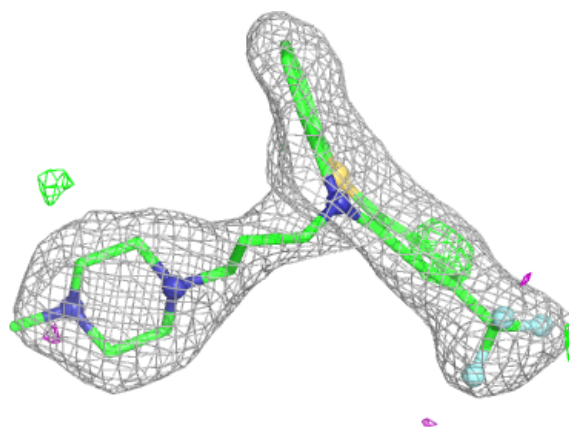
**Electron density around TFP G 201:**

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



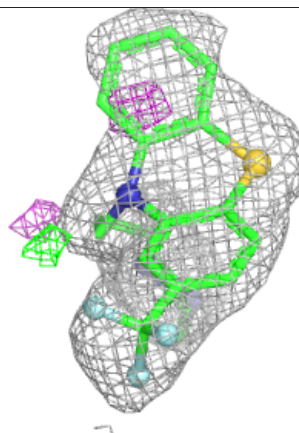
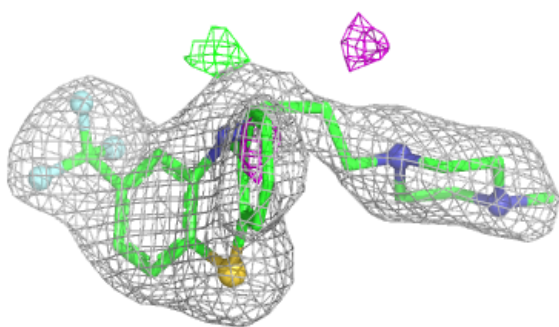
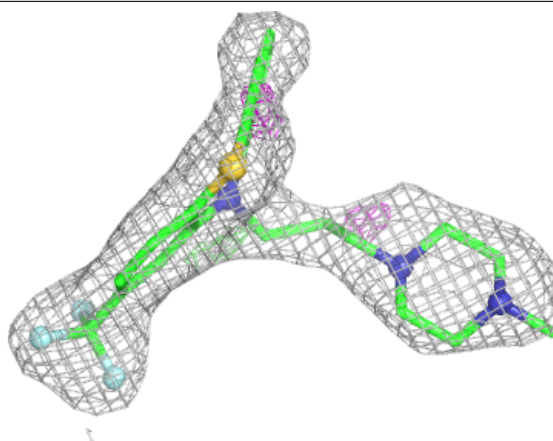
**Electron density around TFP H 201:**

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

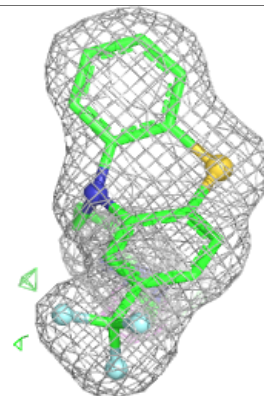
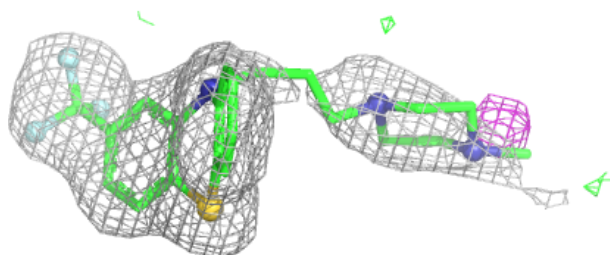
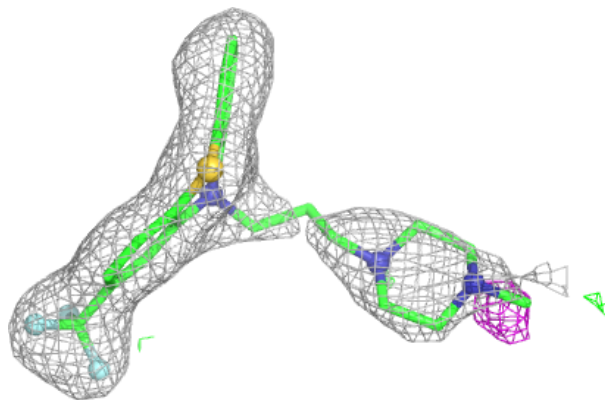


**Electron density around TFP O 201:**

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

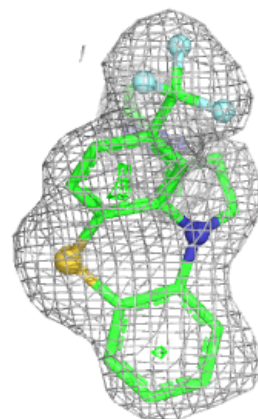
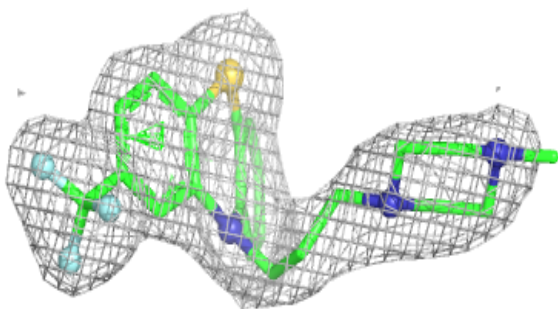
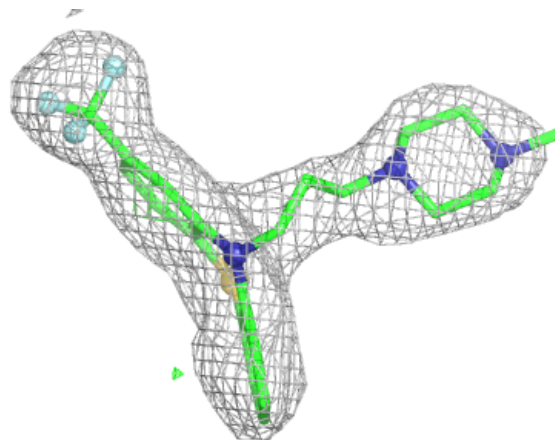
**Electron density around TFP P 201:**

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



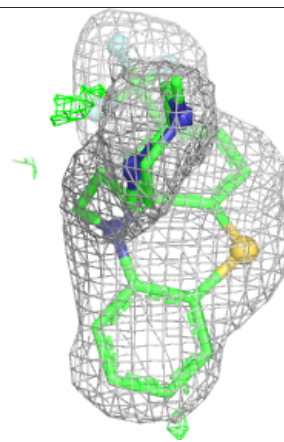
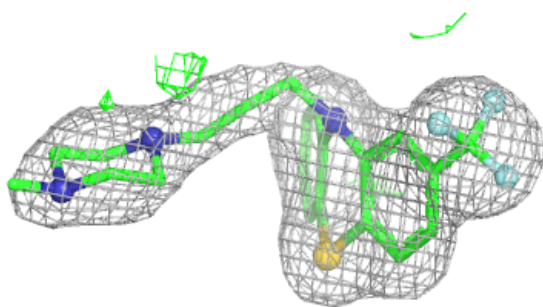
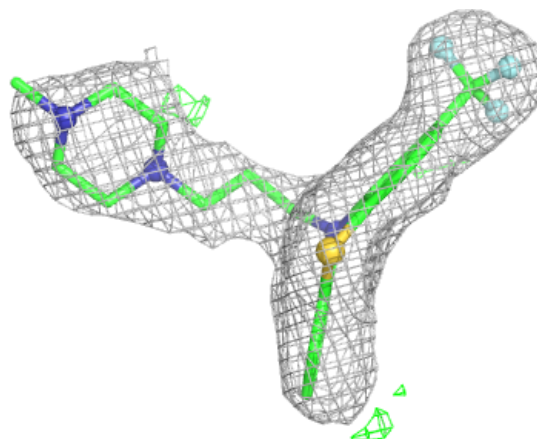
**Electron density around TFP B 201:**

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



**Electron density around TFP D 201:**

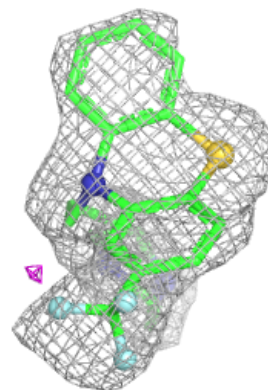
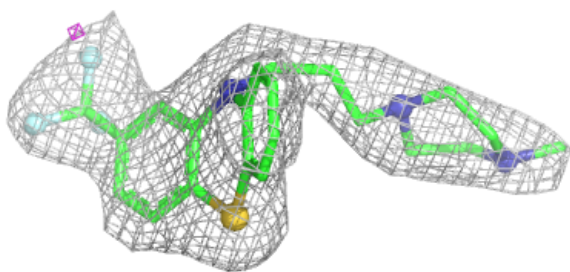
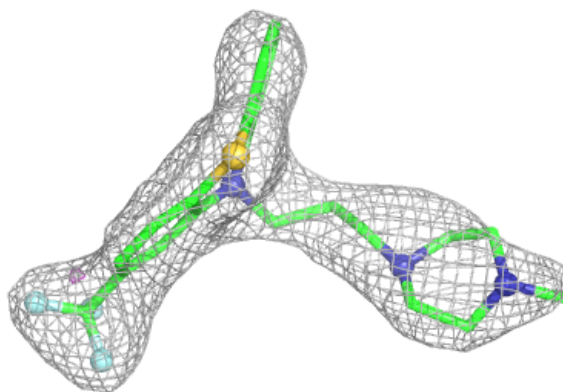
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





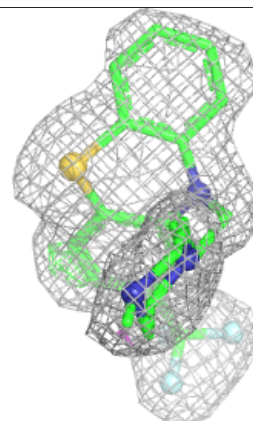
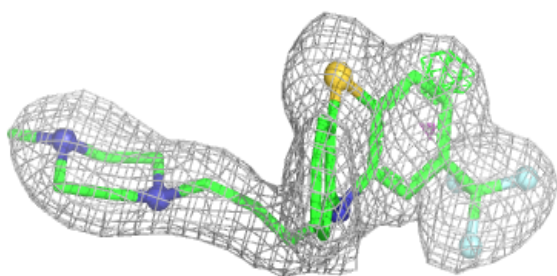
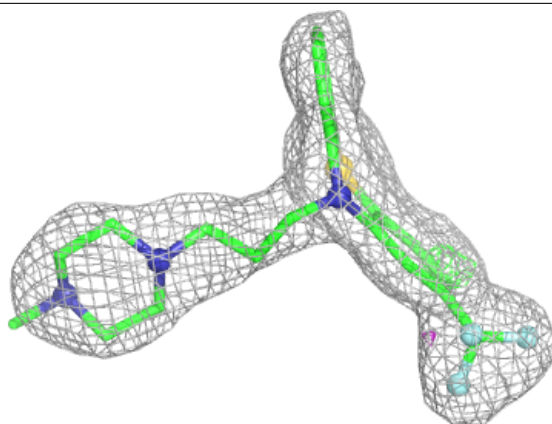
**Electron density around TFP E 201:**

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



**Electron density around TFP J 201:**

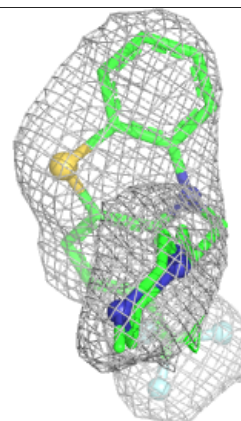
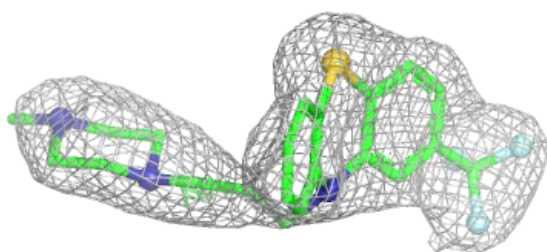
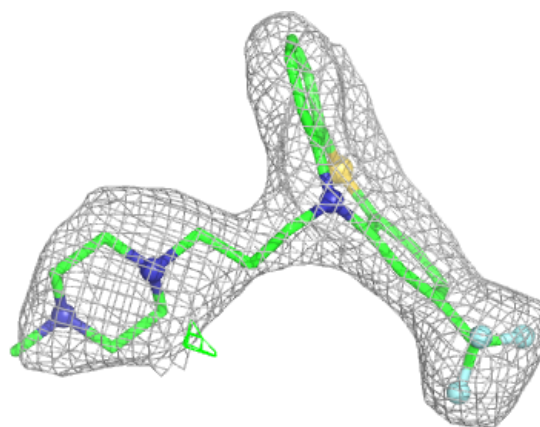
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



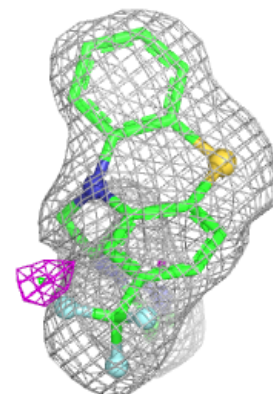
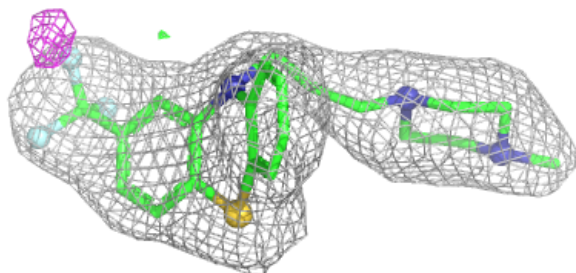
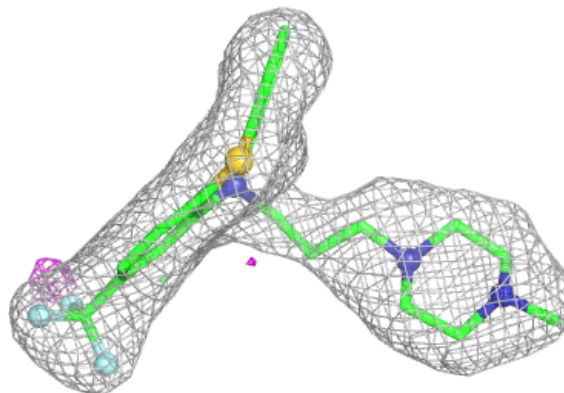


**Electron density around TFP Q 201:**

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

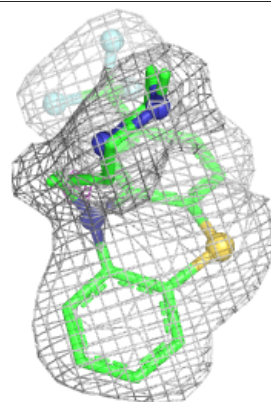
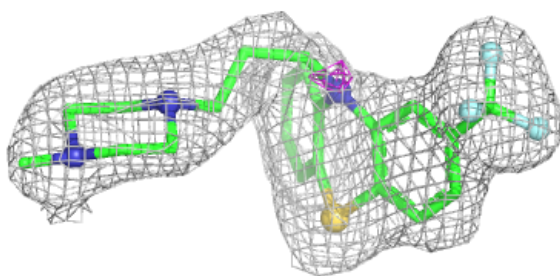
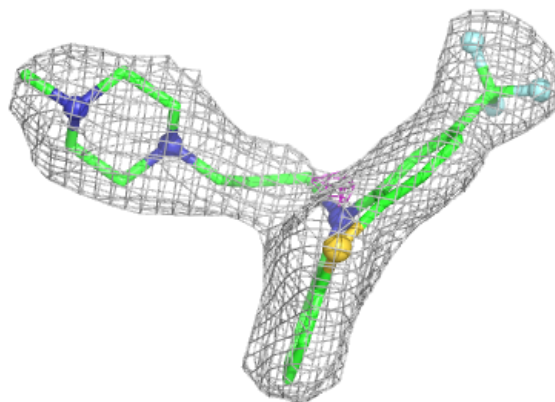
**Electron density around TFP R 201:**

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and green (positive)



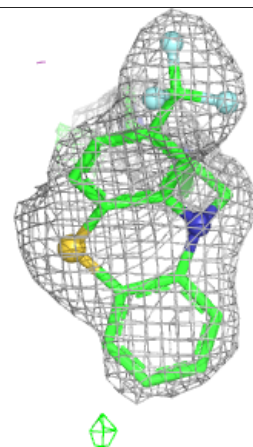
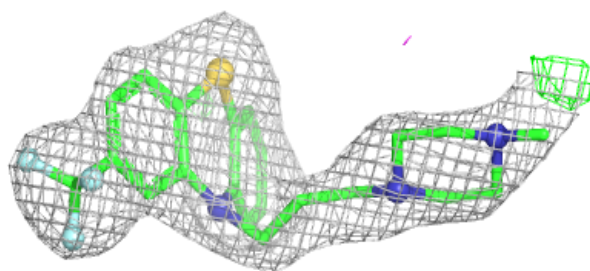
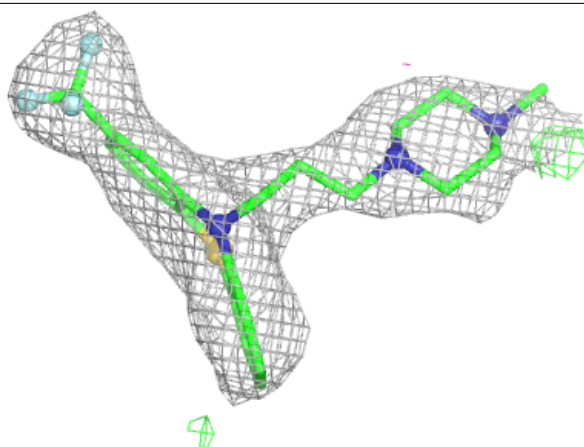
**Electron density around TFP L 201:**

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



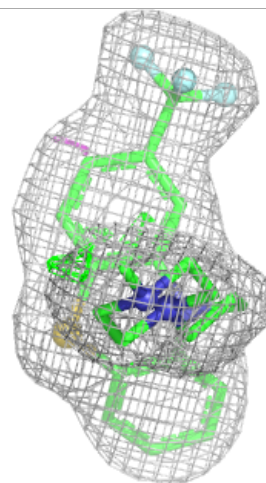
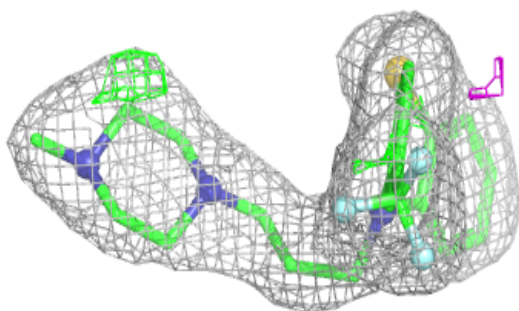
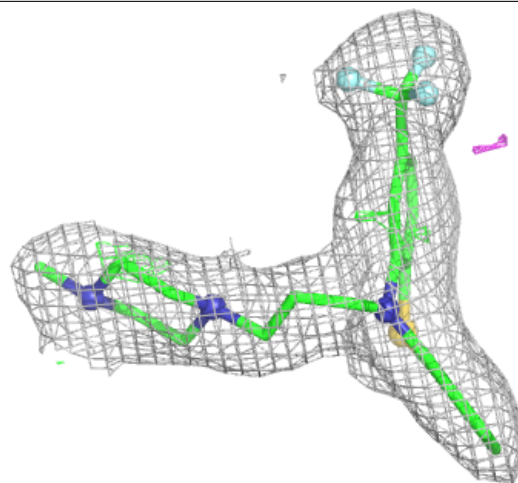
**Electron density around TFP M 201:**

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



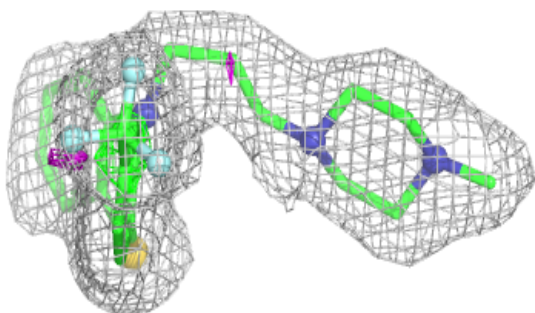
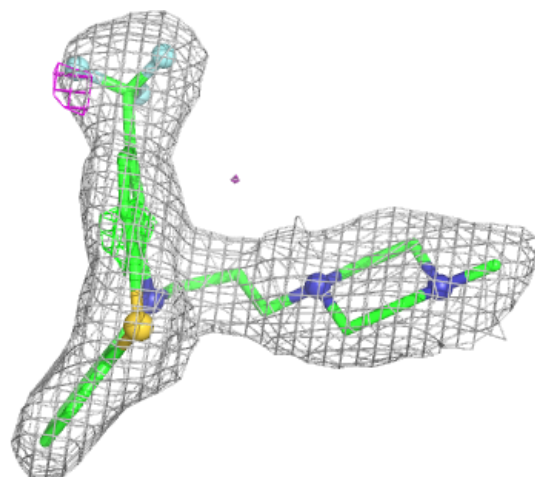
**Electron density around TFP F 202:**

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



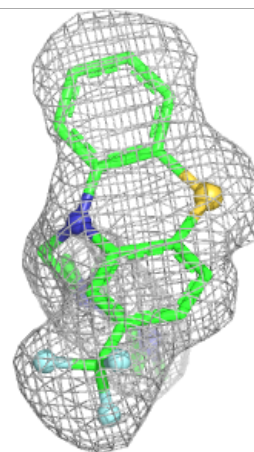
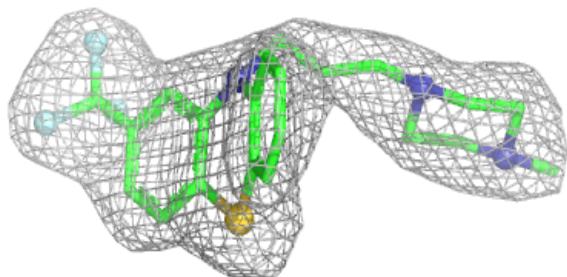
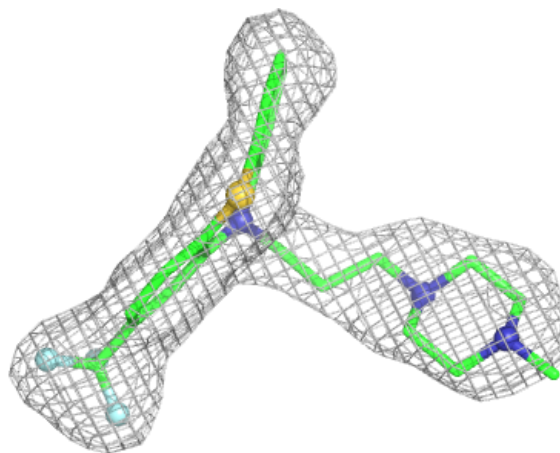
**Electron density around TFP O 202:**

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



**Electron density around TFP T 201:**

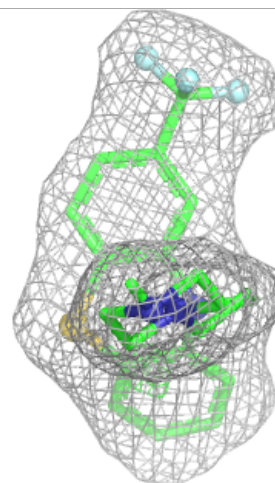
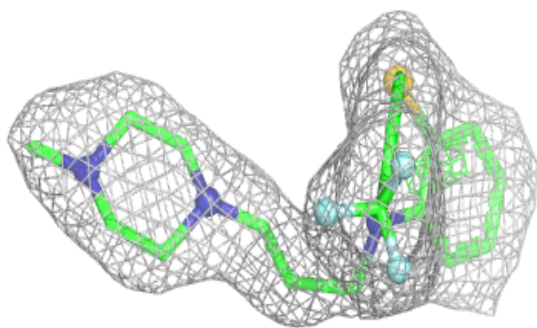
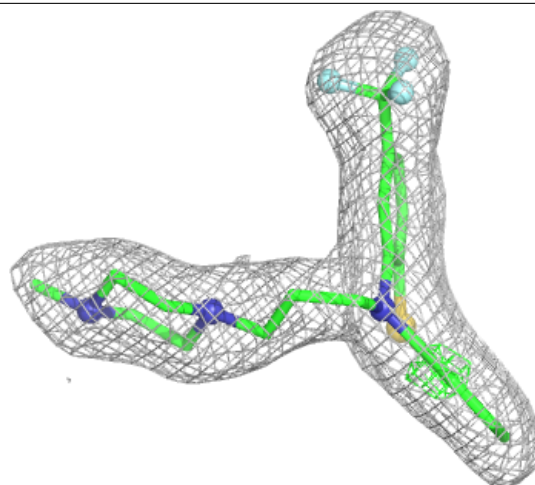
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





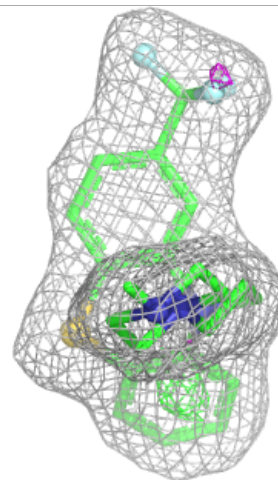
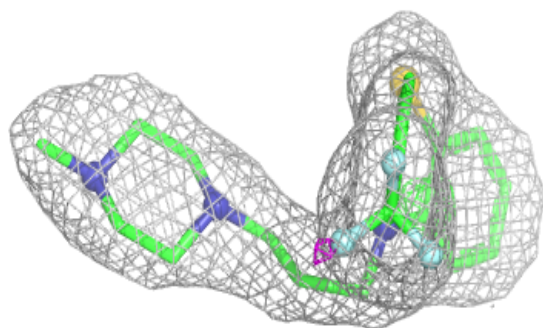
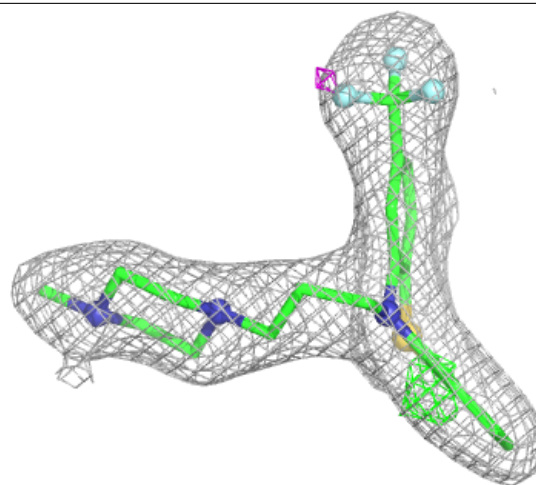
**Electron density around TFP P 202:**

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



**Electron density around TFP E 202:**

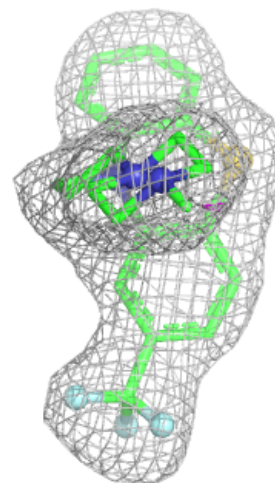
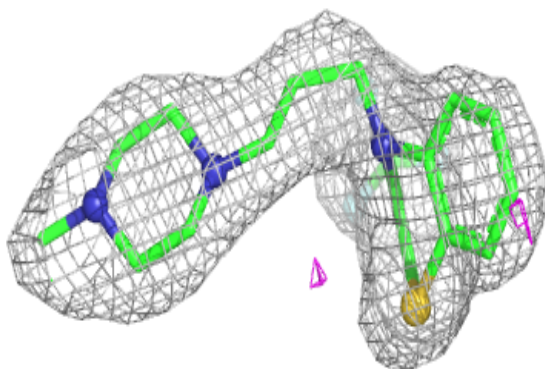
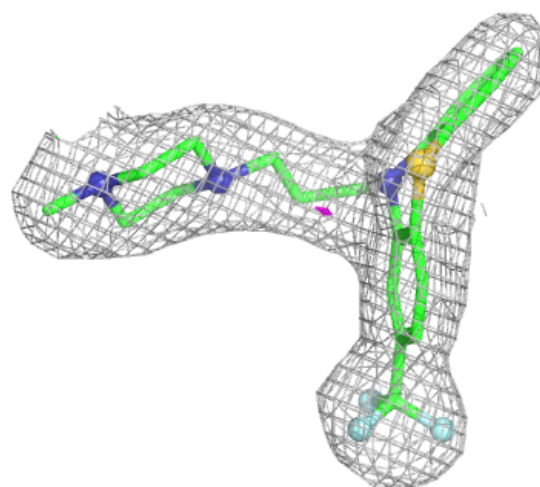
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





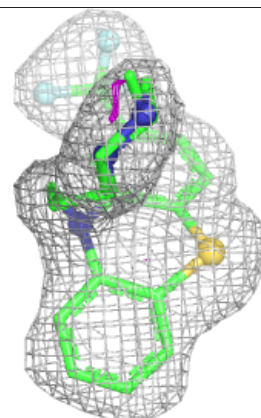
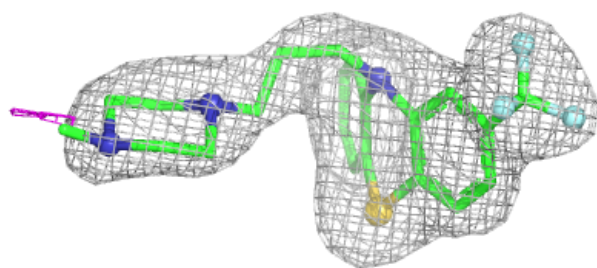
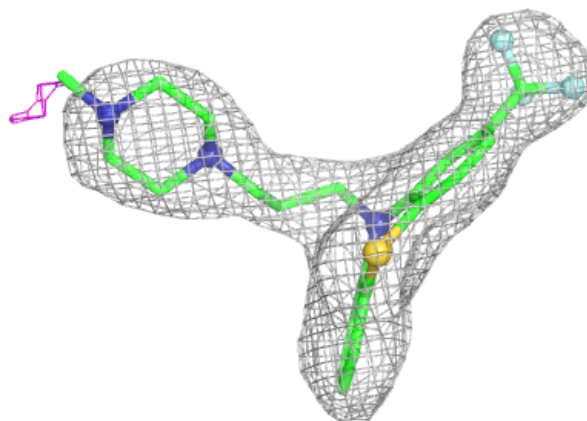
**Electron density around TFP Q 202:**

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



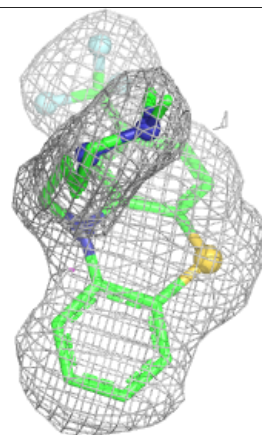
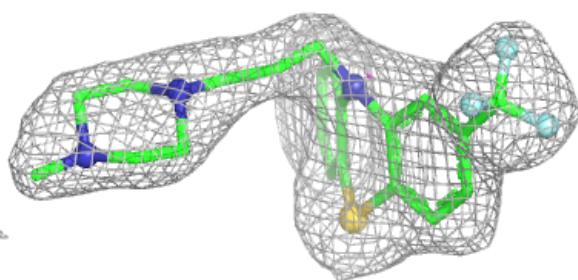
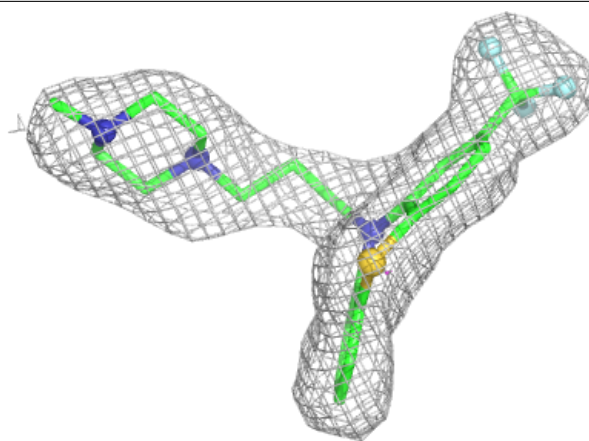
**Electron density around TFP K 201:**

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



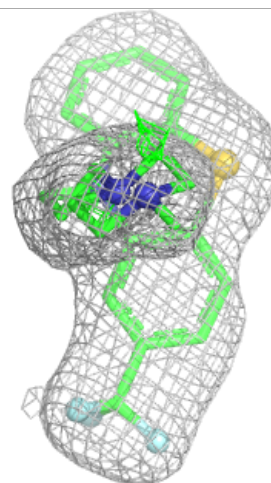
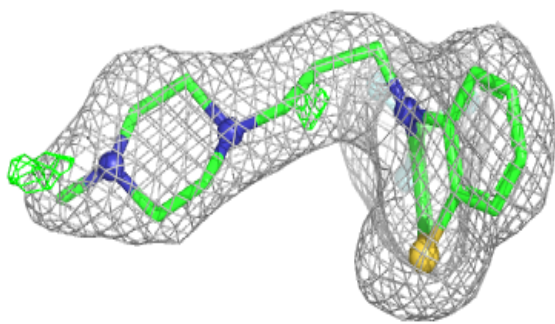
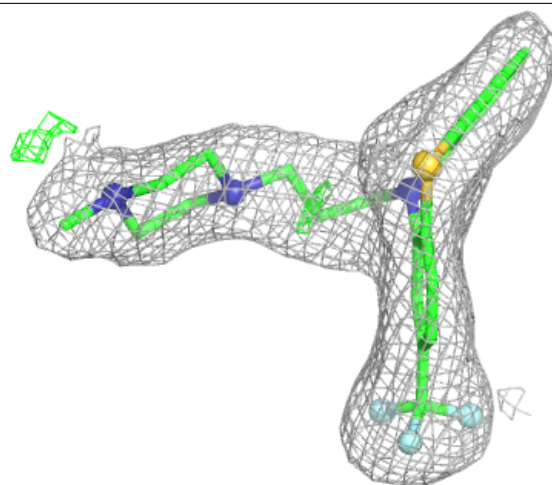
**Electron density around TFP I 201:**

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



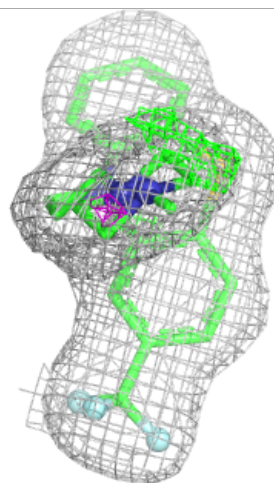
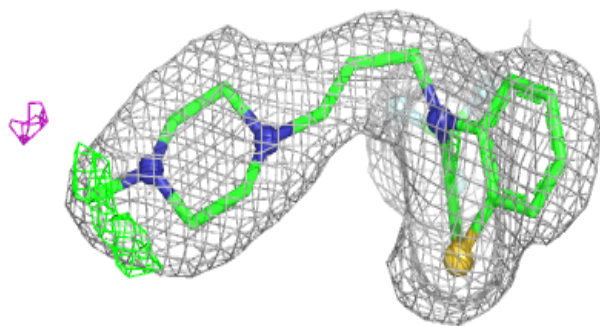
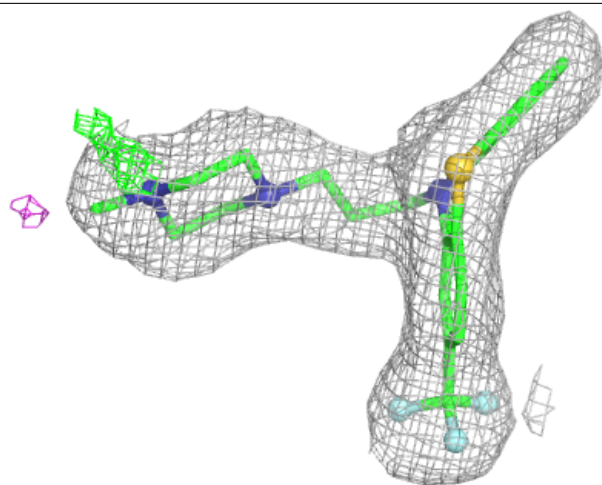
**Electron density around TFP M 202:**

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



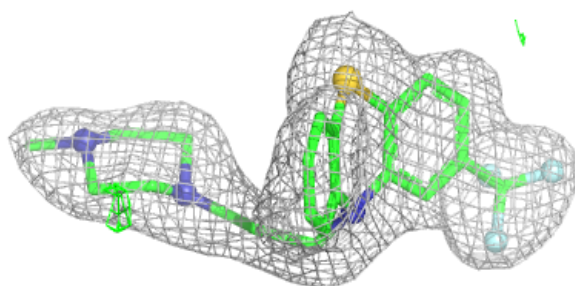
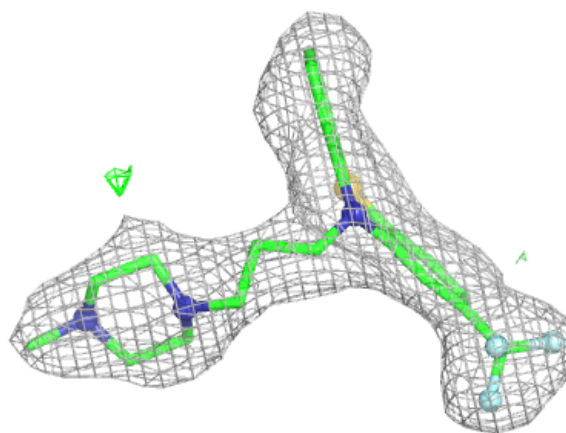
**Electron density around TFP I 202:**

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



**Electron density around TFP C 201:**

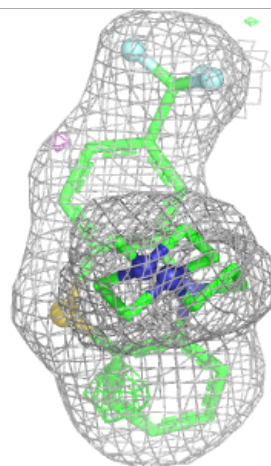
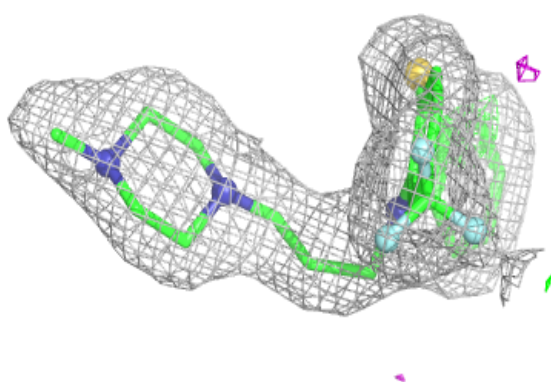
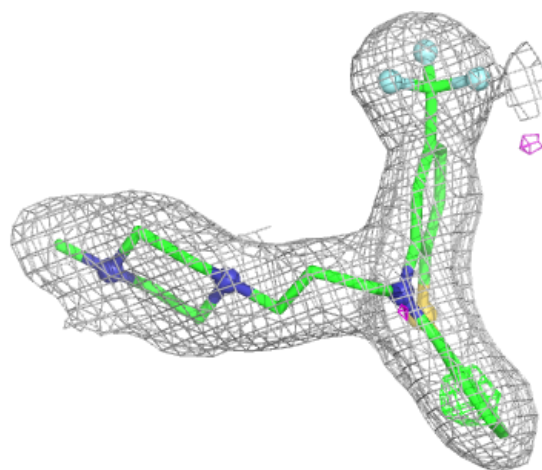
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





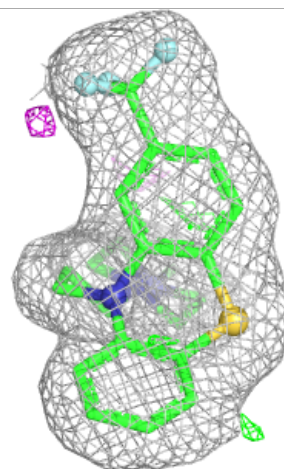
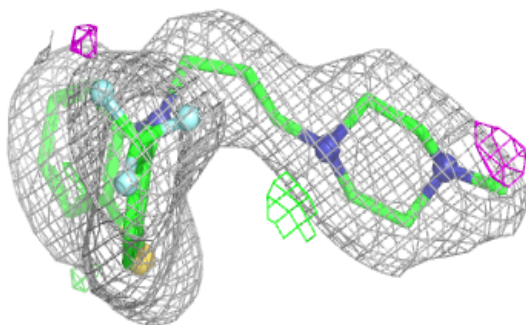
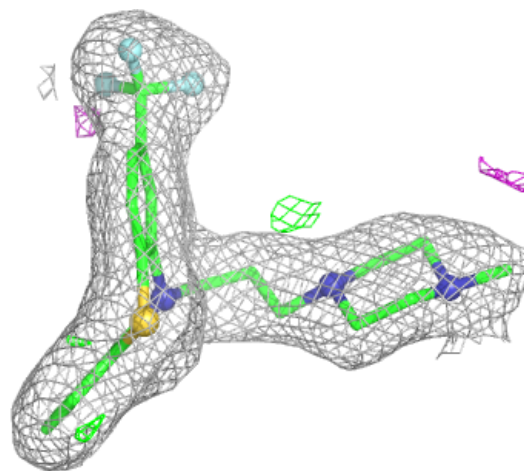
**Electron density around TFP H 202:**

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



**Electron density around TFP N 202:**

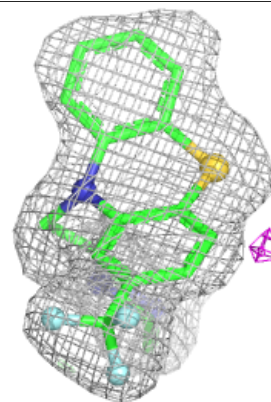
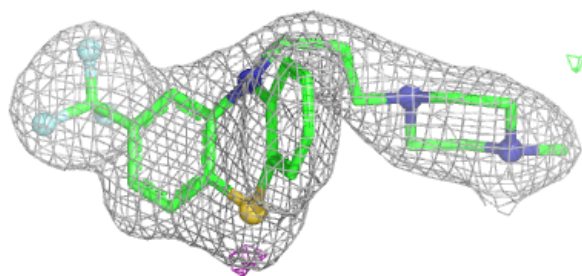
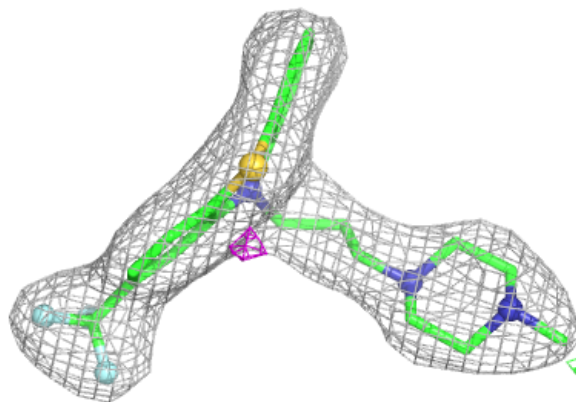
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





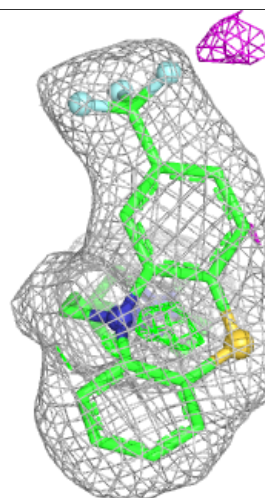
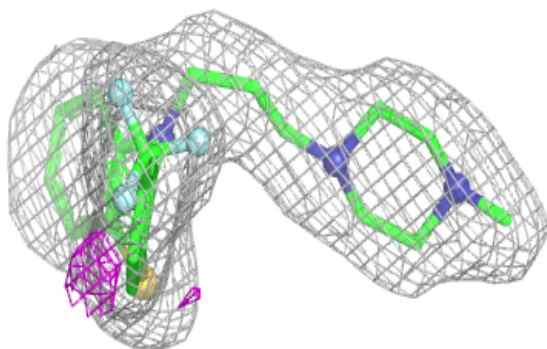
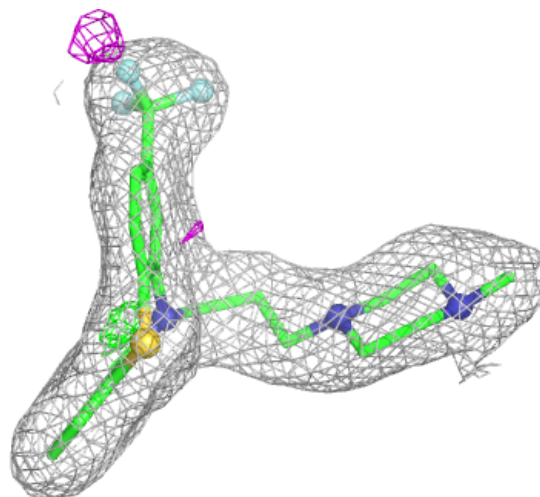
**Electron density around TFP N 201:**

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



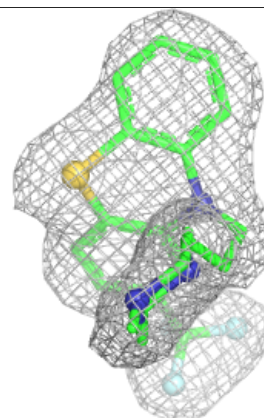
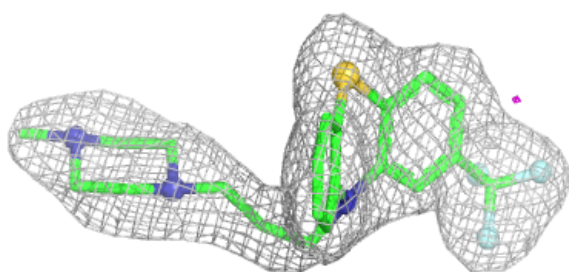
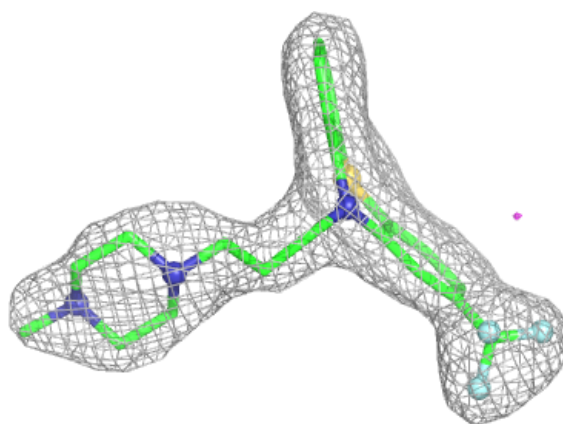
**Electron density around TFP A 202:**

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



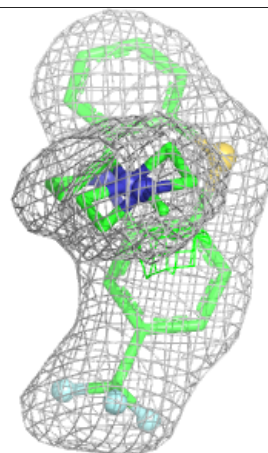
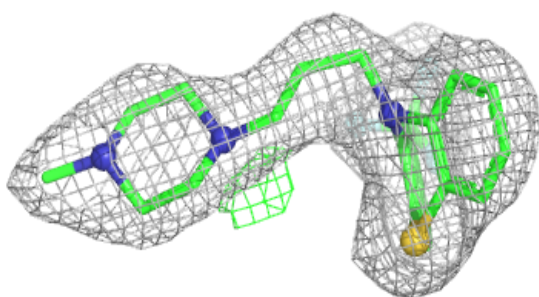
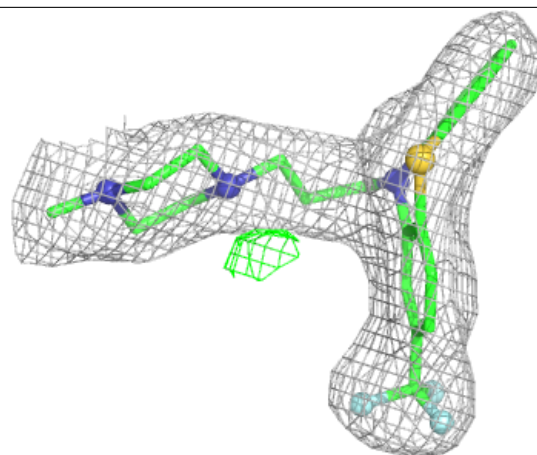
**Electron density around TFP S 201:**

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



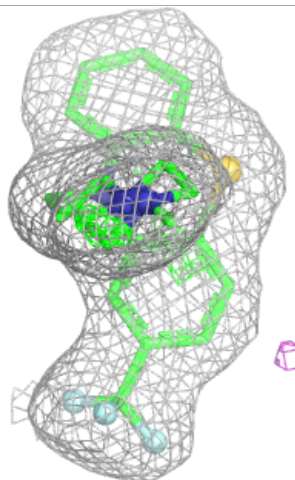
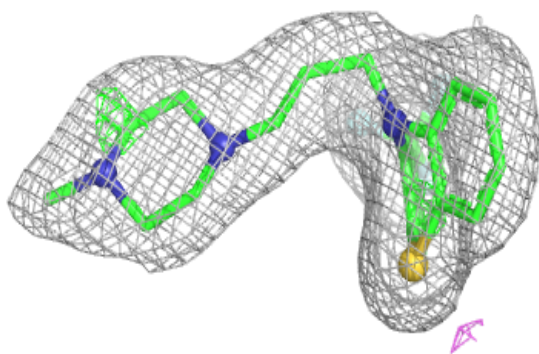
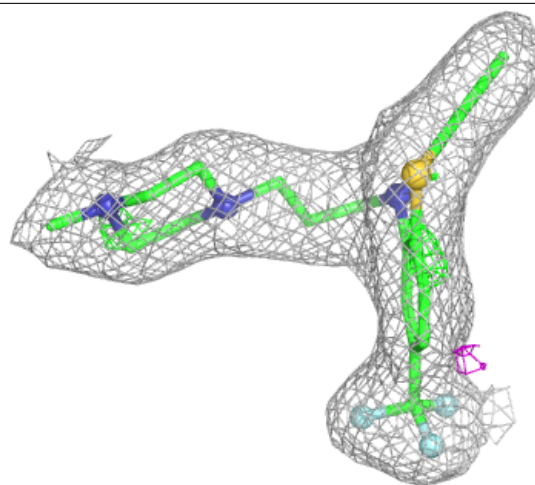
**Electron density around TFP G 202:**

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



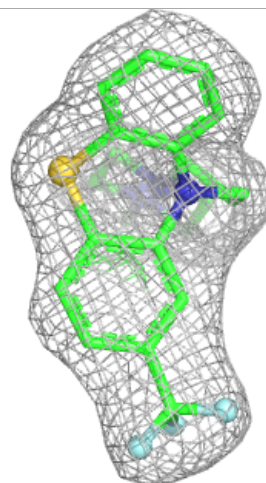
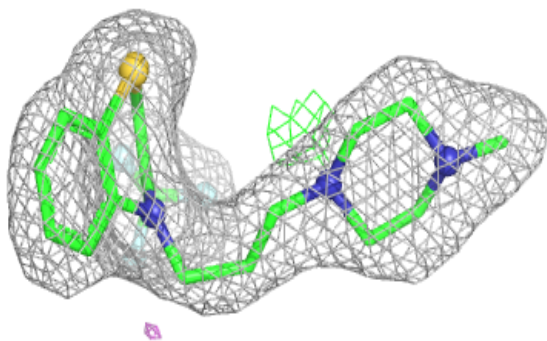
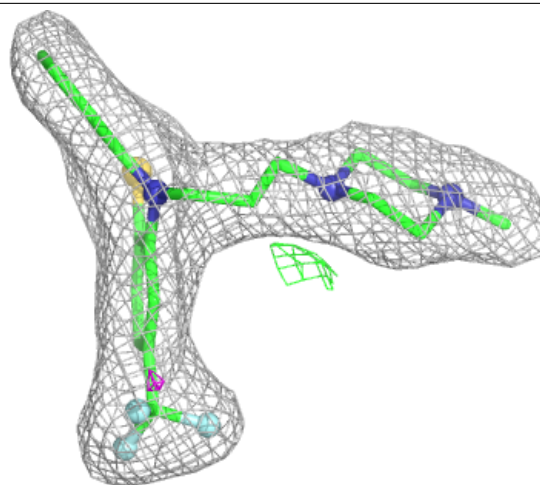
**Electron density around TFP C 202:**

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



**Electron density around TFP D 202:**

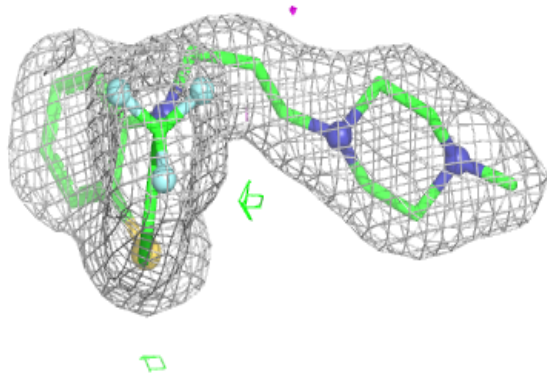
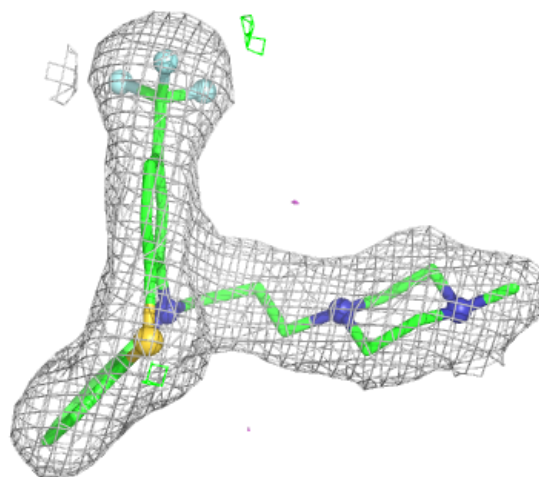
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





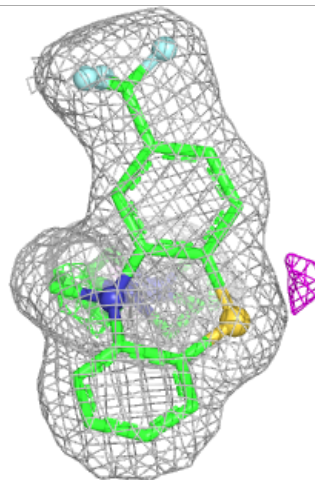
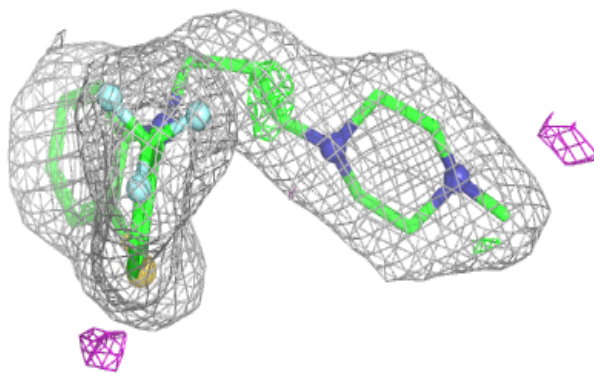
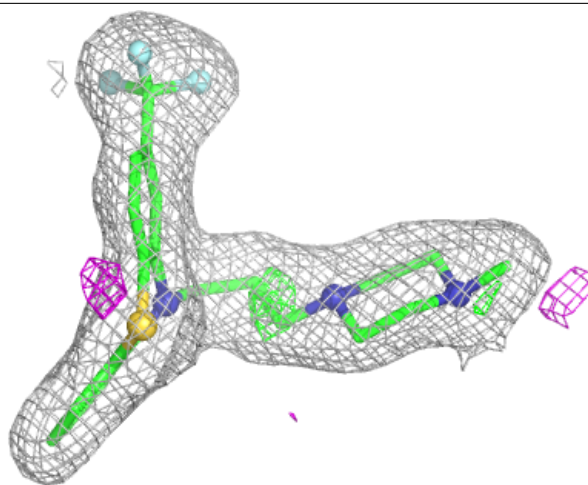
**Electron density around TFP T 202:**

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



**Electron density around TFP J 202:**

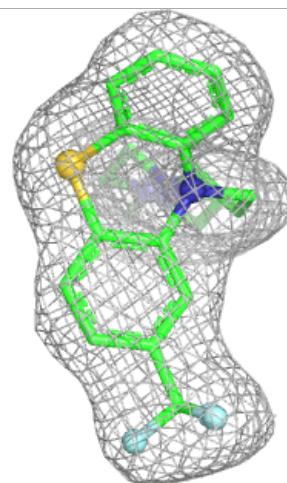
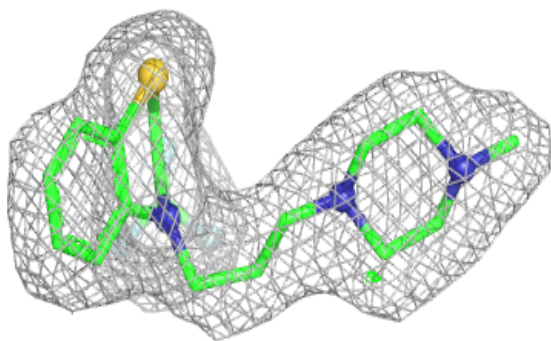
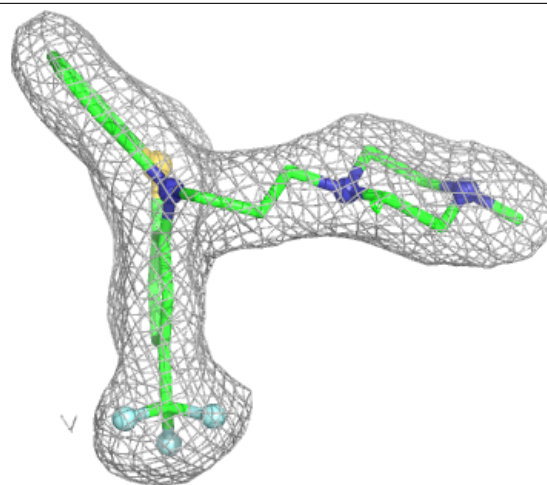
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





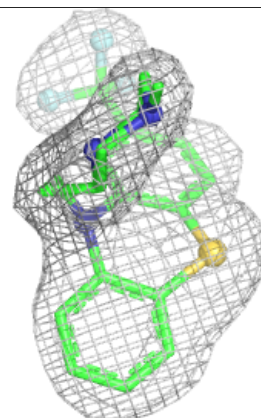
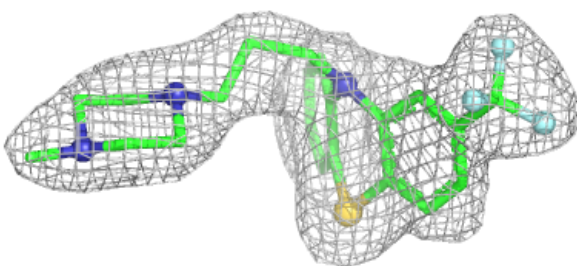
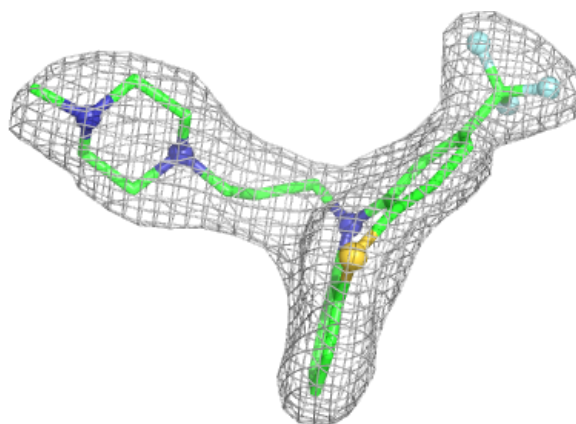
**Electron density around TFP K 202:**

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



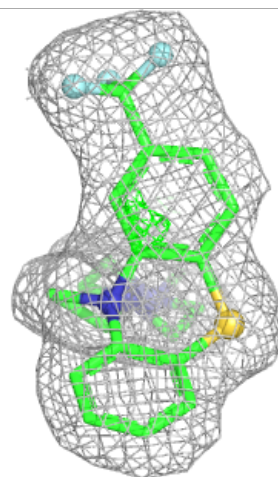
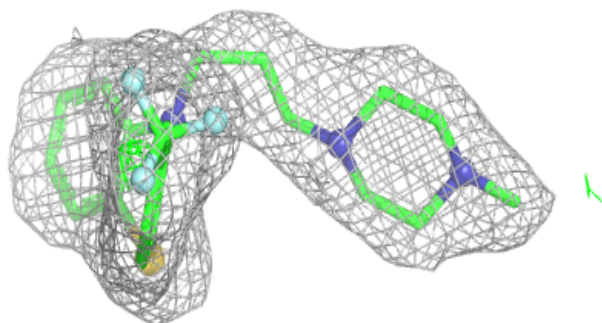
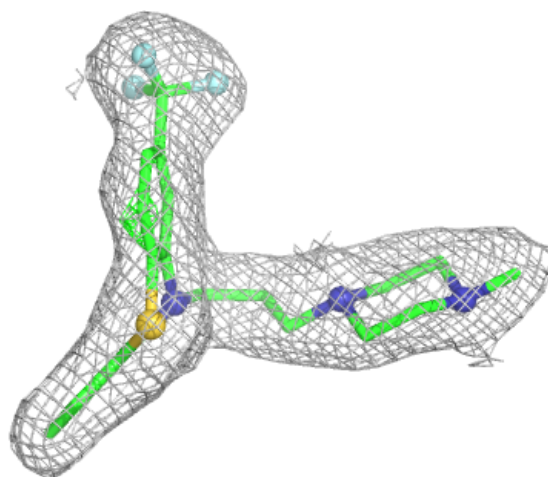
**Electron density around TFP A 201:**

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



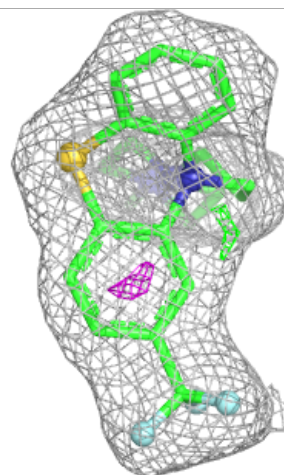
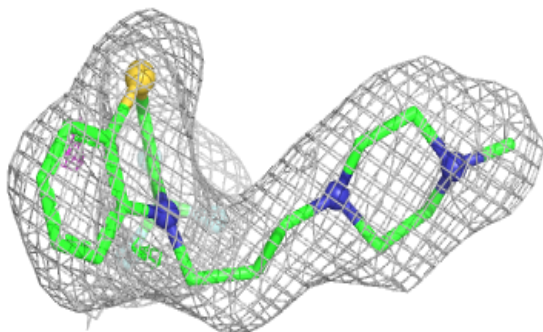
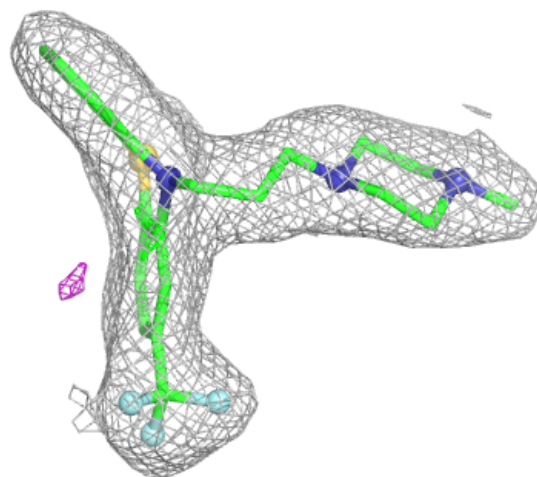
**Electron density around TFP S 202:**

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



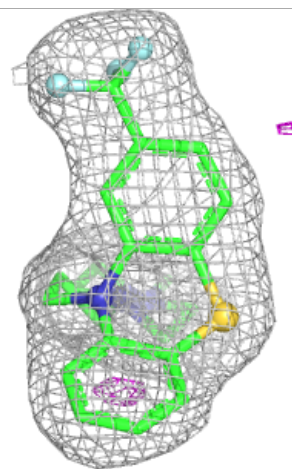
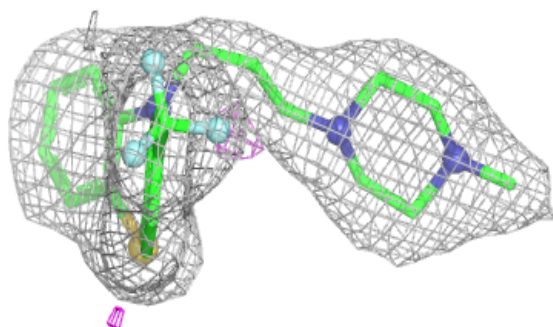
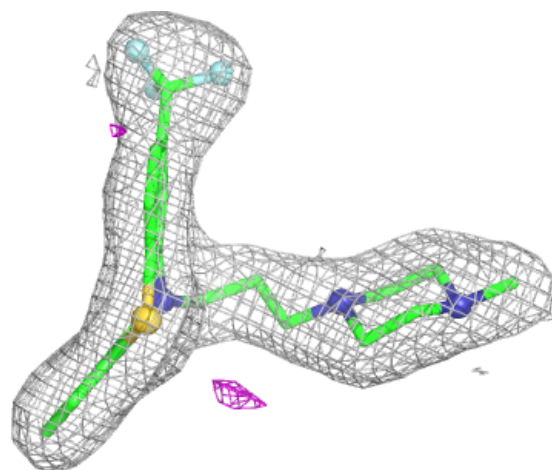
**Electron density around TFP L 202:**

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



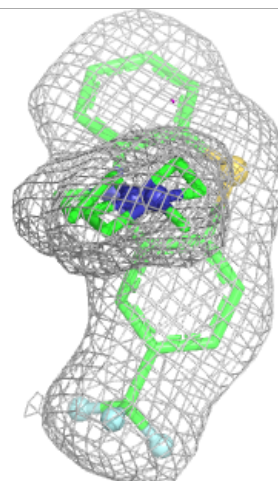
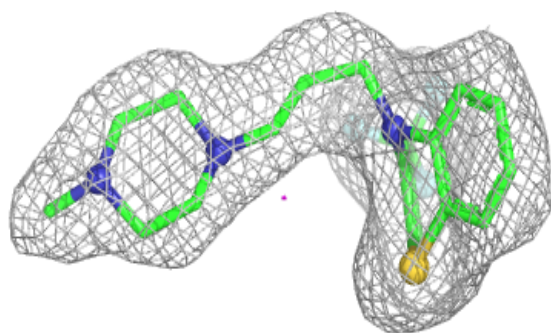
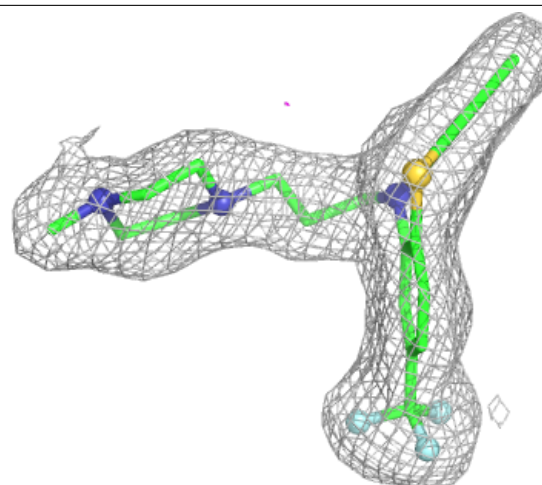
**Electron density around TFP R 202:**

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



**Electron density around TFP B 202:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.