



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:17 AM UTC

PDB ID : 4BF4 / pdb\_00004bf4  
Title : PikC D50N mutant in complex with the engineered cycloalkane substrate mimic bearing a terminal N,N-dimethylamino group  
Authors : Podust, L.M.  
Deposited on : 2013-03-14  
Resolution : 2.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

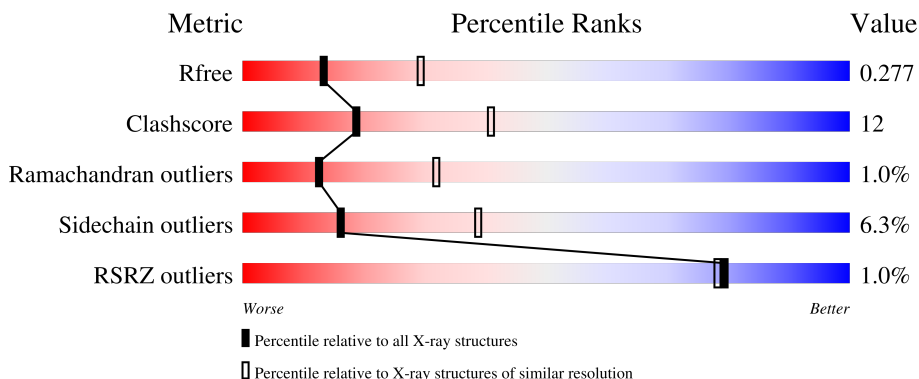
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |

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     | 436    | <br>64% 25% 9%   |
| 1   | B     | 436    | <br>64% 26% 9%   |
| 1   | C     | 436    | <br>68% 20% 9%   |
| 1   | D     | 436    | <br>64% 23% 9%   |
| 1   | E     | 436    | <br>66% 22% 9%   |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | F     | 436    |  66% 24% 9%    |
| 1   | G     | 436    |  68% 20% 9%    |
| 1   | H     | 436    |  68% 22% 9%    |
| 1   | I     | 436    |  70% 18% 9%    |
| 1   | J     | 436    |  67% 22% 9%    |
| 1   | K     | 436    |  65% 24% 9%    |
| 1   | L     | 436    |  1% 66% 23% 9% |
| 1   | M     | 436    |  61% 27% 9%    |
| 1   | N     | 436    |  2% 67% 20% 9% |
| 1   | O     | 436    |  3% 65% 24% 9% |
| 1   | P     | 436    |  4% 64% 25% 9% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | SO4  | A     | 1408 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50342 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 HYDROXYLASE PIKC.

| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
|     |       |          | Total         | C         | N        | O        | S       |         |         |       |
| 1   | A     | 396      | Total<br>3031 | C<br>1912 | N<br>545 | O<br>561 | S<br>13 | 0       | 0       | 0     |
| 1   | B     | 397      | Total<br>3069 | C<br>1939 | N<br>553 | O<br>564 | S<br>13 | 0       | 2       | 0     |
| 1   | C     | 396      | Total<br>3063 | C<br>1937 | N<br>549 | O<br>564 | S<br>13 | 0       | 1       | 0     |
| 1   | D     | 397      | Total<br>3076 | C<br>1942 | N<br>552 | O<br>569 | S<br>13 | 0       | 2       | 0     |
| 1   | E     | 397      | Total<br>3068 | C<br>1938 | N<br>550 | O<br>567 | S<br>13 | 0       | 1       | 0     |
| 1   | F     | 396      | Total<br>3075 | C<br>1944 | N<br>552 | O<br>566 | S<br>13 | 0       | 4       | 0     |
| 1   | G     | 396      | Total<br>3093 | C<br>1952 | N<br>557 | O<br>571 | S<br>13 | 0       | 4       | 0     |
| 1   | H     | 396      | Total<br>3057 | C<br>1935 | N<br>549 | O<br>560 | S<br>13 | 0       | 1       | 0     |
| 1   | I     | 396      | Total<br>3066 | C<br>1939 | N<br>550 | O<br>564 | S<br>13 | 0       | 2       | 0     |
| 1   | J     | 397      | Total<br>3060 | C<br>1934 | N<br>551 | O<br>562 | S<br>13 | 0       | 1       | 0     |
| 1   | K     | 397      | Total<br>3076 | C<br>1944 | N<br>551 | O<br>568 | S<br>13 | 0       | 2       | 0     |
| 1   | L     | 397      | Total<br>3065 | C<br>1938 | N<br>551 | O<br>563 | S<br>13 | 0       | 2       | 0     |
| 1   | M     | 397      | Total<br>3065 | C<br>1936 | N<br>551 | O<br>565 | S<br>13 | 0       | 1       | 0     |
| 1   | N     | 397      | Total<br>3064 | C<br>1938 | N<br>550 | O<br>563 | S<br>13 | 0       | 1       | 0     |
| 1   | O     | 397      | Total<br>3052 | C<br>1931 | N<br>548 | O<br>560 | S<br>13 | 0       | 0       | 0     |
| 1   | P     | 396      | Total<br>3058 | C<br>1932 | N<br>548 | O<br>565 | S<br>13 | 0       | 1       | 0     |

There are 336 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | -19     | MET      | -      | expression tag      | UNP O87605 |
| A     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| A     | -17     | SER      | -      | expression tag      | UNP O87605 |
| A     | -16     | SER      | -      | expression tag      | UNP O87605 |
| A     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| A     | -14     | HIS      | -      | expression tag      | UNP O87605 |
| A     | -13     | HIS      | -      | expression tag      | UNP O87605 |
| A     | -12     | HIS      | -      | expression tag      | UNP O87605 |
| A     | -11     | HIS      | -      | expression tag      | UNP O87605 |
| A     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| A     | -9      | SER      | -      | expression tag      | UNP O87605 |
| A     | -8      | SER      | -      | expression tag      | UNP O87605 |
| A     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| A     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| A     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| A     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| A     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| A     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| A     | -1      | SER      | -      | expression tag      | UNP O87605 |
| A     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| A     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |
| B     | -19     | MET      | -      | expression tag      | UNP O87605 |
| B     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| B     | -17     | SER      | -      | expression tag      | UNP O87605 |
| B     | -16     | SER      | -      | expression tag      | UNP O87605 |
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| B     | -9      | SER      | -      | expression tag      | UNP O87605 |
| B     | -8      | SER      | -      | expression tag      | UNP O87605 |
| B     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| B     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| B     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| B     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| B     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| B     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| B     | -1      | SER      | -      | expression tag      | UNP O87605 |
| B     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| B     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | -19     | MET      | -      | expression tag      | UNP O87605 |
| C     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| C     | -17     | SER      | -      | expression tag      | UNP O87605 |
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| C     | -1      | SER      | -      | expression tag      | UNP O87605 |
| C     | 0       | HIS      | -      | expression tag      | UNP O87605 |
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| D     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| D     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| D     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| D     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| D     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| D     | -1      | SER      | -      | expression tag      | UNP O87605 |
| D     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| D     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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|-------|---------|----------|--------|---------------------|------------|
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| F     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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| G     | -6      | LEU      | -      | expression tag      | UNP O87605 |
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| H     | -15     | HIS      | -      | expression tag      | UNP O87605 |
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| H     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| H     | -9      | SER      | -      | expression tag      | UNP O87605 |
| H     | -8      | SER      | -      | expression tag      | UNP O87605 |
| H     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| H     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| H     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| H     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| H     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| H     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| H     | -1      | SER      | -      | expression tag      | UNP O87605 |
| H     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| H     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| I     | -19     | MET      | -      | expression tag      | UNP O87605 |
| I     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| I     | -17     | SER      | -      | expression tag      | UNP O87605 |
| I     | -16     | SER      | -      | expression tag      | UNP O87605 |
| I     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| I     | -14     | HIS      | -      | expression tag      | UNP O87605 |
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| I     | -9      | SER      | -      | expression tag      | UNP O87605 |
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| I     | -7      | GLY      | -      | expression tag      | UNP O87605 |
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| I     | -5      | VAL      | -      | expression tag      | UNP O87605 |
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| I     | -3      | ARG      | -      | expression tag      | UNP O87605 |
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| J     | -11     | HIS      | -      | expression tag      | UNP O87605 |
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| J     | -9      | SER      | -      | expression tag      | UNP O87605 |
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| J     | -7      | GLY      | -      | expression tag      | UNP O87605 |
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| J     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| J     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| J     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| J     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| J     | -1      | SER      | -      | expression tag      | UNP O87605 |
| J     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| J     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| K     | -19     | MET      | -      | expression tag      | UNP O87605 |
| K     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| K     | -17     | SER      | -      | expression tag      | UNP O87605 |
| K     | -16     | SER      | -      | expression tag      | UNP O87605 |
| K     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| K     | -14     | HIS      | -      | expression tag      | UNP O87605 |
| K     | -13     | HIS      | -      | expression tag      | UNP O87605 |
| K     | -12     | HIS      | -      | expression tag      | UNP O87605 |
| K     | -11     | HIS      | -      | expression tag      | UNP O87605 |
| K     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| K     | -9      | SER      | -      | expression tag      | UNP O87605 |
| K     | -8      | SER      | -      | expression tag      | UNP O87605 |
| K     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| K     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| K     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| K     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| K     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| K     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| K     | -1      | SER      | -      | expression tag      | UNP O87605 |
| K     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| K     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |
| L     | -19     | MET      | -      | expression tag      | UNP O87605 |
| L     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| L     | -17     | SER      | -      | expression tag      | UNP O87605 |
| L     | -16     | SER      | -      | expression tag      | UNP O87605 |
| L     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| L     | -14     | HIS      | -      | expression tag      | UNP O87605 |
| L     | -13     | HIS      | -      | expression tag      | UNP O87605 |
| L     | -12     | HIS      | -      | expression tag      | UNP O87605 |
| L     | -11     | HIS      | -      | expression tag      | UNP O87605 |
| L     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| L     | -9      | SER      | -      | expression tag      | UNP O87605 |
| L     | -8      | SER      | -      | expression tag      | UNP O87605 |
| L     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| L     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| L     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| L     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| L     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| L     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| L     | -1      | SER      | -      | expression tag      | UNP O87605 |
| L     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| L     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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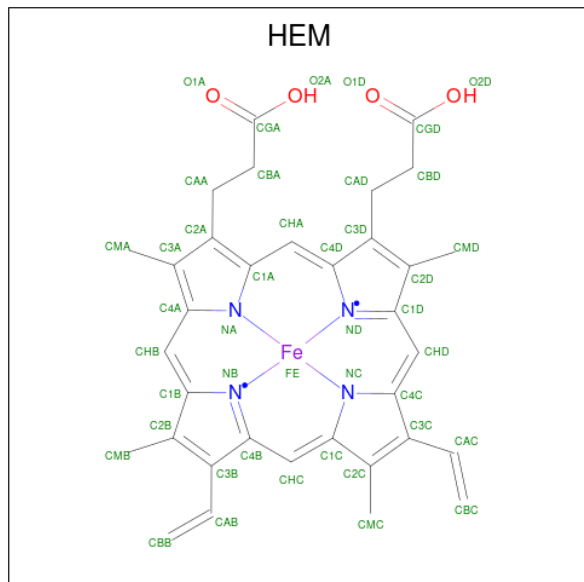
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| M     | -19     | MET      | -      | expression tag      | UNP O87605 |
| M     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| M     | -17     | SER      | -      | expression tag      | UNP O87605 |
| M     | -16     | SER      | -      | expression tag      | UNP O87605 |
| M     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| M     | -14     | HIS      | -      | expression tag      | UNP O87605 |
| M     | -13     | HIS      | -      | expression tag      | UNP O87605 |
| M     | -12     | HIS      | -      | expression tag      | UNP O87605 |
| M     | -11     | HIS      | -      | expression tag      | UNP O87605 |
| M     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| M     | -9      | SER      | -      | expression tag      | UNP O87605 |
| M     | -8      | SER      | -      | expression tag      | UNP O87605 |
| M     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| M     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| M     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| M     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| M     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| M     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| M     | -1      | SER      | -      | expression tag      | UNP O87605 |
| M     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| M     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |
| N     | -19     | MET      | -      | expression tag      | UNP O87605 |
| N     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| N     | -17     | SER      | -      | expression tag      | UNP O87605 |
| N     | -16     | SER      | -      | expression tag      | UNP O87605 |
| N     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| N     | -14     | HIS      | -      | expression tag      | UNP O87605 |
| N     | -13     | HIS      | -      | expression tag      | UNP O87605 |
| N     | -12     | HIS      | -      | expression tag      | UNP O87605 |
| N     | -11     | HIS      | -      | expression tag      | UNP O87605 |
| N     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| N     | -9      | SER      | -      | expression tag      | UNP O87605 |
| N     | -8      | SER      | -      | expression tag      | UNP O87605 |
| N     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| N     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| N     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| N     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| N     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| N     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| N     | -1      | SER      | -      | expression tag      | UNP O87605 |
| N     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| N     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| O     | -19     | MET      | -      | expression tag      | UNP O87605 |
| O     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| O     | -17     | SER      | -      | expression tag      | UNP O87605 |
| O     | -16     | SER      | -      | expression tag      | UNP O87605 |
| O     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| O     | -14     | HIS      | -      | expression tag      | UNP O87605 |
| O     | -13     | HIS      | -      | expression tag      | UNP O87605 |
| O     | -12     | HIS      | -      | expression tag      | UNP O87605 |
| O     | -11     | HIS      | -      | expression tag      | UNP O87605 |
| O     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| O     | -9      | SER      | -      | expression tag      | UNP O87605 |
| O     | -8      | SER      | -      | expression tag      | UNP O87605 |
| O     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| O     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| O     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| O     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| O     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| O     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| O     | -1      | SER      | -      | expression tag      | UNP O87605 |
| O     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| O     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |
| P     | -19     | MET      | -      | expression tag      | UNP O87605 |
| P     | -18     | GLY      | -      | expression tag      | UNP O87605 |
| P     | -17     | SER      | -      | expression tag      | UNP O87605 |
| P     | -16     | SER      | -      | expression tag      | UNP O87605 |
| P     | -15     | HIS      | -      | expression tag      | UNP O87605 |
| P     | -14     | HIS      | -      | expression tag      | UNP O87605 |
| P     | -13     | HIS      | -      | expression tag      | UNP O87605 |
| P     | -12     | HIS      | -      | expression tag      | UNP O87605 |
| P     | -11     | HIS      | -      | expression tag      | UNP O87605 |
| P     | -10     | HIS      | -      | expression tag      | UNP O87605 |
| P     | -9      | SER      | -      | expression tag      | UNP O87605 |
| P     | -8      | SER      | -      | expression tag      | UNP O87605 |
| P     | -7      | GLY      | -      | expression tag      | UNP O87605 |
| P     | -6      | LEU      | -      | expression tag      | UNP O87605 |
| P     | -5      | VAL      | -      | expression tag      | UNP O87605 |
| P     | -4      | PRO      | -      | expression tag      | UNP O87605 |
| P     | -3      | ARG      | -      | expression tag      | UNP O87605 |
| P     | -2      | GLY      | -      | expression tag      | UNP O87605 |
| P     | -1      | SER      | -      | expression tag      | UNP O87605 |
| P     | 0       | HIS      | -      | expression tag      | UNP O87605 |
| P     | 50      | ASN      | ASP    | engineered mutation | UNP O87605 |

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



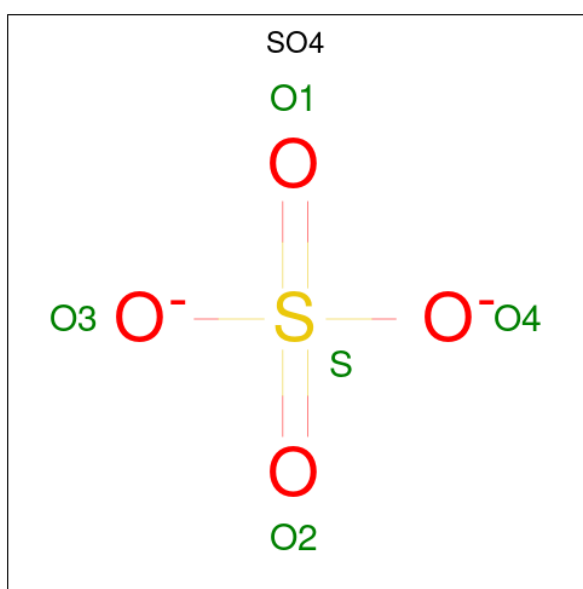
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 2   | A     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 2   | B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

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 2   | M     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 2   | N     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 2   | O     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 2   | P     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



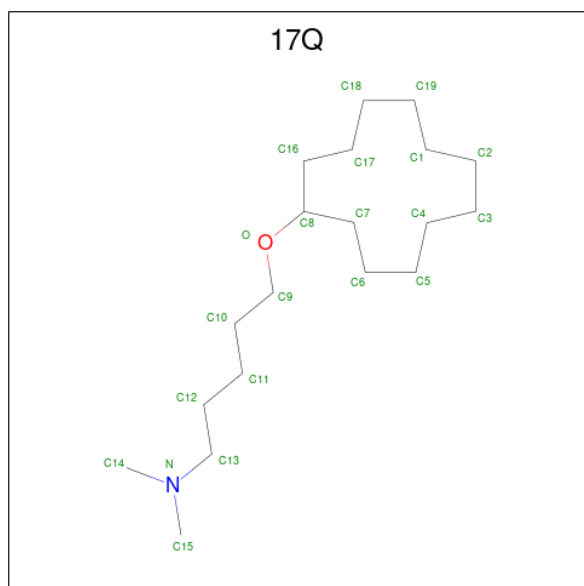
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 1        | Total | O S | 0       | 0       |
|     |       |          | 5     | 4 1 |         |         |
| 3   | B     | 1        | Total | O S | 0       | 0       |
|     |       |          | 5     | 4 1 |         |         |
| 3   | B     | 1        | Total | O S | 0       | 0       |
|     |       |          | 5     | 4 1 |         |         |
| 3   | D     | 1        | Total | O S | 0       | 0       |
|     |       |          | 5     | 4 1 |         |         |
| 3   | F     | 1        | Total | O S | 0       | 0       |
|     |       |          | 5     | 4 1 |         |         |
| 3   | H     | 1        | Total | O S | 0       | 0       |
|     |       |          | 5     | 4 1 |         |         |
| 3   | H     | 1        | Total | O S | 0       | 0       |
|     |       |          | 5     | 4 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is 1.7.6 5-cyclododecyloxy-N,N-dimethyl-pentan-1-amine (CCD ID: 17Q) (formula: C<sub>19</sub>H<sub>39</sub>NO).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 19 | 1 | 1 |         |         |
| 4   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 19 | 1 | 1 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 35       | Total | O  | 0       | 0       |
|     |       |          | 35    | 35 |         |         |
| 5   | B     | 32       | Total | O  | 0       | 0       |
|     |       |          | 32    | 32 |         |         |

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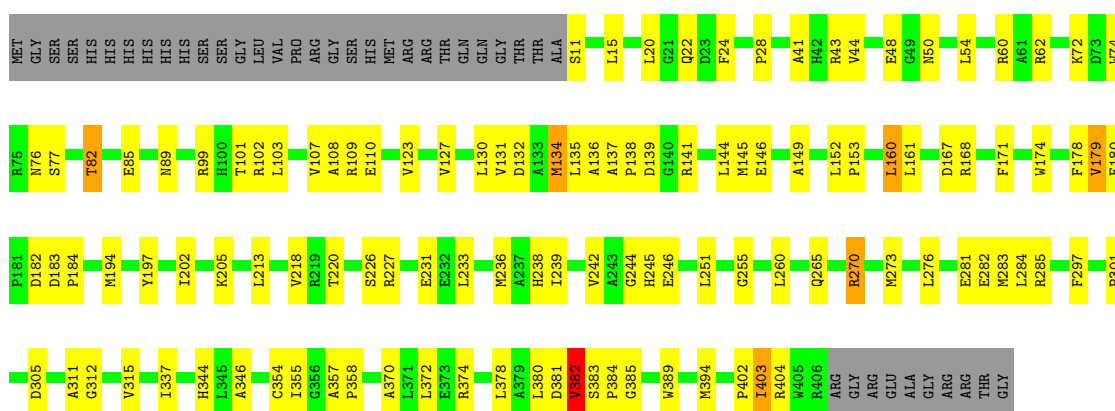
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5   | C     | 43       | Total<br>43 | O<br>43 | 0       | 0       |
| 5   | D     | 46       | Total<br>46 | O<br>46 | 0       | 0       |
| 5   | E     | 37       | Total<br>37 | O<br>37 | 0       | 0       |
| 5   | F     | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 5   | G     | 57       | Total<br>57 | O<br>57 | 0       | 0       |
| 5   | H     | 35       | Total<br>35 | O<br>35 | 0       | 0       |
| 5   | I     | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 5   | J     | 34       | Total<br>34 | O<br>34 | 0       | 0       |
| 5   | K     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 5   | L     | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 5   | M     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 5   | N     | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 5   | O     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 5   | P     | 17       | Total<br>17 | O<br>17 | 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.

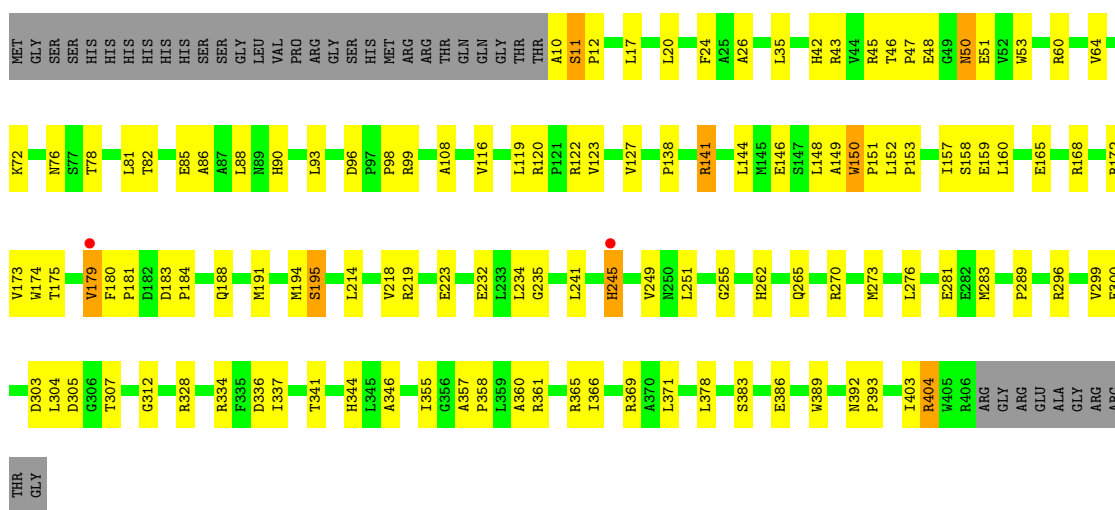
#### • Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain A: 



#### • Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

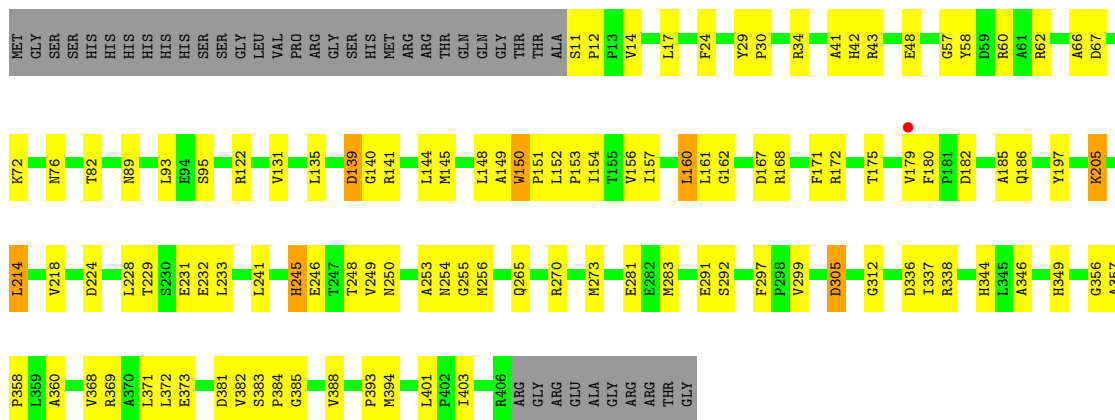
Chain B: 



#### • Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

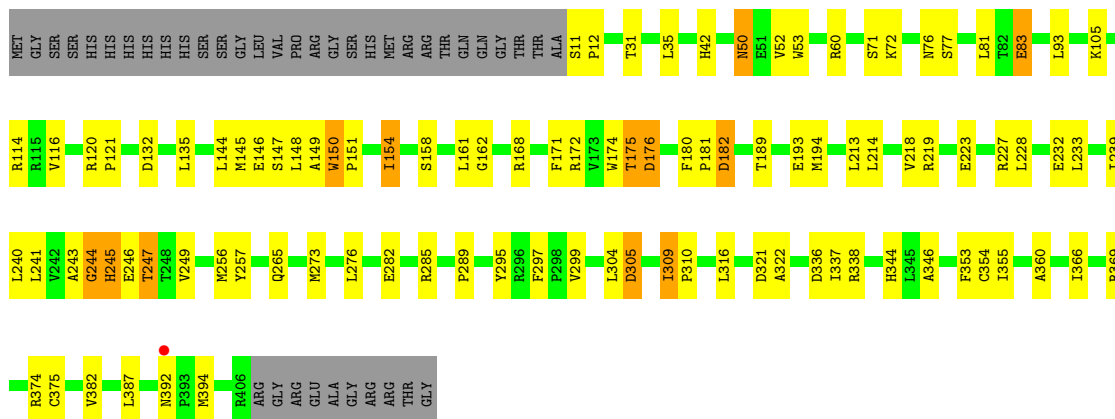
Chain C: 





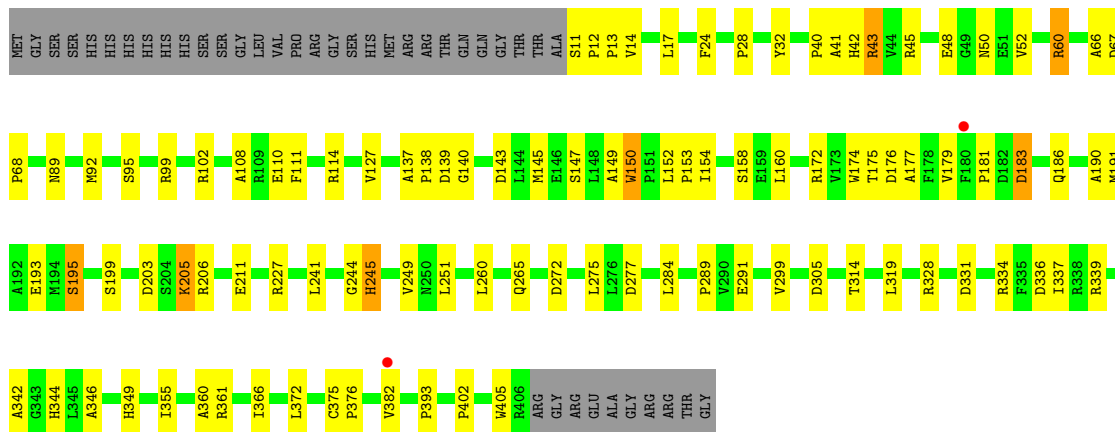
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain G: 68% 20% 9%



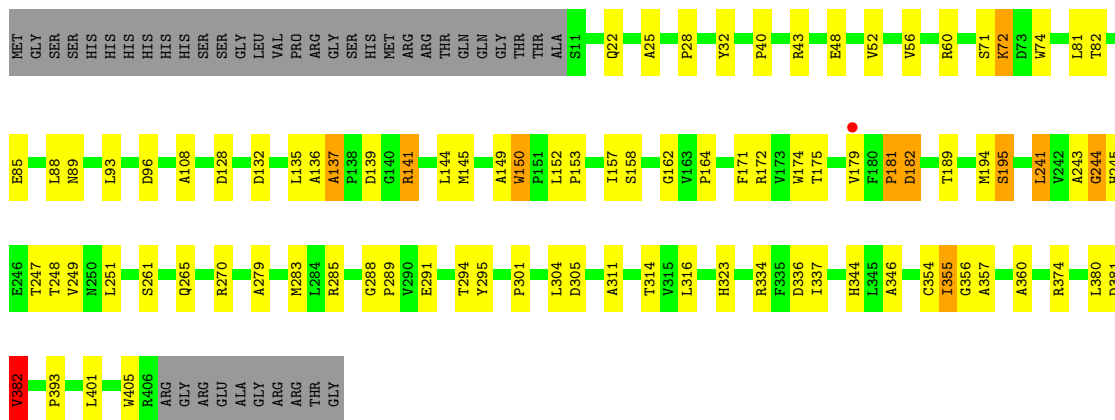
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain H: 68% 22% 9%



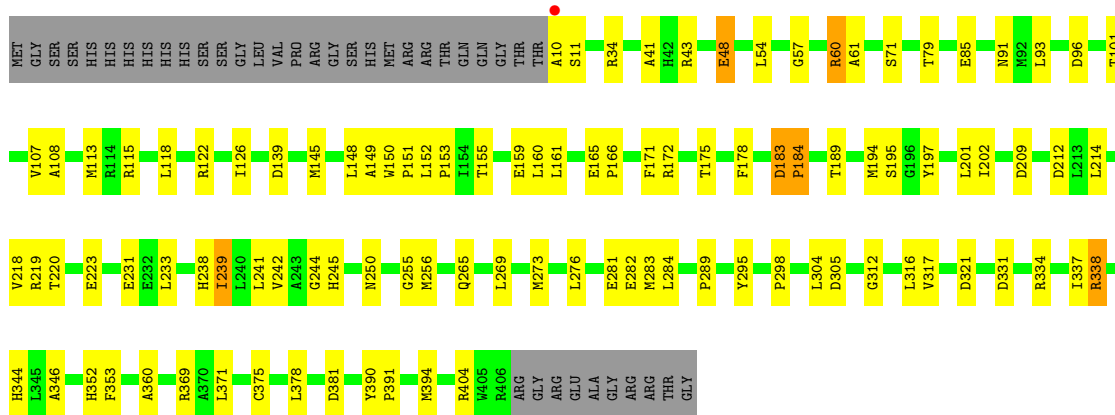
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain I: 70% 18% 9%



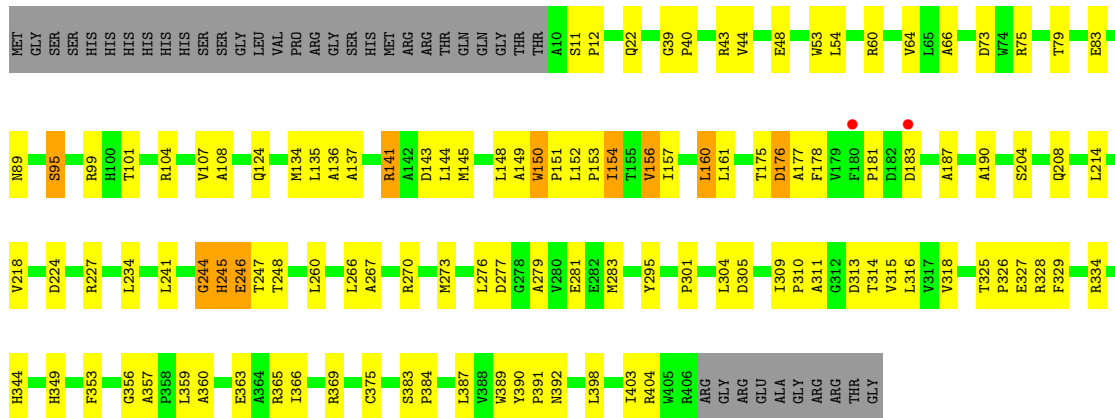
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain J: 67% 22% 9%



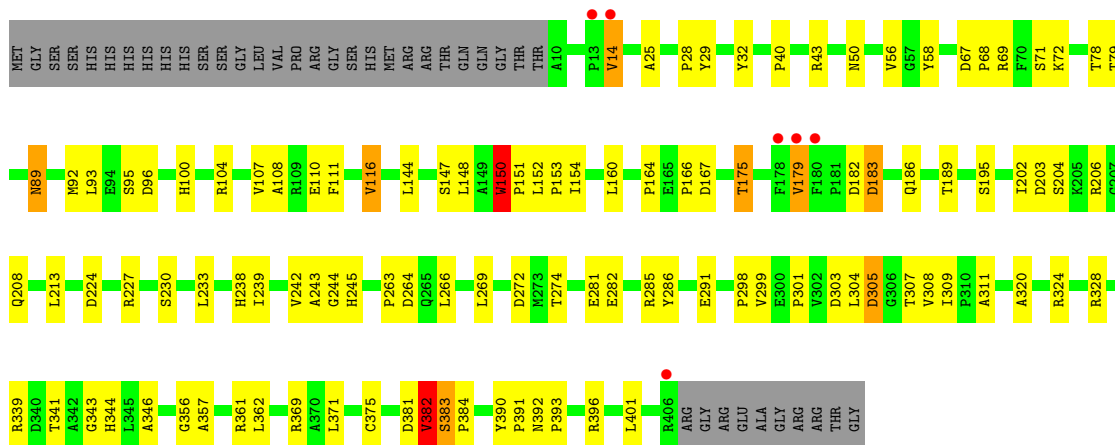
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain K: 65% 24% 9%

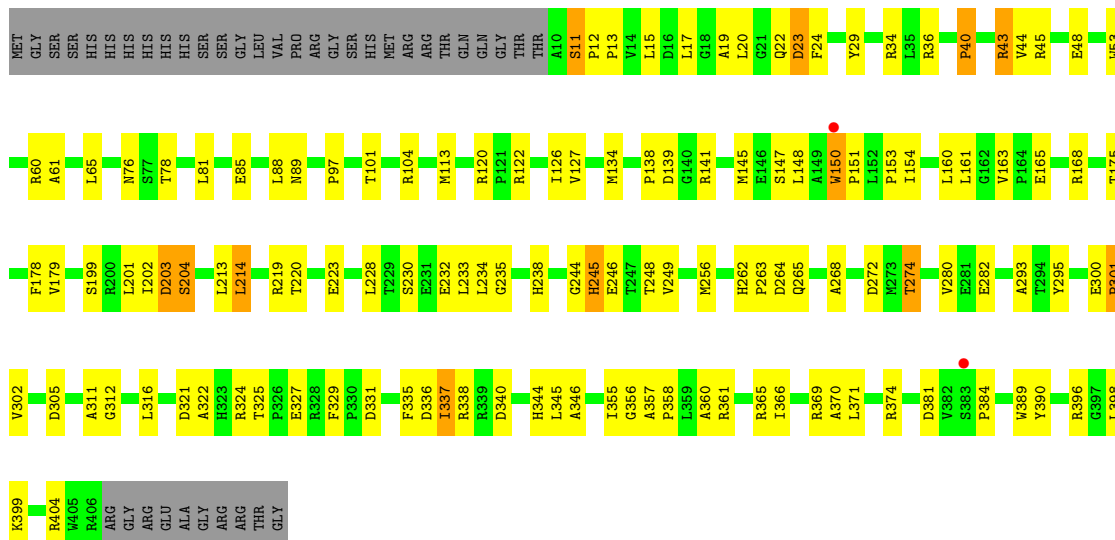


● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

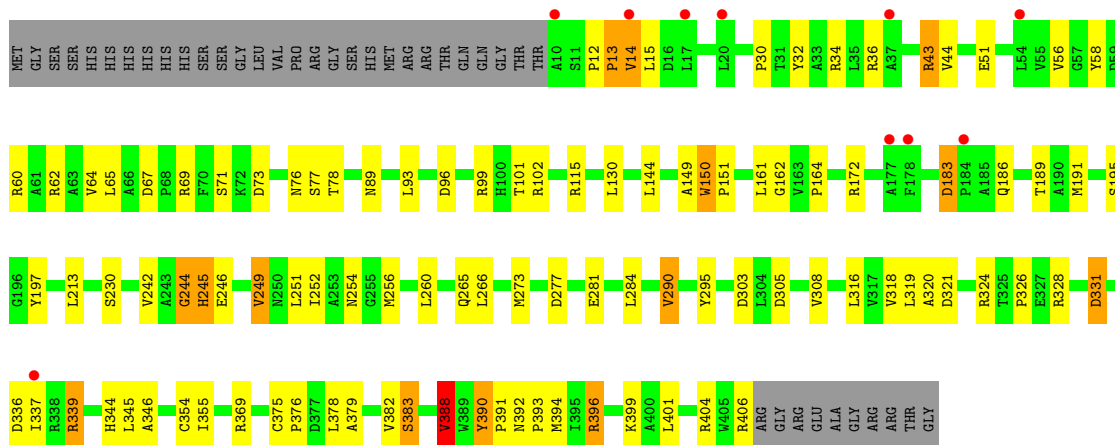
Chain L: 66% 23% 9%



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

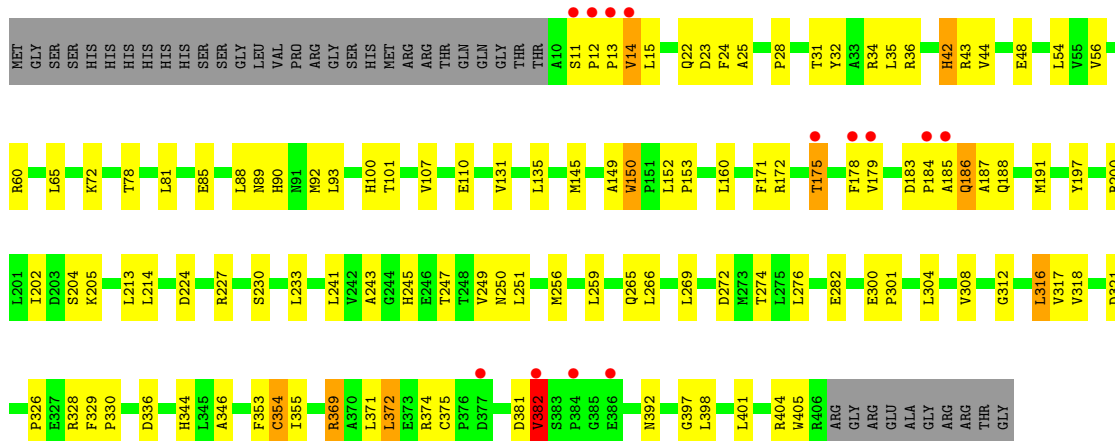


• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



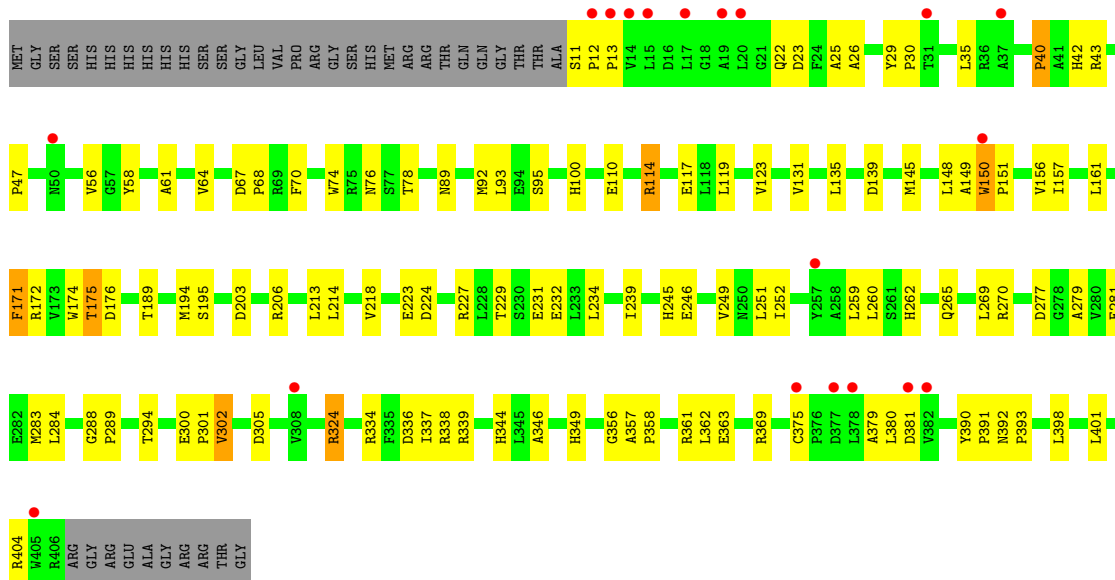
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain O: 3% 65% 24% 9%



● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain P: 4% 64% 25% 9%



## 4 Data and refinement statistics i

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 110.27Å 130.11Å 134.90Å<br>66.48° 70.25° 72.23°             | Depositor        |
| Resolution (Å)  | 119.84 – 2.70<br>119.84 – 2.70                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.3 (119.84-2.70)<br>97.3 (119.84-2.70)                    | Depositor<br>EDS |
| $R_{merge}$   | 0.11  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.73 (at 2.69Å)   | Xtrriage         |
| Refinement program  | REFMAC 5.5.0109   | Depositor        |
| R, $R_{free}$   | 0.196 , 0.279<br>0.199 , 0.277                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8479 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 44.7  | Xtrriage         |
| Anisotropy  | 0.149   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 49.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$ | Xtrriage         |
| Estimated twinning fraction   | 0.030 for -h,-l,-k  | Xtrriage         |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 50342   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 46.0  | 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 23.21 % 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 4.8815e-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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, HEM, 17Q

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         | 0/3100         | 1.07        | 6/4234 (0.1%)   |
| 1   | B     | 0.79         | 0/3142         | 1.02        | 5/4292 (0.1%)   |
| 1   | C     | 0.80         | 0/3136         | 1.06        | 9/4283 (0.2%)   |
| 1   | D     | 0.83         | 1/3149 (0.0%)  | 1.07        | 10/4301 (0.2%)  |
| 1   | E     | 0.82         | 0/3141         | 1.12        | 11/4290 (0.3%)  |
| 1   | F     | 0.78         | 0/3149         | 1.00        | 3/4303 (0.1%)   |
| 1   | G     | 0.79         | 0/3166         | 1.03        | 4/4324 (0.1%)   |
| 1   | H     | 0.82         | 0/3130         | 1.04        | 0/4275          |
| 1   | I     | 0.75         | 0/3139         | 1.01        | 2/4288 (0.0%)   |
| 1   | J     | 0.75         | 0/3133         | 1.00        | 2/4280 (0.0%)   |
| 1   | K     | 0.73         | 1/3149 (0.0%)  | 1.02        | 8/4301 (0.2%)   |
| 1   | L     | 0.72         | 0/3138         | 1.01        | 7/4287 (0.2%)   |
| 1   | M     | 0.70         | 1/3138 (0.0%)  | 1.00        | 11/4286 (0.3%)  |
| 1   | N     | 0.63         | 0/3137         | 0.98        | 8/4285 (0.2%)   |
| 1   | O     | 0.68         | 0/3125         | 0.99        | 4/4269 (0.1%)   |
| 1   | P     | 0.63         | 0/3131         | 0.96        | 4/4276 (0.1%)   |
| All | All   | 0.75         | 3/50203 (0.0%) | 1.02        | 94/68574 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | E     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | D     | 154 | ILE  | CA-CB | 8.53 | 1.64        | 1.54     |
| 1   | M     | 154 | ILE  | CA-CB | 5.54 | 1.61        | 1.54     |
| 1   | K     | 154 | ILE  | CA-CB | 5.36 | 1.60        | 1.54     |

All (94) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 39  | GLY  | CA-C-N | 8.36  | 128.33      | 119.05   |
| 1   | K     | 39  | GLY  | C-N-CA | 8.36  | 128.33      | 119.05   |
| 1   | D     | 390 | TYR  | CA-C-N | 8.09  | 128.18      | 119.28   |
| 1   | D     | 390 | TYR  | C-N-CA | 8.09  | 128.18      | 119.28   |
| 1   | N     | 246 | GLU  | N-CA-C | 7.96  | 119.64      | 110.97   |
| 1   | D     | 39  | GLY  | CA-C-N | 7.83  | 127.47      | 119.56   |
| 1   | D     | 39  | GLY  | C-N-CA | 7.83  | 127.47      | 119.56   |
| 1   | M     | 300 | GLU  | CA-C-N | 7.65  | 129.40      | 119.84   |
| 1   | M     | 300 | GLU  | C-N-CA | 7.65  | 129.40      | 119.84   |
| 1   | K     | 246 | GLU  | N-CA-C | 7.61  | 120.25      | 111.11   |
| 1   | G     | 246 | GLU  | N-CA-C | 6.91  | 119.66      | 111.71   |
| 1   | P     | 390 | TYR  | CA-C-N | 6.69  | 125.93      | 118.97   |
| 1   | P     | 390 | TYR  | C-N-CA | 6.69  | 125.93      | 118.97   |
| 1   | D     | 246 | GLU  | N-CA-C | 6.62  | 120.22      | 111.75   |
| 1   | B     | 386 | GLU  | N-CA-C | -6.59 | 104.81      | 112.92   |
| 1   | C     | 262 | HIS  | CA-C-N | 6.39  | 127.82      | 119.84   |
| 1   | C     | 262 | HIS  | C-N-CA | 6.39  | 127.82      | 119.84   |
| 1   | A     | 182 | ASP  | N-CA-C | -6.28 | 104.35      | 111.07   |
| 1   | P     | 246 | GLU  | N-CA-C | 6.20  | 119.01      | 111.82   |
| 1   | L     | 96  | ASP  | CA-C-N | -6.14 | 115.24      | 119.66   |
| 1   | L     | 96  | ASP  | C-N-CA | -6.14 | 115.24      | 119.66   |
| 1   | G     | 182 | ASP  | N-CA-C | -6.11 | 104.32      | 110.97   |
| 1   | K     | 309 | ILE  | CA-C-N | 5.98  | 126.00      | 119.90   |
| 1   | K     | 309 | ILE  | C-N-CA | 5.98  | 126.00      | 119.90   |
| 1   | M     | 163 | VAL  | N-CA-C | 5.95  | 112.98      | 107.56   |
| 1   | O     | 14  | VAL  | N-CA-C | 5.95  | 117.96      | 111.77   |
| 1   | O     | 42  | HIS  | N-CA-C | 5.88  | 117.85      | 107.61   |
| 1   | E     | 385 | GLY  | N-CA-C | 5.83  | 121.19      | 113.37   |
| 1   | J     | 212 | ASP  | N-CA-C | 5.75  | 117.74      | 110.33   |
| 1   | E     | 110 | GLU  | N-CA-C | 5.64  | 117.43      | 111.28   |
| 1   | F     | 140 | GLY  | N-CA-C | -5.62 | 107.21      | 115.30   |
| 1   | I     | 288 | GLY  | CA-C-N | -5.54 | 114.05      | 119.64   |
| 1   | I     | 288 | GLY  | C-N-CA | -5.54 | 114.05      | 119.64   |
| 1   | L     | 150 | TRP  | CA-C-N | -5.51 | 114.09      | 120.04   |
| 1   | L     | 150 | TRP  | C-N-CA | -5.51 | 114.09      | 120.04   |
| 1   | F     | 224 | ASP  | N-CA-C | 5.48  | 116.38      | 107.23   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | O     | 186 | GLN  | N-CA-C | -5.44 | 105.38      | 112.23   |
| 1   | M     | 302 | VAL  | N-CA-C | 5.42  | 115.66      | 107.75   |
| 1   | A     | 315 | VAL  | N-CA-C | 5.41  | 115.69      | 108.11   |
| 1   | A     | 178 | PHE  | N-CA-C | 5.41  | 119.40      | 112.26   |
| 1   | N     | 44  | VAL  | N-CA-C | 5.41  | 115.13      | 108.53   |
| 1   | K     | 318 | VAL  | N-CA-C | 5.38  | 114.36      | 106.55   |
| 1   | L     | 14  | VAL  | N-CA-C | 5.38  | 116.44      | 111.81   |
| 1   | J     | 171 | PHE  | N-CA-C | 5.37  | 118.93      | 112.38   |
| 1   | G     | 309 | ILE  | CA-C-N | 5.35  | 125.29      | 119.78   |
| 1   | G     | 309 | ILE  | C-N-CA | 5.35  | 125.29      | 119.78   |
| 1   | K     | 383 | SER  | CA-C-N | 5.35  | 126.52      | 119.84   |
| 1   | K     | 383 | SER  | C-N-CA | 5.35  | 126.52      | 119.84   |
| 1   | L     | 383 | SER  | CA-C-N | 5.32  | 126.48      | 119.84   |
| 1   | L     | 383 | SER  | C-N-CA | 5.32  | 126.48      | 119.84   |
| 1   | A     | 103 | LEU  | N-CA-C | 5.31  | 117.15      | 111.36   |
| 1   | N     | 390 | TYR  | CA-C-N | 5.30  | 126.47      | 119.84   |
| 1   | N     | 390 | TYR  | C-N-CA | 5.30  | 126.47      | 119.84   |
| 1   | M     | 97  | PRO  | O-C-N  | 5.29  | 123.63      | 121.15   |
| 1   | P     | 302 | VAL  | N-CA-C | 5.24  | 115.40      | 107.80   |
| 1   | E     | 180 | PHE  | CA-C-N | -5.24 | 114.40      | 119.90   |
| 1   | E     | 180 | PHE  | C-N-CA | -5.24 | 114.40      | 119.90   |
| 1   | N     | 388 | VAL  | N-CA-C | 5.23  | 115.11      | 107.37   |
| 1   | D     | 361 | ARG  | N-CA-C | -5.22 | 105.59      | 111.28   |
| 1   | C     | 331 | ASP  | CA-C-N | 5.21  | 124.83      | 119.56   |
| 1   | C     | 331 | ASP  | C-N-CA | 5.21  | 124.83      | 119.56   |
| 1   | C     | 390 | TYR  | CA-C-N | 5.21  | 124.83      | 119.05   |
| 1   | C     | 390 | TYR  | C-N-CA | 5.21  | 124.83      | 119.05   |
| 1   | M     | 331 | ASP  | CA-C-N | 5.20  | 126.34      | 119.84   |
| 1   | M     | 331 | ASP  | C-N-CA | 5.20  | 126.34      | 119.84   |
| 1   | M     | 329 | PHE  | CA-C-N | 5.19  | 125.49      | 119.93   |
| 1   | M     | 329 | PHE  | C-N-CA | 5.19  | 125.49      | 119.93   |
| 1   | E     | 11  | SER  | CA-C-N | 5.14  | 125.68      | 120.38   |
| 1   | E     | 11  | SER  | C-N-CA | 5.14  | 125.68      | 120.38   |
| 1   | E     | 78  | THR  | N-CA-C | -5.14 | 107.39      | 113.97   |
| 1   | D     | 383 | SER  | CA-C-N | -5.10 | 113.39      | 119.05   |
| 1   | D     | 383 | SER  | C-N-CA | -5.10 | 113.39      | 119.05   |
| 1   | N     | 14  | VAL  | N-CA-C | 5.10  | 119.95      | 109.34   |
| 1   | C     | 357 | ALA  | CA-C-N | -5.09 | 113.79      | 119.19   |
| 1   | C     | 357 | ALA  | C-N-CA | -5.09 | 113.79      | 119.19   |
| 1   | B     | 262 | HIS  | CA-C-N | 5.09  | 126.20      | 119.84   |
| 1   | B     | 262 | HIS  | C-N-CA | 5.09  | 126.20      | 119.84   |
| 1   | O     | 308 | VAL  | N-CA-C | 5.09  | 114.08      | 106.85   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 156 | VAL  | N-CA-C | -5.07 | 105.55      | 110.42   |
| 1   | A     | 246 | GLU  | N-CA-C | 5.07  | 119.73      | 111.37   |
| 1   | E     | 172 | ARG  | N-CA-C | -5.05 | 105.86      | 111.36   |
| 1   | D     | 276 | LEU  | N-CA-C | 5.04  | 116.47      | 111.07   |
| 1   | M     | 246 | GLU  | N-CA-C | 5.03  | 117.14      | 111.11   |
| 1   | E     | 102 | ARG  | N-CA-C | 5.03  | 116.45      | 111.07   |
| 1   | N     | 331 | ASP  | CA-C-N | 5.02  | 124.74      | 119.82   |
| 1   | N     | 331 | ASP  | C-N-CA | 5.02  | 124.74      | 119.82   |
| 1   | B     | 96  | ASP  | CA-C-N | 5.02  | 123.32      | 119.66   |
| 1   | B     | 96  | ASP  | C-N-CA | 5.02  | 123.32      | 119.66   |
| 1   | M     | 295 | TYR  | N-CA-C | 5.02  | 117.62      | 110.24   |
| 1   | E     | 331 | ASP  | CA-C-N | 5.01  | 125.45      | 120.04   |
| 1   | E     | 331 | ASP  | C-N-CA | 5.01  | 125.45      | 120.04   |
| 1   | A     | 233 | LEU  | N-CA-C | -5.00 | 105.91      | 111.36   |
| 1   | C     | 58  | TYR  | N-CA-C | 5.00  | 117.12      | 111.02   |
| 1   | D     | 14  | VAL  | N-CA-C | -5.00 | 107.59      | 112.29   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | E     | 244 | GLY  | Peptide |
| 1   | I     | 179 | VAL  | Peptide |

## 5.2 Too-close contacts [\(i\)](#)

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     | 3031  | 0        | 2990     | 70      | 0            |
| 1   | B     | 3069  | 0        | 3026     | 99      | 0            |
| 1   | C     | 3063  | 0        | 3024     | 75      | 0            |
| 1   | D     | 3076  | 0        | 3027     | 87      | 0            |
| 1   | E     | 3068  | 0        | 3022     | 68      | 0            |
| 1   | F     | 3075  | 0        | 3019     | 79      | 0            |
| 1   | G     | 3093  | 0        | 3049     | 87      | 0            |
| 1   | H     | 3057  | 0        | 3020     | 63      | 0            |
| 1   | I     | 3066  | 0        | 3020     | 67      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | J     | 3060  | 0        | 3016     | 68      | 0            |
| 1   | K     | 3076  | 0        | 3032     | 68      | 0            |
| 1   | L     | 3065  | 0        | 3014     | 67      | 0            |
| 1   | M     | 3065  | 0        | 3014     | 75      | 0            |
| 1   | N     | 3064  | 0        | 3025     | 68      | 0            |
| 1   | O     | 3052  | 0        | 3008     | 74      | 0            |
| 1   | P     | 3058  | 0        | 3006     | 65      | 0            |
| 2   | A     | 43    | 0        | 30       | 1       | 0            |
| 2   | B     | 43    | 0        | 30       | 6       | 0            |
| 2   | C     | 43    | 0        | 30       | 6       | 0            |
| 2   | D     | 43    | 0        | 30       | 8       | 0            |
| 2   | E     | 43    | 0        | 30       | 5       | 0            |
| 2   | F     | 43    | 0        | 30       | 3       | 0            |
| 2   | G     | 43    | 0        | 30       | 6       | 0            |
| 2   | H     | 43    | 0        | 30       | 7       | 0            |
| 2   | I     | 43    | 0        | 30       | 5       | 0            |
| 2   | J     | 43    | 0        | 30       | 4       | 0            |
| 2   | K     | 43    | 0        | 30       | 3       | 0            |
| 2   | L     | 43    | 0        | 30       | 4       | 0            |
| 2   | M     | 43    | 0        | 30       | 5       | 0            |
| 2   | N     | 43    | 0        | 30       | 5       | 0            |
| 2   | O     | 43    | 0        | 30       | 4       | 0            |
| 2   | P     | 43    | 0        | 30       | 5       | 0            |
| 3   | A     | 5     | 0        | 0        | 2       | 0            |
| 3   | B     | 10    | 0        | 0        | 0       | 0            |
| 3   | D     | 5     | 0        | 0        | 0       | 0            |
| 3   | F     | 5     | 0        | 0        | 1       | 0            |
| 3   | H     | 10    | 0        | 0        | 1       | 0            |
| 3   | I     | 10    | 0        | 0        | 0       | 0            |
| 3   | J     | 5     | 0        | 0        | 0       | 0            |
| 3   | O     | 10    | 0        | 0        | 1       | 0            |
| 4   | C     | 21    | 0        | 39       | 6       | 0            |
| 4   | G     | 21    | 0        | 39       | 5       | 0            |
| 5   | A     | 35    | 0        | 0        | 0       | 0            |
| 5   | B     | 32    | 0        | 0        | 0       | 0            |
| 5   | C     | 43    | 0        | 0        | 3       | 0            |
| 5   | D     | 46    | 0        | 0        | 3       | 0            |
| 5   | E     | 37    | 0        | 0        | 1       | 0            |
| 5   | F     | 39    | 0        | 0        | 2       | 0            |
| 5   | G     | 57    | 0        | 0        | 2       | 0            |
| 5   | H     | 35    | 0        | 0        | 4       | 0            |
| 5   | I     | 39    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | J     | 34    | 0        | 0        | 1       | 0            |
| 5   | K     | 28    | 0        | 0        | 1       | 0            |
| 5   | L     | 21    | 0        | 0        | 0       | 0            |
| 5   | M     | 16    | 0        | 0        | 0       | 0            |
| 5   | N     | 15    | 0        | 0        | 0       | 0            |
| 5   | O     | 20    | 0        | 0        | 0       | 0            |
| 5   | P     | 17    | 0        | 0        | 1       | 0            |
| All | All   | 50342 | 0        | 48870    | 1177    | 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 12.

All (1177) 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:C:85:GLU:HG3    | 1:C:191:MET:HE1   | 1.17                     | 1.11              |
| 1:G:273:MET:HE2   | 1:G:369:ARG:HG3   | 1.33                     | 1.10              |
| 1:O:227:ARG:NH1   | 1:O:227:ARG:HB3   | 1.69                     | 1.07              |
| 1:I:128:ASP:HA    | 1:I:374:ARG:HH12  | 1.21                     | 1.06              |
| 1:G:171:PHE:O     | 1:G:175:THR:HG22  | 1.56                     | 1.05              |
| 1:N:390:TYR:HE1   | 1:N:399:LYS:HG3   | 1.20                     | 1.04              |
| 1:A:174:TRP:HE3   | 1:A:194:MET:HE3   | 1.22                     | 1.04              |
| 1:F:171:PHE:O     | 1:F:175:THR:HG22  | 1.59                     | 1.02              |
| 1:K:11:SER:HB2    | 1:K:12:PRO:HD3    | 1.43                     | 1.00              |
| 1:A:174:TRP:CE3   | 1:A:194:MET:HE3   | 1.96                     | 1.00              |
| 3:A:1408:SO4:O1   | 1:E:227:ARG:NH1   | 1.94                     | 0.98              |
| 2:N:1407:HEM:HBC2 | 2:N:1407:HEM:HMC2 | 1.48                     | 0.93              |
| 1:C:11:SER:CB     | 1:C:12:PRO:HD3    | 1.99                     | 0.93              |
| 1:C:150:TRP:HZ3   | 1:C:245:HIS:CE1   | 1.88                     | 0.92              |
| 1:L:150:TRP:HZ3   | 1:L:245:HIS:HE2   | 1.11                     | 0.91              |
| 1:B:165:GLU:HA    | 1:B:168:ARG:HD2   | 1.52                     | 0.89              |
| 1:F:265:GLN:NE2   | 1:F:337:ILE:H     | 1.70                     | 0.89              |
| 1:P:224:ASP:OD2   | 1:P:227:ARG:HG3   | 1.73                     | 0.89              |
| 1:O:227:ARG:HB3   | 1:O:227:ARG:HH11  | 1.26                     | 0.89              |
| 1:D:361:ARG:O     | 1:D:365:ARG:HG3   | 1.73                     | 0.88              |
| 1:N:390:TYR:CE1   | 1:N:399:LYS:HG3   | 2.07                     | 0.87              |
| 1:C:344:HIS:HD2   | 1:C:346:ALA:H     | 1.21                     | 0.87              |
| 1:L:144:LEU:HD23  | 1:L:401:LEU:HD23  | 1.57                     | 0.86              |
| 1:A:381:ASP:O     | 1:A:382:VAL:HB    | 1.75                     | 0.85              |
| 1:C:85:GLU:CG     | 1:C:191:MET:HE1   | 2.05                     | 0.85              |
| 1:A:132:ASP:OD1   | 1:A:374:ARG:NH2   | 2.08                     | 0.85              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:134:MET:HE1    | 1:A:403:ILE:HD11  | 1.57                     | 0.85              |
| 1:I:334:ARG:HE     | 1:I:336:ASP:HB2   | 1.42                     | 0.84              |
| 1:B:245[B]:HIS:CD2 | 1:B:249:VAL:HG21  | 2.11                     | 0.84              |
| 1:E:344:HIS:HD2    | 1:E:346:ALA:H     | 1.25                     | 0.84              |
| 1:J:265:GLN:NE2    | 1:J:337:ILE:H     | 1.75                     | 0.84              |
| 1:A:174:TRP:HE3    | 1:A:194:MET:CE    | 1.90                     | 0.83              |
| 1:G:60:ARG:NH2     | 1:G:305:ASP:OD2   | 2.12                     | 0.82              |
| 1:H:60:ARG:NH2     | 1:H:305:ASP:HB2   | 1.94                     | 0.82              |
| 1:G:189:THR:O      | 1:G:193:GLU:HG3   | 1.79                     | 0.82              |
| 1:L:150:TRP:CZ3    | 1:L:245:HIS:NE2   | 2.46                     | 0.82              |
| 1:E:116:VAL:HG13   | 1:E:362:LEU:HD22  | 1.62                     | 0.82              |
| 1:C:60:ARG:HH22    | 1:C:305:ASP:HB2   | 1.45                     | 0.81              |
| 1:F:11:SER:HB2     | 1:F:12:PRO:HD3    | 1.60                     | 0.81              |
| 1:J:183:ASP:HB2    | 1:J:184:PRO:HD2   | 1.60                     | 0.81              |
| 1:P:114:ARG:HG2    | 1:P:114:ARG:HH11  | 1.45                     | 0.81              |
| 1:E:242:VAL:O      | 1:E:245:HIS:HB3   | 1.81                     | 0.80              |
| 1:N:36:ARG:HH12    | 1:N:326:PRO:HD3   | 1.46                     | 0.80              |
| 1:E:22:GLN:HE22    | 1:E:389:TRP:H     | 1.28                     | 0.80              |
| 1:J:172:ARG:HA     | 1:J:175:THR:HG22  | 1.63                     | 0.79              |
| 1:K:359:LEU:O      | 1:K:363:GLU:HG3   | 1.82                     | 0.79              |
| 1:C:11:SER:HB3     | 1:C:12:PRO:HD3    | 1.62                     | 0.79              |
| 1:L:392:ASN:OD1    | 1:L:393:PRO:HD2   | 1.82                     | 0.78              |
| 1:O:256:MET:HE2    | 1:O:371:LEU:HD13  | 1.65                     | 0.78              |
| 1:A:179:VAL:HG12   | 1:A:180:PHE:H     | 1.47                     | 0.78              |
| 1:B:179:VAL:HG12   | 1:B:180:PHE:H     | 1.48                     | 0.78              |
| 1:L:93:LEU:HD13    | 2:L:1407:HEM:HAD2 | 1.66                     | 0.78              |
| 1:D:244:GLY:HA2    | 2:D:1407:HEM:HMC3 | 1.67                     | 0.77              |
| 1:M:344:HIS:HD2    | 1:M:346:ALA:H     | 1.33                     | 0.77              |
| 1:B:273:MET:HE2    | 1:B:369:ARG:HD2   | 1.66                     | 0.76              |
| 1:K:60:ARG:NH2     | 1:K:305:ASP:HB2   | 2.01                     | 0.76              |
| 1:K:325:THR:HG22   | 1:K:327:GLU:OE1   | 1.85                     | 0.76              |
| 1:D:145:MET:HA     | 1:D:149:ALA:HB3   | 1.68                     | 0.76              |
| 1:B:392:ASN:OD1    | 1:B:393:PRO:HD2   | 1.86                     | 0.75              |
| 1:B:51:GLU:OE2     | 1:L:369:ARG:NH1   | 2.19                     | 0.75              |
| 1:B:82:THR:HG23    | 1:B:85:GLU:OE1    | 1.86                     | 0.75              |
| 1:B:150:TRP:CH2    | 1:B:172:ARG:HB2   | 2.21                     | 0.75              |
| 1:G:171:PHE:O      | 1:G:175:THR:CG2   | 2.35                     | 0.74              |
| 1:H:227:ARG:NH1    | 3:H:1409:SO4:O2   | 2.21                     | 0.73              |
| 1:K:40:PRO:HG3     | 1:K:305:ASP:HB3   | 1.70                     | 0.73              |
| 1:M:161:LEU:HD23   | 1:M:213:LEU:HB3   | 1.70                     | 0.73              |
| 1:P:11:SER:HB2     | 1:P:12:PRO:HD3    | 1.71                     | 0.73              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:I:141:ARG:HD3  | 1:I:381:ASP:OD2     | 1.89                     | 0.73              |
| 1:K:150:TRP:HE3  | 1:K:245:HIS:HE1     | 1.35                     | 0.73              |
| 1:A:265:GLN:NE2  | 1:A:337:ILE:HG12    | 2.03                     | 0.73              |
| 1:D:67:ASP:HB3   | 1:D:70:PHE:HD1      | 1.53                     | 0.72              |
| 1:D:150:TRP:CZ2  | 1:D:172:ARG:HB2     | 2.23                     | 0.72              |
| 1:G:219:ARG:O    | 1:G:223:GLU:HG3     | 1.88                     | 0.72              |
| 1:C:11:SER:HB2   | 1:C:12:PRO:HD3      | 1.70                     | 0.72              |
| 1:A:60:ARG:HH22  | 1:A:305:ASP:HB2     | 1.54                     | 0.72              |
| 1:F:60:ARG:HD3   | 5:F:2007:HOH:O      | 1.90                     | 0.72              |
| 1:G:161:LEU:CD2  | 1:G:213:LEU:HD23    | 2.20                     | 0.72              |
| 1:O:245:HIS:O    | 1:O:249:VAL:HG23    | 1.89                     | 0.72              |
| 1:C:150:TRP:CZ3  | 1:C:245:HIS:CE1     | 2.76                     | 0.71              |
| 1:E:265:GLN:NE2  | 1:E:337:ILE:HG12    | 2.05                     | 0.71              |
| 1:I:344:HIS:HD2  | 1:I:346:ALA:H       | 1.37                     | 0.71              |
| 1:L:154:ILE:HB   | 1:L:245:HIS:HE1     | 1.54                     | 0.71              |
| 1:O:35:LEU:HB3   | 1:O:42:HIS:CD2      | 2.25                     | 0.71              |
| 1:K:150:TRP:CE3  | 1:K:245:HIS:HE1     | 2.09                     | 0.71              |
| 1:B:141:ARG:HH11 | 1:B:141:ARG:HB2     | 1.56                     | 0.71              |
| 1:C:60:ARG:NH2   | 1:C:305:ASP:HB2     | 2.05                     | 0.71              |
| 1:G:243:ALA:O    | 1:G:247:THR:OG1     | 2.09                     | 0.71              |
| 1:K:316[B]:LEU:N | 1:K:316[B]:LEU:HD12 | 2.06                     | 0.70              |
| 1:B:179:VAL:O    | 1:B:181:PRO:HD3     | 1.91                     | 0.70              |
| 1:M:13:PRO:HD2   | 1:P:369:ARG:HH12    | 1.56                     | 0.70              |
| 1:B:344:HIS:HD2  | 1:B:346:ALA:H       | 1.36                     | 0.70              |
| 1:F:344:HIS:HD2  | 1:F:346:ALA:H       | 1.36                     | 0.70              |
| 1:G:214:LEU:O    | 1:G:218:VAL:HG23    | 1.91                     | 0.70              |
| 1:F:150:TRP:CD1  | 1:F:151:PRO:HD3     | 2.27                     | 0.70              |
| 1:E:181:PRO:HB2  | 1:E:183:ASP:O       | 1.91                     | 0.69              |
| 1:P:357:ALA:HB3  | 1:P:358:PRO:HD3     | 1.74                     | 0.69              |
| 1:B:179:VAL:HG12 | 1:B:180:PHE:N       | 2.05                     | 0.69              |
| 1:H:11:SER:HB3   | 1:H:12:PRO:HD3      | 1.74                     | 0.69              |
| 1:J:93:LEU:HD13  | 2:J:1407:HEM:HAD2   | 1.73                     | 0.69              |
| 1:B:265:GLN:NE2  | 1:B:337:ILE:H       | 1.89                     | 0.69              |
| 1:O:227:ARG:HH11 | 1:O:227:ARG:CB      | 2.03                     | 0.69              |
| 1:A:179:VAL:HG12 | 1:A:180:PHE:N       | 2.07                     | 0.69              |
| 1:F:265:GLN:HE22 | 1:F:337:ILE:H       | 1.37                     | 0.69              |
| 1:I:150:TRP:CZ2  | 1:I:172:ARG:HB2     | 2.27                     | 0.69              |
| 1:C:228:LEU:HD12 | 1:C:232:GLU:HB3     | 1.75                     | 0.69              |
| 1:E:265:GLN:NE2  | 1:E:337:ILE:H       | 1.90                     | 0.69              |
| 1:B:11:SER:N     | 1:B:12:PRO:HD3      | 2.08                     | 0.69              |
| 1:B:138:PRO:HB2  | 1:F:185:ALA:HB3     | 1.75                     | 0.69              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:F:241:LEU:O    | 1:F:245[B]:HIS:CE1 | 2.47                     | 0.68              |
| 1:G:360:ALA:HB1  | 2:G:1407:HEM:HAB   | 1.75                     | 0.68              |
| 1:I:128:ASP:HA   | 1:I:374:ARG:NH1    | 2.03                     | 0.68              |
| 1:D:143:ASP:HB2  | 1:G:83:GLU:HG3     | 1.75                     | 0.68              |
| 1:I:22:GLN:HA    | 1:I:25:ALA:HB3     | 1.75                     | 0.68              |
| 1:B:127:VAL:HG21 | 1:B:366:ILE:HG22   | 1.74                     | 0.68              |
| 1:C:344:HIS:CD2  | 1:C:346:ALA:H      | 2.10                     | 0.68              |
| 1:F:145:MET:HE1  | 1:F:253:ALA:CB     | 2.24                     | 0.68              |
| 1:O:282:GLU:HG2  | 1:O:336:ASP:O      | 1.94                     | 0.68              |
| 1:F:139:ASP:HB3  | 1:F:141:ARG:HB2    | 1.76                     | 0.68              |
| 1:D:265:GLN:HE21 | 1:D:337:ILE:H      | 1.40                     | 0.67              |
| 1:F:360:ALA:CB   | 2:F:1407:HEM:HAB   | 2.25                     | 0.67              |
| 1:L:263:PRO:HA   | 1:L:266:LEU:HB3    | 1.75                     | 0.67              |
| 1:D:392:ASN:OD1  | 1:D:393:PRO:HD2    | 1.95                     | 0.67              |
| 1:O:344:HIS:HD2  | 1:O:346:ALA:H      | 1.42                     | 0.67              |
| 1:B:51:GLU:CD    | 1:L:369:ARG:HH22   | 2.03                     | 0.67              |
| 1:C:265:GLN:NE2  | 1:C:337:ILE:H      | 1.92                     | 0.67              |
| 1:D:236:MET:O    | 1:D:239:ILE:HG22   | 1.93                     | 0.67              |
| 1:L:243:ALA:C    | 1:L:245:HIS:H      | 2.02                     | 0.67              |
| 1:D:265:GLN:NE2  | 1:D:337:ILE:H      | 1.93                     | 0.67              |
| 1:G:132:ASP:OD1  | 1:G:374:ARG:NH2    | 2.28                     | 0.67              |
| 1:I:82:THR:HG23  | 1:I:85:GLU:OE1     | 1.94                     | 0.67              |
| 1:A:60:ARG:NH2   | 1:A:305:ASP:HB2    | 2.10                     | 0.67              |
| 1:B:141:ARG:HG3  | 1:B:404:ARG:HB3    | 1.76                     | 0.67              |
| 1:G:265:GLN:NE2  | 1:G:337:ILE:HG12   | 2.08                     | 0.67              |
| 1:M:360:ALA:HB1  | 2:M:1407:HEM:HAB   | 1.76                     | 0.67              |
| 1:L:344:HIS:HD2  | 1:L:346:ALA:H      | 1.40                     | 0.67              |
| 1:B:150:TRP:CE3  | 1:B:245[B]:HIS:NE2 | 2.63                     | 0.67              |
| 1:B:150:TRP:HE3  | 1:B:245[B]:HIS:NE2 | 1.93                     | 0.67              |
| 1:C:11:SER:CB    | 1:C:12:PRO:CD      | 2.73                     | 0.66              |
| 1:G:72:LYS:NZ    | 1:G:72:LYS:HB3     | 2.10                     | 0.66              |
| 1:L:154:ILE:HB   | 1:L:245:HIS:CE1    | 2.31                     | 0.66              |
| 1:F:150:TRP:CZ3  | 1:F:172:ARG:HB2    | 2.31                     | 0.66              |
| 1:N:150:TRP:CE3  | 1:N:245:HIS:HE1    | 2.14                     | 0.66              |
| 1:C:265:GLN:HE21 | 1:C:337:ILE:HG23   | 1.60                     | 0.66              |
| 1:E:289:PRO:HG2  | 2:E:1407:HEM:HMB2  | 1.77                     | 0.66              |
| 1:G:227:ARG:HH21 | 1:O:328:ARG:HH21   | 1.43                     | 0.66              |
| 1:D:244:GLY:CA   | 2:D:1407:HEM:HBC2  | 2.26                     | 0.66              |
| 1:J:250:ASN:HB2  | 1:J:289:PRO:HB3    | 1.77                     | 0.66              |
| 1:L:144:LEU:CD2  | 1:L:401:LEU:HD23   | 2.26                     | 0.65              |
| 1:P:260:LEU:HD22 | 1:P:379:ALA:HA     | 1.77                     | 0.65              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:C:40:PRO:HG3     | 1:C:305:ASP:HB3     | 1.79                     | 0.65              |
| 1:I:40:PRO:HG3     | 1:I:305:ASP:CB      | 2.26                     | 0.65              |
| 1:A:281:GLU:OE1    | 1:A:344:HIS:HE1     | 1.79                     | 0.65              |
| 1:P:114:ARG:HG2    | 1:P:114:ARG:NH1     | 2.11                     | 0.65              |
| 1:M:219:ARG:O      | 1:M:223:GLU:HG3     | 1.96                     | 0.65              |
| 1:P:277:ASP:O      | 1:P:281:GLU:HG2     | 1.96                     | 0.65              |
| 1:O:381:ASP:O      | 1:O:382:VAL:HB      | 1.96                     | 0.65              |
| 1:I:381:ASP:O      | 1:I:382:VAL:HB      | 1.97                     | 0.65              |
| 1:G:360:ALA:CB     | 2:G:1407:HEM:HAB    | 2.27                     | 0.65              |
| 2:H:1407:HEM:HBB2  | 2:H:1407:HEM:HMB2   | 1.77                     | 0.64              |
| 1:K:60:ARG:HD3     | 5:K:2004:HOH:O      | 1.95                     | 0.64              |
| 1:O:282:GLU:OE1    | 1:O:282:GLU:HA      | 1.97                     | 0.64              |
| 1:C:152:LEU:HB3    | 1:C:153:PRO:HD3     | 1.77                     | 0.64              |
| 1:G:50[A]:ASN:HD22 | 1:G:50[A]:ASN:N     | 1.94                     | 0.64              |
| 1:C:344:HIS:HD2    | 1:C:346:ALA:N       | 1.93                     | 0.64              |
| 1:G:161:LEU:HD21   | 1:G:213:LEU:HD23    | 1.80                     | 0.64              |
| 1:O:110:GLU:HG3    | 1:O:213:LEU:HD13    | 1.80                     | 0.64              |
| 1:K:214:LEU:O      | 1:K:218:VAL:HG23    | 1.97                     | 0.64              |
| 1:F:162:GLY:O      | 1:F:205:LYS:NZ      | 2.27                     | 0.64              |
| 1:O:150:TRP:CH2    | 1:O:172:ARG:HB2     | 2.33                     | 0.64              |
| 1:G:172:ARG:O      | 1:G:176:ASP:HB2     | 1.97                     | 0.63              |
| 1:A:265:GLN:HE21   | 1:A:337:ILE:HG12    | 1.62                     | 0.63              |
| 1:D:120:ARG:HB3    | 1:D:121:PRO:HD3     | 1.78                     | 0.63              |
| 1:H:339:ARG:HD3    | 5:H:2031:HOH:O      | 1.97                     | 0.63              |
| 1:N:295:TYR:CD1    | 1:N:316[A]:LEU:HD21 | 2.33                     | 0.63              |
| 1:D:22:GLN:HE22    | 1:D:389:TRP:H       | 1.45                     | 0.63              |
| 1:F:11:SER:CB      | 1:F:12:PRO:HD3      | 2.27                     | 0.63              |
| 1:M:301:PRO:HD3    | 1:M:311:ALA:HB2     | 1.81                     | 0.63              |
| 1:I:301:PRO:HD3    | 1:I:311:ALA:HB2     | 1.80                     | 0.63              |
| 1:C:150:TRP:CH2    | 1:C:172:ARG:HB2     | 2.34                     | 0.63              |
| 1:A:255:GLY:HA2    | 1:A:283:MET:HG2     | 1.80                     | 0.63              |
| 1:G:174:TRP:CB     | 1:G:194:MET:HE3     | 2.28                     | 0.63              |
| 1:O:60:ARG:HD2     | 1:O:304:LEU:HD22    | 1.80                     | 0.63              |
| 1:H:150:TRP:HZ3    | 1:H:245:HIS:CE1     | 2.17                     | 0.63              |
| 1:D:344:HIS:HD2    | 1:D:346:ALA:H       | 1.45                     | 0.63              |
| 1:H:11:SER:HB3     | 1:H:12:PRO:CD       | 2.29                     | 0.62              |
| 1:M:40:PRO:HG3     | 1:M:305:ASP:HB3     | 1.80                     | 0.62              |
| 1:N:344:HIS:HD2    | 1:N:346:ALA:H       | 1.45                     | 0.62              |
| 1:C:265:GLN:NE2    | 1:C:337:ILE:HG12    | 2.14                     | 0.62              |
| 4:G:1410:17Q:H61C  | 4:G:1410:17Q:H172   | 1.82                     | 0.62              |
| 1:N:191:MET:O      | 1:N:195:SER:HB2     | 1.98                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:J:183:ASP:HB2    | 1:J:184:PRO:CD    | 2.27                     | 0.62              |
| 1:J:344:HIS:HD2    | 1:J:346:ALA:H     | 1.47                     | 0.62              |
| 1:A:381:ASP:O      | 1:A:402:PRO:HB2   | 1.99                     | 0.62              |
| 1:H:174:TRP:NE1    | 1:H:193:GLU:OE1   | 2.28                     | 0.62              |
| 1:P:381:ASP:HA     | 1:P:404:ARG:HH11  | 1.64                     | 0.62              |
| 1:B:148:LEU:HD23   | 1:B:371:LEU:HD11  | 1.82                     | 0.62              |
| 1:D:273:MET:HE1    | 1:D:276:LEU:HD13  | 1.82                     | 0.62              |
| 1:G:114:ARG:NH1    | 5:G:2026:HOH:O    | 2.29                     | 0.62              |
| 1:J:244:GLY:HA2    | 2:J:1407:HEM:C3C  | 2.35                     | 0.62              |
| 1:J:265:GLN:HE21   | 1:J:337:ILE:H     | 1.48                     | 0.62              |
| 1:D:328:ARG:NH2    | 1:D:343:GLY:HA3   | 2.15                     | 0.62              |
| 1:M:344:HIS:CD2    | 1:M:346:ALA:H     | 2.16                     | 0.62              |
| 1:B:93:LEU:HD13    | 2:B:1407:HEM:HAD2 | 1.82                     | 0.61              |
| 1:E:72:LYS:HE3     | 1:E:294:THR:OG1   | 1.99                     | 0.61              |
| 1:I:141:ARG:HG3    | 1:I:141:ARG:NH1   | 2.14                     | 0.61              |
| 1:K:360:ALA:CB     | 2:K:1407:HEM:HAB  | 2.30                     | 0.61              |
| 1:C:11:SER:HB3     | 1:C:12:PRO:CD     | 2.31                     | 0.61              |
| 1:C:242:VAL:O      | 1:C:245:HIS:HB3   | 2.00                     | 0.61              |
| 1:I:265:GLN:HE21   | 1:I:337:ILE:H     | 1.48                     | 0.61              |
| 1:J:202:ILE:HG23   | 1:J:218:VAL:HG22  | 1.82                     | 0.61              |
| 1:O:93:LEU:HD13    | 2:O:1407:HEM:HAD2 | 1.81                     | 0.61              |
| 1:K:360:ALA:HB1    | 2:K:1407:HEM:HAB  | 1.83                     | 0.61              |
| 1:B:82:THR:OG1     | 1:B:188:GLN:NE2   | 2.33                     | 0.61              |
| 1:I:40:PRO:HG3     | 1:I:305:ASP:HB2   | 1.83                     | 0.61              |
| 1:B:357:ALA:HB3    | 1:B:358:PRO:HD3   | 1.81                     | 0.61              |
| 1:G:353:PHE:CD1    | 1:P:223:GLU:HG2   | 2.36                     | 0.61              |
| 1:D:244:GLY:HA3    | 2:D:1407:HEM:HBC2 | 1.82                     | 0.61              |
| 1:N:36:ARG:NH1     | 1:N:326:PRO:HD3   | 2.14                     | 0.61              |
| 1:H:145:MET:HA     | 1:H:149:ALA:HB3   | 1.82                     | 0.61              |
| 1:H:152:LEU:HB3    | 1:H:153:PRO:HD3   | 1.82                     | 0.61              |
| 2:C:1407:HEM:NA    | 4:C:1410:17Q:H32C | 2.16                     | 0.61              |
| 1:F:228:LEU:HD12   | 1:F:232:GLU:CB    | 2.31                     | 0.61              |
| 1:B:245[B]:HIS:CD2 | 1:B:249:VAL:CG2   | 2.83                     | 0.60              |
| 1:M:22:GLN:HE22    | 1:M:389:TRP:H     | 1.49                     | 0.60              |
| 1:N:376:PRO:HG2    | 1:N:406:ARG:CB    | 2.30                     | 0.60              |
| 1:B:150:TRP:CZ2    | 1:B:172:ARG:HB2   | 2.37                     | 0.60              |
| 1:B:245[B]:HIS:HD2 | 1:B:249:VAL:CG2   | 2.15                     | 0.60              |
| 1:A:273:MET:HE1    | 1:A:276:LEU:HD13  | 1.84                     | 0.60              |
| 1:C:150:TRP:CZ2    | 1:C:172:ARG:HB2   | 2.37                     | 0.60              |
| 1:D:172:ARG:O      | 1:D:173:VAL:C     | 2.45                     | 0.60              |
| 1:B:214:LEU:O      | 1:B:218:VAL:HG23  | 2.01                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:N:244:GLY:O     | 1:N:245:HIS:C      | 2.45                     | 0.60              |
| 1:D:114:ARG:NH1   | 5:D:2021:HOH:O     | 2.30                     | 0.60              |
| 1:O:88:LEU:C      | 1:O:90:HIS:H       | 2.09                     | 0.60              |
| 1:E:265:GLN:HE21  | 1:E:337:ILE:H      | 1.50                     | 0.59              |
| 1:F:256:MET:HE2   | 1:F:371:LEU:HD13   | 1.83                     | 0.59              |
| 1:D:191:MET:O     | 1:D:195:SER:HB2    | 2.02                     | 0.59              |
| 1:I:149:ALA:O     | 1:I:249:VAL:HG22   | 2.02                     | 0.59              |
| 1:F:62:ARG:NH2    | 3:F:1408:SO4:O3    | 2.33                     | 0.59              |
| 1:L:381:ASP:O     | 1:L:382:VAL:HB     | 2.02                     | 0.59              |
| 2:O:1407:HEM:HBB2 | 2:O:1407:HEM:HMB2  | 1.84                     | 0.59              |
| 1:E:154:ILE:HD13  | 1:E:245:HIS:NE2    | 2.17                     | 0.59              |
| 1:I:150:TRP:CH2   | 1:I:172:ARG:HB2    | 2.38                     | 0.59              |
| 1:N:260:LEU:HD22  | 1:N:379:ALA:HA     | 1.84                     | 0.59              |
| 1:I:141:ARG:HG3   | 1:I:141:ARG:HH11   | 1.68                     | 0.58              |
| 1:I:141:ARG:CG    | 1:I:141:ARG:HH11   | 2.16                     | 0.58              |
| 1:B:26:ALA:HA     | 1:B:389:TRP:CD1    | 2.37                     | 0.58              |
| 1:N:318:VAL:HG12  | 1:N:321:ASP:H      | 1.67                     | 0.58              |
| 1:A:220:THR:HG23  | 1:A:227:ARG:HH11   | 1.67                     | 0.58              |
| 1:M:148:LEU:C     | 1:M:151:PRO:HD2    | 2.28                     | 0.58              |
| 1:D:381:ASP:HB2   | 1:D:404:ARG:HB3    | 1.86                     | 0.58              |
| 1:E:217:LEU:HD11  | 1:E:236:MET:HG2    | 1.85                     | 0.58              |
| 1:O:54:LEU:HD23   | 1:O:316:LEU:HB2    | 1.86                     | 0.58              |
| 1:A:108:ALA:O     | 1:A:109:ARG:C      | 2.47                     | 0.58              |
| 1:B:273:MET:HE1   | 1:B:276:LEU:HD13   | 1.84                     | 0.58              |
| 1:I:144:LEU:HD23  | 1:I:401:LEU:HD23   | 1.85                     | 0.58              |
| 1:N:336:ASP:HB3   | 1:N:339:ARG:HB3    | 1.84                     | 0.58              |
| 1:C:22:GLN:HE22   | 1:C:389:TRP:H      | 1.52                     | 0.58              |
| 1:E:135:LEU:HD21  | 1:E:375:CYS:SG     | 2.43                     | 0.58              |
| 1:F:150:TRP:CZ3   | 1:F:245[A]:HIS:HE1 | 2.21                     | 0.58              |
| 1:P:174:TRP:HB3   | 1:P:194:MET:HE3    | 1.85                     | 0.58              |
| 1:B:82:THR:CG2    | 1:B:85:GLU:OE1     | 2.51                     | 0.58              |
| 1:J:295:TYR:CD1   | 1:J:316:LEU:HD21   | 2.39                     | 0.58              |
| 1:B:148:LEU:C     | 1:B:151:PRO:HD2    | 2.29                     | 0.57              |
| 1:J:48:GLU:CD     | 1:J:48:GLU:H       | 2.10                     | 0.57              |
| 1:G:344:HIS:HD2   | 1:G:346:ALA:H      | 1.50                     | 0.57              |
| 1:I:150:TRP:CZ3   | 1:I:245:HIS:CE1    | 2.92                     | 0.57              |
| 1:M:13:PRO:HD2    | 1:P:369:ARG:NH1    | 2.18                     | 0.57              |
| 1:E:178:PHE:O     | 1:E:179:VAL:HG23   | 2.04                     | 0.57              |
| 2:H:1407:HEM:HBB2 | 2:H:1407:HEM:CMB   | 2.34                     | 0.57              |
| 1:A:251:LEU:HD13  | 1:A:284:LEU:HD23   | 1.85                     | 0.57              |
| 1:M:256:MET:HE2   | 1:M:371:LEU:HD13   | 1.86                     | 0.57              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:B:11:SER:N     | 1:B:12:PRO:CD      | 2.68                     | 0.57              |
| 1:K:152:LEU:HB3  | 1:K:153:PRO:HD3    | 1.86                     | 0.57              |
| 1:C:150:TRP:HZ3  | 1:C:245:HIS:HE1    | 1.51                     | 0.57              |
| 1:E:286:TYR:O    | 1:E:324:ARG:NH2    | 2.37                     | 0.57              |
| 1:I:291:GLU:HB3  | 1:I:393:PRO:O      | 2.03                     | 0.57              |
| 1:J:202:ILE:HG12 | 1:J:214:LEU:HD11   | 1.87                     | 0.57              |
| 1:N:43:ARG:NH1   | 1:N:51:GLU:HB3     | 2.20                     | 0.57              |
| 1:P:22:GLN:HE21  | 1:P:26:ALA:HB2     | 1.70                     | 0.57              |
| 1:P:119:LEU:O    | 1:P:123:VAL:HG23   | 2.05                     | 0.57              |
| 1:B:289:PRO:HG3  | 2:B:1407:HEM:HBB2  | 1.87                     | 0.57              |
| 1:C:244:GLY:HA2  | 2:C:1407:HEM:CMC   | 2.34                     | 0.57              |
| 1:N:93:LEU:HD13  | 2:N:1407:HEM:HAD2  | 1.87                     | 0.57              |
| 1:I:72:LYS:HE2   | 1:I:295:TYR:O      | 2.05                     | 0.57              |
| 1:A:301:PRO:HD3  | 1:A:311:ALA:HB2    | 1.87                     | 0.56              |
| 1:E:53:TRP:CD2   | 1:E:309:ILE:HG12   | 2.40                     | 0.56              |
| 1:D:67:ASP:HB3   | 1:D:70:PHE:CD1     | 2.38                     | 0.56              |
| 1:I:71:SER:OG    | 1:I:96:ASP:OD2     | 2.18                     | 0.56              |
| 1:K:11:SER:HB2   | 1:K:12:PRO:CD      | 2.26                     | 0.56              |
| 1:P:380:LEU:O    | 1:P:404:ARG:NH1    | 2.38                     | 0.56              |
| 1:B:148:LEU:O    | 1:B:151:PRO:HD2    | 2.05                     | 0.56              |
| 1:C:148:LEU:C    | 1:C:151:PRO:HD2    | 2.30                     | 0.56              |
| 1:C:203:ASP:OD1  | 1:C:206:ARG:NH1    | 2.39                     | 0.56              |
| 1:E:361:ARG:O    | 1:E:365:ARG:HG3    | 2.05                     | 0.56              |
| 1:G:135:LEU:HD21 | 1:G:375:CYS:SG     | 2.45                     | 0.56              |
| 1:F:228:LEU:HD12 | 1:F:232:GLU:HB2    | 1.87                     | 0.56              |
| 1:E:304:LEU:HD12 | 1:E:309:ILE:HD12   | 1.87                     | 0.56              |
| 1:G:289:PRO:HG2  | 2:G:1407:HEM:HMB3  | 1.87                     | 0.56              |
| 1:H:244:GLY:HA2  | 2:H:1407:HEM:C3C   | 2.41                     | 0.56              |
| 1:F:383:SER:C    | 1:F:385:GLY:H      | 2.13                     | 0.56              |
| 1:G:171:PHE:CE2  | 1:G:241:LEU:HD13   | 2.41                     | 0.56              |
| 1:I:360:ALA:HB1  | 2:I:1407:HEM:HAB   | 1.88                     | 0.56              |
| 1:J:241:LEU:O    | 1:J:245:HIS:HD2    | 1.89                     | 0.56              |
| 1:P:336:ASP:O    | 1:P:339:ARG:HG2    | 2.06                     | 0.56              |
| 1:I:244:GLY:HA2  | 2:I:1407:HEM:C2C   | 2.40                     | 0.56              |
| 1:K:150:TRP:HE3  | 1:K:245:HIS:CE1    | 2.22                     | 0.56              |
| 1:B:150:TRP:CZ3  | 1:B:245[B]:HIS:CE1 | 2.94                     | 0.56              |
| 1:H:60:ARG:HH22  | 1:H:305:ASP:HB2    | 1.70                     | 0.56              |
| 1:O:227:ARG:HB3  | 1:O:227:ARG:CZ     | 2.35                     | 0.56              |
| 1:B:255:GLY:HA2  | 1:B:283:MET:HG2    | 1.88                     | 0.55              |
| 1:C:243:ALA:HB2  | 4:C:1410:17Q:H52C  | 1.87                     | 0.55              |
| 1:H:328:ARG:NH1  | 1:H:342:ALA:O      | 2.39                     | 0.55              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:D:150:TRP:HZ3  | 1:D:245:HIS:CE1     | 2.24                     | 0.55              |
| 1:M:282:GLU:HG3  | 1:M:335:PHE:CE1     | 2.41                     | 0.55              |
| 1:M:360:ALA:CB   | 2:M:1407:HEM:HAB    | 2.36                     | 0.55              |
| 1:N:183:ASP:OD1  | 1:N:186:GLN:HB2     | 2.05                     | 0.55              |
| 1:B:120:ARG:HG3  | 1:B:366:ILE:HD11    | 1.89                     | 0.55              |
| 1:F:154:ILE:HD12 | 1:F:245[B]:HIS:CE1  | 2.42                     | 0.55              |
| 1:F:265:GLN:NE2  | 1:F:337:ILE:HG12    | 2.21                     | 0.55              |
| 1:P:93:LEU:HD13  | 2:P:1407:HEM:HAD2   | 1.87                     | 0.55              |
| 1:C:243:ALA:CB   | 4:C:1410:17Q:H52C   | 2.37                     | 0.55              |
| 1:G:52:VAL:HG21  | 1:G:316[B]:LEU:HD22 | 1.89                     | 0.55              |
| 1:B:17:LEU:HB2   | 1:B:47:PRO:HD3      | 1.88                     | 0.55              |
| 1:F:145:MET:HE1  | 1:F:253:ALA:HB1     | 1.88                     | 0.55              |
| 1:N:396:ARG:HG3  | 1:N:396:ARG:HH11    | 1.72                     | 0.55              |
| 1:C:244:GLY:HA2  | 2:C:1407:HEM:HMC2   | 1.89                     | 0.54              |
| 1:L:150:TRP:HZ3  | 1:L:245:HIS:NE2     | 1.89                     | 0.54              |
| 1:N:375:CYS:HB3  | 1:N:378:LEU:HB2     | 1.89                     | 0.54              |
| 1:O:22:GLN:HA    | 1:O:25:ALA:HB3      | 1.88                     | 0.54              |
| 1:A:24:PHE:CE1   | 1:A:28:PRO:HB3      | 2.42                     | 0.54              |
| 1:I:265:GLN:NE2  | 1:I:337:ILE:H       | 2.04                     | 0.54              |
| 1:J:250:ASN:CB   | 1:J:289:PRO:HB3     | 2.36                     | 0.54              |
| 1:O:35:LEU:O     | 1:O:42:HIS:NE2      | 2.40                     | 0.54              |
| 1:P:259:LEU:HD21 | 1:P:269:LEU:HD23    | 1.89                     | 0.54              |
| 1:B:11:SER:H     | 1:B:12:PRO:HD3      | 1.72                     | 0.54              |
| 1:B:35:LEU:HD22  | 1:B:42:HIS:CG       | 2.43                     | 0.54              |
| 1:B:88:LEU:HD21  | 1:B:195:SER:HB2     | 1.89                     | 0.54              |
| 1:L:224:ASP:OD2  | 1:L:227:ARG:HG3     | 2.07                     | 0.54              |
| 1:O:110:GLU:HG3  | 1:O:213:LEU:CD1     | 2.36                     | 0.54              |
| 1:E:338:ARG:HG2  | 1:E:338:ARG:HH11    | 1.73                     | 0.54              |
| 1:H:272:ASP:HB3  | 1:H:275:LEU:HD12    | 1.88                     | 0.54              |
| 1:K:60:ARG:HD2   | 1:K:304:LEU:HD22    | 1.88                     | 0.54              |
| 1:M:161:LEU:HD22 | 1:M:214:LEU:HD13    | 1.89                     | 0.54              |
| 1:M:244:GLY:HA2  | 2:M:1407:HEM:C2C    | 2.42                     | 0.54              |
| 1:B:10:ALA:HB1   | 1:B:53:TRP:HH2      | 1.71                     | 0.54              |
| 1:B:265:GLN:NE2  | 1:B:337:ILE:HG12    | 2.23                     | 0.54              |
| 1:G:228:LEU:HD12 | 1:G:232:GLU:HB3     | 1.90                     | 0.54              |
| 1:M:336:ASP:C    | 1:M:338:ARG:H       | 2.14                     | 0.54              |
| 1:E:265:GLN:HE21 | 1:E:337:ILE:HG12    | 1.72                     | 0.54              |
| 1:G:174:TRP:HB3  | 1:G:194:MET:HE3     | 1.90                     | 0.54              |
| 1:B:149:ALA:O    | 1:B:249:VAL:HG13    | 2.08                     | 0.54              |
| 1:J:375:CYS:HB2  | 1:J:378:LEU:HB2     | 1.90                     | 0.54              |
| 1:M:23:ASP:OD1   | 1:M:23:ASP:N        | 2.33                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:O:31:THR:HG23   | 1:O:34:ARG:HH22    | 1.73                     | 0.54              |
| 1:O:145:MET:HA    | 1:O:149:ALA:HB3    | 1.88                     | 0.54              |
| 1:A:354:CYS:HB2   | 2:A:1407:HEM:NA    | 2.22                     | 0.54              |
| 1:C:150:TRP:HZ3   | 1:C:245:HIS:NE2    | 2.06                     | 0.54              |
| 1:C:150:TRP:CE2   | 1:C:172:ARG:HD2    | 2.43                     | 0.54              |
| 1:H:382:VAL:HG11  | 1:H:402:PRO:HD2    | 1.90                     | 0.54              |
| 1:I:171:PHE:CE2   | 1:I:194:MET:HE2    | 2.43                     | 0.54              |
| 1:L:93:LEU:HD11   | 2:L:1407:HEM:HBA1  | 1.90                     | 0.54              |
| 1:O:15:LEU:HB3    | 1:O:44:VAL:HG12    | 1.90                     | 0.54              |
| 1:E:60:ARG:HH22   | 1:E:305:ASP:HB2    | 1.73                     | 0.54              |
| 1:H:265:GLN:NE2   | 1:H:337:ILE:H      | 2.05                     | 0.54              |
| 1:J:269:LEU:HD11  | 1:J:276:LEU:HA     | 1.90                     | 0.54              |
| 1:C:60:ARG:HD2    | 1:C:304:LEU:HD22   | 1.89                     | 0.53              |
| 1:D:150:TRP:CH2   | 1:D:172:ARG:HB2    | 2.43                     | 0.53              |
| 1:P:150:TRP:CE3   | 1:P:245:HIS:CE1    | 2.96                     | 0.53              |
| 1:A:152:LEU:HB3   | 1:A:153:PRO:HD3    | 1.89                     | 0.53              |
| 1:B:150:TRP:HE3   | 1:B:245[B]:HIS:HE2 | 1.56                     | 0.53              |
| 1:L:71:SER:HB2    | 1:L:299:VAL:CG1    | 2.38                     | 0.53              |
| 1:H:154:ILE:O     | 1:H:158:SER:HB2    | 2.07                     | 0.53              |
| 1:J:238:HIS:CE1   | 1:J:242:VAL:HG21   | 2.44                     | 0.53              |
| 2:O:1407:HEM:HBB2 | 2:O:1407:HEM:CMB   | 2.38                     | 0.53              |
| 1:I:88:LEU:HD21   | 1:I:195:SER:HB2    | 1.90                     | 0.53              |
| 1:J:61:ALA:HB1    | 1:J:317:VAL:HG13   | 1.91                     | 0.53              |
| 1:K:73:ASP:OD2    | 1:K:75:ARG:NH2     | 2.42                     | 0.53              |
| 1:M:29:TYR:CD1    | 1:M:324:ARG:HG3    | 2.44                     | 0.53              |
| 1:M:265:GLN:HE21  | 1:M:337:ILE:HG12   | 1.73                     | 0.53              |
| 1:P:294:THR:OG1   | 2:P:1407:HEM:O1A   | 2.25                     | 0.53              |
| 1:D:41:ALA:HA     | 1:D:54:LEU:O       | 2.09                     | 0.53              |
| 1:E:11:SER:N      | 1:E:12:PRO:HD2     | 2.24                     | 0.53              |
| 1:E:145:MET:HE3   | 1:E:398:LEU:O      | 2.08                     | 0.53              |
| 1:A:183:ASP:HB2   | 1:A:184:PRO:CD     | 2.39                     | 0.52              |
| 1:B:122:ARG:NH2   | 1:B:159:GLU:OE2    | 2.42                     | 0.52              |
| 1:C:387:LEU:HD22  | 1:C:398:LEU:HD22   | 1.91                     | 0.52              |
| 1:M:245:HIS:O     | 1:M:249:VAL:HG23   | 2.09                     | 0.52              |
| 1:F:14:VAL:HG22   | 1:F:43:ARG:O       | 2.09                     | 0.52              |
| 1:H:181:PRO:C     | 1:H:183:ASP:N      | 2.66                     | 0.52              |
| 1:C:178:PHE:HZ    | 1:C:194:MET:HE3    | 1.75                     | 0.52              |
| 1:L:243:ALA:C     | 1:L:245:HIS:N      | 2.66                     | 0.52              |
| 1:O:282:GLU:HG2   | 1:O:336:ASP:C      | 2.34                     | 0.52              |
| 1:J:34:ARG:HD3    | 5:J:2006:HOH:O     | 2.09                     | 0.52              |
| 1:D:144:LEU:HD11  | 1:D:371:LEU:HD11   | 1.90                     | 0.52              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:G:180:PHE:O    | 1:G:182:ASP:N       | 2.42                     | 0.52              |
| 1:G:338:ARG:HG2  | 1:G:338:ARG:HH11    | 1.75                     | 0.52              |
| 1:I:145:MET:HA   | 1:I:149:ALA:HB3     | 1.90                     | 0.52              |
| 1:M:78:THR:HG23  | 1:M:312:GLY:HA3     | 1.91                     | 0.52              |
| 1:D:89:ASN:CG    | 1:D:89:ASN:O        | 2.52                     | 0.52              |
| 1:D:174:TRP:CE3  | 1:D:194:MET:HG3     | 2.45                     | 0.52              |
| 1:F:336:ASP:C    | 1:F:338:ARG:H       | 2.18                     | 0.52              |
| 1:I:241:LEU:O    | 1:I:245:HIS:HB3     | 2.10                     | 0.52              |
| 1:I:244:GLY:HA2  | 2:I:1407:HEM:C3C    | 2.45                     | 0.52              |
| 1:L:204:SER:O    | 1:L:208:GLN:HG3     | 2.10                     | 0.52              |
| 1:O:78:THR:HG23  | 1:O:312:GLY:HA3     | 1.91                     | 0.52              |
| 1:B:98:PRO:O     | 1:B:99:ARG:C        | 2.53                     | 0.52              |
| 1:D:139:ASP:HB3  | 1:D:141:ARG:HB2     | 1.92                     | 0.52              |
| 1:E:150:TRP:CD1  | 1:E:151:PRO:HD3     | 2.45                     | 0.52              |
| 1:H:277:ASP:HB3  | 5:H:2027:HOH:O      | 2.08                     | 0.52              |
| 1:I:251:LEU:HB2  | 1:I:289:PRO:HG3     | 1.91                     | 0.52              |
| 1:B:165:GLU:HA   | 1:B:168:ARG:CD      | 2.34                     | 0.52              |
| 1:G:273:MET:CE   | 1:G:276:LEU:HD22    | 2.39                     | 0.52              |
| 1:G:295:TYR:CE1  | 1:G:316[B]:LEU:HD11 | 2.45                     | 0.52              |
| 1:H:17:LEU:HD22  | 1:H:24:PHE:CZ       | 2.45                     | 0.52              |
| 1:O:152:LEU:HB3  | 1:O:153:PRO:HD3     | 1.93                     | 0.52              |
| 1:J:126:ILE:HD13 | 1:J:155:THR:HG22    | 1.92                     | 0.51              |
| 1:O:171:PHE:O    | 1:O:175:THR:HB      | 2.09                     | 0.51              |
| 1:A:179:VAL:CG1  | 1:A:180:PHE:H       | 2.14                     | 0.51              |
| 1:G:11:SER:HB2   | 1:G:12:PRO:HD3      | 1.91                     | 0.51              |
| 1:G:60:ARG:HD2   | 1:G:304:LEU:HD22    | 1.92                     | 0.51              |
| 1:K:260:LEU:HD23 | 1:K:266:LEU:HD22    | 1.91                     | 0.51              |
| 1:N:149:ALA:O    | 1:N:249:VAL:HG22    | 2.10                     | 0.51              |
| 1:P:150:TRP:CH2  | 1:P:172:ARG:HB2     | 2.46                     | 0.51              |
| 1:D:78:THR:HG23  | 1:D:312:GLY:HA3     | 1.92                     | 0.51              |
| 1:H:28:PRO:HB2   | 1:H:32:TYR:CE2      | 2.45                     | 0.51              |
| 1:N:320:ALA:O    | 1:N:324:ARG:HG2     | 2.10                     | 0.51              |
| 1:P:150:TRP:HE3  | 1:P:245:HIS:CE1     | 2.28                     | 0.51              |
| 1:F:360:ALA:HB1  | 2:F:1407:HEM:HAB    | 1.92                     | 0.51              |
| 1:N:58:TYR:CD2   | 1:N:328:ARG:HG2     | 2.46                     | 0.51              |
| 1:N:295:TYR:HD1  | 1:N:316[A]:LEU:HD21 | 1.75                     | 0.51              |
| 1:B:10:ALA:HB1   | 1:B:53:TRP:CH2      | 2.45                     | 0.51              |
| 1:D:150:TRP:O    | 1:D:153:PRO:HD2     | 2.11                     | 0.51              |
| 1:D:161:LEU:CD2  | 1:D:213:LEU:HD23    | 2.40                     | 0.51              |
| 1:E:17:LEU:HA    | 1:E:20:LEU:HD12     | 1.92                     | 0.51              |
| 1:M:282:GLU:HG2  | 1:M:336:ASP:C       | 2.36                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:47:PRO:HG2   | 1:D:393:PRO:HD3   | 1.92                     | 0.51              |
| 1:D:289:PRO:HG2  | 2:D:1407:HEM:HMB3 | 1.92                     | 0.51              |
| 1:F:171:PHE:O    | 1:F:175:THR:CG2   | 2.46                     | 0.51              |
| 1:N:62:ARG:HH11  | 1:N:345:LEU:HD21  | 1.76                     | 0.51              |
| 1:D:228:LEU:HD12 | 1:D:232:GLU:HB3   | 1.93                     | 0.51              |
| 1:L:152:LEU:HB3  | 1:L:153:PRO:HD3   | 1.92                     | 0.51              |
| 1:I:150:TRP:CE3  | 1:I:245:HIS:HE1   | 2.28                     | 0.51              |
| 1:K:295:TYR:CE2  | 1:K:314:THR:HG21  | 2.46                     | 0.51              |
| 1:L:150:TRP:CZ3  | 1:L:245:HIS:CE1   | 2.98                     | 0.51              |
| 1:O:150:TRP:CZ2  | 1:O:172:ARG:HB2   | 2.45                     | 0.51              |
| 1:O:243:ALA:O    | 1:O:247:THR:OG1   | 2.25                     | 0.51              |
| 1:A:378:LEU:HD12 | 1:A:404:ARG:O     | 2.11                     | 0.51              |
| 1:E:228:LEU:CD1  | 1:E:232:GLU:HB3   | 2.41                     | 0.51              |
| 1:E:244:GLY:HA2  | 2:E:1407:HEM:C3C  | 2.46                     | 0.51              |
| 1:G:72:LYS:HB3   | 1:G:72:LYS:HZ2    | 1.76                     | 0.51              |
| 1:J:381:ASP:OD1  | 1:J:404:ARG:NH1   | 2.44                     | 0.51              |
| 1:K:273:MET:HE2  | 1:K:369:ARG:HG3   | 1.93                     | 0.51              |
| 1:A:270:ARG:NH1  | 1:A:372:LEU:O     | 2.43                     | 0.51              |
| 1:D:161:LEU:HD21 | 1:D:213:LEU:HD23  | 1.93                     | 0.51              |
| 1:I:40:PRO:HG3   | 1:I:305:ASP:HB3   | 1.92                     | 0.50              |
| 1:L:282:GLU:OE1  | 1:L:285:ARG:HB3   | 2.11                     | 0.50              |
| 1:N:99:ARG:HG3   | 1:N:102:ARG:NH2   | 2.26                     | 0.50              |
| 1:H:244:GLY:HA2  | 2:H:1407:HEM:C2C  | 2.46                     | 0.50              |
| 1:P:40:PRO:HG3   | 1:P:305:ASP:HB3   | 1.92                     | 0.50              |
| 1:K:148:LEU:C    | 1:K:151:PRO:HD2   | 2.36                     | 0.50              |
| 1:M:325:THR:HG23 | 1:M:327:GLU:OE1   | 2.11                     | 0.50              |
| 1:N:130:LEU:HD11 | 1:N:151:PRO:HB2   | 1.93                     | 0.50              |
| 1:C:104:ARG:NH1  | 2:C:1407:HEM:O2D  | 2.44                     | 0.50              |
| 1:K:136:ALA:O    | 1:K:137:ALA:C     | 2.54                     | 0.50              |
| 1:N:77:SER:OG    | 1:N:78:THR:N      | 2.44                     | 0.50              |
| 1:A:15:LEU:HD11  | 1:A:20:LEU:HD11   | 1.93                     | 0.50              |
| 1:B:90:HIS:HB3   | 1:B:232:GLU:HG3   | 1.94                     | 0.50              |
| 1:D:281:GLU:OE1  | 1:D:344:HIS:HE1   | 1.94                     | 0.50              |
| 1:F:291:GLU:HB3  | 1:F:393:PRO:O     | 2.11                     | 0.50              |
| 1:G:35:LEU:HB3   | 1:G:42:HIS:CD2    | 2.46                     | 0.50              |
| 1:L:281:GLU:OE1  | 1:L:361:ARG:NH2   | 2.45                     | 0.50              |
| 1:A:357:ALA:HB3  | 1:A:358:PRO:HD3   | 1.94                     | 0.50              |
| 1:I:248:THR:O    | 1:I:249:VAL:C     | 2.53                     | 0.50              |
| 1:L:392:ASN:OD1  | 1:L:393:PRO:CD    | 2.58                     | 0.50              |
| 1:D:244:GLY:HA2  | 2:D:1407:HEM:HBC2 | 1.93                     | 0.50              |
| 1:K:135:LEU:HD21 | 1:K:375:CYS:SG    | 2.52                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:P:148:LEU:C     | 1:P:151:PRO:HD2    | 2.36                     | 0.50              |
| 1:C:67:ASP:HB3    | 1:C:70:PHE:HD2     | 1.77                     | 0.50              |
| 1:F:265:GLN:HE21  | 1:F:337:ILE:HG23   | 1.77                     | 0.50              |
| 1:J:281:GLU:OE1   | 1:J:344:HIS:HE1    | 1.95                     | 0.50              |
| 1:J:338:ARG:HG2   | 1:J:338:ARG:HH11   | 1.77                     | 0.50              |
| 1:L:14:VAL:HG22   | 1:L:43:ARG:O       | 2.12                     | 0.50              |
| 1:L:320:ALA:O     | 1:L:324:ARG:HG2    | 2.12                     | 0.50              |
| 2:N:1407:HEM:HBC2 | 2:N:1407:HEM:CMC   | 2.29                     | 0.50              |
| 1:C:352:HIS:O     | 1:C:353:PHE:C      | 2.55                     | 0.50              |
| 1:E:279:ALA:O     | 1:E:283:MET:HG3    | 2.12                     | 0.50              |
| 1:F:154:ILE:CD1   | 1:F:245[B]:HIS:CE1 | 2.95                     | 0.50              |
| 1:H:92:MET:O      | 1:H:95:SER:HB2     | 2.12                     | 0.50              |
| 1:H:191:MET:O     | 1:H:195:SER:HB2    | 2.12                     | 0.50              |
| 1:N:162:GLY:O     | 1:N:164:PRO:HD3    | 2.12                     | 0.50              |
| 1:N:213:LEU:O     | 1:N:213:LEU:HG     | 2.12                     | 0.50              |
| 1:D:344:HIS:CD2   | 1:D:346:ALA:H      | 2.29                     | 0.49              |
| 1:G:174:TRP:HB2   | 1:G:194:MET:HE3    | 1.92                     | 0.49              |
| 1:M:120:ARG:HG3   | 1:M:366:ILE:HD11   | 1.94                     | 0.49              |
| 1:C:121:PRO:HD2   | 5:C:2017:HOH:O     | 2.12                     | 0.49              |
| 1:F:255:GLY:HA3   | 1:F:283:MET:SD     | 2.52                     | 0.49              |
| 1:N:60:ARG:NH1    | 1:N:305:ASP:HB2    | 2.26                     | 0.49              |
| 1:O:65:LEU:HG     | 1:O:317:VAL:HG11   | 1.93                     | 0.49              |
| 1:A:273:MET:HE3   | 1:A:276:LEU:HB2    | 1.93                     | 0.49              |
| 1:C:47:PRO:HD2    | 1:C:393:PRO:HD3    | 1.92                     | 0.49              |
| 1:C:273:MET:HE2   | 1:C:369:ARG:HG3    | 1.94                     | 0.49              |
| 1:J:60:ARG:NH2    | 1:J:305:ASP:HB2    | 2.27                     | 0.49              |
| 1:J:250:ASN:HB2   | 1:J:289:PRO:CB     | 2.41                     | 0.49              |
| 1:B:344:HIS:HD2   | 1:B:346:ALA:N      | 2.06                     | 0.49              |
| 1:O:81:LEU:HD22   | 1:O:85:GLU:HB3     | 1.94                     | 0.49              |
| 1:A:48:GLU:CD     | 1:A:48:GLU:H       | 2.19                     | 0.49              |
| 1:E:64:VAL:O      | 1:E:65:LEU:C       | 2.56                     | 0.49              |
| 1:G:161:LEU:HD12  | 1:G:241:LEU:HG     | 1.93                     | 0.49              |
| 1:K:11:SER:CB     | 1:K:12:PRO:HD3     | 2.28                     | 0.49              |
| 1:D:244:GLY:HA2   | 2:D:1407:HEM:CMC   | 2.39                     | 0.49              |
| 1:D:369:ARG:O     | 1:D:373:GLU:HG3    | 2.13                     | 0.49              |
| 1:O:24:PHE:CD1    | 1:O:28:PRO:HA      | 2.47                     | 0.49              |
| 1:D:29:TYR:O      | 1:D:30:PRO:C       | 2.54                     | 0.49              |
| 1:F:34:ARG:NH1    | 5:F:2004:HOH:O     | 2.44                     | 0.49              |
| 1:F:93:LEU:HD13   | 2:F:1407:HEM:HAD2  | 1.95                     | 0.49              |
| 1:F:228:LEU:HD12  | 1:F:232:GLU:HB3    | 1.92                     | 0.49              |
| 1:I:150:TRP:CD2   | 1:I:172:ARG:HD2    | 2.47                     | 0.49              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:I:243:ALA:C    | 1:I:245:HIS:H      | 2.20                     | 0.49              |
| 1:J:48:GLU:CD    | 1:J:48:GLU:N       | 2.71                     | 0.49              |
| 1:K:387:LEU:HD22 | 1:K:398:LEU:HD22   | 1.94                     | 0.49              |
| 1:M:262:HIS:O    | 1:M:264:ASP:N      | 2.45                     | 0.49              |
| 1:M:344:HIS:CD2  | 1:M:344:HIS:C      | 2.90                     | 0.49              |
| 1:D:273:MET:HE2  | 1:D:369:ARG:HG3    | 1.94                     | 0.49              |
| 1:E:376:PRO:O    | 1:E:377:ASP:HB2    | 2.13                     | 0.49              |
| 1:E:390:TYR:CE1  | 1:E:399:LYS:HG2    | 2.47                     | 0.49              |
| 1:I:279:ALA:O    | 1:I:283:MET:HG3    | 2.13                     | 0.49              |
| 1:J:298:PRO:HD2  | 1:J:312:GLY:H      | 1.78                     | 0.49              |
| 1:D:157:ILE:HD12 | 1:D:160:LEU:HD23   | 1.94                     | 0.49              |
| 1:D:344:HIS:CD2  | 1:D:344:HIS:C      | 2.91                     | 0.49              |
| 1:G:273:MET:HE2  | 1:G:369:ARG:CG     | 2.24                     | 0.49              |
| 1:N:144:LEU:HD23 | 1:N:401:LEU:HD23   | 1.95                     | 0.49              |
| 1:B:175:THR:HG21 | 1:B:245[B]:HIS:CE1 | 2.48                     | 0.49              |
| 1:E:244:GLY:HA2  | 2:E:1407:HEM:CAC   | 2.43                     | 0.49              |
| 1:H:289:PRO:HG2  | 2:H:1407:HEM:HMB2  | 1.95                     | 0.49              |
| 1:L:58:TYR:C     | 1:L:58:TYR:CD1     | 2.90                     | 0.49              |
| 1:B:51:GLU:OE2   | 1:L:369:ARG:NH2    | 2.45                     | 0.48              |
| 1:C:72:LYS:HE2   | 1:C:296:ARG:NH1    | 2.28                     | 0.48              |
| 1:C:236:MET:O    | 1:C:239:ILE:HG22   | 2.12                     | 0.48              |
| 1:C:260:LEU:HD21 | 1:C:378:LEU:HD23   | 1.94                     | 0.48              |
| 1:E:67:ASP:HB3   | 1:E:70:PHE:HD2     | 1.76                     | 0.48              |
| 1:E:152:LEU:HB3  | 1:E:153:PRO:HD3    | 1.95                     | 0.48              |
| 1:E:243:ALA:O    | 2:E:1407:HEM:C4C   | 2.67                     | 0.48              |
| 1:J:115:ARG:HD3  | 1:J:118:LEU:HD12   | 1.94                     | 0.48              |
| 1:J:360:ALA:HB1  | 2:J:1407:HEM:CBB   | 2.43                     | 0.48              |
| 1:K:279:ALA:O    | 1:K:283:MET:HG3    | 2.13                     | 0.48              |
| 1:O:250:ASN:O    | 1:O:251:LEU:C      | 2.56                     | 0.48              |
| 1:P:135:LEU:HD21 | 1:P:375:CYS:SG     | 2.53                     | 0.48              |
| 1:B:245[B]:HIS:O | 1:B:249:VAL:HG23   | 2.13                     | 0.48              |
| 1:B:336:ASP:C    | 1:B:336:ASP:OD1    | 2.55                     | 0.48              |
| 1:D:153:PRO:HG2  | 1:D:249:VAL:HG22   | 1.96                     | 0.48              |
| 1:F:281:GLU:OE1  | 1:F:344:HIS:HE1    | 1.96                     | 0.48              |
| 1:H:13:PRO:HG2   | 1:H:45:ARG:HH21    | 1.78                     | 0.48              |
| 1:I:60:ARG:HD2   | 1:I:304:LEU:HD22   | 1.95                     | 0.48              |
| 1:L:32:TYR:OH    | 1:L:291:GLU:OE2    | 2.29                     | 0.48              |
| 1:M:203:ASP:O    | 1:M:204:SER:C      | 2.56                     | 0.48              |
| 1:O:265:GLN:HE21 | 1:O:336:ASP:HA     | 1.77                     | 0.48              |
| 1:B:175:THR:HG21 | 1:B:245[B]:HIS:ND1 | 2.29                     | 0.48              |
| 1:K:66:ALA:HB2   | 1:K:349:HIS:CD2    | 2.48                     | 0.48              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:C:360:ALA:HB1  | 2:C:1407:HEM:HAB    | 1.95                     | 0.48              |
| 1:D:66:ALA:HB2   | 1:D:349:HIS:CD2     | 2.48                     | 0.48              |
| 1:E:183:ASP:OD1  | 1:E:183:ASP:N       | 2.32                     | 0.48              |
| 1:G:321:ASP:O    | 1:G:322:ALA:C       | 2.57                     | 0.48              |
| 1:M:201:LEU:O    | 1:M:204:SER:HB3     | 2.13                     | 0.48              |
| 1:O:272:ASP:OD1  | 1:O:274:THR:HG23    | 2.13                     | 0.48              |
| 1:B:270:ARG:HH22 | 1:B:378:LEU:HB3     | 1.77                     | 0.48              |
| 1:E:29:TYR:CD1   | 1:E:324:ARG:HG3     | 2.48                     | 0.48              |
| 1:F:150:TRP:CE3  | 1:F:245[A]:HIS:CE1  | 3.01                     | 0.48              |
| 1:G:158:SER:O    | 1:G:162:GLY:N       | 2.47                     | 0.48              |
| 1:N:290:VAL:HB   | 1:N:319:LEU:HD12    | 1.94                     | 0.48              |
| 1:A:174:TRP:CE3  | 1:A:194:MET:CE      | 2.75                     | 0.48              |
| 1:B:85:GLU:HG3   | 1:B:191:MET:HE1     | 1.94                     | 0.48              |
| 1:J:145:MET:HA   | 1:J:149:ALA:HB3     | 1.95                     | 0.48              |
| 1:J:295:TYR:CE1  | 1:J:316:LEU:HD21    | 2.49                     | 0.48              |
| 1:G:180:PHE:HA   | 1:G:392[B]:ASN:HD21 | 1.79                     | 0.48              |
| 1:G:257:TYR:CE1  | 1:G:387:LEU:HD11    | 2.49                     | 0.48              |
| 1:I:295:TYR:CD1  | 1:I:316[B]:LEU:HD11 | 2.49                     | 0.48              |
| 1:J:338:ARG:HG2  | 1:J:338:ARG:NH1     | 2.29                     | 0.48              |
| 1:N:260:LEU:HD23 | 1:N:266:LEU:HD22    | 1.95                     | 0.48              |
| 1:O:88:LEU:C     | 1:O:90:HIS:N        | 2.72                     | 0.48              |
| 1:B:299:VAL:HG23 | 1:B:300:GLU:N       | 2.28                     | 0.48              |
| 1:C:275:LEU:HD13 | 1:C:337:ILE:HD11    | 1.95                     | 0.48              |
| 1:D:265:GLN:NE2  | 1:D:337:ILE:HG12    | 2.28                     | 0.48              |
| 1:E:88:LEU:HD22  | 1:E:238:HIS:CG      | 2.49                     | 0.48              |
| 1:H:344:HIS:C    | 1:H:344:HIS:CD2     | 2.92                     | 0.48              |
| 1:M:43:ARG:HG2   | 1:M:53:TRP:CE2      | 2.49                     | 0.48              |
| 1:M:381:ASP:CG   | 1:M:381:ASP:O       | 2.56                     | 0.48              |
| 1:O:88:LEU:O     | 1:O:90:HIS:N        | 2.46                     | 0.48              |
| 1:O:183:ASP:C    | 1:O:185:ALA:H       | 2.21                     | 0.48              |
| 1:H:251:LEU:HD22 | 1:H:284:LEU:HD21    | 1.95                     | 0.47              |
| 1:I:136:ALA:O    | 1:I:137:ALA:C       | 2.57                     | 0.47              |
| 1:P:13:PRO:HB3   | 1:P:43:ARG:HH11     | 1.79                     | 0.47              |
| 1:A:370:ALA:O    | 1:A:374:ARG:HG3     | 2.13                     | 0.47              |
| 1:B:281:GLU:HB3  | 1:B:341:THR:OG1     | 2.14                     | 0.47              |
| 1:C:285:ARG:NH1  | 1:C:332:PRO:O       | 2.39                     | 0.47              |
| 1:F:17:LEU:HD22  | 1:F:24:PHE:CZ       | 2.49                     | 0.47              |
| 1:G:265:GLN:HE21 | 1:G:337:ILE:HG23    | 1.79                     | 0.47              |
| 1:K:234:LEU:HD12 | 1:K:234:LEU:O       | 2.13                     | 0.47              |
| 1:E:176:ASP:O    | 1:E:177:ALA:C       | 2.57                     | 0.47              |
| 1:N:150:TRP:HE3  | 1:N:245:HIS:HE1     | 1.57                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:269:LEU:HD11  | 1:O:276:LEU:HA    | 1.95                     | 0.47              |
| 1:P:214:LEU:O     | 1:P:218:VAL:HG23  | 2.14                     | 0.47              |
| 1:E:154:ILE:HD13  | 1:E:245:HIS:CD2   | 2.49                     | 0.47              |
| 1:G:265:GLN:NE2   | 1:G:337:ILE:H     | 2.11                     | 0.47              |
| 1:K:244:GLY:O     | 1:K:245:HIS:C     | 2.58                     | 0.47              |
| 1:N:71:SER:OG     | 1:N:96:ASP:OD2    | 2.28                     | 0.47              |
| 1:E:48:GLU:CD     | 1:E:48:GLU:H      | 2.22                     | 0.47              |
| 1:K:281:GLU:OE1   | 1:K:344:HIS:HE1   | 1.97                     | 0.47              |
| 1:L:148:LEU:C     | 1:L:151:PRO:HD2   | 2.39                     | 0.47              |
| 1:M:357:ALA:HB3   | 1:M:358:PRO:HD3   | 1.96                     | 0.47              |
| 1:B:265:GLN:HE21  | 1:B:337:ILE:H     | 1.61                     | 0.47              |
| 1:F:67:ASP:C      | 1:F:67:ASP:OD1    | 2.57                     | 0.47              |
| 4:G:1410:17Q:H91C | 4:G:1410:17Q:H72C | 1.65                     | 0.47              |
| 1:N:273:MET:HE2   | 1:N:369:ARG:HG3   | 1.97                     | 0.47              |
| 1:N:396:ARG:HH11  | 1:N:396:ARG:CG    | 2.27                     | 0.47              |
| 1:A:107:VAL:O     | 1:A:110:GLU:HB2   | 2.13                     | 0.47              |
| 1:A:127:VAL:O     | 1:A:131:VAL:HG23  | 2.14                     | 0.47              |
| 1:C:339:ARG:HG3   | 1:C:341:THR:HG23  | 1.95                     | 0.47              |
| 1:D:69:ARG:NH1    | 1:D:302:VAL:HG13  | 2.29                     | 0.47              |
| 1:F:131:VAL:O     | 1:F:135:LEU:HG    | 2.14                     | 0.47              |
| 1:I:162:GLY:O     | 1:I:164:PRO:HD3   | 2.14                     | 0.47              |
| 1:K:22:GLN:HE22   | 1:K:389:TRP:H     | 1.63                     | 0.47              |
| 1:L:183:ASP:N     | 1:L:183:ASP:OD1   | 2.48                     | 0.47              |
| 1:M:88:LEU:HD22   | 1:M:238:HIS:ND1   | 2.29                     | 0.47              |
| 1:M:122:ARG:O     | 1:M:126:ILE:HG13  | 2.14                     | 0.47              |
| 1:O:36:ARG:HH12   | 1:O:326:PRO:HD3   | 1.80                     | 0.47              |
| 1:O:250:ASN:OD1   | 1:O:397:GLY:HA2   | 2.15                     | 0.47              |
| 1:P:29:TYR:N      | 1:P:30:PRO:HD2    | 2.29                     | 0.47              |
| 1:A:273:MET:CE    | 1:A:276:LEU:HD22  | 2.45                     | 0.47              |
| 1:G:145:MET:HA    | 1:G:149:ALA:HB3   | 1.97                     | 0.47              |
| 1:I:150:TRP:CE2   | 1:I:172:ARG:HD2   | 2.50                     | 0.47              |
| 1:N:115:ARG:HA    | 1:N:115:ARG:HD3   | 1.77                     | 0.47              |
| 1:P:58:TYR:CD1    | 1:P:58:TYR:C      | 2.92                     | 0.47              |
| 1:A:62:ARG:NH2    | 3:A:1408:SO4:O4   | 2.40                     | 0.47              |
| 1:A:381:ASP:O     | 1:A:382:VAL:CB    | 2.53                     | 0.47              |
| 1:B:82:THR:OG1    | 1:B:85:GLU:OE1    | 2.32                     | 0.47              |
| 1:C:29:TYR:N      | 1:C:30:PRO:HD2    | 2.29                     | 0.47              |
| 1:H:114:ARG:NH1   | 5:H:2017:HOH:O    | 2.47                     | 0.47              |
| 1:H:127:VAL:HG21  | 1:H:366:ILE:HG22  | 1.97                     | 0.47              |
| 1:H:360:ALA:O     | 1:H:361:ARG:C     | 2.56                     | 0.47              |
| 1:I:381:ASP:O     | 1:I:382:VAL:CB    | 2.62                     | 0.47              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:F:167:ASP:OD2  | 1:F:197:TYR:OH     | 2.30                     | 0.47              |
| 1:H:291:GLU:HB3  | 1:H:393:PRO:O      | 2.15                     | 0.47              |
| 1:M:19:ALA:HB3   | 1:P:117:GLU:HG2    | 1.97                     | 0.47              |
| 1:B:60:ARG:O     | 1:B:64:VAL:HG23    | 2.15                     | 0.46              |
| 1:B:158:SER:HB3  | 1:B:168:ARG:NE     | 2.30                     | 0.46              |
| 1:E:152:LEU:O    | 1:E:156:VAL:HG23   | 2.15                     | 0.46              |
| 1:L:301:PRO:HD3  | 1:L:311:ALA:HB2    | 1.97                     | 0.46              |
| 1:B:183:ASP:HB2  | 1:B:184:PRO:CD     | 2.45                     | 0.46              |
| 1:B:241:LEU:O    | 1:B:245[A]:HIS:CE1 | 2.68                     | 0.46              |
| 1:C:344:HIS:CD2  | 1:C:344:HIS:C      | 2.94                     | 0.46              |
| 1:F:150:TRP:O    | 1:F:153:PRO:HD2    | 2.14                     | 0.46              |
| 1:G:149:ALA:O    | 1:G:249:VAL:HG22   | 2.16                     | 0.46              |
| 1:I:128:ASP:CA   | 1:I:374:ARG:HH12   | 2.09                     | 0.46              |
| 1:K:187:ALA:O    | 1:K:190:ALA:HB3    | 2.15                     | 0.46              |
| 1:N:13:PRO:O     | 1:N:15:LEU:N       | 2.48                     | 0.46              |
| 1:N:281:GLU:HA   | 1:N:284:LEU:HD12   | 1.97                     | 0.46              |
| 1:N:390:TYR:HA   | 1:N:391:PRO:HD3    | 1.77                     | 0.46              |
| 1:O:36:ARG:NH1   | 1:O:326:PRO:HD3    | 2.30                     | 0.46              |
| 1:A:344:HIS:CD2  | 1:A:346:ALA:HB3    | 2.51                     | 0.46              |
| 1:G:150:TRP:CZ3  | 1:G:154:ILE:HG21   | 2.50                     | 0.46              |
| 1:J:150:TRP:HZ3  | 1:J:245:HIS:CE1    | 2.33                     | 0.46              |
| 1:K:267:ALA:HA   | 1:K:270:ARG:HB2    | 1.97                     | 0.46              |
| 1:M:145:MET:HE1  | 1:M:398:LEU:HB2    | 1.96                     | 0.46              |
| 1:C:282:GLU:HG3  | 1:C:335:PHE:CE1    | 2.50                     | 0.46              |
| 1:E:392:ASN:OD1  | 1:E:393:PRO:HD2    | 2.15                     | 0.46              |
| 1:J:178:PHE:HE1  | 1:J:194:MET:HE1    | 1.81                     | 0.46              |
| 1:B:81:LEU:HD13  | 1:B:86:ALA:HA      | 1.96                     | 0.46              |
| 1:K:327:GLU:H    | 1:K:327:GLU:CD     | 2.23                     | 0.46              |
| 1:P:171:PHE:O    | 1:P:175:THR:HB     | 2.15                     | 0.46              |
| 1:J:183:ASP:OD1  | 1:J:183:ASP:N      | 2.49                     | 0.46              |
| 1:J:273:MET:HE2  | 1:J:369:ARG:HG3    | 1.98                     | 0.46              |
| 1:L:298:PRO:HG2  | 1:L:309:ILE:HG22   | 1.98                     | 0.46              |
| 1:N:150:TRP:CD1  | 1:N:151:PRO:HD3    | 2.51                     | 0.46              |
| 1:A:123:VAL:O    | 1:A:127:VAL:HG23   | 2.16                     | 0.46              |
| 1:B:179:VAL:CG1  | 1:B:180:PHE:N      | 2.73                     | 0.46              |
| 1:C:24:PHE:O     | 1:C:25:ALA:C       | 2.59                     | 0.46              |
| 1:C:82:THR:OG1   | 1:C:188:GLN:NE2    | 2.48                     | 0.46              |
| 1:E:228:LEU:HD12 | 1:E:232:GLU:HB3    | 1.97                     | 0.46              |
| 1:G:394:MET:HE2  | 1:G:394:MET:HB3    | 1.83                     | 0.46              |
| 1:H:227:ARG:NH2  | 5:H:2025:HOH:O     | 2.48                     | 0.46              |
| 1:I:354:CYS:HB2  | 2:I:1407:HEM:NA    | 2.30                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:J:122:ARG:NH2    | 1:J:159:GLU:OE2    | 2.48                     | 0.46              |
| 1:K:175:THR:C      | 1:K:177:ALA:N      | 2.73                     | 0.46              |
| 1:K:301:PRO:HD3    | 1:K:311:ALA:HB2    | 1.97                     | 0.46              |
| 1:P:35:LEU:HD13    | 1:P:42:HIS:HB2     | 1.98                     | 0.46              |
| 1:P:279:ALA:O      | 1:P:283:MET:HG3    | 2.16                     | 0.46              |
| 1:F:76:ASN:O       | 1:F:312:GLY:HA2    | 2.15                     | 0.46              |
| 1:F:265:GLN:HE22   | 1:F:337:ILE:HG12   | 1.81                     | 0.46              |
| 1:F:356:GLY:O      | 1:F:357:ALA:C      | 2.59                     | 0.46              |
| 1:I:356:GLY:O      | 1:I:357:ALA:C      | 2.59                     | 0.46              |
| 1:J:352:HIS:O      | 1:J:353:PHE:C      | 2.59                     | 0.46              |
| 1:M:36:ARG:HH21    | 1:M:321:ASP:CG     | 2.23                     | 0.46              |
| 1:O:179:VAL:O      | 1:O:392:ASN:HB2    | 2.16                     | 0.46              |
| 1:A:161:LEU:CD2    | 1:A:213:LEU:HB3    | 2.46                     | 0.46              |
| 1:B:273:MET:HE2    | 1:B:369:ARG:CD     | 2.40                     | 0.46              |
| 1:C:178:PHE:HZ     | 1:C:194:MET:CE     | 2.28                     | 0.46              |
| 1:E:114:ARG:NH2    | 5:E:2018:HOH:O     | 2.48                     | 0.46              |
| 1:K:161:LEU:CD1    | 1:K:241:LEU:HG     | 2.45                     | 0.46              |
| 1:K:390:TYR:HA     | 1:K:391:PRO:HD3    | 1.81                     | 0.46              |
| 1:M:248:THR:HA     | 2:M:1407:HEM:HBB1  | 1.98                     | 0.46              |
| 1:P:203[A]:ASP:OD1 | 1:P:206:ARG:NH1    | 2.45                     | 0.46              |
| 1:C:145:MET:HE3    | 1:C:398:LEU:O      | 2.16                     | 0.46              |
| 1:H:331:ASP:OD2    | 1:H:334:ARG:HD3    | 2.16                     | 0.46              |
| 1:I:150:TRP:CE3    | 1:I:245:HIS:CE1    | 3.04                     | 0.46              |
| 1:J:150:TRP:HB3    | 1:J:151:PRO:HD3    | 1.97                     | 0.46              |
| 1:D:119:LEU:O      | 1:D:120:ARG:C      | 2.57                     | 0.45              |
| 1:F:265:GLN:HE22   | 1:F:337:ILE:N      | 2.11                     | 0.45              |
| 1:F:357:ALA:HB3    | 1:F:358:PRO:HD3    | 1.97                     | 0.45              |
| 1:J:331:ASP:OD2    | 1:J:334:ARG:HD3    | 2.16                     | 0.45              |
| 1:K:145:MET:HA     | 1:K:149:ALA:HB3    | 1.97                     | 0.45              |
| 1:M:81:LEU:HD22    | 1:M:85:GLU:HB3     | 1.99                     | 0.45              |
| 1:N:354:CYS:HB2    | 2:N:1407:HEM:NA    | 2.31                     | 0.45              |
| 1:O:318:VAL:HG12   | 1:O:321:ASP:H      | 1.81                     | 0.45              |
| 1:O:344:HIS:HD2    | 1:O:346:ALA:N      | 2.13                     | 0.45              |
| 1:C:64:VAL:HG13    | 1:C:70:PHE:CD2     | 2.50                     | 0.45              |
| 1:G:353:PHE:CE1    | 1:P:223:GLU:HG2    | 2.51                     | 0.45              |
| 1:H:375:CYS:HA     | 1:H:376:PRO:HD2    | 1.74                     | 0.45              |
| 1:J:71:SER:OG      | 1:J:96:ASP:OD2     | 2.32                     | 0.45              |
| 1:P:174:TRP:CB     | 1:P:194:MET:HE3    | 2.45                     | 0.45              |
| 1:P:231:GLU:O      | 1:P:234:LEU:HB3    | 2.16                     | 0.45              |
| 1:F:150:TRP:CE3    | 1:F:245[A]:HIS:HE1 | 2.34                     | 0.45              |
| 1:J:148:LEU:HD23   | 1:J:371:LEU:HD21   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:152:LEU:HB3  | 1:J:153:PRO:HD3   | 1.99                     | 0.45              |
| 1:A:131:VAL:O    | 1:A:135:LEU:HG    | 2.15                     | 0.45              |
| 1:B:344:HIS:CD2  | 1:B:346:ALA:HB3   | 2.51                     | 0.45              |
| 1:C:94:GLU:OE1   | 4:C:1410:17Q:H112 | 2.17                     | 0.45              |
| 1:D:381:ASP:CG   | 1:D:381:ASP:O     | 2.58                     | 0.45              |
| 1:H:137:ALA:HA   | 1:H:138:PRO:HD3   | 1.85                     | 0.45              |
| 1:D:11:SER:HB3   | 1:O:369:ARG:NH2   | 2.32                     | 0.45              |
| 1:D:181:PRO:HA   | 1:D:186:GLN:OE1   | 2.17                     | 0.45              |
| 1:H:40:PRO:HG3   | 1:H:305:ASP:HB3   | 1.99                     | 0.45              |
| 1:I:181:PRO:O    | 1:I:182:ASP:C     | 2.59                     | 0.45              |
| 1:K:141:ARG:HG3  | 1:K:404:ARG:HB3   | 1.99                     | 0.45              |
| 1:L:110:GLU:HG3  | 1:L:213:LEU:HD13  | 1.98                     | 0.45              |
| 1:N:303:ASP:HA   | 1:N:308:VAL:HA    | 1.99                     | 0.45              |
| 1:B:281:GLU:OE1  | 1:B:344:HIS:HE1   | 1.99                     | 0.45              |
| 1:C:244:GLY:HA2  | 2:C:1407:HEM:C2C  | 2.51                     | 0.45              |
| 1:H:344:HIS:CD2  | 1:H:346:ALA:H     | 2.35                     | 0.45              |
| 1:L:29:TYR:HE1   | 1:L:320:ALA:HB1   | 1.82                     | 0.45              |
| 1:N:252:ILE:O    | 1:N:256:MET:HB2   | 2.16                     | 0.45              |
| 1:N:254:ASN:ND2  | 1:N:396:ARG:O     | 2.44                     | 0.45              |
| 1:D:219:ARG:O    | 1:D:223:GLU:HG3   | 2.17                     | 0.45              |
| 1:G:93:LEU:HD13  | 2:G:1407:HEM:HAD2 | 1.98                     | 0.45              |
| 1:H:140:GLY:HA2  | 1:H:405:TRP:CE2   | 2.51                     | 0.45              |
| 1:M:148:LEU:O    | 1:M:151:PRO:HD2   | 2.16                     | 0.45              |
| 1:P:229:THR:OG1  | 1:P:232:GLU:HG3   | 2.17                     | 0.45              |
| 1:B:152:LEU:HB3  | 1:B:153:PRO:HD3   | 1.98                     | 0.45              |
| 1:D:153:PRO:HG2  | 1:D:249:VAL:CG2   | 2.47                     | 0.45              |
| 1:D:324:ARG:HA   | 1:D:332:PRO:HB2   | 1.99                     | 0.45              |
| 1:E:13:PRO:HA    | 1:E:43:ARG:O      | 2.17                     | 0.45              |
| 1:E:294:THR:HA   | 1:E:394:MET:HE3   | 1.99                     | 0.45              |
| 1:F:29:TYR:N     | 1:F:30:PRO:CD     | 2.80                     | 0.45              |
| 1:G:168:ARG:O    | 1:G:171:PHE:HB2   | 2.17                     | 0.45              |
| 1:K:326:PRO:HA   | 1:K:329:PHE:O     | 2.17                     | 0.45              |
| 1:N:150:TRP:CZ3  | 1:N:245:HIS:CE1   | 3.04                     | 0.45              |
| 1:P:284:LEU:O    | 1:P:346:ALA:HB2   | 2.15                     | 0.45              |
| 1:J:202:ILE:HD13 | 1:J:233:LEU:HG    | 1.98                     | 0.45              |
| 1:J:390:TYR:HA   | 1:J:391:PRO:HD3   | 1.84                     | 0.45              |
| 1:O:107:VAL:HG23 | 1:O:355:ILE:CD1   | 2.46                     | 0.45              |
| 1:O:197:TYR:HA   | 1:O:200:ARG:NH2   | 2.32                     | 0.45              |
| 1:H:52:VAL:HG12  | 1:H:314:THR:HB    | 2.00                     | 0.45              |
| 1:J:150:TRP:CZ3  | 1:J:245:HIS:CE1   | 3.05                     | 0.45              |
| 1:M:228:LEU:HD12 | 1:M:232:GLU:HB2   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:73:ASP:HB3   | 1:N:76:ASN:ND2   | 2.32                     | 0.45              |
| 1:N:388:VAL:HG23 | 1:N:399:LYS:HB2  | 1.99                     | 0.45              |
| 1:P:74:TRP:C     | 1:P:76:ASN:H     | 2.24                     | 0.45              |
| 1:P:245:HIS:O    | 1:P:249:VAL:HG23 | 2.17                     | 0.45              |
| 1:P:324:ARG:HA   | 1:P:324:ARG:HD3  | 1.64                     | 0.45              |
| 1:A:41:ALA:HA    | 1:A:54:LEU:O     | 2.17                     | 0.44              |
| 1:D:47:PRO:C     | 1:D:49:GLY:H     | 2.24                     | 0.44              |
| 1:D:391:PRO:O    | 1:D:392:ASN:C    | 2.60                     | 0.44              |
| 1:D:394:MET:HE2  | 1:D:394:MET:HB3  | 1.94                     | 0.44              |
| 1:F:148:LEU:C    | 1:F:151:PRO:HD2  | 2.42                     | 0.44              |
| 1:G:148:LEU:C    | 1:G:151:PRO:HD2  | 2.43                     | 0.44              |
| 1:K:53:TRP:HB2   | 1:K:315:VAL:HG22 | 1.99                     | 0.44              |
| 1:M:11:SER:N     | 1:M:12:PRO:HD2   | 2.32                     | 0.44              |
| 1:O:36:ARG:HA    | 1:O:56:VAL:HG21  | 1.99                     | 0.44              |
| 1:P:92:MET:O     | 1:P:100:HIS:HD2  | 2.00                     | 0.44              |
| 1:P:110:GLU:HG3  | 1:P:213:LEU:HD13 | 1.99                     | 0.44              |
| 1:E:78:THR:HG23  | 1:E:312:GLY:HA3  | 1.98                     | 0.44              |
| 1:E:150:TRP:HD1  | 1:E:151:PRO:HD3  | 1.81                     | 0.44              |
| 1:E:344:HIS:CD2  | 1:E:346:ALA:H    | 2.17                     | 0.44              |
| 1:F:66:ALA:HB2   | 1:F:349:HIS:CD2  | 2.52                     | 0.44              |
| 1:F:245[B]:HIS:O | 1:F:246:GLU:C    | 2.60                     | 0.44              |
| 1:H:203:ASP:C    | 1:H:205:LYS:H    | 2.25                     | 0.44              |
| 1:J:281:GLU:HA   | 1:J:284:LEU:HD12 | 1.98                     | 0.44              |
| 1:K:204:SER:O    | 1:K:208:GLN:HG3  | 2.17                     | 0.44              |
| 1:K:273:MET:CE   | 1:K:276:LEU:HD22 | 2.48                     | 0.44              |
| 1:M:40:PRO:HG3   | 1:M:305:ASP:CB   | 2.44                     | 0.44              |
| 1:A:22:GLN:HE22  | 1:A:389:TRP:H    | 1.66                     | 0.44              |
| 1:A:251:LEU:HD13 | 1:A:284:LEU:CD2  | 2.47                     | 0.44              |
| 1:B:46:THR:OG1   | 1:B:50:ASN:N     | 2.50                     | 0.44              |
| 1:G:344:HIS:CD2  | 1:G:346:ALA:HB3  | 2.52                     | 0.44              |
| 1:L:25:ALA:HB2   | 1:L:391:PRO:HA   | 1.99                     | 0.44              |
| 1:M:272:ASP:OD1  | 1:M:274:THR:OG1  | 2.36                     | 0.44              |
| 1:N:150:TRP:CE3  | 1:N:245:HIS:CE1  | 3.01                     | 0.44              |
| 1:P:145:MET:HA   | 1:P:149:ALA:HB3  | 1.99                     | 0.44              |
| 1:F:180:PHE:O    | 1:F:180:PHE:CG   | 2.70                     | 0.44              |
| 1:F:368:VAL:O    | 1:F:369:ARG:C    | 2.60                     | 0.44              |
| 1:G:265:GLN:HE21 | 1:G:337:ILE:HG12 | 1.83                     | 0.44              |
| 1:G:354:CYS:HA   | 2:G:1407:HEM:CHA | 2.48                     | 0.44              |
| 1:I:152:LEU:HB3  | 1:I:153:PRO:HD3  | 1.98                     | 0.44              |
| 1:L:179:VAL:HG11 | 1:L:390:TYR:CD2  | 2.52                     | 0.44              |
| 1:L:238:HIS:O    | 1:L:239:ILE:C    | 2.60                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:M:17:LEU:HD22  | 1:M:24:PHE:CE1     | 2.53                     | 0.44              |
| 1:M:202:ILE:HD13 | 1:M:233:LEU:HG     | 1.99                     | 0.44              |
| 1:M:356:GLY:O    | 1:M:357:ALA:C      | 2.61                     | 0.44              |
| 1:O:202:ILE:HD13 | 1:O:233:LEU:HG     | 1.98                     | 0.44              |
| 1:O:381:ASP:O    | 1:O:382:VAL:CB     | 2.65                     | 0.44              |
| 1:E:298:PRO:HG2  | 1:E:309:ILE:HG22   | 2.00                     | 0.44              |
| 1:H:172:ARG:O    | 1:H:175:THR:HG22   | 2.18                     | 0.44              |
| 1:H:244:GLY:HA2  | 2:H:1407:HEM:CAC   | 2.47                     | 0.44              |
| 1:O:72:LYS:HD3   | 1:O:93:LEU:O       | 2.18                     | 0.44              |
| 1:O:107:VAL:HG23 | 1:O:355:ILE:HD13   | 1.99                     | 0.44              |
| 1:A:136:ALA:HB2  | 1:M:268:ALA:HA     | 2.00                     | 0.44              |
| 1:A:282:GLU:CD   | 1:A:285:ARG:HH21   | 2.26                     | 0.44              |
| 1:H:99:ARG:HG3   | 1:H:102:ARG:HH21   | 1.82                     | 0.44              |
| 1:L:175:THR:O    | 1:L:179:VAL:HG23   | 2.17                     | 0.44              |
| 1:D:175:THR:C    | 1:D:177:ALA:N      | 2.75                     | 0.44              |
| 1:F:60:ARG:HH12  | 1:F:305:ASP:HB2    | 1.81                     | 0.44              |
| 1:F:145:MET:HA   | 1:F:149:ALA:HB3    | 1.99                     | 0.44              |
| 1:G:146:GLU:OE2  | 1:G:172:ARG:NH1    | 2.50                     | 0.44              |
| 1:G:265:GLN:HE22 | 1:G:337:ILE:HG12   | 1.81                     | 0.44              |
| 1:I:28:PRO:HB2   | 1:I:32:TYR:CE2     | 2.52                     | 0.44              |
| 1:J:295:TYR:HD1  | 1:J:316:LEU:CD2    | 2.29                     | 0.44              |
| 1:M:134:MET:HG3  | 1:M:147:SER:HB3    | 2.00                     | 0.44              |
| 1:O:92:MET:O     | 1:O:100:HIS:HD2    | 2.01                     | 0.44              |
| 1:P:356:GLY:HA3  | 2:P:1407:HEM:C3C   | 2.53                     | 0.44              |
| 1:P:392:ASN:HA   | 1:P:393:PRO:HD3    | 1.70                     | 0.44              |
| 1:B:76:ASN:O     | 1:B:312:GLY:HA2    | 2.18                     | 0.44              |
| 1:F:57:GLY:O     | 1:F:58:TYR:C       | 2.61                     | 0.44              |
| 1:G:120:ARG:HB3  | 1:G:121:PRO:HD3    | 1.99                     | 0.44              |
| 1:G:144:LEU:HD21 | 1:G:256:MET:HG3    | 2.00                     | 0.44              |
| 1:O:28:PRO:HB2   | 1:O:32:TYR:CE2     | 2.53                     | 0.44              |
| 1:B:150:TRP:HZ3  | 1:B:245[B]:HIS:CE1 | 2.35                     | 0.44              |
| 1:B:344:HIS:CD2  | 1:B:346:ALA:H      | 2.25                     | 0.44              |
| 1:I:144:LEU:HB3  | 1:I:401:LEU:HB3    | 2.00                     | 0.44              |
| 1:L:71:SER:HB2   | 1:L:299:VAL:HG13   | 1.98                     | 0.44              |
| 1:N:382:VAL:HG22 | 1:N:383:SER:H      | 1.83                     | 0.44              |
| 1:O:183:ASP:OD1  | 1:O:186:GLN:N      | 2.51                     | 0.44              |
| 1:B:72:LYS:HE2   | 1:B:296:ARG:NH1    | 2.33                     | 0.43              |
| 1:D:175:THR:HG21 | 1:D:246:GLU:HG2    | 2.00                     | 0.43              |
| 1:D:242:VAL:O    | 1:D:243:ALA:C      | 2.60                     | 0.43              |
| 1:E:74:TRP:C     | 1:E:76:ASN:N       | 2.75                     | 0.43              |
| 1:G:239:ILE:HD11 | 4:G:1410:17Q:H51C  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:156:VAL:HG12  | 1:K:157:ILE:N     | 2.33                     | 0.43              |
| 1:L:28:PRO:HB2    | 1:L:32:TYR:CE2    | 2.53                     | 0.43              |
| 1:L:371:LEU:O     | 1:L:375:CYS:HB2   | 2.17                     | 0.43              |
| 1:M:282:GLU:HG3   | 1:M:335:PHE:CD1   | 2.53                     | 0.43              |
| 1:N:251:LEU:HD22  | 2:N:1407:HEM:HBB1 | 2.00                     | 0.43              |
| 1:O:265:GLN:NE2   | 1:O:336:ASP:HA    | 2.32                     | 0.43              |
| 1:C:29:TYR:CE1    | 1:C:320:ALA:HB1   | 2.53                     | 0.43              |
| 1:P:252:ILE:H     | 1:P:252:ILE:HG13  | 1.65                     | 0.43              |
| 1:B:219:ARG:O     | 1:B:223:GLU:HG3   | 2.18                     | 0.43              |
| 1:C:152:LEU:CB    | 1:C:153:PRO:HD3   | 2.48                     | 0.43              |
| 1:F:161:LEU:O     | 1:F:214:LEU:HB2   | 2.19                     | 0.43              |
| 1:G:71:SER:CB     | 1:G:76:ASN:HD22   | 2.31                     | 0.43              |
| 1:P:64:VAL:HG13   | 1:P:70:PHE:CD2    | 2.54                     | 0.43              |
| 1:P:157:ILE:HG13  | 1:P:161:LEU:HD12  | 2.00                     | 0.43              |
| 1:B:251:LEU:HB2   | 2:B:1407:HEM:HBB1 | 2.00                     | 0.43              |
| 1:F:273:MET:HG3   | 1:F:373:GLU:OE2   | 2.19                     | 0.43              |
| 1:N:186:GLN:O     | 1:N:189:THR:HB    | 2.18                     | 0.43              |
| 1:B:360:ALA:CB    | 2:B:1407:HEM:HAB  | 2.49                     | 0.43              |
| 1:F:152:LEU:HB3   | 1:F:153:PRO:HD3   | 2.01                     | 0.43              |
| 1:H:140:GLY:HA2   | 1:H:405:TRP:CZ2   | 2.53                     | 0.43              |
| 1:I:108:ALA:HA    | 1:I:355:ILE:HD11  | 2.01                     | 0.43              |
| 1:M:293:ALA:O     | 1:M:316:LEU:HD22  | 2.18                     | 0.43              |
| 1:M:390:TYR:CZ    | 1:M:399:LYS:HG2   | 2.54                     | 0.43              |
| 1:O:205:LYS:HD2   | 1:O:214:LEU:HD23  | 1.99                     | 0.43              |
| 1:B:328:ARG:O     | 1:B:328:ARG:NH1   | 2.46                     | 0.43              |
| 1:D:175:THR:C     | 1:D:177:ALA:H     | 2.27                     | 0.43              |
| 1:F:381:ASP:HB2   | 1:F:403:ILE:C     | 2.44                     | 0.43              |
| 1:K:143:ASP:O     | 1:K:144:LEU:C     | 2.62                     | 0.43              |
| 1:K:356:GLY:O     | 1:K:357:ALA:C     | 2.60                     | 0.43              |
| 1:L:244:GLY:HA2   | 2:L:1407:HEM:HMC3 | 2.01                     | 0.43              |
| 1:B:51:GLU:OE2    | 1:L:369:ARG:CZ    | 2.66                     | 0.43              |
| 1:D:82:THR:O      | 1:D:83:GLU:C      | 2.61                     | 0.43              |
| 1:G:50[A]:ASN:N   | 1:G:50[A]:ASN:ND2 | 2.66                     | 0.43              |
| 1:H:137:ALA:C     | 1:H:139:ASP:H     | 2.26                     | 0.43              |
| 1:H:145:MET:O     | 1:H:150:TRP:HB3   | 2.18                     | 0.43              |
| 1:J:107:VAL:O     | 1:J:108:ALA:C     | 2.61                     | 0.43              |
| 1:N:30:PRO:O      | 1:N:34:ARG:HB2    | 2.19                     | 0.43              |
| 1:P:300:GLU:O     | 1:P:302:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:130:LEU:O     | 1:A:134:MET:HB2   | 2.18                     | 0.43              |
| 1:A:242:VAL:C     | 1:A:244:GLY:H     | 2.26                     | 0.43              |
| 4:C:1410:17Q:H11C | 4:C:1410:17Q:H42C | 1.56                     | 0.43              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:E:119:LEU:O    | 1:E:123:VAL:HG23   | 2.19                     | 0.43              |
| 1:F:218:VAL:HG22 | 1:F:233:LEU:HD21   | 2.01                     | 0.43              |
| 1:G:228:LEU:HD12 | 1:G:232:GLU:CB     | 2.49                     | 0.43              |
| 1:K:44:VAL:HG11  | 1:K:54:LEU:HD12    | 2.00                     | 0.43              |
| 1:K:181:PRO:C    | 1:K:183:ASP:N      | 2.74                     | 0.43              |
| 1:O:178:PHE:HB3  | 1:O:187:ALA:CB     | 2.48                     | 0.43              |
| 1:E:270:ARG:NH1  | 1:E:372:LEU:O      | 2.45                     | 0.43              |
| 1:J:91:ASN:OD1   | 1:J:239:ILE:HD13   | 2.18                     | 0.43              |
| 1:J:165:GLU:N    | 1:J:166:PRO:CD     | 2.81                     | 0.43              |
| 1:N:197:TYR:CD1  | 1:N:197:TYR:C      | 2.97                     | 0.43              |
| 1:N:396:ARG:CG   | 1:N:396:ARG:NH1    | 2.81                     | 0.43              |
| 1:A:82:THR:HG23  | 1:A:85:GLU:OE1     | 2.19                     | 0.43              |
| 1:C:163:VAL:O    | 1:C:164:PRO:C      | 2.60                     | 0.43              |
| 1:E:41:ALA:HA    | 1:E:54:LEU:O       | 2.19                     | 0.43              |
| 1:F:160:LEU:HD12 | 1:F:160:LEU:HA     | 1.86                     | 0.43              |
| 1:G:53:TRP:CD1   | 1:G:309:ILE:HG23   | 2.54                     | 0.43              |
| 1:I:60:ARG:HH11  | 1:I:304:LEU:HD22   | 1.84                     | 0.43              |
| 1:O:300:GLU:O    | 1:O:301:PRO:C      | 2.59                     | 0.43              |
| 1:P:337:ILE:O    | 5:P:2016:HOH:O     | 2.22                     | 0.43              |
| 1:A:76:ASN:O     | 1:A:312:GLY:HA2    | 2.19                     | 0.42              |
| 1:A:77:SER:HB2   | 1:A:297:PHE:CE2    | 2.54                     | 0.42              |
| 1:A:145:MET:HA   | 1:A:149:ALA:HB3    | 2.01                     | 0.42              |
| 1:G:72:LYS:HB3   | 1:G:72:LYS:HZ3     | 1.84                     | 0.42              |
| 1:I:285:ARG:O    | 1:I:323:HIS:HB3    | 2.19                     | 0.42              |
| 1:M:139:ASP:O    | 1:M:141:ARG:HG3    | 2.19                     | 0.42              |
| 1:N:67:ASP:OD1   | 1:N:69:ARG:N       | 2.52                     | 0.42              |
| 1:O:178:PHE:HB3  | 1:O:187:ALA:HB1    | 2.00                     | 0.42              |
| 1:B:20:LEU:HB3   | 1:B:24:PHE:HB2     | 2.00                     | 0.42              |
| 1:C:150:TRP:CZ3  | 1:C:245:HIS:HE1    | 2.29                     | 0.42              |
| 1:D:114:ARG:NH1  | 1:D:114:ARG:HG2    | 2.34                     | 0.42              |
| 1:D:114:ARG:HG2  | 1:D:114:ARG:HH11   | 1.84                     | 0.42              |
| 1:G:245:HIS:CE1  | 5:G:2042:HOH:O     | 2.72                     | 0.42              |
| 1:I:132:ASP:OD1  | 1:I:374:ARG:NH2    | 2.51                     | 0.42              |
| 1:J:256:MET:HE2  | 1:J:371:LEU:HD13   | 2.00                     | 0.42              |
| 1:K:95:SER:HB3   | 1:K:99:ARG:HB3     | 2.00                     | 0.42              |
| 1:K:316[B]:LEU:N | 1:K:316[B]:LEU:CD1 | 2.80                     | 0.42              |
| 1:P:251:LEU:HD22 | 2:P:1407:HEM:HBB1  | 2.01                     | 0.42              |
| 1:A:74:TRP:C     | 1:A:76:ASN:N       | 2.77                     | 0.42              |
| 1:A:161:LEU:HD21 | 1:A:213:LEU:HD23   | 2.01                     | 0.42              |
| 1:D:82:THR:OG1   | 1:D:188:GLN:NE2    | 2.51                     | 0.42              |
| 1:D:218:VAL:HG22 | 1:D:233:LEU:HD21   | 2.02                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:J:282:GLU:OE1    | 1:J:282:GLU:HA    | 2.20                     | 0.42              |
| 1:L:148:LEU:O      | 1:L:151:PRO:HD2   | 2.18                     | 0.42              |
| 1:N:60:ARG:HH12    | 1:N:305:ASP:HB2   | 1.84                     | 0.42              |
| 1:P:288:GLY:HA2    | 1:P:289:PRO:HD3   | 1.88                     | 0.42              |
| 1:A:238:HIS:O      | 1:A:239:ILE:C     | 2.62                     | 0.42              |
| 1:A:344:HIS:HD2    | 1:A:346:ALA:H     | 1.68                     | 0.42              |
| 1:B:108:ALA:HA     | 1:B:355:ILE:HD11  | 2.01                     | 0.42              |
| 1:B:360:ALA:HB1    | 2:B:1407:HEM:HAB  | 2.00                     | 0.42              |
| 1:C:68:PRO:HA      | 5:C:2002:HOH:O    | 2.19                     | 0.42              |
| 1:C:78:THR:HG23    | 1:C:312:GLY:HA3   | 2.01                     | 0.42              |
| 1:D:139:ASP:CB     | 1:D:141:ARG:HB2   | 2.49                     | 0.42              |
| 1:E:174:TRP:O      | 1:E:177:ALA:HB3   | 2.20                     | 0.42              |
| 1:F:168:ARG:O      | 1:F:171:PHE:HB2   | 2.19                     | 0.42              |
| 1:H:336:ASP:OD1    | 1:H:336:ASP:C     | 2.62                     | 0.42              |
| 1:J:219:ARG:O      | 1:J:223:GLU:HG3   | 2.19                     | 0.42              |
| 1:K:60:ARG:O       | 1:K:64:VAL:HG23   | 2.19                     | 0.42              |
| 1:K:175:THR:O      | 1:K:176:ASP:C     | 2.62                     | 0.42              |
| 1:K:277:ASP:OD1    | 1:K:365:ARG:HD3   | 2.19                     | 0.42              |
| 1:C:175:THR:CG2    | 1:C:176:ASP:N     | 2.82                     | 0.42              |
| 1:D:174:TRP:HB3    | 1:D:194:MET:HE2   | 2.00                     | 0.42              |
| 1:D:325:THR:HA     | 1:D:326:PRO:HD3   | 1.94                     | 0.42              |
| 1:E:280:VAL:HA     | 1:E:283:MET:HG3   | 2.01                     | 0.42              |
| 1:J:57:GLY:N       | 1:J:321:ASP:OD2   | 2.50                     | 0.42              |
| 1:J:61:ALA:HB1     | 1:J:317:VAL:CG1   | 2.50                     | 0.42              |
| 1:L:92:MET:HE1     | 1:L:104:ARG:HA    | 2.00                     | 0.42              |
| 1:M:150:TRP:O      | 1:M:153:PRO:HD2   | 2.20                     | 0.42              |
| 1:F:382:VAL:HG22   | 1:F:383:SER:H     | 1.84                     | 0.42              |
| 1:I:174:TRP:CB     | 1:I:194:MET:HE3   | 2.49                     | 0.42              |
| 1:J:60:ARG:NH1     | 1:J:305:ASP:HB2   | 2.35                     | 0.42              |
| 1:M:370:ALA:O      | 1:M:374:ARG:HG3   | 2.20                     | 0.42              |
| 1:A:168:ARG:O      | 1:A:171:PHE:HB2   | 2.19                     | 0.42              |
| 1:B:90:HIS:O       | 1:B:232:GLU:HA    | 2.19                     | 0.42              |
| 1:B:119:LEU:O      | 1:B:123:VAL:HG23  | 2.19                     | 0.42              |
| 1:B:174:TRP:HE3    | 1:B:194:MET:HE3   | 1.85                     | 0.42              |
| 1:D:115:ARG:HD3    | 1:D:115:ARG:HA    | 1.77                     | 0.42              |
| 1:D:168:ARG:O      | 1:D:171:PHE:HB2   | 2.20                     | 0.42              |
| 1:E:203[B]:ASP:OD1 | 1:E:203[B]:ASP:O  | 2.37                     | 0.42              |
| 1:F:122:ARG:HA     | 1:F:122:ARG:HD2   | 1.92                     | 0.42              |
| 1:G:60:ARG:HH11    | 1:G:304:LEU:HD22  | 1.85                     | 0.42              |
| 1:G:243:ALA:HB2    | 4:G:1410:17Q:H41C | 2.00                     | 0.42              |
| 1:G:336:ASP:OD1    | 1:G:336:ASP:C     | 2.62                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:H:175:THR:O    | 1:H:179:VAL:HG23   | 2.20                     | 0.42              |
| 1:I:251:LEU:CB   | 2:I:1407:HEM:HBB1  | 2.50                     | 0.42              |
| 1:J:150:TRP:CZ2  | 1:J:172:ARG:HB2    | 2.55                     | 0.42              |
| 1:J:197:TYR:OH   | 1:J:201:LEU:HD13   | 2.19                     | 0.42              |
| 1:L:164:PRO:HB2  | 1:L:166:PRO:HD2    | 2.02                     | 0.42              |
| 1:N:161:LEU:HD21 | 1:N:213:LEU:HD23   | 2.01                     | 0.42              |
| 1:O:259:LEU:O    | 1:O:266:LEU:HB2    | 2.20                     | 0.42              |
| 1:E:241:LEU:O    | 1:E:245:HIS:HB2    | 2.19                     | 0.42              |
| 1:F:41:ALA:C     | 1:F:42:HIS:CG      | 2.98                     | 0.42              |
| 1:F:144:LEU:HD23 | 1:F:401:LEU:HD23   | 2.02                     | 0.42              |
| 1:I:74:TRP:CD2   | 1:I:81:LEU:HD21    | 2.55                     | 0.42              |
| 1:L:92:MET:O     | 1:L:100:HIS:HD2    | 2.02                     | 0.42              |
| 1:M:61:ALA:O     | 1:M:65:LEU:HG      | 2.19                     | 0.42              |
| 1:M:203:ASP:N    | 1:M:203:ASP:OD1    | 2.53                     | 0.42              |
| 1:N:392:ASN:HA   | 1:N:393:PRO:HD2    | 1.92                     | 0.42              |
| 1:E:46:THR:HB    | 1:E:48:GLU:OE2     | 2.19                     | 0.42              |
| 1:F:11:SER:CB    | 1:F:12:PRO:CD      | 2.94                     | 0.42              |
| 1:H:67:ASP:OD1   | 1:H:68:PRO:HD2     | 2.20                     | 0.42              |
| 1:K:60:ARG:HH21  | 1:K:305:ASP:HB2    | 1.83                     | 0.42              |
| 1:L:339:ARG:HG3  | 1:L:341:THR:HG22   | 2.01                     | 0.42              |
| 1:N:394:MET:HE2  | 1:N:394:MET:HB3    | 1.96                     | 0.42              |
| 1:C:243:ALA:HB2  | 4:C:1410:17Q:C5    | 2.50                     | 0.42              |
| 1:F:150:TRP:HZ3  | 1:F:245[A]:HIS:HE1 | 1.65                     | 0.42              |
| 1:H:260:LEU:HD23 | 1:H:260:LEU:HA     | 1.87                     | 0.42              |
| 1:J:60:ARG:HH22  | 1:J:305:ASP:HB2    | 1.85                     | 0.42              |
| 1:K:154:ILE:HD12 | 1:K:154:ILE:HA     | 1.86                     | 0.42              |
| 1:L:67:ASP:HA    | 1:L:68:PRO:HD3     | 1.94                     | 0.42              |
| 1:P:67:ASP:HA    | 1:P:68:PRO:HD3     | 1.77                     | 0.42              |
| 1:A:202:ILE:HG23 | 1:A:218:VAL:HG22   | 2.02                     | 0.41              |
| 1:A:265:GLN:NE2  | 1:A:337:ILE:H      | 2.18                     | 0.41              |
| 1:B:289:PRO:HG2  | 2:B:1407:HEM:HMB3  | 2.02                     | 0.41              |
| 1:B:361:ARG:HD3  | 1:B:365:ARG:NH2    | 2.35                     | 0.41              |
| 1:C:376:PRO:O    | 1:C:377:ASP:HB2    | 2.19                     | 0.41              |
| 1:G:154:ILE:HD12 | 1:G:154:ILE:HA     | 1.93                     | 0.41              |
| 1:H:110:GLU:HB2  | 1:H:111:PHE:CD2    | 2.55                     | 0.41              |
| 1:H:203:ASP:C    | 1:H:205:LYS:N      | 2.76                     | 0.41              |
| 1:P:25:ALA:CB    | 1:P:391:PRO:HA     | 2.50                     | 0.41              |
| 1:P:361:ARG:O    | 1:P:362:LEU:C      | 2.64                     | 0.41              |
| 1:A:160:LEU:O    | 1:A:161:LEU:HD23   | 2.20                     | 0.41              |
| 1:C:392:ASN:O    | 5:C:2038:HOH:O     | 2.21                     | 0.41              |
| 1:H:41:ALA:C     | 1:H:42:HIS:CG      | 2.98                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:H:1407:HEM:HMB2  | 2:H:1407:HEM:CBB | 2.49                     | 0.41              |
| 1:K:107:VAL:O      | 1:K:108:ALA:C    | 2.63                     | 0.41              |
| 1:A:242:VAL:C      | 1:A:244:GLY:N    | 2.77                     | 0.41              |
| 1:B:144:LEU:HD13   | 1:B:403:ILE:HD13 | 2.01                     | 0.41              |
| 1:B:299:VAL:HG23   | 1:B:300:GLU:H    | 1.84                     | 0.41              |
| 1:D:98:PRO:HD2     | 5:D:2017:HOH:O   | 2.19                     | 0.41              |
| 1:E:103:LEU:O      | 1:E:104:ARG:C    | 2.64                     | 0.41              |
| 1:G:77:SER:HB2     | 1:G:297:PHE:CE1  | 2.55                     | 0.41              |
| 1:G:120:ARG:HG3    | 1:G:366:ILE:HD11 | 2.02                     | 0.41              |
| 1:K:310:PRO:HB2    | 1:K:313:ASP:OD1  | 2.19                     | 0.41              |
| 1:M:60:ARG:HD3     | 1:M:60:ARG:HA    | 1.85                     | 0.41              |
| 1:M:104:ARG:NH1    | 2:M:1407:HEM:O2D | 2.53                     | 0.41              |
| 1:N:265:GLN:NE2    | 1:N:337:ILE:H    | 2.18                     | 0.41              |
| 1:O:336:ASP:C      | 1:O:336:ASP:OD1  | 2.63                     | 0.41              |
| 1:O:353:PHE:O      | 1:O:354:CYS:C    | 2.63                     | 0.41              |
| 1:A:99:ARG:HG3     | 1:A:102:ARG:NH2  | 2.35                     | 0.41              |
| 1:B:60:ARG:HA      | 1:B:60:ARG:HD3   | 1.89                     | 0.41              |
| 1:B:304:LEU:O      | 1:B:305:ASP:C    | 2.63                     | 0.41              |
| 1:D:67:ASP:HA      | 1:D:68:PRO:HD2   | 1.90                     | 0.41              |
| 1:F:292:SER:HB2    | 1:F:394:MET:HA   | 2.02                     | 0.41              |
| 1:G:257:TYR:CE1    | 1:G:387:LEU:CD1  | 3.04                     | 0.41              |
| 1:G:392[A]:ASN:OD1 | 1:G:394:MET:HB2  | 2.20                     | 0.41              |
| 1:J:126:ILE:HD13   | 1:J:155:THR:CG2  | 2.49                     | 0.41              |
| 1:K:124:GLN:HA     | 1:K:366:ILE:HG21 | 2.02                     | 0.41              |
| 1:L:29:TYR:CE1     | 1:L:320:ALA:HB1  | 2.55                     | 0.41              |
| 1:L:67:ASP:OD2     | 1:L:69:ARG:NH2   | 2.49                     | 0.41              |
| 1:M:234:LEU:O      | 1:M:235:GLY:C    | 2.62                     | 0.41              |
| 1:N:390:TYR:C      | 1:N:392:ASN:H    | 2.29                     | 0.41              |
| 1:A:236:MET:HA     | 1:A:239:ILE:HG22 | 2.01                     | 0.41              |
| 1:C:135:LEU:HD21   | 1:C:375:CYS:SG   | 2.61                     | 0.41              |
| 1:E:244:GLY:HA2    | 2:E:1407:HEM:C2C | 2.55                     | 0.41              |
| 1:I:135:LEU:HA     | 1:I:405:TRP:CZ2  | 2.56                     | 0.41              |
| 1:I:265:GLN:HE21   | 1:I:337:ILE:HG23 | 1.85                     | 0.41              |
| 1:L:202:ILE:HD13   | 1:L:233:LEU:HG   | 2.02                     | 0.41              |
| 1:O:398:LEU:HD13   | 1:O:401:LEU:HB2  | 2.02                     | 0.41              |
| 1:D:13:PRO:HA      | 1:D:43:ARG:HB3   | 2.01                     | 0.41              |
| 1:D:150:TRP:CE2    | 1:D:172:ARG:HD2  | 2.55                     | 0.41              |
| 1:D:390:TYR:HA     | 1:D:391:PRO:HD3  | 1.80                     | 0.41              |
| 1:E:175:THR:HG22   | 1:E:176:ASP:N    | 2.35                     | 0.41              |
| 1:F:250:ASN:O      | 1:F:254:ASN:HB2  | 2.20                     | 0.41              |
| 1:H:99:ARG:HG3     | 1:H:102:ARG:NH2  | 2.35                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:L:111:PHE:CE1    | 2:L:1407:HEM:HBC1  | 2.55                     | 0.41              |
| 1:L:328:ARG:NH2    | 1:L:343:GLY:HA3    | 2.36                     | 0.41              |
| 1:M:48:GLU:H       | 1:M:48:GLU:CD      | 2.27                     | 0.41              |
| 1:M:122:ARG:HE     | 1:M:126:ILE:HD11   | 1.85                     | 0.41              |
| 1:M:336:ASP:C      | 1:M:338:ARG:N      | 2.78                     | 0.41              |
| 1:N:150:TRP:CH2    | 1:N:172:ARG:HB2    | 2.55                     | 0.41              |
| 1:O:224:ASP:OD2    | 1:O:227:ARG:HG3    | 2.21                     | 0.41              |
| 1:O:329:PHE:HA     | 1:O:330:PRO:HD3    | 1.94                     | 0.41              |
| 1:C:239:ILE:O      | 1:C:243:ALA:HB3    | 2.20                     | 0.41              |
| 1:D:309:ILE:HA     | 1:D:310:PRO:HD3    | 1.91                     | 0.41              |
| 1:F:150:TRP:HE3    | 1:F:245[A]:HIS:CE1 | 2.38                     | 0.41              |
| 1:H:265:GLN:HE21   | 1:H:337:ILE:H      | 1.69                     | 0.41              |
| 1:K:160:LEU:HD12   | 1:K:160:LEU:HA     | 1.85                     | 0.41              |
| 1:K:224:ASP:OD2    | 1:K:227:ARG:HG3    | 2.20                     | 0.41              |
| 1:K:353:PHE:CD1    | 1:K:353:PHE:C      | 2.98                     | 0.41              |
| 1:L:89:ASN:O       | 1:L:89:ASN:CG      | 2.63                     | 0.41              |
| 1:M:76:ASN:O       | 1:M:312:GLY:HA2    | 2.19                     | 0.41              |
| 1:P:300:GLU:O      | 1:P:301:PRO:C      | 2.64                     | 0.41              |
| 1:A:137:ALA:HA     | 1:A:138:PRO:HD3    | 1.93                     | 0.41              |
| 1:A:197:TYR:CD1    | 1:A:197:TYR:C      | 2.98                     | 0.41              |
| 1:C:119:LEU:O      | 1:C:120:ARG:C      | 2.64                     | 0.41              |
| 1:F:248:THR:O      | 1:F:249:VAL:C      | 2.64                     | 0.41              |
| 1:F:344:HIS:CD2    | 1:F:346:ALA:HB3    | 2.56                     | 0.41              |
| 1:G:223:GLU:O      | 3:O:1409:SO4:O2    | 2.38                     | 0.41              |
| 1:G:309:ILE:HA     | 1:G:310:PRO:HD3    | 1.93                     | 0.41              |
| 1:H:150:TRP:CE2    | 1:H:172:ARG:HD2    | 2.56                     | 0.41              |
| 1:J:10:ALA:O       | 1:J:43:ARG:HG3     | 2.20                     | 0.41              |
| 1:J:255:GLY:CA     | 1:J:283:MET:HG2    | 2.50                     | 0.41              |
| 1:L:107:VAL:O      | 1:L:108:ALA:C      | 2.64                     | 0.41              |
| 1:O:135:LEU:HA     | 1:O:405:TRP:CZ2    | 2.56                     | 0.41              |
| 1:A:260:LEU:HD21   | 1:A:378:LEU:HD23   | 2.03                     | 0.41              |
| 1:D:88:LEU:HD22    | 1:D:238:HIS:CG     | 2.55                     | 0.41              |
| 1:D:361:ARG:O      | 1:D:365:ARG:CG     | 2.57                     | 0.41              |
| 2:D:1407:HEM:HMB1  | 2:D:1407:HEM:HBB2  | 2.03                     | 0.41              |
| 1:F:229:THR:O      | 1:F:232:GLU:N      | 2.52                     | 0.41              |
| 1:G:273:MET:HE1    | 1:G:276:LEU:HD13   | 2.03                     | 0.41              |
| 1:G:392[B]:ASN:OD1 | 1:G:392[B]:ASN:N   | 2.54                     | 0.41              |
| 1:H:13:PRO:HA      | 1:H:43:ARG:HB3     | 2.02                     | 0.41              |
| 1:H:108:ALA:HA     | 1:H:355:ILE:HD11   | 2.03                     | 0.41              |
| 1:H:150:TRP:HA     | 1:H:249:VAL:HG22   | 2.02                     | 0.41              |
| 1:I:243:ALA:O      | 1:I:245:HIS:N      | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:209:ASP:OD2   | 1:M:101:THR:OG1   | 2.30                     | 0.41              |
| 1:J:244:GLY:HA2   | 2:J:1407:HEM:C2C  | 2.56                     | 0.41              |
| 1:K:104:ARG:NH1   | 2:K:1407:HEM:O2D  | 2.53                     | 0.41              |
| 1:L:203[A]:ASP:HA | 1:L:206:ARG:NH1   | 2.36                     | 0.41              |
| 1:L:356:GLY:O     | 1:L:357:ALA:C     | 2.64                     | 0.41              |
| 1:M:322:ALA:CB    | 1:M:345:LEU:HD12  | 2.51                     | 0.41              |
| 1:M:390:TYR:CE1   | 1:M:399:LYS:HG2   | 2.56                     | 0.41              |
| 1:P:58:TYR:O      | 1:P:61:ALA:HB3    | 2.21                     | 0.41              |
| 1:P:149:ALA:C     | 1:P:249:VAL:HG13  | 2.46                     | 0.41              |
| 1:P:156:VAL:HG11  | 1:P:363:GLU:OE2   | 2.21                     | 0.41              |
| 1:D:154:ILE:HD12  | 1:D:154:ILE:HA    | 1.92                     | 0.41              |
| 1:D:382:VAL:HG22  | 1:D:383:SER:N     | 2.36                     | 0.41              |
| 1:G:240:LEU:HD23  | 1:G:240:LEU:HA    | 1.93                     | 0.41              |
| 1:G:282:GLU:CD    | 1:G:285:ARG:HH21  | 2.29                     | 0.41              |
| 1:H:143:ASP:O     | 1:H:147:SER:HB2   | 2.21                     | 0.41              |
| 1:J:304:LEU:O     | 1:J:305:ASP:C     | 2.63                     | 0.41              |
| 1:L:154:ILE:HD13  | 1:L:245:HIS:CE1   | 2.56                     | 0.41              |
| 1:L:269:LEU:HD12  | 1:L:269:LEU:HA    | 1.89                     | 0.41              |
| 1:L:390:TYR:HA    | 1:L:391:PRO:HD3   | 1.80                     | 0.41              |
| 1:M:122:ARG:NE    | 1:M:126:ILE:HD11  | 2.36                     | 0.41              |
| 1:N:32:TYR:HB3    | 1:N:321:ASP:OD2   | 2.21                     | 0.41              |
| 1:O:12:PRO:HA     | 1:O:13:PRO:HD2    | 1.92                     | 0.41              |
| 1:O:131:VAL:HG11  | 1:O:374:ARG:HD3   | 2.03                     | 0.41              |
| 1:P:74:TRP:C      | 1:P:76:ASN:N      | 2.77                     | 0.41              |
| 1:B:127:VAL:HG23  | 1:B:152:LEU:HD13  | 2.03                     | 0.40              |
| 1:D:89:ASN:ND2    | 5:D:2014:HOH:O    | 2.52                     | 0.40              |
| 1:E:82:THR:HG23   | 1:E:85:GLU:OE1    | 2.21                     | 0.40              |
| 1:E:344:HIS:CD2   | 1:E:344:HIS:C     | 2.99                     | 0.40              |
| 1:G:289:PRO:HG3   | 2:G:1407:HEM:HBB2 | 2.02                     | 0.40              |
| 1:I:52:VAL:HG12   | 1:I:314:THR:HB    | 2.03                     | 0.40              |
| 1:I:157:ILE:HD12  | 1:I:157:ILE:HA    | 1.91                     | 0.40              |
| 1:J:41:ALA:HA     | 1:J:54:LEU:O      | 2.21                     | 0.40              |
| 1:N:12:PRO:HA     | 1:N:13:PRO:HD3    | 1.79                     | 0.40              |
| 1:N:60:ARG:HH12   | 1:N:305:ASP:N     | 2.19                     | 0.40              |
| 1:O:36:ARG:HH21   | 1:O:321:ASP:CG    | 2.30                     | 0.40              |
| 1:P:265:GLN:NE2   | 1:P:337:ILE:H     | 2.19                     | 0.40              |
| 1:B:78:THR:HG23   | 1:B:312:GLY:HA3   | 2.03                     | 0.40              |
| 1:C:265:GLN:HE21  | 1:C:337:ILE:HG12  | 1.81                     | 0.40              |
| 1:C:319:LEU:N     | 1:C:319:LEU:HD23  | 2.36                     | 0.40              |
| 1:D:171:PHE:HE1   | 1:D:197:TYR:CE2   | 2.39                     | 0.40              |
| 1:G:239:ILE:CD1   | 4:G:1410:17Q:H51C | 2.52                     | 0.40              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:G:244:GLY:O     | 1:G:245:HIS:C       | 2.64                     | 0.40              |
| 1:H:145:MET:HE2   | 1:H:145:MET:HB2     | 1.90                     | 0.40              |
| 1:I:158:SER:O     | 1:I:162:GLY:N       | 2.51                     | 0.40              |
| 1:K:295:TYR:CD2   | 1:K:314:THR:CG2     | 3.05                     | 0.40              |
| 1:K:391:PRO:O     | 1:K:392:ASN:C       | 2.65                     | 0.40              |
| 1:L:92:MET:CE     | 1:L:104:ARG:HA      | 2.52                     | 0.40              |
| 1:L:272:ASP:C     | 1:L:274:THR:H       | 2.30                     | 0.40              |
| 1:M:165:GLU:HA    | 1:M:168:ARG:HD2     | 2.01                     | 0.40              |
| 1:N:64:VAL:O      | 1:N:65:LEU:C        | 2.64                     | 0.40              |
| 1:P:262:HIS:HB3   | 1:P:265:GLN:HG3     | 2.04                     | 0.40              |
| 1:B:234:LEU:O     | 1:B:235:GLY:C       | 2.65                     | 0.40              |
| 1:D:364:ALA:O     | 1:D:368:VAL:HG23    | 2.21                     | 0.40              |
| 1:E:99:ARG:HG3    | 1:E:102:ARG:HH21    | 1.86                     | 0.40              |
| 1:F:11:SER:HB2    | 1:F:12:PRO:CD       | 2.41                     | 0.40              |
| 1:F:157:ILE:HD12  | 1:F:157:ILE:HA      | 1.84                     | 0.40              |
| 1:F:228:LEU:CD1   | 1:F:232:GLU:HB3     | 2.51                     | 0.40              |
| 1:G:295:TYR:CD1   | 1:G:316[B]:LEU:HD11 | 2.55                     | 0.40              |
| 1:H:177:ALA:CB    | 1:H:190:ALA:HB2     | 2.52                     | 0.40              |
| 1:K:295:TYR:CD2   | 1:K:314:THR:HG23    | 2.56                     | 0.40              |
| 1:L:116:VAL:HG13  | 1:L:362:LEU:HD22    | 2.02                     | 0.40              |
| 1:M:381:ASP:HB2   | 1:M:404:ARG:HG2     | 2.03                     | 0.40              |
| 1:O:269:LEU:HD23  | 1:O:372:LEU:HD22    | 2.03                     | 0.40              |
| 1:C:390:TYR:HA    | 1:C:391:PRO:HD3     | 1.87                     | 0.40              |
| 1:D:157:ILE:HD12  | 1:D:157:ILE:HA      | 1.94                     | 0.40              |
| 2:D:1407:HEM:HBB2 | 2:D:1407:HEM:CMB    | 2.51                     | 0.40              |
| 1:G:228:LEU:CD1   | 1:G:232:GLU:HB3     | 2.50                     | 0.40              |
| 1:H:66:ALA:HB2    | 1:H:349:HIS:CD2     | 2.57                     | 0.40              |
| 1:I:93:LEU:HD21   | 1:I:294:THR:HG21    | 2.03                     | 0.40              |
| 1:K:161:LEU:HD13  | 1:K:241:LEU:HG      | 2.04                     | 0.40              |
| 1:M:15:LEU:O      | 1:M:44:VAL:HB       | 2.21                     | 0.40              |
| 1:M:127:VAL:HG21  | 1:M:366:ILE:HG22    | 2.02                     | 0.40              |
| 1:M:280:VAL:HG21  | 1:M:365:ARG:HG3     | 2.04                     | 0.40              |
| 1:N:277:ASP:N     | 1:N:277:ASP:OD1     | 2.54                     | 0.40              |
| 1:P:251:LEU:CD2   | 2:P:1407:HEM:HBB1   | 2.52                     | 0.40              |
| 1:A:136:ALA:CB    | 1:M:268:ALA:HA      | 2.52                     | 0.40              |
| 1:A:239:ILE:HD12  | 1:A:239:ILE:HA      | 1.92                     | 0.40              |
| 1:A:383:SER:O     | 1:A:385:GLY:N       | 2.54                     | 0.40              |
| 1:E:44:VAL:O      | 1:E:51:GLU:HA       | 2.21                     | 0.40              |
| 1:I:150:TRP:HZ3   | 1:I:245:HIS:NE2     | 2.19                     | 0.40              |
| 1:K:273:MET:HE1   | 1:K:276:LEU:HD22    | 2.02                     | 0.40              |
| 1:L:339:ARG:HH11  | 1:L:339:ARG:HD3     | 1.75                     | 0.40              |

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| Atom-1        | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------|--------------------------|-------------------|
| 1:M:361:ARG:O | 1:M:365:ARG:HD2  | 2.22                     | 0.40              |
| 1:O:93:LEU:HA | 2:O:1407:HEM:O1D | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 394/436 (90%)   | 370 (94%)  | 20 (5%)  | 4 (1%)   | 12          | 32 |
| 1   | B     | 397/436 (91%)   | 367 (92%)  | 29 (7%)  | 1 (0%)   | 36          | 60 |
| 1   | C     | 395/436 (91%)   | 370 (94%)  | 23 (6%)  | 2 (0%)   | 24          | 48 |
| 1   | D     | 397/436 (91%)   | 366 (92%)  | 28 (7%)  | 3 (1%)   | 16          | 37 |
| 1   | E     | 396/436 (91%)   | 367 (93%)  | 26 (7%)  | 3 (1%)   | 16          | 37 |
| 1   | F     | 398/436 (91%)   | 362 (91%)  | 30 (8%)  | 6 (2%)   | 8           | 22 |
| 1   | G     | 398/436 (91%)   | 373 (94%)  | 22 (6%)  | 3 (1%)   | 16          | 37 |
| 1   | H     | 395/436 (91%)   | 368 (93%)  | 26 (7%)  | 1 (0%)   | 36          | 60 |
| 1   | I     | 396/436 (91%)   | 363 (92%)  | 29 (7%)  | 4 (1%)   | 12          | 32 |
| 1   | J     | 396/436 (91%)   | 370 (93%)  | 24 (6%)  | 2 (0%)   | 24          | 48 |
| 1   | K     | 397/436 (91%)   | 362 (91%)  | 30 (8%)  | 5 (1%)   | 9           | 25 |
| 1   | L     | 397/436 (91%)   | 357 (90%)  | 33 (8%)  | 7 (2%)   | 6           | 18 |
| 1   | M     | 396/436 (91%)   | 367 (93%)  | 22 (6%)  | 7 (2%)   | 6           | 18 |
| 1   | N     | 396/436 (91%)   | 355 (90%)  | 37 (9%)  | 4 (1%)   | 12          | 32 |
| 1   | O     | 395/436 (91%)   | 343 (87%)  | 47 (12%) | 5 (1%)   | 9           | 25 |
| 1   | P     | 395/436 (91%)   | 356 (90%)  | 35 (9%)  | 4 (1%)   | 12          | 32 |
| All | All   | 6338/6976 (91%) | 5816 (92%) | 461 (7%) | 61 (1%)  | 12          | 32 |

All (61) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 382    | VAL  |
| 1   | E     | 179    | VAL  |
| 1   | E     | 305    | ASP  |
| 1   | F     | 245[A] | HIS  |
| 1   | F     | 245[B] | HIS  |
| 1   | G     | 245    | HIS  |
| 1   | I     | 382    | VAL  |
| 1   | J     | 183    | ASP  |
| 1   | K     | 245    | HIS  |
| 1   | L     | 305    | ASP  |
| 1   | L     | 382    | VAL  |
| 1   | M     | 138    | PRO  |
| 1   | M     | 245    | HIS  |
| 1   | N     | 14     | VAL  |
| 1   | N     | 245    | HIS  |
| 1   | O     | 382    | VAL  |
| 1   | A     | 179    | VAL  |
| 1   | B     | 179    | VAL  |
| 1   | C     | 244    | GLY  |
| 1   | C     | 245    | HIS  |
| 1   | D     | 176    | ASP  |
| 1   | F     | 182    | ASP  |
| 1   | F     | 305    | ASP  |
| 1   | G     | 244    | GLY  |
| 1   | I     | 244    | GLY  |
| 1   | K     | 134    | MET  |
| 1   | M     | 301    | PRO  |
| 1   | N     | 244    | GLY  |
| 1   | P     | 40     | PRO  |
| 1   | A     | 245    | HIS  |
| 1   | A     | 384    | PRO  |
| 1   | F     | 139    | ASP  |
| 1   | G     | 181    | PRO  |
| 1   | K     | 83     | GLU  |
| 1   | K     | 244    | GLY  |
| 1   | L     | 286    | TYR  |
| 1   | M     | 40     | PRO  |
| 1   | O     | 89     | ASN  |
| 1   | O     | 191    | MET  |
| 1   | O     | 354    | CYS  |
| 1   | P     | 349    | HIS  |
| 1   | D     | 83     | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 244 | GLY  |
| 1   | I     | 137 | ALA  |
| 1   | J     | 184 | PRO  |
| 1   | D     | 173 | VAL  |
| 1   | K     | 384 | PRO  |
| 1   | L     | 182 | ASP  |
| 1   | M     | 263 | PRO  |
| 1   | N     | 13  | PRO  |
| 1   | P     | 344 | HIS  |
| 1   | F     | 384 | PRO  |
| 1   | H     | 176 | ASP  |
| 1   | L     | 40  | PRO  |
| 1   | L     | 303 | ASP  |
| 1   | I     | 181 | PRO  |
| 1   | L     | 384 | PRO  |
| 1   | M     | 337 | ILE  |
| 1   | M     | 384 | PRO  |
| 1   | O     | 184 | PRO  |
| 1   | P     | 47  | PRO  |

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

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     | 312/355 (88%) | 288 (92%) | 24 (8%)  | 12          | 30 |
| 1   | B     | 316/355 (89%) | 296 (94%) | 20 (6%)  | 16          | 39 |
| 1   | C     | 317/355 (89%) | 298 (94%) | 19 (6%)  | 17          | 41 |
| 1   | D     | 318/355 (90%) | 297 (93%) | 21 (7%)  | 15          | 36 |
| 1   | E     | 317/355 (89%) | 300 (95%) | 17 (5%)  | 20          | 45 |
| 1   | F     | 317/355 (89%) | 300 (95%) | 17 (5%)  | 20          | 45 |
| 1   | G     | 321/355 (90%) | 303 (94%) | 18 (6%)  | 19          | 44 |
| 1   | H     | 315/355 (89%) | 295 (94%) | 20 (6%)  | 16          | 39 |
| 1   | I     | 316/355 (89%) | 297 (94%) | 19 (6%)  | 17          | 41 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | J     | 315/355 (89%)   | 298 (95%)  | 17 (5%)  | 20          | 45 |
| 1   | K     | 318/355 (90%)   | 300 (94%)  | 18 (6%)  | 18          | 43 |
| 1   | L     | 314/355 (88%)   | 286 (91%)  | 28 (9%)  | 9           | 23 |
| 1   | M     | 315/355 (89%)   | 291 (92%)  | 24 (8%)  | 12          | 30 |
| 1   | N     | 316/355 (89%)   | 299 (95%)  | 17 (5%)  | 20          | 45 |
| 1   | O     | 313/355 (88%)   | 294 (94%)  | 19 (6%)  | 17          | 40 |
| 1   | P     | 315/355 (89%)   | 294 (93%)  | 21 (7%)  | 15          | 36 |
| All | All   | 5055/5680 (89%) | 4736 (94%) | 319 (6%) | 16          | 39 |

All (319) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | SER  |
| 1   | A     | 43  | ARG  |
| 1   | A     | 44  | VAL  |
| 1   | A     | 50  | ASN  |
| 1   | A     | 72  | LYS  |
| 1   | A     | 82  | THR  |
| 1   | A     | 89  | ASN  |
| 1   | A     | 101 | THR  |
| 1   | A     | 134 | MET  |
| 1   | A     | 139 | ASP  |
| 1   | A     | 141 | ARG  |
| 1   | A     | 144 | LEU  |
| 1   | A     | 146 | GLU  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 167 | ASP  |
| 1   | A     | 205 | LYS  |
| 1   | A     | 226 | SER  |
| 1   | A     | 231 | GLU  |
| 1   | A     | 270 | ARG  |
| 1   | A     | 355 | ILE  |
| 1   | A     | 380 | LEU  |
| 1   | A     | 382 | VAL  |
| 1   | A     | 394 | MET  |
| 1   | A     | 403 | ILE  |
| 1   | B     | 11  | SER  |
| 1   | B     | 43  | ARG  |
| 1   | B     | 45  | ARG  |
| 1   | B     | 48  | GLU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 50         | ASN         |
| 1          | B            | 116        | VAL         |
| 1          | B            | 141        | ARG         |
| 1          | B            | 146        | GLU         |
| 1          | B            | 150        | TRP         |
| 1          | B            | 157        | ILE         |
| 1          | B            | 160        | LEU         |
| 1          | B            | 173        | VAL         |
| 1          | B            | 195        | SER         |
| 1          | B            | 245[A]     | HIS         |
| 1          | B            | 245[B]     | HIS         |
| 1          | B            | 303        | ASP         |
| 1          | B            | 307        | THR         |
| 1          | B            | 334        | ARG         |
| 1          | B            | 383        | SER         |
| 1          | B            | 404        | ARG         |
| 1          | C            | 43         | ARG         |
| 1          | C            | 48         | GLU         |
| 1          | C            | 72         | LYS         |
| 1          | C            | 101        | THR         |
| 1          | C            | 115        | ARG         |
| 1          | C            | 139        | ASP         |
| 1          | C            | 150        | TRP         |
| 1          | C            | 175        | THR         |
| 1          | C            | 178        | PHE         |
| 1          | C            | 183        | ASP         |
| 1          | C            | 189        | THR         |
| 1          | C            | 203        | ASP         |
| 1          | C            | 239        | ILE         |
| 1          | C            | 274        | THR         |
| 1          | C            | 307        | THR         |
| 1          | C            | 319        | LEU         |
| 1          | C            | 341        | THR         |
| 1          | C            | 355        | ILE         |
| 1          | C            | 372        | LEU         |
| 1          | D            | 43         | ARG         |
| 1          | D            | 54         | LEU         |
| 1          | D            | 72         | LYS         |
| 1          | D            | 85         | GLU         |
| 1          | D            | 89         | ASN         |
| 1          | D            | 101        | THR         |
| 1          | D            | 105        | LYS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | D            | 116        | VAL         |
| 1          | D            | 160        | LEU         |
| 1          | D            | 175        | THR         |
| 1          | D            | 178        | PHE         |
| 1          | D            | 195        | SER         |
| 1          | D            | 206        | ARG         |
| 1          | D            | 239        | ILE         |
| 1          | D            | 245        | HIS         |
| 1          | D            | 247        | THR         |
| 1          | D            | 292        | SER         |
| 1          | D            | 316        | LEU         |
| 1          | D            | 355        | ILE         |
| 1          | D            | 373        | GLU         |
| 1          | D            | 394        | MET         |
| 1          | E            | 45         | ARG         |
| 1          | E            | 48         | GLU         |
| 1          | E            | 50         | ASN         |
| 1          | E            | 72         | LYS         |
| 1          | E            | 116        | VAL         |
| 1          | E            | 150        | TRP         |
| 1          | E            | 160        | LEU         |
| 1          | E            | 175        | THR         |
| 1          | E            | 179        | VAL         |
| 1          | E            | 182        | ASP         |
| 1          | E            | 183        | ASP         |
| 1          | E            | 230        | SER         |
| 1          | E            | 246        | GLU         |
| 1          | E            | 248        | THR         |
| 1          | E            | 292        | SER         |
| 1          | E            | 334        | ARG         |
| 1          | E            | 372        | LEU         |
| 1          | F            | 48         | GLU         |
| 1          | F            | 72         | LYS         |
| 1          | F            | 82         | THR         |
| 1          | F            | 89         | ASN         |
| 1          | F            | 95         | SER         |
| 1          | F            | 150        | TRP         |
| 1          | F            | 160        | LEU         |
| 1          | F            | 179        | VAL         |
| 1          | F            | 186        | GLN         |
| 1          | F            | 205        | LYS         |
| 1          | F            | 214        | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | F            | 231        | GLU         |
| 1          | F            | 270        | ARG         |
| 1          | F            | 297        | PHE         |
| 1          | F            | 299        | VAL         |
| 1          | F            | 372        | LEU         |
| 1          | F            | 388        | VAL         |
| 1          | G            | 31         | THR         |
| 1          | G            | 50[A]      | ASN         |
| 1          | G            | 50[B]      | ASN         |
| 1          | G            | 81         | LEU         |
| 1          | G            | 83         | GLU         |
| 1          | G            | 105        | LYS         |
| 1          | G            | 116        | VAL         |
| 1          | G            | 147        | SER         |
| 1          | G            | 150        | TRP         |
| 1          | G            | 154        | ILE         |
| 1          | G            | 175        | THR         |
| 1          | G            | 176        | ASP         |
| 1          | G            | 233        | LEU         |
| 1          | G            | 247        | THR         |
| 1          | G            | 299        | VAL         |
| 1          | G            | 305        | ASP         |
| 1          | G            | 355        | ILE         |
| 1          | G            | 382        | VAL         |
| 1          | H            | 14         | VAL         |
| 1          | H            | 43         | ARG         |
| 1          | H            | 48         | GLU         |
| 1          | H            | 50         | ASN         |
| 1          | H            | 60         | ARG         |
| 1          | H            | 89         | ASN         |
| 1          | H            | 150        | TRP         |
| 1          | H            | 160        | LEU         |
| 1          | H            | 183        | ASP         |
| 1          | H            | 186        | GLN         |
| 1          | H            | 195        | SER         |
| 1          | H            | 199        | SER         |
| 1          | H            | 205        | LYS         |
| 1          | H            | 206        | ARG         |
| 1          | H            | 211        | GLU         |
| 1          | H            | 241        | LEU         |
| 1          | H            | 245        | HIS         |
| 1          | H            | 299        | VAL         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | H            | 319        | LEU         |
| 1          | H            | 372        | LEU         |
| 1          | I            | 43         | ARG         |
| 1          | I            | 48         | GLU         |
| 1          | I            | 56         | VAL         |
| 1          | I            | 72         | LYS         |
| 1          | I            | 89         | ASN         |
| 1          | I            | 139        | ASP         |
| 1          | I            | 141        | ARG         |
| 1          | I            | 150        | TRP         |
| 1          | I            | 175        | THR         |
| 1          | I            | 182        | ASP         |
| 1          | I            | 189        | THR         |
| 1          | I            | 195        | SER         |
| 1          | I            | 241        | LEU         |
| 1          | I            | 247        | THR         |
| 1          | I            | 261        | SER         |
| 1          | I            | 270        | ARG         |
| 1          | I            | 355        | ILE         |
| 1          | I            | 380        | LEU         |
| 1          | I            | 382        | VAL         |
| 1          | J            | 11         | SER         |
| 1          | J            | 48         | GLU         |
| 1          | J            | 60         | ARG         |
| 1          | J            | 79         | THR         |
| 1          | J            | 85         | GLU         |
| 1          | J            | 101        | THR         |
| 1          | J            | 113        | MET         |
| 1          | J            | 139        | ASP         |
| 1          | J            | 160        | LEU         |
| 1          | J            | 161        | LEU         |
| 1          | J            | 189        | THR         |
| 1          | J            | 195        | SER         |
| 1          | J            | 220        | THR         |
| 1          | J            | 231        | GLU         |
| 1          | J            | 239        | ILE         |
| 1          | J            | 338        | ARG         |
| 1          | J            | 394        | MET         |
| 1          | K            | 43         | ARG         |
| 1          | K            | 48         | GLU         |
| 1          | K            | 79         | THR         |
| 1          | K            | 89         | ASN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | K            | 95         | SER         |
| 1          | K            | 101        | THR         |
| 1          | K            | 141        | ARG         |
| 1          | K            | 150        | TRP         |
| 1          | K            | 156        | VAL         |
| 1          | K            | 160        | LEU         |
| 1          | K            | 176        | ASP         |
| 1          | K            | 178        | PHE         |
| 1          | K            | 246        | GLU         |
| 1          | K            | 247        | THR         |
| 1          | K            | 248        | THR         |
| 1          | K            | 328        | ARG         |
| 1          | K            | 334        | ARG         |
| 1          | K            | 403        | ILE         |
| 1          | L            | 50         | ASN         |
| 1          | L            | 56         | VAL         |
| 1          | L            | 72         | LYS         |
| 1          | L            | 78         | THR         |
| 1          | L            | 79         | THR         |
| 1          | L            | 89         | ASN         |
| 1          | L            | 95         | SER         |
| 1          | L            | 116        | VAL         |
| 1          | L            | 147        | SER         |
| 1          | L            | 150        | TRP         |
| 1          | L            | 160        | LEU         |
| 1          | L            | 167        | ASP         |
| 1          | L            | 175        | THR         |
| 1          | L            | 179        | VAL         |
| 1          | L            | 183        | ASP         |
| 1          | L            | 186        | GLN         |
| 1          | L            | 189        | THR         |
| 1          | L            | 195        | SER         |
| 1          | L            | 230        | SER         |
| 1          | L            | 242        | VAL         |
| 1          | L            | 264        | ASP         |
| 1          | L            | 304        | LEU         |
| 1          | L            | 305        | ASP         |
| 1          | L            | 307        | THR         |
| 1          | L            | 308        | VAL         |
| 1          | L            | 382        | VAL         |
| 1          | L            | 383        | SER         |
| 1          | L            | 396        | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | M            | 11         | SER         |
| 1          | M            | 20         | LEU         |
| 1          | M            | 23         | ASP         |
| 1          | M            | 34         | ARG         |
| 1          | M            | 43         | ARG         |
| 1          | M            | 45         | ARG         |
| 1          | M            | 89         | ASN         |
| 1          | M            | 113        | MET         |
| 1          | M            | 150        | TRP         |
| 1          | M            | 160        | LEU         |
| 1          | M            | 175        | THR         |
| 1          | M            | 178        | PHE         |
| 1          | M            | 179        | VAL         |
| 1          | M            | 199        | SER         |
| 1          | M            | 203        | ASP         |
| 1          | M            | 204        | SER         |
| 1          | M            | 214        | LEU         |
| 1          | M            | 220        | THR         |
| 1          | M            | 230        | SER         |
| 1          | M            | 274        | THR         |
| 1          | M            | 340        | ASP         |
| 1          | M            | 355        | ILE         |
| 1          | M            | 369        | ARG         |
| 1          | M            | 396        | ARG         |
| 1          | N            | 43         | ARG         |
| 1          | N            | 56         | VAL         |
| 1          | N            | 89         | ASN         |
| 1          | N            | 101        | THR         |
| 1          | N            | 150        | TRP         |
| 1          | N            | 183        | ASP         |
| 1          | N            | 230        | SER         |
| 1          | N            | 242        | VAL         |
| 1          | N            | 249        | VAL         |
| 1          | N            | 290        | VAL         |
| 1          | N            | 331        | ASP         |
| 1          | N            | 339        | ARG         |
| 1          | N            | 355        | ILE         |
| 1          | N            | 383        | SER         |
| 1          | N            | 388        | VAL         |
| 1          | N            | 396        | ARG         |
| 1          | N            | 404        | ARG         |
| 1          | O            | 11         | SER         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 14  | VAL  |
| 1   | O     | 23  | ASP  |
| 1   | O     | 43  | ARG  |
| 1   | O     | 48  | GLU  |
| 1   | O     | 101 | THR  |
| 1   | O     | 150 | TRP  |
| 1   | O     | 160 | LEU  |
| 1   | O     | 175 | THR  |
| 1   | O     | 188 | GLN  |
| 1   | O     | 204 | SER  |
| 1   | O     | 230 | SER  |
| 1   | O     | 241 | LEU  |
| 1   | O     | 316 | LEU  |
| 1   | O     | 369 | ARG  |
| 1   | O     | 372 | LEU  |
| 1   | O     | 375 | CYS  |
| 1   | O     | 382 | VAL  |
| 1   | O     | 404 | ARG  |
| 1   | P     | 23  | ASP  |
| 1   | P     | 56  | VAL  |
| 1   | P     | 78  | THR  |
| 1   | P     | 89  | ASN  |
| 1   | P     | 95  | SER  |
| 1   | P     | 114 | ARG  |
| 1   | P     | 131 | VAL  |
| 1   | P     | 139 | ASP  |
| 1   | P     | 150 | TRP  |
| 1   | P     | 171 | PHE  |
| 1   | P     | 175 | THR  |
| 1   | P     | 176 | ASP  |
| 1   | P     | 189 | THR  |
| 1   | P     | 195 | SER  |
| 1   | P     | 239 | ILE  |
| 1   | P     | 270 | ARG  |
| 1   | P     | 324 | ARG  |
| 1   | P     | 334 | ARG  |
| 1   | P     | 338 | ARG  |
| 1   | P     | 398 | LEU  |
| 1   | P     | 401 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | GLN  |
| 1   | A     | 50  | ASN  |
| 1   | A     | 238 | HIS  |
| 1   | A     | 265 | GLN  |
| 1   | A     | 344 | HIS  |
| 1   | B     | 188 | GLN  |
| 1   | B     | 265 | GLN  |
| 1   | B     | 344 | HIS  |
| 1   | C     | 22  | GLN  |
| 1   | C     | 89  | ASN  |
| 1   | C     | 90  | HIS  |
| 1   | C     | 188 | GLN  |
| 1   | C     | 238 | HIS  |
| 1   | C     | 245 | HIS  |
| 1   | C     | 265 | GLN  |
| 1   | C     | 344 | HIS  |
| 1   | D     | 22  | GLN  |
| 1   | D     | 89  | ASN  |
| 1   | D     | 90  | HIS  |
| 1   | D     | 188 | GLN  |
| 1   | D     | 245 | HIS  |
| 1   | D     | 265 | GLN  |
| 1   | D     | 344 | HIS  |
| 1   | E     | 22  | GLN  |
| 1   | E     | 50  | ASN  |
| 1   | E     | 188 | GLN  |
| 1   | E     | 265 | GLN  |
| 1   | E     | 344 | HIS  |
| 1   | F     | 265 | GLN  |
| 1   | F     | 344 | HIS  |
| 1   | F     | 349 | HIS  |
| 1   | G     | 22  | GLN  |
| 1   | G     | 76  | ASN  |
| 1   | G     | 89  | ASN  |
| 1   | G     | 124 | GLN  |
| 1   | G     | 186 | GLN  |
| 1   | G     | 188 | GLN  |
| 1   | G     | 208 | GLN  |
| 1   | G     | 238 | HIS  |
| 1   | G     | 245 | HIS  |
| 1   | G     | 265 | GLN  |
| 1   | G     | 344 | HIS  |
| 1   | H     | 50  | ASN  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | H            | 89         | ASN         |
| 1          | H            | 245        | HIS         |
| 1          | H            | 265        | GLN         |
| 1          | H            | 344        | HIS         |
| 1          | H            | 349        | HIS         |
| 1          | I            | 22         | GLN         |
| 1          | I            | 89         | ASN         |
| 1          | I            | 238        | HIS         |
| 1          | I            | 245        | HIS         |
| 1          | I            | 265        | GLN         |
| 1          | I            | 344        | HIS         |
| 1          | I            | 349        | HIS         |
| 1          | J            | 186        | GLN         |
| 1          | J            | 238        | HIS         |
| 1          | J            | 245        | HIS         |
| 1          | J            | 250        | ASN         |
| 1          | J            | 265        | GLN         |
| 1          | J            | 344        | HIS         |
| 1          | K            | 22         | GLN         |
| 1          | K            | 89         | ASN         |
| 1          | K            | 90         | HIS         |
| 1          | K            | 188        | GLN         |
| 1          | K            | 245        | HIS         |
| 1          | K            | 344        | HIS         |
| 1          | K            | 392        | ASN         |
| 1          | L            | 22         | GLN         |
| 1          | L            | 50         | ASN         |
| 1          | L            | 265        | GLN         |
| 1          | L            | 344        | HIS         |
| 1          | M            | 22         | GLN         |
| 1          | M            | 188        | GLN         |
| 1          | M            | 265        | GLN         |
| 1          | M            | 344        | HIS         |
| 1          | N            | 50         | ASN         |
| 1          | N            | 76         | ASN         |
| 1          | N            | 188        | GLN         |
| 1          | N            | 245        | HIS         |
| 1          | N            | 265        | GLN         |
| 1          | N            | 344        | HIS         |
| 1          | N            | 352        | HIS         |
| 1          | O            | 91         | ASN         |
| 1          | O            | 188        | GLN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 245 | HIS  |
| 1   | O     | 265 | GLN  |
| 1   | O     | 344 | HIS  |
| 1   | P     | 22  | GLN  |
| 1   | P     | 186 | GLN  |
| 1   | P     | 188 | GLN  |
| 1   | P     | 238 | HIS  |
| 1   | P     | 254 | ASN  |
| 1   | P     | 262 | HIS  |
| 1   | P     | 265 | GLN  |
| 1   | P     | 344 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | SO4  | F     | 1408 | -    | 4,4,4        | 0.60 | 0        | 6,6,6       | 0.54 | 0        |
| 2   | HEM  | D     | 1407 | 1    | 50,50,50     | 1.85 | 9 (18%)  | 67,82,82    | 1.24 | 8 (11%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | HEM  | F     | 1407 | 1    | 50,50,50     | 1.83 | 11 (22%) | 67,82,82    | 1.30 | 6 (8%)   |
| 2   | HEM  | L     | 1407 | 1    | 50,50,50     | 1.68 | 7 (14%)  | 67,82,82    | 1.36 | 10 (14%) |
| 3   | SO4  | A     | 1408 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.54 | 0        |
| 3   | SO4  | I     | 1409 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.37 | 0        |
| 3   | SO4  | O     | 1409 | -    | 4,4,4        | 0.55 | 0        | 6,6,6       | 0.80 | 0        |
| 2   | HEM  | I     | 1407 | 1    | 50,50,50     | 1.90 | 8 (16%)  | 67,82,82    | 1.48 | 8 (11%)  |
| 3   | SO4  | J     | 1408 | -    | 4,4,4        | 0.68 | 0        | 6,6,6       | 0.49 | 0        |
| 2   | HEM  | M     | 1407 | 1    | 50,50,50     | 1.88 | 10 (20%) | 67,82,82    | 1.34 | 6 (8%)   |
| 2   | HEM  | G     | 1407 | 1    | 50,50,50     | 1.88 | 8 (16%)  | 67,82,82    | 1.38 | 8 (11%)  |
| 3   | SO4  | B     | 1409 | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.22 | 0        |
| 2   | HEM  | O     | 1407 | 1    | 50,50,50     | 1.90 | 9 (18%)  | 67,82,82    | 1.23 | 6 (8%)   |
| 3   | SO4  | H     | 1409 | -    | 4,4,4        | 0.39 | 0        | 6,6,6       | 0.31 | 0        |
| 4   | 17Q  | C     | 1410 | -    | 21,21,21     | 0.30 | 0        | 23,23,23    | 1.02 | 2 (8%)   |
| 2   | HEM  | J     | 1407 | 1    | 50,50,50     | 1.78 | 9 (18%)  | 67,82,82    | 1.16 | 4 (5%)   |
| 2   | HEM  | A     | 1407 | 1    | 50,50,50     | 1.78 | 7 (14%)  | 67,82,82    | 1.27 | 6 (8%)   |
| 3   | SO4  | D     | 1408 | -    | 4,4,4        | 0.73 | 0        | 6,6,6       | 0.77 | 0        |
| 2   | HEM  | P     | 1407 | 1    | 50,50,50     | 1.87 | 9 (18%)  | 67,82,82    | 1.30 | 8 (11%)  |
| 2   | HEM  | K     | 1407 | 1    | 50,50,50     | 1.75 | 11 (22%) | 67,82,82    | 1.33 | 11 (16%) |
| 3   | SO4  | B     | 1408 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.28 | 0        |
| 4   | 17Q  | G     | 1410 | -    | 21,21,21     | 0.48 | 0        | 23,23,23    | 0.75 | 0        |
| 3   | SO4  | H     | 1408 | -    | 4,4,4        | 0.56 | 0        | 6,6,6       | 0.49 | 0        |
| 2   | HEM  | E     | 1407 | 1    | 50,50,50     | 1.71 | 7 (14%)  | 67,82,82    | 1.45 | 11 (16%) |
| 2   | HEM  | C     | 1407 | 1    | 50,50,50     | 1.85 | 8 (16%)  | 67,82,82    | 1.47 | 11 (16%) |
| 3   | SO4  | I     | 1408 | -    | 4,4,4        | 0.75 | 0        | 6,6,6       | 0.77 | 0        |
| 2   | HEM  | N     | 1407 | 1    | 50,50,50     | 1.74 | 6 (12%)  | 67,82,82    | 1.21 | 8 (11%)  |
| 2   | HEM  | B     | 1407 | 1    | 50,50,50     | 1.85 | 7 (14%)  | 67,82,82    | 1.51 | 13 (19%) |
| 3   | SO4  | O     | 1408 | -    | 4,4,4        | 0.64 | 0        | 6,6,6       | 0.49 | 0        |
| 2   | HEM  | H     | 1407 | 1    | 50,50,50     | 1.79 | 7 (14%)  | 67,82,82    | 1.06 | 3 (4%)   |

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     | 1407 | 1    | -       | 2/14/54/54 | -     |
| 2   | HEM  | C     | 1407 | 1    | -       | 3/14/54/54 | -     |
| 2   | HEM  | I     | 1407 | 1    | -       | 4/14/54/54 | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 2   | HEM  | L     | 1407 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEM  | P     | 1407 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEM  | K     | 1407 | 1    | -       | 6/14/54/54  | -       |
| 2   | HEM  | M     | 1407 | 1    | -       | 6/14/54/54  | -       |
| 4   | 17Q  | G     | 1410 | -    | -       | 14/23/23/23 | 1/1/1/1 |
| 2   | HEM  | F     | 1407 | 1    | -       | 2/14/54/54  | -       |
| 2   | HEM  | E     | 1407 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEM  | G     | 1407 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEM  | J     | 1407 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEM  | N     | 1407 | 1    | -       | 0/14/54/54  | -       |
| 2   | HEM  | B     | 1407 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEM  | O     | 1407 | 1    | -       | 1/14/54/54  | -       |
| 4   | 17Q  | C     | 1410 | -    | -       | 14/23/23/23 | 1/1/1/1 |
| 2   | HEM  | H     | 1407 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEM  | A     | 1407 | 1    | -       | 3/14/54/54  | -       |

All (133) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | A     | 1407 | HEM  | C3D-C2D | 8.15 | 1.54        | 1.36     |
| 2   | M     | 1407 | HEM  | C3D-C2D | 8.07 | 1.54        | 1.36     |
| 2   | P     | 1407 | HEM  | C3D-C2D | 7.76 | 1.53        | 1.36     |
| 2   | C     | 1407 | HEM  | C3D-C2D | 7.73 | 1.53        | 1.36     |
| 2   | O     | 1407 | HEM  | C3D-C2D | 7.61 | 1.53        | 1.36     |
| 2   | F     | 1407 | HEM  | C3D-C2D | 7.57 | 1.53        | 1.36     |
| 2   | E     | 1407 | HEM  | C3D-C2D | 7.56 | 1.53        | 1.36     |
| 2   | G     | 1407 | HEM  | C3D-C2D | 7.53 | 1.53        | 1.36     |
| 2   | I     | 1407 | HEM  | C3D-C2D | 7.31 | 1.52        | 1.36     |
| 2   | D     | 1407 | HEM  | C3D-C2D | 7.30 | 1.52        | 1.36     |
| 2   | N     | 1407 | HEM  | C3D-C2D | 7.30 | 1.52        | 1.36     |
| 2   | J     | 1407 | HEM  | C3D-C2D | 7.26 | 1.52        | 1.36     |
| 2   | K     | 1407 | HEM  | C3D-C2D | 7.24 | 1.52        | 1.36     |
| 2   | H     | 1407 | HEM  | C3D-C2D | 7.22 | 1.52        | 1.36     |
| 2   | L     | 1407 | HEM  | C3D-C2D | 7.14 | 1.52        | 1.36     |
| 2   | B     | 1407 | HEM  | C3D-C2D | 6.82 | 1.51        | 1.36     |
| 2   | B     | 1407 | HEM  | FE-ND   | 5.98 | 2.13        | 1.94     |
| 2   | P     | 1407 | HEM  | FE-NB   | 5.44 | 2.11        | 1.94     |
| 2   | D     | 1407 | HEM  | FE-ND   | 5.35 | 2.11        | 1.94     |
| 2   | I     | 1407 | HEM  | FE-NB   | 5.30 | 2.11        | 1.94     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | O     | 1407 | HEM  | FE-ND   | 5.09 | 2.10        | 1.94     |
| 2   | J     | 1407 | HEM  | FE-ND   | 4.96 | 2.10        | 1.94     |
| 2   | I     | 1407 | HEM  | FE-ND   | 4.92 | 2.10        | 1.94     |
| 2   | O     | 1407 | HEM  | FE-NA   | 4.56 | 2.10        | 1.95     |
| 2   | F     | 1407 | HEM  | FE-ND   | 4.47 | 2.08        | 1.94     |
| 2   | H     | 1407 | HEM  | FE-ND   | 4.46 | 2.08        | 1.94     |
| 2   | E     | 1407 | HEM  | FE-ND   | 4.27 | 2.08        | 1.94     |
| 2   | N     | 1407 | HEM  | FE-ND   | 4.24 | 2.08        | 1.94     |
| 2   | P     | 1407 | HEM  | FE-ND   | 4.18 | 2.07        | 1.94     |
| 2   | A     | 1407 | HEM  | FE-ND   | 4.12 | 2.07        | 1.94     |
| 2   | M     | 1407 | HEM  | FE-NB   | 4.08 | 2.07        | 1.94     |
| 2   | G     | 1407 | HEM  | FE-NA   | 3.98 | 2.08        | 1.95     |
| 2   | G     | 1407 | HEM  | FE-NC   | 3.96 | 2.08        | 1.95     |
| 2   | B     | 1407 | HEM  | FE-NC   | 3.96 | 2.08        | 1.95     |
| 2   | C     | 1407 | HEM  | CAB-C3B | 3.66 | 1.57        | 1.47     |
| 2   | M     | 1407 | HEM  | FE-ND   | 3.57 | 2.05        | 1.94     |
| 2   | L     | 1407 | HEM  | FE-NA   | 3.44 | 2.06        | 1.95     |
| 2   | C     | 1407 | HEM  | FE-ND   | 3.35 | 2.05        | 1.94     |
| 2   | I     | 1407 | HEM  | CAC-C3C | 3.34 | 1.56        | 1.47     |
| 2   | B     | 1407 | HEM  | CAC-C3C | 3.31 | 1.56        | 1.47     |
| 2   | J     | 1407 | HEM  | CAC-C3C | 3.29 | 1.56        | 1.47     |
| 2   | K     | 1407 | HEM  | CAB-C3B | 3.18 | 1.55        | 1.47     |
| 2   | H     | 1407 | HEM  | CAC-C3C | 3.17 | 1.55        | 1.47     |
| 2   | N     | 1407 | HEM  | FE-NA   | 3.14 | 2.05        | 1.95     |
| 2   | A     | 1407 | HEM  | FE-NB   | 3.14 | 2.04        | 1.94     |
| 2   | B     | 1407 | HEM  | CAB-C3B | 3.13 | 1.55        | 1.47     |
| 2   | G     | 1407 | HEM  | CAC-C3C | 3.12 | 1.55        | 1.47     |
| 2   | F     | 1407 | HEM  | FE-NC   | 3.11 | 2.05        | 1.95     |
| 2   | D     | 1407 | HEM  | CAC-C3C | 3.00 | 1.55        | 1.47     |
| 2   | D     | 1407 | HEM  | CAB-C3B | 3.00 | 1.55        | 1.47     |
| 2   | M     | 1407 | HEM  | CAC-C3C | 2.98 | 1.55        | 1.47     |
| 2   | A     | 1407 | HEM  | CAB-C3B | 2.95 | 1.55        | 1.47     |
| 2   | D     | 1407 | HEM  | FE-NB   | 2.94 | 2.04        | 1.94     |
| 2   | G     | 1407 | HEM  | CAB-C3B | 2.94 | 1.55        | 1.47     |
| 2   | P     | 1407 | HEM  | CAC-C3C | 2.92 | 1.55        | 1.47     |
| 2   | K     | 1407 | HEM  | CAC-C3C | 2.91 | 1.55        | 1.47     |
| 2   | E     | 1407 | HEM  | CMC-C2C | 2.91 | 1.56        | 1.50     |
| 2   | L     | 1407 | HEM  | FE-ND   | 2.89 | 2.03        | 1.94     |
| 2   | C     | 1407 | HEM  | FE-NA   | 2.87 | 2.04        | 1.95     |
| 2   | N     | 1407 | HEM  | CAC-C3C | 2.87 | 1.55        | 1.47     |
| 2   | B     | 1407 | HEM  | FE-NB   | 2.85 | 2.03        | 1.94     |
| 2   | A     | 1407 | HEM  | CAC-C3C | 2.85 | 1.55        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | O     | 1407 | HEM  | FE-NB   | 2.84  | 2.03        | 1.94     |
| 2   | F     | 1407 | HEM  | CAC-C3C | 2.83  | 1.54        | 1.47     |
| 2   | G     | 1407 | HEM  | FE-NB   | 2.81  | 2.03        | 1.94     |
| 2   | H     | 1407 | HEM  | FE-NB   | 2.75  | 2.03        | 1.94     |
| 2   | H     | 1407 | HEM  | CMC-C2C | 2.73  | 1.56        | 1.50     |
| 2   | N     | 1407 | HEM  | CAB-C3B | 2.72  | 1.54        | 1.47     |
| 2   | O     | 1407 | HEM  | CAB-C3B | 2.70  | 1.54        | 1.47     |
| 2   | M     | 1407 | HEM  | FE-NA   | 2.70  | 2.04        | 1.95     |
| 2   | K     | 1407 | HEM  | FE-NA   | 2.69  | 2.04        | 1.95     |
| 2   | L     | 1407 | HEM  | C2A-C3A | -2.68 | 1.31        | 1.38     |
| 2   | O     | 1407 | HEM  | CAC-C3C | 2.68  | 1.54        | 1.47     |
| 2   | C     | 1407 | HEM  | CAC-C3C | 2.65  | 1.54        | 1.47     |
| 2   | M     | 1407 | HEM  | CMC-C2C | 2.65  | 1.56        | 1.50     |
| 2   | I     | 1407 | HEM  | CAB-C3B | 2.62  | 1.54        | 1.47     |
| 2   | O     | 1407 | HEM  | CMC-C2C | 2.60  | 1.56        | 1.50     |
| 2   | K     | 1407 | HEM  | FE-NB   | 2.60  | 2.02        | 1.94     |
| 2   | K     | 1407 | HEM  | FE-NC   | 2.59  | 2.03        | 1.95     |
| 2   | F     | 1407 | HEM  | CAB-C3B | 2.56  | 1.54        | 1.47     |
| 2   | L     | 1407 | HEM  | CAC-C3C | 2.56  | 1.54        | 1.47     |
| 2   | L     | 1407 | HEM  | CAB-C3B | 2.56  | 1.54        | 1.47     |
| 2   | G     | 1407 | HEM  | FE-ND   | 2.54  | 2.02        | 1.94     |
| 2   | E     | 1407 | HEM  | CAC-C3C | 2.54  | 1.54        | 1.47     |
| 2   | F     | 1407 | HEM  | CMB-C2B | 2.51  | 1.55        | 1.50     |
| 2   | I     | 1407 | HEM  | CMA-C3A | 2.51  | 1.55        | 1.50     |
| 2   | O     | 1407 | HEM  | CMA-C3A | 2.48  | 1.55        | 1.50     |
| 2   | F     | 1407 | HEM  | CMA-C3A | 2.47  | 1.55        | 1.50     |
| 2   | P     | 1407 | HEM  | FE-NA   | 2.42  | 2.03        | 1.95     |
| 2   | H     | 1407 | HEM  | CAB-C3B | 2.41  | 1.53        | 1.47     |
| 2   | G     | 1407 | HEM  | CMA-C3A | 2.41  | 1.55        | 1.50     |
| 2   | J     | 1407 | HEM  | CAB-C3B | 2.39  | 1.53        | 1.47     |
| 2   | E     | 1407 | HEM  | FE-NB   | 2.39  | 2.02        | 1.94     |
| 2   | I     | 1407 | HEM  | CMD-C2D | 2.39  | 1.55        | 1.50     |
| 2   | K     | 1407 | HEM  | FE-ND   | 2.39  | 2.02        | 1.94     |
| 2   | F     | 1407 | HEM  | CMD-C2D | 2.39  | 1.55        | 1.50     |
| 2   | O     | 1407 | HEM  | CMD-C2D | 2.38  | 1.55        | 1.50     |
| 2   | H     | 1407 | HEM  | FE-NA   | 2.38  | 2.03        | 1.95     |
| 2   | P     | 1407 | HEM  | CMC-C2C | 2.37  | 1.55        | 1.50     |
| 2   | D     | 1407 | HEM  | CMB-C2B | 2.36  | 1.55        | 1.50     |
| 2   | D     | 1407 | HEM  | FE-NC   | 2.34  | 2.02        | 1.95     |
| 2   | K     | 1407 | HEM  | CMA-C3A | 2.32  | 1.55        | 1.50     |
| 2   | A     | 1407 | HEM  | FE-NA   | 2.30  | 2.02        | 1.95     |
| 2   | C     | 1407 | HEM  | CMD-C2D | 2.29  | 1.55        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | E     | 1407 | HEM  | CAB-C3B | 2.28  | 1.53        | 1.47     |
| 2   | P     | 1407 | HEM  | CAB-C3B | 2.28  | 1.53        | 1.47     |
| 2   | J     | 1407 | HEM  | CMA-C3A | 2.27  | 1.55        | 1.50     |
| 2   | M     | 1407 | HEM  | CAB-C3B | 2.27  | 1.53        | 1.47     |
| 2   | K     | 1407 | HEM  | C2A-C3A | -2.25 | 1.33        | 1.38     |
| 2   | D     | 1407 | HEM  | CMA-C3A | 2.22  | 1.55        | 1.50     |
| 2   | K     | 1407 | HEM  | CMD-C2D | 2.21  | 1.55        | 1.50     |
| 2   | C     | 1407 | HEM  | C4D-ND  | -2.21 | 1.36        | 1.40     |
| 2   | J     | 1407 | HEM  | CMC-C2C | 2.20  | 1.55        | 1.50     |
| 2   | B     | 1407 | HEM  | CMB-C2B | 2.20  | 1.55        | 1.50     |
| 2   | F     | 1407 | HEM  | FE-NB   | 2.19  | 2.01        | 1.94     |
| 2   | N     | 1407 | HEM  | CMC-C2C | 2.18  | 1.55        | 1.50     |
| 2   | F     | 1407 | HEM  | CMC-C2C | 2.18  | 1.55        | 1.50     |
| 2   | K     | 1407 | HEM  | CMC-C2C | 2.18  | 1.55        | 1.50     |
| 2   | J     | 1407 | HEM  | FE-NB   | 2.15  | 2.01        | 1.94     |
| 2   | C     | 1407 | HEM  | C3C-C2C | -2.15 | 1.32        | 1.37     |
| 2   | M     | 1407 | HEM  | CAA-C2A | 2.13  | 1.56        | 1.51     |
| 2   | M     | 1407 | HEM  | CMA-C3A | 2.13  | 1.55        | 1.50     |
| 2   | P     | 1407 | HEM  | C3B-C2B | -2.12 | 1.32        | 1.37     |
| 2   | F     | 1407 | HEM  | FE-NA   | 2.12  | 2.02        | 1.95     |
| 2   | M     | 1407 | HEM  | CMB-C2B | 2.11  | 1.55        | 1.50     |
| 2   | P     | 1407 | HEM  | CMA-C3A | 2.10  | 1.55        | 1.50     |
| 2   | D     | 1407 | HEM  | CMC-C2C | 2.09  | 1.55        | 1.50     |
| 2   | J     | 1407 | HEM  | CMB-C2B | 2.08  | 1.55        | 1.50     |
| 2   | L     | 1407 | HEM  | CMC-C2C | 2.06  | 1.55        | 1.50     |
| 2   | I     | 1407 | HEM  | CMC-C2C | 2.05  | 1.55        | 1.50     |
| 2   | E     | 1407 | HEM  | CMD-C2D | 2.04  | 1.55        | 1.50     |
| 2   | J     | 1407 | HEM  | C2A-C3A | -2.02 | 1.33        | 1.38     |
| 2   | A     | 1407 | HEM  | FE-NC   | 2.01  | 2.01        | 1.95     |

All (129) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 2   | G     | 1407 | HEM  | C4D-ND-C1D | 5.14 | 111.29      | 105.21   |
| 2   | P     | 1407 | HEM  | C4D-ND-C1D | 5.07 | 111.21      | 105.21   |
| 2   | A     | 1407 | HEM  | C4D-ND-C1D | 4.80 | 110.89      | 105.21   |
| 2   | O     | 1407 | HEM  | C4D-ND-C1D | 4.80 | 110.89      | 105.21   |
| 2   | F     | 1407 | HEM  | C4D-ND-C1D | 4.54 | 110.58      | 105.21   |
| 2   | M     | 1407 | HEM  | C4D-ND-C1D | 4.47 | 110.50      | 105.21   |
| 2   | K     | 1407 | HEM  | C4D-ND-C1D | 4.41 | 110.42      | 105.21   |
| 2   | I     | 1407 | HEM  | CHD-C4C-NC | 4.37 | 129.21      | 124.45   |
| 2   | B     | 1407 | HEM  | C4D-ND-C1D | 4.30 | 110.30      | 105.21   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | H     | 1407 | HEM  | C4D-ND-C1D  | 4.23  | 110.21      | 105.21   |
| 2   | C     | 1407 | HEM  | C4D-ND-C1D  | 4.17  | 110.15      | 105.21   |
| 2   | E     | 1407 | HEM  | CHD-C4C-NC  | 4.09  | 128.91      | 124.45   |
| 2   | E     | 1407 | HEM  | C4D-ND-C1D  | 4.00  | 109.94      | 105.21   |
| 2   | J     | 1407 | HEM  | C4D-ND-C1D  | 3.93  | 109.86      | 105.21   |
| 2   | I     | 1407 | HEM  | C4D-ND-C1D  | 3.84  | 109.75      | 105.21   |
| 2   | L     | 1407 | HEM  | C4D-ND-C1D  | 3.80  | 109.71      | 105.21   |
| 2   | N     | 1407 | HEM  | C4D-ND-C1D  | 3.74  | 109.63      | 105.21   |
| 2   | I     | 1407 | HEM  | CMD-C2D-C1D | 3.68  | 130.79      | 125.03   |
| 2   | C     | 1407 | HEM  | C1D-C2D-C3D | -3.67 | 103.12      | 106.98   |
| 2   | F     | 1407 | HEM  | CMD-C2D-C1D | 3.54  | 130.57      | 125.03   |
| 2   | E     | 1407 | HEM  | C4C-C3C-C2C | 3.50  | 109.85      | 106.81   |
| 2   | C     | 1407 | HEM  | C3B-C2B-C1B | 3.45  | 109.00      | 106.41   |
| 2   | D     | 1407 | HEM  | CHD-C4C-NC  | 3.35  | 128.10      | 124.45   |
| 2   | D     | 1407 | HEM  | C4D-ND-C1D  | 3.33  | 109.15      | 105.21   |
| 2   | F     | 1407 | HEM  | CBD-CAD-C3D | -3.32 | 103.36      | 112.53   |
| 2   | I     | 1407 | HEM  | CBD-CAD-C3D | -3.27 | 103.48      | 112.53   |
| 2   | E     | 1407 | HEM  | C1D-C2D-C3D | -3.27 | 103.54      | 106.98   |
| 2   | C     | 1407 | HEM  | CBD-CAD-C3D | -3.25 | 103.55      | 112.53   |
| 2   | G     | 1407 | HEM  | CBD-CAD-C3D | -3.23 | 103.60      | 112.53   |
| 2   | J     | 1407 | HEM  | CHD-C4C-NC  | 3.14  | 127.87      | 124.45   |
| 2   | L     | 1407 | HEM  | CHD-C1D-ND  | 3.10  | 127.76      | 124.42   |
| 2   | E     | 1407 | HEM  | CMD-C2D-C1D | 3.10  | 129.88      | 125.03   |
| 2   | I     | 1407 | HEM  | C1D-C2D-C3D | -3.08 | 103.74      | 106.98   |
| 2   | M     | 1407 | HEM  | CAD-C3D-C4D | 3.05  | 130.01      | 124.70   |
| 2   | C     | 1407 | HEM  | CHD-C1D-ND  | 3.00  | 127.65      | 124.42   |
| 2   | G     | 1407 | HEM  | CHD-C1D-ND  | 2.94  | 127.59      | 124.42   |
| 2   | B     | 1407 | HEM  | CAA-CBA-CGA | -2.93 | 105.89      | 113.67   |
| 2   | J     | 1407 | HEM  | CAD-C3D-C4D | 2.88  | 129.71      | 124.70   |
| 2   | B     | 1407 | HEM  | C1B-NB-C4B  | 2.86  | 108.59      | 105.21   |
| 2   | G     | 1407 | HEM  | C1B-NB-C4B  | 2.84  | 108.57      | 105.21   |
| 2   | C     | 1407 | HEM  | CHB-C1B-NB  | 2.84  | 127.88      | 124.37   |
| 2   | C     | 1407 | HEM  | CHD-C1D-C2D | -2.81 | 120.59      | 125.03   |
| 2   | L     | 1407 | HEM  | CBD-CAD-C3D | -2.80 | 104.78      | 112.53   |
| 2   | B     | 1407 | HEM  | CHA-C1A-NA  | 2.80  | 128.94      | 123.86   |
| 2   | A     | 1407 | HEM  | CHC-C1C-NC  | 2.79  | 127.49      | 124.45   |
| 2   | B     | 1407 | HEM  | CAD-CBD-CGD | -2.77 | 106.31      | 113.67   |
| 2   | E     | 1407 | HEM  | CHC-C4B-NB  | 2.75  | 127.38      | 124.42   |
| 2   | I     | 1407 | HEM  | CAD-C3D-C4D | 2.68  | 129.36      | 124.70   |
| 2   | O     | 1407 | HEM  | CAD-C3D-C4D | 2.67  | 129.35      | 124.70   |
| 2   | B     | 1407 | HEM  | CBD-CAD-C3D | -2.67 | 105.16      | 112.53   |
| 2   | N     | 1407 | HEM  | C1D-C2D-C3D | -2.66 | 104.18      | 106.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | I     | 1407 | HEM  | CHC-C1C-NC  | 2.66  | 127.35      | 124.45   |
| 4   | C     | 1410 | 17Q  | C12-C13-N   | -2.65 | 106.87      | 113.71   |
| 2   | B     | 1407 | HEM  | CHD-C4C-NC  | 2.64  | 127.33      | 124.45   |
| 2   | G     | 1407 | HEM  | C3B-C4B-NB  | -2.62 | 107.59      | 109.47   |
| 2   | N     | 1407 | HEM  | C3B-C2B-C1B | 2.61  | 108.37      | 106.41   |
| 2   | P     | 1407 | HEM  | CAD-C3D-C4D | 2.60  | 129.22      | 124.70   |
| 2   | O     | 1407 | HEM  | C1D-C2D-C3D | -2.60 | 104.25      | 106.98   |
| 2   | P     | 1407 | HEM  | CHD-C1D-ND  | 2.59  | 127.21      | 124.42   |
| 2   | N     | 1407 | HEM  | CHB-C1B-NB  | 2.58  | 127.55      | 124.37   |
| 2   | L     | 1407 | HEM  | CMC-C2C-C1C | 2.57  | 129.25      | 124.73   |
| 2   | N     | 1407 | HEM  | CHD-C4C-NC  | 2.50  | 127.18      | 124.45   |
| 2   | C     | 1407 | HEM  | CMB-C2B-C1B | -2.49 | 121.14      | 125.03   |
| 2   | E     | 1407 | HEM  | C3B-C4B-NB  | -2.48 | 107.69      | 109.47   |
| 2   | D     | 1407 | HEM  | O1A-CGA-CBA | -2.48 | 115.24      | 123.09   |
| 2   | B     | 1407 | HEM  | CMD-C2D-C1D | 2.47  | 128.89      | 125.03   |
| 2   | F     | 1407 | HEM  | C1D-C2D-C3D | -2.46 | 104.39      | 106.98   |
| 2   | A     | 1407 | HEM  | O1A-CGA-CBA | -2.46 | 115.29      | 123.09   |
| 2   | J     | 1407 | HEM  | C1D-C2D-C3D | -2.45 | 104.40      | 106.98   |
| 2   | N     | 1407 | HEM  | CMD-C2D-C1D | 2.45  | 128.87      | 125.03   |
| 2   | L     | 1407 | HEM  | CAD-C3D-C4D | 2.44  | 128.95      | 124.70   |
| 2   | O     | 1407 | HEM  | CMD-C2D-C1D | 2.43  | 128.83      | 125.03   |
| 2   | M     | 1407 | HEM  | C1B-NB-C4B  | 2.42  | 108.07      | 105.21   |
| 2   | L     | 1407 | HEM  | CHC-C1C-NC  | -2.42 | 121.82      | 124.45   |
| 2   | E     | 1407 | HEM  | CBD-CAD-C3D | -2.42 | 105.85      | 112.53   |
| 2   | K     | 1407 | HEM  | O2A-CGA-CBA | 2.41  | 121.63      | 114.00   |
| 2   | C     | 1407 | HEM  | C1B-NB-C4B  | 2.40  | 108.05      | 105.21   |
| 2   | P     | 1407 | HEM  | O1A-CGA-CBA | -2.38 | 115.55      | 123.09   |
| 2   | K     | 1407 | HEM  | CHA-C4D-ND  | 2.37  | 127.30      | 124.37   |
| 2   | B     | 1407 | HEM  | C3B-C4B-NB  | -2.37 | 107.77      | 109.47   |
| 2   | A     | 1407 | HEM  | CBA-CAA-C2A | -2.36 | 106.01      | 112.53   |
| 2   | A     | 1407 | HEM  | O2A-CGA-CBA | 2.36  | 121.44      | 114.00   |
| 2   | K     | 1407 | HEM  | C4C-C3C-C2C | 2.35  | 108.85      | 106.81   |
| 2   | L     | 1407 | HEM  | CHC-C4B-NB  | 2.35  | 126.95      | 124.42   |
| 2   | B     | 1407 | HEM  | CAD-C3D-C4D | 2.34  | 128.78      | 124.70   |
| 2   | D     | 1407 | HEM  | CHA-C1A-NA  | 2.33  | 128.08      | 123.86   |
| 2   | C     | 1407 | HEM  | CHD-C4C-NC  | 2.32  | 126.98      | 124.45   |
| 2   | E     | 1407 | HEM  | CHC-C1C-NC  | 2.31  | 126.97      | 124.45   |
| 2   | B     | 1407 | HEM  | C3B-C2B-C1B | 2.30  | 108.14      | 106.41   |
| 2   | D     | 1407 | HEM  | C1D-C2D-C3D | -2.29 | 104.57      | 106.98   |
| 2   | O     | 1407 | HEM  | CHD-C4C-NC  | 2.29  | 126.94      | 124.45   |
| 2   | H     | 1407 | HEM  | C4A-C3A-C2A | 2.27  | 109.42      | 106.82   |
| 2   | M     | 1407 | HEM  | O2A-CGA-CBA | 2.26  | 121.15      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1407 | HEM  | CBD-CAD-C3D | -2.26 | 106.28      | 112.53   |
| 2   | I     | 1407 | HEM  | CAA-CBA-CGA | -2.26 | 107.68      | 113.67   |
| 2   | P     | 1407 | HEM  | C3B-C2B-C1B | 2.24  | 108.09      | 106.41   |
| 4   | C     | 1410 | 17Q  | C6-C7-C8    | -2.23 | 106.92      | 114.66   |
| 2   | F     | 1407 | HEM  | O2A-CGA-CBA | 2.22  | 121.01      | 114.00   |
| 2   | L     | 1407 | HEM  | CAA-CBA-CGA | -2.22 | 107.79      | 113.67   |
| 2   | K     | 1407 | HEM  | CMD-C2D-C1D | 2.20  | 128.47      | 125.03   |
| 2   | F     | 1407 | HEM  | C4C-C3C-C2C | 2.19  | 108.71      | 106.81   |
| 2   | K     | 1407 | HEM  | CBD-CAD-C3D | -2.17 | 106.54      | 112.53   |
| 2   | C     | 1407 | HEM  | CMD-C2D-C3D | 2.16  | 131.99      | 126.15   |
| 2   | O     | 1407 | HEM  | O2A-CGA-CBA | 2.14  | 120.77      | 114.00   |
| 2   | K     | 1407 | HEM  | C1D-C2D-C3D | -2.14 | 104.73      | 106.98   |
| 2   | M     | 1407 | HEM  | CHD-C4C-NC  | 2.13  | 126.77      | 124.45   |
| 2   | K     | 1407 | HEM  | CAA-C2A-C1A | 2.12  | 129.07      | 124.94   |
| 2   | K     | 1407 | HEM  | C3B-C4B-NB  | -2.12 | 107.95      | 109.47   |
| 2   | P     | 1407 | HEM  | O2A-CGA-CBA | 2.11  | 120.68      | 114.00   |
| 2   | M     | 1407 | HEM  | CHC-C1C-NC  | 2.10  | 126.74      | 124.45   |
| 2   | N     | 1407 | HEM  | CHC-C4B-NB  | 2.10  | 126.68      | 124.42   |
| 2   | G     | 1407 | HEM  | O2A-CGA-CBA | 2.09  | 120.61      | 114.00   |
| 2   | P     | 1407 | HEM  | CBD-CAD-C3D | -2.09 | 106.75      | 112.53   |
| 2   | D     | 1407 | HEM  | CAA-CBA-CGA | -2.08 | 108.14      | 113.67   |
| 2   | L     | 1407 | HEM  | CHD-C4C-NC  | 2.08  | 126.72      | 124.45   |
| 2   | B     | 1407 | HEM  | O1D-CGD-CBD | -2.07 | 116.54      | 123.09   |
| 2   | E     | 1407 | HEM  | C1C-CHC-C4B | -2.07 | 121.63      | 126.02   |
| 2   | H     | 1407 | HEM  | O2D-CGD-CBD | 2.05  | 120.49      | 114.00   |
| 2   | D     | 1407 | HEM  | C1B-NB-C4B  | 2.05  | 107.64      | 105.21   |
| 2   | A     | 1407 | HEM  | C4D-C3D-C2D | -2.04 | 103.92      | 106.89   |
| 2   | P     | 1407 | HEM  | CHB-C4A-NA  | 2.04  | 127.56      | 123.86   |
| 2   | G     | 1407 | HEM  | O1A-CGA-CBA | -2.03 | 116.66      | 123.09   |
| 2   | K     | 1407 | HEM  | C1B-NB-C4B  | 2.02  | 107.60      | 105.21   |
| 2   | G     | 1407 | HEM  | C3D-C4D-ND  | -2.02 | 107.95      | 110.17   |
| 2   | E     | 1407 | HEM  | CBB-CAB-C3B | -2.02 | 117.43      | 127.53   |
| 2   | K     | 1407 | HEM  | CHD-C1D-ND  | 2.02  | 126.59      | 124.42   |
| 2   | B     | 1407 | HEM  | C3A-C4A-NA  | -2.01 | 106.92      | 110.14   |
| 2   | N     | 1407 | HEM  | O2A-CGA-CBA | 2.01  | 120.34      | 114.00   |
| 2   | L     | 1407 | HEM  | CHD-C1D-C2D | -2.00 | 121.86      | 125.03   |

There are no chirality outliers.

All (83) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 1407 | HEM  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | C     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | C     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | E     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | F     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | G     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | G     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | H     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | H     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | J     | 1407 | HEM  | C2B-C3B-CAB-CBB |
| 2   | J     | 1407 | HEM  | C4B-C3B-CAB-CBB |
| 2   | K     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | K     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | L     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | L     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | M     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | P     | 1407 | HEM  | C2B-C3B-CAB-CBB |
| 2   | P     | 1407 | HEM  | C4B-C3B-CAB-CBB |
| 4   | C     | 1410 | 17Q  | C7-C8-O-C9      |
| 4   | C     | 1410 | 17Q  | C6-C7-C8-O      |
| 4   | G     | 1410 | 17Q  | C7-C8-O-C9      |
| 4   | C     | 1410 | 17Q  | C2-C1-C19-C18   |
| 4   | G     | 1410 | 17Q  | C11-C12-C13-N   |
| 4   | C     | 1410 | 17Q  | C1-C2-C3-C4     |
| 4   | G     | 1410 | 17Q  | C11-C10-C9-O    |
| 4   | C     | 1410 | 17Q  | C6-C7-C8-C16    |
| 4   | G     | 1410 | 17Q  | C10-C9-O-C8     |
| 4   | C     | 1410 | 17Q  | C9-C10-C11-C12  |
| 4   | C     | 1410 | 17Q  | C19-C1-C2-C3    |
| 4   | G     | 1410 | 17Q  | C19-C1-C2-C3    |
| 4   | G     | 1410 | 17Q  | C2-C3-C4-C5     |
| 4   | C     | 1410 | 17Q  | C2-C3-C4-C5     |
| 4   | G     | 1410 | 17Q  | C1-C2-C3-C4     |
| 4   | C     | 1410 | 17Q  | C16-C17-C18-C19 |
| 4   | G     | 1410 | 17Q  | C9-C10-C11-C12  |
| 2   | M     | 1407 | HEM  | C2B-C3B-CAB-CBB |
| 2   | E     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | F     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 4   | C     | 1410 | 17Q  | C4-C5-C6-C7     |
| 4   | G     | 1410 | 17Q  | C3-C4-C5-C6     |
| 4   | G     | 1410 | 17Q  | C17-C18-C19-C1  |
| 4   | G     | 1410 | 17Q  | C2-C1-C19-C18   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | C     | 1410 | 17Q  | C17-C16-C8-C7   |
| 4   | G     | 1410 | 17Q  | C16-C17-C18-C19 |
| 4   | G     | 1410 | 17Q  | C10-C11-C12-C13 |
| 2   | A     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | I     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | J     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | P     | 1407 | HEM  | C2C-C3C-CAC-CBC |
| 2   | A     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | M     | 1407 | HEM  | C4B-C3B-CAB-CBB |
| 2   | M     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 4   | C     | 1410 | 17Q  | C17-C16-C8-O    |
| 2   | K     | 1407 | HEM  | C2B-C3B-CAB-CBB |
| 2   | I     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | P     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | G     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | K     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | M     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | K     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 2   | L     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | B     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | E     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 4   | C     | 1410 | 17Q  | C5-C6-C7-C8     |
| 2   | M     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 2   | E     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 2   | G     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 2   | C     | 1407 | HEM  | C2B-C3B-CAB-CBB |
| 2   | L     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 4   | C     | 1410 | 17Q  | C17-C18-C19-C1  |
| 2   | J     | 1407 | HEM  | C4C-C3C-CAC-CBC |
| 2   | K     | 1407 | HEM  | C4B-C3B-CAB-CBB |
| 2   | B     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 2   | H     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 4   | G     | 1410 | 17Q  | C6-C7-C8-O      |
| 2   | D     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | H     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 2   | O     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | I     | 1407 | HEM  | C2B-C3B-CAB-CBB |
| 2   | A     | 1407 | HEM  | CAA-CBA-CGA-O2A |
| 2   | D     | 1407 | HEM  | CAA-CBA-CGA-O1A |
| 2   | I     | 1407 | HEM  | CAA-CBA-CGA-O2A |

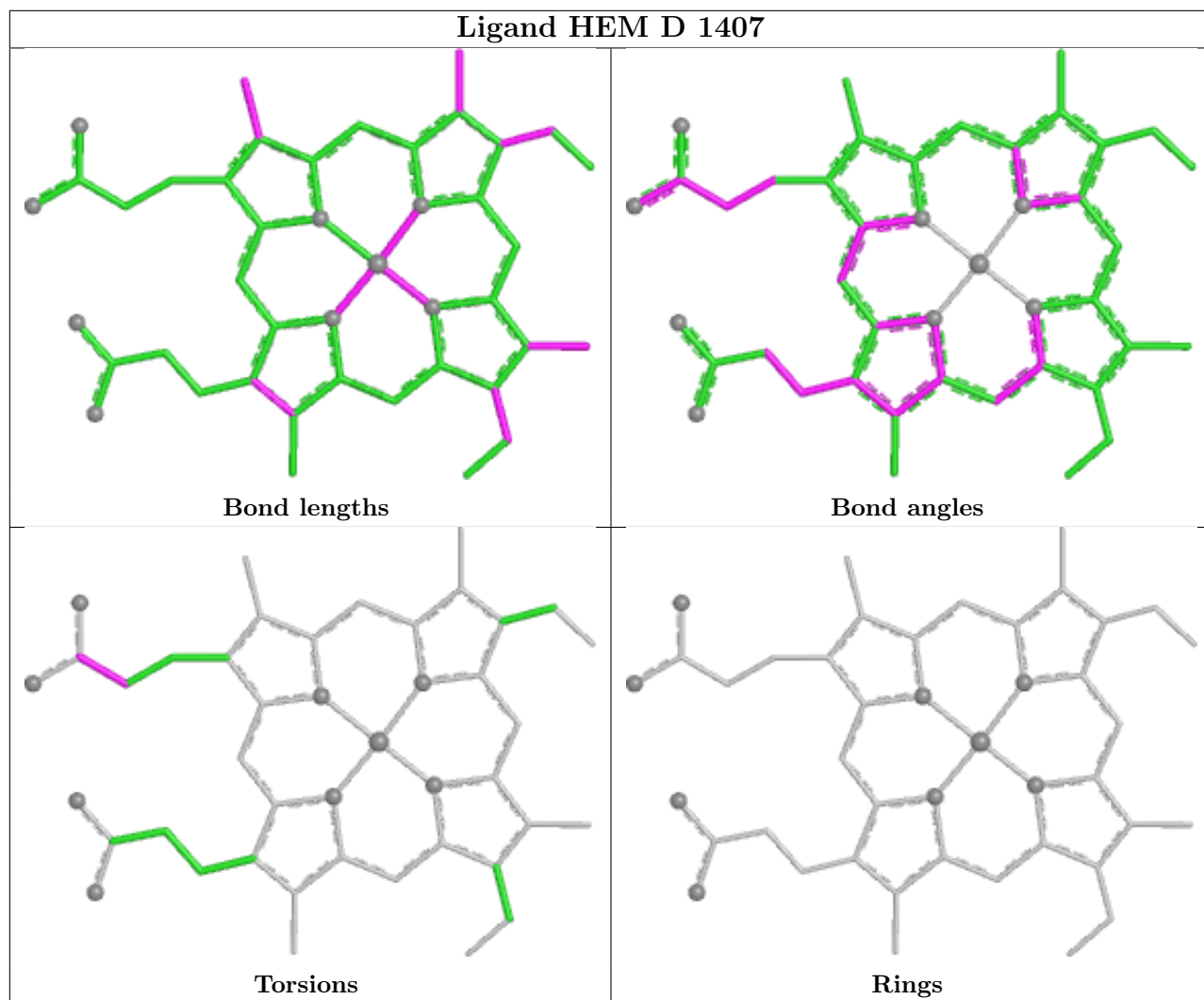
All (2) ring outliers are listed below:

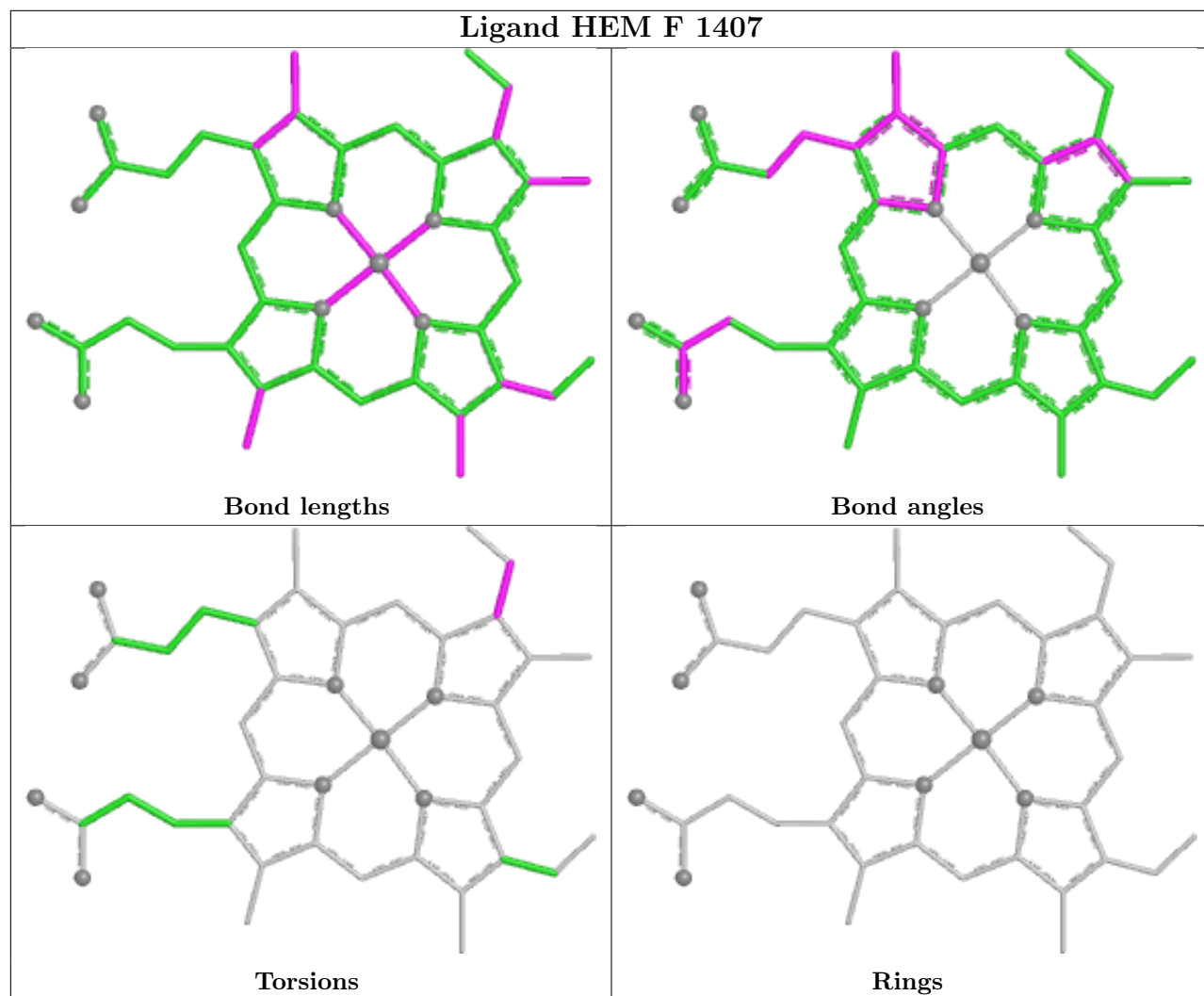
| Mol | Chain | Res  | Type | Atoms                                   |
|-----|-------|------|------|---|
| 4   | C     | 1410 | 17Q  | C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8 |
| 4   | G     | 1410 | 17Q  | C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8 |

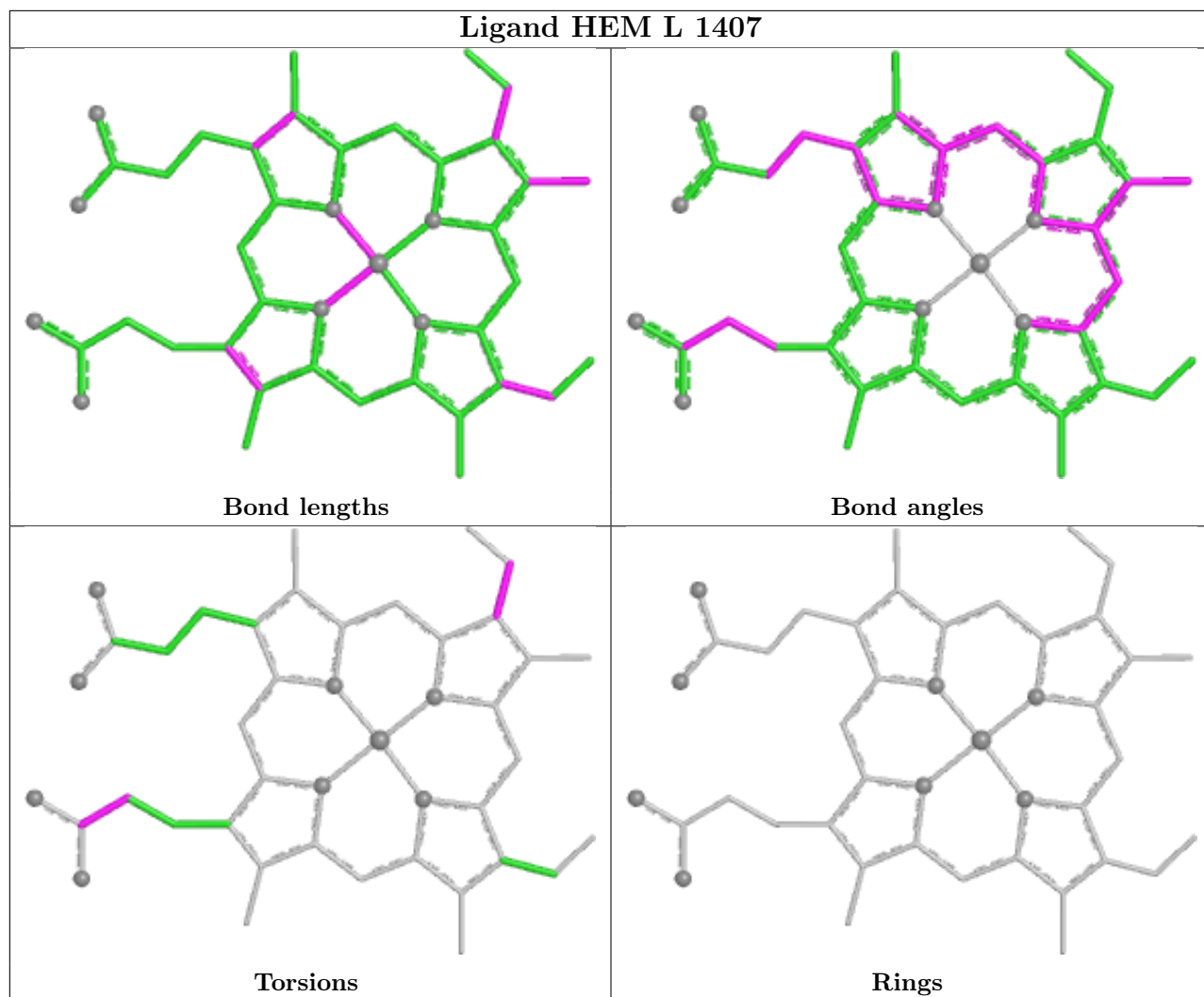
22 monomers are involved in 92 short contacts:

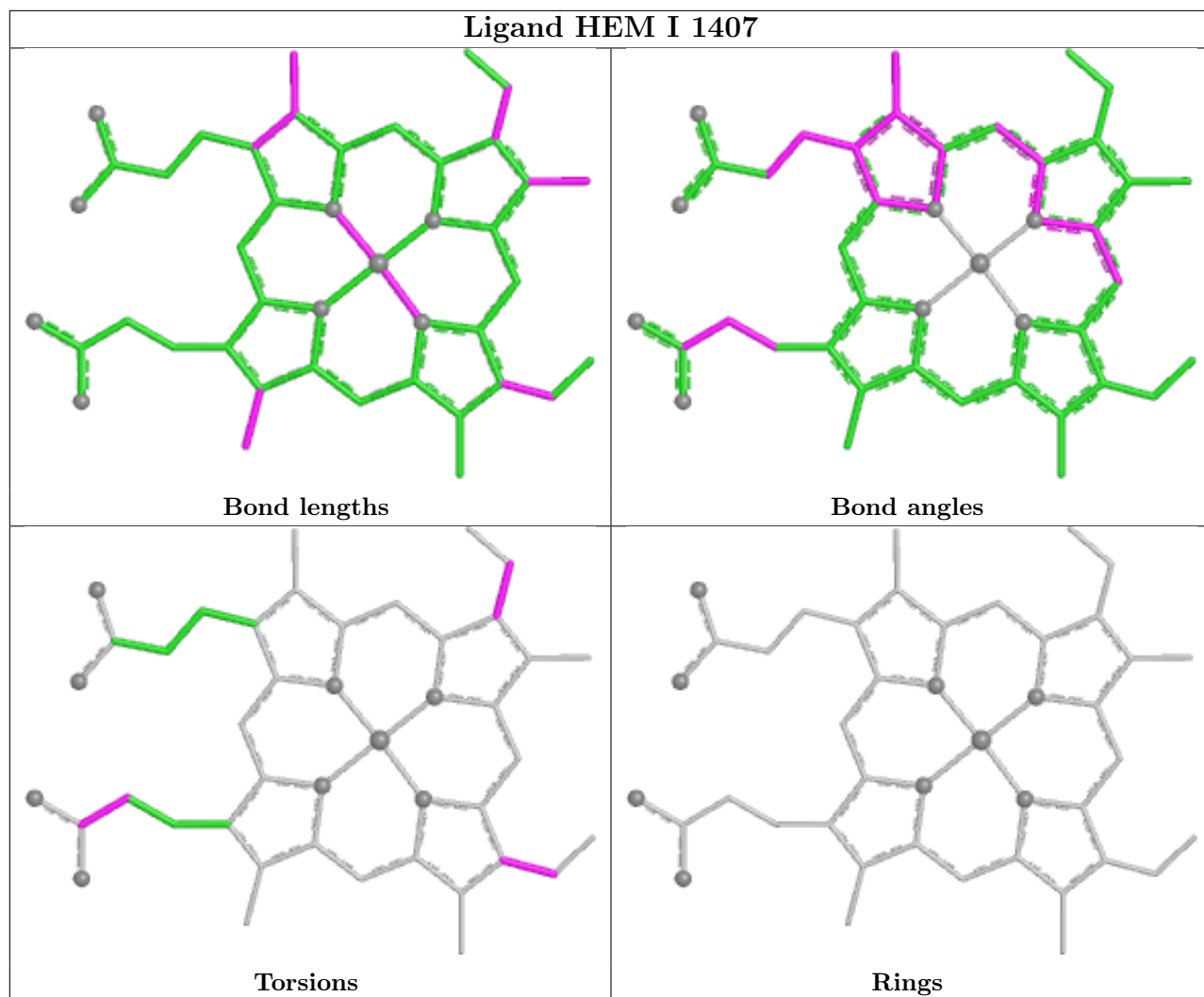
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | F     | 1408 | SO4  | 1       | 0            |
| 2   | D     | 1407 | HEM  | 8       | 0            |
| 2   | F     | 1407 | HEM  | 3       | 0            |
| 2   | L     | 1407 | HEM  | 4       | 0            |
| 3   | A     | 1408 | SO4  | 2       | 0            |
| 3   | O     | 1409 | SO4  | 1       | 0            |
| 2   | I     | 1407 | HEM  | 5       | 0            |
| 2   | M     | 1407 | HEM  | 5       | 0            |
| 2   | G     | 1407 | HEM  | 6       | 0            |
| 2   | O     | 1407 | HEM  | 4       | 0            |
| 3   | H     | 1409 | SO4  | 1       | 0            |
| 4   | C     | 1410 | 17Q  | 6       | 0            |
| 2   | J     | 1407 | HEM  | 4       | 0            |
| 2   | A     | 1407 | HEM  | 1       | 0            |
| 2   | P     | 1407 | HEM  | 5       | 0            |
| 2   | K     | 1407 | HEM  | 3       | 0            |
| 4   | G     | 1410 | 17Q  | 5       | 0            |
| 2   | E     | 1407 | HEM  | 5       | 0            |
| 2   | C     | 1407 | HEM  | 6       | 0            |
| 2   | N     | 1407 | HEM  | 5       | 0            |
| 2   | B     | 1407 | HEM  | 6       | 0            |
| 2   | H     | 1407 | HEM  | 7       | 0            |

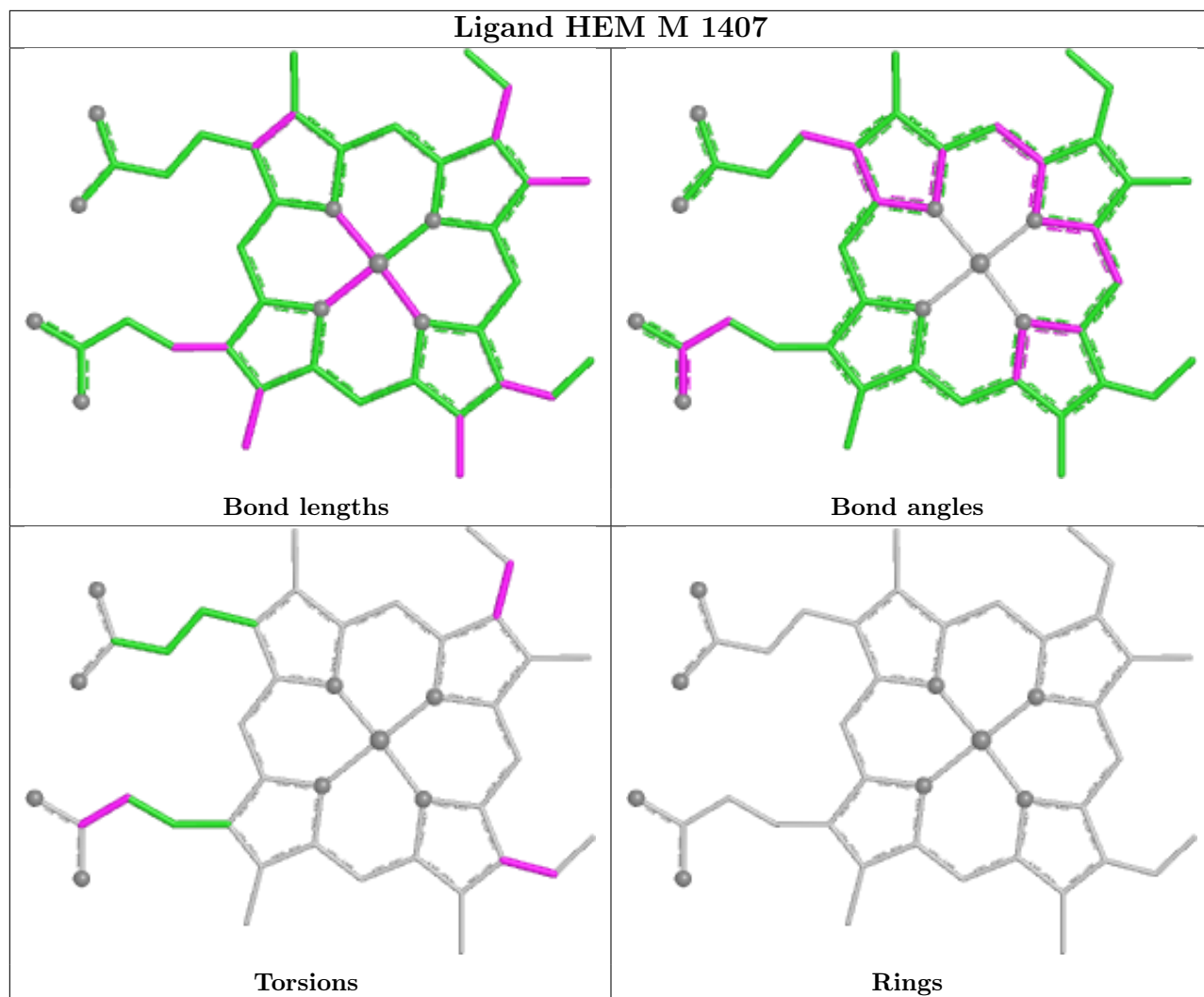
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

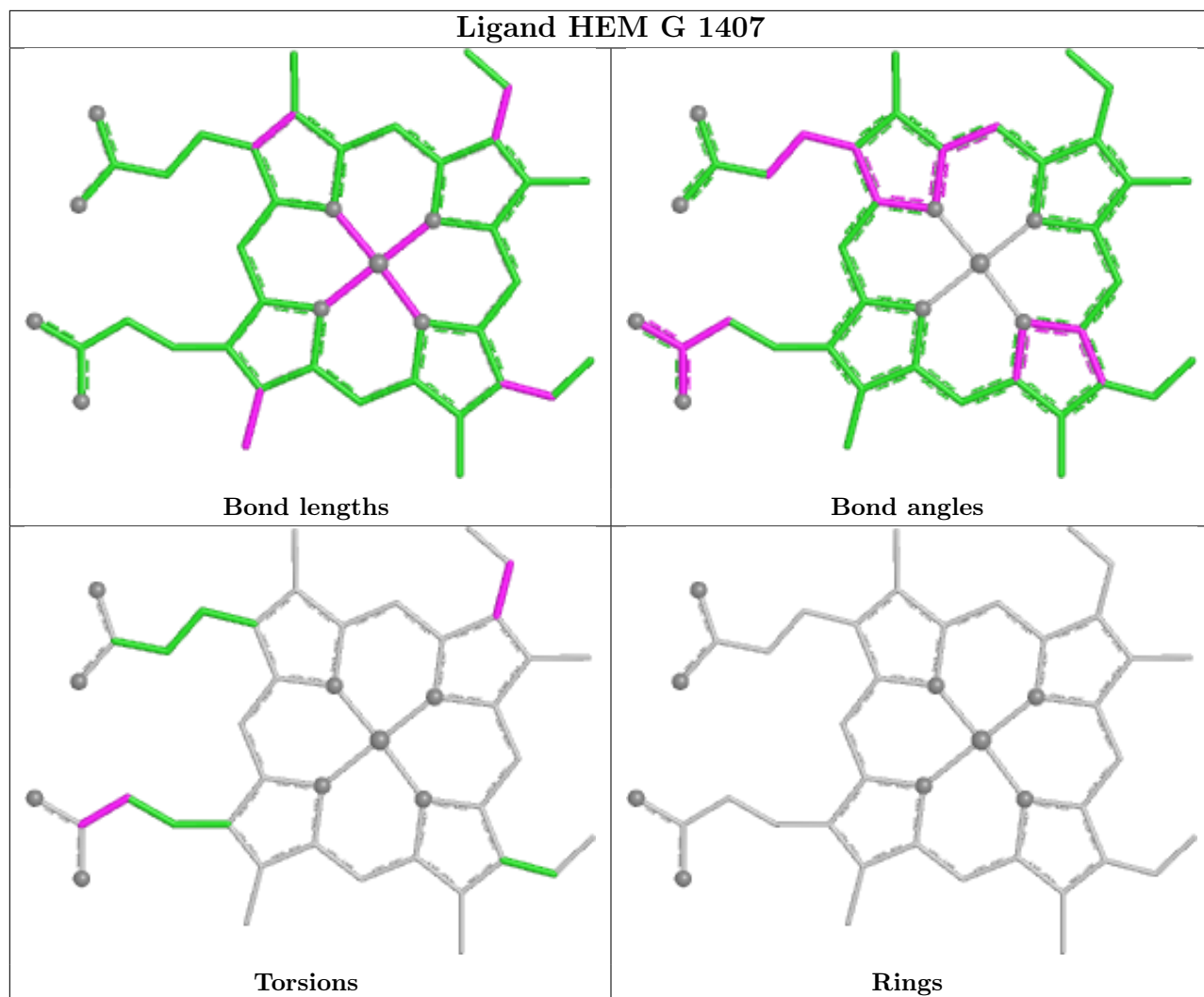


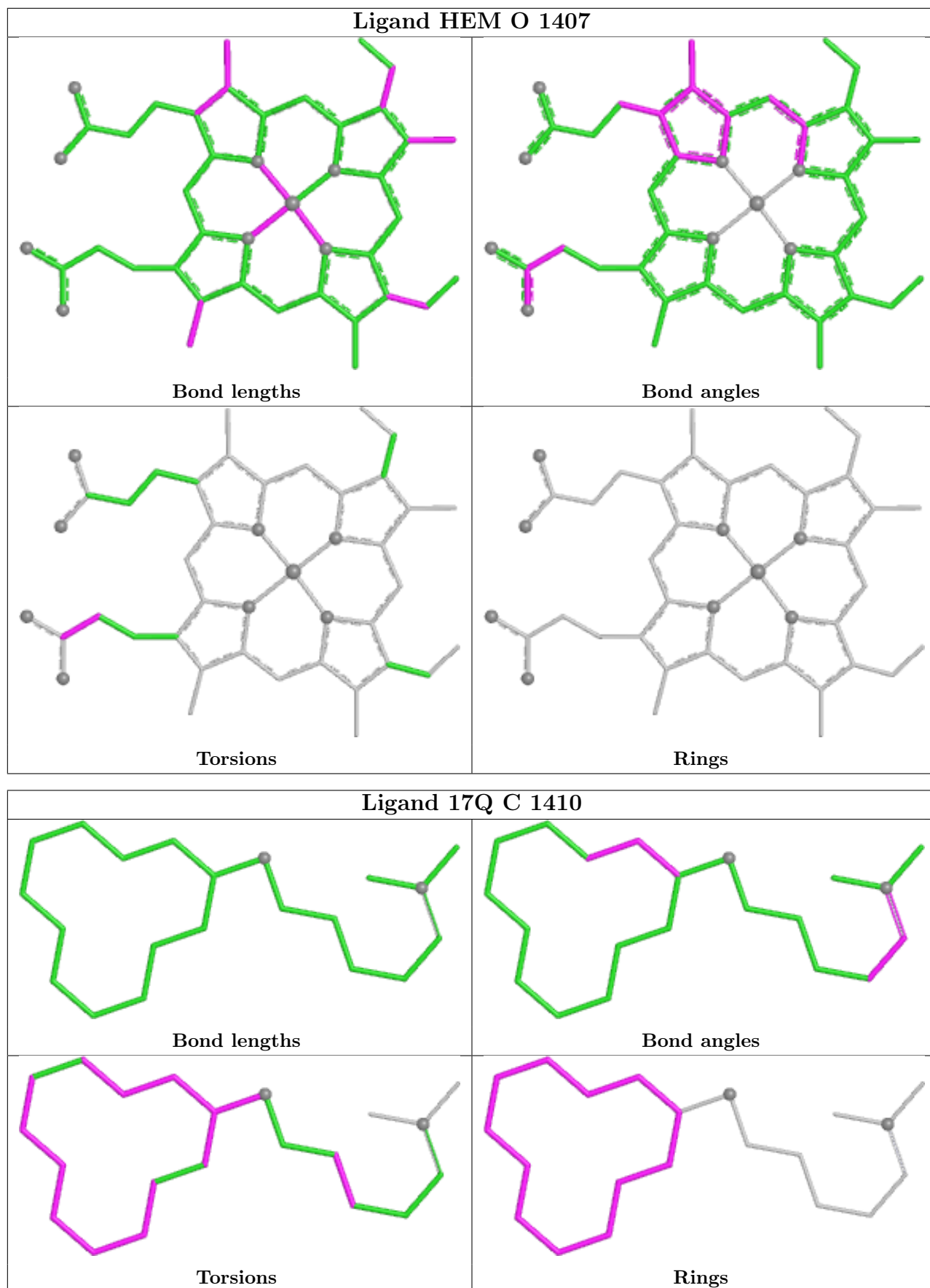


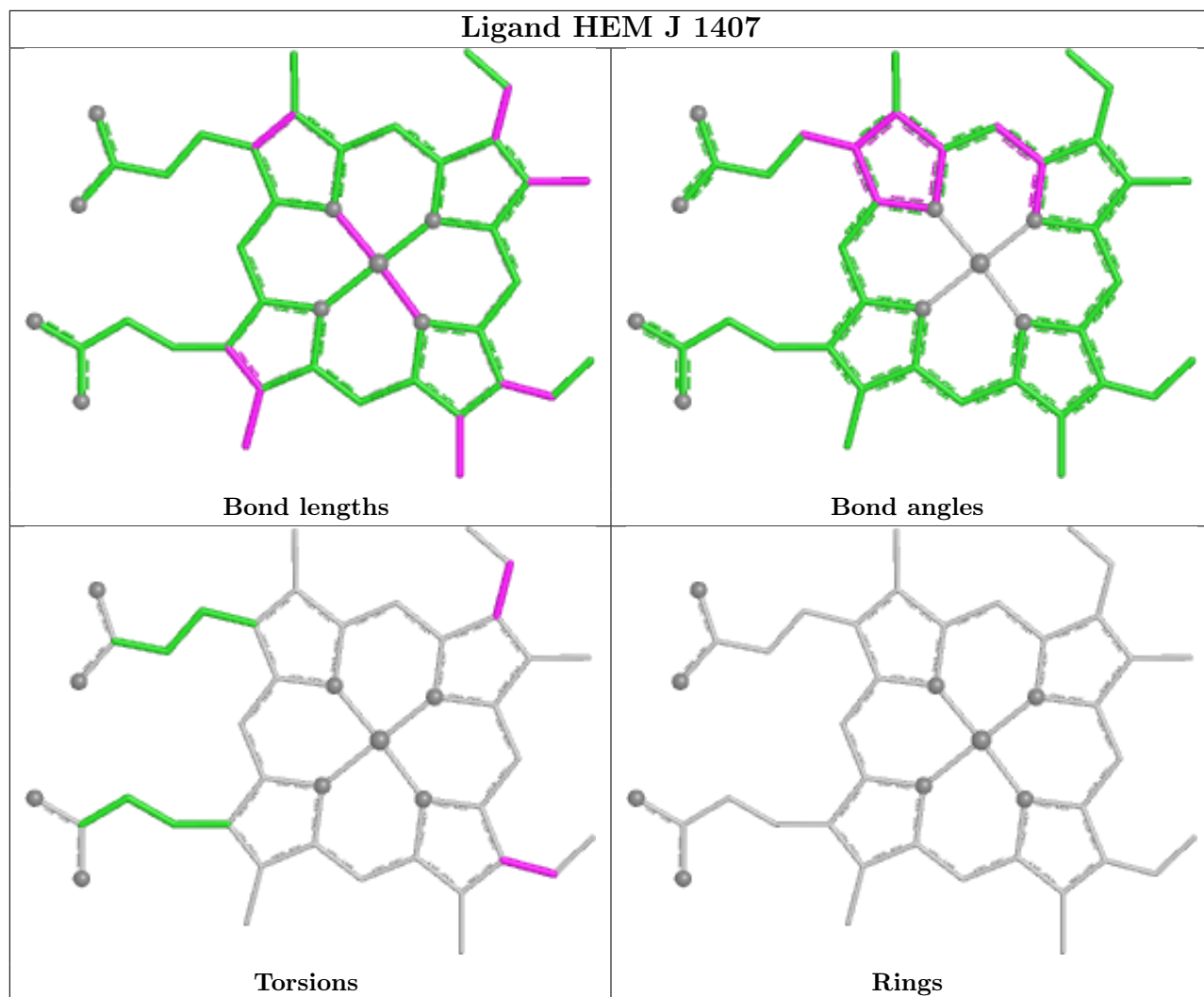


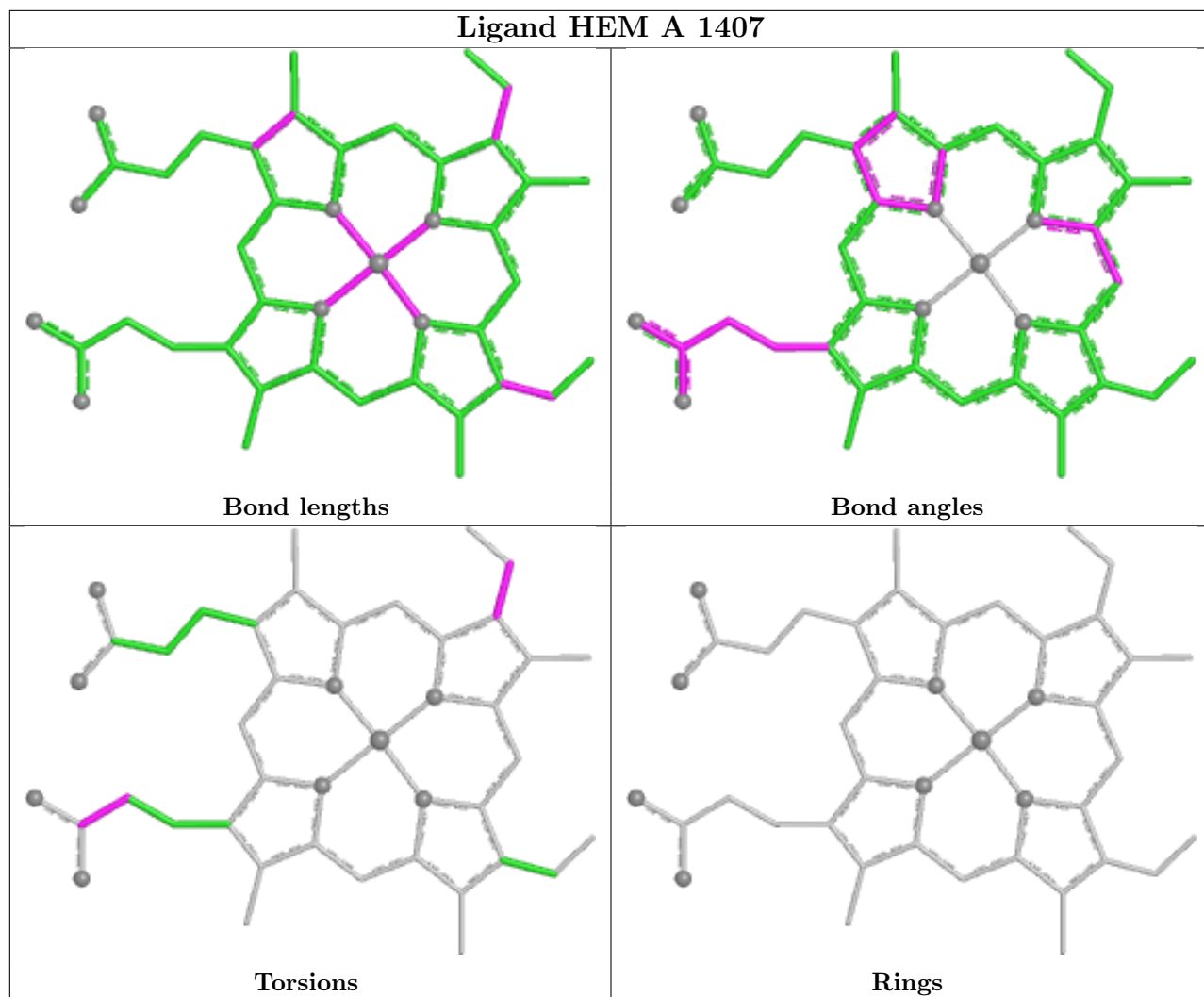


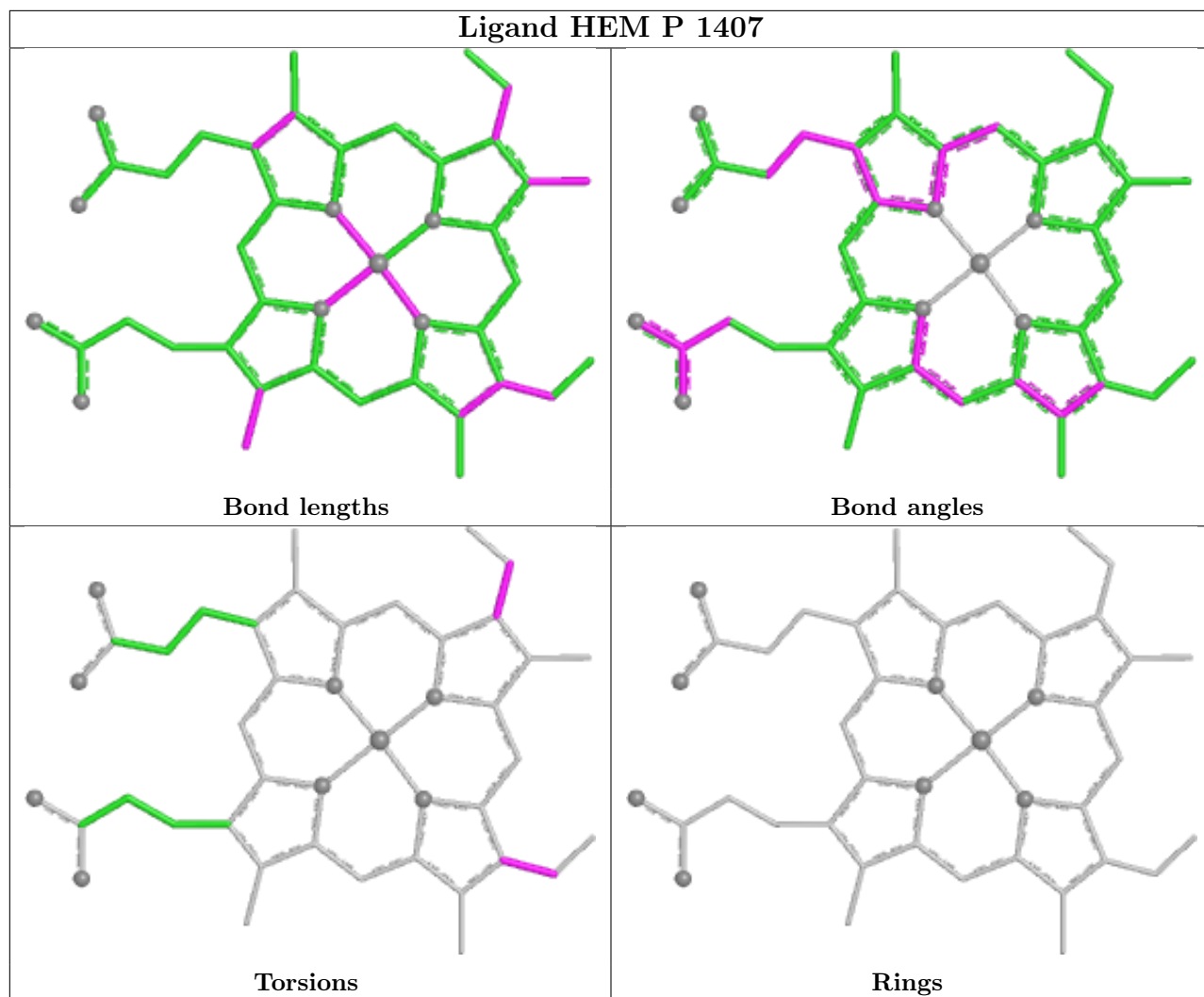


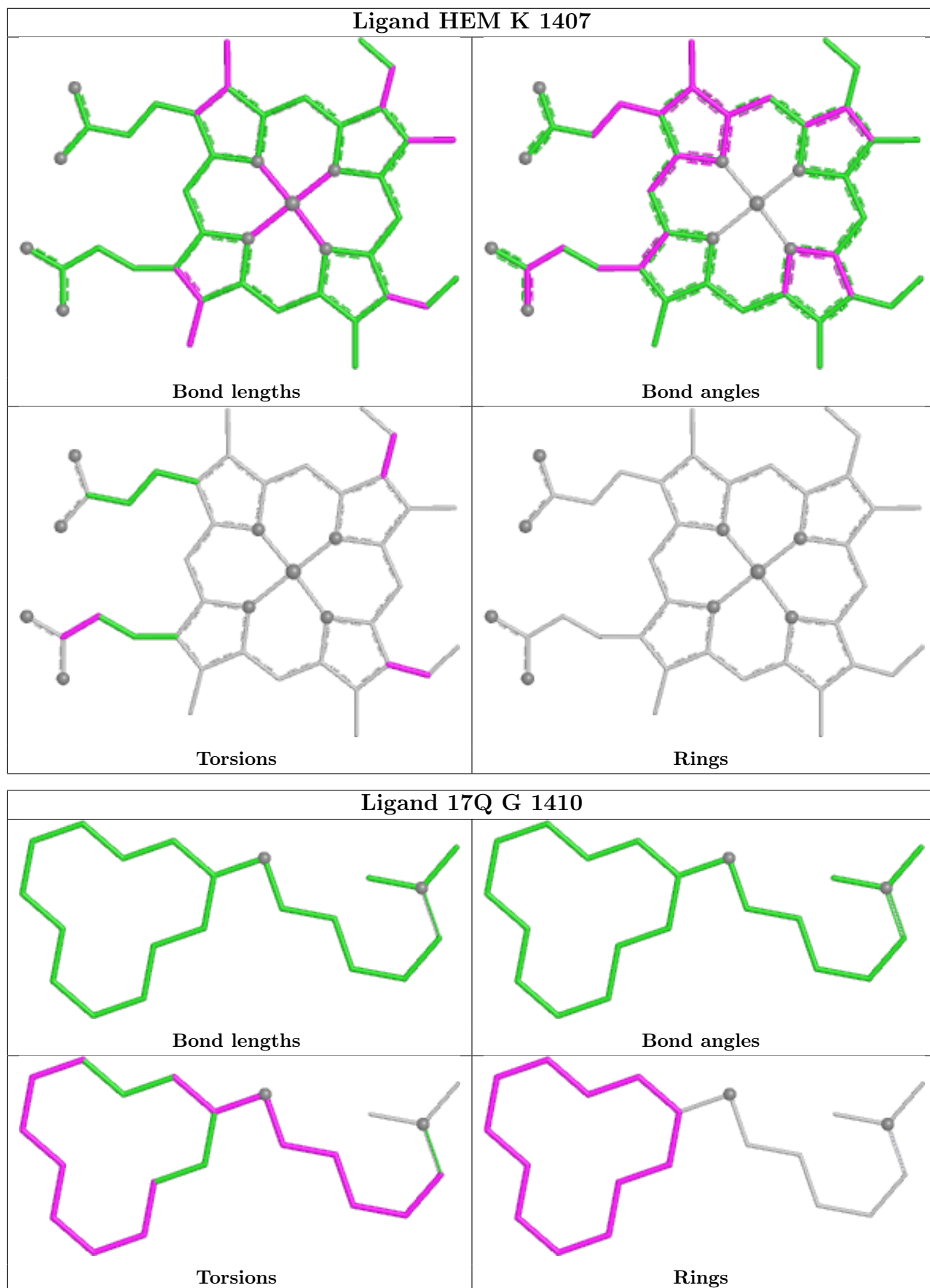


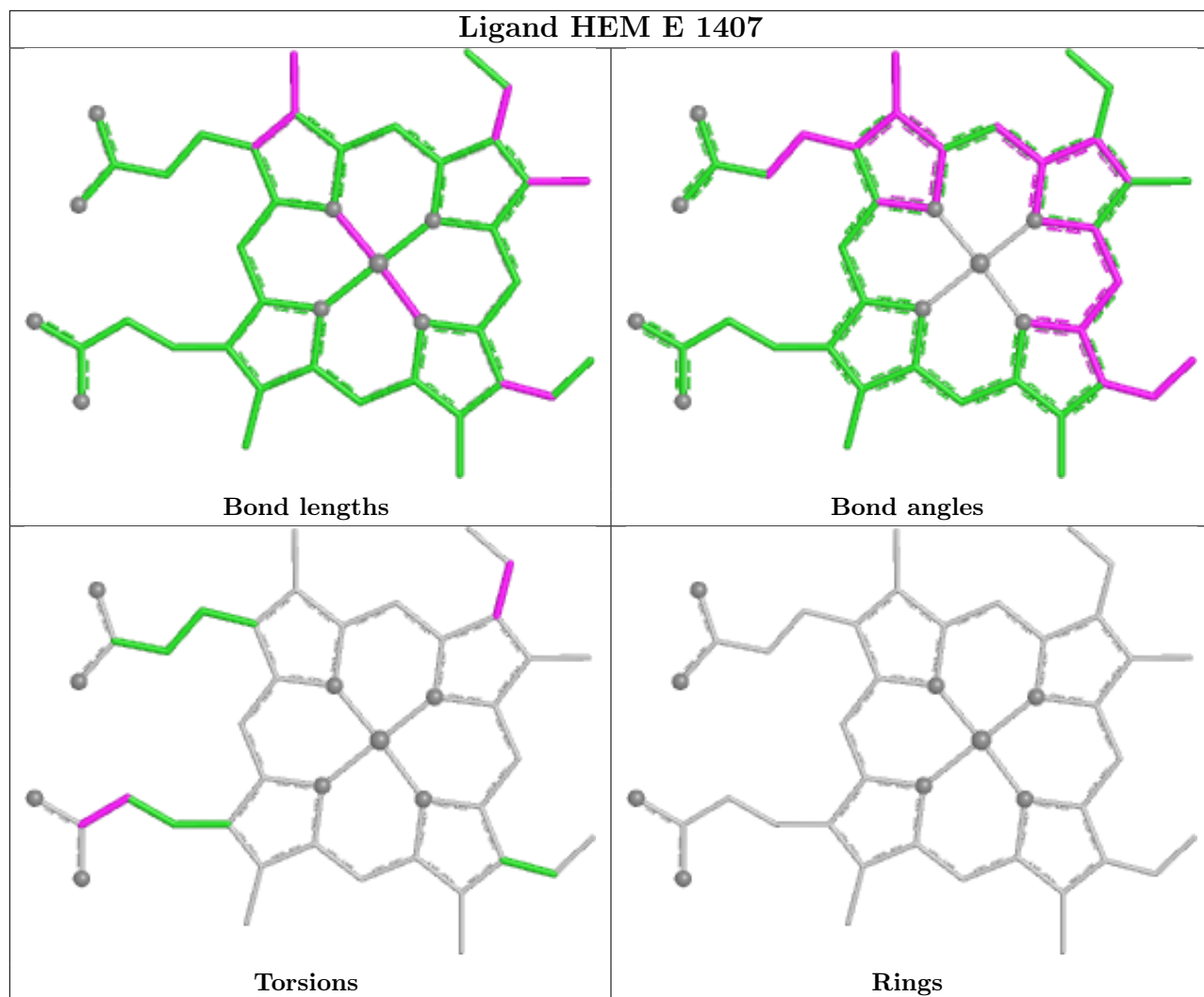


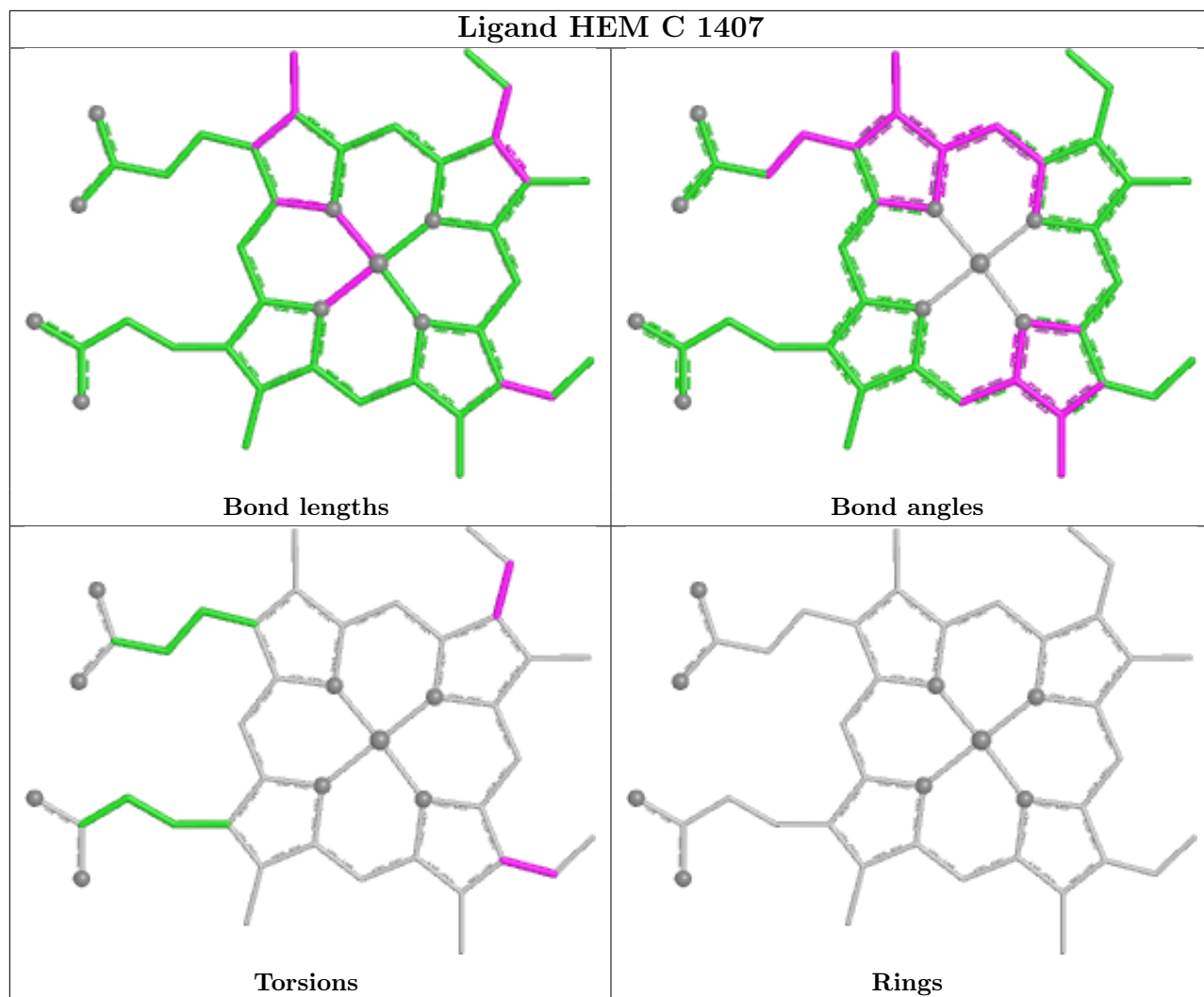


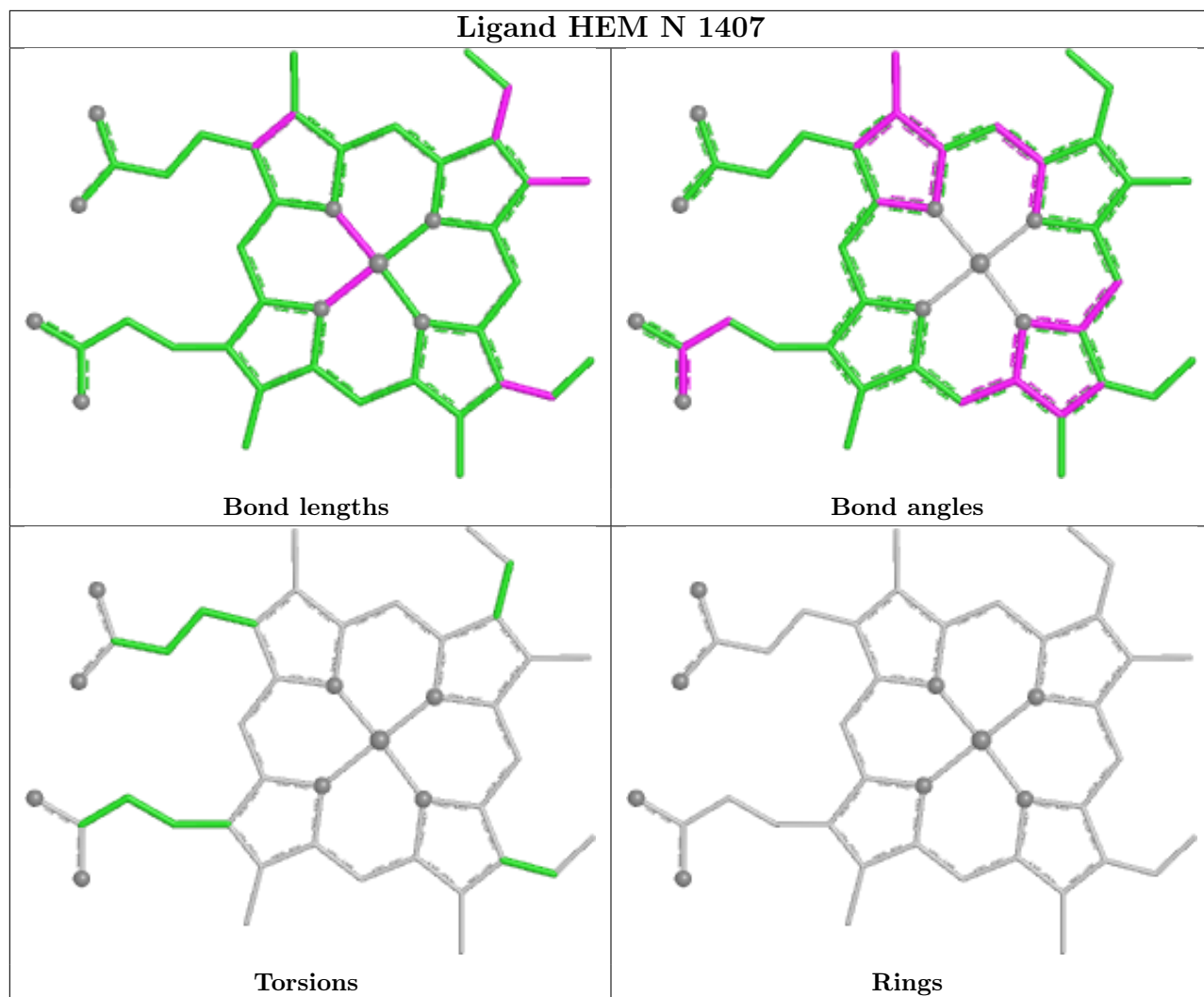


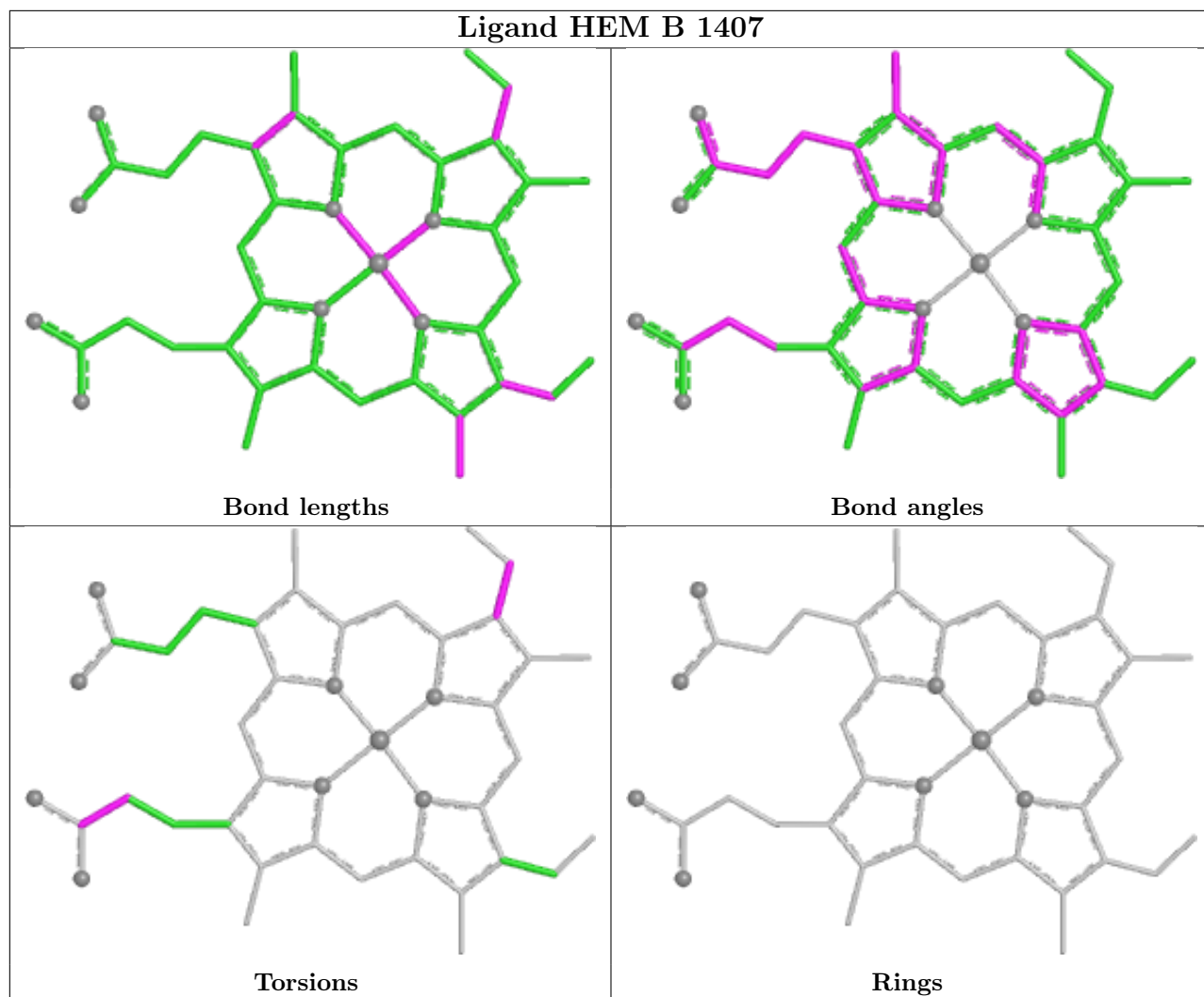


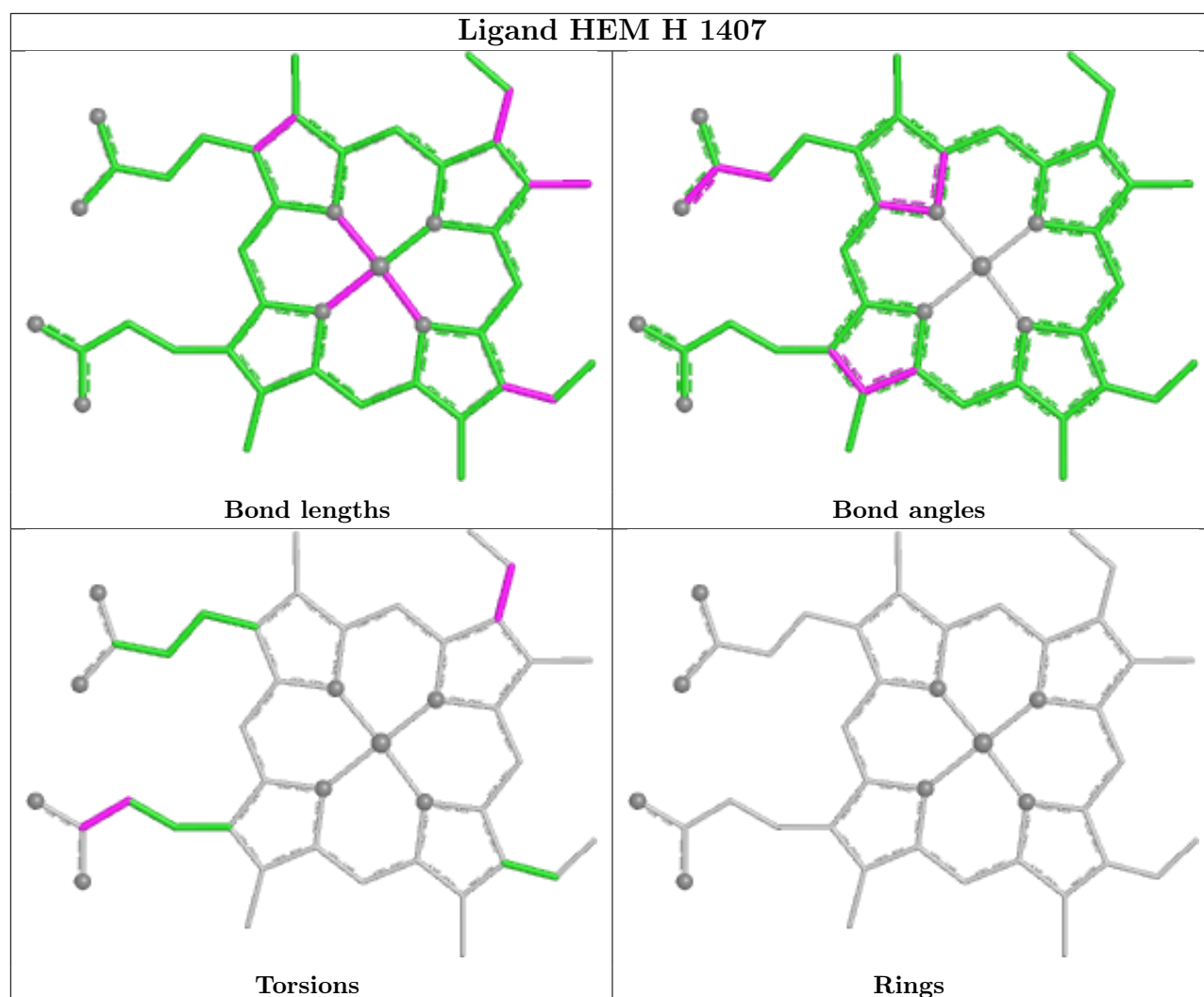












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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     | 396/436 (90%)   | -0.54  | 0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>     | 17, 33, 55, 71        | 0       |
| 1   | B     | 397/436 (91%)   | -0.43  | 2 (0%) <span style="border: 1px solid blue; padding: 0 2px;">87</span> <span style="border: 1px solid blue; padding: 0 2px;">86</span>  | 15, 35, 57, 76        | 2 (0%)  |
| 1   | C     | 396/436 (90%)   | -0.51  | 1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">89</span>  | 13, 33, 55, 73        | 1 (0%)  |
| 1   | D     | 397/436 (91%)   | -0.49  | 2 (0%) <span style="border: 1px solid blue; padding: 0 2px;">87</span> <span style="border: 1px solid blue; padding: 0 2px;">86</span>  | 18, 32, 55, 81        | 2 (0%)  |
| 1   | E     | 397/436 (91%)   | -0.44  | 1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">89</span>  | 16, 33, 55, 73        | 1 (0%)  |
| 1   | F     | 396/436 (90%)   | -0.36  | 1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">89</span>  | 14, 39, 66, 84        | 4 (1%)  |
| 1   | G     | 396/436 (90%)   | -0.47  | 1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">89</span>  | 12, 35, 52, 61        | 4 (1%)  |
| 1   | H     | 396/436 (90%)   | -0.42  | 2 (0%) <span style="border: 1px solid blue; padding: 0 2px;">87</span> <span style="border: 1px solid blue; padding: 0 2px;">86</span>  | 12, 35, 61, 87        | 1 (0%)  |
| 1   | I     | 396/436 (90%)   | -0.41  | 1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">89</span>  | 12, 38, 66, 79        | 2 (0%)  |
| 1   | J     | 397/436 (91%)   | -0.30  | 1 (0%) <span style="border: 1px solid blue; padding: 0 2px;">90</span> <span style="border: 1px solid blue; padding: 0 2px;">89</span>  | 21, 42, 68, 91        | 1 (0%)  |
| 1   | K     | 397/436 (91%)   | -0.20  | 2 (0%) <span style="border: 1px solid blue; padding: 0 2px;">87</span> <span style="border: 1px solid blue; padding: 0 2px;">86</span>  | 17, 46, 72, 90        | 2 (0%)  |
| 1   | L     | 397/436 (91%)   | -0.09  | 6 (1%) <span style="border: 1px solid blue; padding: 0 2px;">72</span> <span style="border: 1px solid blue; padding: 0 2px;">70</span>  | 18, 50, 86, 99        | 2 (0%)  |
| 1   | M     | 397/436 (91%)   | -0.02  | 2 (0%) <span style="border: 1px solid blue; padding: 0 2px;">87</span> <span style="border: 1px solid blue; padding: 0 2px;">86</span>  | 30, 53, 85, 91        | 1 (0%)  |
| 1   | N     | 397/436 (91%)   | 0.30   | 10 (2%) <span style="border: 1px solid blue; padding: 0 2px;">58</span> <span style="border: 1px solid blue; padding: 0 2px;">55</span> | 34, 72, 116, 158      | 1 (0%)  |
| 1   | O     | 397/436 (91%)   | 0.14   | 13 (3%) <span style="border: 1px solid red; padding: 0 2px;">49</span> <span style="border: 1px solid red; padding: 0 2px;">45</span>   | 28, 57, 105, 133      | 0       |
| 1   | P     | 396/436 (90%)   | 0.47   | 19 (4%) <span style="border: 1px solid red; padding: 0 2px;">35</span> <span style="border: 1px solid red; padding: 0 2px;">32</span>   | 20, 78, 129, 155      | 1 (0%)  |
| All | All   | 6345/6976 (90%) | -0.24  | 64 (1%) <span style="border: 1px solid blue; padding: 0 2px;">79</span> <span style="border: 1px solid blue; padding: 0 2px;">78</span> | 12, 41, 91, 158       | 25 (0%) |

All (64) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 179 | VAL  | 4.8  |
| 1   | N     | 10  | ALA  | 3.8  |
| 1   | M     | 150 | TRP  | 3.3  |
| 1   | O     | 13  | PRO  | 3.2  |
| 1   | O     | 184 | PRO  | 3.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | N            | 14         | VAL         | 3.1         |
| 1          | O            | 12         | PRO         | 3.1         |
| 1          | P            | 377        | ASP         | 3.1         |
| 1          | N            | 17         | LEU         | 3.0         |
| 1          | P            | 375        | CYS         | 3.0         |
| 1          | P            | 15         | LEU         | 2.9         |
| 1          | O            | 179        | VAL         | 2.9         |
| 1          | P            | 14         | VAL         | 2.9         |
| 1          | B            | 245[A]     | HIS         | 2.9         |
| 1          | P            | 12         | PRO         | 2.9         |
| 1          | M            | 383        | SER         | 2.9         |
| 1          | L            | 180        | PHE         | 2.9         |
| 1          | P            | 382        | VAL         | 2.9         |
| 1          | O            | 382        | VAL         | 2.8         |
| 1          | P            | 378        | LEU         | 2.8         |
| 1          | E            | 179        | VAL         | 2.8         |
| 1          | O            | 14         | VAL         | 2.7         |
| 1          | P            | 308        | VAL         | 2.7         |
| 1          | L            | 406        | ARG         | 2.6         |
| 1          | D            | 10         | ALA         | 2.6         |
| 1          | P            | 37         | ALA         | 2.6         |
| 1          | P            | 17         | LEU         | 2.6         |
| 1          | O            | 377        | ASP         | 2.5         |
| 1          | N            | 20         | LEU         | 2.5         |
| 1          | P            | 20         | LEU         | 2.5         |
| 1          | N            | 37         | ALA         | 2.5         |
| 1          | G            | 392[A]     | ASN         | 2.5         |
| 1          | P            | 150        | TRP         | 2.4         |
| 1          | O            | 185        | ALA         | 2.4         |
| 1          | P            | 257        | TYR         | 2.4         |
| 1          | H            | 382        | VAL         | 2.4         |
| 1          | P            | 381        | ASP         | 2.3         |
| 1          | N            | 177        | ALA         | 2.3         |
| 1          | B            | 179        | VAL         | 2.3         |
| 1          | P            | 13         | PRO         | 2.3         |
| 1          | L            | 178        | PHE         | 2.3         |
| 1          | O            | 175        | THR         | 2.2         |
| 1          | J            | 10         | ALA         | 2.2         |
| 1          | P            | 19         | ALA         | 2.2         |
| 1          | P            | 50         | ASN         | 2.2         |
| 1          | N            | 178        | PHE         | 2.2         |
| 1          | O            | 11         | SER         | 2.2         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 179 | VAL  | 2.2  |
| 1   | O     | 178 | PHE  | 2.2  |
| 1   | P     | 405 | TRP  | 2.2  |
| 1   | K     | 183 | ASP  | 2.1  |
| 1   | C     | 178 | PHE  | 2.1  |
| 1   | H     | 180 | PHE  | 2.1  |
| 1   | N     | 184 | PRO  | 2.1  |
| 1   | O     | 384 | PRO  | 2.1  |
| 1   | N     | 337 | ILE  | 2.1  |
| 1   | L     | 14  | VAL  | 2.1  |
| 1   | O     | 386 | GLU  | 2.0  |
| 1   | L     | 13  | PRO  | 2.0  |
| 1   | N     | 54  | LEU  | 2.0  |
| 1   | I     | 179 | VAL  | 2.0  |
| 1   | L     | 179 | VAL  | 2.0  |
| 1   | K     | 180 | PHE  | 2.0  |
| 1   | P     | 31  | THR  | 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   | SO4  | D     | 1408 | 5/5   | 0.89 | 0.18 | 37,37,39,40                 | 0     |
| 3   | SO4  | O     | 1409 | 5/5   | 0.90 | 0.19 | 39,39,40,40                 | 0     |
| 4   | 17Q  | C     | 1410 | 21/21 | 0.90 | 0.14 | 53,57,60,60                 | 0     |
| 3   | SO4  | O     | 1408 | 5/5   | 0.91 | 0.20 | 41,41,42,42                 | 0     |
| 3   | SO4  | B     | 1408 | 5/5   | 0.91 | 0.12 | 61,62,63,63                 | 0     |
| 3   | SO4  | J     | 1408 | 5/5   | 0.91 | 0.17 | 41,42,42,43                 | 0     |

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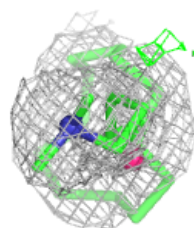
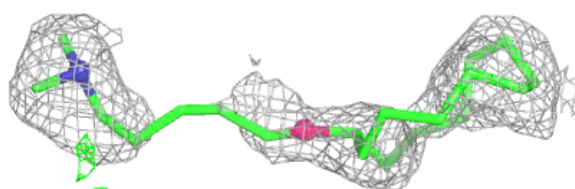
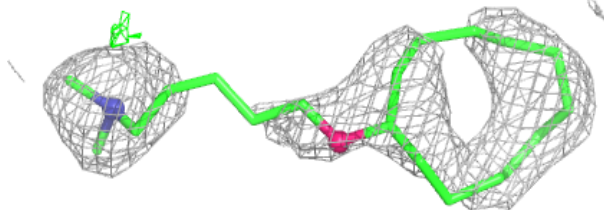
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | 17Q  | G     | 1410 | 21/21 | 0.91 | 0.13 | 39,49,55,55                 | 0     |
| 3   | SO4  | I     | 1408 | 5/5   | 0.93 | 0.20 | 39,41,42,43                 | 0     |
| 3   | SO4  | B     | 1409 | 5/5   | 0.93 | 0.12 | 49,49,51,51                 | 0     |
| 3   | SO4  | H     | 1408 | 5/5   | 0.94 | 0.15 | 42,42,44,45                 | 0     |
| 3   | SO4  | A     | 1408 | 5/5   | 0.95 | 0.09 | 41,42,43,43                 | 0     |
| 3   | SO4  | I     | 1409 | 5/5   | 0.96 | 0.07 | 53,54,55,55                 | 0     |
| 2   | HEM  | P     | 1407 | 43/43 | 0.96 | 0.08 | 36,46,51,54                 | 0     |
| 3   | SO4  | F     | 1408 | 5/5   | 0.96 | 0.15 | 38,39,40,41                 | 0     |
| 2   | HEM  | E     | 1407 | 43/43 | 0.97 | 0.06 | 13,18,21,23                 | 0     |
| 3   | SO4  | H     | 1409 | 5/5   | 0.97 | 0.10 | 38,39,40,40                 | 0     |
| 2   | HEM  | O     | 1407 | 43/43 | 0.97 | 0.07 | 29,33,38,41                 | 0     |
| 2   | HEM  | G     | 1407 | 43/43 | 0.98 | 0.06 | 17,23,24,28                 | 0     |
| 2   | HEM  | H     | 1407 | 43/43 | 0.98 | 0.06 | 15,19,21,22                 | 0     |
| 2   | HEM  | I     | 1407 | 43/43 | 0.98 | 0.07 | 23,25,29,31                 | 0     |
| 2   | HEM  | J     | 1407 | 43/43 | 0.98 | 0.06 | 26,28,31,32                 | 0     |
| 2   | HEM  | K     | 1407 | 43/43 | 0.98 | 0.06 | 21,25,27,29                 | 0     |
| 2   | HEM  | L     | 1407 | 43/43 | 0.98 | 0.06 | 19,24,27,31                 | 0     |
| 2   | HEM  | M     | 1407 | 43/43 | 0.98 | 0.06 | 18,23,26,31                 | 0     |
| 2   | HEM  | N     | 1407 | 43/43 | 0.98 | 0.07 | 29,33,44,49                 | 0     |
| 2   | HEM  | B     | 1407 | 43/43 | 0.98 | 0.06 | 19,25,27,29                 | 0     |
| 2   | HEM  | C     | 1407 | 43/43 | 0.98 | 0.06 | 12,14,19,24                 | 0     |
| 2   | HEM  | A     | 1407 | 43/43 | 0.98 | 0.05 | 14,20,24,28                 | 0     |
| 2   | HEM  | F     | 1407 | 43/43 | 0.98 | 0.06 | 17,22,24,26                 | 0     |
| 2   | HEM  | D     | 1407 | 43/43 | 0.99 | 0.05 | 13,18,22,23                 | 0     |

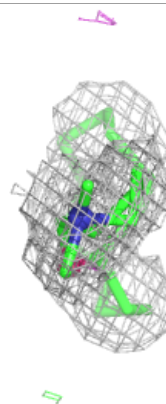
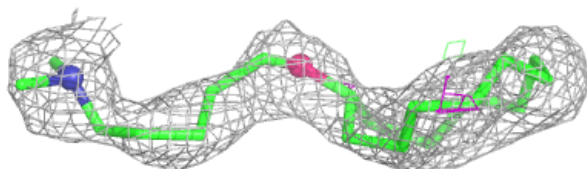
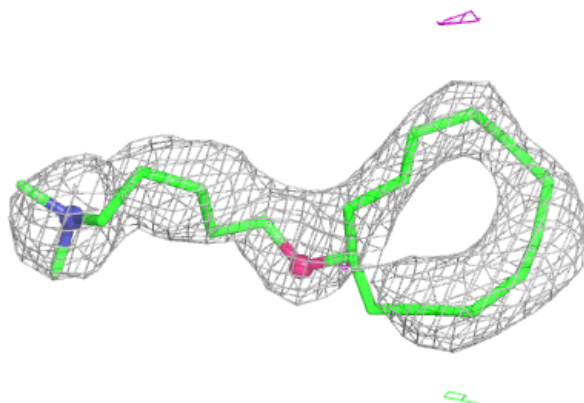
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 17Q C 1410:**

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

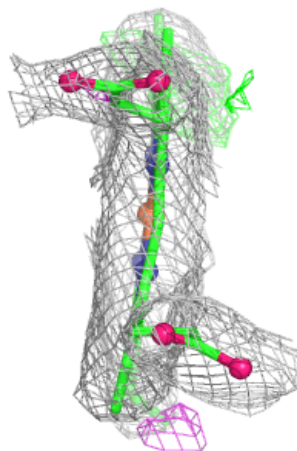
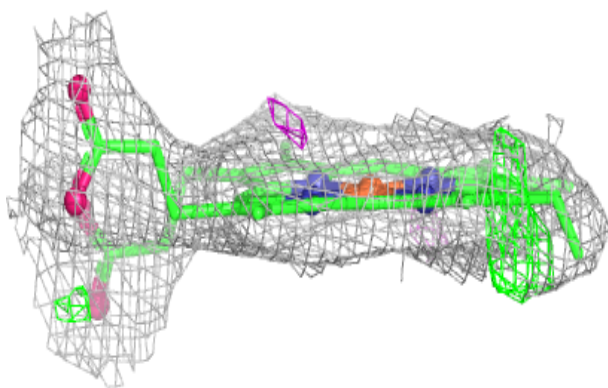
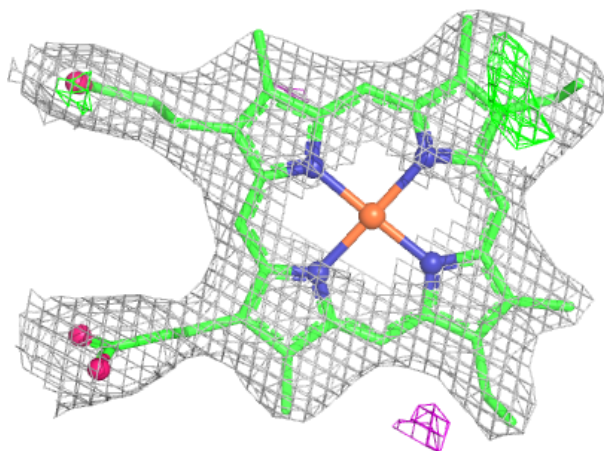
**Electron density around 17Q G 1410:**

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



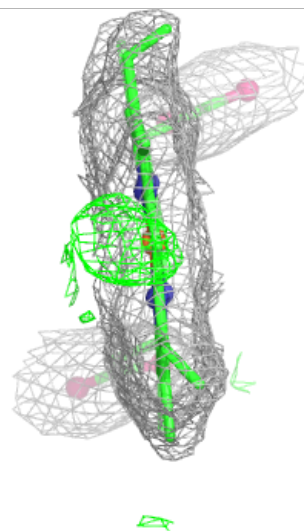
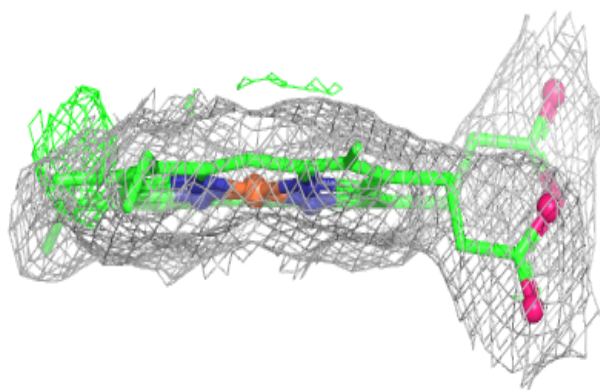
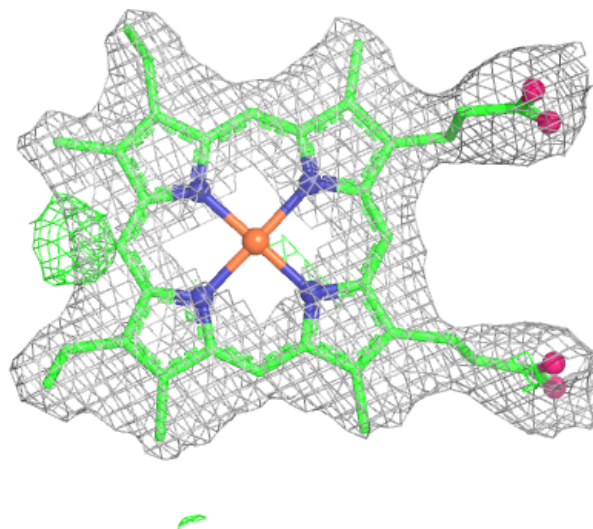
**Electron density around HEM P 1407:**

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



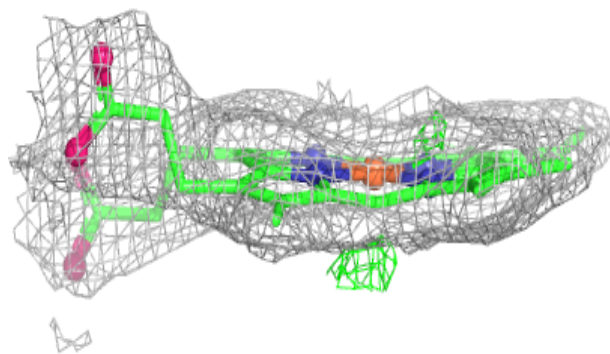
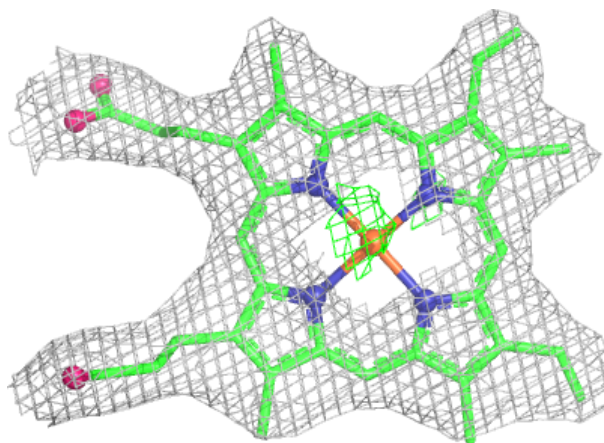
**Electron density around HEM E 1407:**

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



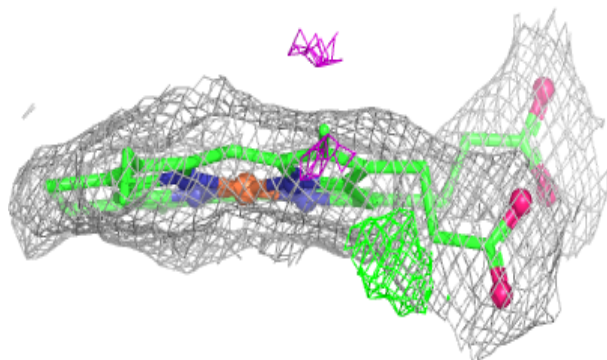
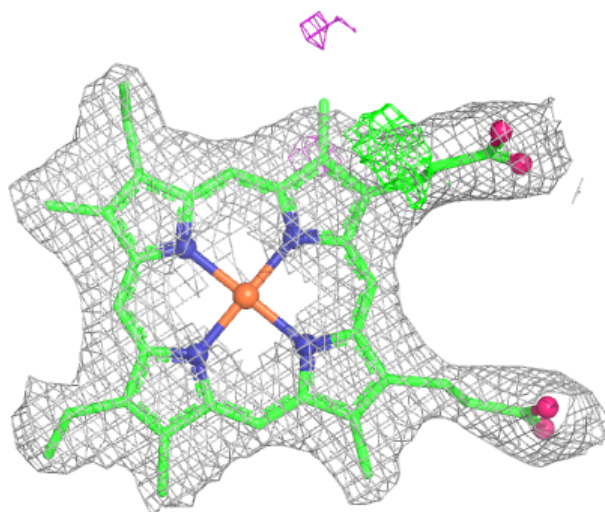
**Electron density around HEM O 1407:**

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



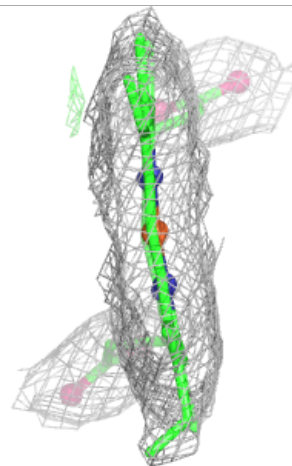
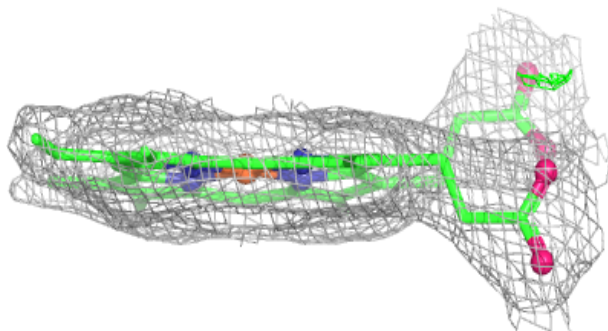
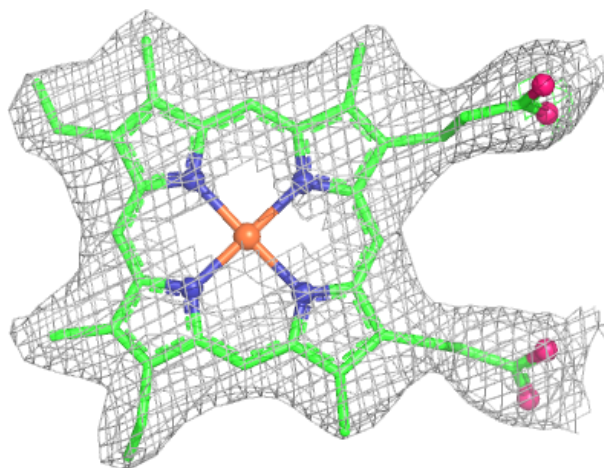
**Electron density around HEM G 1407:**

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and green (positive)



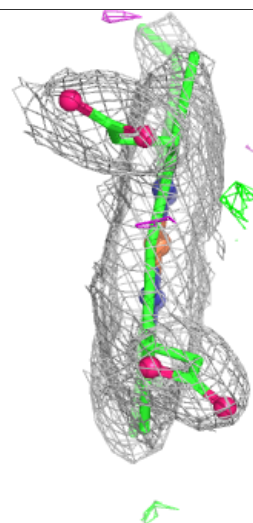
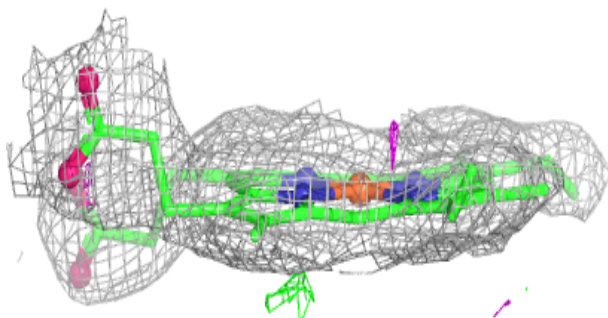
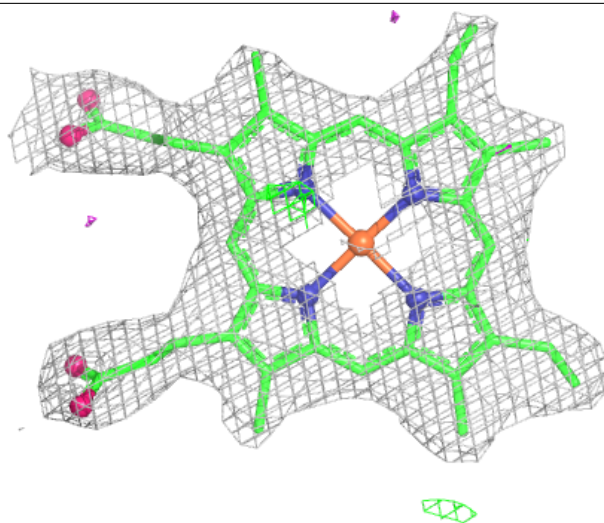
**Electron density around HEM H 1407:**

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and green (positive)



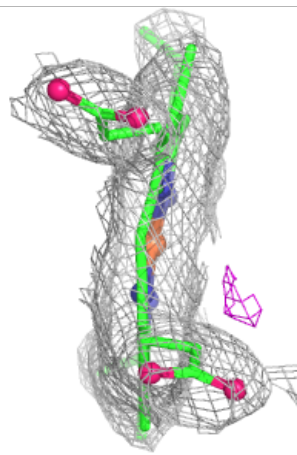
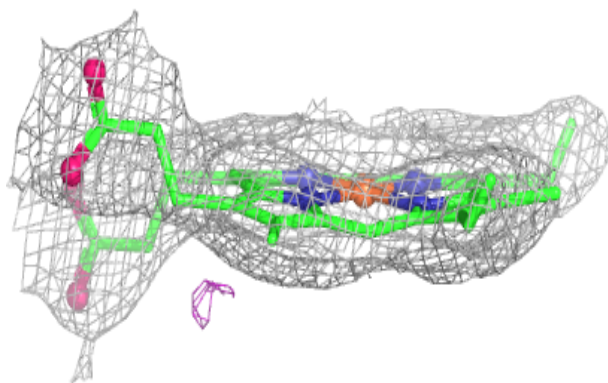
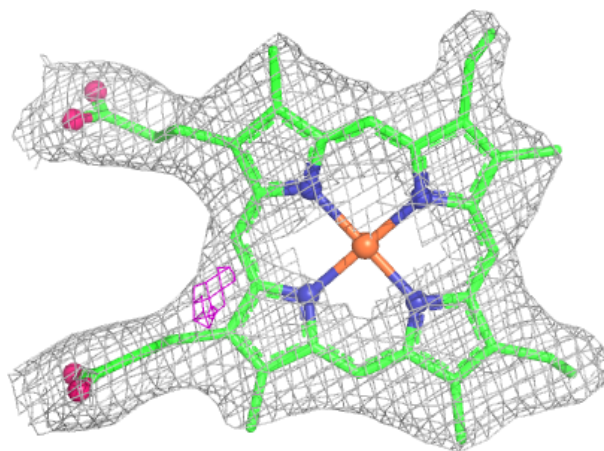
**Electron density around HEM I 1407:**

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



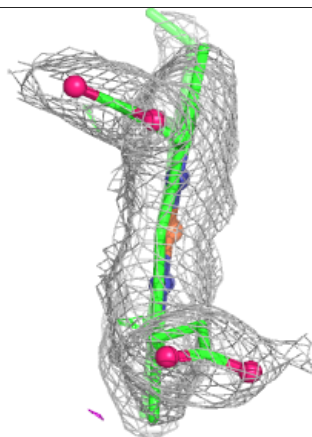
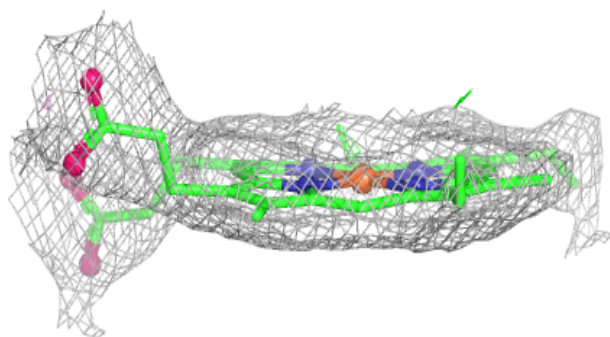
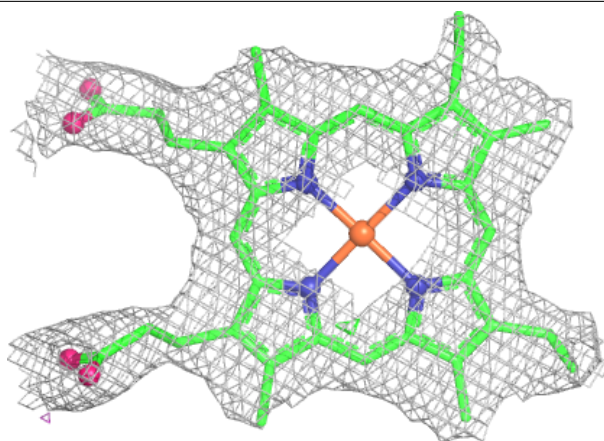
**Electron density around HEM J 1407:**

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



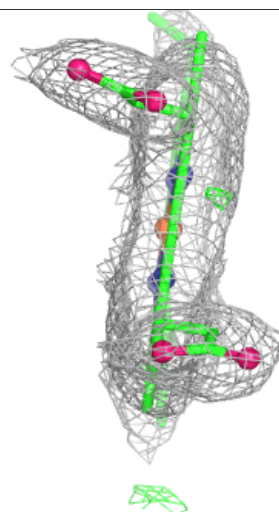
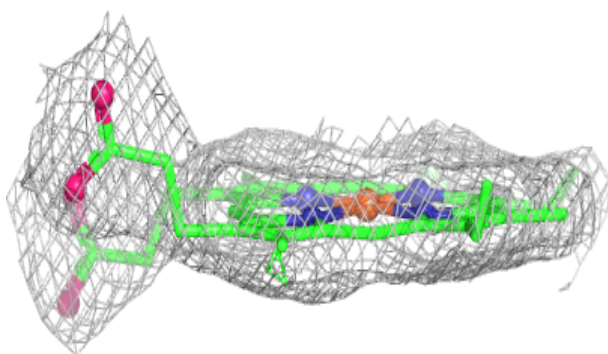
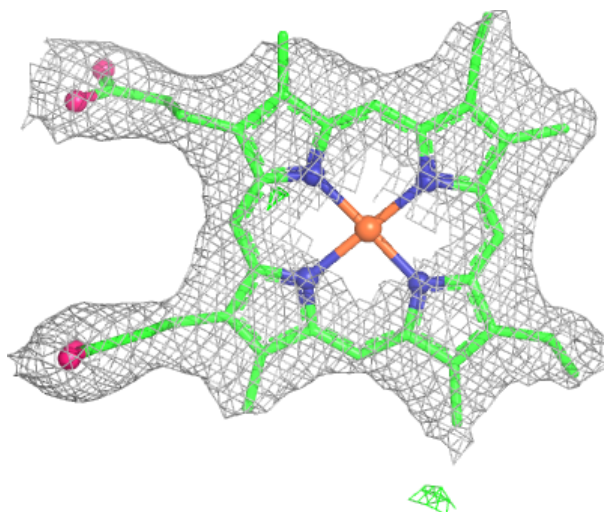
**Electron density around HEM K 1407:**

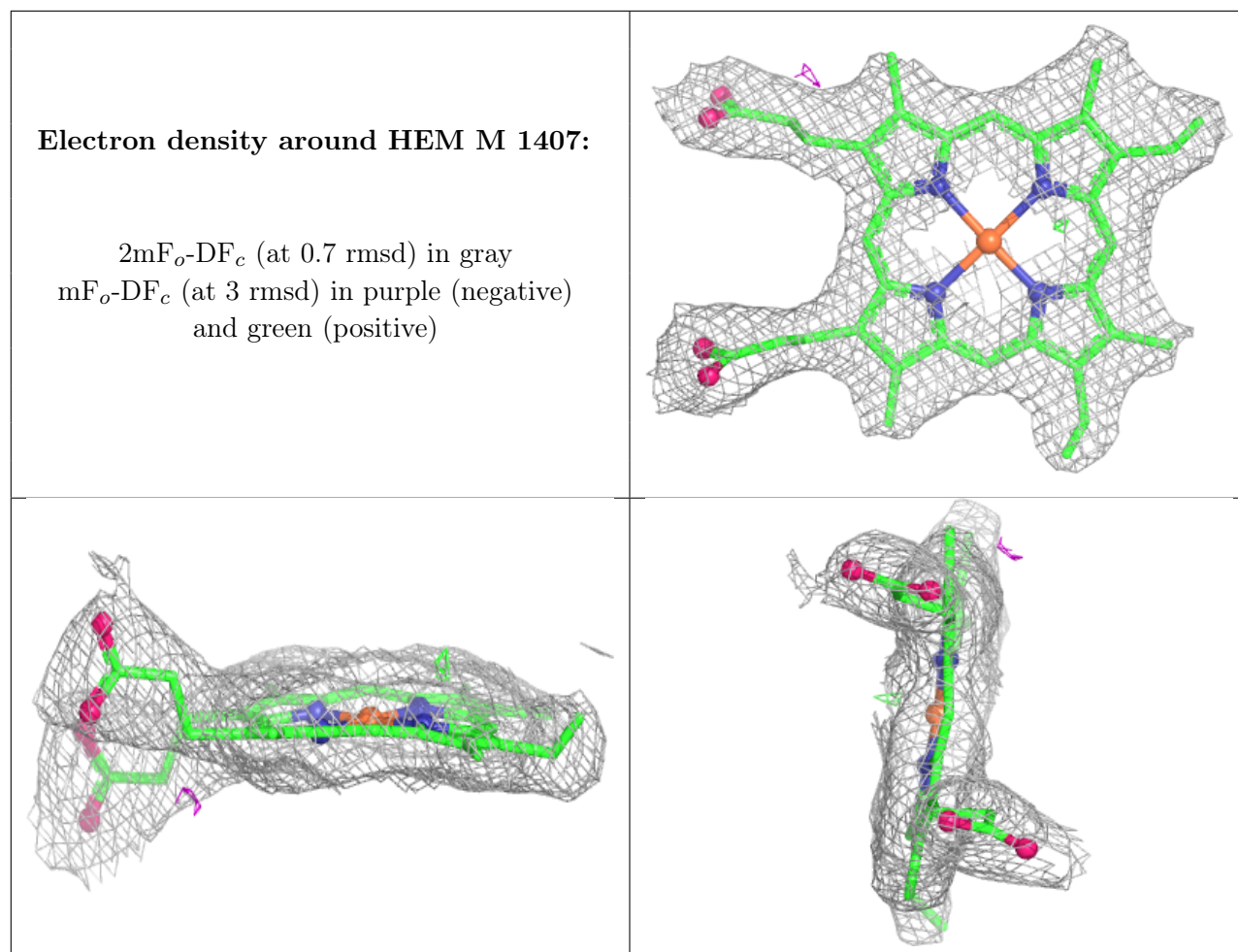
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM L 1407:**

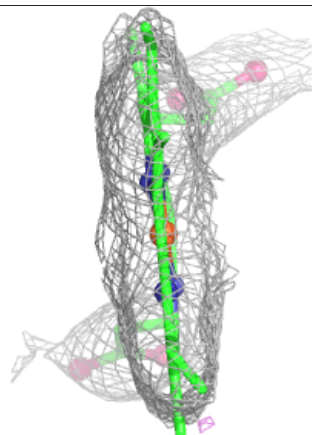
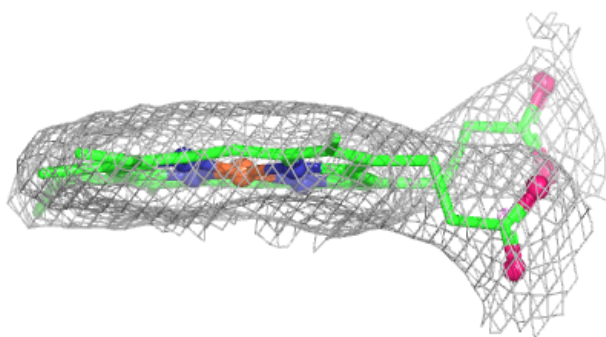
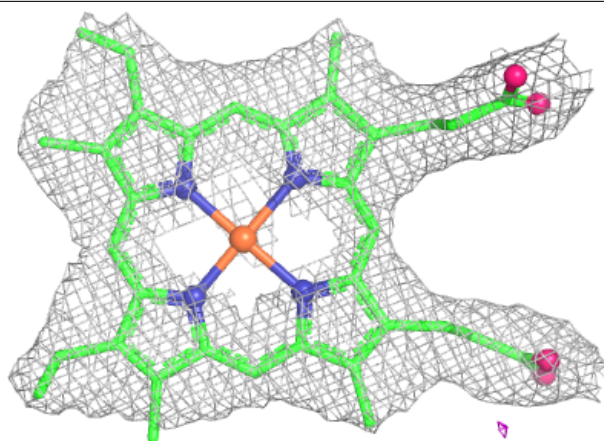
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





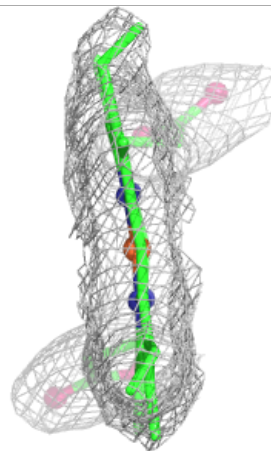
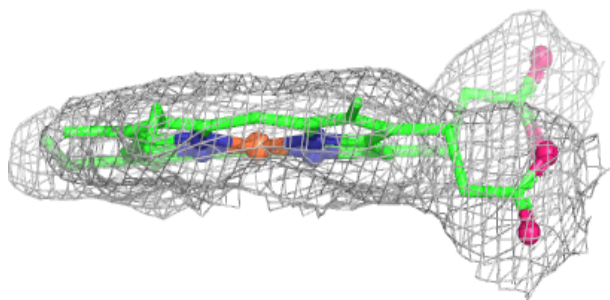
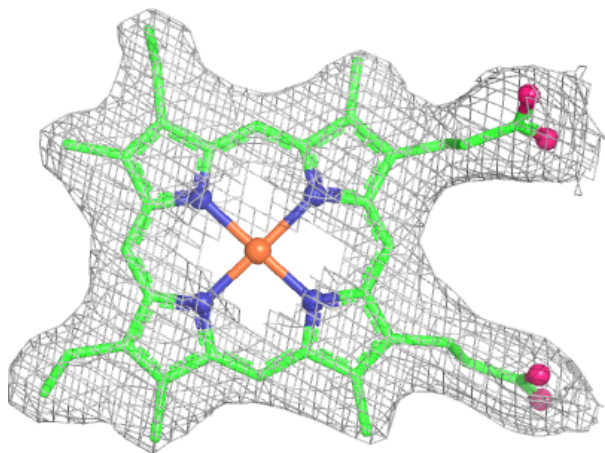
**Electron density around HEM N 1407:**

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



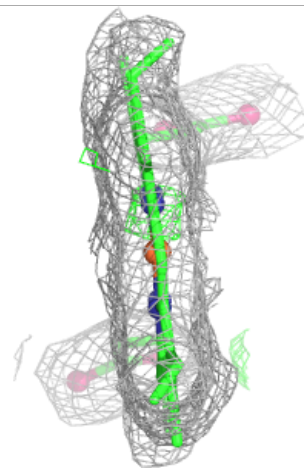
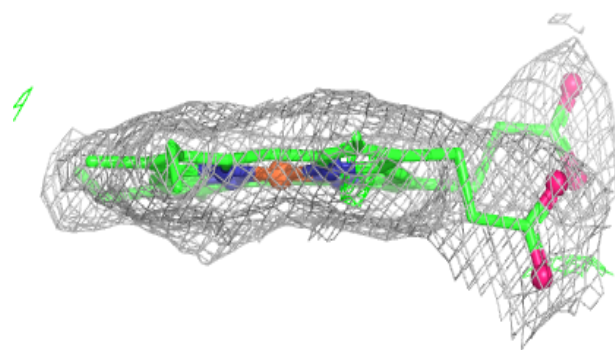
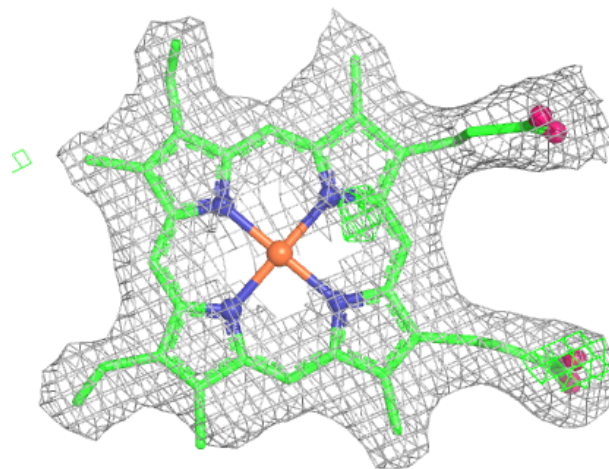
**Electron density around HEM B 1407:**

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



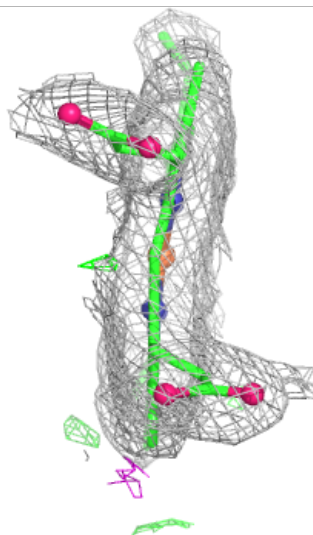
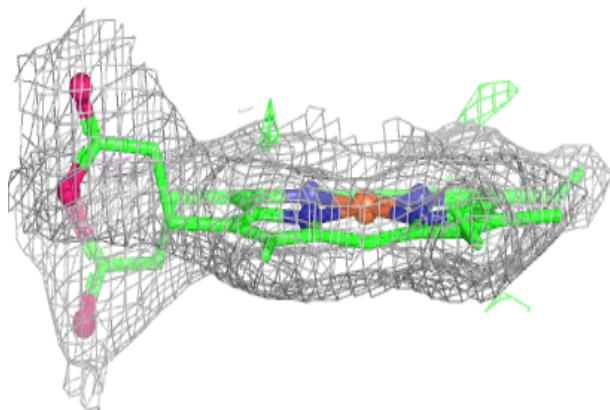
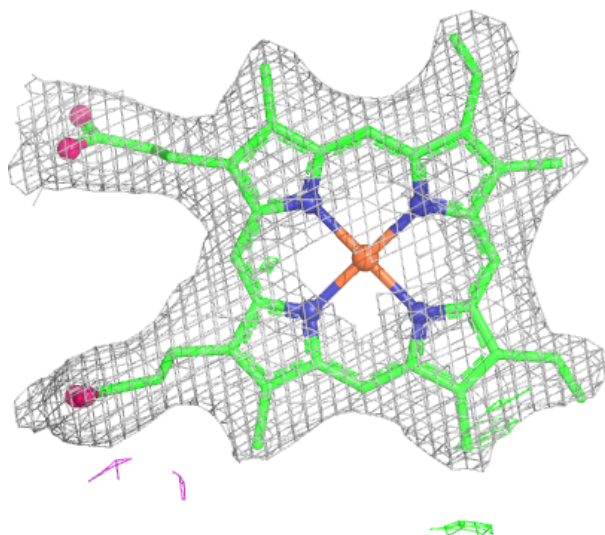
**Electron density around HEM C 1407:**

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



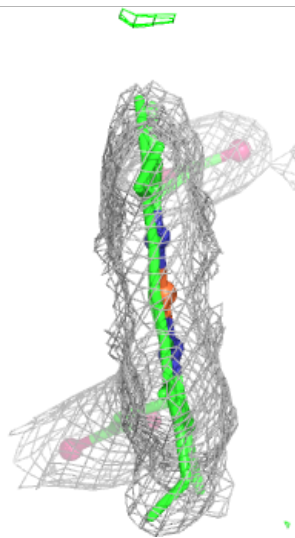
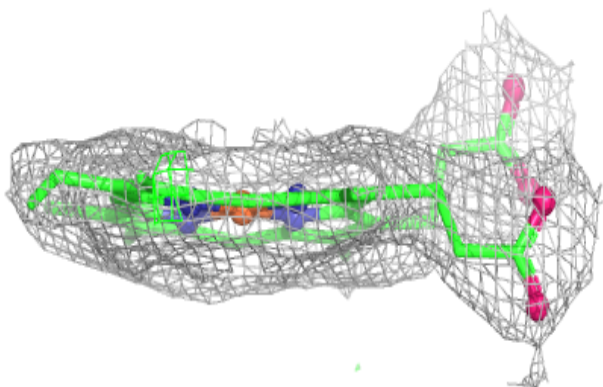
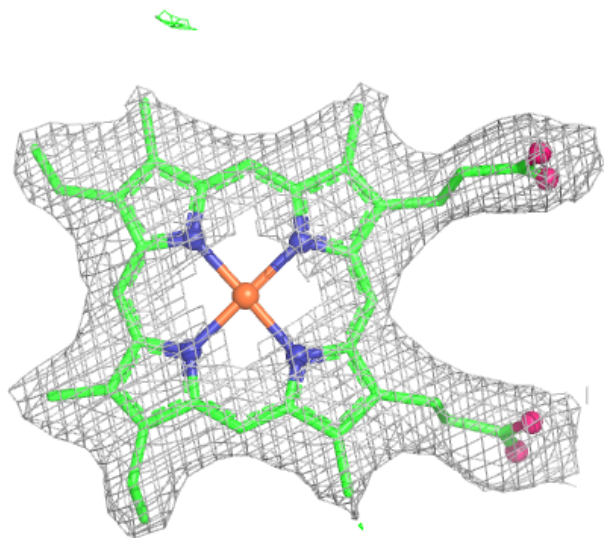
**Electron density around HEM A 1407:**

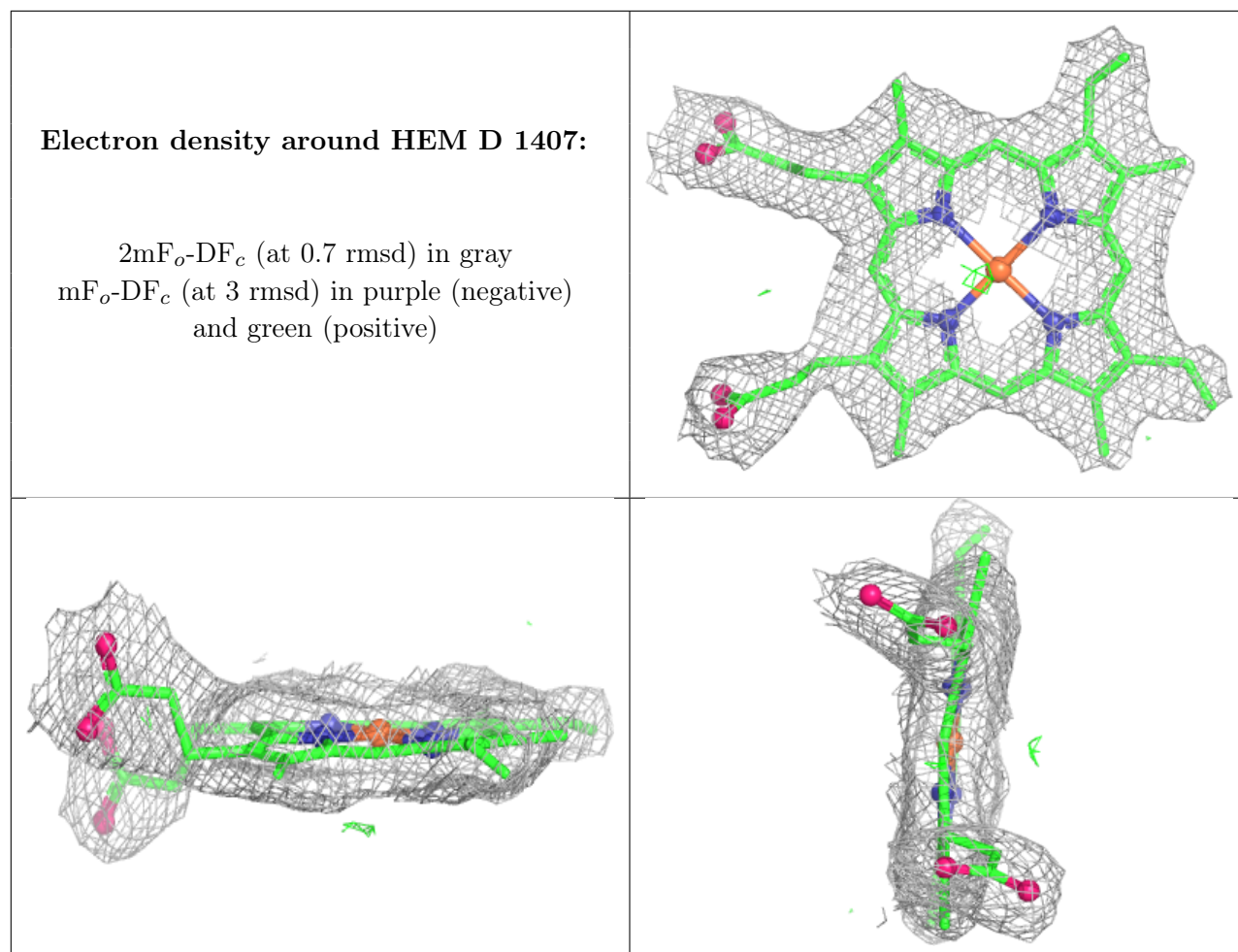
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM F 1407:**

$2mF_o-DF_c$  (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.