



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:57 PM UTC

PDB ID : 4ZGX / pdb\_00004zgx  
Title : Structure of aldosterone synthase (CYP11B2) in complex with (+)-(R)-N-(4-(4-chloro-3-fluorophenyl)-5,6,7,8-tetrahydroisoquinolin-8-yl)propionamide  
Authors : Kuglstatter, A.; Joseph, C.  
Deposited on : 2015-04-24  
Resolution : 3.20 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                                                             |

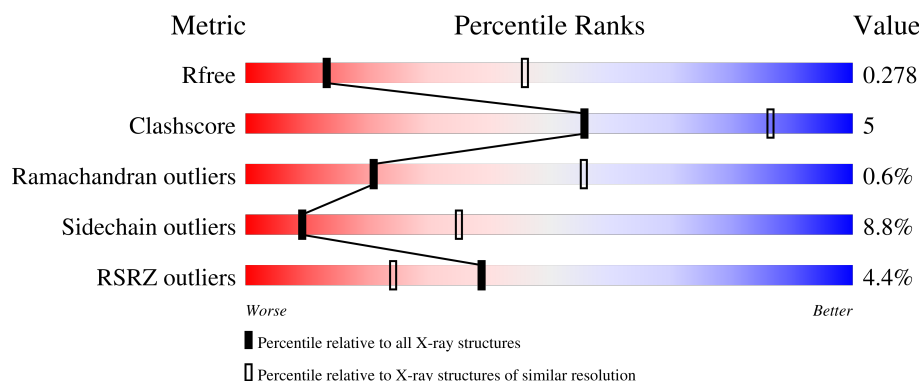
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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     | 489    |                  |
| 1   | B     | 489    |                  |
| 1   | C     | 489    |                  |
| 1   | D     | 489    |                  |
| 1   | E     | 489    |                  |

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| Mol | Chain | Length | Quality of chain                                                                          |
|-----|-------|--------|-------------------------------------------------------------------------------------------|
| 1   | F     | 489    | <div><div>4%</div><div><div></div><div>77%</div><div>15%</div><div>• 5%</div></div></div> |
| 1   | G     | 489    | <div><div>3%</div><div><div></div><div>78%</div><div>14%</div><div>• 5%</div></div></div> |
| 1   | H     | 489    | <div><div>8%</div><div><div></div><div>76%</div><div>16%</div><div>• 5%</div></div></div> |
| 1   | I     | 489    | <div><div>5%</div><div><div></div><div>73%</div><div>18%</div><div>• 6%</div></div></div> |
| 1   | J     | 489    | <div><div>7%</div><div><div></div><div>74%</div><div>17%</div><div>• 5%</div></div></div> |
| 1   | K     | 489    | <div><div>5%</div><div><div></div><div>76%</div><div>15%</div><div>• 6%</div></div></div> |
| 1   | L     | 489    | <div><div>9%</div><div><div></div><div>75%</div><div>18%</div><div>• 6%</div></div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46675 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 Cytochrome P450 11B2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3774  | 2439 | 666 | 649 | 20 |         |         |       |
| 1   | B     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3774  | 2439 | 666 | 649 | 20 |         |         |       |
| 1   | C     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3774  | 2439 | 666 | 649 | 20 |         |         |       |
| 1   | D     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3774  | 2439 | 666 | 649 | 20 |         |         |       |
| 1   | E     | 459      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3731  | 2412 | 658 | 641 | 20 |         |         |       |
| 1   | F     | 464      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3770  | 2437 | 665 | 648 | 20 |         |         |       |
| 1   | G     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3774  | 2439 | 666 | 649 | 20 |         |         |       |
| 1   | H     | 465      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3774  | 2439 | 666 | 649 | 20 |         |         |       |
| 1   | I     | 458      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3721  | 2406 | 655 | 640 | 20 |         |         |       |
| 1   | J     | 463      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3762  | 2431 | 664 | 647 | 20 |         |         |       |
| 1   | K     | 461      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3737  | 2416 | 657 | 644 | 20 |         |         |       |
| 1   | L     | 462      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3747  | 2422 | 661 | 644 | 20 |         |         |       |

There are 156 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 24      | MET      | -      | expression tag | UNP P19099 |
| A     | 25      | ALA      | -      | expression tag | UNP P19099 |
| A     | 26      | THR      | -      | expression tag | UNP P19099 |
| A     | 27      | LYS      | -      | expression tag | UNP P19099 |
| A     | 504     | GLY      | -      | expression tag | UNP P19099 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 505     | GLY      | -      | expression tag | UNP P19099 |
| A     | 506     | ARG      | -      | expression tag | UNP P19099 |
| A     | 507     | HIS      | -      | expression tag | UNP P19099 |
| A     | 508     | HIS      | -      | expression tag | UNP P19099 |
| A     | 509     | HIS      | -      | expression tag | UNP P19099 |
| A     | 510     | HIS      | -      | expression tag | UNP P19099 |
| A     | 511     | HIS      | -      | expression tag | UNP P19099 |
| A     | 512     | HIS      | -      | expression tag | UNP P19099 |
| B     | 24      | MET      | -      | expression tag | UNP P19099 |
| B     | 25      | ALA      | -      | expression tag | UNP P19099 |
| B     | 26      | THR      | -      | expression tag | UNP P19099 |
| B     | 27      | LYS      | -      | expression tag | UNP P19099 |
| B     | 504     | GLY      | -      | expression tag | UNP P19099 |
| B     | 505     | GLY      | -      | expression tag | UNP P19099 |
| B     | 506     | ARG      | -      | expression tag | UNP P19099 |
| B     | 507     | HIS      | -      | expression tag | UNP P19099 |
| B     | 508     | HIS      | -      | expression tag | UNP P19099 |
| B     | 509     | HIS      | -      | expression tag | UNP P19099 |
| B     | 510     | HIS      | -      | expression tag | UNP P19099 |
| B     | 511     | HIS      | -      | expression tag | UNP P19099 |
| B     | 512     | HIS      | -      | expression tag | UNP P19099 |
| C     | 24      | MET      | -      | expression tag | UNP P19099 |
| C     | 25      | ALA      | -      | expression tag | UNP P19099 |
| C     | 26      | THR      | -      | expression tag | UNP P19099 |
| C     | 27      | LYS      | -      | expression tag | UNP P19099 |
| C     | 504     | GLY      | -      | expression tag | UNP P19099 |
| C     | 505     | GLY      | -      | expression tag | UNP P19099 |
| C     | 506     | ARG      | -      | expression tag | UNP P19099 |
| C     | 507     | HIS      | -      | expression tag | UNP P19099 |
| C     | 508     | HIS      | -      | expression tag | UNP P19099 |
| C     | 509     | HIS      | -      | expression tag | UNP P19099 |
| C     | 510     | HIS      | -      | expression tag | UNP P19099 |
| C     | 511     | HIS      | -      | expression tag | UNP P19099 |
| C     | 512     | HIS      | -      | expression tag | UNP P19099 |
| D     | 24      | MET      | -      | expression tag | UNP P19099 |
| D     | 25      | ALA      | -      | expression tag | UNP P19099 |
| D     | 26      | THR      | -      | expression tag | UNP P19099 |
| D     | 27      | LYS      | -      | expression tag | UNP P19099 |
| D     | 504     | GLY      | -      | expression tag | UNP P19099 |
| D     | 505     | GLY      | -      | expression tag | UNP P19099 |
| D     | 506     | ARG      | -      | expression tag | UNP P19099 |
| D     | 507     | HIS      | -      | expression tag | UNP P19099 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 508     | HIS      | -      | expression tag | UNP P19099 |
| D     | 509     | HIS      | -      | expression tag | UNP P19099 |
| D     | 510     | HIS      | -      | expression tag | UNP P19099 |
| D     | 511     | HIS      | -      | expression tag | UNP P19099 |
| D     | 512     | HIS      | -      | expression tag | UNP P19099 |
| E     | 24      | MET      | -      | expression tag | UNP P19099 |
| E     | 25      | ALA      | -      | expression tag | UNP P19099 |
| E     | 26      | THR      | -      | expression tag | UNP P19099 |
| E     | 27      | LYS      | -      | expression tag | UNP P19099 |
| E     | 504     | GLY      | -      | expression tag | UNP P19099 |
| E     | 505     | GLY      | -      | expression tag | UNP P19099 |
| E     | 506     | ARG      | -      | expression tag | UNP P19099 |
| E     | 507     | HIS      | -      | expression tag | UNP P19099 |
| E     | 508     | HIS      | -      | expression tag | UNP P19099 |
| E     | 509     | HIS      | -      | expression tag | UNP P19099 |
| E     | 510     | HIS      | -      | expression tag | UNP P19099 |
| E     | 511     | HIS      | -      | expression tag | UNP P19099 |
| E     | 512     | HIS      | -      | expression tag | UNP P19099 |
| F     | 24      | MET      | -      | expression tag | UNP P19099 |
| F     | 25      | ALA      | -      | expression tag | UNP P19099 |
| F     | 26      | THR      | -      | expression tag | UNP P19099 |
| F     | 27      | LYS      | -      | expression tag | UNP P19099 |
| F     | 504     | GLY      | -      | expression tag | UNP P19099 |
| F     | 505     | GLY      | -      | expression tag | UNP P19099 |
| F     | 506     | ARG      | -      | expression tag | UNP P19099 |
| F     | 507     | HIS      | -      | expression tag | UNP P19099 |
| F     | 508     | HIS      | -      | expression tag | UNP P19099 |
| F     | 509     | HIS      | -      | expression tag | UNP P19099 |
| F     | 510     | HIS      | -      | expression tag | UNP P19099 |
| F     | 511     | HIS      | -      | expression tag | UNP P19099 |
| F     | 512     | HIS      | -      | expression tag | UNP P19099 |
| G     | 24      | MET      | -      | expression tag | UNP P19099 |
| G     | 25      | ALA      | -      | expression tag | UNP P19099 |
| G     | 26      | THR      | -      | expression tag | UNP P19099 |
| G     | 27      | LYS      | -      | expression tag | UNP P19099 |
| G     | 504     | GLY      | -      | expression tag | UNP P19099 |
| G     | 505     | GLY      | -      | expression tag | UNP P19099 |
| G     | 506     | ARG      | -      | expression tag | UNP P19099 |
| G     | 507     | HIS      | -      | expression tag | UNP P19099 |
| G     | 508     | HIS      | -      | expression tag | UNP P19099 |
| G     | 509     | HIS      | -      | expression tag | UNP P19099 |
| G     | 510     | HIS      | -      | expression tag | UNP P19099 |

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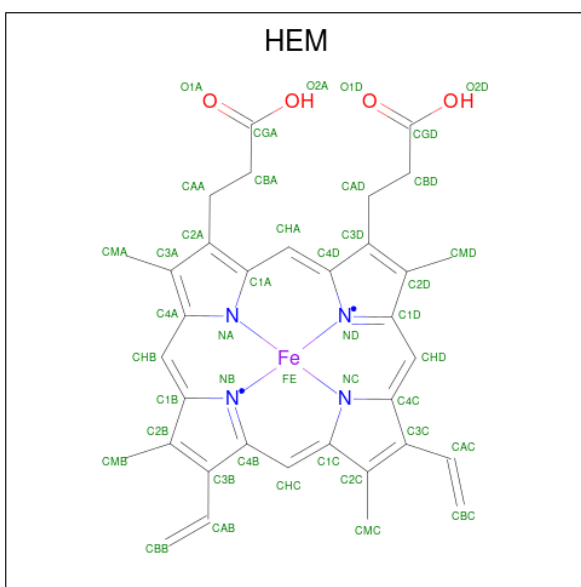
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 511     | HIS      | -      | expression tag | UNP P19099 |
| G     | 512     | HIS      | -      | expression tag | UNP P19099 |
| H     | 24      | MET      | -      | expression tag | UNP P19099 |
| H     | 25      | ALA      | -      | expression tag | UNP P19099 |
| H     | 26      | THR      | -      | expression tag | UNP P19099 |
| H     | 27      | LYS      | -      | expression tag | UNP P19099 |
| H     | 504     | GLY      | -      | expression tag | UNP P19099 |
| H     | 505     | GLY      | -      | expression tag | UNP P19099 |
| H     | 506     | ARG      | -      | expression tag | UNP P19099 |
| H     | 507     | HIS      | -      | expression tag | UNP P19099 |
| H     | 508     | HIS      | -      | expression tag | UNP P19099 |
| H     | 509     | HIS      | -      | expression tag | UNP P19099 |
| H     | 510     | HIS      | -      | expression tag | UNP P19099 |
| H     | 511     | HIS      | -      | expression tag | UNP P19099 |
| H     | 512     | HIS      | -      | expression tag | UNP P19099 |
| I     | 24      | MET      | -      | expression tag | UNP P19099 |
| I     | 25      | ALA      | -      | expression tag | UNP P19099 |
| I     | 26      | THR      | -      | expression tag | UNP P19099 |
| I     | 27      | LYS      | -      | expression tag | UNP P19099 |
| I     | 504     | GLY      | -      | expression tag | UNP P19099 |
| I     | 505     | GLY      | -      | expression tag | UNP P19099 |
| I     | 506     | ARG      | -      | expression tag | UNP P19099 |
| I     | 507     | HIS      | -      | expression tag | UNP P19099 |
| I     | 508     | HIS      | -      | expression tag | UNP P19099 |
| I     | 509     | HIS      | -      | expression tag | UNP P19099 |
| I     | 510     | HIS      | -      | expression tag | UNP P19099 |
| I     | 511     | HIS      | -      | expression tag | UNP P19099 |
| I     | 512     | HIS      | -      | expression tag | UNP P19099 |
| J     | 24      | MET      | -      | expression tag | UNP P19099 |
| J     | 25      | ALA      | -      | expression tag | UNP P19099 |
| J     | 26      | THR      | -      | expression tag | UNP P19099 |
| J     | 27      | LYS      | -      | expression tag | UNP P19099 |
| J     | 504     | GLY      | -      | expression tag | UNP P19099 |
| J     | 505     | GLY      | -      | expression tag | UNP P19099 |
| J     | 506     | ARG      | -      | expression tag | UNP P19099 |
| J     | 507     | HIS      | -      | expression tag | UNP P19099 |
| J     | 508     | HIS      | -      | expression tag | UNP P19099 |
| J     | 509     | HIS      | -      | expression tag | UNP P19099 |
| J     | 510     | HIS      | -      | expression tag | UNP P19099 |
| J     | 511     | HIS      | -      | expression tag | UNP P19099 |
| J     | 512     | HIS      | -      | expression tag | UNP P19099 |
| K     | 24      | MET      | -      | expression tag | UNP P19099 |

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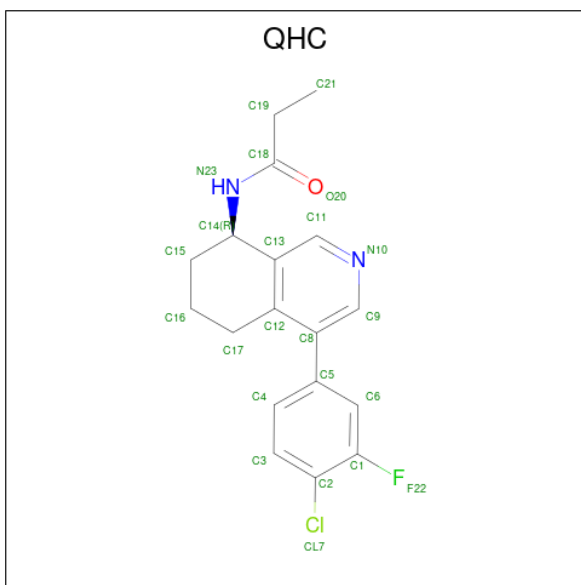
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | 25      | ALA      | -      | expression tag | UNP P19099 |
| K     | 26      | THR      | -      | expression tag | UNP P19099 |
| K     | 27      | LYS      | -      | expression tag | UNP P19099 |
| K     | 504     | GLY      | -      | expression tag | UNP P19099 |
| K     | 505     | GLY      | -      | expression tag | UNP P19099 |
| K     | 506     | ARG      | -      | expression tag | UNP P19099 |
| K     | 507     | HIS      | -      | expression tag | UNP P19099 |
| K     | 508     | HIS      | -      | expression tag | UNP P19099 |
| K     | 509     | HIS      | -      | expression tag | UNP P19099 |
| K     | 510     | HIS      | -      | expression tag | UNP P19099 |
| K     | 511     | HIS      | -      | expression tag | UNP P19099 |
| K     | 512     | HIS      | -      | expression tag | UNP P19099 |
| L     | 24      | MET      | -      | expression tag | UNP P19099 |
| L     | 25      | ALA      | -      | expression tag | UNP P19099 |
| L     | 26      | THR      | -      | expression tag | UNP P19099 |
| L     | 27      | LYS      | -      | expression tag | UNP P19099 |
| L     | 504     | GLY      | -      | expression tag | UNP P19099 |
| L     | 505     | GLY      | -      | expression tag | UNP P19099 |
| L     | 506     | ARG      | -      | expression tag | UNP P19099 |
| L     | 507     | HIS      | -      | expression tag | UNP P19099 |
| L     | 508     | HIS      | -      | expression tag | UNP P19099 |
| L     | 509     | HIS      | -      | expression tag | UNP P19099 |
| L     | 510     | HIS      | -      | expression tag | UNP P19099 |
| L     | 511     | HIS      | -      | expression tag | UNP P19099 |
| L     | 512     | HIS      | -      | expression tag | UNP P19099 |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |

- Molecule 3 is N-[(8R)-4-(4-chloro-3-fluorophenyl)-5,6,7,8-tetrahydroisoquinolin-8-yl]propanamide (CCD ID: QHC) (formula: C<sub>18</sub>H<sub>18</sub>ClFN<sub>2</sub>O).



| Mol | Chain | Residues | Atoms       |         |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|--------|---------|---------|
| 3   | A     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | B     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | C     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | D     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | E     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | F     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | I     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | J     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | K     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |
| 3   | L     | 1        | Total<br>23 | C<br>18 | Cl<br>1 | F<br>1 | N<br>2 | O<br>1 | 0       | 0       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 108      | Total | O   | 0       | 0       |
|     |       |          | 108   | 108 |         |         |
| 4   | B     | 81       | Total | O   | 0       | 0       |
|     |       |          | 81    | 81  |         |         |

*Continued on next page...*

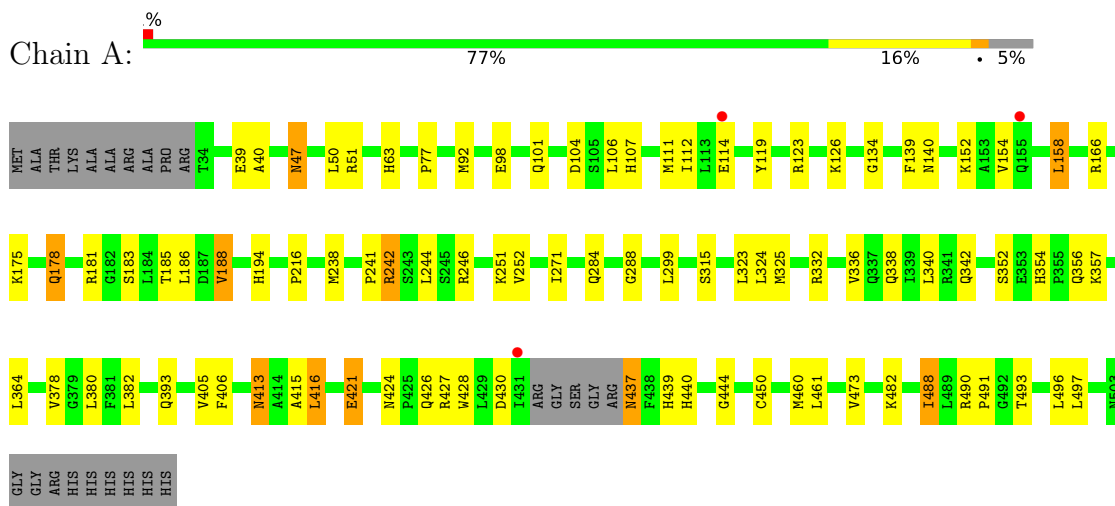
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | C     | 64       | Total<br>64  | O<br>64  | 0       | 0       |
| 4   | D     | 100      | Total<br>100 | O<br>100 | 0       | 0       |
| 4   | E     | 54       | Total<br>54  | O<br>54  | 0       | 0       |
| 4   | F     | 73       | Total<br>73  | O<br>73  | 0       | 0       |
| 4   | G     | 45       | Total<br>45  | O<br>45  | 0       | 0       |
| 4   | H     | 68       | Total<br>68  | O<br>68  | 0       | 0       |
| 4   | I     | 54       | Total<br>54  | O<br>54  | 0       | 0       |
| 4   | J     | 50       | Total<br>50  | O<br>50  | 0       | 0       |
| 4   | K     | 53       | Total<br>53  | O<br>53  | 0       | 0       |
| 4   | L     | 67       | Total<br>67  | O<br>67  | 0       | 0       |

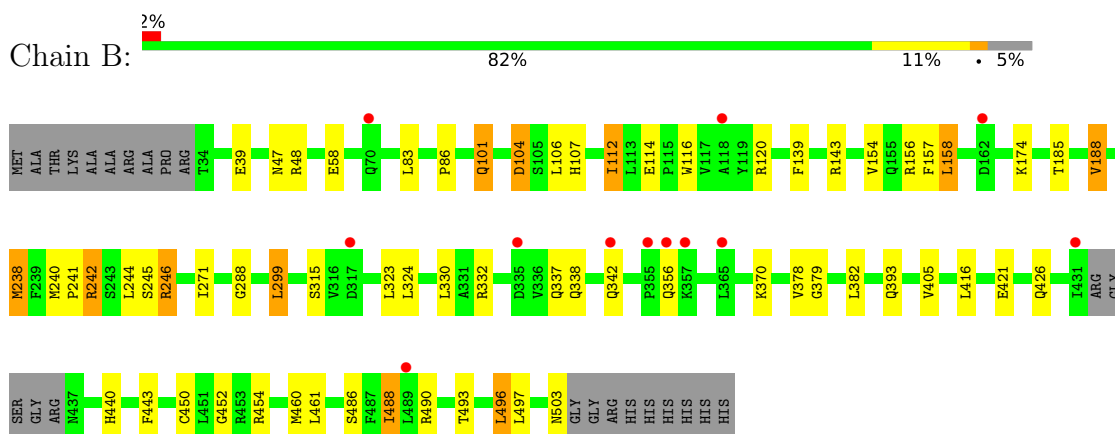
### 3 Residue-property plots

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.

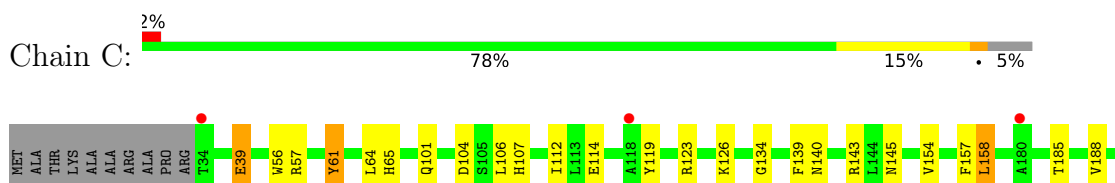
- Molecule 1: Cytochrome P450 11B2, mitochondrial

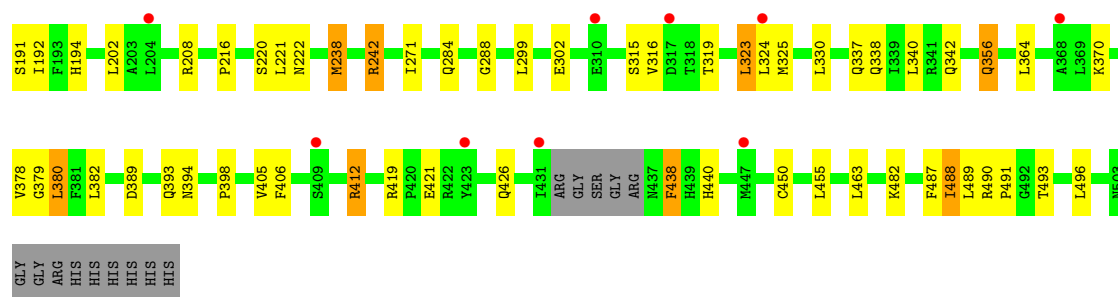


- Molecule 1: Cytochrome P450 11B2, mitochondrial

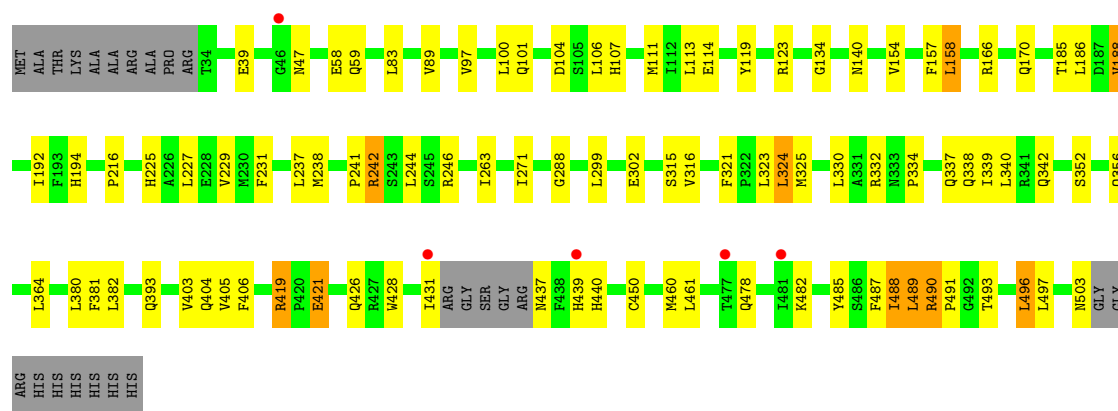
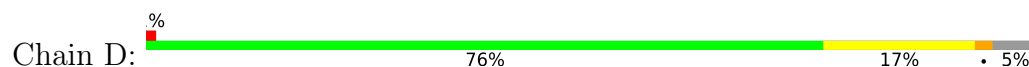


- Molecule 1: Cytochrome P450 11B2, mitochondrial

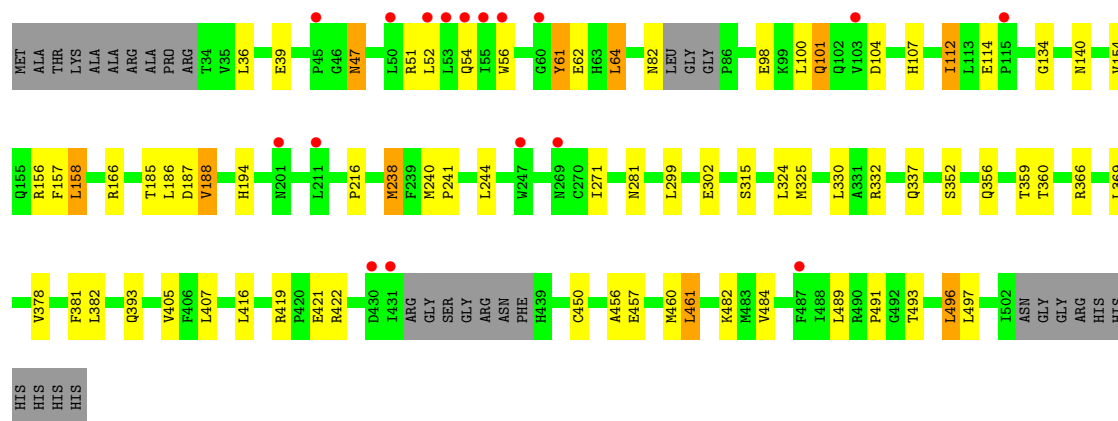
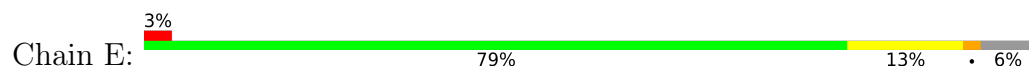




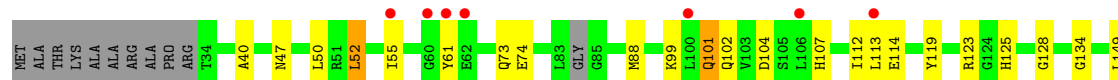
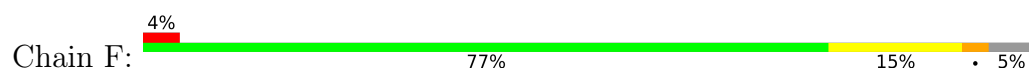
- Molecule 1: Cytochrome P450 11B2, mitochondrial

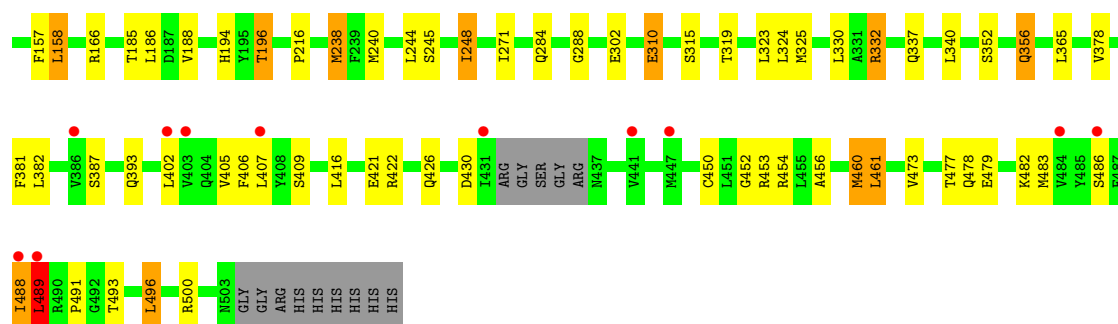


- Molecule 1: Cytochrome P450 11B2, mitochondrial



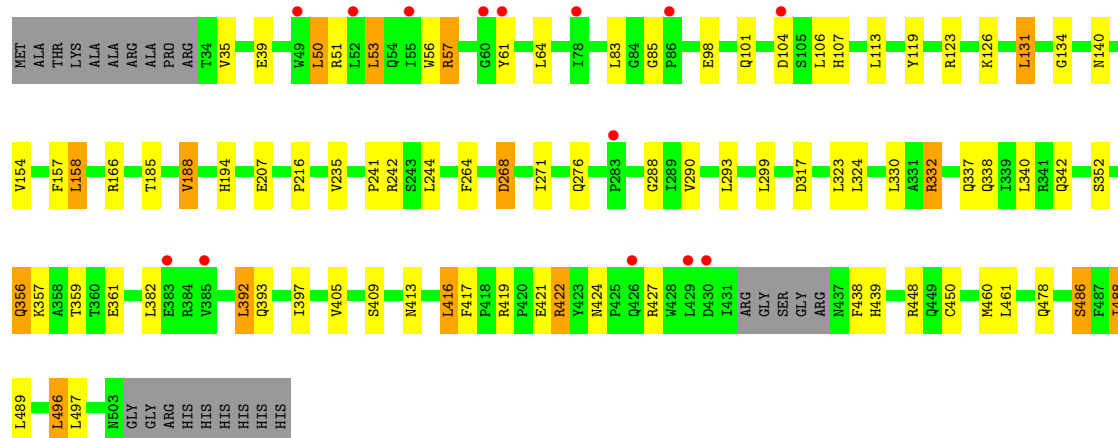
- Molecule 1: Cytochrome P450 11B2, mitochondrial





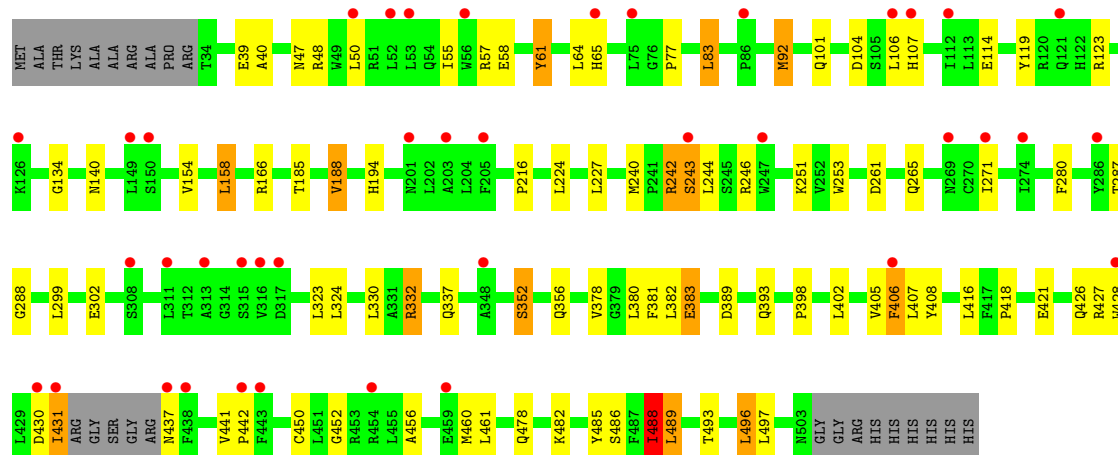
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain G: 3% 78% 14% 5%



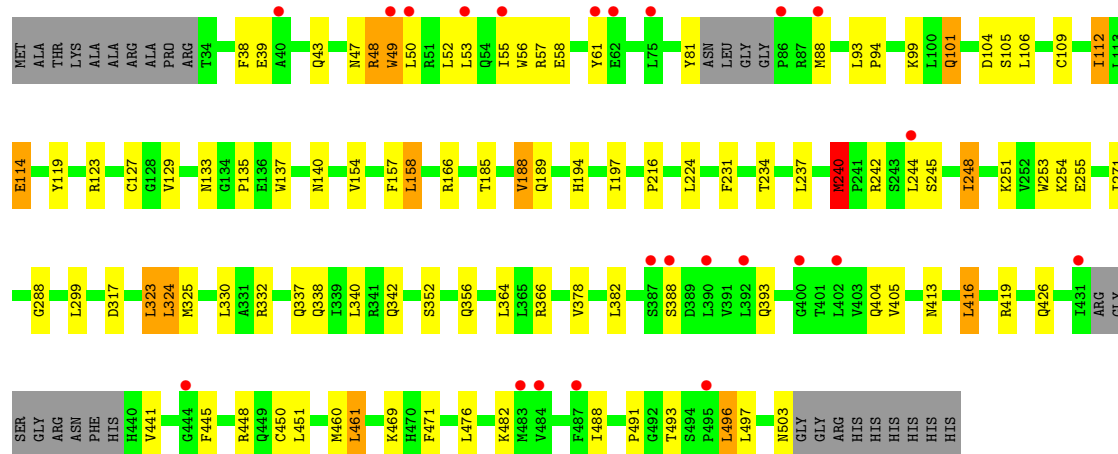
• Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain H: 8% 76% 16% 5%

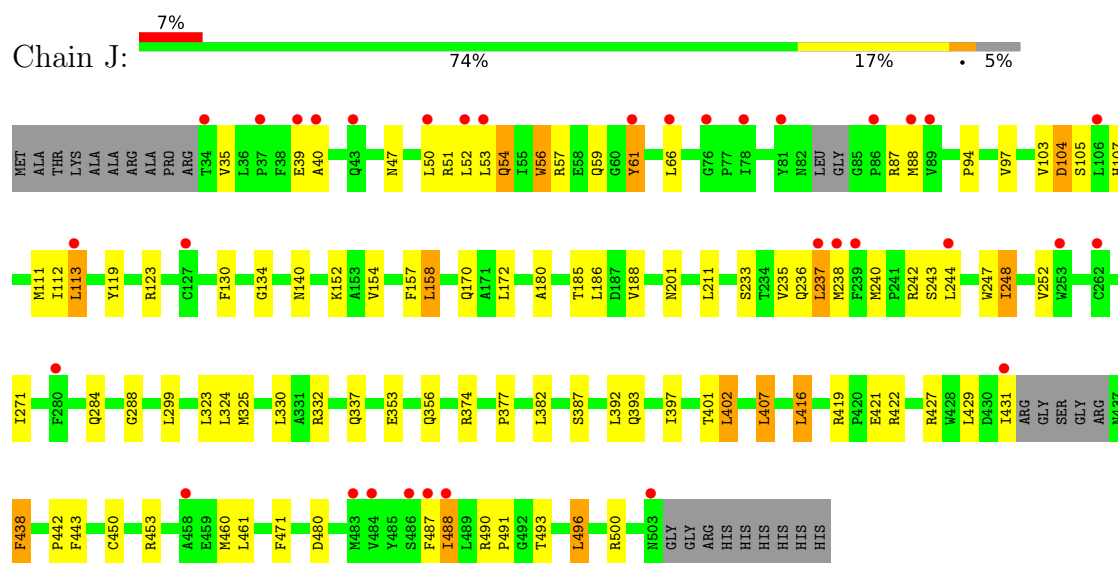


• Molecule 1: Cytochrome P450 11B2, mitochondrial

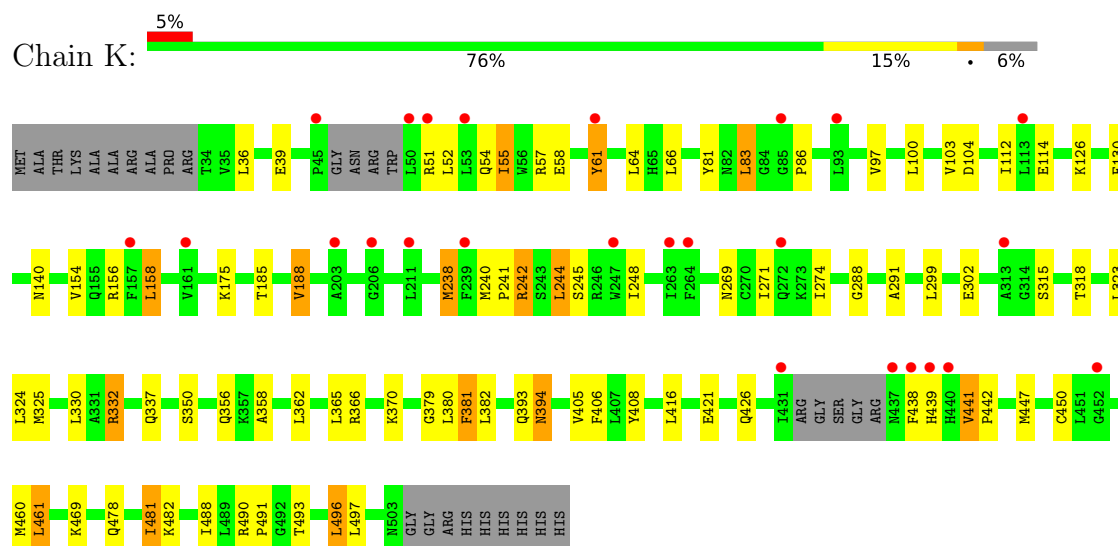
Chain I: 5% 73% 18% 6%



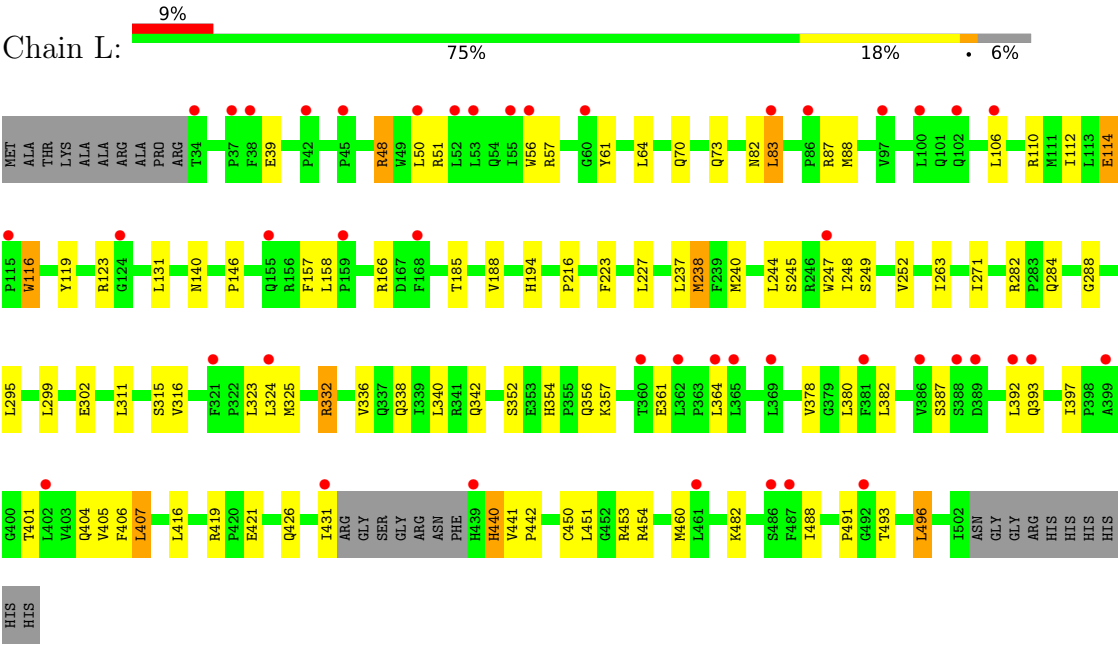
- Molecule 1: Cytochrome P450 11B2, mitochondrial



- Molecule 1: Cytochrome P450 11B2, mitochondrial



- Molecule 1: Cytochrome P450 11B2, mitochondrial



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 104.70Å 125.96Å 155.23Å<br>70.25° 85.87° 73.84°             | Depositor        |
| Resolution (Å)                                                          | 88.20 – 3.20<br>88.20 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.2 (88.20-3.20)<br>97.2 (88.20-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.70 (at 3.19Å)                                             | Xtrriage         |
| Refinement program                                                      | BUSTER 2.11.4                                               | Depositor        |
| R, $R_{free}$                                                           | 0.212 , 0.255<br>0.234 , 0.278                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5769 reflections (4.88%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 60.1                                                        | Xtrriage         |
| Anisotropy                                                              | 0.246                                                       | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 79.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtrriage         |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation                                                  | 0.88                                                        | EDS              |
| Total number of atoms                                                   | 46675                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 72.0                                                        | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.13 % 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 7.4821e-03. 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: HEM, QHC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | A     | 0.80         | 0/3874  | 1.35        | 15/5257 (0.3%)   |
| 1   | B     | 0.76         | 0/3874  | 1.33        | 9/5257 (0.2%)    |
| 1   | C     | 0.77         | 0/3874  | 1.36        | 18/5257 (0.3%)   |
| 1   | D     | 0.79         | 0/3874  | 1.33        | 15/5257 (0.3%)   |
| 1   | E     | 0.78         | 0/3829  | 1.34        | 13/5194 (0.3%)   |
| 1   | F     | 0.77         | 0/3869  | 1.35        | 13/5249 (0.2%)   |
| 1   | G     | 0.77         | 0/3874  | 1.33        | 10/5257 (0.2%)   |
| 1   | H     | 0.76         | 0/3874  | 1.34        | 8/5257 (0.2%)    |
| 1   | I     | 0.77         | 0/3818  | 1.35        | 16/5179 (0.3%)   |
| 1   | J     | 0.76         | 0/3861  | 1.34        | 10/5238 (0.2%)   |
| 1   | K     | 0.76         | 0/3834  | 1.34        | 18/5201 (0.3%)   |
| 1   | L     | 0.78         | 0/3846  | 1.35        | 18/5219 (0.3%)   |
| All | All   | 0.77         | 0/46301 | 1.34        | 163/62822 (0.3%) |

There are no bond length outliers.

All (163) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | K     | 381 | PHE  | CA-CB-CG | 8.60  | 122.40      | 113.80   |
| 1   | I     | 55  | ILE  | N-CA-C   | -7.58 | 105.04      | 111.56   |
| 1   | K     | 394 | ASN  | CA-CB-CG | 7.06  | 119.66      | 112.60   |
| 1   | F     | 40  | ALA  | N-CA-C   | -6.99 | 105.37      | 114.04   |
| 1   | E     | 54  | GLN  | N-CA-C   | -6.91 | 103.53      | 112.23   |
| 1   | J     | 157 | PHE  | CA-CB-CG | 6.59  | 120.39      | 113.80   |
| 1   | E     | 100 | LEU  | CA-C-N   | 6.58  | 129.10      | 120.28   |
| 1   | E     | 100 | LEU  | C-N-CA   | 6.58  | 129.10      | 120.28   |
| 1   | J     | 97  | VAL  | CA-C-N   | 6.41  | 128.87      | 120.28   |
| 1   | J     | 97  | VAL  | C-N-CA   | 6.41  | 128.87      | 120.28   |
| 1   | D     | 237 | LEU  | CA-C-N   | 6.28  | 129.32      | 120.28   |
| 1   | D     | 237 | LEU  | C-N-CA   | 6.28  | 129.32      | 120.28   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 288 | GLY  | CA-C-N   | 6.27  | 128.98      | 120.77   |
| 1   | A     | 288 | GLY  | C-N-CA   | 6.27  | 128.98      | 120.77   |
| 1   | F     | 55  | ILE  | N-CA-C   | -6.22 | 106.46      | 111.81   |
| 1   | D     | 437 | ASN  | CA-CB-CG | 6.18  | 118.78      | 112.60   |
| 1   | C     | 56  | TRP  | CA-C-N   | 6.16  | 129.00      | 120.63   |
| 1   | C     | 56  | TRP  | C-N-CA   | 6.16  | 129.00      | 120.63   |
| 1   | K     | 238 | MET  | N-CA-C   | 6.09  | 118.00      | 111.36   |
| 1   | C     | 222 | ASN  | CA-C-N   | 6.07  | 128.34      | 120.44   |
| 1   | C     | 222 | ASN  | C-N-CA   | 6.07  | 128.34      | 120.44   |
| 1   | I     | 48  | ARG  | CA-C-N   | 6.07  | 128.91      | 120.29   |
| 1   | I     | 48  | ARG  | C-N-CA   | 6.07  | 128.91      | 120.29   |
| 1   | E     | 238 | MET  | N-CA-C   | 6.07  | 117.97      | 111.36   |
| 1   | C     | 220 | SER  | CA-C-N   | 6.07  | 128.69      | 120.38   |
| 1   | C     | 220 | SER  | C-N-CA   | 6.07  | 128.69      | 120.38   |
| 1   | J     | 238 | MET  | N-CA-C   | 6.01  | 119.09      | 111.69   |
| 1   | F     | 288 | GLY  | CA-C-N   | 6.00  | 128.12      | 120.56   |
| 1   | F     | 288 | GLY  | C-N-CA   | 6.00  | 128.12      | 120.56   |
| 1   | G     | 288 | GLY  | CA-C-N   | 5.98  | 128.18      | 120.70   |
| 1   | G     | 288 | GLY  | C-N-CA   | 5.98  | 128.18      | 120.70   |
| 1   | H     | 288 | GLY  | CA-C-N   | 5.92  | 128.02      | 120.56   |
| 1   | H     | 288 | GLY  | C-N-CA   | 5.92  | 128.02      | 120.56   |
| 1   | C     | 319 | THR  | CA-C-N   | 5.92  | 128.21      | 120.28   |
| 1   | C     | 319 | THR  | C-N-CA   | 5.92  | 128.21      | 120.28   |
| 1   | B     | 288 | GLY  | CA-C-N   | 5.91  | 128.09      | 120.70   |
| 1   | B     | 288 | GLY  | C-N-CA   | 5.91  | 128.09      | 120.70   |
| 1   | B     | 47  | ASN  | CA-C-N   | 5.90  | 128.99      | 120.38   |
| 1   | B     | 47  | ASN  | C-N-CA   | 5.90  | 128.99      | 120.38   |
| 1   | L     | 406 | PHE  | CA-C-N   | 5.88  | 128.74      | 120.28   |
| 1   | L     | 406 | PHE  | C-N-CA   | 5.88  | 128.74      | 120.28   |
| 1   | B     | 112 | ILE  | N-CA-CB  | 5.86  | 117.33      | 110.82   |
| 1   | K     | 97  | VAL  | CA-C-N   | 5.83  | 128.10      | 120.28   |
| 1   | K     | 97  | VAL  | C-N-CA   | 5.83  | 128.10      | 120.28   |
| 1   | K     | 242 | ARG  | CA-C-N   | 5.83  | 128.41      | 120.54   |
| 1   | K     | 242 | ARG  | C-N-CA   | 5.83  | 128.41      | 120.54   |
| 1   | J     | 438 | PHE  | CA-CB-CG | 5.81  | 119.61      | 113.80   |
| 1   | E     | 381 | PHE  | CA-CB-CG | 5.80  | 119.60      | 113.80   |
| 1   | F     | 238 | MET  | N-CA-C   | 5.78  | 117.66      | 111.36   |
| 1   | F     | 157 | PHE  | CA-CB-CG | 5.75  | 119.55      | 113.80   |
| 1   | D     | 288 | GLY  | CA-C-N   | 5.74  | 127.87      | 120.70   |
| 1   | D     | 288 | GLY  | C-N-CA   | 5.74  | 127.87      | 120.70   |
| 1   | A     | 437 | ASN  | CA-CB-CG | 5.74  | 118.33      | 112.60   |
| 1   | L     | 288 | GLY  | N-CA-C   | 5.73  | 117.40      | 111.95   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 288 | GLY  | CA-C-N     | 5.73  | 127.78      | 120.56   |
| 1   | K     | 288 | GLY  | C-N-CA     | 5.73  | 127.78      | 120.56   |
| 1   | I     | 471 | PHE  | N-CA-C     | 5.71  | 118.09      | 109.41   |
| 1   | L     | 237 | LEU  | CA-C-N     | 5.71  | 128.39      | 120.29   |
| 1   | L     | 237 | LEU  | C-N-CA     | 5.71  | 128.39      | 120.29   |
| 1   | E     | 157 | PHE  | CA-CB-CG   | 5.69  | 119.49      | 113.80   |
| 1   | A     | 252 | VAL  | N-CA-C     | -5.69 | 104.80      | 111.00   |
| 1   | G     | 83  | LEU  | N-CA-C     | -5.67 | 106.14      | 113.16   |
| 1   | K     | 175 | LYS  | CA-C-N     | 5.66  | 128.22      | 120.46   |
| 1   | K     | 175 | LYS  | C-N-CA     | 5.66  | 128.22      | 120.46   |
| 1   | L     | 302 | GLU  | CB-CG-CD   | 5.66  | 122.22      | 112.60   |
| 1   | E     | 112 | ILE  | N-CA-CB    | 5.62  | 117.06      | 110.82   |
| 1   | F     | 430 | ASP  | CA-C-N     | 5.62  | 131.82      | 121.70   |
| 1   | F     | 430 | ASP  | C-N-CA     | 5.62  | 131.82      | 121.70   |
| 1   | A     | 430 | ASP  | CA-C-N     | 5.62  | 131.81      | 121.70   |
| 1   | A     | 430 | ASP  | C-N-CA     | 5.62  | 131.81      | 121.70   |
| 1   | I     | 255 | GLU  | CA-C-N     | 5.61  | 127.74      | 120.44   |
| 1   | I     | 255 | GLU  | C-N-CA     | 5.61  | 127.74      | 120.44   |
| 1   | A     | 98  | GLU  | CA-C-N     | 5.60  | 127.79      | 120.28   |
| 1   | A     | 98  | GLU  | C-N-CA     | 5.60  | 127.79      | 120.28   |
| 1   | F     | 430 | ASP  | N-CA-C     | 5.56  | 115.18      | 107.73   |
| 1   | C     | 288 | GLY  | CA-C-N     | 5.52  | 127.60      | 120.70   |
| 1   | C     | 288 | GLY  | C-N-CA     | 5.52  | 127.60      | 120.70   |
| 1   | I     | 48  | ARG  | N-CA-C     | -5.52 | 105.35      | 111.36   |
| 1   | C     | 238 | MET  | N-CA-C     | 5.51  | 117.36      | 111.36   |
| 1   | A     | 421 | GLU  | CB-CG-CD   | 5.50  | 121.94      | 112.60   |
| 1   | G     | 51  | ARG  | CA-C-N     | 5.49  | 127.90      | 120.38   |
| 1   | G     | 51  | ARG  | C-N-CA     | 5.49  | 127.90      | 120.38   |
| 1   | D     | 242 | ARG  | CA-C-N     | 5.49  | 127.95      | 120.54   |
| 1   | D     | 242 | ARG  | C-N-CA     | 5.49  | 127.95      | 120.54   |
| 1   | C     | 140 | ASN  | CA-C-N     | 5.47  | 127.61      | 120.28   |
| 1   | C     | 140 | ASN  | C-N-CA     | 5.47  | 127.61      | 120.28   |
| 1   | I     | 288 | GLY  | CA-C-N     | 5.46  | 127.44      | 120.56   |
| 1   | I     | 288 | GLY  | C-N-CA     | 5.46  | 127.44      | 120.56   |
| 1   | A     | 415 | ALA  | N-CA-C     | -5.46 | 107.17      | 113.88   |
| 1   | A     | 112 | ILE  | CB-CG1-CD1 | 5.45  | 125.24      | 113.80   |
| 1   | B     | 486 | SER  | CA-C-N     | 5.43  | 131.91      | 121.54   |
| 1   | B     | 486 | SER  | C-N-CA     | 5.43  | 131.91      | 121.54   |
| 1   | L     | 157 | PHE  | CA-CB-CG   | 5.42  | 119.22      | 113.80   |
| 1   | L     | 336 | VAL  | CA-C-N     | 5.42  | 127.55      | 120.28   |
| 1   | L     | 336 | VAL  | C-N-CA     | 5.42  | 127.55      | 120.28   |
| 1   | B     | 157 | PHE  | CA-CB-CG   | 5.42  | 119.22      | 113.80   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | J     | 288 | GLY  | CA-C-N   | 5.41  | 127.46      | 120.70   |
| 1   | J     | 288 | GLY  | C-N-CA   | 5.41  | 127.46      | 120.70   |
| 1   | F     | 101 | GLN  | CA-C-N   | 5.40  | 128.26      | 120.38   |
| 1   | F     | 101 | GLN  | C-N-CA   | 5.40  | 128.26      | 120.38   |
| 1   | B     | 238 | MET  | N-CA-C   | 5.39  | 117.23      | 111.36   |
| 1   | G     | 241 | PRO  | CA-C-N   | 5.38  | 131.81      | 121.54   |
| 1   | G     | 241 | PRO  | C-N-CA   | 5.38  | 131.81      | 121.54   |
| 1   | A     | 336 | VAL  | CA-C-N   | 5.37  | 127.80      | 120.54   |
| 1   | A     | 336 | VAL  | C-N-CA   | 5.37  | 127.80      | 120.54   |
| 1   | G     | 340 | LEU  | CA-C-N   | 5.37  | 127.48      | 120.28   |
| 1   | G     | 340 | LEU  | C-N-CA   | 5.37  | 127.48      | 120.28   |
| 1   | D     | 97  | VAL  | CA-C-N   | 5.36  | 127.47      | 120.28   |
| 1   | D     | 97  | VAL  | C-N-CA   | 5.36  | 127.47      | 120.28   |
| 1   | D     | 316 | VAL  | CA-C-N   | 5.35  | 127.89      | 120.29   |
| 1   | D     | 316 | VAL  | C-N-CA   | 5.35  | 127.89      | 120.29   |
| 1   | L     | 114 | GLU  | CA-C-O   | -5.31 | 113.19      | 118.34   |
| 1   | L     | 116 | TRP  | CA-C-N   | 5.31  | 127.74      | 120.46   |
| 1   | L     | 116 | TRP  | C-N-CA   | 5.31  | 127.74      | 120.46   |
| 1   | L     | 238 | MET  | N-CA-C   | 5.30  | 117.14      | 111.36   |
| 1   | I     | 157 | PHE  | CA-CB-CG | 5.29  | 119.09      | 113.80   |
| 1   | D     | 47  | ASN  | CA-CB-CG | 5.23  | 117.83      | 112.60   |
| 1   | G     | 157 | PHE  | CA-CB-CG | 5.22  | 119.02      | 113.80   |
| 1   | I     | 323 | LEU  | CA-C-N   | 5.22  | 127.27      | 120.28   |
| 1   | I     | 323 | LEU  | C-N-CA   | 5.22  | 127.27      | 120.28   |
| 1   | D     | 58  | GLU  | CA-C-N   | 5.21  | 131.50      | 121.54   |
| 1   | D     | 58  | GLU  | C-N-CA   | 5.21  | 131.50      | 121.54   |
| 1   | K     | 370 | LYS  | CA-C-N   | 5.20  | 128.22      | 120.31   |
| 1   | K     | 370 | LYS  | C-N-CA   | 5.20  | 128.22      | 120.31   |
| 1   | I     | 254 | LYS  | CA-C-N   | 5.20  | 128.62      | 120.82   |
| 1   | I     | 254 | LYS  | C-N-CA   | 5.20  | 128.62      | 120.82   |
| 1   | J     | 353 | GLU  | CB-CG-CD | 5.20  | 121.44      | 112.60   |
| 1   | L     | 288 | GLY  | CA-C-N   | 5.20  | 127.30      | 120.60   |
| 1   | L     | 288 | GLY  | C-N-CA   | 5.20  | 127.30      | 120.60   |
| 1   | C     | 242 | ARG  | CA-C-N   | 5.19  | 127.19      | 120.44   |
| 1   | C     | 242 | ARG  | C-N-CA   | 5.19  | 127.19      | 120.44   |
| 1   | C     | 406 | PHE  | CA-C-N   | 5.17  | 127.72      | 120.28   |
| 1   | C     | 406 | PHE  | C-N-CA   | 5.17  | 127.72      | 120.28   |
| 1   | F     | 460 | MET  | CA-C-N   | 5.16  | 127.20      | 120.28   |
| 1   | F     | 460 | MET  | C-N-CA   | 5.16  | 127.20      | 120.28   |
| 1   | I     | 38  | PHE  | CA-C-N   | 5.16  | 127.19      | 120.28   |
| 1   | I     | 38  | PHE  | C-N-CA   | 5.16  | 127.19      | 120.28   |
| 1   | K     | 438 | PHE  | CA-CB-CG | 5.16  | 118.96      | 113.80   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | L     | 440 | HIS  | CA-C-N   | 5.14  | 131.63      | 122.13   |
| 1   | L     | 440 | HIS  | C-N-CA   | 5.14  | 131.63      | 122.13   |
| 1   | D     | 157 | PHE  | CA-CB-CG | 5.14  | 118.94      | 113.80   |
| 1   | E     | 359 | THR  | CA-C-N   | 5.11  | 127.55      | 120.29   |
| 1   | E     | 359 | THR  | C-N-CA   | 5.11  | 127.55      | 120.29   |
| 1   | K     | 100 | LEU  | CA-C-N   | 5.08  | 127.05      | 120.44   |
| 1   | K     | 100 | LEU  | C-N-CA   | 5.08  | 127.05      | 120.44   |
| 1   | H     | 406 | PHE  | CA-CB-CG | -5.07 | 108.73      | 113.80   |
| 1   | E     | 56  | TRP  | CA-C-N   | 5.07  | 127.52      | 120.63   |
| 1   | E     | 56  | TRP  | C-N-CA   | 5.07  | 127.52      | 120.63   |
| 1   | L     | 407 | LEU  | N-CA-C   | 5.06  | 117.53      | 111.71   |
| 1   | H     | 352 | SER  | CA-C-N   | 5.05  | 127.31      | 120.44   |
| 1   | H     | 352 | SER  | C-N-CA   | 5.05  | 127.31      | 120.44   |
| 1   | K     | 269 | ASN  | CA-C-N   | 5.05  | 127.04      | 120.28   |
| 1   | K     | 269 | ASN  | C-N-CA   | 5.05  | 127.04      | 120.28   |
| 1   | E     | 457 | GLU  | CA-C-N   | 5.04  | 127.03      | 120.28   |
| 1   | E     | 457 | GLU  | C-N-CA   | 5.04  | 127.03      | 120.28   |
| 1   | H     | 488 | ILE  | CB-CA-C  | 5.04  | 117.22      | 110.42   |
| 1   | C     | 157 | PHE  | CA-CB-CG | 5.02  | 118.82      | 113.80   |
| 1   | A     | 40  | ALA  | CA-C-N   | 5.02  | 127.36      | 120.39   |
| 1   | A     | 40  | ALA  | C-N-CA   | 5.02  | 127.36      | 120.39   |
| 1   | H     | 40  | ALA  | CA-C-N   | 5.01  | 127.36      | 120.39   |
| 1   | H     | 40  | ALA  | C-N-CA   | 5.01  | 127.36      | 120.39   |
| 1   | J     | 40  | ALA  | CA-C-N   | 5.01  | 127.36      | 120.39   |
| 1   | J     | 40  | ALA  | C-N-CA   | 5.01  | 127.36      | 120.39   |

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     | 3774  | 0        | 3808     | 35      | 0            |
| 1   | B     | 3774  | 0        | 3808     | 24      | 0            |
| 1   | C     | 3774  | 0        | 3808     | 34      | 0            |
| 1   | D     | 3774  | 0        | 3808     | 40      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 3731  | 0        | 3770     | 30      | 0            |
| 1   | F     | 3770  | 0        | 3804     | 38      | 0            |
| 1   | G     | 3774  | 0        | 3809     | 30      | 0            |
| 1   | H     | 3774  | 0        | 3809     | 42      | 0            |
| 1   | I     | 3721  | 0        | 3763     | 41      | 0            |
| 1   | J     | 3762  | 0        | 3793     | 30      | 0            |
| 1   | K     | 3737  | 0        | 3775     | 39      | 0            |
| 1   | L     | 3747  | 0        | 3787     | 42      | 0            |
| 2   | A     | 43    | 0        | 30       | 6       | 0            |
| 2   | B     | 43    | 0        | 30       | 5       | 0            |
| 2   | C     | 43    | 0        | 30       | 5       | 0            |
| 2   | D     | 43    | 0        | 30       | 2       | 0            |
| 2   | E     | 43    | 0        | 30       | 4       | 0            |
| 2   | F     | 43    | 0        | 30       | 8       | 0            |
| 2   | G     | 43    | 0        | 30       | 1       | 0            |
| 2   | H     | 43    | 0        | 30       | 7       | 0            |
| 2   | I     | 43    | 0        | 30       | 3       | 0            |
| 2   | J     | 43    | 0        | 30       | 1       | 0            |
| 2   | K     | 43    | 0        | 30       | 5       | 0            |
| 2   | L     | 43    | 0        | 30       | 4       | 0            |
| 3   | A     | 23    | 0        | 18       | 7       | 0            |
| 3   | B     | 23    | 0        | 18       | 5       | 0            |
| 3   | C     | 23    | 0        | 18       | 5       | 0            |
| 3   | D     | 23    | 0        | 18       | 0       | 0            |
| 3   | E     | 23    | 0        | 18       | 2       | 0            |
| 3   | F     | 23    | 0        | 18       | 5       | 0            |
| 3   | I     | 23    | 0        | 18       | 4       | 0            |
| 3   | J     | 23    | 0        | 18       | 4       | 0            |
| 3   | K     | 23    | 0        | 18       | 5       | 0            |
| 3   | L     | 23    | 0        | 18       | 3       | 0            |
| 4   | A     | 108   | 0        | 0        | 0       | 0            |
| 4   | B     | 81    | 0        | 0        | 0       | 0            |
| 4   | C     | 64    | 0        | 0        | 1       | 0            |
| 4   | D     | 100   | 0        | 0        | 0       | 0            |
| 4   | E     | 54    | 0        | 0        | 1       | 0            |
| 4   | F     | 73    | 0        | 0        | 1       | 0            |
| 4   | G     | 45    | 0        | 0        | 0       | 0            |
| 4   | H     | 68    | 0        | 0        | 0       | 0            |
| 4   | I     | 54    | 0        | 0        | 0       | 0            |
| 4   | J     | 50    | 0        | 0        | 0       | 0            |
| 4   | K     | 53    | 0        | 0        | 1       | 0            |
| 4   | L     | 67    | 0        | 0        | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 46675 | 0        | 46082    | 432     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (432) 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:K:52:LEU:HD11  | 1:K:240:MET:HB3  | 1.33                     | 1.08              |
| 1:K:323:LEU:HG   | 1:K:460:MET:HG2  | 1.46                     | 0.97              |
| 1:C:323:LEU:HD21 | 1:C:463:LEU:HD22 | 1.54                     | 0.89              |
| 2:K:601:HEM:HMA3 | 3:K:602:QHC:H14  | 1.60                     | 0.84              |
| 1:A:242:ARG:HD3  | 1:A:246:ARG:HD2  | 1.60                     | 0.83              |
| 2:I:601:HEM:HMA2 | 3:I:602:QHC:H14  | 1.66                     | 0.78              |
| 1:C:412:ARG:HH11 | 1:C:412:ARG:HB2  | 1.49                     | 0.77              |
| 1:D:488:ILE:HD12 | 1:D:490:ARG:HG2  | 1.65                     | 0.77              |
| 1:E:62:GLU:HG2   | 1:E:484:VAL:HG13 | 1.66                     | 0.76              |
| 1:I:189:GLN:HA   | 1:I:324:LEU:HD21 | 1.65                     | 0.76              |
| 1:K:441:VAL:H    | 1:K:442:PRO:HD3  | 1.51                     | 0.76              |
| 1:A:315:SER:HA   | 2:A:601:HEM:HMC2 | 1.68                     | 0.75              |
| 3:A:602:QHC:H12  | 3:A:602:QHC:H2   | 1.70                     | 0.74              |
| 1:B:378:VAL:HG21 | 2:B:601:HEM:HAB  | 1.70                     | 0.72              |
| 3:A:602:QHC:H12  | 3:A:602:QHC:C4   | 2.20                     | 0.71              |
| 1:E:382:LEU:HG   | 1:E:407:LEU:HD11 | 1.71                     | 0.71              |
| 1:E:281:ASN:HB3  | 1:F:500:ARG:HH12 | 1.55                     | 0.71              |
| 2:A:601:HEM:HMA2 | 3:A:602:QHC:H14  | 1.74                     | 0.70              |
| 1:G:235:VAL:HG21 | 1:G:486:SER:HA   | 1.74                     | 0.70              |
| 1:H:383:GLU:HG2  | 1:H:402:LEU:HD11 | 1.74                     | 0.70              |
| 1:G:61:TYR:HB3   | 1:G:64:LEU:HB2   | 1.74                     | 0.69              |
| 1:C:380:LEU:HD23 | 1:C:489:LEU:HD13 | 1.76                     | 0.68              |
| 1:L:382:LEU:HG   | 1:L:407:LEU:HD11 | 1.76                     | 0.68              |
| 1:D:421:GLU:OE1  | 1:I:388:SER:HB3  | 1.94                     | 0.67              |
| 2:C:601:HEM:HMA2 | 3:C:602:QHC:H14  | 1.78                     | 0.66              |
| 1:D:242:ARG:HD2  | 1:D:246:ARG:HH21 | 1.60                     | 0.66              |
| 1:D:485:TYR:HD1  | 1:D:489:LEU:HD12 | 1.61                     | 0.66              |
| 1:I:47:ASN:HB3   | 1:I:49:TRP:HD1   | 1.61                     | 0.65              |
| 1:D:478:GLN:HG3  | 1:I:135:PRO:HG2  | 1.78                     | 0.65              |
| 1:D:315:SER:HA   | 2:D:601:HEM:HMC2 | 1.78                     | 0.64              |
| 1:C:65:HIS:HB3   | 1:C:380:LEU:HD21 | 1.77                     | 0.64              |
| 1:E:281:ASN:CB   | 1:F:500:ARG:HH12 | 2.11                     | 0.64              |
| 1:K:460:MET:HE1  | 2:K:601:HEM:HBB1 | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:601:HEM:HBB2 | 2:F:601:HEM:HHC  | 1.79                     | 0.64              |
| 1:E:241:PRO:HD2  | 1:E:244:LEU:HD12 | 1.80                     | 0.63              |
| 1:J:88:MET:HG3   | 1:J:402:LEU:HD23 | 1.79                     | 0.63              |
| 1:D:225:HIS:O    | 1:D:229:VAL:HG23 | 1.99                     | 0.63              |
| 1:B:83:LEU:HD23  | 1:B:86:PRO:HB2   | 1.82                     | 0.61              |
| 2:C:601:HEM:CMA  | 3:C:602:QHC:H14  | 2.30                     | 0.61              |
| 1:D:421:GLU:CD   | 1:I:388:SER:HB3  | 2.25                     | 0.61              |
| 1:L:382:LEU:HB2  | 1:L:405:VAL:HB   | 1.81                     | 0.61              |
| 1:J:111:MET:HG3  | 1:J:402:LEU:HD13 | 1.82                     | 0.60              |
| 1:D:166:ARG:HH22 | 1:D:352:SER:HA   | 1.64                     | 0.60              |
| 1:I:245:SER:HA   | 1:I:248:ILE:HG22 | 1.84                     | 0.60              |
| 1:B:107:HIS:CE1  | 1:K:36:LEU:HD11  | 2.36                     | 0.60              |
| 1:H:456:ALA:HB2  | 2:H:601:HEM:HMC3 | 1.84                     | 0.60              |
| 1:L:110:ARG:HD3  | 2:L:601:HEM:O1A  | 2.00                     | 0.60              |
| 1:C:412:ARG:HB2  | 1:C:412:ARG:NH1  | 2.15                     | 0.60              |
| 1:H:452:GLY:HA3  | 2:H:601:HEM:HBC2 | 1.83                     | 0.60              |
| 1:L:64:LEU:HG    | 1:L:380:LEU:HD21 | 1.83                     | 0.59              |
| 1:I:240:MET:HE2  | 1:I:248:ILE:HG21 | 1.85                     | 0.59              |
| 1:K:61:TYR:HD1   | 1:K:64:LEU:HD22  | 1.67                     | 0.59              |
| 1:E:378:VAL:HG21 | 2:E:601:HEM:HAB  | 1.83                     | 0.59              |
| 1:K:416:LEU:HB3  | 1:K:439:HIS:NE2  | 2.17                     | 0.59              |
| 1:A:378:VAL:HG21 | 2:A:601:HEM:HAB  | 1.84                     | 0.58              |
| 1:K:441:VAL:N    | 1:K:442:PRO:HD3  | 2.19                     | 0.58              |
| 1:K:52:LEU:CD1   | 1:K:240:MET:HB3  | 2.22                     | 0.58              |
| 1:K:83:LEU:HD23  | 1:K:86:PRO:HB2   | 1.86                     | 0.58              |
| 1:L:378:VAL:HG13 | 1:L:488:ILE:HG23 | 1.85                     | 0.58              |
| 1:J:233:SER:HA   | 1:J:236:GLN:HE21 | 1.69                     | 0.58              |
| 1:A:354:HIS:HB2  | 1:A:357:LYS:HD2  | 1.86                     | 0.58              |
| 1:F:52:LEU:HD21  | 1:F:240:MET:HB3  | 1.86                     | 0.58              |
| 1:G:392:LEU:HD12 | 1:G:397:ILE:HG13 | 1.86                     | 0.57              |
| 1:B:370:LYS:HA   | 1:B:440:HIS:CE1  | 2.39                     | 0.57              |
| 1:F:483:MET:HE3  | 1:F:489:LEU:HB3  | 1.85                     | 0.57              |
| 1:L:244:LEU:HG   | 1:L:248:ILE:HD12 | 1.87                     | 0.57              |
| 1:D:490:ARG:HB2  | 1:D:490:ARG:NH2  | 2.20                     | 0.57              |
| 1:F:196:THR:CG2  | 1:F:319:THR:HB   | 2.35                     | 0.57              |
| 1:I:101:GLN:HG2  | 1:I:445:PHE:CD1  | 2.39                     | 0.57              |
| 1:F:158:LEU:HD22 | 1:F:356:GLN:HA   | 1.87                     | 0.56              |
| 1:C:488:ILE:HG23 | 3:C:602:QHC:H9   | 1.87                     | 0.56              |
| 1:E:456:ALA:O    | 1:E:460:MET:HG3  | 2.05                     | 0.56              |
| 1:I:101:GLN:O    | 1:I:104:ASP:HB2  | 2.05                     | 0.56              |
| 1:J:374:ARG:NE   | 1:J:427:ARG:HH12 | 2.04                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:240:MET:HG3  | 1:L:245:SER:HB3  | 1.86                     | 0.56              |
| 1:H:65:HIS:HB3   | 1:H:380:LEU:HD11 | 1.88                     | 0.56              |
| 1:C:192:ILE:HD12 | 1:C:323:LEU:HD22 | 1.87                     | 0.56              |
| 1:H:389:ASP:OD1  | 1:H:398:PRO:HA   | 2.05                     | 0.56              |
| 1:E:61:TYR:CD1   | 1:E:64:LEU:HG    | 2.41                     | 0.56              |
| 1:B:488:ILE:HD12 | 1:B:490:ARG:HD3  | 1.88                     | 0.56              |
| 1:D:166:ARG:NH2  | 1:D:352:SER:HA   | 2.21                     | 0.56              |
| 1:H:406:PHE:CE2  | 1:H:408:TYR:HB3  | 2.41                     | 0.56              |
| 1:C:315:SER:HA   | 2:C:601:HEM:HMC2 | 1.87                     | 0.55              |
| 1:J:56:TRP:HE1   | 1:J:248:ILE:HG12 | 1.71                     | 0.55              |
| 1:K:240:MET:HE1  | 1:K:248:ILE:HG21 | 1.89                     | 0.55              |
| 1:K:441:VAL:N    | 1:K:442:PRO:CD   | 2.69                     | 0.55              |
| 1:D:188:VAL:HG21 | 1:D:497:LEU:HD12 | 1.89                     | 0.55              |
| 1:H:406:PHE:HE2  | 1:H:408:TYR:HB3  | 1.72                     | 0.54              |
| 1:J:87:ARG:HB3   | 1:J:401:THR:HG23 | 1.88                     | 0.54              |
| 1:L:392:LEU:HD12 | 1:L:397:ILE:HG13 | 1.88                     | 0.54              |
| 1:A:382:LEU:HB2  | 1:A:405:VAL:HB   | 1.89                     | 0.54              |
| 1:G:188:VAL:HG21 | 1:G:497:LEU:HD12 | 1.89                     | 0.54              |
| 1:D:323:LEU:HG   | 1:D:460:MET:HG2  | 1.88                     | 0.54              |
| 1:C:378:VAL:HG21 | 2:C:601:HEM:HAB  | 1.90                     | 0.54              |
| 1:G:413:ASN:HD22 | 1:G:416:LEU:HG   | 1.72                     | 0.54              |
| 1:G:323:LEU:HG   | 1:G:460:MET:HG2  | 1.90                     | 0.54              |
| 1:L:227:LEU:HD22 | 1:L:263:ILE:HG12 | 1.90                     | 0.54              |
| 3:A:602:QHC:C4   | 3:A:602:QHC:C17  | 2.83                     | 0.54              |
| 1:I:330:LEU:HB3  | 1:I:337:GLN:HG3  | 1.88                     | 0.54              |
| 1:I:57:ARG:HH11  | 1:I:58:GLU:HG3   | 1.73                     | 0.54              |
| 2:E:601:HEM:CMA  | 3:E:602:QHC:H14  | 2.38                     | 0.53              |
| 1:J:392:LEU:HD12 | 1:J:397:ILE:HG13 | 1.89                     | 0.53              |
| 1:I:323:LEU:HG   | 1:I:460:MET:HG2  | 1.91                     | 0.53              |
| 1:I:378:VAL:HG21 | 2:I:601:HEM:HAB  | 1.90                     | 0.53              |
| 1:K:52:LEU:HD11  | 1:K:240:MET:CB   | 2.24                     | 0.53              |
| 1:L:146:PRO:HD2  | 4:L:701:HOH:O    | 2.09                     | 0.53              |
| 1:D:241:PRO:HD2  | 1:D:244:LEU:HD12 | 1.90                     | 0.53              |
| 1:J:47:ASN:H     | 1:J:50:LEU:HD12  | 1.74                     | 0.53              |
| 1:A:323:LEU:HG   | 1:A:460:MET:HG2  | 1.91                     | 0.53              |
| 1:C:107:HIS:HE1  | 1:E:36:LEU:HD11  | 1.73                     | 0.53              |
| 1:D:428:TRP:CZ3  | 1:D:440:HIS:HB2  | 2.43                     | 0.53              |
| 2:F:601:HEM:HMA3 | 3:F:602:QHC:H14  | 1.90                     | 0.53              |
| 1:J:130:PHE:CD1  | 3:J:602:QHC:H2   | 2.45                     | 0.52              |
| 1:G:419:ARG:HD3  | 1:G:422:ARG:HD3  | 1.89                     | 0.52              |
| 1:J:323:LEU:HG   | 1:J:460:MET:HG2  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:488:ILE:HG23 | 3:A:602:QHC:H9   | 1.90                     | 0.52              |
| 1:C:143:ARG:HB3  | 1:C:299:LEU:HD11 | 1.91                     | 0.52              |
| 1:G:113:LEU:HB3  | 1:G:131:LEU:HD11 | 1.91                     | 0.52              |
| 2:I:601:HEM:CMA  | 3:I:602:QHC:H14  | 2.36                     | 0.52              |
| 1:F:332:ARG:HA   | 1:F:478:GLN:HE22 | 1.73                     | 0.52              |
| 1:L:488:ILE:HG12 | 3:L:602:QHC:H9   | 1.89                     | 0.52              |
| 2:E:601:HEM:HMA2 | 3:E:602:QHC:H14  | 1.92                     | 0.52              |
| 1:H:441:VAL:N    | 1:H:442:PRO:HD3  | 2.25                     | 0.52              |
| 1:A:47:ASN:HD21  | 1:A:50:LEU:HD12  | 1.74                     | 0.52              |
| 1:H:378:VAL:HG21 | 2:H:601:HEM:HBB2 | 1.91                     | 0.52              |
| 1:H:382:LEU:HG   | 1:H:407:LEU:HD11 | 1.91                     | 0.52              |
| 1:L:282:ARG:HG3  | 1:L:295:LEU:HD22 | 1.92                     | 0.52              |
| 1:F:240:MET:HE3  | 1:F:245:SER:HB3  | 1.92                     | 0.52              |
| 1:H:188:VAL:HG21 | 1:H:497:LEU:HD12 | 1.92                     | 0.52              |
| 1:K:330:LEU:HB3  | 1:K:337:GLN:HG3  | 1.92                     | 0.52              |
| 1:B:452:GLY:HA3  | 2:B:601:HEM:HBC2 | 1.92                     | 0.51              |
| 1:A:188:VAL:HG21 | 1:A:497:LEU:HD12 | 1.91                     | 0.51              |
| 1:F:378:VAL:HG21 | 2:F:601:HEM:HAB  | 1.92                     | 0.51              |
| 1:B:323:LEU:HG   | 1:B:460:MET:HG2  | 1.93                     | 0.51              |
| 1:G:417:PHE:HZ   | 1:G:439:HIS:HB3  | 1.75                     | 0.51              |
| 1:D:194:HIS:NE2  | 1:D:216:PRO:HB3  | 2.25                     | 0.51              |
| 1:B:143:ARG:HB3  | 1:B:299:LEU:HD11 | 1.93                     | 0.51              |
| 1:C:107:HIS:CE1  | 1:E:36:LEU:HD11  | 2.46                     | 0.51              |
| 1:C:330:LEU:HB3  | 1:C:337:GLN:HG3  | 1.93                     | 0.51              |
| 1:L:315:SER:HA   | 2:L:601:HEM:HMC2 | 1.92                     | 0.51              |
| 1:B:188:VAL:HG21 | 1:B:497:LEU:HD12 | 1.93                     | 0.51              |
| 1:L:323:LEU:HG   | 1:L:460:MET:HG2  | 1.93                     | 0.51              |
| 1:A:194:HIS:NE2  | 1:A:216:PRO:HB3  | 2.26                     | 0.51              |
| 1:L:223:PHE:HE2  | 1:L:316:VAL:HG21 | 1.75                     | 0.51              |
| 1:C:488:ILE:HD12 | 1:C:490:ARG:HD3  | 1.93                     | 0.51              |
| 1:I:317:ASP:HB3  | 1:I:488:ILE:HD13 | 1.92                     | 0.50              |
| 1:J:94:PRO:HG3   | 1:J:416:LEU:HD11 | 1.93                     | 0.50              |
| 1:L:441:VAL:N    | 1:L:442:PRO:HD3  | 2.27                     | 0.50              |
| 1:I:194:HIS:NE2  | 1:I:216:PRO:HB3  | 2.26                     | 0.50              |
| 1:E:330:LEU:HB3  | 1:E:337:GLN:HG3  | 1.93                     | 0.50              |
| 1:F:406:PHE:HD2  | 1:F:409:SER:HB2  | 1.77                     | 0.50              |
| 1:I:88:MET:HE3   | 1:I:404:GLN:OE1  | 2.12                     | 0.50              |
| 1:L:223:PHE:CE2  | 1:L:316:VAL:HG21 | 2.46                     | 0.50              |
| 1:E:194:HIS:NE2  | 1:E:216:PRO:HB3  | 2.27                     | 0.50              |
| 1:K:315:SER:HA   | 2:K:601:HEM:HMC2 | 1.94                     | 0.50              |
| 1:G:113:LEU:H    | 1:G:131:LEU:HD21 | 1.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:382:LEU:HB2  | 1:C:405:VAL:HB   | 1.93                     | 0.50              |
| 1:D:421:GLU:OE1  | 1:I:388:SER:CB   | 2.58                     | 0.50              |
| 1:H:323:LEU:HG   | 1:H:460:MET:HG2  | 1.93                     | 0.50              |
| 1:I:137:TRP:NE1  | 1:I:448:ARG:HD3  | 2.27                     | 0.50              |
| 1:B:382:LEU:HB2  | 1:B:405:VAL:HB   | 1.94                     | 0.49              |
| 1:G:194:HIS:NE2  | 1:G:216:PRO:HB3  | 2.27                     | 0.49              |
| 1:B:107:HIS:HE1  | 1:K:36:LEU:CD1   | 2.26                     | 0.49              |
| 1:B:241:PRO:HD2  | 1:B:244:LEU:HD12 | 1.94                     | 0.49              |
| 1:F:488:ILE:HG23 | 3:F:602:QHC:H9   | 1.95                     | 0.49              |
| 1:J:330:LEU:HB3  | 1:J:337:GLN:HG3  | 1.95                     | 0.49              |
| 1:B:488:ILE:HG23 | 3:B:602:QHC:H9   | 1.94                     | 0.49              |
| 1:G:330:LEU:HB3  | 1:G:337:GLN:HG3  | 1.94                     | 0.49              |
| 1:B:330:LEU:HB3  | 1:B:337:GLN:HG3  | 1.95                     | 0.49              |
| 1:L:453:ARG:HH12 | 1:L:454:ARG:HH21 | 1.59                     | 0.49              |
| 1:L:440:HIS:C    | 1:L:442:PRO:HD3  | 2.37                     | 0.49              |
| 1:A:380:LEU:HG   | 1:A:406:PHE:CE1  | 2.47                     | 0.49              |
| 1:E:281:ASN:CB   | 1:F:500:ARG:NH1  | 2.75                     | 0.49              |
| 1:K:188:VAL:HG21 | 1:K:497:LEU:HD12 | 1.93                     | 0.49              |
| 1:A:126:LYS:HG2  | 1:H:418:PRO:HG2  | 1.94                     | 0.49              |
| 1:K:382:LEU:HB2  | 1:K:405:VAL:HB   | 1.94                     | 0.49              |
| 1:I:366:ARG:HG3  | 1:I:461:LEU:HD21 | 1.95                     | 0.49              |
| 1:A:315:SER:CA   | 2:A:601:HEM:HMC2 | 2.40                     | 0.48              |
| 1:E:51:ARG:HG3   | 1:E:61:TYR:CE1   | 2.48                     | 0.48              |
| 1:K:441:VAL:H    | 1:K:442:PRO:CD   | 2.22                     | 0.48              |
| 1:L:87:ARG:HB2   | 1:L:401:THR:HG23 | 1.94                     | 0.48              |
| 1:F:194:HIS:NE2  | 1:F:216:PRO:HB3  | 2.27                     | 0.48              |
| 1:F:323:LEU:HG   | 1:F:460:MET:HG2  | 1.95                     | 0.48              |
| 1:H:77:PRO:HB3   | 1:H:92:MET:HE2   | 1.96                     | 0.48              |
| 1:H:428:TRP:HE3  | 1:H:431:ILE:HG12 | 1.79                     | 0.48              |
| 1:I:112:ILE:HD11 | 1:I:114:GLU:HG2  | 1.94                     | 0.48              |
| 1:L:378:VAL:CG1  | 1:L:488:ILE:HG23 | 2.44                     | 0.48              |
| 1:E:140:ASN:HA   | 1:E:299:LEU:HD21 | 1.95                     | 0.48              |
| 1:H:140:ASN:HA   | 1:H:299:LEU:HD21 | 1.96                     | 0.48              |
| 1:L:357:LYS:O    | 1:L:361:GLU:HB2  | 2.13                     | 0.48              |
| 1:B:379:GLY:HA3  | 3:B:602:QHC:C18  | 2.44                     | 0.48              |
| 1:E:382:LEU:HB2  | 1:E:405:VAL:HB   | 1.95                     | 0.48              |
| 1:H:382:LEU:HB2  | 1:H:405:VAL:HB   | 1.96                     | 0.48              |
| 1:I:49:TRP:H     | 1:I:49:TRP:CD1   | 2.30                     | 0.48              |
| 1:C:194:HIS:NE2  | 1:C:216:PRO:HB3  | 2.28                     | 0.48              |
| 1:E:315:SER:HA   | 2:E:601:HEM:HMC2 | 1.95                     | 0.48              |
| 1:A:63:HIS:CD2   | 1:A:63:HIS:H     | 2.30                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:50:LEU:HG    | 1:G:53:LEU:HD21  | 1.94                     | 0.48              |
| 1:L:440:HIS:CG   | 1:L:441:VAL:H    | 2.29                     | 0.48              |
| 1:F:381:PHE:HA   | 1:F:405:VAL:O    | 2.14                     | 0.47              |
| 1:E:98:GLU:HA    | 1:E:101:GLN:OE1  | 2.14                     | 0.47              |
| 1:H:194:HIS:NE2  | 1:H:216:PRO:HB3  | 2.28                     | 0.47              |
| 1:I:140:ASN:HA   | 1:I:299:LEU:HD21 | 1.96                     | 0.47              |
| 1:J:488:ILE:HD12 | 1:J:490:ARG:HD3  | 1.95                     | 0.47              |
| 1:L:194:HIS:NE2  | 1:L:216:PRO:HB3  | 2.29                     | 0.47              |
| 1:D:140:ASN:HA   | 1:D:299:LEU:HD21 | 1.96                     | 0.47              |
| 1:D:192:ILE:HG13 | 1:D:324:LEU:HD23 | 1.95                     | 0.47              |
| 1:D:340:LEU:CD2  | 1:D:364:LEU:HB3  | 2.44                     | 0.47              |
| 1:L:140:ASN:HA   | 1:L:299:LEU:HD21 | 1.96                     | 0.47              |
| 1:F:245:SER:HA   | 1:F:248:ILE:HG22 | 1.96                     | 0.47              |
| 1:G:119:TYR:CZ   | 1:G:123:ARG:HG3  | 2.49                     | 0.47              |
| 1:L:48:ARG:HD3   | 1:L:83:LEU:HA    | 1.95                     | 0.47              |
| 1:A:424:ASN:O    | 1:A:427:ARG:HG2  | 2.14                     | 0.47              |
| 1:G:276:GLN:HG3  | 1:I:476:LEU:HG   | 1.97                     | 0.47              |
| 1:H:330:LEU:HB3  | 1:H:337:GLN:HG3  | 1.95                     | 0.47              |
| 1:L:116:TRP:HE3  | 1:L:131:LEU:HD21 | 1.79                     | 0.47              |
| 1:E:188:VAL:HG21 | 1:E:497:LEU:HD12 | 1.96                     | 0.47              |
| 1:H:65:HIS:HB3   | 1:H:380:LEU:CD1  | 2.44                     | 0.47              |
| 1:H:242:ARG:HG2  | 1:H:253:TRP:CZ2  | 2.49                     | 0.47              |
| 1:K:380:LEU:HD23 | 1:K:381:PHE:CE1  | 2.49                     | 0.47              |
| 1:E:281:ASN:HB3  | 1:F:500:ARG:NH1  | 2.26                     | 0.47              |
| 1:F:382:LEU:HD12 | 1:F:405:VAL:HB   | 1.97                     | 0.47              |
| 1:H:452:GLY:HA3  | 2:H:601:HEM:CBC  | 2.44                     | 0.47              |
| 1:I:237:LEU:HD22 | 1:I:253:TRP:NE1  | 2.30                     | 0.47              |
| 1:G:185:THR:HG22 | 1:G:496:LEU:HG   | 1.97                     | 0.47              |
| 1:A:241:PRO:HD2  | 1:A:244:LEU:HD12 | 1.96                     | 0.47              |
| 1:F:315:SER:HA   | 2:F:601:HEM:HMC2 | 1.96                     | 0.47              |
| 1:F:452:GLY:HA3  | 2:F:601:HEM:HBC2 | 1.95                     | 0.47              |
| 2:K:601:HEM:CMA  | 3:K:602:QHC:H14  | 2.37                     | 0.47              |
| 1:A:413:ASN:HB3  | 1:A:416:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:140:ASN:HA   | 1:A:299:LEU:HD21 | 1.97                     | 0.46              |
| 1:G:264:PHE:O    | 1:G:268:ASP:HB3  | 2.16                     | 0.46              |
| 1:K:245:SER:HA   | 1:K:248:ILE:HG22 | 1.97                     | 0.46              |
| 1:J:407:LEU:HD11 | 1:J:442:PRO:HA   | 1.96                     | 0.46              |
| 1:A:488:ILE:HD12 | 1:A:490:ARG:HD3  | 1.97                     | 0.46              |
| 1:G:357:LYS:O    | 1:G:361:GLU:HB2  | 2.16                     | 0.46              |
| 1:I:197:ILE:HD11 | 1:I:224:LEU:HD21 | 1.96                     | 0.46              |
| 1:K:381:PHE:HB2  | 4:K:722:HOH:O    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:119:TYR:CZ   | 1:F:123:ARG:HG3  | 2.50                     | 0.46              |
| 1:I:382:LEU:HB2  | 1:I:405:VAL:HB   | 1.97                     | 0.46              |
| 1:B:315:SER:HA   | 2:B:601:HEM:HMC2 | 1.98                     | 0.46              |
| 1:F:128:GLY:HA3  | 1:F:310:GLU:CD   | 2.40                     | 0.46              |
| 1:F:166:ARG:HH22 | 1:F:352:SER:HA   | 1.80                     | 0.46              |
| 1:L:378:VAL:HG12 | 3:L:602:QHC:H6   | 1.98                     | 0.46              |
| 3:B:602:QHC:H12  | 3:B:602:QHC:C4   | 2.45                     | 0.46              |
| 1:G:382:LEU:HB2  | 1:G:405:VAL:HB   | 1.97                     | 0.46              |
| 1:H:185:THR:HG22 | 1:H:496:LEU:HG   | 1.97                     | 0.46              |
| 3:I:602:QHC:C4   | 3:I:602:QHC:H12  | 2.46                     | 0.46              |
| 1:B:242:ARG:NH2  | 1:B:246:ARG:HH21 | 2.14                     | 0.46              |
| 1:C:487:PHE:CD2  | 3:C:602:QHC:H10  | 2.51                     | 0.46              |
| 1:F:486:SER:C    | 1:F:488:ILE:H    | 2.23                     | 0.46              |
| 2:F:601:HEM:CMA  | 3:F:602:QHC:H14  | 2.45                     | 0.46              |
| 1:G:424:ASN:O    | 1:G:427:ARG:HG2  | 2.16                     | 0.46              |
| 1:H:48:ARG:HD3   | 1:H:83:LEU:HG    | 1.98                     | 0.46              |
| 1:H:378:VAL:HG21 | 2:H:601:HEM:CBB  | 2.46                     | 0.46              |
| 1:I:93:LEU:HD23  | 1:I:413:ASN:HD21 | 1.80                     | 0.45              |
| 1:I:188:VAL:HG21 | 1:I:497:LEU:HD12 | 1.97                     | 0.45              |
| 1:J:107:HIS:HB3  | 1:J:134:GLY:HA2  | 1.99                     | 0.45              |
| 1:E:166:ARG:HH22 | 1:E:352:SER:HA   | 1.82                     | 0.45              |
| 2:G:601:HEM:HMB1 | 2:G:601:HEM:HBB2 | 1.98                     | 0.45              |
| 1:E:369:LEU:HD22 | 1:E:460:MET:HE3  | 1.97                     | 0.45              |
| 1:K:140:ASN:HA   | 1:K:299:LEU:HD21 | 1.99                     | 0.45              |
| 1:K:185:THR:HG22 | 1:K:496:LEU:HG   | 1.98                     | 0.45              |
| 1:K:325:MET:HE3  | 1:K:491:PRO:HG3  | 1.98                     | 0.45              |
| 2:L:601:HEM:HMA3 | 3:L:602:QHC:H14  | 1.99                     | 0.45              |
| 1:E:185:THR:HG22 | 1:E:496:LEU:HG   | 1.99                     | 0.45              |
| 1:I:325:MET:HE3  | 1:I:491:PRO:HG3  | 1.99                     | 0.45              |
| 1:L:354:HIS:O    | 1:L:357:LYS:HB2  | 2.17                     | 0.45              |
| 1:H:456:ALA:HB2  | 2:H:601:HEM:CMC  | 2.47                     | 0.45              |
| 1:A:175:LYS:HA   | 1:A:178:GLN:HG3  | 1.98                     | 0.45              |
| 1:D:321:PHE:CZ   | 1:D:490:ARG:HB3  | 2.51                     | 0.45              |
| 1:E:154:VAL:O    | 1:E:158:LEU:HB2  | 2.16                     | 0.45              |
| 1:G:417:PHE:CZ   | 1:G:439:HIS:HB3  | 2.52                     | 0.45              |
| 1:C:389:ASP:OD2  | 1:C:398:PRO:HA   | 2.17                     | 0.45              |
| 1:D:119:TYR:CZ   | 1:D:123:ARG:HG3  | 2.52                     | 0.45              |
| 1:D:381:PHE:HA   | 1:D:405:VAL:O    | 2.17                     | 0.45              |
| 1:F:330:LEU:HD21 | 1:F:340:LEU:HD12 | 1.99                     | 0.45              |
| 1:H:452:GLY:CA   | 2:H:601:HEM:HBC2 | 2.46                     | 0.45              |
| 1:J:54:GLN:HG3   | 1:J:61:TYR:CZ    | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:185:THR:HG22 | 1:L:496:LEU:HG   | 1.98                     | 0.45              |
| 1:G:158:LEU:HD22 | 1:G:356:GLN:HA   | 1.99                     | 0.45              |
| 1:L:88:MET:HE3   | 1:L:404:GLN:NE2  | 2.32                     | 0.45              |
| 1:A:166:ARG:HH22 | 1:A:352:SER:HA   | 1.81                     | 0.44              |
| 1:D:185:THR:HG22 | 1:D:496:LEU:HG   | 1.98                     | 0.44              |
| 1:D:490:ARG:HB2  | 1:D:490:ARG:HH21 | 1.82                     | 0.44              |
| 1:F:407:LEU:CD1  | 3:F:602:QHC:H15  | 2.47                     | 0.44              |
| 1:H:224:LEU:HA   | 1:H:227:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:154:VAL:O    | 1:A:158:LEU:HB2  | 2.17                     | 0.44              |
| 1:C:158:LEU:HD22 | 1:C:356:GLN:HA   | 2.00                     | 0.44              |
| 1:B:185:THR:HG22 | 1:B:496:LEU:HG   | 2.00                     | 0.44              |
| 1:I:166:ARG:HH22 | 1:I:352:SER:HA   | 1.82                     | 0.44              |
| 3:I:602:QHC:H12  | 3:I:602:QHC:H2   | 1.99                     | 0.44              |
| 1:D:107:HIS:HB3  | 1:D:134:GLY:HA2  | 2.00                     | 0.44              |
| 1:K:274:ILE:HD11 | 1:K:291:ALA:HB2  | 2.00                     | 0.44              |
| 1:L:166:ARG:HH22 | 1:L:352:SER:HA   | 1.83                     | 0.44              |
| 1:C:185:THR:HG22 | 1:C:496:LEU:HG   | 1.99                     | 0.44              |
| 1:A:119:TYR:CZ   | 1:A:123:ARG:HG3  | 2.53                     | 0.44              |
| 1:E:107:HIS:HB3  | 1:E:134:GLY:HA2  | 2.00                     | 0.44              |
| 1:H:61:TYR:O     | 1:H:485:TYR:HB3  | 2.18                     | 0.44              |
| 1:D:330:LEU:HB3  | 1:D:337:GLN:HG3  | 2.00                     | 0.44              |
| 1:H:486:SER:C    | 1:H:488:ILE:H    | 2.26                     | 0.44              |
| 1:K:379:GLY:HA3  | 3:K:602:QHC:H17  | 1.99                     | 0.44              |
| 1:G:107:HIS:HB3  | 1:G:134:GLY:HA2  | 2.00                     | 0.43              |
| 1:J:488:ILE:HG23 | 3:J:602:QHC:H9   | 1.99                     | 0.43              |
| 1:A:185:THR:HG22 | 1:A:496:LEU:HG   | 2.00                     | 0.43              |
| 1:C:323:LEU:CD2  | 1:C:463:LEU:HD22 | 2.36                     | 0.43              |
| 1:L:83:LEU:HD11  | 4:L:709:HOH:O    | 2.17                     | 0.43              |
| 1:F:330:LEU:HD21 | 1:F:340:LEU:CD1  | 2.48                     | 0.43              |
| 1:G:140:ASN:HA   | 1:G:299:LEU:HD21 | 2.00                     | 0.43              |
| 1:L:119:TYR:CZ   | 1:L:123:ARG:HG3  | 2.53                     | 0.43              |
| 2:B:601:HEM:CMA  | 3:B:602:QHC:H13  | 2.48                     | 0.43              |
| 1:K:481:ILE:HD12 | 1:K:481:ILE:H    | 1.82                     | 0.43              |
| 1:C:370:LYS:HA   | 1:C:440:HIS:CE1  | 2.54                     | 0.43              |
| 1:D:154:VAL:O    | 1:D:158:LEU:HB2  | 2.18                     | 0.43              |
| 1:D:324:LEU:HD22 | 1:D:324:LEU:HA   | 1.86                     | 0.43              |
| 1:K:366:ARG:HG2  | 1:K:461:LEU:HD11 | 1.99                     | 0.43              |
| 1:A:325:MET:HE3  | 1:A:491:PRO:HG3  | 1.99                     | 0.43              |
| 1:A:378:VAL:HG12 | 3:A:602:QHC:H6   | 2.00                     | 0.43              |
| 1:H:332:ARG:HD3  | 1:H:478:GLN:HA   | 2.01                     | 0.43              |
| 1:I:185:THR:HG22 | 1:I:496:LEU:HG   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:154:VAL:O    | 1:B:158:LEU:HB2  | 2.18                     | 0.43              |
| 1:C:154:VAL:O    | 1:C:158:LEU:HB2  | 2.18                     | 0.43              |
| 1:D:315:SER:HB3  | 2:D:601:HEM:CBC  | 2.48                     | 0.43              |
| 1:E:325:MET:HE3  | 1:E:491:PRO:HG3  | 2.00                     | 0.43              |
| 1:F:456:ALA:HB2  | 2:F:601:HEM:HMC3 | 2.01                     | 0.43              |
| 1:D:227:LEU:HA   | 1:D:263:ILE:HD11 | 2.01                     | 0.43              |
| 1:D:382:LEU:HB2  | 1:D:405:VAL:HB   | 1.99                     | 0.43              |
| 1:F:365:LEU:HD23 | 1:F:461:LEU:HD13 | 2.00                     | 0.43              |
| 1:I:338:GLN:HG3  | 1:I:342:GLN:HE21 | 1.84                     | 0.43              |
| 1:J:113:LEU:HD21 | 1:J:487:PHE:HZ   | 1.84                     | 0.43              |
| 1:J:154:VAL:O    | 1:J:158:LEU:HB2  | 2.18                     | 0.43              |
| 1:J:407:LEU:HD12 | 3:J:602:QHC:H15  | 2.01                     | 0.43              |
| 1:K:51:ARG:HB2   | 1:K:61:TYR:OH    | 2.19                     | 0.43              |
| 1:F:330:LEU:HB3  | 1:F:337:GLN:HG3  | 2.01                     | 0.42              |
| 1:J:377:PRO:HB3  | 1:J:407:LEU:HD13 | 2.00                     | 0.42              |
| 2:A:601:HEM:CMA  | 3:A:602:QHC:H14  | 2.46                     | 0.42              |
| 1:B:240:MET:HG3  | 1:B:245:SER:HB3  | 2.01                     | 0.42              |
| 1:C:379:GLY:HA3  | 3:C:602:QHC:C18  | 2.48                     | 0.42              |
| 1:D:419:ARG:HD2  | 1:I:388:SER:OG   | 2.19                     | 0.42              |
| 1:H:61:TYR:HB3   | 1:H:64:LEU:HB2   | 2.02                     | 0.42              |
| 1:D:325:MET:HE3  | 1:D:491:PRO:HG3  | 2.00                     | 0.42              |
| 1:D:380:LEU:HD11 | 1:D:406:PHE:CE1  | 2.54                     | 0.42              |
| 1:J:185:THR:HG22 | 1:J:496:LEU:HG   | 2.00                     | 0.42              |
| 1:K:416:LEU:HB3  | 1:K:439:HIS:CE1  | 2.54                     | 0.42              |
| 1:A:107:HIS:HB3  | 1:A:134:GLY:HA2  | 2.01                     | 0.42              |
| 1:C:61:TYR:CD1   | 1:C:64:LEU:HD13  | 2.54                     | 0.42              |
| 1:C:438:PHE:HE2  | 4:C:728:HOH:O    | 2.02                     | 0.42              |
| 1:C:455:LEU:HD23 | 2:C:601:HEM:CBC  | 2.50                     | 0.42              |
| 1:B:116:TRP:O    | 1:B:120:ARG:HG2  | 2.19                     | 0.42              |
| 1:C:107:HIS:HB3  | 1:C:134:GLY:HA2  | 2.01                     | 0.42              |
| 1:E:47:ASN:HB3   | 1:E:82:ASN:HD22  | 1.84                     | 0.42              |
| 1:I:129:VAL:HG11 | 1:I:451:LEU:HD22 | 2.02                     | 0.42              |
| 1:I:231:PHE:O    | 1:I:234:THR:HB   | 2.19                     | 0.42              |
| 1:C:202:LEU:HD22 | 1:C:208:ARG:HD3  | 2.01                     | 0.42              |
| 1:J:325:MET:HE3  | 1:J:491:PRO:HG3  | 2.00                     | 0.42              |
| 1:F:149:LEU:HD23 | 4:F:747:HOH:O    | 2.20                     | 0.42              |
| 1:G:290:VAL:HA   | 1:G:293:LEU:HD12 | 2.01                     | 0.42              |
| 1:J:140:ASN:HA   | 1:J:299:LEU:HD21 | 2.02                     | 0.42              |
| 1:A:77:PRO:HA    | 1:A:92:MET:HE2   | 2.01                     | 0.42              |
| 1:D:334:PRO:HD2  | 1:I:106:LEU:HD21 | 2.01                     | 0.42              |
| 1:E:52:LEU:HD11  | 1:E:240:MET:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:172:LEU:HD23 | 1:J:471:PHE:CE1  | 2.54                     | 0.42              |
| 1:J:237:LEU:HD12 | 1:J:252:VAL:HG12 | 2.02                     | 0.42              |
| 1:G:154:VAL:O    | 1:G:158:LEU:HB2  | 2.19                     | 0.42              |
| 1:I:119:TYR:CZ   | 1:I:123:ARG:HG3  | 2.55                     | 0.42              |
| 1:F:325:MET:HE3  | 1:F:491:PRO:HG3  | 2.02                     | 0.41              |
| 1:H:166:ARG:HH22 | 1:H:352:SER:HA   | 1.85                     | 0.41              |
| 1:A:444:GLY:HA3  | 2:A:601:HEM:HBA1 | 2.02                     | 0.41              |
| 1:E:187:ASP:HB3  | 4:E:711:HOH:O    | 2.18                     | 0.41              |
| 1:F:88:MET:HG3   | 1:F:402:LEU:HD23 | 2.01                     | 0.41              |
| 1:F:453:ARG:HH12 | 1:F:454:ARG:HH21 | 1.69                     | 0.41              |
| 1:F:99:LYS:O     | 1:F:102:GLN:HB2  | 2.19                     | 0.41              |
| 1:H:287:THR:HG22 | 1:J:180:ALA:HB1  | 2.01                     | 0.41              |
| 1:H:380:LEU:HD13 | 1:H:489:LEU:HD11 | 2.02                     | 0.41              |
| 1:K:154:VAL:O    | 1:K:158:LEU:HB2  | 2.20                     | 0.41              |
| 1:E:366:ARG:HG2  | 1:E:461:LEU:HD11 | 2.03                     | 0.41              |
| 1:I:94:PRO:HG3   | 1:I:416:LEU:HG   | 2.02                     | 0.41              |
| 1:A:242:ARG:HH21 | 1:A:246:ARG:NH2  | 2.18                     | 0.41              |
| 1:C:338:GLN:HG3  | 1:C:342:GLN:HE21 | 1.85                     | 0.41              |
| 1:D:231:PHE:CD1  | 1:D:487:PHE:HD2  | 2.39                     | 0.41              |
| 2:F:601:HEM:HHC  | 2:F:601:HEM:CBB  | 2.47                     | 0.41              |
| 1:K:55:ILE:HG12  | 1:K:61:TYR:CE2   | 2.56                     | 0.41              |
| 1:L:249:SER:HB3  | 1:L:252:VAL:HB   | 2.01                     | 0.41              |
| 1:D:89:VAL:CG1   | 1:D:403:VAL:HG22 | 2.50                     | 0.41              |
| 1:F:185:THR:HG22 | 1:F:496:LEU:HG   | 2.02                     | 0.41              |
| 1:G:332:ARG:HD3  | 1:G:478:GLN:HA   | 2.01                     | 0.41              |
| 3:K:602:QHC:C6   | 3:K:602:QHC:H12  | 2.51                     | 0.41              |
| 1:L:340:LEU:HD23 | 1:L:364:LEU:HB3  | 2.02                     | 0.41              |
| 1:C:119:TYR:CZ   | 1:C:123:ARG:HG3  | 2.56                     | 0.41              |
| 1:D:338:GLN:HG3  | 1:D:342:GLN:HE21 | 1.86                     | 0.41              |
| 1:H:107:HIS:HB3  | 1:H:134:GLY:HA2  | 2.02                     | 0.41              |
| 1:I:109:CYS:HA   | 1:I:133:ASN:OD1  | 2.21                     | 0.41              |
| 1:K:241:PRO:HD2  | 1:K:244:LEU:HD12 | 2.03                     | 0.41              |
| 1:K:332:ARG:HD3  | 1:K:478:GLN:HA   | 2.02                     | 0.41              |
| 1:K:358:ALA:O    | 1:K:362:LEU:HB2  | 2.21                     | 0.41              |
| 1:K:406:PHE:CZ   | 1:K:408:TYR:HB3  | 2.56                     | 0.41              |
| 1:L:442:PRO:O    | 2:L:601:HEM:HMB3 | 2.20                     | 0.41              |
| 1:D:340:LEU:HD23 | 1:D:364:LEU:HB3  | 2.02                     | 0.41              |
| 1:I:154:VAL:O    | 1:I:158:LEU:HB2  | 2.20                     | 0.41              |
| 1:J:119:TYR:CZ   | 1:J:123:ARG:HG3  | 2.55                     | 0.41              |
| 1:A:139:PHE:CZ   | 1:H:430:ASP:HA   | 2.56                     | 0.41              |
| 1:A:338:GLN:HG3  | 1:A:342:GLN:HE21 | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:380:LEU:HG   | 1:A:406:PHE:HE1  | 1.85                     | 0.41              |
| 1:C:325:MET:HE3  | 1:C:491:PRO:HG3  | 2.03                     | 0.41              |
| 1:G:317:ASP:HB3  | 1:G:488:ILE:HD13 | 2.02                     | 0.41              |
| 1:L:311:LEU:HD21 | 1:L:451:LEU:HD23 | 2.02                     | 0.41              |
| 1:B:338:GLN:HG3  | 1:B:342:GLN:HE21 | 1.86                     | 0.41              |
| 1:C:39:GLU:H     | 1:C:39:GLU:HG2   | 1.73                     | 0.41              |
| 1:F:107:HIS:HB3  | 1:F:134:GLY:HA2  | 2.03                     | 0.41              |
| 1:H:158:LEU:HD22 | 1:H:356:GLN:HA   | 2.01                     | 0.41              |
| 1:H:261:ASP:O    | 1:H:265:GLN:HB2  | 2.21                     | 0.41              |
| 2:J:601:HEM:C1B  | 3:J:602:QHC:H5   | 2.56                     | 0.41              |
| 1:L:338:GLN:HG3  | 1:L:342:GLN:HE21 | 1.86                     | 0.41              |
| 1:H:280:PHE:HB2  | 1:J:500:ARG:HH21 | 1.86                     | 0.40              |
| 3:B:602:QHC:H12  | 3:B:602:QHC:H2   | 2.03                     | 0.40              |
| 1:C:340:LEU:HD23 | 1:C:364:LEU:HB3  | 2.02                     | 0.40              |
| 1:H:154:VAL:O    | 1:H:158:LEU:HB2  | 2.20                     | 0.40              |
| 1:I:340:LEU:HD23 | 1:I:364:LEU:HB3  | 2.03                     | 0.40              |
| 1:L:116:TRP:CE3  | 1:L:131:LEU:HD21 | 2.55                     | 0.40              |
| 1:L:325:MET:HE3  | 1:L:491:PRO:HG3  | 2.04                     | 0.40              |
| 1:A:340:LEU:HD23 | 1:A:364:LEU:HB3  | 2.02                     | 0.40              |
| 1:A:428:TRP:CZ3  | 1:A:440:HIS:HB2  | 2.56                     | 0.40              |
| 1:J:443:PHE:CG   | 1:J:453:ARG:HG3  | 2.57                     | 0.40              |
| 1:K:318:THR:O    | 2:K:601:HEM:HAB  | 2.22                     | 0.40              |
| 1:B:101:GLN:O    | 1:B:104:ASP:HB2  | 2.22                     | 0.40              |
| 1:B:443:PHE:C    | 2:B:601:HEM:HMA3 | 2.46                     | 0.40              |
| 1:G:338:GLN:HG3  | 1:G:342:GLN:HE21 | 1.87                     | 0.40              |
| 1:H:119:TYR:CZ   | 1:H:123:ARG:HG3  | 2.57                     | 0.40              |
| 1:K:130:PHE:CD1  | 3:K:602:QHC:H2   | 2.56                     | 0.40              |
| 1:L:332:ARG:HH21 | 1:L:332:ARG:HB3  | 1.87                     | 0.40              |
| 1:F:407:LEU:HD13 | 3:F:602:QHC:H15  | 2.02                     | 0.40              |
| 1:G:166:ARG:HH22 | 1:G:352:SER:HA   | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 461/489 (94%)   | 447 (97%)  | 13 (3%)  | 1 (0%)   | 43          | 73 |
| 1   | B     | 461/489 (94%)   | 446 (97%)  | 14 (3%)  | 1 (0%)   | 43          | 73 |
| 1   | C     | 461/489 (94%)   | 448 (97%)  | 11 (2%)  | 2 (0%)   | 30          | 62 |
| 1   | D     | 461/489 (94%)   | 441 (96%)  | 18 (4%)  | 2 (0%)   | 30          | 62 |
| 1   | E     | 453/489 (93%)   | 440 (97%)  | 12 (3%)  | 1 (0%)   | 43          | 73 |
| 1   | F     | 458/489 (94%)   | 441 (96%)  | 15 (3%)  | 2 (0%)   | 30          | 62 |
| 1   | G     | 461/489 (94%)   | 440 (95%)  | 16 (4%)  | 5 (1%)   | 11          | 43 |
| 1   | H     | 461/489 (94%)   | 440 (95%)  | 17 (4%)  | 4 (1%)   | 14          | 47 |
| 1   | I     | 452/489 (92%)   | 433 (96%)  | 16 (4%)  | 3 (1%)   | 18          | 52 |
| 1   | J     | 457/489 (94%)   | 433 (95%)  | 17 (4%)  | 7 (2%)   | 8           | 37 |
| 1   | K     | 455/489 (93%)   | 437 (96%)  | 15 (3%)  | 3 (1%)   | 18          | 52 |
| 1   | L     | 458/489 (94%)   | 436 (95%)  | 18 (4%)  | 4 (1%)   | 14          | 47 |
| All | All   | 5499/5868 (94%) | 5282 (96%) | 182 (3%) | 35 (1%)  | 21          | 56 |

All (35) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 59  | GLN  |
| 1   | G     | 242 | ARG  |
| 1   | J     | 105 | SER  |
| 1   | L     | 57  | ARG  |
| 1   | F     | 489 | LEU  |
| 1   | G     | 57  | ARG  |
| 1   | J     | 103 | VAL  |
| 1   | J     | 104 | ASP  |
| 1   | L     | 48  | ARG  |
| 1   | A     | 450 | CYS  |
| 1   | B     | 450 | CYS  |
| 1   | E     | 450 | CYS  |
| 1   | H     | 57  | ARG  |
| 1   | H     | 450 | CYS  |
| 1   | I     | 450 | CYS  |
| 1   | J     | 450 | CYS  |
| 1   | L     | 82  | ASN  |
| 1   | C     | 450 | CYS  |
| 1   | D     | 450 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 450 | CYS  |
| 1   | G     | 489 | LEU  |
| 1   | H     | 489 | LEU  |
| 1   | J     | 243 | SER  |
| 1   | K     | 450 | CYS  |
| 1   | L     | 450 | CYS  |
| 1   | F     | 450 | CYS  |
| 1   | H     | 243 | SER  |
| 1   | J     | 242 | ARG  |
| 1   | K     | 441 | VAL  |
| 1   | C     | 316 | VAL  |
| 1   | G     | 85  | GLY  |
| 1   | I     | 105 | SER  |
| 1   | J     | 57  | ARG  |
| 1   | K     | 103 | VAL  |
| 1   | I     | 240 | MET  |

### 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     | 410/426 (96%) | 375 (92%) | 35 (8%)  | 10          | 37 |
| 1   | B     | 410/426 (96%) | 379 (92%) | 31 (8%)  | 12          | 42 |
| 1   | C     | 410/426 (96%) | 376 (92%) | 34 (8%)  | 10          | 38 |
| 1   | D     | 410/426 (96%) | 375 (92%) | 35 (8%)  | 10          | 37 |
| 1   | E     | 406/426 (95%) | 377 (93%) | 29 (7%)  | 13          | 44 |
| 1   | F     | 410/426 (96%) | 369 (90%) | 41 (10%) | 7           | 30 |
| 1   | G     | 410/426 (96%) | 376 (92%) | 34 (8%)  | 10          | 38 |
| 1   | H     | 410/426 (96%) | 372 (91%) | 38 (9%)  | 8           | 33 |
| 1   | I     | 405/426 (95%) | 368 (91%) | 37 (9%)  | 9           | 34 |
| 1   | J     | 409/426 (96%) | 361 (88%) | 48 (12%) | 5           | 23 |
| 1   | K     | 407/426 (96%) | 368 (90%) | 39 (10%) | 8           | 32 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | L     | 407/426 (96%)   | 377 (93%)  | 30 (7%)  | 13          | 43 |
| All | All   | 4904/5112 (96%) | 4473 (91%) | 431 (9%) | 9           | 35 |

All (431) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 39  | GLU  |
| 1   | A     | 47  | ASN  |
| 1   | A     | 51  | ARG  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 104 | ASP  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 111 | MET  |
| 1   | A     | 114 | GLU  |
| 1   | A     | 152 | LYS  |
| 1   | A     | 158 | LEU  |
| 1   | A     | 178 | GLN  |
| 1   | A     | 181 | ARG  |
| 1   | A     | 183 | SER  |
| 1   | A     | 186 | LEU  |
| 1   | A     | 188 | VAL  |
| 1   | A     | 238 | MET  |
| 1   | A     | 242 | ARG  |
| 1   | A     | 251 | LYS  |
| 1   | A     | 271 | ILE  |
| 1   | A     | 284 | GLN  |
| 1   | A     | 324 | LEU  |
| 1   | A     | 332 | ARG  |
| 1   | A     | 356 | GLN  |
| 1   | A     | 393 | GLN  |
| 1   | A     | 413 | ASN  |
| 1   | A     | 416 | LEU  |
| 1   | A     | 421 | GLU  |
| 1   | A     | 426 | GLN  |
| 1   | A     | 437 | ASN  |
| 1   | A     | 439 | HIS  |
| 1   | A     | 461 | LEU  |
| 1   | A     | 473 | VAL  |
| 1   | A     | 482 | LYS  |
| 1   | A     | 488 | ILE  |
| 1   | A     | 493 | THR  |
| 1   | B     | 39  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 48  | ARG  |
| 1   | B     | 58  | GLU  |
| 1   | B     | 101 | GLN  |
| 1   | B     | 104 | ASP  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 112 | ILE  |
| 1   | B     | 114 | GLU  |
| 1   | B     | 139 | PHE  |
| 1   | B     | 156 | ARG  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 174 | LYS  |
| 1   | B     | 188 | VAL  |
| 1   | B     | 238 | MET  |
| 1   | B     | 242 | ARG  |
| 1   | B     | 246 | ARG  |
| 1   | B     | 271 | ILE  |
| 1   | B     | 299 | LEU  |
| 1   | B     | 324 | LEU  |
| 1   | B     | 332 | ARG  |
| 1   | B     | 356 | GLN  |
| 1   | B     | 393 | GLN  |
| 1   | B     | 416 | LEU  |
| 1   | B     | 421 | GLU  |
| 1   | B     | 426 | GLN  |
| 1   | B     | 454 | ARG  |
| 1   | B     | 461 | LEU  |
| 1   | B     | 488 | ILE  |
| 1   | B     | 493 | THR  |
| 1   | B     | 496 | LEU  |
| 1   | B     | 503 | ASN  |
| 1   | C     | 39  | GLU  |
| 1   | C     | 57  | ARG  |
| 1   | C     | 61  | TYR  |
| 1   | C     | 101 | GLN  |
| 1   | C     | 104 | ASP  |
| 1   | C     | 106 | LEU  |
| 1   | C     | 112 | ILE  |
| 1   | C     | 114 | GLU  |
| 1   | C     | 126 | LYS  |
| 1   | C     | 139 | PHE  |
| 1   | C     | 145 | ASN  |
| 1   | C     | 158 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 188 | VAL  |
| 1   | C     | 191 | SER  |
| 1   | C     | 221 | LEU  |
| 1   | C     | 238 | MET  |
| 1   | C     | 242 | ARG  |
| 1   | C     | 271 | ILE  |
| 1   | C     | 284 | GLN  |
| 1   | C     | 302 | GLU  |
| 1   | C     | 323 | LEU  |
| 1   | C     | 324 | LEU  |
| 1   | C     | 356 | GLN  |
| 1   | C     | 380 | LEU  |
| 1   | C     | 393 | GLN  |
| 1   | C     | 394 | ASN  |
| 1   | C     | 412 | ARG  |
| 1   | C     | 419 | ARG  |
| 1   | C     | 421 | GLU  |
| 1   | C     | 426 | GLN  |
| 1   | C     | 438 | PHE  |
| 1   | C     | 482 | LYS  |
| 1   | C     | 488 | ILE  |
| 1   | C     | 493 | THR  |
| 1   | D     | 39  | GLU  |
| 1   | D     | 83  | LEU  |
| 1   | D     | 100 | LEU  |
| 1   | D     | 101 | GLN  |
| 1   | D     | 104 | ASP  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 111 | MET  |
| 1   | D     | 113 | LEU  |
| 1   | D     | 114 | GLU  |
| 1   | D     | 158 | LEU  |
| 1   | D     | 170 | GLN  |
| 1   | D     | 186 | LEU  |
| 1   | D     | 188 | VAL  |
| 1   | D     | 238 | MET  |
| 1   | D     | 271 | ILE  |
| 1   | D     | 302 | GLU  |
| 1   | D     | 324 | LEU  |
| 1   | D     | 332 | ARG  |
| 1   | D     | 339 | ILE  |
| 1   | D     | 356 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 393 | GLN  |
| 1   | D     | 404 | GLN  |
| 1   | D     | 419 | ARG  |
| 1   | D     | 421 | GLU  |
| 1   | D     | 426 | GLN  |
| 1   | D     | 431 | ILE  |
| 1   | D     | 439 | HIS  |
| 1   | D     | 461 | LEU  |
| 1   | D     | 482 | LYS  |
| 1   | D     | 488 | ILE  |
| 1   | D     | 489 | LEU  |
| 1   | D     | 490 | ARG  |
| 1   | D     | 493 | THR  |
| 1   | D     | 496 | LEU  |
| 1   | D     | 503 | ASN  |
| 1   | E     | 39  | GLU  |
| 1   | E     | 47  | ASN  |
| 1   | E     | 61  | TYR  |
| 1   | E     | 64  | LEU  |
| 1   | E     | 101 | GLN  |
| 1   | E     | 104 | ASP  |
| 1   | E     | 112 | ILE  |
| 1   | E     | 114 | GLU  |
| 1   | E     | 156 | ARG  |
| 1   | E     | 158 | LEU  |
| 1   | E     | 186 | LEU  |
| 1   | E     | 188 | VAL  |
| 1   | E     | 238 | MET  |
| 1   | E     | 271 | ILE  |
| 1   | E     | 302 | GLU  |
| 1   | E     | 324 | LEU  |
| 1   | E     | 332 | ARG  |
| 1   | E     | 356 | GLN  |
| 1   | E     | 360 | THR  |
| 1   | E     | 393 | GLN  |
| 1   | E     | 416 | LEU  |
| 1   | E     | 419 | ARG  |
| 1   | E     | 421 | GLU  |
| 1   | E     | 422 | ARG  |
| 1   | E     | 461 | LEU  |
| 1   | E     | 482 | LYS  |
| 1   | E     | 489 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 493 | THR  |
| 1   | E     | 496 | LEU  |
| 1   | F     | 47  | ASN  |
| 1   | F     | 50  | LEU  |
| 1   | F     | 52  | LEU  |
| 1   | F     | 61  | TYR  |
| 1   | F     | 73  | GLN  |
| 1   | F     | 74  | GLU  |
| 1   | F     | 101 | GLN  |
| 1   | F     | 104 | ASP  |
| 1   | F     | 112 | ILE  |
| 1   | F     | 113 | LEU  |
| 1   | F     | 114 | GLU  |
| 1   | F     | 125 | HIS  |
| 1   | F     | 158 | LEU  |
| 1   | F     | 186 | LEU  |
| 1   | F     | 188 | VAL  |
| 1   | F     | 196 | THR  |
| 1   | F     | 238 | MET  |
| 1   | F     | 244 | LEU  |
| 1   | F     | 248 | ILE  |
| 1   | F     | 271 | ILE  |
| 1   | F     | 284 | GLN  |
| 1   | F     | 302 | GLU  |
| 1   | F     | 310 | GLU  |
| 1   | F     | 324 | LEU  |
| 1   | F     | 332 | ARG  |
| 1   | F     | 356 | GLN  |
| 1   | F     | 387 | SER  |
| 1   | F     | 393 | GLN  |
| 1   | F     | 416 | LEU  |
| 1   | F     | 421 | GLU  |
| 1   | F     | 422 | ARG  |
| 1   | F     | 426 | GLN  |
| 1   | F     | 461 | LEU  |
| 1   | F     | 473 | VAL  |
| 1   | F     | 477 | THR  |
| 1   | F     | 479 | GLU  |
| 1   | F     | 482 | LYS  |
| 1   | F     | 488 | ILE  |
| 1   | F     | 489 | LEU  |
| 1   | F     | 493 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 496 | LEU  |
| 1   | G     | 35  | VAL  |
| 1   | G     | 39  | GLU  |
| 1   | G     | 50  | LEU  |
| 1   | G     | 53  | LEU  |
| 1   | G     | 56  | TRP  |
| 1   | G     | 57  | ARG  |
| 1   | G     | 98  | GLU  |
| 1   | G     | 101 | GLN  |
| 1   | G     | 104 | ASP  |
| 1   | G     | 106 | LEU  |
| 1   | G     | 126 | LYS  |
| 1   | G     | 131 | LEU  |
| 1   | G     | 158 | LEU  |
| 1   | G     | 188 | VAL  |
| 1   | G     | 207 | GLU  |
| 1   | G     | 244 | LEU  |
| 1   | G     | 268 | ASP  |
| 1   | G     | 271 | ILE  |
| 1   | G     | 324 | LEU  |
| 1   | G     | 332 | ARG  |
| 1   | G     | 356 | GLN  |
| 1   | G     | 359 | THR  |
| 1   | G     | 392 | LEU  |
| 1   | G     | 393 | GLN  |
| 1   | G     | 409 | SER  |
| 1   | G     | 416 | LEU  |
| 1   | G     | 421 | GLU  |
| 1   | G     | 422 | ARG  |
| 1   | G     | 438 | PHE  |
| 1   | G     | 448 | ARG  |
| 1   | G     | 461 | LEU  |
| 1   | G     | 486 | SER  |
| 1   | G     | 488 | ILE  |
| 1   | G     | 496 | LEU  |
| 1   | H     | 39  | GLU  |
| 1   | H     | 47  | ASN  |
| 1   | H     | 50  | LEU  |
| 1   | H     | 55  | ILE  |
| 1   | H     | 58  | GLU  |
| 1   | H     | 61  | TYR  |
| 1   | H     | 83  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 92  | MET  |
| 1   | H     | 101 | GLN  |
| 1   | H     | 104 | ASP  |
| 1   | H     | 106 | LEU  |
| 1   | H     | 114 | GLU  |
| 1   | H     | 158 | LEU  |
| 1   | H     | 188 | VAL  |
| 1   | H     | 240 | MET  |
| 1   | H     | 242 | ARG  |
| 1   | H     | 243 | SER  |
| 1   | H     | 244 | LEU  |
| 1   | H     | 246 | ARG  |
| 1   | H     | 251 | LYS  |
| 1   | H     | 271 | ILE  |
| 1   | H     | 302 | GLU  |
| 1   | H     | 324 | LEU  |
| 1   | H     | 332 | ARG  |
| 1   | H     | 381 | PHE  |
| 1   | H     | 383 | GLU  |
| 1   | H     | 393 | GLN  |
| 1   | H     | 416 | LEU  |
| 1   | H     | 421 | GLU  |
| 1   | H     | 426 | GLN  |
| 1   | H     | 427 | ARG  |
| 1   | H     | 431 | ILE  |
| 1   | H     | 437 | ASN  |
| 1   | H     | 461 | LEU  |
| 1   | H     | 482 | LYS  |
| 1   | H     | 488 | ILE  |
| 1   | H     | 493 | THR  |
| 1   | H     | 496 | LEU  |
| 1   | I     | 39  | GLU  |
| 1   | I     | 43  | GLN  |
| 1   | I     | 48  | ARG  |
| 1   | I     | 49  | TRP  |
| 1   | I     | 50  | LEU  |
| 1   | I     | 52  | LEU  |
| 1   | I     | 53  | LEU  |
| 1   | I     | 56  | TRP  |
| 1   | I     | 61  | TYR  |
| 1   | I     | 81  | TYR  |
| 1   | I     | 99  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 101 | GLN  |
| 1   | I     | 112 | ILE  |
| 1   | I     | 114 | GLU  |
| 1   | I     | 127 | CYS  |
| 1   | I     | 158 | LEU  |
| 1   | I     | 188 | VAL  |
| 1   | I     | 240 | MET  |
| 1   | I     | 242 | ARG  |
| 1   | I     | 244 | LEU  |
| 1   | I     | 248 | ILE  |
| 1   | I     | 251 | LYS  |
| 1   | I     | 271 | ILE  |
| 1   | I     | 324 | LEU  |
| 1   | I     | 332 | ARG  |
| 1   | I     | 356 | GLN  |
| 1   | I     | 393 | GLN  |
| 1   | I     | 416 | LEU  |
| 1   | I     | 419 | ARG  |
| 1   | I     | 426 | GLN  |
| 1   | I     | 441 | VAL  |
| 1   | I     | 461 | LEU  |
| 1   | I     | 469 | LYS  |
| 1   | I     | 482 | LYS  |
| 1   | I     | 493 | THR  |
| 1   | I     | 496 | LEU  |
| 1   | I     | 503 | ASN  |
| 1   | J     | 35  | VAL  |
| 1   | J     | 39  | GLU  |
| 1   | J     | 51  | ARG  |
| 1   | J     | 52  | LEU  |
| 1   | J     | 53  | LEU  |
| 1   | J     | 54  | GLN  |
| 1   | J     | 56  | TRP  |
| 1   | J     | 59  | GLN  |
| 1   | J     | 61  | TYR  |
| 1   | J     | 66  | LEU  |
| 1   | J     | 104 | ASP  |
| 1   | J     | 112 | ILE  |
| 1   | J     | 113 | LEU  |
| 1   | J     | 152 | LYS  |
| 1   | J     | 158 | LEU  |
| 1   | J     | 170 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 186 | LEU  |
| 1   | J     | 188 | VAL  |
| 1   | J     | 201 | ASN  |
| 1   | J     | 211 | LEU  |
| 1   | J     | 235 | VAL  |
| 1   | J     | 237 | LEU  |
| 1   | J     | 240 | MET  |
| 1   | J     | 244 | LEU  |
| 1   | J     | 247 | TRP  |
| 1   | J     | 248 | ILE  |
| 1   | J     | 271 | ILE  |
| 1   | J     | 284 | GLN  |
| 1   | J     | 324 | LEU  |
| 1   | J     | 332 | ARG  |
| 1   | J     | 356 | GLN  |
| 1   | J     | 382 | LEU  |
| 1   | J     | 387 | SER  |
| 1   | J     | 393 | GLN  |
| 1   | J     | 402 | LEU  |
| 1   | J     | 407 | LEU  |
| 1   | J     | 416 | LEU  |
| 1   | J     | 419 | ARG  |
| 1   | J     | 421 | GLU  |
| 1   | J     | 422 | ARG  |
| 1   | J     | 429 | LEU  |
| 1   | J     | 431 | ILE  |
| 1   | J     | 438 | PHE  |
| 1   | J     | 461 | LEU  |
| 1   | J     | 480 | ASP  |
| 1   | J     | 488 | ILE  |
| 1   | J     | 493 | THR  |
| 1   | J     | 496 | LEU  |
| 1   | K     | 39  | GLU  |
| 1   | K     | 54  | GLN  |
| 1   | K     | 55  | ILE  |
| 1   | K     | 57  | ARG  |
| 1   | K     | 58  | GLU  |
| 1   | K     | 61  | TYR  |
| 1   | K     | 66  | LEU  |
| 1   | K     | 81  | TYR  |
| 1   | K     | 83  | LEU  |
| 1   | K     | 104 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 112 | ILE  |
| 1   | K     | 114 | GLU  |
| 1   | K     | 126 | LYS  |
| 1   | K     | 156 | ARG  |
| 1   | K     | 158 | LEU  |
| 1   | K     | 188 | VAL  |
| 1   | K     | 238 | MET  |
| 1   | K     | 242 | ARG  |
| 1   | K     | 244 | LEU  |
| 1   | K     | 271 | ILE  |
| 1   | K     | 302 | GLU  |
| 1   | K     | 324 | LEU  |
| 1   | K     | 332 | ARG  |
| 1   | K     | 350 | SER  |
| 1   | K     | 356 | GLN  |
| 1   | K     | 365 | LEU  |
| 1   | K     | 393 | GLN  |
| 1   | K     | 394 | ASN  |
| 1   | K     | 421 | GLU  |
| 1   | K     | 426 | GLN  |
| 1   | K     | 447 | MET  |
| 1   | K     | 461 | LEU  |
| 1   | K     | 469 | LYS  |
| 1   | K     | 481 | ILE  |
| 1   | K     | 482 | LYS  |
| 1   | K     | 488 | ILE  |
| 1   | K     | 490 | ARG  |
| 1   | K     | 493 | THR  |
| 1   | K     | 496 | LEU  |
| 1   | L     | 39  | GLU  |
| 1   | L     | 50  | LEU  |
| 1   | L     | 51  | ARG  |
| 1   | L     | 56  | TRP  |
| 1   | L     | 61  | TYR  |
| 1   | L     | 70  | GLN  |
| 1   | L     | 73  | GLN  |
| 1   | L     | 83  | LEU  |
| 1   | L     | 106 | LEU  |
| 1   | L     | 112 | ILE  |
| 1   | L     | 114 | GLU  |
| 1   | L     | 158 | LEU  |
| 1   | L     | 188 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 238 | MET  |
| 1   | L     | 247 | TRP  |
| 1   | L     | 271 | ILE  |
| 1   | L     | 284 | GLN  |
| 1   | L     | 324 | LEU  |
| 1   | L     | 332 | ARG  |
| 1   | L     | 356 | GLN  |
| 1   | L     | 387 | SER  |
| 1   | L     | 393 | GLN  |
| 1   | L     | 416 | LEU  |
| 1   | L     | 419 | ARG  |
| 1   | L     | 421 | GLU  |
| 1   | L     | 426 | GLN  |
| 1   | L     | 431 | ILE  |
| 1   | L     | 482 | LYS  |
| 1   | L     | 493 | THR  |
| 1   | L     | 496 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | ASN  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 125 | HIS  |
| 1   | A     | 155 | GLN  |
| 1   | A     | 189 | GLN  |
| 1   | A     | 236 | GLN  |
| 1   | A     | 338 | GLN  |
| 1   | A     | 342 | GLN  |
| 1   | A     | 393 | GLN  |
| 1   | A     | 440 | HIS  |
| 1   | A     | 449 | GLN  |
| 1   | B     | 47  | ASN  |
| 1   | B     | 82  | ASN  |
| 1   | B     | 107 | HIS  |
| 1   | B     | 125 | HIS  |
| 1   | B     | 338 | GLN  |
| 1   | B     | 342 | GLN  |
| 1   | B     | 393 | GLN  |
| 1   | B     | 439 | HIS  |
| 1   | B     | 440 | HIS  |
| 1   | C     | 44  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 47  | ASN  |
| 1   | C     | 73  | GLN  |
| 1   | C     | 107 | HIS  |
| 1   | C     | 125 | HIS  |
| 1   | C     | 155 | GLN  |
| 1   | C     | 189 | GLN  |
| 1   | C     | 222 | ASN  |
| 1   | C     | 338 | GLN  |
| 1   | C     | 342 | GLN  |
| 1   | C     | 393 | GLN  |
| 1   | C     | 404 | GLN  |
| 1   | C     | 440 | HIS  |
| 1   | C     | 449 | GLN  |
| 1   | D     | 101 | GLN  |
| 1   | D     | 125 | HIS  |
| 1   | D     | 155 | GLN  |
| 1   | D     | 178 | GLN  |
| 1   | D     | 236 | GLN  |
| 1   | D     | 338 | GLN  |
| 1   | D     | 342 | GLN  |
| 1   | D     | 393 | GLN  |
| 1   | D     | 404 | GLN  |
| 1   | E     | 47  | ASN  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 178 | GLN  |
| 1   | E     | 338 | GLN  |
| 1   | E     | 393 | GLN  |
| 1   | E     | 440 | HIS  |
| 1   | F     | 125 | HIS  |
| 1   | F     | 155 | GLN  |
| 1   | F     | 178 | GLN  |
| 1   | F     | 236 | GLN  |
| 1   | F     | 338 | GLN  |
| 1   | F     | 393 | GLN  |
| 1   | F     | 394 | ASN  |
| 1   | F     | 437 | ASN  |
| 1   | F     | 449 | GLN  |
| 1   | F     | 478 | GLN  |
| 1   | G     | 59  | GLN  |
| 1   | G     | 63  | HIS  |
| 1   | G     | 125 | HIS  |
| 1   | G     | 338 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 342 | GLN  |
| 1   | G     | 393 | GLN  |
| 1   | G     | 413 | ASN  |
| 1   | G     | 424 | ASN  |
| 1   | G     | 439 | HIS  |
| 1   | G     | 440 | HIS  |
| 1   | G     | 503 | ASN  |
| 1   | H     | 44  | HIS  |
| 1   | H     | 54  | GLN  |
| 1   | H     | 102 | GLN  |
| 1   | H     | 125 | HIS  |
| 1   | H     | 178 | GLN  |
| 1   | H     | 214 | HIS  |
| 1   | H     | 236 | GLN  |
| 1   | H     | 338 | GLN  |
| 1   | H     | 342 | GLN  |
| 1   | H     | 393 | GLN  |
| 1   | H     | 394 | ASN  |
| 1   | H     | 424 | ASN  |
| 1   | H     | 439 | HIS  |
| 1   | I     | 43  | GLN  |
| 1   | I     | 73  | GLN  |
| 1   | I     | 125 | HIS  |
| 1   | I     | 155 | GLN  |
| 1   | I     | 178 | GLN  |
| 1   | I     | 284 | GLN  |
| 1   | I     | 338 | GLN  |
| 1   | I     | 342 | GLN  |
| 1   | I     | 393 | GLN  |
| 1   | I     | 413 | ASN  |
| 1   | I     | 449 | GLN  |
| 1   | J     | 43  | GLN  |
| 1   | J     | 59  | GLN  |
| 1   | J     | 125 | HIS  |
| 1   | J     | 155 | GLN  |
| 1   | J     | 284 | GLN  |
| 1   | J     | 338 | GLN  |
| 1   | J     | 342 | GLN  |
| 1   | J     | 393 | GLN  |
| 1   | J     | 396 | HIS  |
| 1   | J     | 426 | GLN  |
| 1   | J     | 437 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 440 | HIS  |
| 1   | J     | 503 | ASN  |
| 1   | K     | 44  | HIS  |
| 1   | K     | 54  | GLN  |
| 1   | K     | 82  | ASN  |
| 1   | K     | 155 | GLN  |
| 1   | K     | 178 | GLN  |
| 1   | K     | 189 | GLN  |
| 1   | K     | 236 | GLN  |
| 1   | K     | 338 | GLN  |
| 1   | K     | 354 | HIS  |
| 1   | K     | 437 | ASN  |
| 1   | K     | 465 | HIS  |
| 1   | K     | 503 | ASN  |
| 1   | L     | 43  | GLN  |
| 1   | L     | 47  | ASN  |
| 1   | L     | 121 | GLN  |
| 1   | L     | 125 | HIS  |
| 1   | L     | 155 | GLN  |
| 1   | L     | 178 | GLN  |
| 1   | L     | 189 | GLN  |
| 1   | L     | 284 | GLN  |
| 1   | L     | 338 | GLN  |
| 1   | L     | 342 | GLN  |
| 1   | L     | 393 | GLN  |

### 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

22 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | HEM  | D     | 601 | 3,1  | 50,50,50     | 1.40 | 8 (16%)     | 67,82,82    | 1.46 | 12 (17%)    |
| 2   | HEM  | I     | 601 | 3,1  | 50,50,50     | 1.36 | 6 (12%)     | 67,82,82    | 1.59 | 15 (22%)    |
| 3   | QHC  | K     | 602 | 2    | 25,25,25     | 0.76 | 0           | 31,35,35    | 1.40 | 4 (12%)     |
| 3   | QHC  | L     | 602 | 2    | 25,25,25     | 0.74 | 0           | 31,35,35    | 1.47 | 7 (22%)     |
| 2   | HEM  | E     | 601 | 3,1  | 50,50,50     | 1.69 | 9 (18%)     | 67,82,82    | 1.57 | 14 (20%)    |
| 3   | QHC  | E     | 602 | 2    | 25,25,25     | 0.80 | 0           | 31,35,35    | 1.81 | 10 (32%)    |
| 2   | HEM  | J     | 601 | 3    | 50,50,50     | 1.34 | 6 (12%)     | 67,82,82    | 1.56 | 15 (22%)    |
| 2   | HEM  | K     | 601 | 3,1  | 50,50,50     | 1.38 | 7 (14%)     | 67,82,82    | 1.44 | 10 (14%)    |
| 2   | HEM  | A     | 601 | 3,1  | 50,50,50     | 1.36 | 7 (14%)     | 67,82,82    | 1.45 | 9 (13%)     |
| 2   | HEM  | H     | 601 | -    | 50,50,50     | 1.29 | 6 (12%)     | 67,82,82    | 1.65 | 18 (26%)    |
| 3   | QHC  | C     | 602 | 2    | 25,25,25     | 0.78 | 0           | 31,35,35    | 1.47 | 5 (16%)     |
| 3   | QHC  | B     | 602 | 2    | 25,25,25     | 1.01 | 1 (4%)      | 31,35,35    | 1.67 | 6 (19%)     |
| 3   | QHC  | A     | 602 | 2    | 25,25,25     | 0.73 | 0           | 31,35,35    | 1.81 | 11 (35%)    |
| 3   | QHC  | J     | 602 | 2    | 25,25,25     | 0.84 | 1 (4%)      | 31,35,35    | 1.83 | 7 (22%)     |
| 3   | QHC  | F     | 602 | 2    | 25,25,25     | 0.82 | 0           | 31,35,35    | 2.23 | 8 (25%)     |
| 2   | HEM  | L     | 601 | 3,1  | 50,50,50     | 1.23 | 5 (10%)     | 67,82,82    | 1.60 | 14 (20%)    |
| 2   | HEM  | C     | 601 | 3,1  | 50,50,50     | 1.53 | 10 (20%)    | 67,82,82    | 1.49 | 10 (14%)    |
| 3   | QHC  | I     | 602 | 2    | 25,25,25     | 0.93 | 1 (4%)      | 31,35,35    | 1.57 | 5 (16%)     |
| 3   | QHC  | D     | 602 | 2    | 25,25,25     | 0.86 | 1 (4%)      | 31,35,35    | 1.85 | 7 (22%)     |
| 2   | HEM  | G     | 601 | -    | 50,50,50     | 1.40 | 8 (16%)     | 67,82,82    | 1.65 | 15 (22%)    |
| 2   | HEM  | F     | 601 | 3,1  | 50,50,50     | 1.43 | 10 (20%)    | 67,82,82    | 1.22 | 7 (10%)     |
| 2   | HEM  | B     | 601 | 3,1  | 50,50,50     | 1.32 | 6 (12%)     | 67,82,82    | 1.30 | 9 (13%)     |

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   | HEM  | D     | 601 | 3,1  | -       | 2/14/54/54 | -       |
| 2   | HEM  | I     | 601 | 3,1  | -       | 5/14/54/54 | -       |
| 3   | QHC  | K     | 602 | 2    | -       | 2/10/20/20 | 0/3/3/3 |
| 3   | QHC  | L     | 602 | 2    | -       | 2/10/20/20 | 0/3/3/3 |
| 2   | HEM  | E     | 601 | 3,1  | -       | 6/14/54/54 | -       |
| 3   | QHC  | E     | 602 | 2    | -       | 2/10/20/20 | 0/3/3/3 |
| 2   | HEM  | J     | 601 | 3    | -       | 3/14/54/54 | -       |
| 2   | HEM  | K     | 601 | 3,1  | -       | 4/14/54/54 | -       |
| 2   | HEM  | A     | 601 | 3,1  | -       | 6/14/54/54 | -       |
| 2   | HEM  | H     | 601 | -    | -       | 4/14/54/54 | -       |
| 3   | QHC  | C     | 602 | 2    | -       | 1/10/20/20 | 0/3/3/3 |
| 3   | QHC  | B     | 602 | 2    | -       | 3/10/20/20 | 0/3/3/3 |
| 3   | QHC  | A     | 602 | 2    | -       | 2/10/20/20 | 0/3/3/3 |
| 3   | QHC  | J     | 602 | 2    | -       | 1/10/20/20 | 0/3/3/3 |
| 3   | QHC  | F     | 602 | 2    | -       | 1/10/20/20 | 0/3/3/3 |
| 2   | HEM  | L     | 601 | 3,1  | -       | 9/14/54/54 | -       |
| 2   | HEM  | C     | 601 | 3,1  | -       | 5/14/54/54 | -       |
| 3   | QHC  | I     | 602 | 2    | -       | 2/10/20/20 | 0/3/3/3 |
| 3   | QHC  | D     | 602 | 2    | -       | 1/10/20/20 | 0/3/3/3 |
| 2   | HEM  | G     | 601 | -    | -       | 2/14/54/54 | -       |
| 2   | HEM  | F     | 601 | 3,1  | -       | 5/14/54/54 | -       |
| 2   | HEM  | B     | 601 | 3,1  | -       | 7/14/54/54 | -       |

All (92) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 601 | HEM  | C4D-ND  | -5.33 | 1.31        | 1.40     |
| 2   | I     | 601 | HEM  | C3B-C4B | 4.34  | 1.53        | 1.44     |
| 2   | E     | 601 | HEM  | C1B-NB  | -4.31 | 1.32        | 1.40     |
| 2   | D     | 601 | HEM  | C1D-C2D | 4.27  | 1.53        | 1.44     |
| 2   | A     | 601 | HEM  | C1D-C2D | 4.00  | 1.52        | 1.44     |
| 2   | C     | 601 | HEM  | C3B-C4B | 3.99  | 1.52        | 1.44     |
| 2   | F     | 601 | HEM  | C1C-C2C | -3.74 | 1.37        | 1.45     |
| 2   | J     | 601 | HEM  | C1D-C2D | 3.72  | 1.52        | 1.44     |
| 2   | B     | 601 | HEM  | C1D-C2D | 3.58  | 1.51        | 1.44     |
| 2   | C     | 601 | HEM  | C1B-NB  | -3.45 | 1.34        | 1.40     |
| 2   | L     | 601 | HEM  | C4D-ND  | -3.33 | 1.34        | 1.40     |
| 2   | K     | 601 | HEM  | C1D-ND  | -3.31 | 1.32        | 1.38     |
| 2   | B     | 601 | HEM  | C4D-C3D | 3.25  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 601 | HEM  | C4D-ND  | -3.17 | 1.34        | 1.40     |
| 2   | A     | 601 | HEM  | C3B-C4B | 3.17  | 1.51        | 1.44     |
| 2   | J     | 601 | HEM  | C1B-NB  | -3.16 | 1.34        | 1.40     |
| 2   | E     | 601 | HEM  | C3B-C4B | 3.16  | 1.51        | 1.44     |
| 2   | K     | 601 | HEM  | C1B-NB  | -3.15 | 1.34        | 1.40     |
| 2   | C     | 601 | HEM  | C1D-C2D | 3.05  | 1.50        | 1.44     |
| 2   | K     | 601 | HEM  | C4D-ND  | -3.05 | 1.35        | 1.40     |
| 2   | F     | 601 | HEM  | C3C-C4C | -2.97 | 1.40        | 1.46     |
| 2   | G     | 601 | HEM  | C1B-NB  | -2.97 | 1.35        | 1.40     |
| 2   | B     | 601 | HEM  | C1B-NB  | -2.93 | 1.35        | 1.40     |
| 2   | E     | 601 | HEM  | C4B-NB  | -2.90 | 1.33        | 1.38     |
| 2   | D     | 601 | HEM  | C1B-NB  | -2.87 | 1.35        | 1.40     |
| 2   | B     | 601 | HEM  | C3B-C4B | 2.86  | 1.50        | 1.44     |
| 2   | G     | 601 | HEM  | C1D-C2D | 2.86  | 1.50        | 1.44     |
| 2   | I     | 601 | HEM  | C1D-C2D | 2.84  | 1.50        | 1.44     |
| 2   | H     | 601 | HEM  | C3B-C4B | 2.82  | 1.50        | 1.44     |
| 2   | F     | 601 | HEM  | C2A-C3A | -2.81 | 1.31        | 1.38     |
| 3   | B     | 602 | QHC  | C14-N23 | 2.79  | 1.50        | 1.46     |
| 2   | G     | 601 | HEM  | C4D-ND  | -2.78 | 1.35        | 1.40     |
| 2   | D     | 601 | HEM  | C4B-NB  | -2.76 | 1.33        | 1.38     |
| 2   | C     | 601 | HEM  | FE-NB   | 2.75  | 2.03        | 1.94     |
| 2   | H     | 601 | HEM  | C1D-ND  | -2.72 | 1.33        | 1.38     |
| 2   | A     | 601 | HEM  | C4D-ND  | -2.70 | 1.35        | 1.40     |
| 2   | C     | 601 | HEM  | C1D-ND  | -2.69 | 1.33        | 1.38     |
| 2   | G     | 601 | HEM  | CMB-C2B | 2.69  | 1.56        | 1.50     |
| 2   | E     | 601 | HEM  | C1D-C2D | 2.63  | 1.49        | 1.44     |
| 2   | F     | 601 | HEM  | C1D-ND  | -2.63 | 1.33        | 1.38     |
| 3   | J     | 602 | QHC  | C14-N23 | 2.58  | 1.49        | 1.46     |
| 2   | K     | 601 | HEM  | C1D-C2D | 2.56  | 1.49        | 1.44     |
| 2   | J     | 601 | HEM  | C4D-ND  | -2.56 | 1.35        | 1.40     |
| 2   | E     | 601 | HEM  | CHA-C1A | -2.54 | 1.33        | 1.39     |
| 2   | C     | 601 | HEM  | O2A-CGA | 2.53  | 1.39        | 1.30     |
| 2   | F     | 601 | HEM  | C1A-C2A | -2.51 | 1.39        | 1.44     |
| 2   | F     | 601 | HEM  | C4D-ND  | -2.50 | 1.35        | 1.40     |
| 2   | A     | 601 | HEM  | CMC-C2C | -2.49 | 1.45        | 1.50     |
| 2   | H     | 601 | HEM  | C1C-C2C | -2.49 | 1.40        | 1.45     |
| 2   | I     | 601 | HEM  | C3B-C2B | -2.48 | 1.32        | 1.37     |
| 2   | D     | 601 | HEM  | C4D-C3D | 2.47  | 1.49        | 1.45     |
| 2   | H     | 601 | HEM  | C1D-C2D | 2.45  | 1.49        | 1.44     |
| 2   | A     | 601 | HEM  | C2A-C3A | -2.44 | 1.32        | 1.38     |
| 2   | K     | 601 | HEM  | C3B-C2B | -2.43 | 1.32        | 1.37     |
| 2   | C     | 601 | HEM  | CBD-CGD | 2.43  | 1.56        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 601 | HEM  | C4D-C3D | 2.41  | 1.49        | 1.45     |
| 2   | D     | 601 | HEM  | C1C-C2C | -2.41 | 1.40        | 1.45     |
| 2   | L     | 601 | HEM  | C3C-C4C | -2.41 | 1.41        | 1.46     |
| 2   | L     | 601 | HEM  | C1B-NB  | -2.36 | 1.36        | 1.40     |
| 2   | D     | 601 | HEM  | CHA-C1A | -2.36 | 1.34        | 1.39     |
| 2   | E     | 601 | HEM  | O2A-CGA | 2.35  | 1.38        | 1.30     |
| 2   | I     | 601 | HEM  | C4B-NB  | -2.32 | 1.34        | 1.38     |
| 2   | F     | 601 | HEM  | CHA-C1A | -2.31 | 1.34        | 1.39     |
| 2   | L     | 601 | HEM  | C1C-C2C | -2.31 | 1.40        | 1.45     |
| 2   | F     | 601 | HEM  | C3B-C4B | 2.31  | 1.49        | 1.44     |
| 2   | E     | 601 | HEM  | C1A-NA  | -2.28 | 1.35        | 1.39     |
| 2   | D     | 601 | HEM  | C3B-C4B | 2.28  | 1.49        | 1.44     |
| 2   | G     | 601 | HEM  | CBA-CGA | 2.27  | 1.55        | 1.50     |
| 2   | C     | 601 | HEM  | CHA-C4D | -2.27 | 1.34        | 1.38     |
| 2   | J     | 601 | HEM  | C3D-C2D | -2.26 | 1.31        | 1.36     |
| 2   | H     | 601 | HEM  | CBA-CAA | 2.25  | 1.59        | 1.51     |
| 2   | I     | 601 | HEM  | C2A-C3A | -2.25 | 1.33        | 1.38     |
| 2   | A     | 601 | HEM  | C1B-C2B | -2.25 | 1.40        | 1.44     |
| 2   | K     | 601 | HEM  | CHA-C1A | -2.24 | 1.34        | 1.39     |
| 2   | D     | 601 | HEM  | C3B-C2B | -2.23 | 1.32        | 1.37     |
| 3   | I     | 602 | QHC  | C14-N23 | 2.20  | 1.49        | 1.46     |
| 2   | G     | 601 | HEM  | CHA-C1A | -2.18 | 1.34        | 1.39     |
| 2   | G     | 601 | HEM  | C3B-C4B | 2.18  | 1.49        | 1.44     |
| 3   | D     | 602 | QHC  | C8-C12  | 2.15  | 1.44        | 1.41     |
| 2   | A     | 601 | HEM  | C3B-C2B | -2.10 | 1.32        | 1.37     |
| 2   | G     | 601 | HEM  | C1D-ND  | -2.09 | 1.34        | 1.38     |
| 2   | I     | 601 | HEM  | C1D-ND  | -2.09 | 1.34        | 1.38     |
| 2   | H     | 601 | HEM  | C4D-ND  | -2.08 | 1.36        | 1.40     |
| 2   | F     | 601 | HEM  | C1D-C2D | 2.08  | 1.48        | 1.44     |
| 2   | B     | 601 | HEM  | C1C-C2C | -2.08 | 1.41        | 1.45     |
| 2   | C     | 601 | HEM  | CHB-C4A | -2.07 | 1.34        | 1.39     |
| 2   | B     | 601 | HEM  | FE-NB   | 2.07  | 2.01        | 1.94     |
| 2   | F     | 601 | HEM  | C1B-NB  | -2.06 | 1.36        | 1.40     |
| 2   | K     | 601 | HEM  | CHA-C4D | -2.04 | 1.34        | 1.38     |
| 2   | J     | 601 | HEM  | CBA-CGA | 2.03  | 1.55        | 1.50     |
| 2   | J     | 601 | HEM  | O2D-CGD | 2.02  | 1.37        | 1.30     |
| 2   | L     | 601 | HEM  | C2A-C3A | -2.00 | 1.33        | 1.38     |

All (218) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3   | F     | 602 | QHC  | C15-C14-N23 | 7.00 | 117.44      | 110.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | F     | 602 | QHC  | C14-N23-C18 | 6.20  | 132.69      | 123.44   |
| 3   | I     | 602 | QHC  | C14-N23-C18 | 5.70  | 131.94      | 123.44   |
| 3   | B     | 602 | QHC  | C14-N23-C18 | 5.38  | 131.47      | 123.44   |
| 2   | C     | 601 | HEM  | C2B-C1B-NB  | 5.23  | 115.85      | 109.84   |
| 3   | J     | 602 | QHC  | C14-N23-C18 | 5.10  | 131.06      | 123.44   |
| 3   | D     | 602 | QHC  | C13-C14-N23 | 4.89  | 117.71      | 110.22   |
| 3   | J     | 602 | QHC  | C13-C14-N23 | 4.47  | 117.06      | 110.22   |
| 2   | D     | 601 | HEM  | CMA-C3A-C4A | 4.34  | 132.02      | 125.42   |
| 3   | E     | 602 | QHC  | C14-N23-C18 | 4.33  | 129.90      | 123.44   |
| 3   | C     | 602 | QHC  | C11-N10-C9  | 4.23  | 123.26      | 117.51   |
| 2   | H     | 601 | HEM  | C2B-C1B-NB  | 4.21  | 114.68      | 109.84   |
| 3   | B     | 602 | QHC  | C11-N10-C9  | 4.14  | 123.14      | 117.51   |
| 3   | D     | 602 | QHC  | C11-N10-C9  | 4.08  | 123.06      | 117.51   |
| 2   | G     | 601 | HEM  | C3B-C4B-NB  | 4.05  | 112.38      | 109.47   |
| 2   | A     | 601 | HEM  | C2A-C1A-NA  | 4.01  | 114.60      | 110.15   |
| 2   | J     | 601 | HEM  | CMD-C2D-C1D | 3.94  | 131.19      | 125.03   |
| 3   | C     | 602 | QHC  | C14-N23-C18 | 3.87  | 129.21      | 123.44   |
| 3   | L     | 602 | QHC  | C11-N10-C9  | 3.87  | 122.77      | 117.51   |
| 2   | E     | 601 | HEM  | C3D-C4D-ND  | 3.76  | 114.30      | 110.17   |
| 2   | I     | 601 | HEM  | C3B-C4B-NB  | -3.72 | 106.79      | 109.47   |
| 2   | I     | 601 | HEM  | C4A-NA-C1A  | -3.71 | 99.78       | 105.82   |
| 2   | E     | 601 | HEM  | C2B-C1B-NB  | 3.70  | 114.10      | 109.84   |
| 3   | A     | 602 | QHC  | C11-N10-C9  | 3.69  | 122.53      | 117.51   |
| 3   | E     | 602 | QHC  | C1-C2-CL7   | -3.67 | 115.16      | 119.79   |
| 2   | F     | 601 | HEM  | C4A-NA-C1A  | -3.66 | 99.86       | 105.82   |
| 3   | F     | 602 | QHC  | C11-N10-C9  | 3.61  | 122.42      | 117.51   |
| 3   | E     | 602 | QHC  | C3-C2-CL7   | 3.60  | 125.52      | 118.42   |
| 2   | L     | 601 | HEM  | CBA-CAA-C2A | 3.57  | 122.42      | 112.53   |
| 3   | I     | 602 | QHC  | C11-N10-C9  | 3.54  | 122.32      | 117.51   |
| 3   | J     | 602 | QHC  | C11-N10-C9  | 3.52  | 122.29      | 117.51   |
| 2   | K     | 601 | HEM  | CHA-C4D-C3D | -3.51 | 118.75      | 125.23   |
| 2   | L     | 601 | HEM  | CHC-C4B-NB  | 3.50  | 128.19      | 124.42   |
| 2   | E     | 601 | HEM  | C4B-C3B-C2B | -3.50 | 104.07      | 107.28   |
| 2   | A     | 601 | HEM  | C3D-C4D-ND  | 3.49  | 114.00      | 110.17   |
| 2   | A     | 601 | HEM  | C4A-NA-C1A  | -3.45 | 100.19      | 105.82   |
| 2   | A     | 601 | HEM  | CHA-C4D-C3D | -3.43 | 118.89      | 125.23   |
| 3   | K     | 602 | QHC  | C11-N10-C9  | 3.41  | 122.14      | 117.51   |
| 2   | L     | 601 | HEM  | CHD-C1D-ND  | 3.38  | 128.06      | 124.42   |
| 3   | D     | 602 | QHC  | C19-C18-N23 | 3.37  | 120.19      | 115.78   |
| 2   | L     | 601 | HEM  | C2A-C1A-NA  | 3.37  | 113.89      | 110.15   |
| 2   | J     | 601 | HEM  | CHC-C4B-NB  | 3.36  | 128.04      | 124.42   |
| 3   | E     | 602 | QHC  | C11-N10-C9  | 3.35  | 122.07      | 117.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | G     | 601 | HEM  | CHA-C4D-C3D | -3.35 | 119.05      | 125.23   |
| 2   | I     | 601 | HEM  | C3B-C2B-C1B | -3.30 | 103.94      | 106.41   |
| 2   | I     | 601 | HEM  | C2B-C1B-NB  | 3.27  | 113.60      | 109.84   |
| 2   | G     | 601 | HEM  | C2B-C1B-NB  | 3.25  | 113.58      | 109.84   |
| 3   | A     | 602 | QHC  | C3-C2-C1    | 3.24  | 121.82      | 119.04   |
| 3   | K     | 602 | QHC  | C14-N23-C18 | 3.22  | 128.25      | 123.44   |
| 2   | J     | 601 | HEM  | C1D-C2D-C3D | -3.21 | 103.61      | 106.98   |
| 2   | K     | 601 | HEM  | C2B-C1B-NB  | 3.20  | 113.52      | 109.84   |
| 2   | B     | 601 | HEM  | C2B-C1B-NB  | 3.19  | 113.51      | 109.84   |
| 2   | L     | 601 | HEM  | CHD-C1D-C2D | -3.19 | 119.99      | 125.03   |
| 2   | K     | 601 | HEM  | C4A-NA-C1A  | -3.14 | 100.70      | 105.82   |
| 2   | J     | 601 | HEM  | CHD-C1D-C2D | -3.14 | 120.08      | 125.03   |
| 2   | B     | 601 | HEM  | C4B-C3B-C2B | -3.13 | 104.40      | 107.28   |
| 3   | F     | 602 | QHC  | C11-C13-C12 | 3.13  | 120.43      | 117.84   |
| 3   | J     | 602 | QHC  | C19-C18-N23 | 3.11  | 119.84      | 115.78   |
| 2   | D     | 601 | HEM  | CHA-C4D-C3D | -3.11 | 119.50      | 125.23   |
| 2   | I     | 601 | HEM  | CHA-C4D-C3D | -3.10 | 119.51      | 125.23   |
| 2   | D     | 601 | HEM  | CAD-CBD-CGD | -3.10 | 105.44      | 113.67   |
| 2   | K     | 601 | HEM  | C3D-C4D-ND  | 3.10  | 113.57      | 110.17   |
| 2   | G     | 601 | HEM  | C2A-C1A-NA  | 3.09  | 113.58      | 110.15   |
| 2   | K     | 601 | HEM  | C2A-C1A-NA  | 3.03  | 113.52      | 110.15   |
| 2   | C     | 601 | HEM  | CMB-C2B-C1B | 3.00  | 129.72      | 125.03   |
| 2   | E     | 601 | HEM  | C2A-C1A-NA  | 3.00  | 113.48      | 110.15   |
| 2   | G     | 601 | HEM  | C3B-C2B-C1B | -2.96 | 104.19      | 106.41   |
| 2   | C     | 601 | HEM  | O2D-CGD-O1D | -2.96 | 115.73      | 123.33   |
| 3   | B     | 602 | QHC  | C8-C9-N10   | -2.95 | 120.11      | 124.27   |
| 2   | F     | 601 | HEM  | CHA-C4D-C3D | -2.94 | 119.81      | 125.23   |
| 3   | I     | 602 | QHC  | C13-C14-N23 | 2.91  | 114.68      | 110.22   |
| 2   | F     | 601 | HEM  | C2A-C1A-NA  | 2.91  | 113.38      | 110.15   |
| 3   | D     | 602 | QHC  | C14-N23-C18 | 2.89  | 127.75      | 123.44   |
| 2   | E     | 601 | HEM  | C3C-C2C-C1C | -2.89 | 104.31      | 107.05   |
| 2   | G     | 601 | HEM  | O2D-CGD-CBD | 2.88  | 123.11      | 114.00   |
| 2   | K     | 601 | HEM  | CBA-CAA-C2A | 2.88  | 120.50      | 112.53   |
| 2   | E     | 601 | HEM  | CMD-C2D-C1D | 2.88  | 129.54      | 125.03   |
| 2   | H     | 601 | HEM  | CHC-C4B-NB  | 2.88  | 127.52      | 124.42   |
| 3   | D     | 602 | QHC  | C15-C14-N23 | -2.86 | 107.86      | 110.64   |
| 2   | I     | 601 | HEM  | C3D-C4D-ND  | 2.86  | 113.30      | 110.17   |
| 3   | B     | 602 | QHC  | C15-C14-N23 | 2.84  | 113.40      | 110.64   |
| 2   | H     | 601 | HEM  | C3B-C4B-NB  | 2.84  | 111.51      | 109.47   |
| 3   | B     | 602 | QHC  | C19-C18-N23 | 2.82  | 119.46      | 115.78   |
| 2   | D     | 601 | HEM  | C2B-C1B-NB  | 2.81  | 113.06      | 109.84   |
| 2   | J     | 601 | HEM  | CMA-C3A-C4A | 2.79  | 129.67      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 601 | HEM  | CMC-C2C-C1C | 2.77  | 129.61      | 124.73   |
| 2   | D     | 601 | HEM  | C3D-C4D-ND  | 2.77  | 113.21      | 110.17   |
| 3   | K     | 602 | QHC  | C11-C13-C12 | 2.76  | 120.12      | 117.84   |
| 2   | G     | 601 | HEM  | C3D-C4D-ND  | 2.73  | 113.16      | 110.17   |
| 3   | A     | 602 | QHC  | C5-C6-C1    | -2.72 | 117.46      | 119.61   |
| 2   | B     | 601 | HEM  | C4C-C3C-C2C | 2.71  | 109.17      | 106.81   |
| 2   | D     | 601 | HEM  | CHD-C1D-ND  | 2.71  | 127.34      | 124.42   |
| 2   | H     | 601 | HEM  | C2D-C1D-ND  | 2.70  | 113.02      | 109.90   |
| 2   | J     | 601 | HEM  | CHA-C4D-C3D | -2.69 | 120.26      | 125.23   |
| 2   | H     | 601 | HEM  | C4A-NA-C1A  | -2.68 | 101.45      | 105.82   |
| 2   | C     | 601 | HEM  | C3B-C4B-NB  | 2.68  | 111.39      | 109.47   |
| 2   | D     | 601 | HEM  | C4A-NA-C1A  | -2.68 | 101.45      | 105.82   |
| 2   | A     | 601 | HEM  | CMA-C3A-C4A | 2.67  | 129.49      | 125.42   |
| 2   | L     | 601 | HEM  | CHA-C4D-C3D | -2.65 | 120.34      | 125.23   |
| 2   | G     | 601 | HEM  | C4B-C3B-C2B | -2.63 | 104.86      | 107.28   |
| 3   | L     | 602 | QHC  | C14-N23-C18 | 2.62  | 127.35      | 123.44   |
| 2   | B     | 601 | HEM  | C3D-C4D-ND  | 2.61  | 113.04      | 110.17   |
| 2   | J     | 601 | HEM  | C2A-C1A-NA  | 2.61  | 113.05      | 110.15   |
| 3   | A     | 602 | QHC  | C13-C11-N10 | -2.61 | 120.25      | 124.41   |
| 2   | H     | 601 | HEM  | C3D-C4D-ND  | 2.61  | 113.03      | 110.17   |
| 2   | K     | 601 | HEM  | CHC-C4B-NB  | 2.61  | 127.23      | 124.42   |
| 2   | I     | 601 | HEM  | CBB-CAB-C3B | -2.61 | 114.50      | 127.53   |
| 2   | D     | 601 | HEM  | C2A-C1A-NA  | 2.61  | 113.04      | 110.15   |
| 2   | L     | 601 | HEM  | C4B-C3B-C2B | -2.60 | 104.89      | 107.28   |
| 2   | I     | 601 | HEM  | C2A-C1A-NA  | 2.59  | 113.03      | 110.15   |
| 2   | A     | 601 | HEM  | C4C-CHD-C1D | -2.59 | 120.52      | 126.02   |
| 2   | I     | 601 | HEM  | CHB-C1B-C2B | -2.57 | 119.66      | 126.95   |
| 3   | A     | 602 | QHC  | C15-C14-N23 | 2.56  | 113.13      | 110.64   |
| 2   | E     | 601 | HEM  | O2A-CGA-CBA | 2.54  | 122.04      | 114.00   |
| 2   | J     | 601 | HEM  | C2D-C1D-ND  | 2.53  | 112.83      | 109.90   |
| 3   | C     | 602 | QHC  | C13-C11-N10 | -2.53 | 120.38      | 124.41   |
| 2   | J     | 601 | HEM  | O2D-CGD-CBD | 2.52  | 121.96      | 114.00   |
| 2   | L     | 601 | HEM  | C3D-C4D-ND  | 2.51  | 112.92      | 110.17   |
| 3   | K     | 602 | QHC  | C13-C11-N10 | -2.50 | 120.43      | 124.41   |
| 2   | H     | 601 | HEM  | C3A-C4A-NA  | 2.48  | 114.12      | 110.14   |
| 3   | F     | 602 | QHC  | C13-C11-N10 | -2.48 | 120.46      | 124.41   |
| 3   | D     | 602 | QHC  | C8-C9-N10   | -2.48 | 120.78      | 124.27   |
| 3   | E     | 602 | QHC  | C13-C11-N10 | -2.47 | 120.47      | 124.41   |
| 3   | L     | 602 | QHC  | C13-C11-N10 | -2.46 | 120.49      | 124.41   |
| 2   | D     | 601 | HEM  | CMA-C3A-C2A | -2.46 | 120.42      | 125.62   |
| 2   | K     | 601 | HEM  | CHA-C4D-ND  | 2.46  | 127.40      | 124.37   |
| 2   | I     | 601 | HEM  | CMB-C2B-C1B | 2.45  | 128.86      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | J     | 601 | HEM  | C4A-NA-C1A  | -2.44 | 101.83      | 105.82   |
| 3   | C     | 602 | QHC  | C8-C9-N10   | -2.44 | 120.83      | 124.27   |
| 2   | C     | 601 | HEM  | C1B-NB-C4B  | -2.44 | 102.32      | 105.21   |
| 2   | L     | 601 | HEM  | C4A-NA-C1A  | -2.43 | 101.86      | 105.82   |
| 2   | E     | 601 | HEM  | C4A-NA-C1A  | -2.43 | 101.87      | 105.82   |
| 2   | J     | 601 | HEM  | C2B-C1B-NB  | 2.42  | 112.62      | 109.84   |
| 2   | H     | 601 | HEM  | C3B-C2B-C1B | -2.41 | 104.60      | 106.41   |
| 2   | L     | 601 | HEM  | C4C-CHD-C1D | -2.41 | 120.89      | 126.02   |
| 3   | E     | 602 | QHC  | C16-C17-C12 | -2.41 | 107.94      | 112.84   |
| 2   | L     | 601 | HEM  | CAD-C3D-C2D | 2.41  | 132.38      | 127.87   |
| 2   | G     | 601 | HEM  | C4A-NA-C1A  | -2.40 | 101.91      | 105.82   |
| 2   | L     | 601 | HEM  | O2A-CGA-CBA | 2.39  | 121.55      | 114.00   |
| 3   | L     | 602 | QHC  | C8-C9-N10   | -2.39 | 120.91      | 124.27   |
| 2   | I     | 601 | HEM  | C4B-C3B-C2B | 2.37  | 109.46      | 107.28   |
| 2   | F     | 601 | HEM  | C3D-C4D-ND  | 2.37  | 112.77      | 110.17   |
| 3   | E     | 602 | QHC  | C15-C14-C13 | 2.35  | 115.20      | 111.83   |
| 3   | J     | 602 | QHC  | C15-C14-C13 | -2.35 | 108.47      | 111.83   |
| 2   | G     | 601 | HEM  | CHA-C4D-ND  | 2.35  | 127.28      | 124.37   |
| 2   | E     | 601 | HEM  | C2D-C1D-ND  | 2.35  | 112.62      | 109.90   |
| 2   | E     | 601 | HEM  | CHA-C4D-C3D | -2.35 | 120.90      | 125.23   |
| 2   | D     | 601 | HEM  | CHA-C4D-ND  | 2.35  | 127.27      | 124.37   |
| 3   | A     | 602 | QHC  | C4-C3-C2    | -2.34 | 116.74      | 119.98   |
| 2   | B     | 601 | HEM  | C2D-C1D-ND  | 2.34  | 112.61      | 109.90   |
| 2   | I     | 601 | HEM  | CHD-C1D-ND  | 2.34  | 126.94      | 124.42   |
| 2   | E     | 601 | HEM  | C3B-C4B-NB  | 2.33  | 111.14      | 109.47   |
| 2   | J     | 601 | HEM  | CAA-CBA-CGA | 2.33  | 119.83      | 113.67   |
| 2   | H     | 601 | HEM  | C1C-CHC-C4B | -2.31 | 121.10      | 126.02   |
| 2   | C     | 601 | HEM  | C4B-C3B-C2B | -2.31 | 105.15      | 107.28   |
| 2   | K     | 601 | HEM  | CMA-C3A-C4A | 2.31  | 128.94      | 125.42   |
| 2   | F     | 601 | HEM  | CHA-C4D-ND  | 2.29  | 127.20      | 124.37   |
| 2   | H     | 601 | HEM  | CHD-C1D-C2D | -2.28 | 121.42      | 125.03   |
| 2   | G     | 601 | HEM  | CHC-C4B-NB  | 2.28  | 126.87      | 124.42   |
| 2   | A     | 601 | HEM  | C2B-C1B-NB  | 2.27  | 112.45      | 109.84   |
| 3   | A     | 602 | QHC  | C1-C2-CL7   | -2.25 | 116.94      | 119.79   |
| 2   | B     | 601 | HEM  | C4A-NA-C1A  | -2.25 | 102.15      | 105.82   |
| 2   | D     | 601 | HEM  | C4C-CHD-C1D | -2.25 | 121.23      | 126.02   |
| 2   | H     | 601 | HEM  | C4C-NC-C1C  | -2.25 | 102.16      | 105.82   |
| 3   | A     | 602 | QHC  | C8-C9-N10   | -2.25 | 121.11      | 124.27   |
| 2   | G     | 601 | HEM  | CBC-CAC-C3C | -2.23 | 116.38      | 127.53   |
| 3   | C     | 602 | QHC  | C15-C14-N23 | 2.22  | 112.80      | 110.64   |
| 2   | G     | 601 | HEM  | C1A-CHA-C4D | -2.22 | 121.03      | 126.25   |
| 2   | I     | 601 | HEM  | CHA-C4D-ND  | 2.22  | 127.11      | 124.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | F     | 602 | QHC  | C3-C2-C1    | 2.22  | 120.94      | 119.04   |
| 3   | F     | 602 | QHC  | C15-C16-C17 | 2.21  | 116.65      | 110.69   |
| 2   | A     | 601 | HEM  | CHA-C4D-ND  | 2.21  | 127.10      | 124.37   |
| 2   | E     | 601 | HEM  | O2D-CGD-O1D | -2.20 | 117.68      | 123.33   |
| 2   | H     | 601 | HEM  | O2D-CGD-O1D | -2.20 | 117.68      | 123.33   |
| 2   | C     | 601 | HEM  | C3D-C4D-ND  | 2.20  | 112.58      | 110.17   |
| 2   | I     | 601 | HEM  | CHD-C1D-C2D | -2.19 | 121.57      | 125.03   |
| 2   | H     | 601 | HEM  | CHB-C1B-C2B | -2.18 | 120.75      | 126.95   |
| 2   | G     | 601 | HEM  | CHC-C4B-C3B | -2.17 | 120.74      | 125.07   |
| 3   | B     | 602 | QHC  | O20-C18-C19 | -2.17 | 116.28      | 122.13   |
| 2   | L     | 601 | HEM  | CMD-C2D-C3D | 2.17  | 132.01      | 126.15   |
| 2   | C     | 601 | HEM  | C1D-C2D-C3D | -2.16 | 104.71      | 106.98   |
| 2   | B     | 601 | HEM  | CBC-CAC-C3C | -2.16 | 116.75      | 127.53   |
| 3   | J     | 602 | QHC  | C13-C11-N10 | -2.16 | 120.97      | 124.41   |
| 3   | I     | 602 | QHC  | C13-C11-N10 | -2.15 | 120.98      | 124.41   |
| 3   | I     | 602 | QHC  | C8-C9-N10   | -2.15 | 121.24      | 124.27   |
| 2   | J     | 601 | HEM  | CHA-C4D-ND  | 2.15  | 127.03      | 124.37   |
| 2   | H     | 601 | HEM  | CAB-C3B-C2B | 2.15  | 135.42      | 128.43   |
| 2   | E     | 601 | HEM  | C1D-C2D-C3D | -2.15 | 104.72      | 106.98   |
| 3   | E     | 602 | QHC  | C17-C12-C13 | -2.15 | 118.07      | 121.44   |
| 2   | H     | 601 | HEM  | CAC-C3C-C4C | 2.14  | 129.93      | 124.82   |
| 2   | A     | 601 | HEM  | CHB-C1B-C2B | -2.14 | 120.87      | 126.95   |
| 2   | J     | 601 | HEM  | CHD-C1D-ND  | 2.13  | 126.72      | 124.42   |
| 3   | L     | 602 | QHC  | C3-C2-C1    | 2.13  | 120.87      | 119.04   |
| 2   | F     | 601 | HEM  | O2D-CGD-O1D | -2.12 | 117.87      | 123.33   |
| 2   | J     | 601 | HEM  | C1C-CHC-C4B | -2.12 | 121.51      | 126.02   |
| 3   | A     | 602 | QHC  | C4-C5-C8    | -2.12 | 117.40      | 120.91   |
| 3   | D     | 602 | QHC  | C3-C2-C1    | 2.10  | 120.84      | 119.04   |
| 3   | E     | 602 | QHC  | F22-C1-C2   | -2.10 | 116.42      | 118.96   |
| 3   | E     | 602 | QHC  | C5-C8-C12   | 2.09  | 125.93      | 122.88   |
| 2   | C     | 601 | HEM  | O2A-CGA-CBA | 2.09  | 120.59      | 114.00   |
| 3   | A     | 602 | QHC  | C5-C8-C12   | -2.08 | 119.84      | 122.88   |
| 2   | C     | 601 | HEM  | CHB-C1B-C2B | -2.08 | 121.04      | 126.95   |
| 2   | B     | 601 | HEM  | C3C-C2C-C1C | -2.07 | 105.08      | 107.05   |
| 2   | H     | 601 | HEM  | CHC-C4B-C3B | -2.07 | 120.94      | 125.07   |
| 3   | F     | 602 | QHC  | C8-C9-N10   | -2.06 | 121.36      | 124.27   |
| 2   | D     | 601 | HEM  | C1A-CHA-C4D | -2.05 | 121.42      | 126.25   |
| 3   | L     | 602 | QHC  | C11-C13-C12 | 2.05  | 119.53      | 117.84   |
| 2   | K     | 601 | HEM  | CAD-C3D-C2D | 2.04  | 131.69      | 127.87   |
| 2   | I     | 601 | HEM  | C4C-CHD-C1D | -2.04 | 121.69      | 126.02   |
| 2   | F     | 601 | HEM  | O2D-CGD-CBD | 2.03  | 120.42      | 114.00   |
| 2   | G     | 601 | HEM  | C3C-C2C-C1C | -2.03 | 105.12      | 107.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | L     | 602 | QHC  | C19-C18-N23 | 2.02  | 118.42      | 115.78   |
| 2   | H     | 601 | HEM  | C1D-C2D-C3D | -2.02 | 104.86      | 106.98   |
| 2   | B     | 601 | HEM  | CHB-C1B-C2B | -2.02 | 121.22      | 126.95   |
| 3   | A     | 602 | QHC  | C14-N23-C18 | 2.02  | 126.45      | 123.44   |
| 3   | J     | 602 | QHC  | C8-C9-N10   | -2.01 | 121.44      | 124.27   |
| 2   | E     | 601 | HEM  | CHB-C1B-C2B | -2.01 | 121.24      | 126.95   |
| 2   | L     | 601 | HEM  | CBC-CAC-C3C | -2.00 | 117.51      | 127.53   |

There are no chirality outliers.

All (75) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | A     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | E     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 2   | H     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | L     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 3   | A     | 602 | QHC  | C15-C14-N23-C18 |
| 3   | B     | 602 | QHC  | C15-C14-N23-C18 |
| 3   | C     | 602 | QHC  | C15-C14-N23-C18 |
| 3   | D     | 602 | QHC  | C13-C14-N23-C18 |
| 3   | E     | 602 | QHC  | C13-C14-N23-C18 |
| 3   | F     | 602 | QHC  | C15-C14-N23-C18 |
| 3   | I     | 602 | QHC  | C13-C14-N23-C18 |
| 3   | I     | 602 | QHC  | C15-C14-N23-C18 |
| 3   | J     | 602 | QHC  | C13-C14-N23-C18 |
| 3   | K     | 602 | QHC  | C13-C14-N23-C18 |
| 3   | L     | 602 | QHC  | C13-C14-N23-C18 |
| 2   | L     | 601 | HEM  | C1A-C2A-CAA-CBA |
| 2   | B     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 2   | F     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | I     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 2   | B     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | E     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 3   | B     | 602 | QHC  | O20-C18-C19-C21 |
| 3   | B     | 602 | QHC  | N23-C18-C19-C21 |
| 3   | K     | 602 | QHC  | C15-C14-N23-C18 |
| 3   | L     | 602 | QHC  | C15-C14-N23-C18 |
| 2   | L     | 601 | HEM  | C3A-C2A-CAA-CBA |
| 2   | A     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 2   | B     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | C     | 601 | HEM  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | G     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | I     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | K     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 2   | K     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 2   | L     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 3   | A     | 602 | QHC  | C13-C14-N23-C18 |
| 2   | C     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 2   | I     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 2   | L     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | C     | 601 | HEM  | C2A-CAA-CBA-CGA |
| 2   | A     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 2   | B     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 2   | C     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | E     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | F     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | G     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | H     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | I     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | K     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | L     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | B     | 601 | HEM  | C3D-CAD-CBD-CGD |
| 2   | H     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | D     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | F     | 601 | HEM  | C2A-CAA-CBA-CGA |
| 2   | D     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | H     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | L     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | J     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 2   | K     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 2   | E     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | J     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | L     | 601 | HEM  | CAA-CBA-CGA-O1A |
| 2   | B     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | B     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | F     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | E     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | J     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | F     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | A     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | L     | 601 | HEM  | CAA-CBA-CGA-O2A |
| 2   | I     | 601 | HEM  | C3D-CAD-CBD-CGD |

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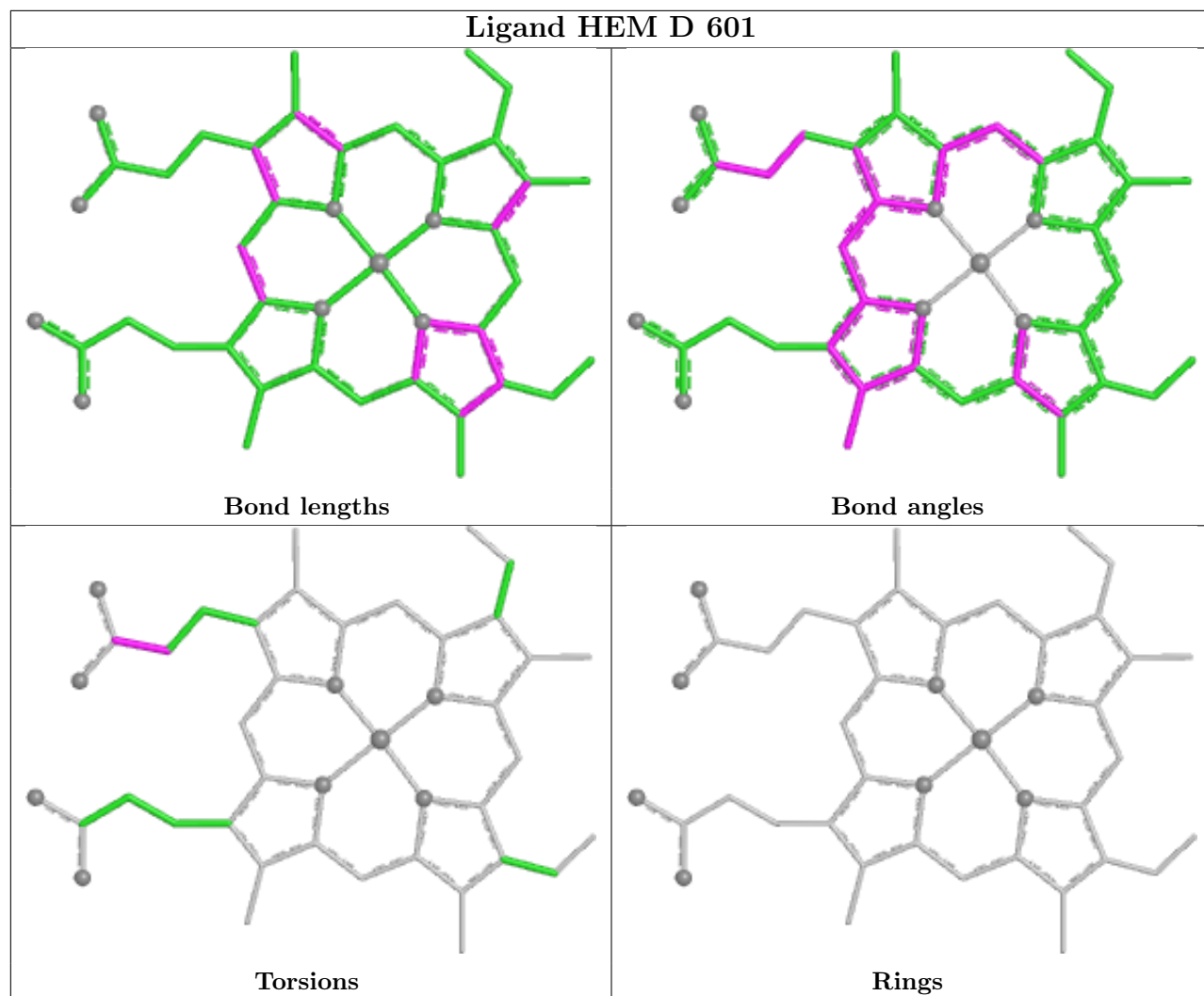
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 3   | E     | 602 | QHC  | C15-C14-N23-C18 |
| 2   | E     | 601 | HEM  | C2C-C3C-CAC-CBC |

There are no ring outliers.

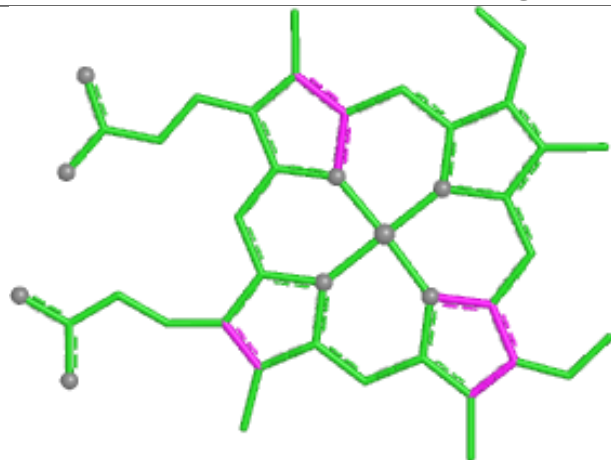
21 monomers are involved in 76 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | D     | 601 | HEM  | 2       | 0            |
| 2   | I     | 601 | HEM  | 3       | 0            |
| 3   | K     | 602 | QHC  | 5       | 0            |
| 3   | L     | 602 | QHC  | 3       | 0            |
| 2   | E     | 601 | HEM  | 4       | 0            |
| 3   | E     | 602 | QHC  | 2       | 0            |
| 2   | J     | 601 | HEM  | 1       | 0            |
| 2   | K     | 601 | HEM  | 5       | 0            |
| 2   | A     | 601 | HEM  | 6       | 0            |
| 2   | H     | 601 | HEM  | 7       | 0            |
| 3   | C     | 602 | QHC  | 5       | 0            |
| 3   | B     | 602 | QHC  | 5       | 0            |
| 3   | A     | 602 | QHC  | 7       | 0            |
| 3   | J     | 602 | QHC  | 4       | 0            |
| 3   | F     | 602 | QHC  | 5       | 0            |
| 2   | L     | 601 | HEM  | 4       | 0            |
| 2   | C     | 601 | HEM  | 5       | 0            |
| 3   | I     | 602 | QHC  | 4       | 0            |
| 2   | G     | 601 | HEM  | 1       | 0            |
| 2   | F     | 601 | HEM  | 8       | 0            |
| 2   | B     | 601 | HEM  | 5       | 0            |

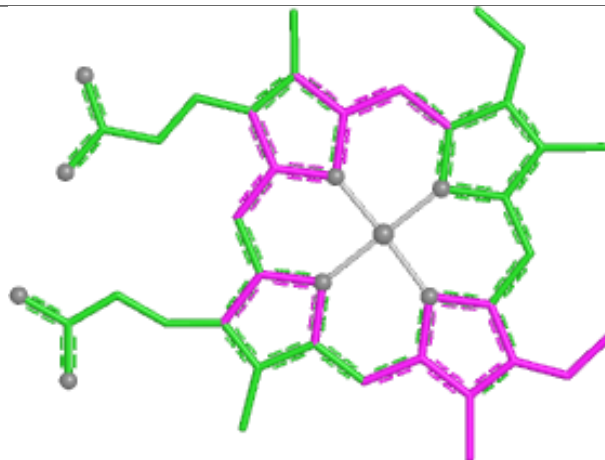
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



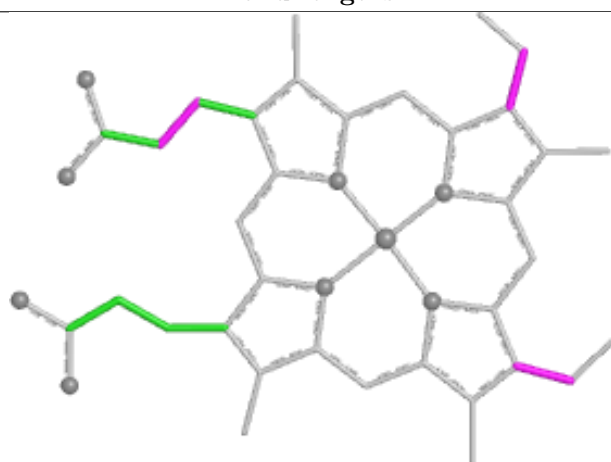
## Ligand HEM I 601



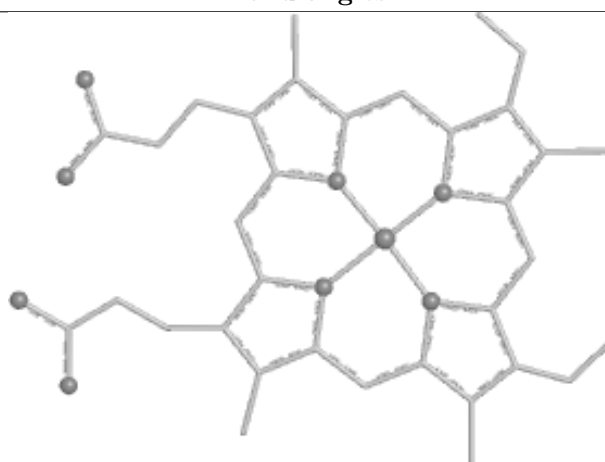
Bond lengths



Bond angles

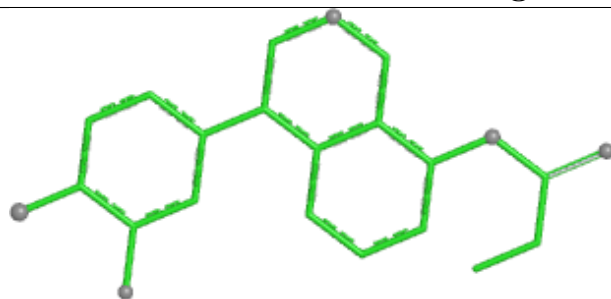


Torsions

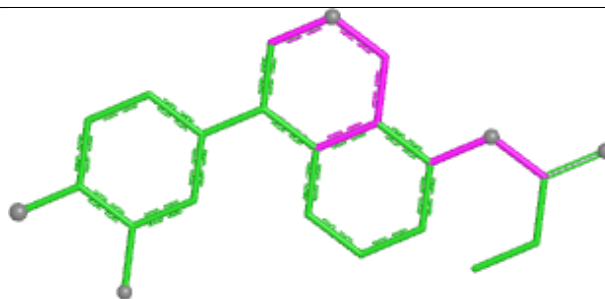


Rings

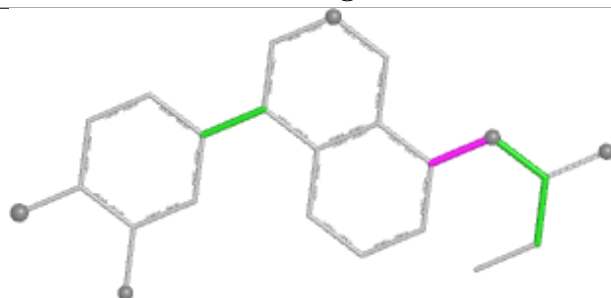
## Ligand QHC K 602



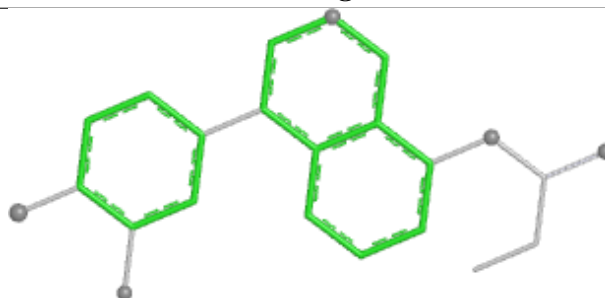
Bond lengths



Bond angles

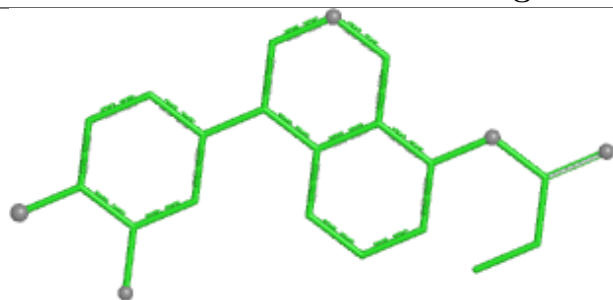


Torsions

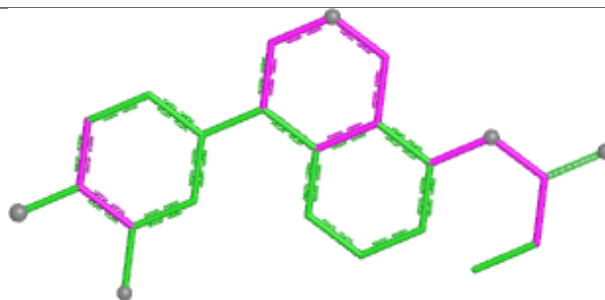


Rings

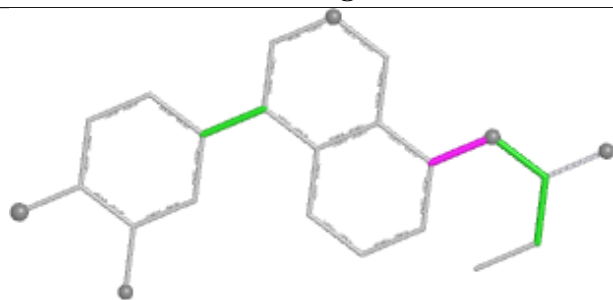
## Ligand QHC L 602



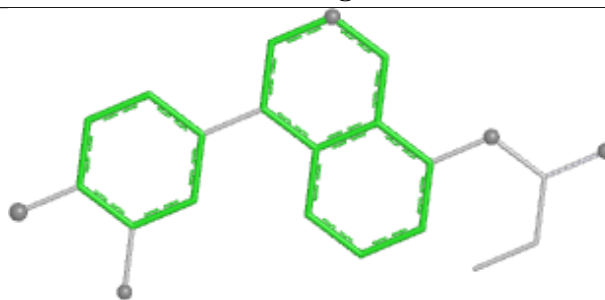
Bond lengths



Bond angles

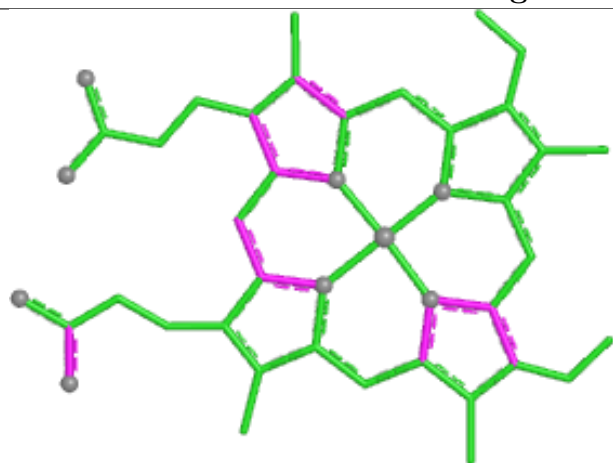


Torsions

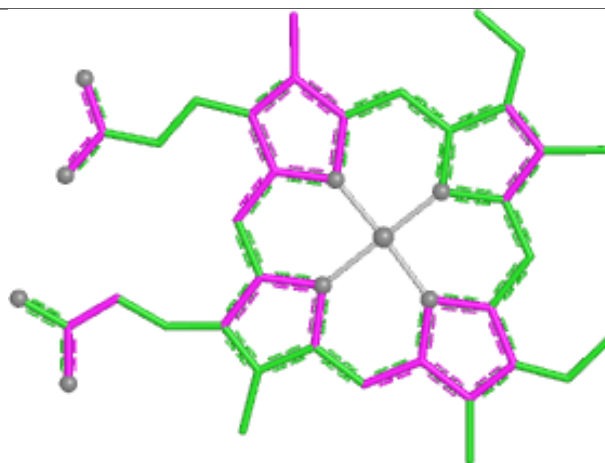


Rings

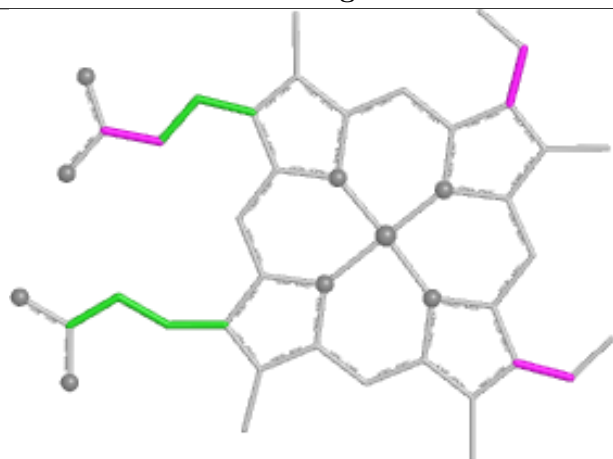
## Ligand HEM E 601



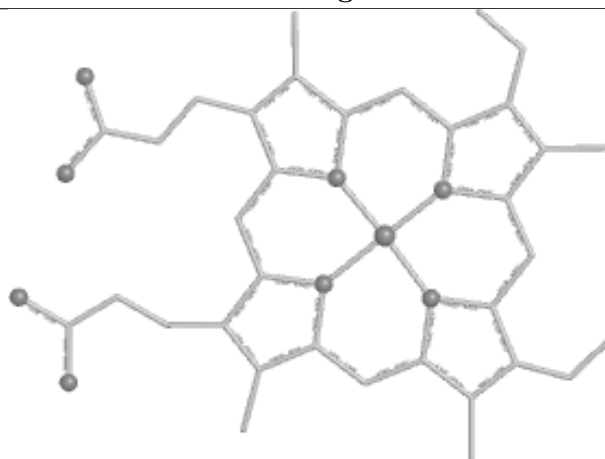
Bond lengths



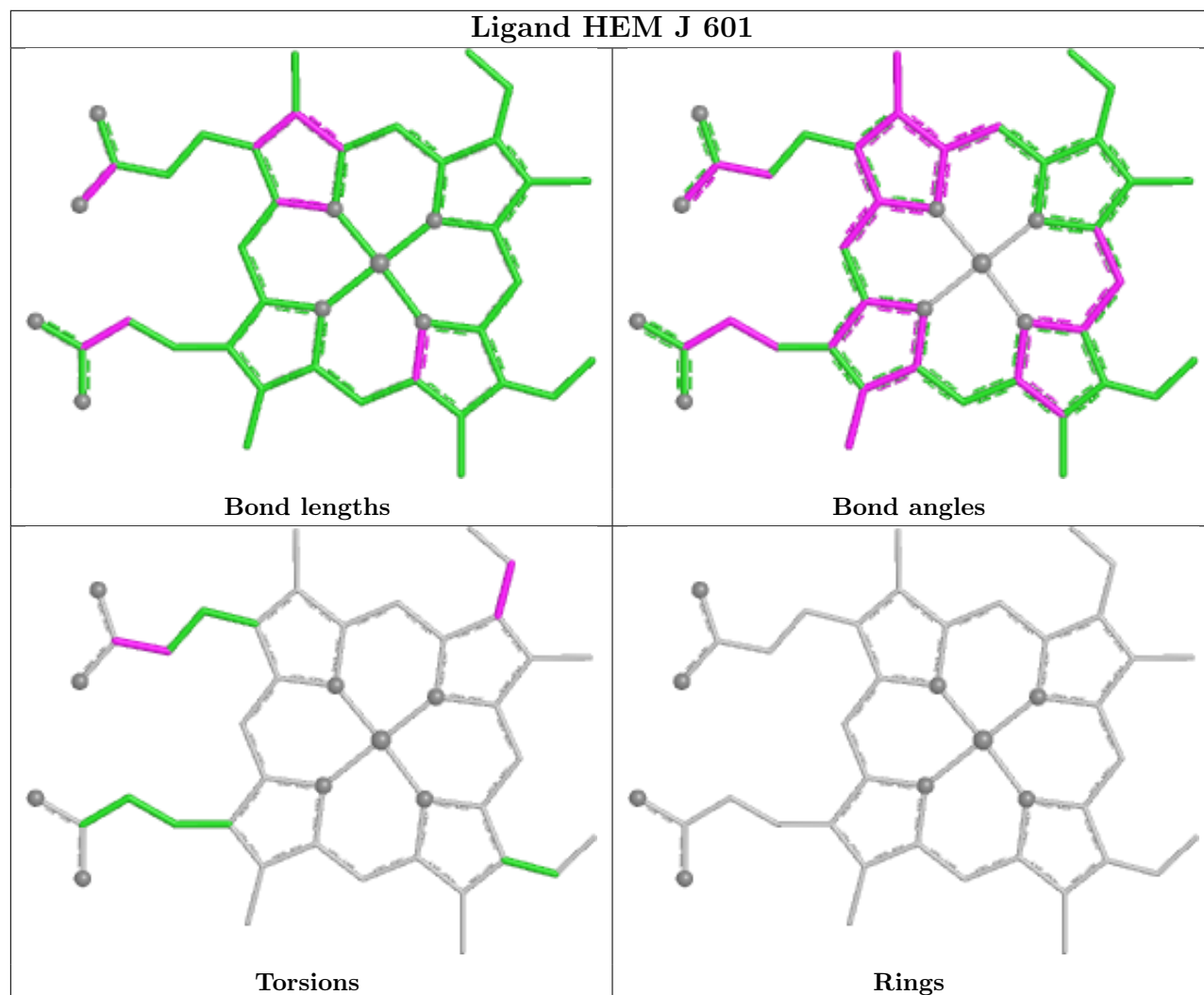
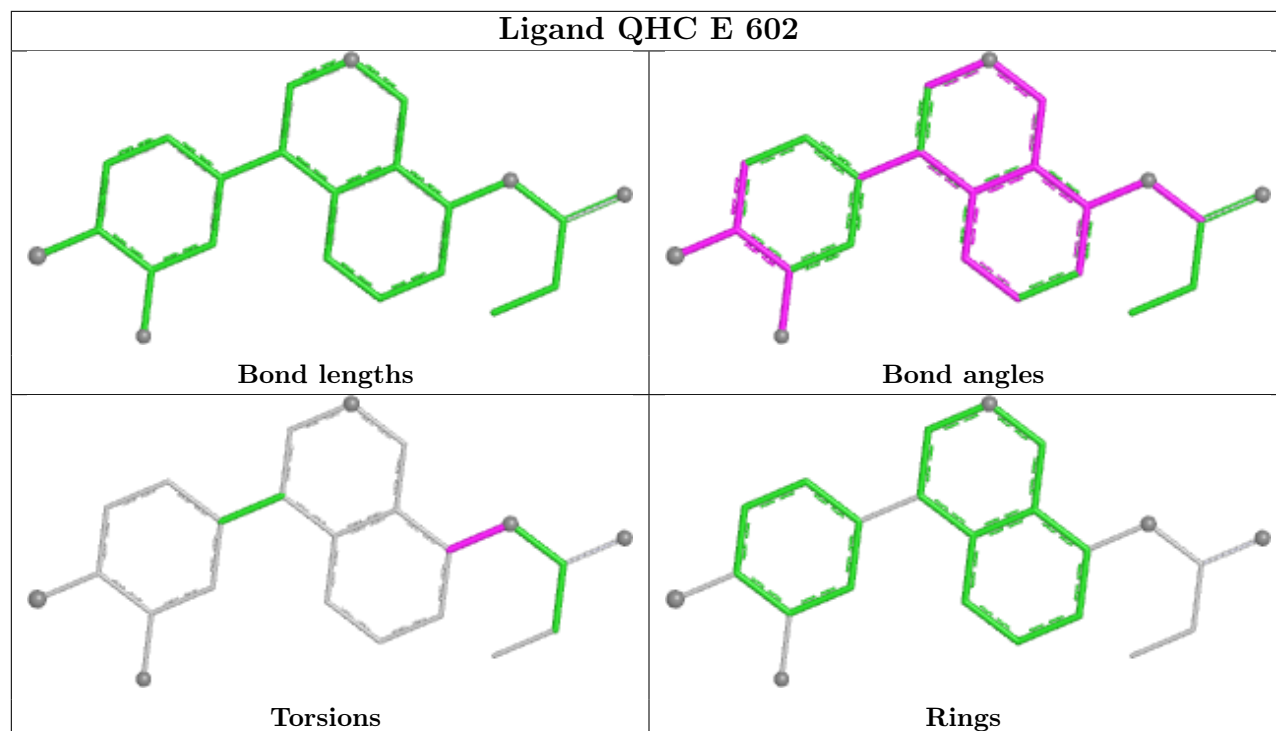
Bond angles

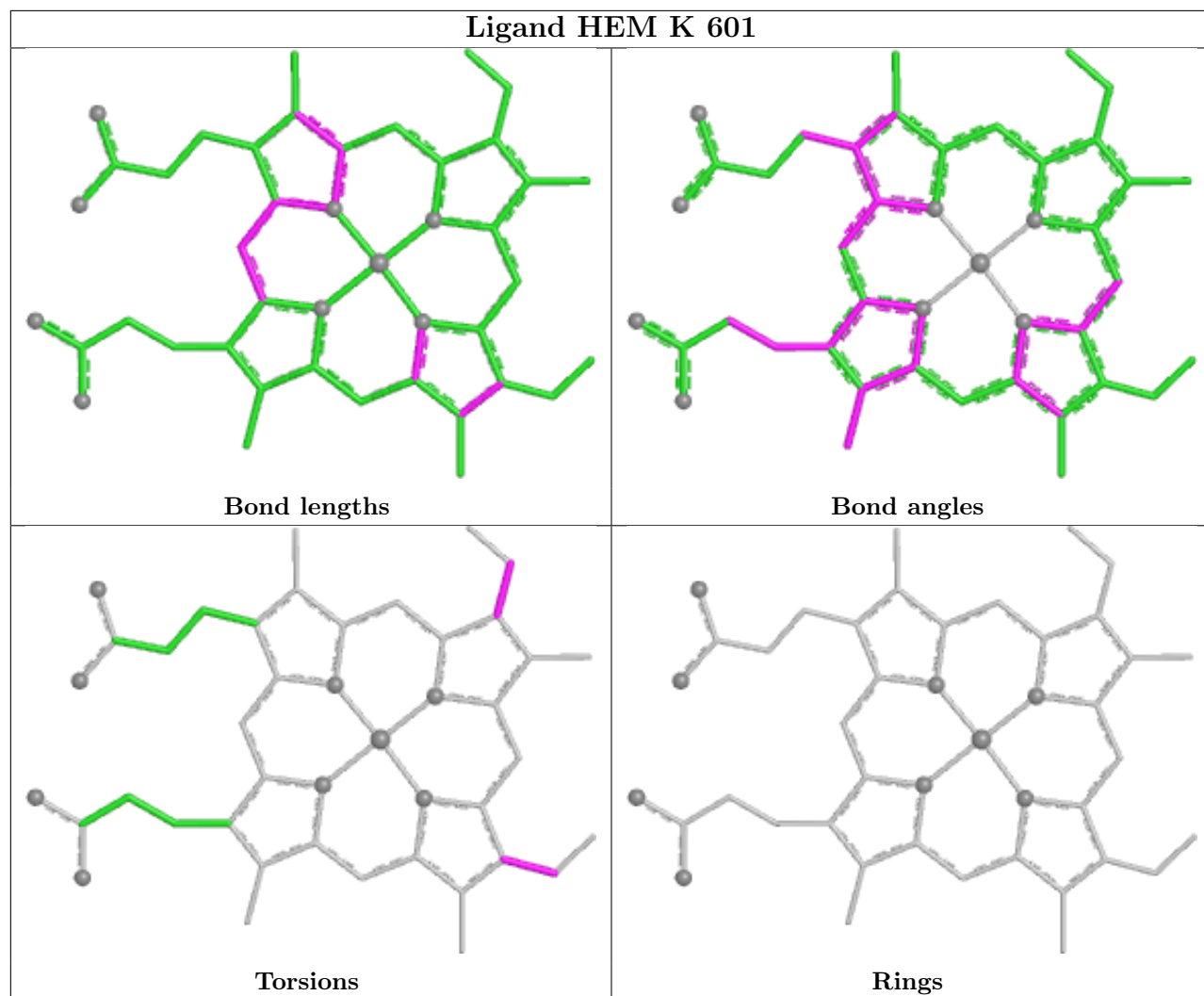


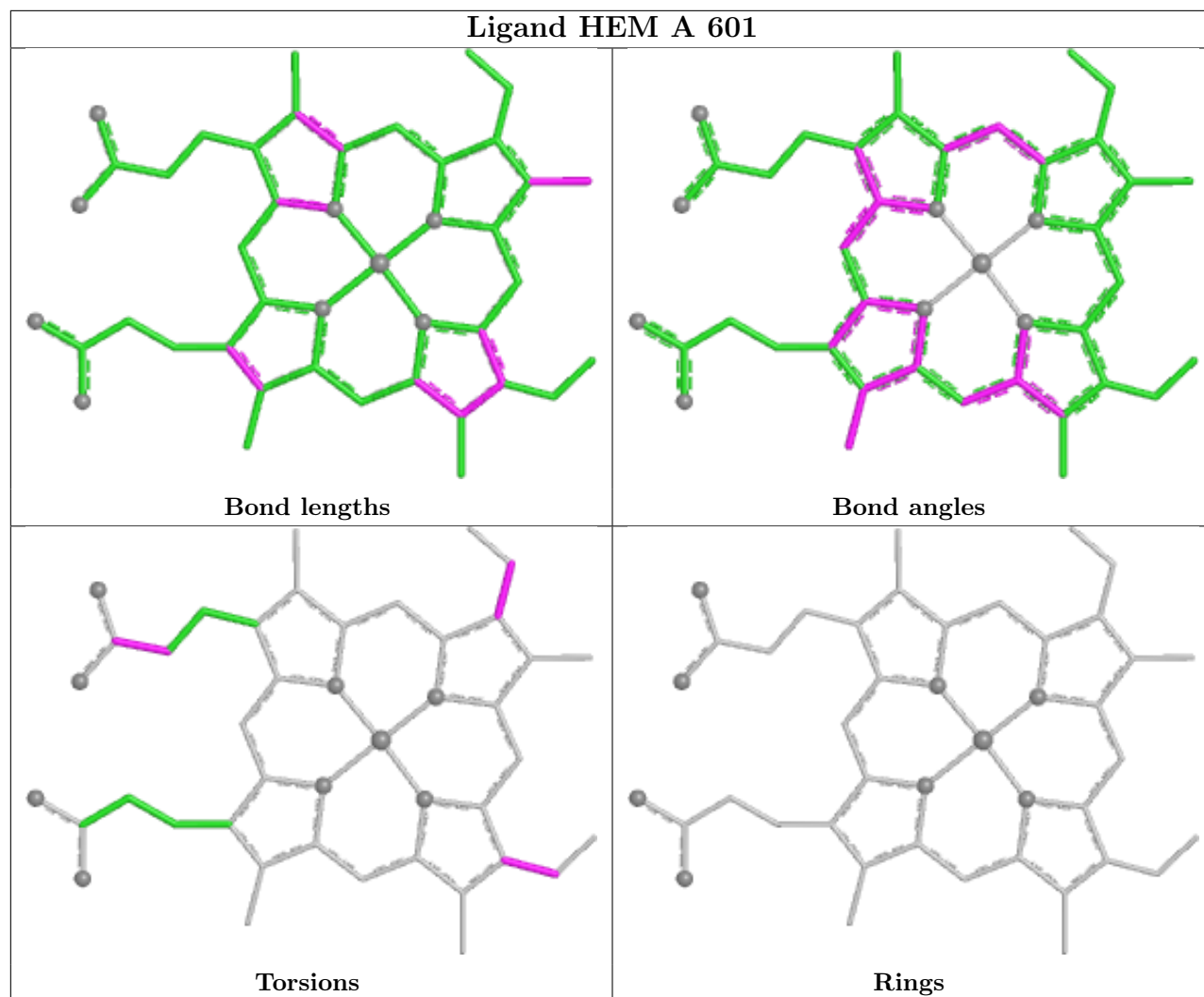
Torsions

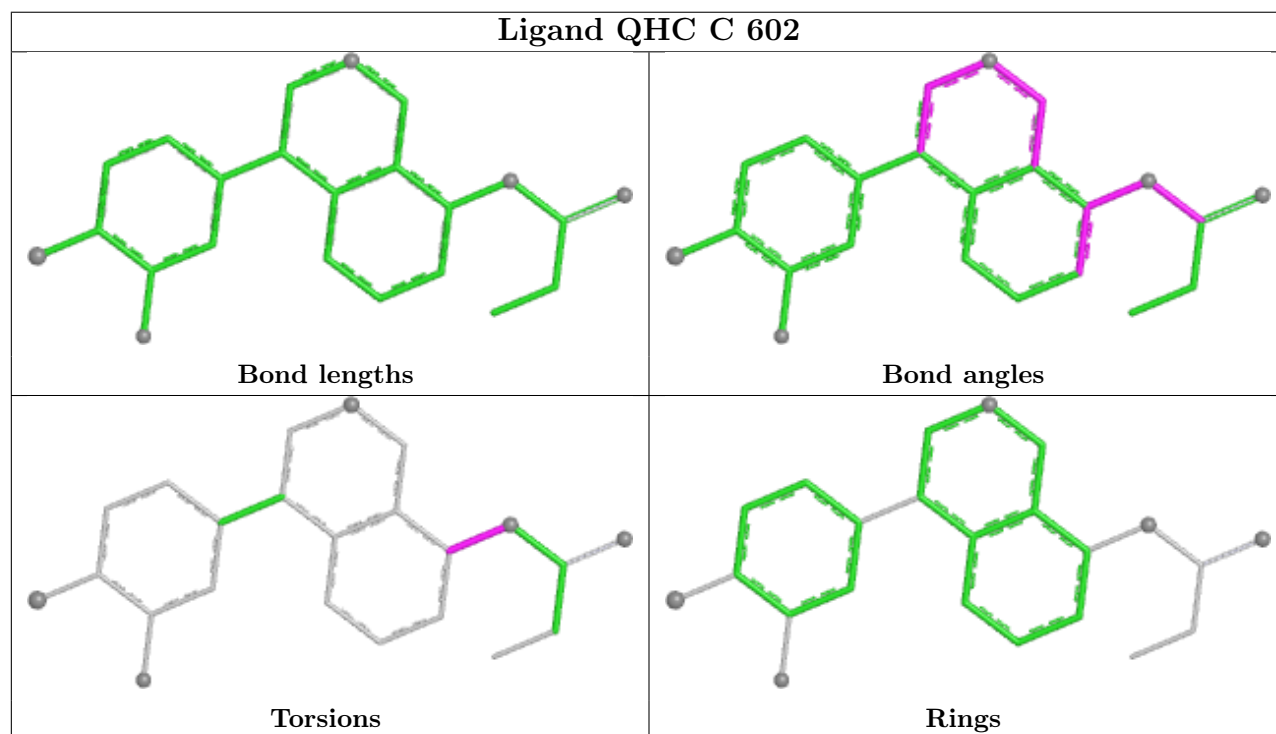
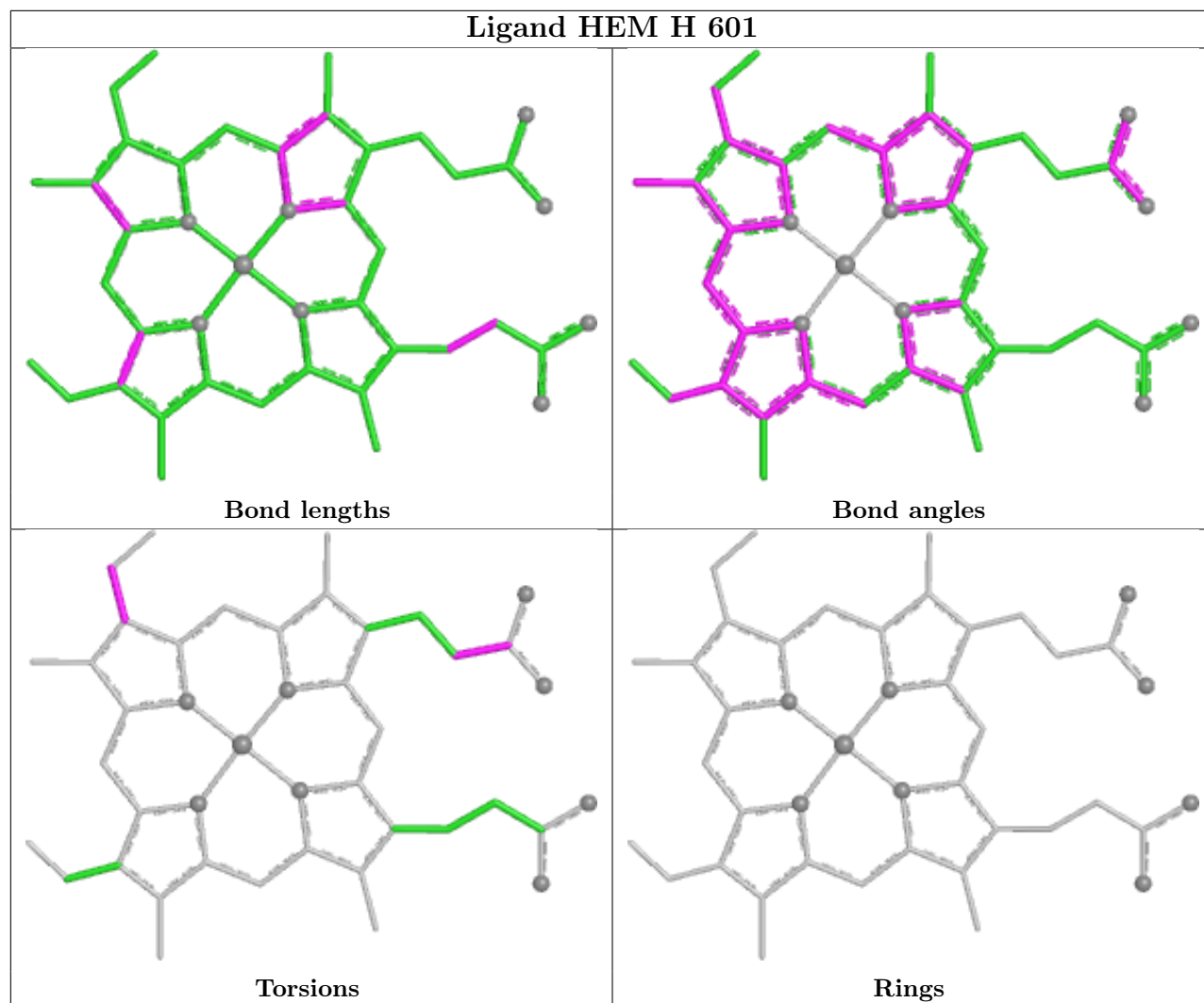


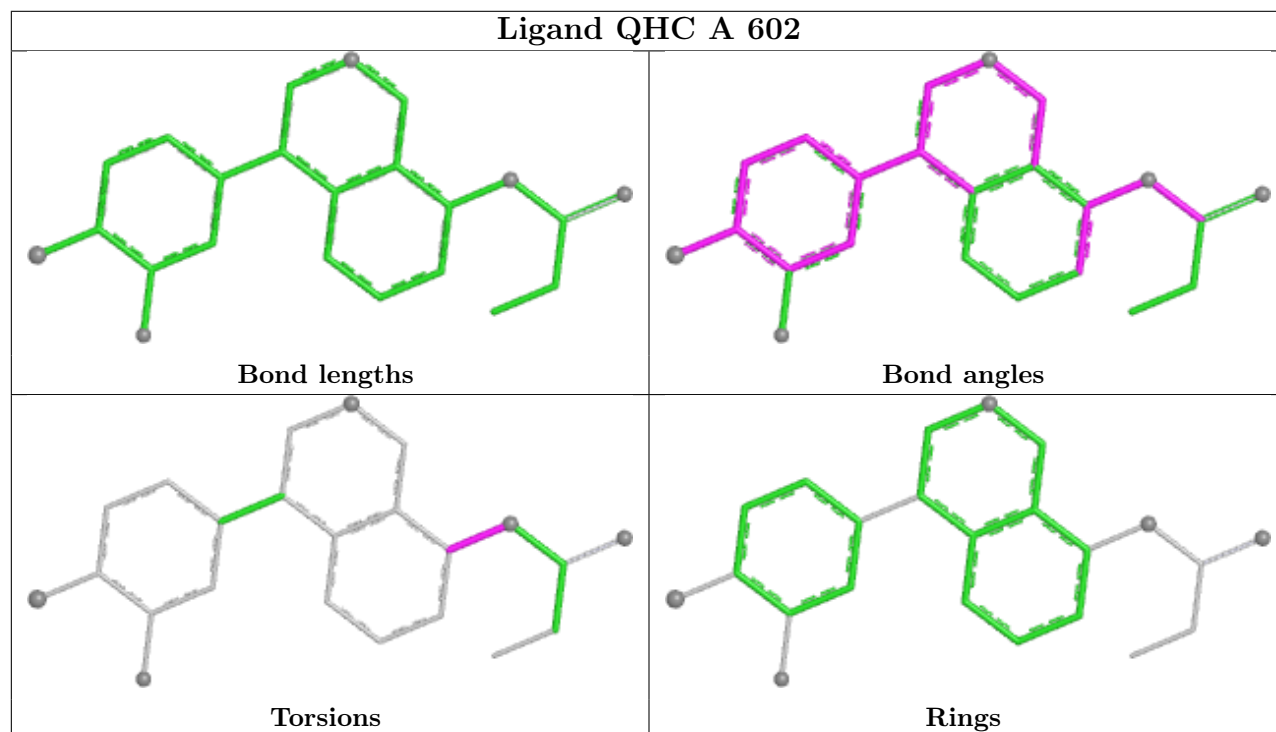
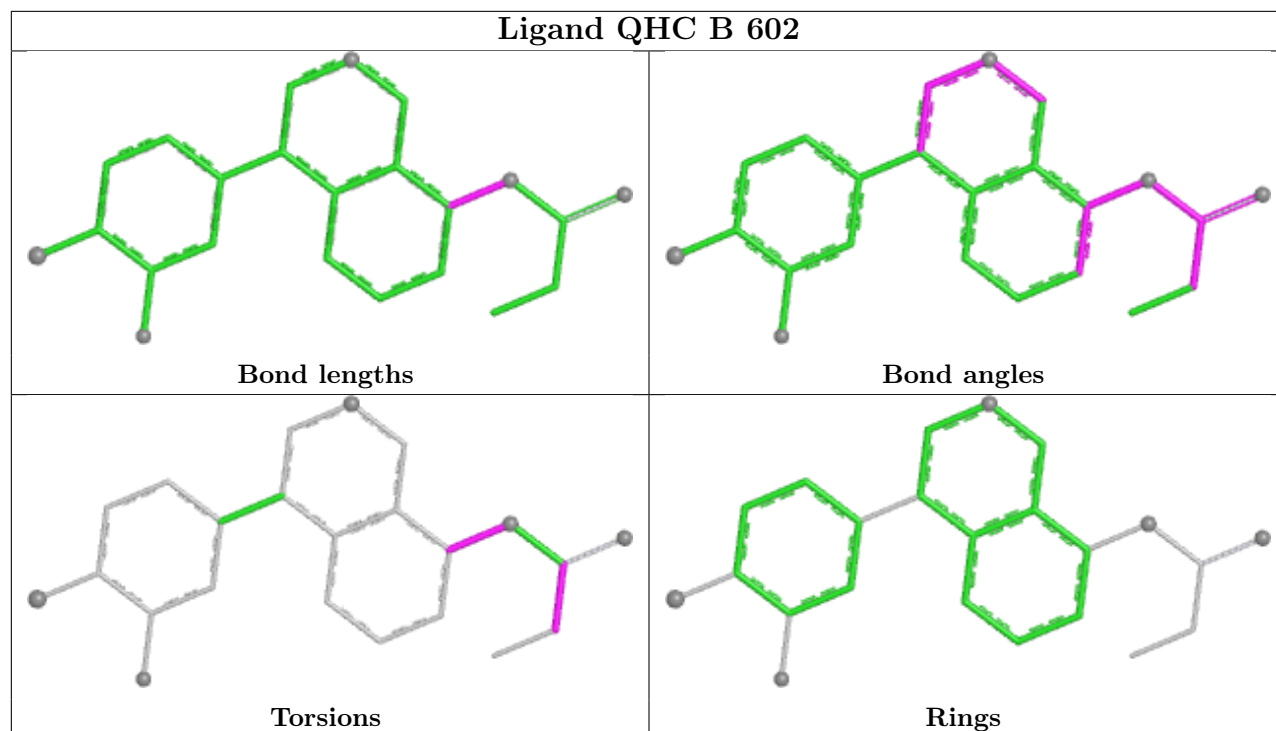
Rings



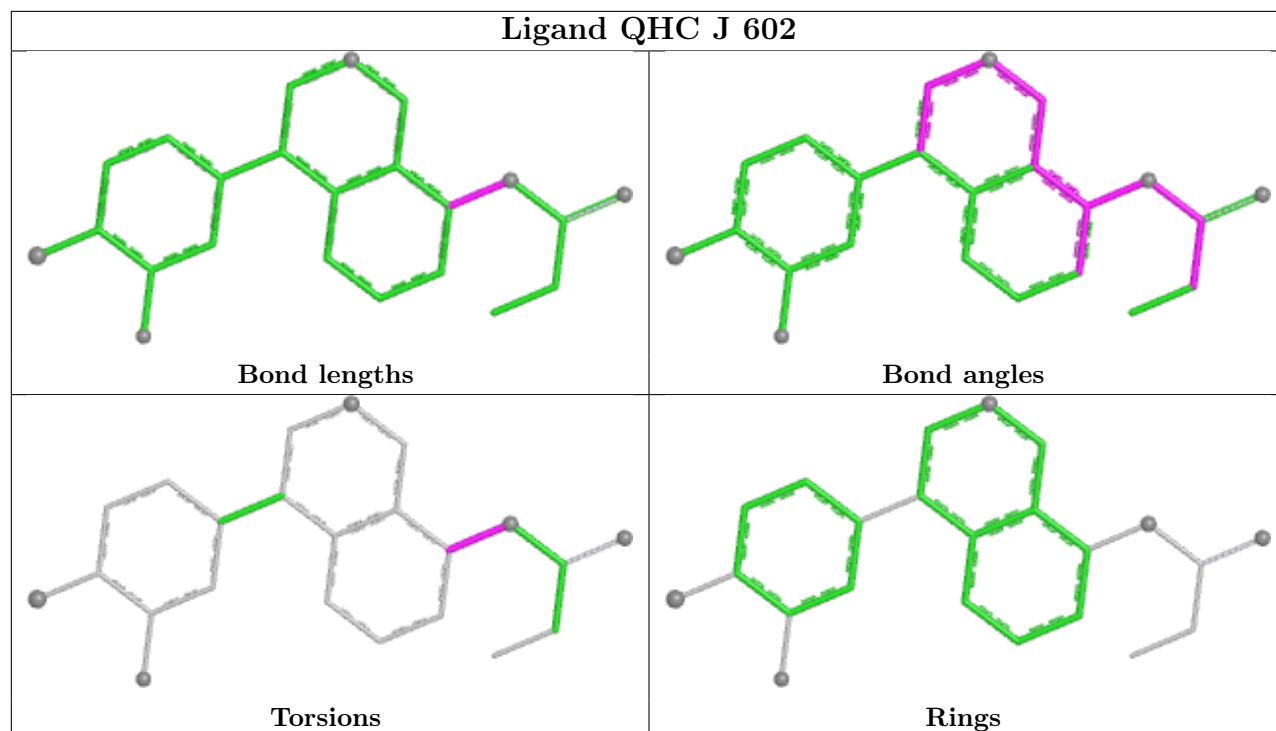




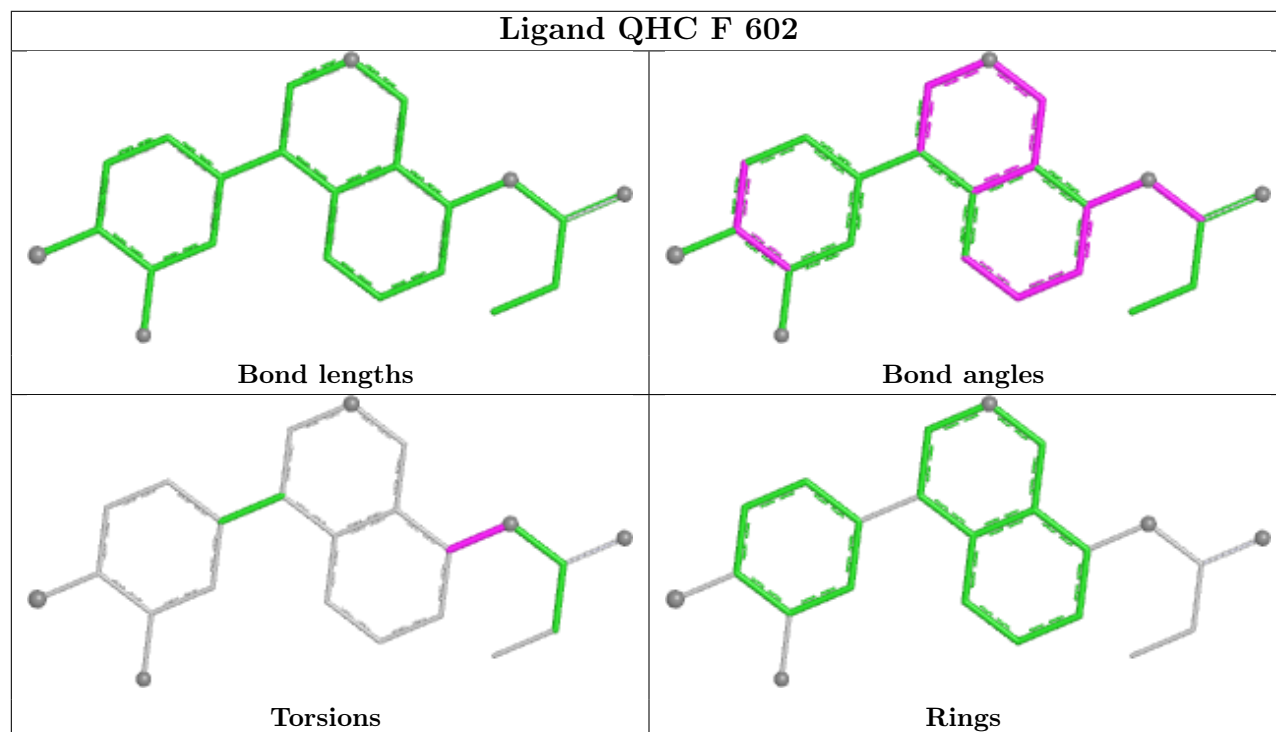


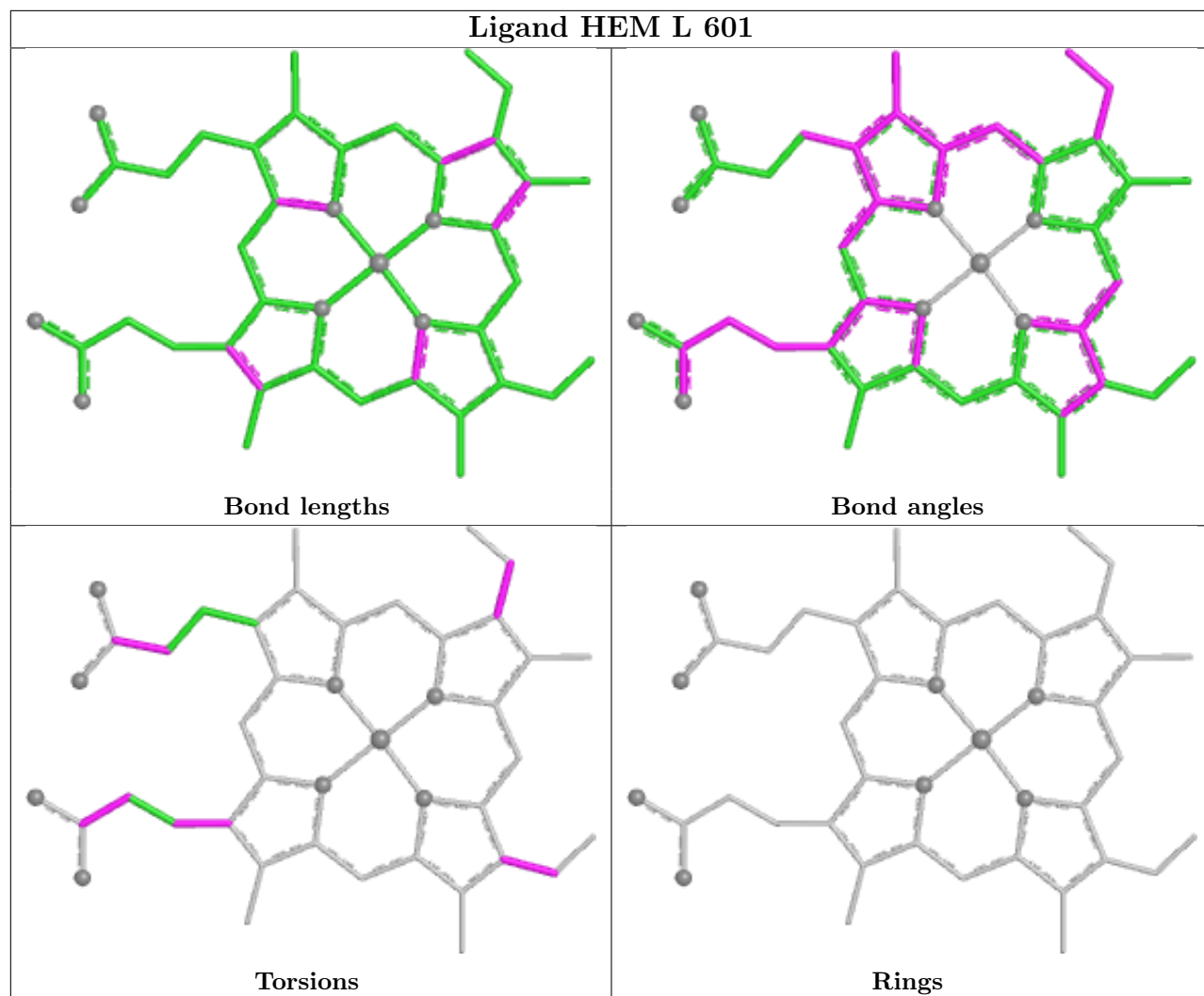


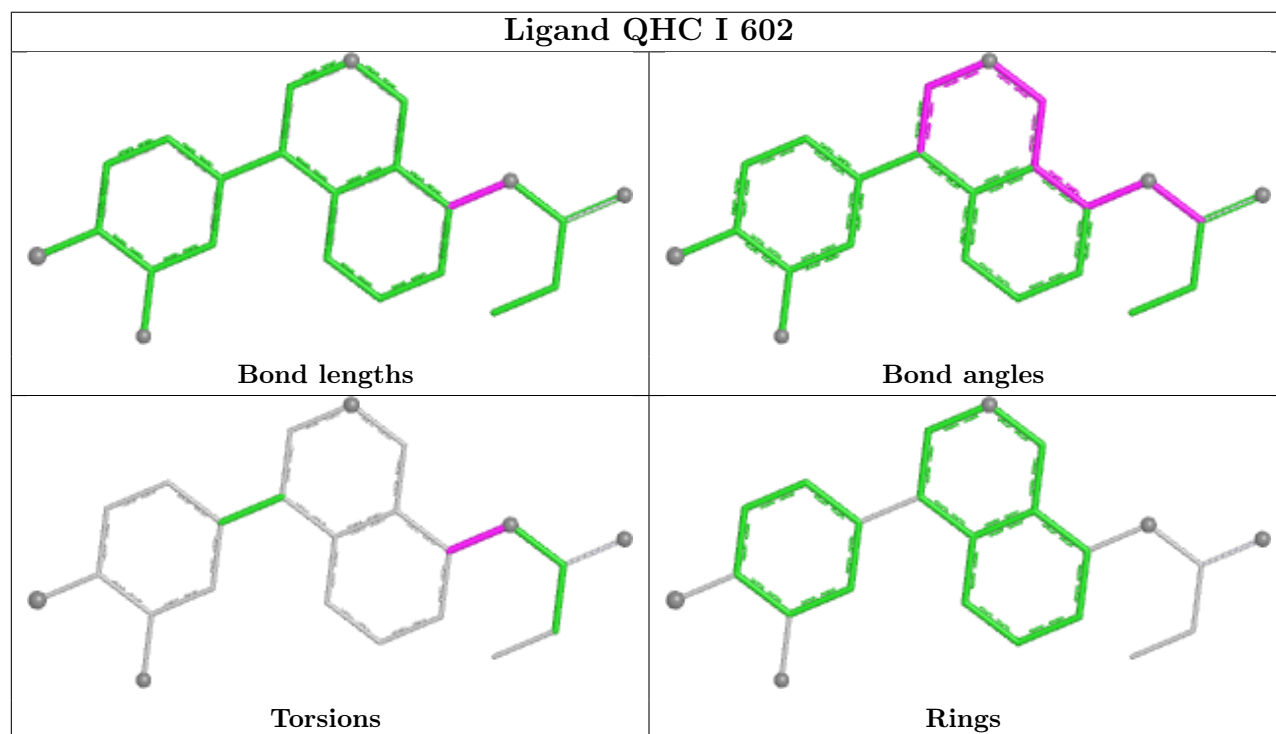
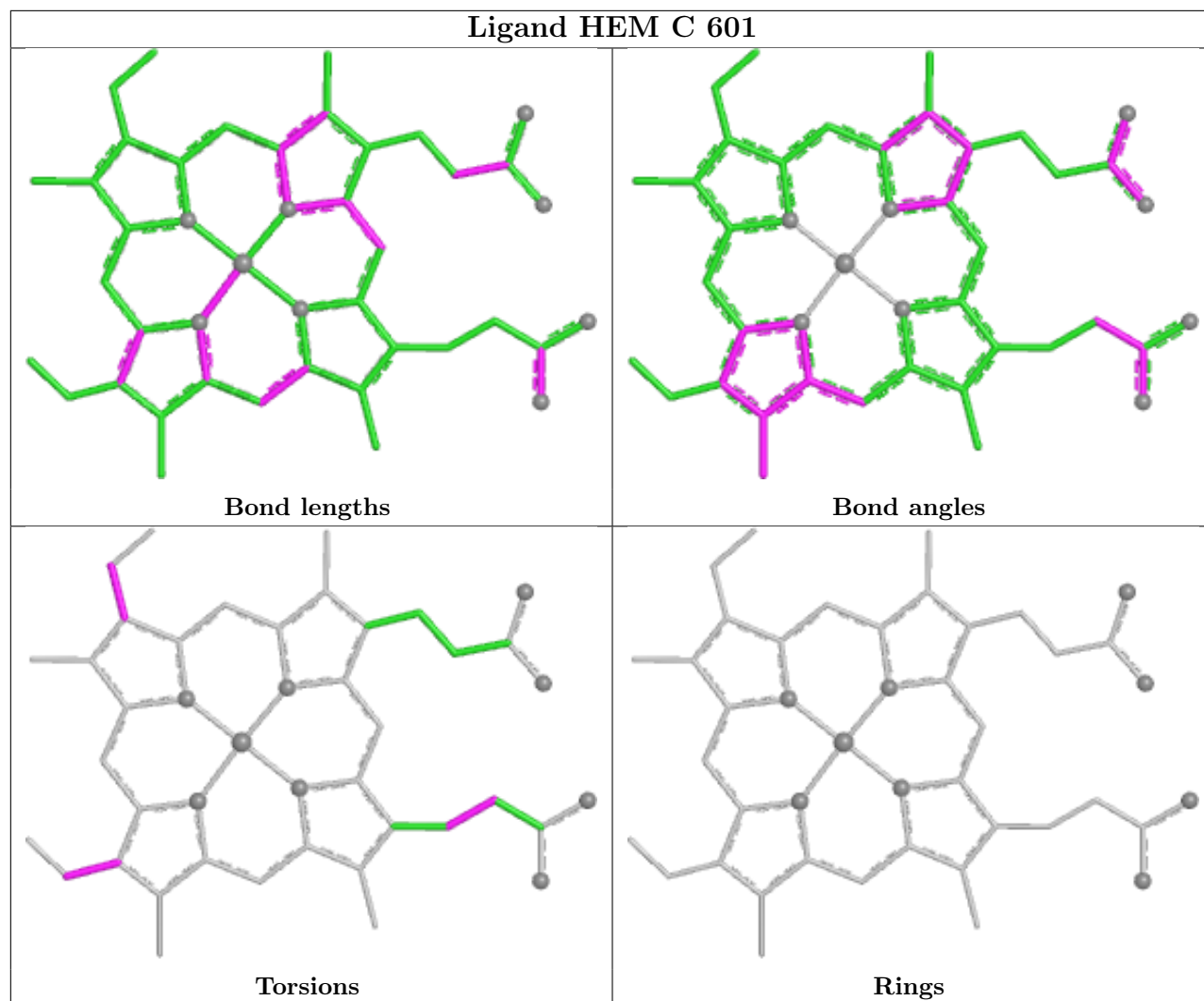
## Ligand QHC J 602

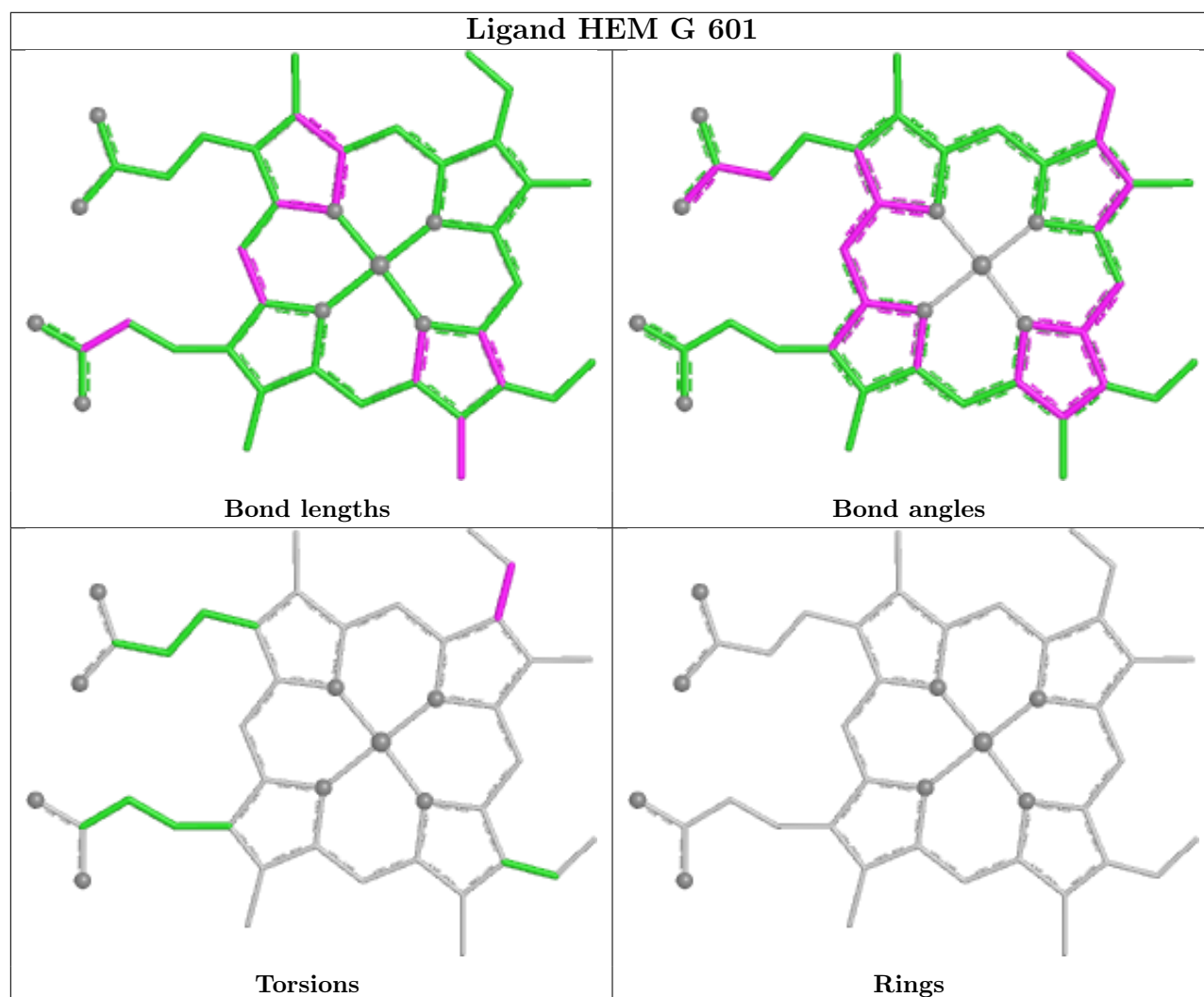
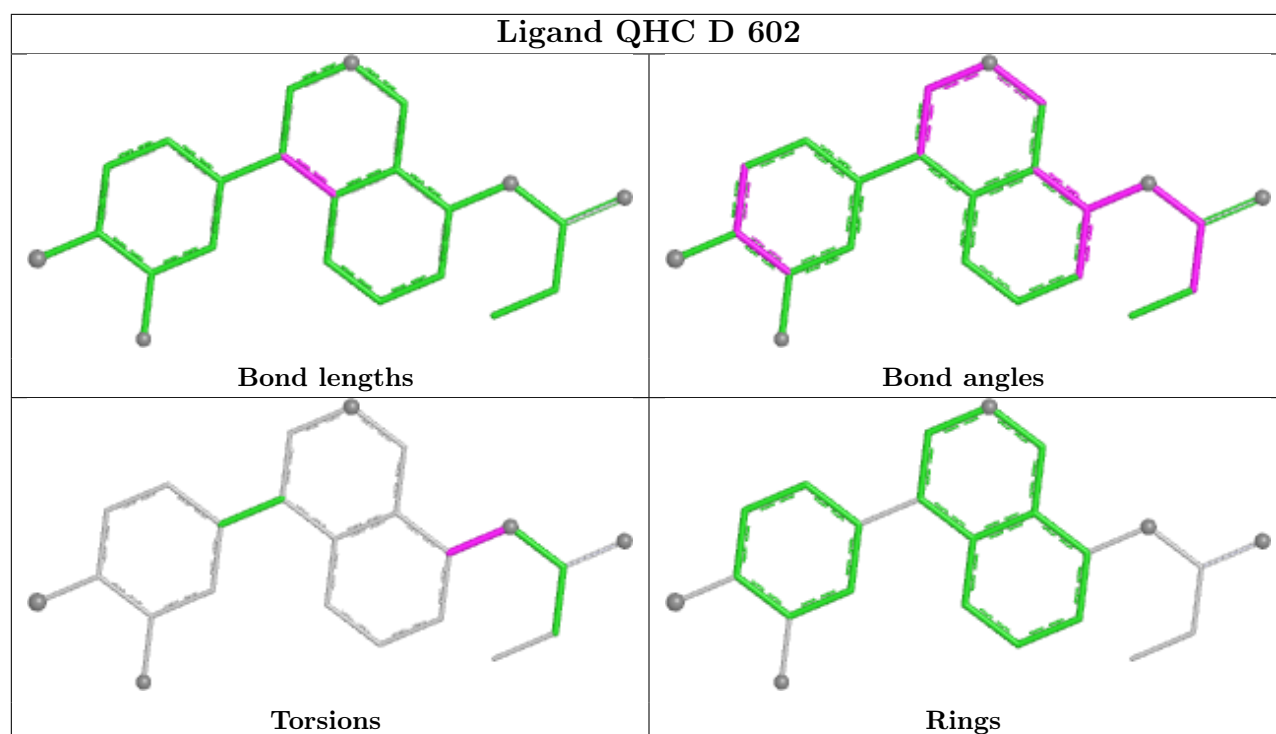


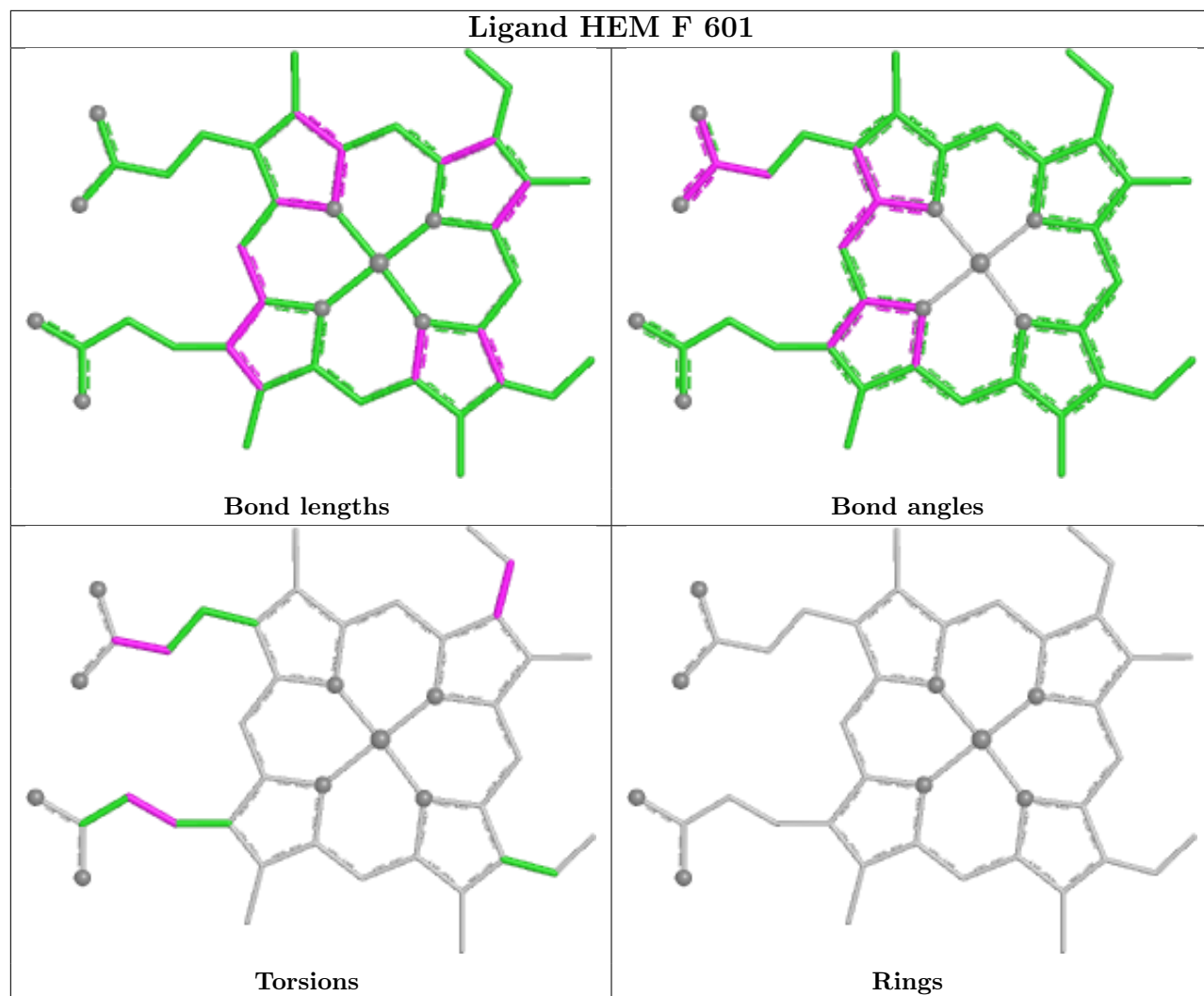
## Ligand QHC F 602

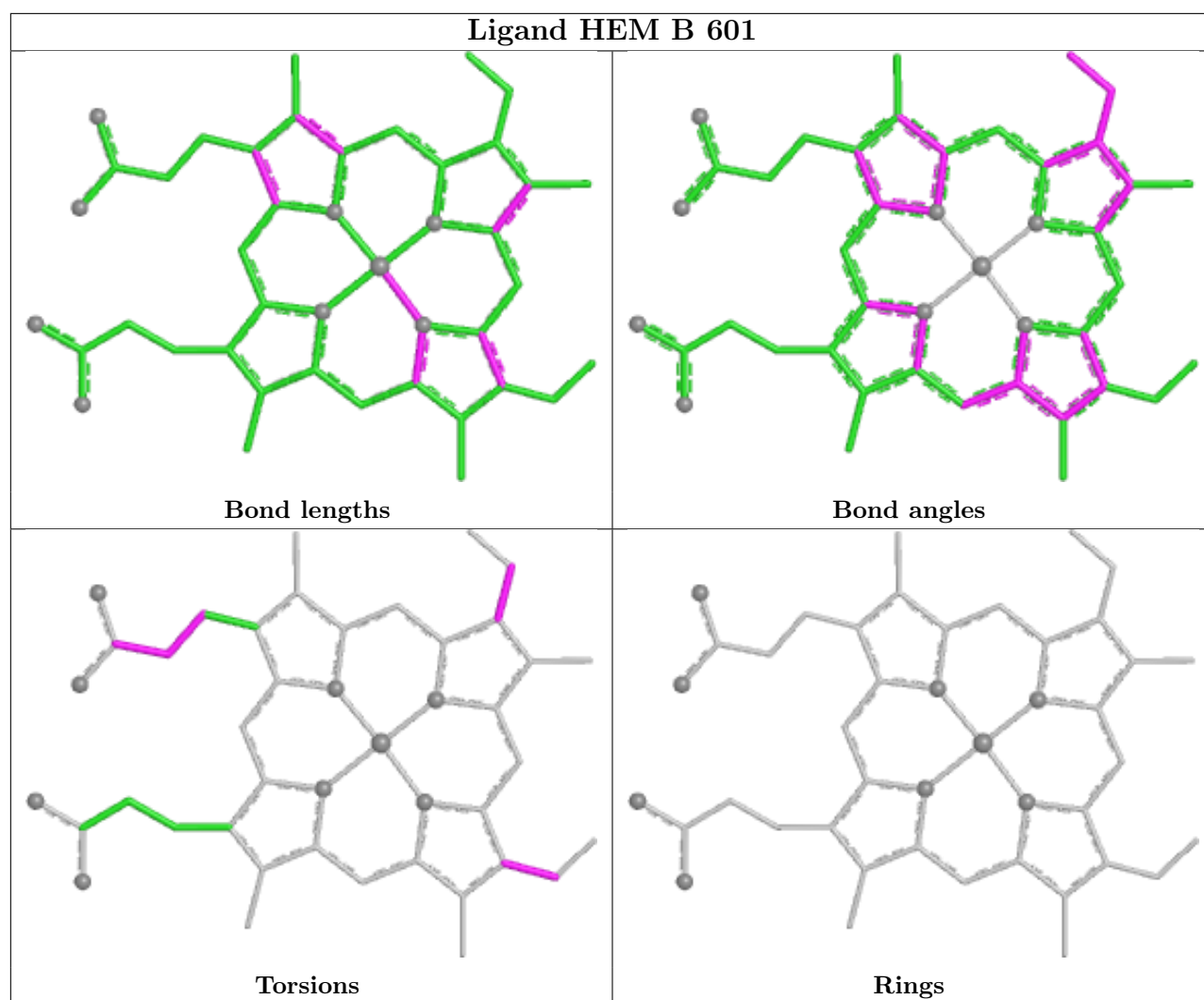












## 5.7 Other polymers [i](#)

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     | 465/489 (95%)   | 0.28   | 3 (0%) 85 73   | 25, 50, 78, 112       | 0     |
| 1   | B     | 465/489 (95%)   | 0.60   | 12 (2%) 57 37  | 27, 64, 99, 126       | 0     |
| 1   | C     | 465/489 (95%)   | 0.69   | 12 (2%) 57 37  | 34, 70, 106, 138      | 0     |
| 1   | D     | 465/489 (95%)   | 0.49   | 5 (1%) 78 61   | 27, 58, 99, 136       | 0     |
| 1   | E     | 459/489 (93%)   | 0.48   | 17 (3%) 45 28  | 31, 58, 105, 140      | 0     |
| 1   | F     | 464/489 (94%)   | 0.68   | 18 (3%) 43 27  | 35, 68, 106, 125      | 0     |
| 1   | G     | 465/489 (95%)   | 0.76   | 14 (3%) 52 33  | 44, 76, 124, 145      | 0     |
| 1   | H     | 465/489 (95%)   | 0.92   | 40 (8%) 16 11  | 43, 78, 122, 173      | 0     |
| 1   | I     | 458/489 (93%)   | 0.73   | 23 (5%) 34 22  | 33, 74, 143, 216      | 0     |
| 1   | J     | 463/489 (94%)   | 0.91   | 34 (7%) 21 13  | 44, 82, 145, 230      | 0     |
| 1   | K     | 461/489 (94%)   | 0.70   | 25 (5%) 31 20  | 35, 68, 107, 127      | 0     |
| 1   | L     | 462/489 (94%)   | 1.03   | 44 (9%) 14 9   | 44, 82, 149, 239      | 0     |
| All | All   | 5557/5868 (94%) | 0.69   | 247 (4%) 39 24 | 25, 69, 118, 239      | 0     |

All (247) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 484 | VAL  | 4.6  |
| 1   | K     | 452 | GLY  | 4.4  |
| 1   | B     | 431 | ILE  | 4.4  |
| 1   | G     | 429 | LEU  | 4.4  |
| 1   | L     | 431 | ILE  | 4.0  |
| 1   | L     | 55  | ILE  | 4.0  |
| 1   | H     | 317 | ASP  | 3.9  |
| 1   | I     | 431 | ILE  | 3.9  |
| 1   | F     | 431 | ILE  | 3.9  |
| 1   | G     | 430 | ASP  | 3.9  |
| 1   | L     | 115 | PRO  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 383 | GLU  | 3.8  |
| 1   | H     | 316 | VAL  | 3.8  |
| 1   | K     | 439 | HIS  | 3.7  |
| 1   | E     | 55  | ILE  | 3.7  |
| 1   | L     | 34  | THR  | 3.7  |
| 1   | C     | 368 | ALA  | 3.6  |
| 1   | H     | 454 | ARG  | 3.6  |
| 1   | B     | 118 | ALA  | 3.5  |
| 1   | B     | 356 | GLN  | 3.5  |
| 1   | D     | 431 | ILE  | 3.5  |
| 1   | C     | 431 | ILE  | 3.4  |
| 1   | A     | 431 | ILE  | 3.4  |
| 1   | K     | 263 | ILE  | 3.4  |
| 1   | F     | 402 | LEU  | 3.3  |
| 1   | L     | 365 | LEU  | 3.3  |
| 1   | E     | 431 | ILE  | 3.3  |
| 1   | H     | 269 | ASN  | 3.2  |
| 1   | H     | 431 | ILE  | 3.2  |
| 1   | J     | 237 | LEU  | 3.2  |
| 1   | L     | 399 | ALA  | 3.2  |
| 1   | E     | 115 | PRO  | 3.2  |
| 1   | G     | 86  | PRO  | 3.2  |
| 1   | H     | 203 | ALA  | 3.2  |
| 1   | H     | 52  | LEU  | 3.2  |
| 1   | F     | 55  | ILE  | 3.2  |
| 1   | J     | 483 | MET  | 3.2  |
| 1   | J     | 61  | TYR  | 3.1  |
| 1   | F     | 441 | VAL  | 3.1  |
| 1   | K     | 431 | ILE  | 3.1  |
| 1   | F     | 386 | VAL  | 3.0  |
| 1   | E     | 50  | LEU  | 3.0  |
| 1   | H     | 65  | HIS  | 3.0  |
| 1   | L     | 42  | PRO  | 3.0  |
| 1   | E     | 53  | LEU  | 3.0  |
| 1   | G     | 52  | LEU  | 3.0  |
| 1   | E     | 269 | ASN  | 3.0  |
| 1   | H     | 430 | ASP  | 2.9  |
| 1   | J     | 88  | MET  | 2.9  |
| 1   | L     | 52  | LEU  | 2.9  |
| 1   | L     | 247 | TRP  | 2.9  |
| 1   | H     | 311 | LEU  | 2.9  |
| 1   | J     | 89  | VAL  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 53  | LEU  | 2.9  |
| 1   | F     | 403 | VAL  | 2.9  |
| 1   | L     | 389 | ASP  | 2.9  |
| 1   | L     | 83  | LEU  | 2.9  |
| 1   | L     | 56  | TRP  | 2.8  |
| 1   | L     | 487 | PHE  | 2.8  |
| 1   | I     | 483 | MET  | 2.8  |
| 1   | C     | 118 | ALA  | 2.8  |
| 1   | A     | 114 | GLU  | 2.8  |
| 1   | H     | 50  | LEU  | 2.8  |
| 1   | B     | 162 | ASP  | 2.8  |
| 1   | I     | 49  | TRP  | 2.8  |
| 1   | J     | 458 | ALA  | 2.8  |
| 1   | J     | 53  | LEU  | 2.8  |
| 1   | H     | 274 | ILE  | 2.8  |
| 1   | L     | 360 | THR  | 2.8  |
| 1   | K     | 61  | TYR  | 2.7  |
| 1   | H     | 437 | ASN  | 2.7  |
| 1   | B     | 342 | GLN  | 2.7  |
| 1   | J     | 66  | LEU  | 2.7  |
| 1   | L     | 60  | GLY  | 2.7  |
| 1   | G     | 61  | TYR  | 2.7  |
| 1   | F     | 100 | LEU  | 2.7  |
| 1   | H     | 406 | PHE  | 2.7  |
| 1   | K     | 85  | GLY  | 2.7  |
| 1   | H     | 315 | SER  | 2.7  |
| 1   | L     | 388 | SER  | 2.7  |
| 1   | J     | 244 | LEU  | 2.7  |
| 1   | K     | 50  | LEU  | 2.7  |
| 1   | L     | 86  | PRO  | 2.7  |
| 1   | G     | 60  | GLY  | 2.7  |
| 1   | C     | 180 | ALA  | 2.7  |
| 1   | F     | 106 | LEU  | 2.7  |
| 1   | I     | 61  | TYR  | 2.7  |
| 1   | D     | 439 | HIS  | 2.7  |
| 1   | I     | 88  | MET  | 2.6  |
| 1   | K     | 53  | LEU  | 2.6  |
| 1   | H     | 86  | PRO  | 2.6  |
| 1   | L     | 155 | GLN  | 2.6  |
| 1   | G     | 385 | VAL  | 2.6  |
| 1   | K     | 157 | PHE  | 2.6  |
| 1   | L     | 38  | PHE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 60  | GLY  | 2.6  |
| 1   | G     | 49  | TRP  | 2.6  |
| 1   | J     | 127 | CYS  | 2.6  |
| 1   | K     | 51  | ARG  | 2.6  |
| 1   | K     | 438 | PHE  | 2.6  |
| 1   | I     | 388 | SER  | 2.6  |
| 1   | F     | 489 | LEU  | 2.5  |
| 1   | L     | 324 | LEU  | 2.5  |
| 1   | L     | 386 | VAL  | 2.5  |
| 1   | J     | 40  | ALA  | 2.5  |
| 1   | H     | 150 | SER  | 2.5  |
| 1   | H     | 243 | SER  | 2.5  |
| 1   | L     | 97  | VAL  | 2.5  |
| 1   | G     | 55  | ILE  | 2.5  |
| 1   | J     | 239 | PHE  | 2.5  |
| 1   | L     | 168 | PHE  | 2.5  |
| 1   | G     | 283 | PRO  | 2.5  |
| 1   | I     | 50  | LEU  | 2.5  |
| 1   | J     | 106 | LEU  | 2.5  |
| 1   | L     | 362 | LEU  | 2.5  |
| 1   | I     | 55  | ILE  | 2.5  |
| 1   | H     | 442 | PRO  | 2.5  |
| 1   | L     | 492 | GLY  | 2.5  |
| 1   | B     | 70  | GLN  | 2.5  |
| 1   | I     | 487 | PHE  | 2.5  |
| 1   | E     | 45  | PRO  | 2.5  |
| 1   | K     | 211 | LEU  | 2.4  |
| 1   | J     | 86  | PRO  | 2.4  |
| 1   | L     | 45  | PRO  | 2.4  |
| 1   | L     | 159 | PRO  | 2.4  |
| 1   | I     | 484 | VAL  | 2.4  |
| 1   | L     | 124 | GLY  | 2.4  |
| 1   | K     | 203 | ALA  | 2.4  |
| 1   | E     | 487 | PHE  | 2.4  |
| 1   | L     | 381 | PHE  | 2.4  |
| 1   | E     | 211 | LEU  | 2.4  |
| 1   | H     | 75  | LEU  | 2.4  |
| 1   | J     | 81  | TYR  | 2.4  |
| 1   | J     | 39  | GLU  | 2.4  |
| 1   | H     | 308 | SER  | 2.4  |
| 1   | I     | 390 | LEU  | 2.4  |
| 1   | L     | 461 | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 106 | LEU  | 2.4  |
| 1   | J     | 34  | THR  | 2.4  |
| 1   | E     | 430 | ASP  | 2.4  |
| 1   | K     | 206 | GLY  | 2.4  |
| 1   | F     | 113 | LEU  | 2.4  |
| 1   | A     | 155 | GLN  | 2.3  |
| 1   | B     | 365 | LEU  | 2.3  |
| 1   | H     | 121 | GLN  | 2.3  |
| 1   | H     | 438 | PHE  | 2.3  |
| 1   | J     | 487 | PHE  | 2.3  |
| 1   | H     | 271 | ILE  | 2.3  |
| 1   | J     | 431 | ILE  | 2.3  |
| 1   | H     | 313 | ALA  | 2.3  |
| 1   | L     | 486 | SER  | 2.3  |
| 1   | E     | 52  | LEU  | 2.3  |
| 1   | I     | 402 | LEU  | 2.3  |
| 1   | L     | 50  | LEU  | 2.3  |
| 1   | F     | 62  | GLU  | 2.3  |
| 1   | I     | 62  | GLU  | 2.3  |
| 1   | B     | 357 | LYS  | 2.3  |
| 1   | J     | 486 | SER  | 2.3  |
| 1   | L     | 369 | LEU  | 2.3  |
| 1   | H     | 286 | TYR  | 2.3  |
| 1   | G     | 78  | ILE  | 2.3  |
| 1   | J     | 488 | ILE  | 2.3  |
| 1   | H     | 106 | LEU  | 2.3  |
| 1   | F     | 486 | SER  | 2.3  |
| 1   | L     | 321 | PHE  | 2.3  |
| 1   | C     | 317 | ASP  | 2.3  |
| 1   | F     | 407 | LEU  | 2.2  |
| 1   | H     | 247 | TRP  | 2.2  |
| 1   | H     | 428 | TRP  | 2.2  |
| 1   | H     | 107 | HIS  | 2.2  |
| 1   | K     | 264 | PHE  | 2.2  |
| 1   | L     | 439 | HIS  | 2.2  |
| 1   | J     | 503 | ASN  | 2.2  |
| 1   | B     | 335 | ASP  | 2.2  |
| 1   | C     | 204 | LEU  | 2.2  |
| 1   | J     | 253 | TRP  | 2.2  |
| 1   | C     | 423 | TYR  | 2.2  |
| 1   | F     | 484 | VAL  | 2.2  |
| 1   | J     | 43  | GLN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 78  | ILE  | 2.2  |
| 1   | C     | 447 | MET  | 2.2  |
| 1   | E     | 60  | GLY  | 2.2  |
| 1   | J     | 52  | LEU  | 2.2  |
| 1   | L     | 100 | LEU  | 2.2  |
| 1   | H     | 201 | ASN  | 2.2  |
| 1   | H     | 459 | GLU  | 2.2  |
| 1   | B     | 317 | ASP  | 2.2  |
| 1   | G     | 104 | ASP  | 2.2  |
| 1   | E     | 247 | TRP  | 2.2  |
| 1   | H     | 112 | ILE  | 2.2  |
| 1   | K     | 272 | GLN  | 2.2  |
| 1   | I     | 392 | LEU  | 2.2  |
| 1   | J     | 238 | MET  | 2.2  |
| 1   | D     | 46  | GLY  | 2.2  |
| 1   | I     | 400 | GLY  | 2.2  |
| 1   | E     | 56  | TRP  | 2.2  |
| 1   | I     | 244 | LEU  | 2.1  |
| 1   | C     | 310 | GLU  | 2.1  |
| 1   | I     | 86  | PRO  | 2.1  |
| 1   | H     | 205 | PHE  | 2.1  |
| 1   | D     | 477 | THR  | 2.1  |
| 1   | C     | 324 | LEU  | 2.1  |
| 1   | H     | 126 | LYS  | 2.1  |
| 1   | K     | 93  | LEU  | 2.1  |
| 1   | G     | 426 | GLN  | 2.1  |
| 1   | K     | 313 | ALA  | 2.1  |
| 1   | I     | 387 | SER  | 2.1  |
| 1   | J     | 280 | PHE  | 2.1  |
| 1   | K     | 239 | PHE  | 2.1  |
| 1   | F     | 61  | TYR  | 2.1  |
| 1   | H     | 53  | LEU  | 2.1  |
| 1   | J     | 50  | LEU  | 2.1  |
| 1   | L     | 402 | LEU  | 2.1  |
| 1   | F     | 447 | MET  | 2.1  |
| 1   | I     | 40  | ALA  | 2.1  |
| 1   | E     | 201 | ASN  | 2.1  |
| 1   | K     | 161 | VAL  | 2.1  |
| 1   | H     | 56  | TRP  | 2.1  |
| 1   | J     | 262 | CYS  | 2.1  |
| 1   | K     | 440 | HIS  | 2.1  |
| 1   | H     | 348 | ALA  | 2.1  |

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*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 489 | LEU  | 2.1  |
| 1   | J     | 113 | LEU  | 2.1  |
| 1   | K     | 113 | LEU  | 2.1  |
| 1   | L     | 392 | LEU  | 2.1  |
| 1   | I     | 444 | GLY  | 2.1  |
| 1   | B     | 355 | PRO  | 2.1  |
| 1   | J     | 37  | PRO  | 2.1  |
| 1   | L     | 37  | PRO  | 2.1  |
| 1   | I     | 75  | LEU  | 2.0  |
| 1   | K     | 247 | TRP  | 2.0  |
| 1   | C     | 34  | THR  | 2.0  |
| 1   | E     | 54  | GLN  | 2.0  |
| 1   | L     | 102 | GLN  | 2.0  |
| 1   | E     | 103 | VAL  | 2.0  |
| 1   | H     | 149 | LEU  | 2.0  |
| 1   | I     | 53  | LEU  | 2.0  |
| 1   | C     | 409 | SER  | 2.0  |
| 1   | D     | 481 | ILE  | 2.0  |
| 1   | F     | 488 | ILE  | 2.0  |
| 1   | K     | 437 | ASN  | 2.0  |
| 1   | H     | 443 | PHE  | 2.0  |
| 1   | J     | 76  | GLY  | 2.0  |
| 1   | I     | 495 | PRO  | 2.0  |
| 1   | K     | 45  | PRO  | 2.0  |
| 1   | L     | 393 | GLN  | 2.0  |
| 1   | L     | 364 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

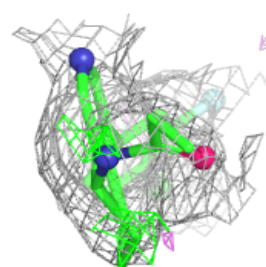
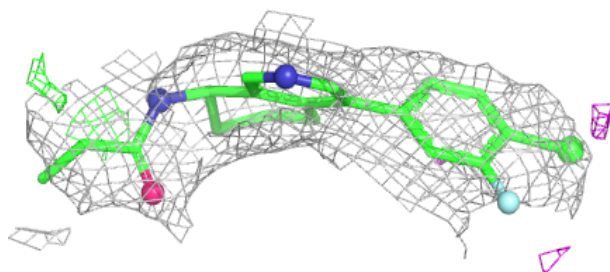
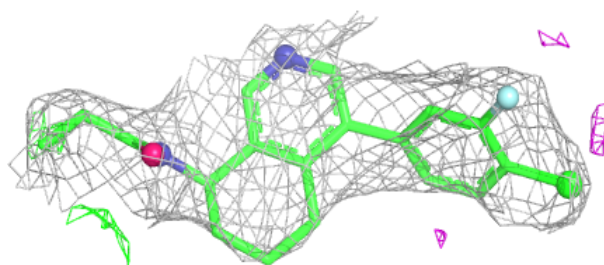
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | QHC  | C     | 602 | 23/23 | 0.84 | 0.20 | 84,85,89,91                 | 0     |
| 3   | QHC  | D     | 602 | 23/23 | 0.85 | 0.17 | 54,60,61,61                 | 0     |
| 3   | QHC  | L     | 602 | 23/23 | 0.85 | 0.16 | 65,74,84,86                 | 0     |
| 3   | QHC  | I     | 602 | 23/23 | 0.86 | 0.16 | 56,66,73,75                 | 0     |
| 3   | QHC  | J     | 602 | 23/23 | 0.87 | 0.14 | 50,54,68,74                 | 0     |
| 3   | QHC  | B     | 602 | 23/23 | 0.87 | 0.16 | 56,62,69,72                 | 0     |
| 3   | QHC  | F     | 602 | 23/23 | 0.90 | 0.13 | 51,61,68,68                 | 0     |
| 3   | QHC  | E     | 602 | 23/23 | 0.90 | 0.12 | 44,49,53,54                 | 0     |
| 3   | QHC  | K     | 602 | 23/23 | 0.91 | 0.13 | 51,60,72,72                 | 0     |
| 2   | HEM  | H     | 601 | 43/43 | 0.91 | 0.15 | 62,64,67,68                 | 0     |
| 2   | HEM  | L     | 601 | 43/43 | 0.92 | 0.13 | 59,60,64,64                 | 0     |
| 2   | HEM  | B     | 601 | 43/43 | 0.92 | 0.14 | 54,56,60,61                 | 0     |
| 2   | HEM  | J     | 601 | 43/43 | 0.94 | 0.12 | 51,52,56,58                 | 0     |
| 2   | HEM  | K     | 601 | 43/43 | 0.94 | 0.12 | 55,56,60,64                 | 0     |
| 2   | HEM  | G     | 601 | 43/43 | 0.94 | 0.11 | 51,52,56,58                 | 0     |
| 2   | HEM  | I     | 601 | 43/43 | 0.94 | 0.12 | 53,54,58,65                 | 0     |
| 2   | HEM  | F     | 601 | 43/43 | 0.95 | 0.11 | 46,48,52,52                 | 0     |
| 2   | HEM  | A     | 601 | 43/43 | 0.95 | 0.11 | 39,39,44,51                 | 0     |
| 2   | HEM  | E     | 601 | 43/43 | 0.96 | 0.10 | 43,44,48,49                 | 0     |
| 2   | HEM  | C     | 601 | 43/43 | 0.96 | 0.10 | 39,41,46,48                 | 0     |
| 3   | QHC  | A     | 602 | 23/23 | 0.96 | 0.07 | 3,13,32,37                  | 0     |
| 2   | HEM  | D     | 601 | 43/43 | 0.96 | 0.10 | 32,33,38,43                 | 0     |

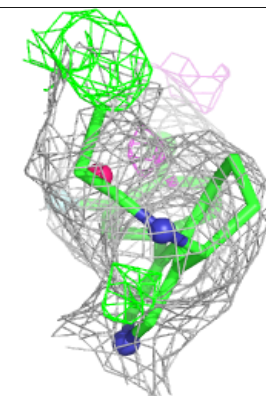
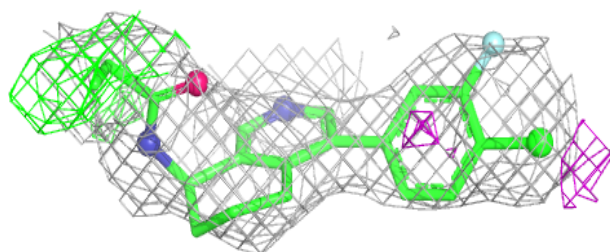
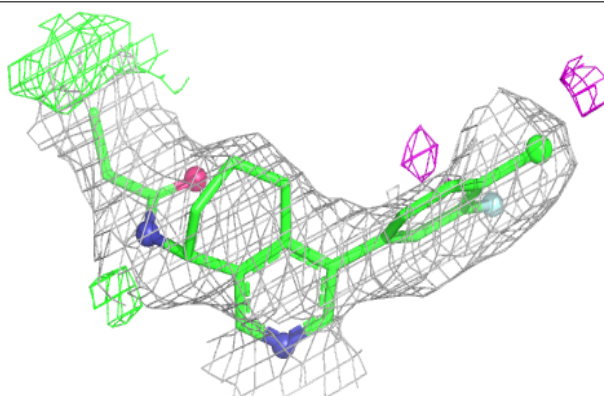
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around QHC C 602:**

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

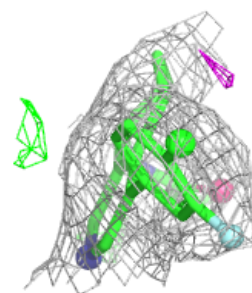
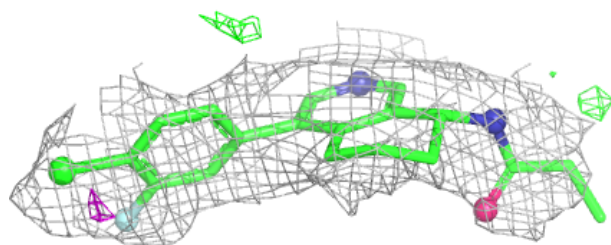
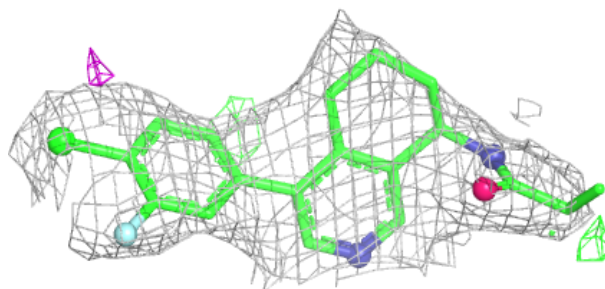
**Electron density around QHC D 602:**

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

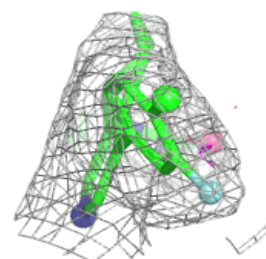
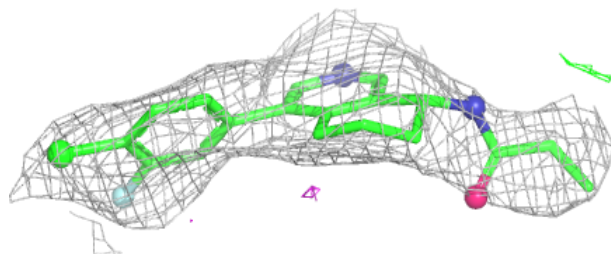
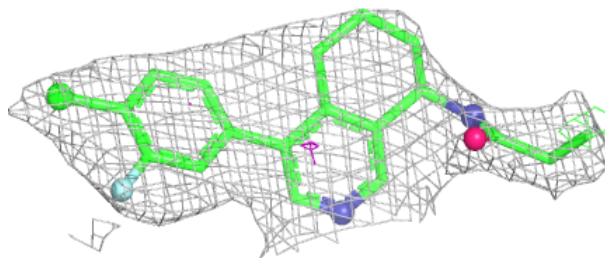


**Electron density around QHC L 602:**

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

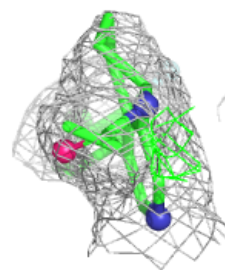
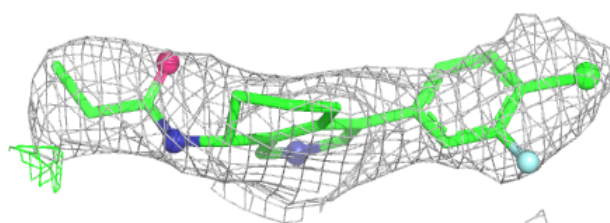
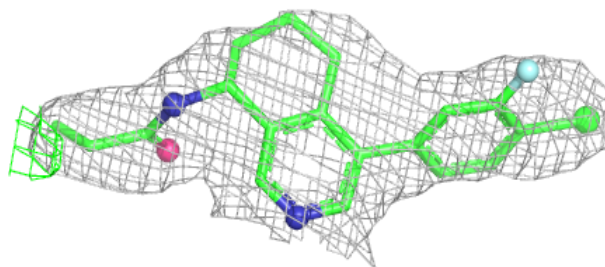
**Electron density around QHC I 602:**

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and green (positive)

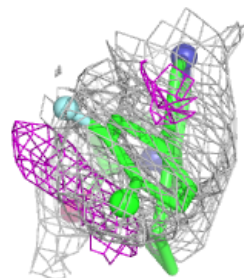
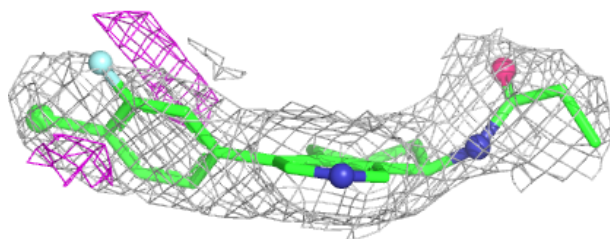
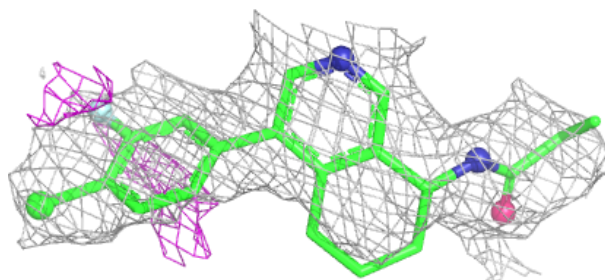


**Electron density around QHC J 602:**

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

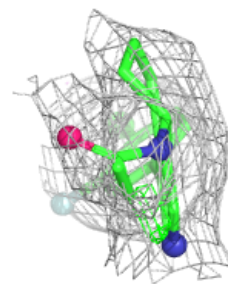
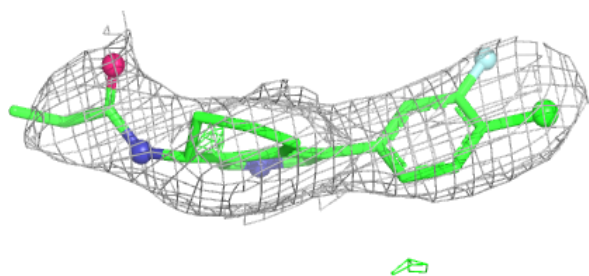
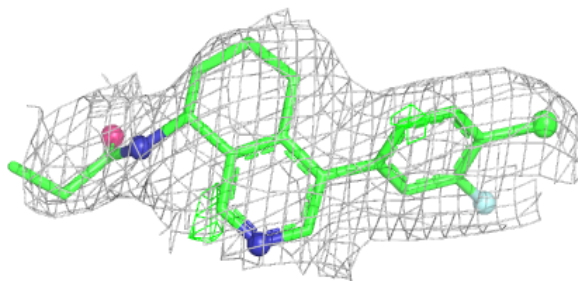
**Electron density around QHC B 602:**

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and green (positive)

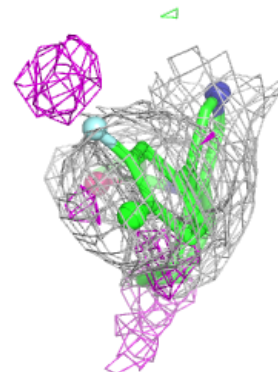
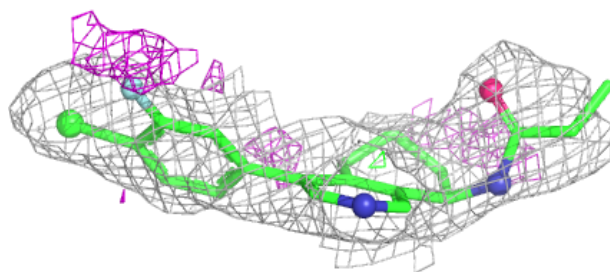
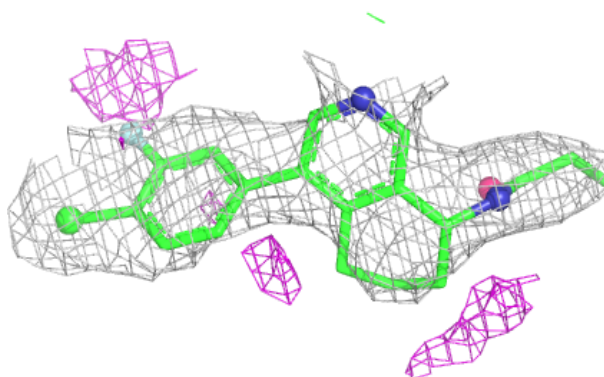


**Electron density around QHC F 602:**

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and green (positive)

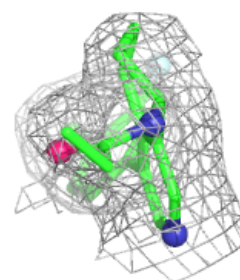
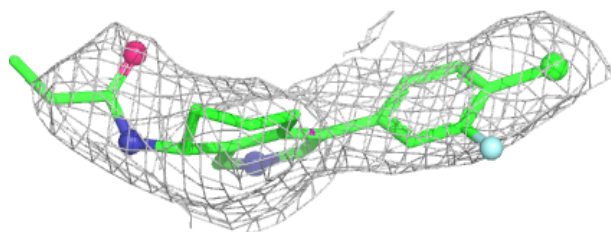
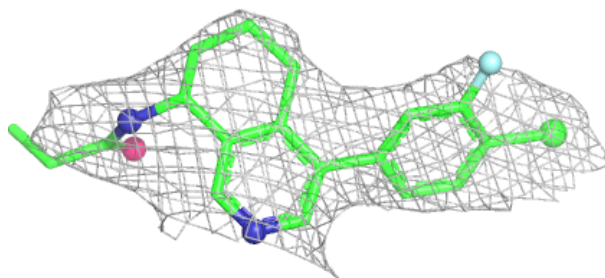
**Electron density around QHC E 602:**

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and green (positive)



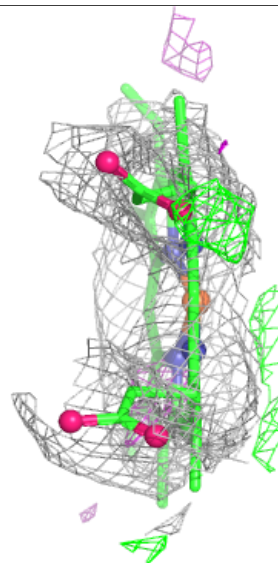
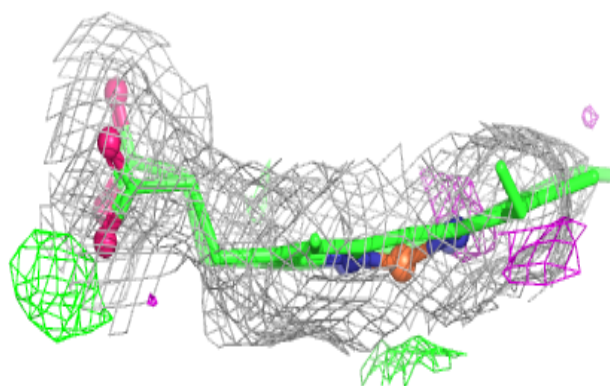
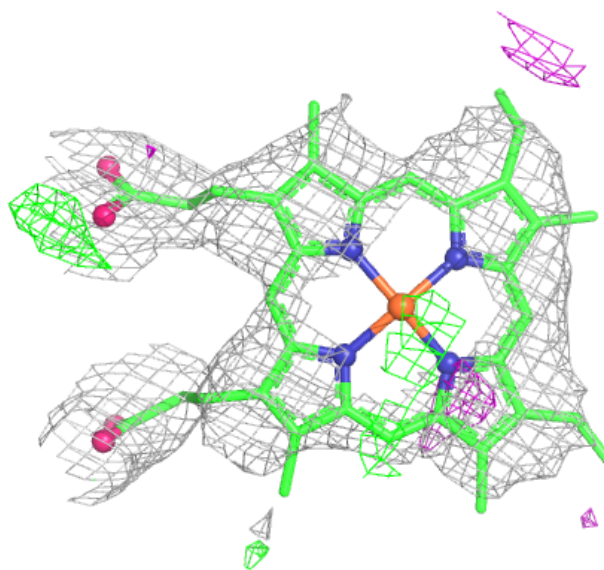
**Electron density around QHC K 602:**

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and green (positive)



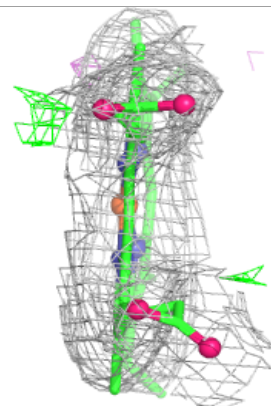
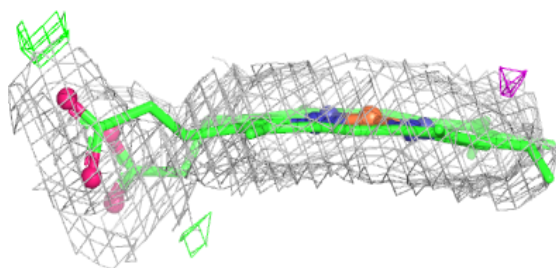
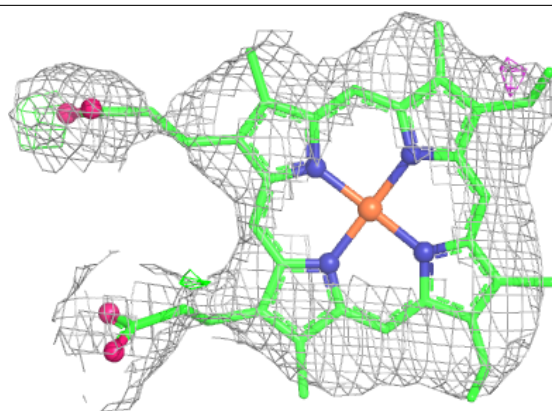
**Electron density around HEM H 601:**

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



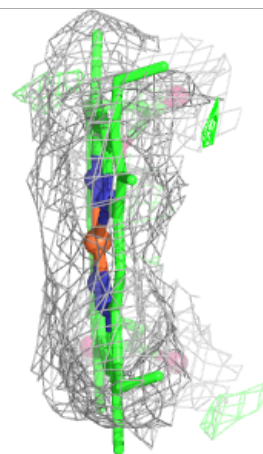
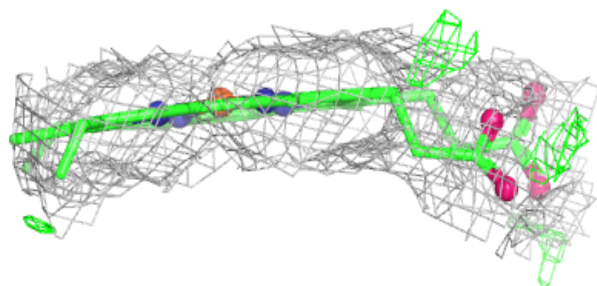
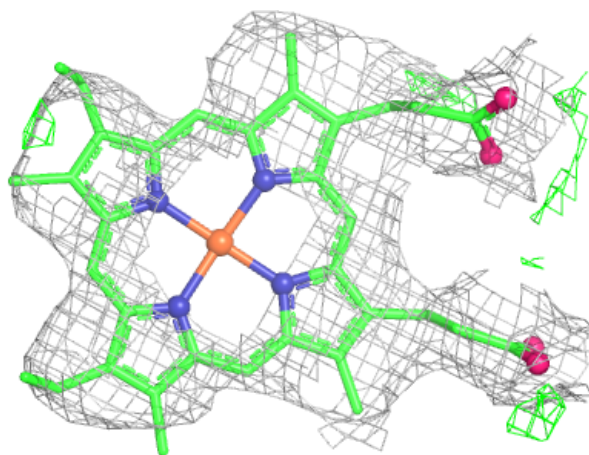
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and green (positive)



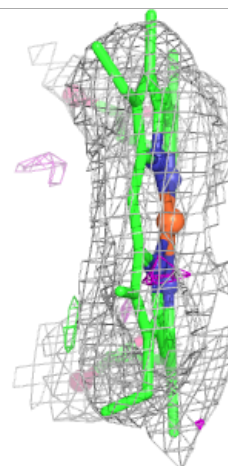
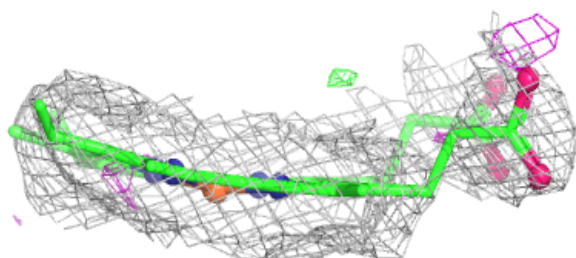
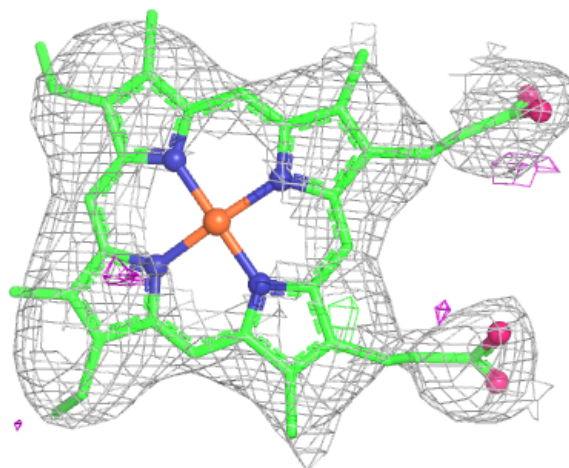
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and green (positive)



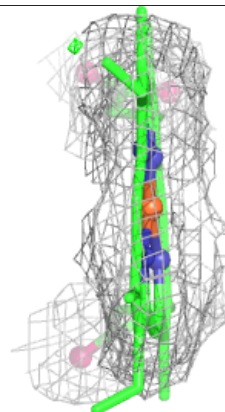
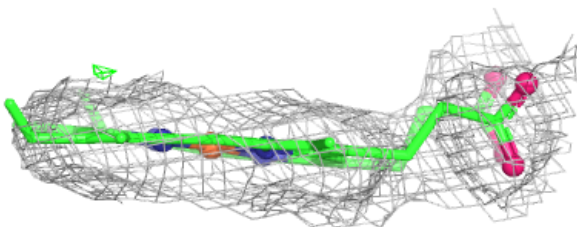
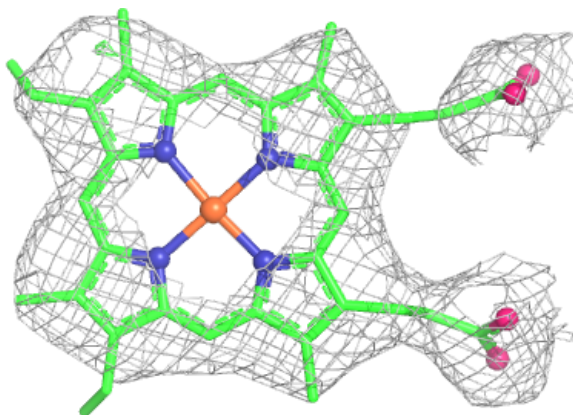
**Electron density around HEM J 601:**

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and green (positive)



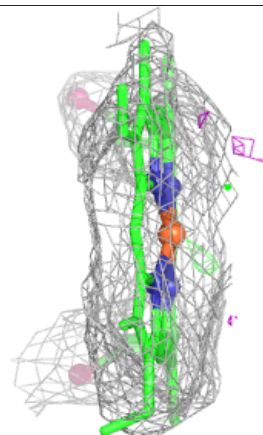
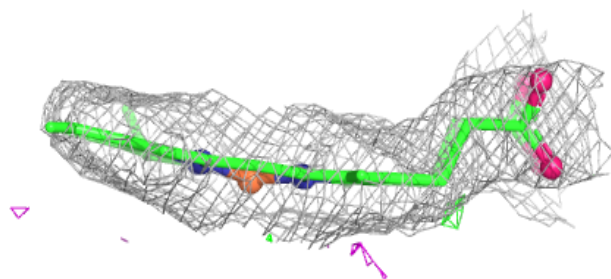
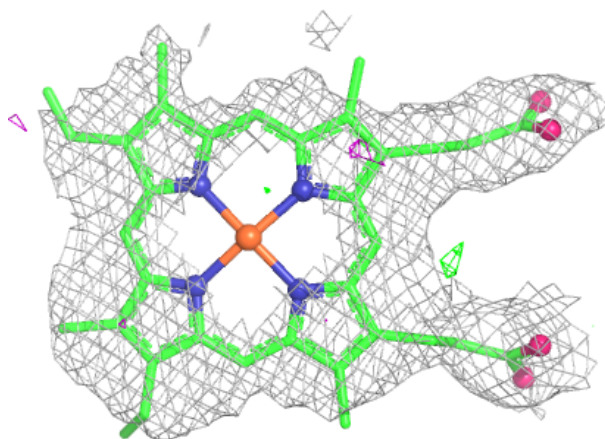
**Electron density around HEM K 601:**

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and green (positive)



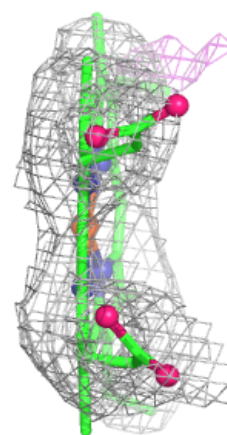
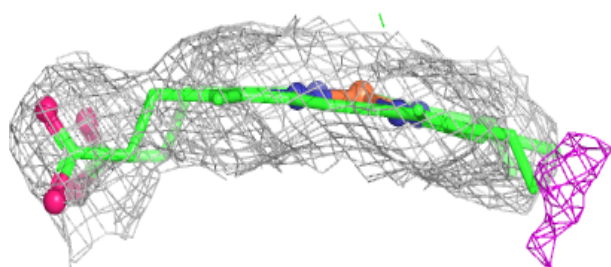
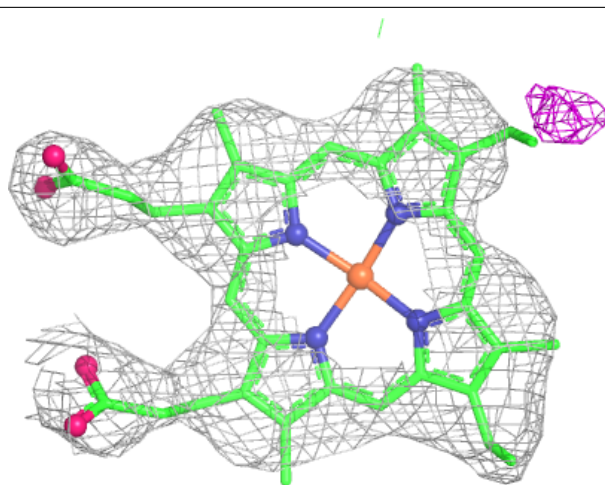
**Electron density around HEM G 601:**

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



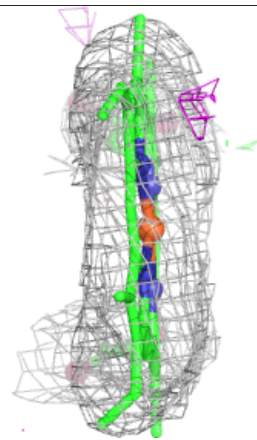
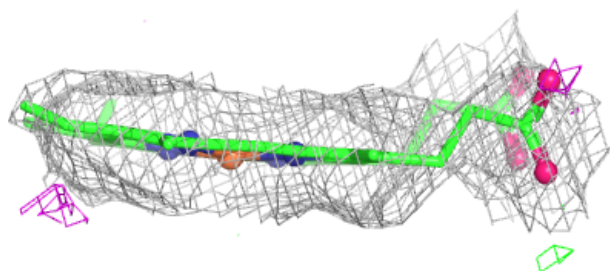
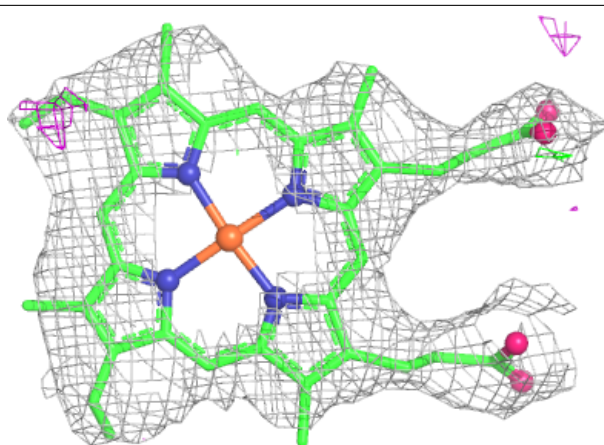
**Electron density around HEM I 601:**

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



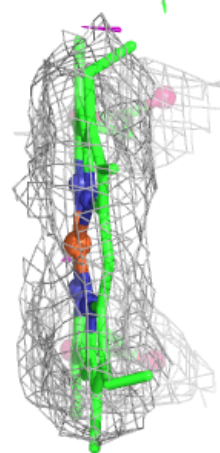
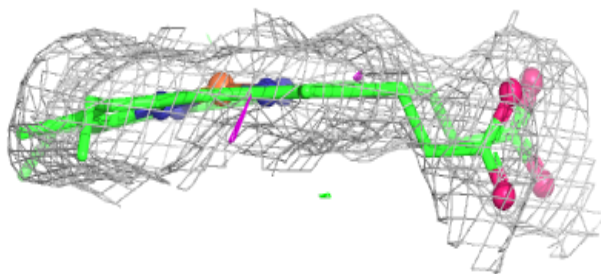
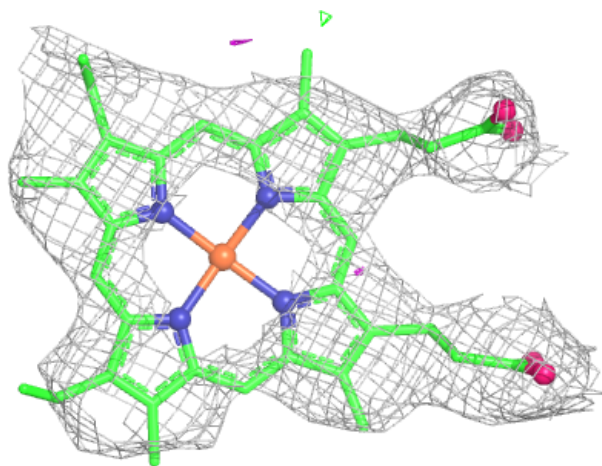
**Electron density around HEM F 601:**

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



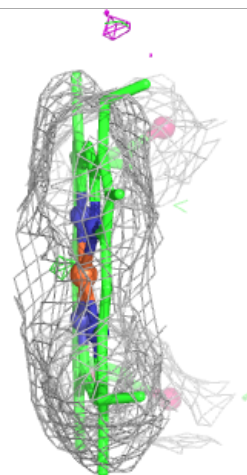
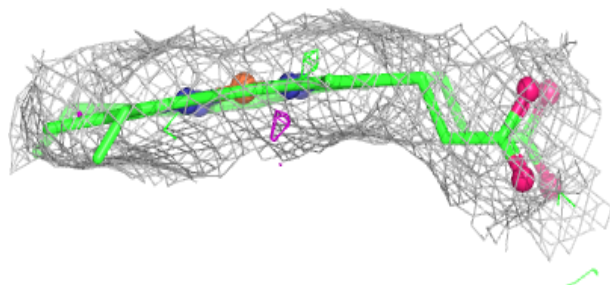
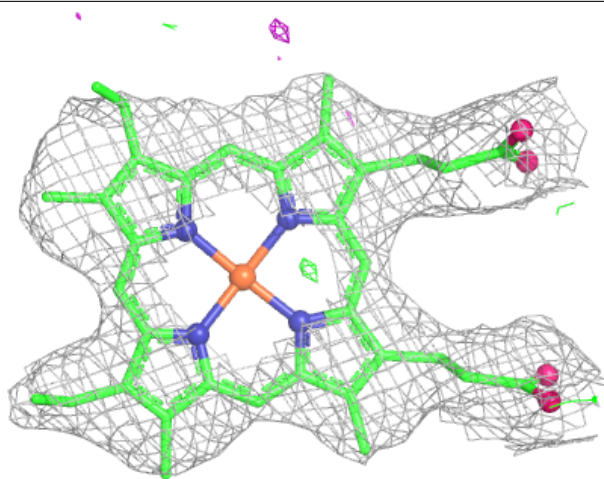
**Electron density around HEM A 601:**

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



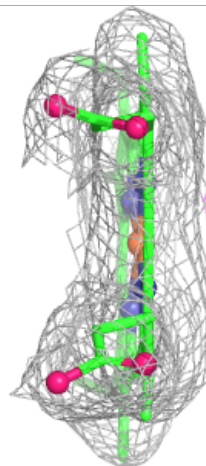
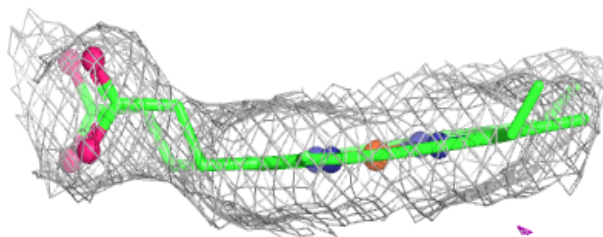
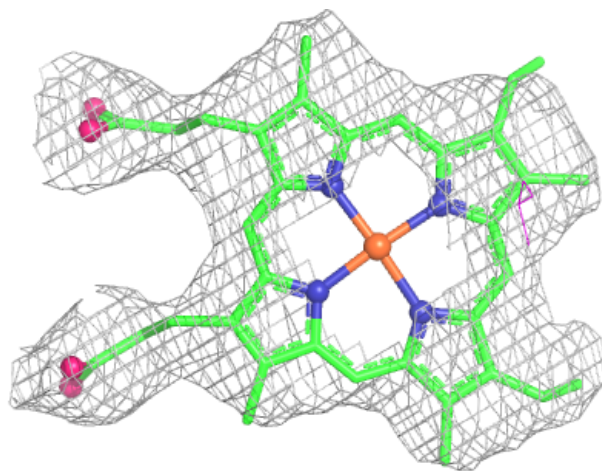
**Electron density around HEM E 601:**

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



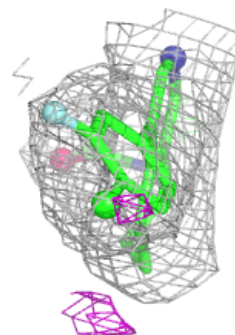
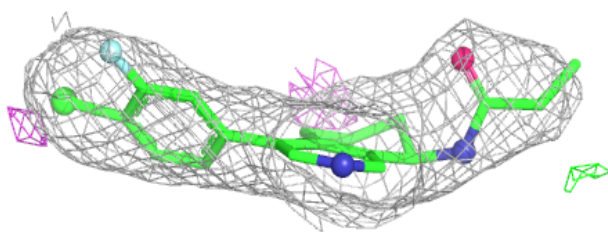
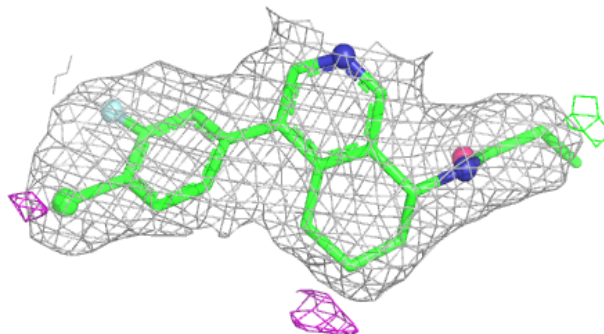
**Electron density around HEM C 601:**

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

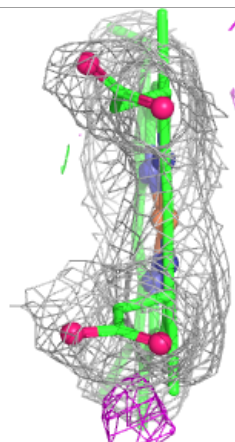
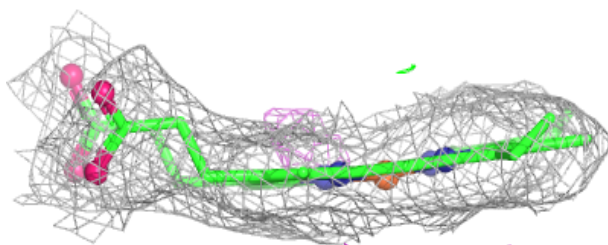
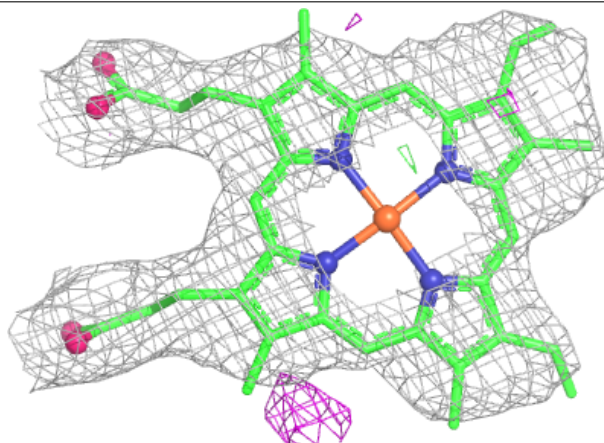


**Electron density around QHC A 602:**

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

**Electron density around HEM D 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.