



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 11:42 am GMT

PDB ID : 5DJQ
Title : The structure of CBB3 cytochrome oxidase.
Authors : Buschmann, S.; Warkentin, E.; Xie, H.; Kohlstaedt, M.; Langer, J.D.; Ermler, U.; Michel, H.
Deposited on : 2015-09-02
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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>.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 3.0 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4 | : | 9.0.003 (Gargrove) |
| Density-Fitness | : | 1.0.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

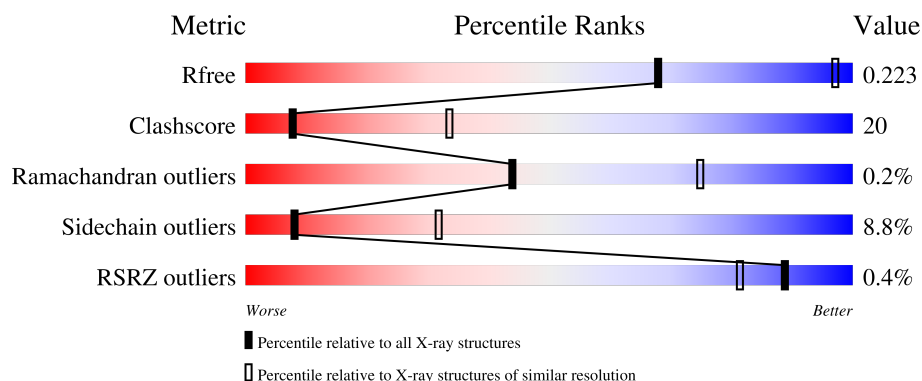
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 164625 | 1370 (3.20-3.20) |
| Clashscore | 180529 | 1497 (3.20-3.20) |
| Ramachandran outliers | 177936 | 1479 (3.20-3.20) |
| Sidechain outliers | 177891 | 1478 (3.20-3.20) |
| RSRZ outliers | 164620 | 1371 (3.20-3.20) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 | 474 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 64%, yellow 30%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 64% 30% </div> </div> |
| 1 | D | 474 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 61%, yellow 34%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 61% 34% </div> </div> |
| 1 | G | 474 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 60%, yellow 34%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 60% 34% </div> </div> |
| 1 | K | 474 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 63%, yellow 31%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 63% 31% </div> </div> |
| 2 | B | 203 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 67%, yellow 26%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 67% 26% </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | E | 203 |  |
| 2 | H | 203 |  |
| 2 | L | 203 |  |
| 3 | C | 311 |  |
| 3 | F | 311 |  |
| 3 | I | 311 |  |
| 3 | M | 311 |  |
| 4 | N | 36 |  |
| 4 | O | 36 |  |
| 4 | P | 36 |  |
| 4 | Q | 36 |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 9 | PO4 | K | 506 | - | - | X | - |

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31974 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 Cbb3-type cytochrome c oxidase subunit CcoN1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 466 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3683 | 2461 | 593 | 607 | 22 | | | |
| 1 | D | 463 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3663 | 2450 | 590 | 601 | 22 | | | |
| 1 | G | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3676 | 2457 | 592 | 605 | 22 | | | |
| 1 | K | 465 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3676 | 2457 | 592 | 605 | 22 | | | |

- Molecule 2 is a protein called Cbb3-type cytochrome c oxidase subunit II.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2 | B | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1548 | 981 | 268 | 289 | 10 | | | |
| 2 | E | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1548 | 981 | 268 | 289 | 10 | | | |
| 2 | H | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1548 | 981 | 268 | 289 | 10 | | | |
| 2 | L | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1548 | 981 | 268 | 289 | 10 | | | |

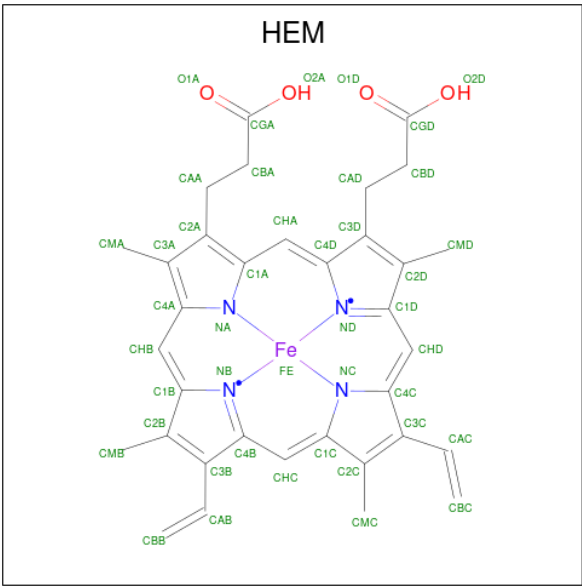
- Molecule 3 is a protein called Cbb3-type cytochrome c oxidase subunit CcoP1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 303 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2312 | 1483 | 391 | 427 | 11 | | | |
| 3 | F | 303 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2312 | 1483 | 391 | 427 | 11 | | | |
| 3 | I | 303 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2312 | 1483 | 391 | 427 | 11 | | | |
| 3 | M | 303 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2312 | 1483 | 391 | 427 | 11 | | | |

- Molecule 4 is a protein called Putative uncharacterized protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 4 | N | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 221 | 154 | 31 | 34 | 2 | | | |
| 4 | O | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 221 | 154 | 31 | 34 | 2 | | | |
| 4 | P | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 221 | 154 | 31 | 34 | 2 | | | |
| 4 | Q | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 221 | 154 | 31 | 34 | 2 | | | |

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 5 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 5 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 5 | D | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 5 | D | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 5 | G | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 5 | G | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 5 | K | 1 | Total | C | Fe | N | O | |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 5 | K | 1 | Total | C | Fe | N | O | |
| | | | 43 | 34 | 1 | 4 | 4 | |

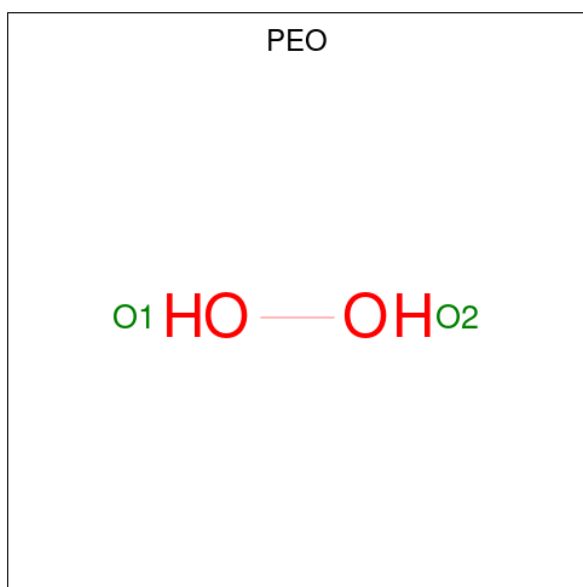
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6 | A | 1 | Total | Cu | | |
| | | | 1 | 1 | 0 | 0 |
| 6 | D | 1 | Total | Cu | | |
| | | | 1 | 1 | 0 | 0 |
| 6 | G | 1 | Total | Cu | | |
| | | | 1 | 1 | 0 | 0 |
| 6 | K | 1 | Total | Cu | | |
| | | | 1 | 1 | 0 | 0 |

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

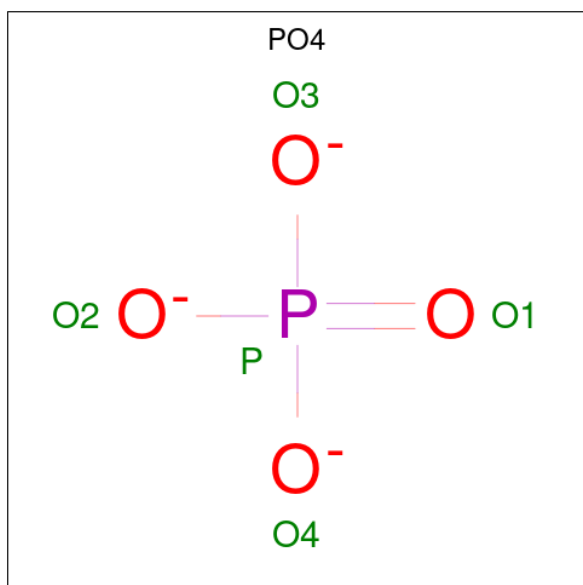
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7 | A | 2 | Total | Ca | | |
| | | | 2 | 2 | 0 | 0 |
| 7 | D | 2 | Total | Ca | | |
| | | | 2 | 2 | 0 | 0 |
| 7 | G | 2 | Total | Ca | | |
| | | | 2 | 2 | 0 | 0 |
| 7 | K | 2 | Total | Ca | | |
| | | | 2 | 2 | 0 | 0 |

- Molecule 8 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



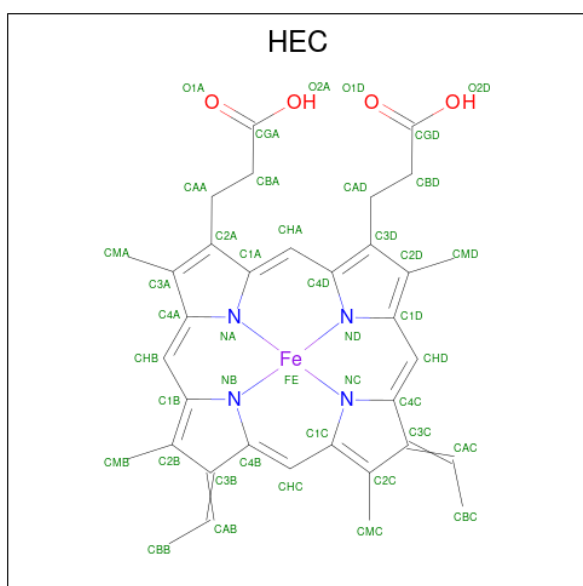
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 8 | A | 1 | Total O 2 2 | 0 | 0 |
| 8 | D | 1 | Total O 2 2 | 0 | 0 |
| 8 | G | 1 | Total O 2 2 | 0 | 0 |
| 8 | K | 1 | Total O 2 2 | 0 | 0 |

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 9 | A | 1 | Total 5 | O 4 | P 1 | 0 | 0 |
| 9 | D | 1 | Total 5 | O 4 | P 1 | 0 | 0 |
| 9 | G | 1 | Total 5 | O 4 | P 1 | 0 | 0 |
| 9 | K | 1 | Total 5 | O 4 | P 1 | 0 | 0 |

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



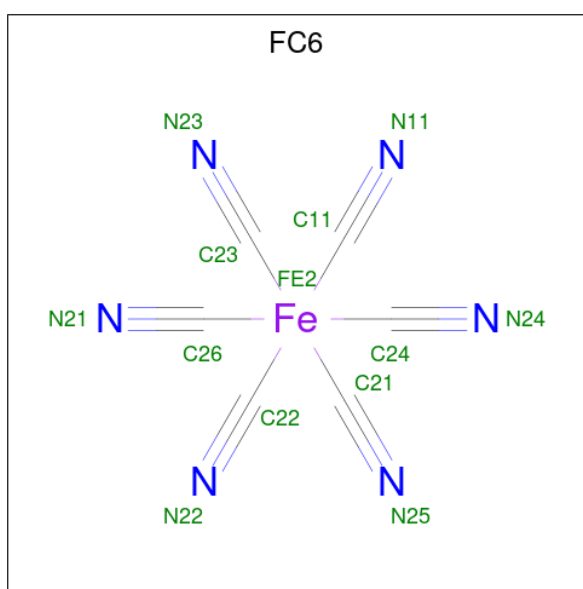
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 10 | B | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 10 | C | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 10 | C | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 10 | E | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 10 | F | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 10 | F | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 10 | H | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 10 | I | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 10 | I | 1 | Total | C | Fe | N | O | |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 10 | L | 1 | Total | C | Fe | N | O | |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 10 | M | 1 | Total | C | Fe | N | O | |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 10 | M | 1 | Total | C | Fe | N | O | |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 11 is HEXACYANOFERRATE(3-) (three-letter code: FC6) (formula: C_6FeN_6).

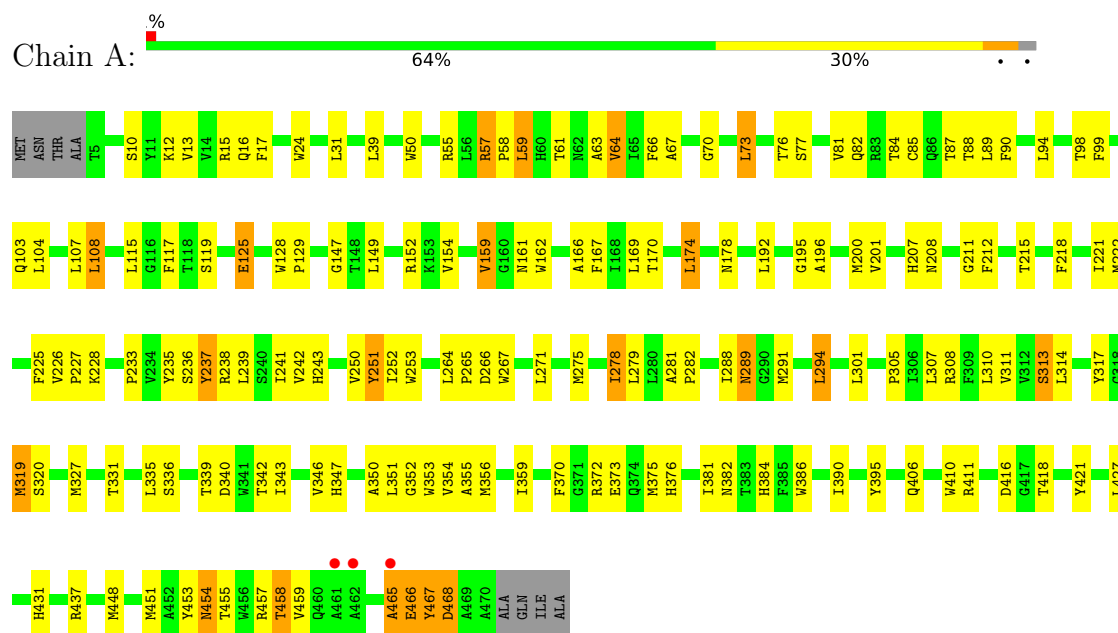


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 11 | C | 1 | Total | C | Fe | N | | |
| | | | 13 | 6 | 1 | 6 | 0 | 0 |
| 11 | F | 1 | Total | C | Fe | N | | |
| | | | 13 | 6 | 1 | 6 | 0 | 0 |
| 11 | I | 1 | Total | C | Fe | N | | |
| | | | 13 | 6 | 1 | 6 | 0 | 0 |
| 11 | M | 1 | Total | C | Fe | N | | |
| | | | 13 | 6 | 1 | 6 | 0 | 0 |

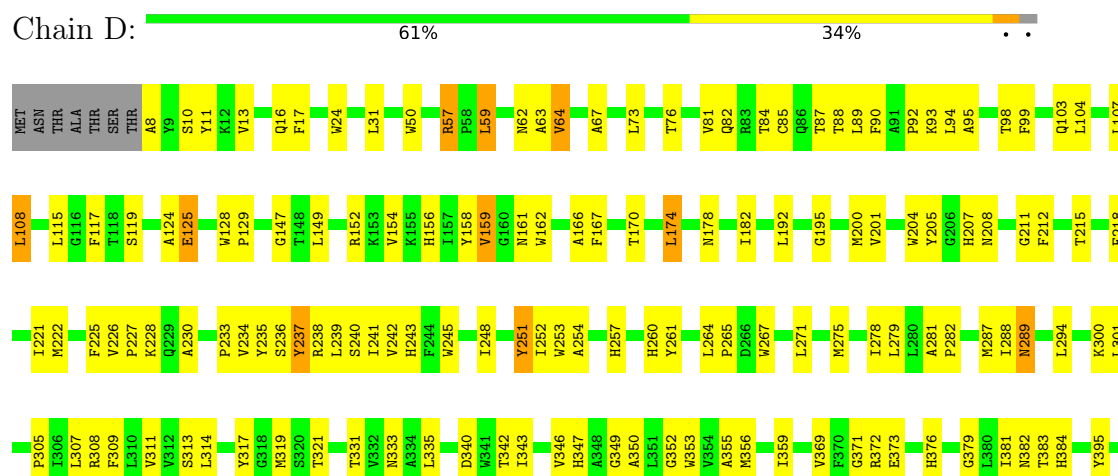
3 Residue-property plots [i](#)

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

- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

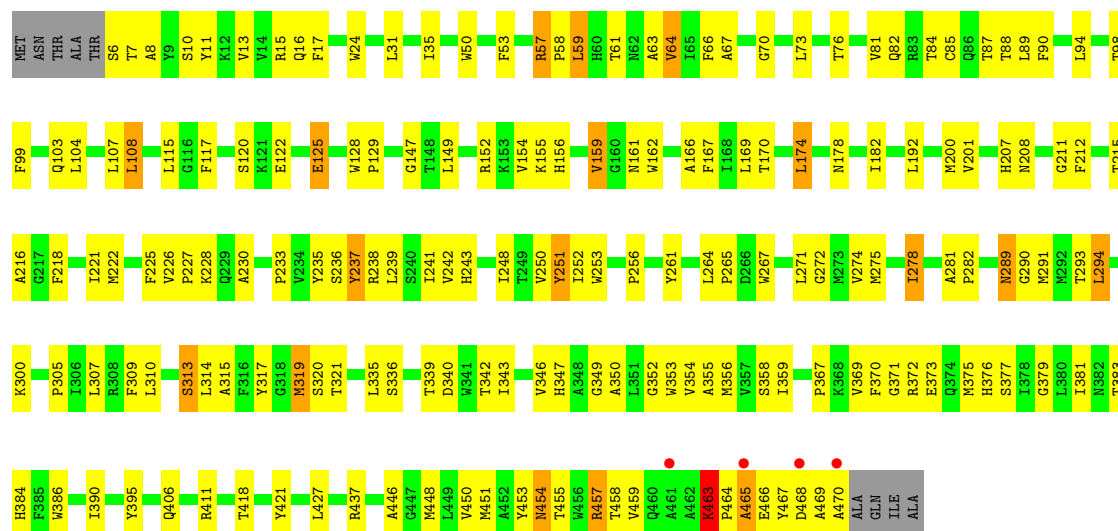


- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

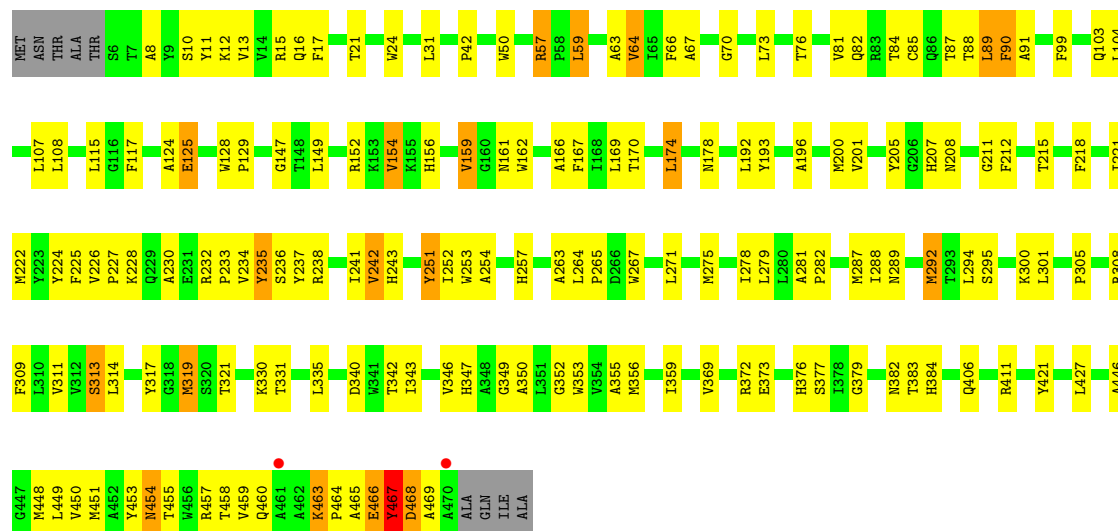




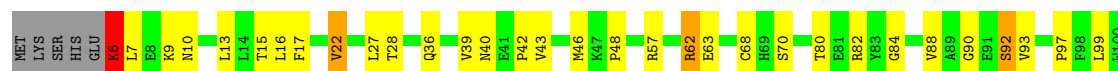
- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

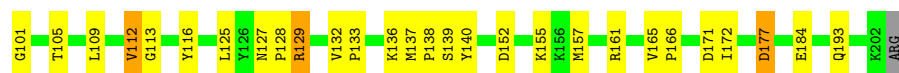


- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

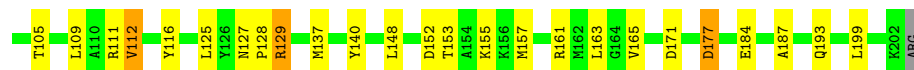


- Molecule 2: Cbb3-type cytochrome c oxidase subunit II





• Molecule 2: Cbb3-type cytochrome c oxidase subunit II



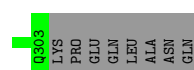
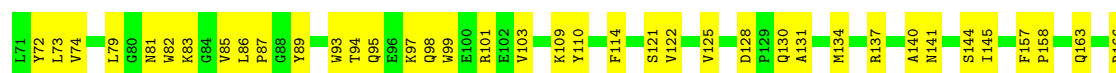
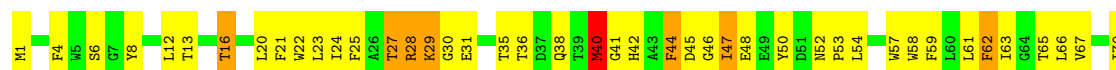
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II



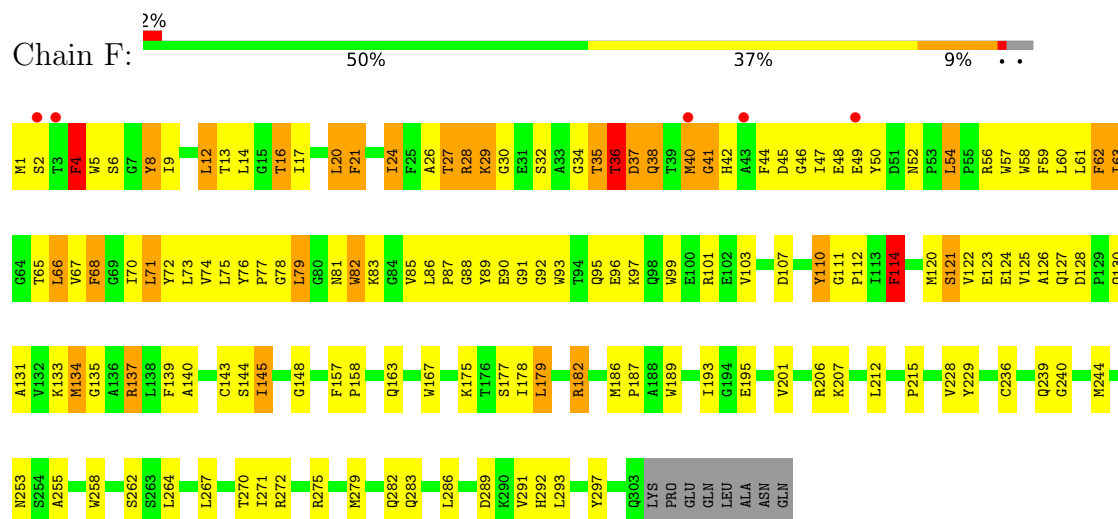
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II



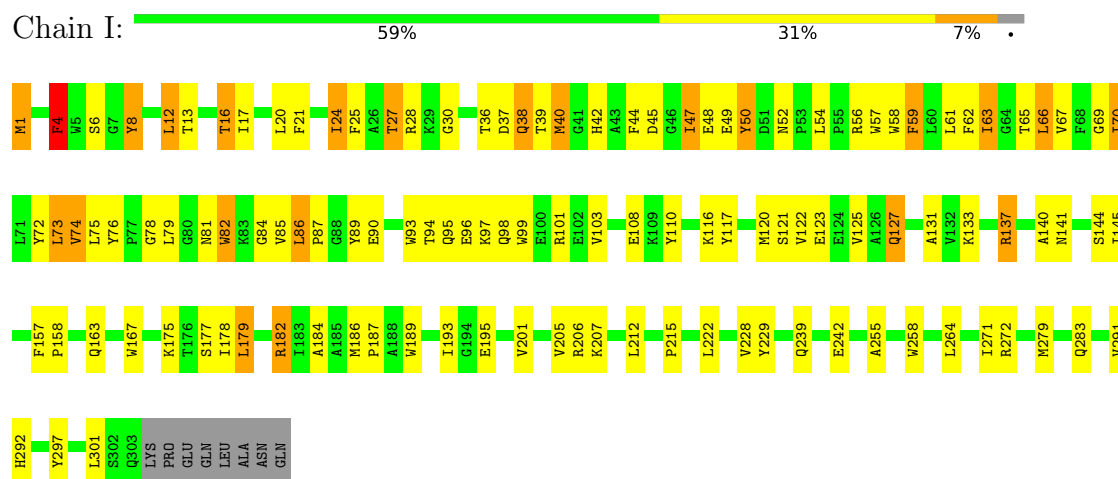
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1



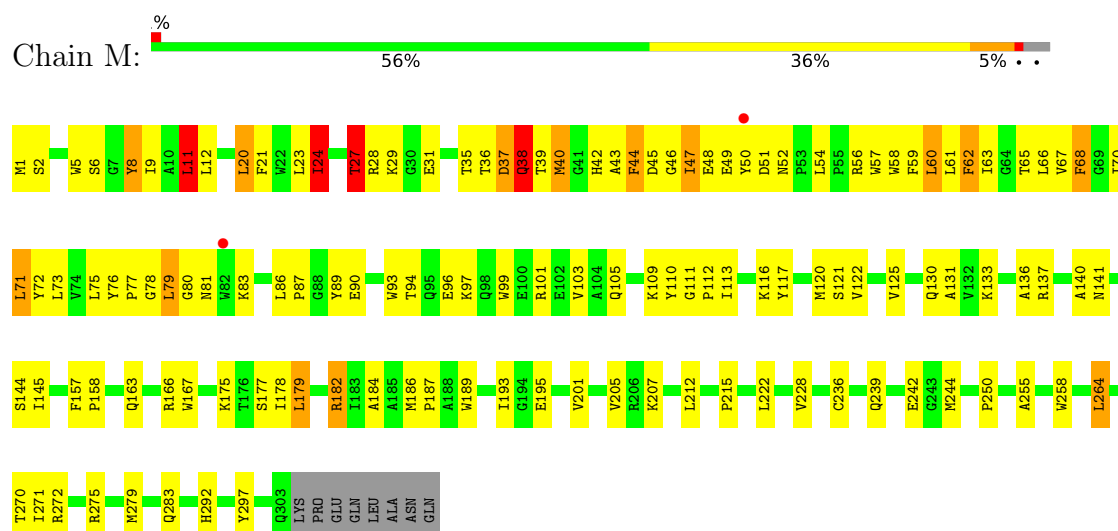
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1



• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1



• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1



- Molecule 4: Putative uncharacterized protein

Chain N:  56% 22% • 19%



- Molecule 4: Putative uncharacterized protein

Chain O:  53% 25% • 19%



- Molecule 4: Putative uncharacterized protein

Chain P:  44% 33% • 19%



- Molecule 4: Putative uncharacterized protein

Chain Q:  50% 22% 6% • 19%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 136.47Å 279.93Å 175.19Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 14.98 – 3.20 14.98 – 3.20 | Depositor EDS |
| % Data completeness (in resolution range) | 98.5 (14.98-3.20) 97.4 (14.98-3.20) | Depositor EDS |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | 0.11 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.69 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX 1.9_1692 | Depositor |
| R, R_{free} | 0.187 , 0.223 0.189 , 0.223 | Depositor DCC |
| R_{free} test set | 5480 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 86.4 | Xtriage |
| Anisotropy | 0.200 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 78.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 31974 | wwPDB-VP |
| Average B, all atoms (Å ²) | 117.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: HEC, FC6, CU, PO4, HEM, PEO, CA

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.39 | 0/3811 | 0.64 | 5/5210 (0.1%) |
| 1 | D | 0.36 | 0/3791 | 0.66 | 9/5182 (0.2%) |
| 1 | G | 0.40 | 1/3804 (0.0%) | 0.60 | 4/5200 (0.1%) |
| 1 | K | 0.37 | 0/3804 | 0.60 | 4/5200 (0.1%) |
| 2 | B | 0.38 | 0/1584 | 0.60 | 1/2146 (0.0%) |
| 2 | E | 0.30 | 0/1584 | 0.53 | 0/2146 |
| 2 | H | 0.34 | 0/1584 | 0.57 | 0/2146 |
| 2 | L | 0.31 | 0/1584 | 0.52 | 0/2146 |
| 3 | C | 0.50 | 0/2374 | 0.89 | 9/3225 (0.3%) |
| 3 | F | 0.56 | 2/2374 (0.1%) | 1.02 | 10/3225 (0.3%) |
| 3 | I | 0.54 | 1/2374 (0.0%) | 0.91 | 12/3225 (0.4%) |
| 3 | M | 0.54 | 0/2374 | 0.89 | 5/3225 (0.2%) |
| 4 | N | 0.50 | 0/227 | 0.85 | 2/309 (0.6%) |
| 4 | O | 0.47 | 0/227 | 0.82 | 2/309 (0.6%) |
| 4 | P | 0.50 | 0/227 | 0.89 | 2/309 (0.6%) |
| 4 | Q | 0.65 | 0/227 | 0.96 | 2/309 (0.6%) |
| All | All | 0.43 | 4/31950 (0.0%) | 0.73 | 67/43512 (0.2%) |

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 | A | 0 | 2 |
| 1 | G | 0 | 1 |
| 3 | C | 0 | 1 |
| 3 | F | 0 | 2 |
| 3 | I | 0 | 2 |
| All | All | 0 | 8 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | F | 110 | TYR | CD2-CE2 | -8.28 | 1.26 | 1.39 |
| 3 | I | 82 | TRP | CB-CG | -7.12 | 1.37 | 1.50 |
| 3 | F | 110 | TYR | CE2-CZ | -5.39 | 1.31 | 1.38 |
| 1 | G | 237 | TYR | CD2-CE2 | -5.10 | 1.31 | 1.39 |

All (67) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | C | 44 | PHE | CB-CG-CD1 | -10.56 | 113.41 | 120.80 |
| 3 | I | 44 | PHE | CB-CG-CD1 | -10.03 | 113.78 | 120.80 |
| 3 | F | 66 | LEU | CB-CG-CD1 | -9.58 | 94.72 | 111.00 |
| 3 | M | 79 | LEU | CB-CG-CD1 | -9.16 | 95.42 | 111.00 |
| 1 | D | 462 | ALA | N-CA-C | 8.96 | 135.18 | 111.00 |
| 1 | A | 468 | ASP | N-CA-C | -8.90 | 86.96 | 111.00 |
| 3 | F | 110 | TYR | CB-CG-CD2 | -8.84 | 115.69 | 121.00 |
| 1 | A | 467 | TYR | N-CA-C | -8.59 | 87.81 | 111.00 |
| 3 | C | 41 | GLY | N-CA-C | 8.35 | 133.97 | 113.10 |
| 3 | C | 28 | ARG | CB-CA-C | -8.08 | 94.24 | 110.40 |
| 4 | P | 27 | PHE | CB-CG-CD1 | -8.05 | 115.17 | 120.80 |
| 3 | I | 44 | PHE | CB-CG-CD2 | 8.03 | 126.42 | 120.80 |
| 3 | F | 110 | TYR | CB-CG-CD1 | 7.90 | 125.74 | 121.00 |
| 1 | G | 237 | TYR | CB-CG-CD2 | -7.89 | 116.26 | 121.00 |
| 3 | M | 24 | ILE | CG1-CB-CG2 | -7.88 | 94.06 | 111.40 |
| 4 | N | 27 | PHE | CB-CG-CD1 | -7.82 | 115.33 | 120.80 |
| 4 | Q | 27 | PHE | CB-CG-CD1 | -7.81 | 115.33 | 120.80 |
| 3 | F | 79 | LEU | CB-CG-CD1 | -7.73 | 97.86 | 111.00 |
| 4 | O | 27 | PHE | CB-CG-CD1 | -7.53 | 115.53 | 120.80 |
| 4 | P | 27 | PHE | CB-CG-CD2 | 7.50 | 126.05 | 120.80 |
| 1 | A | 467 | TYR | C-N-CA | 7.40 | 140.19 | 121.70 |
| 1 | A | 467 | TYR | CA-C-N | -7.18 | 101.39 | 117.20 |
| 4 | N | 27 | PHE | CB-CG-CD2 | 6.80 | 125.56 | 120.80 |
| 1 | G | 237 | TYR | CB-CG-CD1 | 6.79 | 125.07 | 121.00 |
| 3 | C | 42 | HIS | N-CA-CB | 6.77 | 122.78 | 110.60 |
| 1 | D | 457 | ARG | NE-CZ-NH1 | -6.70 | 116.95 | 120.30 |
| 3 | I | 28 | ARG | CB-CA-C | -6.61 | 97.18 | 110.40 |
| 1 | D | 457 | ARG | CG-CD-NE | 6.58 | 125.61 | 111.80 |
| 4 | O | 27 | PHE | CB-CG-CD2 | 6.57 | 125.40 | 120.80 |
| 1 | D | 456 | TRP | CB-CG-CD1 | -6.55 | 118.48 | 127.00 |
| 1 | D | 457 | ARG | NE-CZ-NH2 | 6.44 | 123.52 | 120.30 |
| 1 | D | 462 | ALA | N-CA-CB | -6.40 | 101.14 | 110.10 |
| 3 | I | 4 | PHE | CB-CG-CD2 | -6.33 | 116.37 | 120.80 |
| 3 | I | 1 | MET | CB-CA-C | -6.32 | 97.75 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3 | I | 110 | TYR | CB-CG-CD1 | -6.32 | 117.21 | 121.00 |
| 1 | K | 292 | MET | CA-CB-CG | 6.29 | 124.00 | 113.30 |
| 3 | C | 42 | HIS | N-CA-C | -6.21 | 94.22 | 111.00 |
| 2 | B | 6 | LYS | CD-CE-NZ | -5.91 | 98.11 | 111.70 |
| 3 | F | 36 | THR | OG1-CB-CG2 | 5.83 | 123.41 | 110.00 |
| 3 | C | 40 | MET | C-N-CA | -5.83 | 110.06 | 122.30 |
| 1 | K | 242 | VAL | CB-CA-C | -5.76 | 100.45 | 111.40 |
| 1 | G | 457 | ARG | CD-NE-CZ | 5.76 | 131.66 | 123.60 |
| 3 | F | 41 | GLY | C-N-CA | -5.75 | 107.33 | 121.70 |
| 3 | F | 4 | PHE | CB-CG-CD2 | -5.71 | 116.80 | 120.80 |
| 1 | D | 457 | ARG | CD-NE-CZ | -5.70 | 115.62 | 123.60 |
| 1 | D | 468 | ASP | N-CA-C | -5.62 | 95.84 | 111.00 |
| 3 | C | 29 | LYS | N-CA-C | 5.59 | 126.08 | 111.00 |
| 3 | C | 44 | PHE | N-CA-C | -5.58 | 95.93 | 111.00 |
| 3 | M | 11 | LEU | CA-CB-CG | 5.57 | 128.10 | 115.30 |
| 3 | C | 44 | PHE | CB-CG-CD2 | 5.46 | 124.62 | 120.80 |
| 3 | I | 59 | PHE | CB-CG-CD1 | -5.45 | 116.99 | 120.80 |
| 3 | F | 114 | PHE | CB-CG-CD2 | -5.43 | 117.00 | 120.80 |
| 1 | K | 467 | TYR | N-CA-C | 5.40 | 125.58 | 111.00 |
| 3 | M | 47 | ILE | CG1-CB-CG2 | -5.38 | 99.56 | 111.40 |
| 3 | I | 50 | TYR | CA-CB-CG | 5.38 | 123.62 | 113.40 |
| 4 | Q | 27 | PHE | CB-CG-CD2 | 5.37 | 124.56 | 120.80 |
| 1 | K | 463 | LYS | C-N-CD | -5.32 | 108.89 | 120.60 |
| 3 | I | 70 | ILE | CG1-CB-CG2 | -5.31 | 99.72 | 111.40 |
| 3 | F | 66 | LEU | CB-CG-CD2 | 5.30 | 120.00 | 111.00 |
| 3 | I | 4 | PHE | CB-CG-CD1 | 5.29 | 124.50 | 120.80 |
| 1 | D | 237 | TYR | CB-CG-CD2 | 5.20 | 124.12 | 121.00 |
| 3 | F | 56 | ARG | CB-CG-CD | 5.18 | 125.08 | 111.60 |
| 1 | A | 237 | TYR | CB-CG-CD2 | -5.17 | 117.90 | 121.00 |
| 3 | I | 82 | TRP | CB-CG-CD2 | -5.14 | 119.92 | 126.60 |
| 1 | G | 463 | LYS | O-C-N | -5.08 | 111.44 | 121.10 |
| 3 | M | 27 | THR | CA-CB-CG2 | -5.08 | 105.28 | 112.40 |
| 3 | I | 110 | TYR | CB-CG-CD2 | 5.08 | 124.05 | 121.00 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 465 | ALA | Mainchain |
| 1 | A | 467 | TYR | Peptide |
| 3 | C | 44 | PHE | Sidechain |
| 3 | F | 114 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | F | 37 | ASP | Peptide |
| 1 | G | 463 | LYS | Mainchain |
| 3 | I | 4 | PHE | Sidechain |
| 3 | I | 74 | VAL | Mainchain |

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3683 | 0 | 3663 | 134 | 0 |
| 1 | D | 3663 | 0 | 3644 | 161 | 0 |
| 1 | G | 3676 | 0 | 3656 | 150 | 0 |
| 1 | K | 3676 | 0 | 3656 | 158 | 0 |
| 2 | B | 1548 | 0 | 1526 | 46 | 0 |
| 2 | E | 1548 | 0 | 1526 | 48 | 0 |
| 2 | H | 1548 | 0 | 1526 | 42 | 0 |
| 2 | L | 1548 | 0 | 1526 | 39 | 0 |
| 3 | C | 2312 | 0 | 2237 | 103 | 0 |
| 3 | F | 2312 | 0 | 2237 | 194 | 0 |
| 3 | I | 2312 | 0 | 2237 | 124 | 0 |
| 3 | M | 2312 | 0 | 2237 | 147 | 0 |
| 4 | N | 221 | 0 | 226 | 9 | 0 |
| 4 | O | 221 | 0 | 226 | 11 | 0 |
| 4 | P | 221 | 0 | 226 | 12 | 0 |
| 4 | Q | 221 | 0 | 226 | 12 | 0 |
| 5 | A | 86 | 0 | 60 | 12 | 0 |
| 5 | D | 86 | 0 | 60 | 13 | 0 |
| 5 | G | 86 | 0 | 60 | 13 | 0 |
| 5 | K | 86 | 0 | 60 | 13 | 0 |
| 6 | A | 1 | 0 | 0 | 0 | 0 |
| 6 | D | 1 | 0 | 0 | 0 | 0 |
| 6 | G | 1 | 0 | 0 | 0 | 0 |
| 6 | K | 1 | 0 | 0 | 0 | 0 |
| 7 | A | 2 | 0 | 0 | 0 | 0 |
| 7 | D | 2 | 0 | 0 | 0 | 0 |
| 7 | G | 2 | 0 | 0 | 0 | 0 |
| 7 | K | 2 | 0 | 0 | 0 | 0 |
| 8 | A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8 | D | 2 | 0 | 0 | 0 | 0 |
| 8 | G | 2 | 0 | 0 | 0 | 0 |
| 8 | K | 2 | 0 | 0 | 0 | 0 |
| 9 | A | 5 | 0 | 0 | 1 | 0 |
| 9 | D | 5 | 0 | 0 | 1 | 0 |
| 9 | G | 5 | 0 | 0 | 1 | 0 |
| 9 | K | 5 | 0 | 0 | 4 | 0 |
| 10 | B | 43 | 0 | 30 | 5 | 0 |
| 10 | C | 86 | 0 | 60 | 11 | 0 |
| 10 | E | 43 | 0 | 30 | 6 | 0 |
| 10 | F | 86 | 0 | 60 | 10 | 0 |
| 10 | H | 43 | 0 | 30 | 6 | 0 |
| 10 | I | 86 | 0 | 60 | 11 | 0 |
| 10 | L | 43 | 0 | 30 | 4 | 0 |
| 10 | M | 86 | 0 | 60 | 11 | 0 |
| 11 | C | 13 | 0 | 0 | 2 | 0 |
| 11 | F | 13 | 0 | 0 | 2 | 0 |
| 11 | I | 13 | 0 | 0 | 1 | 0 |
| 11 | M | 13 | 0 | 0 | 2 | 0 |
| All | All | 31974 | 0 | 31175 | 1240 | 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 20.

All (1240) 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:D:207:HIS:NE2 | 1:D:251:TYR:CE1 | 1.70 | 1.59 |
| 1:A:207:HIS:NE2 | 1:A:251:TYR:CE1 | 1.70 | 1.56 |
| 1:G:207:HIS:NE2 | 1:G:251:TYR:CE1 | 1.70 | 1.56 |
| 1:K:207:HIS:NE2 | 1:K:251:TYR:CE1 | 1.70 | 1.53 |
| 1:K:207:HIS:NE2 | 1:K:251:TYR:HE1 | 1.02 | 1.33 |
| 1:D:207:HIS:NE2 | 1:D:251:TYR:HE1 | 1.05 | 1.26 |
| 1:G:207:HIS:CE1 | 1:G:251:TYR:HE1 | 1.55 | 1.25 |
| 1:G:207:HIS:NE2 | 1:G:251:TYR:HE1 | 1.05 | 1.21 |
| 1:K:207:HIS:CE1 | 1:K:251:TYR:HE1 | 1.62 | 1.16 |
| 1:D:207:HIS:CE1 | 1:D:251:TYR:HE1 | 1.63 | 1.15 |
| 1:A:207:HIS:NE2 | 1:A:251:TYR:HE1 | 1.14 | 1.13 |
| 1:G:207:HIS:NE2 | 1:G:251:TYR:CD1 | 2.18 | 1.12 |
| 3:M:43:ALA:HA | 3:M:48:GLU:HB3 | 1.34 | 1.09 |
| 1:A:207:HIS:CE1 | 1:A:251:TYR:HE1 | 1.70 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:207:HIS:NE2 | 1:A:251:TYR:CD1 | 2.21 | 1.07 |
| 1:D:207:HIS:NE2 | 1:D:251:TYR:CD1 | 2.23 | 1.06 |
| 1:D:234:VAL:HB | 3:F:49:GLU:HG2 | 1.37 | 1.05 |
| 1:K:207:HIS:NE2 | 1:K:251:TYR:CD1 | 2.23 | 1.04 |
| 1:A:207:HIS:CE1 | 1:A:251:TYR:CE1 | 2.45 | 1.03 |
| 1:D:462:ALA:HB1 | 1:D:464:PRO:HD2 | 1.37 | 1.03 |
| 1:D:418:THR:OG1 | 3:F:137:ARG:NH1 | 1.91 | 1.02 |
| 3:M:186:MET:HG2 | 10:M:402:HEC:ND | 1.75 | 1.01 |
| 3:F:37:ASP:HB3 | 3:F:38:GLN:HA | 1.43 | 1.00 |
| 1:G:237:TYR:OH | 2:H:8:GLU:OE2 | 1.81 | 0.98 |
| 3:F:6:SER:OG | 3:F:81:ASN:N | 1.97 | 0.97 |
| 1:G:207:HIS:CE1 | 1:G:251:TYR:CE1 | 2.40 | 0.97 |
| 3:C:186:MET:HG2 | 10:C:401:HEC:ND | 1.78 | 0.97 |
| 3:I:186:MET:HG2 | 10:I:402:HEC:ND | 1.79 | 0.96 |
| 3:F:6:SER:HB2 | 3:F:81:ASN:HD22 | 1.28 | 0.95 |
| 1:D:207:HIS:CE1 | 1:D:251:TYR:CE1 | 2.45 | 0.94 |
| 3:I:137:ARG:O | 3:I:141:ASN:ND2 | 2.01 | 0.94 |
| 1:K:207:HIS:CE1 | 1:K:251:TYR:CE1 | 2.46 | 0.93 |
| 1:G:90:PHE:HD1 | 1:G:147:GLY:HA3 | 1.34 | 0.93 |
| 1:D:90:PHE:CD1 | 1:D:147:GLY:HA3 | 2.03 | 0.92 |
| 3:F:186:MET:HG2 | 10:F:401:HEC:ND | 1.85 | 0.92 |
| 3:M:68:PHE:HA | 3:M:71:LEU:HD12 | 1.49 | 0.91 |
| 3:M:137:ARG:O | 3:M:141:ASN:ND2 | 2.05 | 0.90 |
| 1:D:24:TRP:HE1 | 1:D:103:GLN:HE22 | 1.19 | 0.90 |
| 3:M:36:THR:HG22 | 3:M:38:GLN:NE2 | 1.86 | 0.90 |
| 1:K:242:VAL:HG22 | 3:M:27:THR:HG21 | 1.54 | 0.89 |
| 3:I:82:TRP:CZ2 | 3:I:85:VAL:HG23 | 2.05 | 0.89 |
| 3:C:189:TRP:HZ2 | 10:C:401:HEC:HMC2 | 1.35 | 0.89 |
| 1:G:7:THR:O | 1:G:469:ALA:HB1 | 1.71 | 0.89 |
| 3:C:137:ARG:O | 3:C:141:ASN:ND2 | 2.06 | 0.88 |
| 3:F:86:LEU:HG | 3:F:87:PRO:HD2 | 1.57 | 0.87 |
| 1:D:233:PRO:HG2 | 3:F:50:TYR:CE2 | 2.09 | 0.87 |
| 1:D:446:ALA:HA | 1:D:449:LEU:HD12 | 1.55 | 0.87 |
| 1:D:156:HIS:CG | 3:F:42:HIS:HD2 | 1.92 | 0.86 |
| 3:F:50:TYR:HB3 | 3:F:52:ASN:ND2 | 1.90 | 0.86 |
| 1:A:90:PHE:HD1 | 1:A:147:GLY:HA3 | 1.41 | 0.86 |
| 1:G:24:TRP:HE1 | 1:G:103:GLN:HE22 | 1.23 | 0.85 |
| 1:G:233:PRO:HG2 | 3:I:50:TYR:CE2 | 2.11 | 0.85 |
| 1:A:24:TRP:HE1 | 1:A:103:GLN:HE22 | 1.24 | 0.85 |
| 3:F:92:GLY:O | 3:F:97:LYS:NZ | 2.10 | 0.85 |
| 2:L:7:LEU:HA | 2:L:10:ASN:HD22 | 1.42 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:6:SER:OG | 3:M:81:ASN:N | 2.08 | 0.84 |
| 3:C:193:ILE:HD11 | 3:C:228:VAL:HG11 | 1.59 | 0.84 |
| 3:F:12:LEU:O | 3:F:16:THR:OG1 | 1.95 | 0.84 |
| 3:I:193:ILE:HD11 | 3:I:228:VAL:HG11 | 1.58 | 0.83 |
| 1:K:24:TRP:HE1 | 1:K:103:GLN:HE22 | 1.22 | 0.83 |
| 9:K:506:PO4:O1 | 3:M:72:TYR:OH | 1.94 | 0.83 |
| 1:G:15:ARG:NH2 | 1:G:466:GLU:OE2 | 2.12 | 0.83 |
| 1:A:233:PRO:HG2 | 3:C:50:TYR:CE2 | 2.13 | 0.83 |
| 1:D:245:TRP:HZ2 | 2:E:7:LEU:HD11 | 1.44 | 0.83 |
| 3:I:6:SER:OG | 3:I:81:ASN:N | 2.12 | 0.82 |
| 1:A:455:THR:O | 1:A:459:VAL:HG23 | 1.80 | 0.82 |
| 3:I:73:LEU:HB3 | 3:I:79:LEU:HD11 | 1.63 | 0.81 |
| 1:K:234:VAL:HB | 3:M:49:GLU:HB3 | 1.62 | 0.81 |
| 3:F:193:ILE:HD11 | 3:F:228:VAL:HG11 | 1.61 | 0.81 |
| 1:A:90:PHE:CD1 | 1:A:147:GLY:HA3 | 2.15 | 0.80 |
| 3:C:189:TRP:CZ2 | 10:C:401:HEC:HMC2 | 2.17 | 0.80 |
| 3:I:207:LYS:HD3 | 3:I:222:LEU:HD21 | 1.63 | 0.80 |
| 2:H:68:CYS:HB3 | 2:H:105:THR:HB | 1.61 | 0.80 |
| 1:K:232:ARG:NH1 | 1:K:295:SER:O | 2.14 | 0.79 |
| 3:M:193:ILE:HD11 | 3:M:228:VAL:HG11 | 1.63 | 0.79 |
| 1:D:156:HIS:CD2 | 3:F:42:HIS:HD2 | 2.01 | 0.79 |
| 2:B:68:CYS:HB3 | 2:B:105:THR:HB | 1.63 | 0.78 |
| 1:G:8:ALA:HA | 1:G:469:ALA:HA | 1.65 | 0.78 |
| 9:G:506:PO4:O4 | 3:I:72:TYR:OH | 2.00 | 0.78 |
| 2:H:57:ARG:NH2 | 2:H:97:PRO:O | 2.17 | 0.78 |
| 3:I:82:TRP:HZ2 | 3:I:85:VAL:HG23 | 1.45 | 0.78 |
| 1:A:335:LEU:HB2 | 4:N:6:VAL:HG12 | 1.66 | 0.78 |
| 3:M:24:ILE:HD11 | 3:M:59:PHE:CZ | 2.18 | 0.78 |
| 1:D:267:TRP:HA | 3:F:78:GLY:HA2 | 1.65 | 0.78 |
| 1:D:90:PHE:HD1 | 1:D:147:GLY:HA3 | 1.47 | 0.78 |
| 3:I:86:LEU:HD12 | 3:I:87:PRO:HD2 | 1.66 | 0.78 |
| 3:I:90:GLU:O | 3:I:97:LYS:NZ | 2.16 | 0.78 |
| 3:F:90:GLU:O | 3:F:97:LYS:NZ | 2.16 | 0.77 |
| 1:D:207:HIS:CD2 | 1:D:251:TYR:CE1 | 2.71 | 0.77 |
| 3:I:1:MET:HB3 | 3:I:81:ASN:HD21 | 1.49 | 0.77 |
| 1:A:207:HIS:CD2 | 1:A:251:TYR:CE1 | 2.70 | 0.77 |
| 5:D:502:HEM:HHC | 5:D:502:HEM:HBB2 | 1.67 | 0.77 |
| 1:D:455:THR:O | 1:D:459:VAL:HG23 | 1.86 | 0.76 |
| 5:K:502:HEM:HBC2 | 5:K:502:HEM:HHD | 1.64 | 0.76 |
| 1:G:10:SER:H | 1:G:82:GLN:HE22 | 1.33 | 0.76 |
| 3:M:167:TRP:CE2 | 3:M:182:ARG:HG2 | 2.20 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:68:CYS:HB3 | 2:E:105:THR:HB | 1.66 | 0.76 |
| 3:I:6:SER:HB2 | 3:I:81:ASN:HD22 | 1.51 | 0.76 |
| 5:D:502:HEM:HBC2 | 5:D:502:HEM:HHD | 1.68 | 0.76 |
| 3:C:6:SER:OG | 3:C:81:ASN:N | 2.19 | 0.76 |
| 3:I:167:TRP:CE2 | 3:I:182:ARG:HG2 | 2.21 | 0.76 |
| 2:L:57:ARG:NH2 | 2:L:97:PRO:O | 2.19 | 0.75 |
| 3:F:40:MET:HB2 | 3:F:49:GLU:O | 1.85 | 0.75 |
| 3:F:60:LEU:HA | 3:F:63:ILE:HD11 | 1.68 | 0.75 |
| 1:K:335:LEU:HB2 | 4:Q:6:VAL:HG12 | 1.69 | 0.75 |
| 3:M:86:LEU:HD12 | 3:M:87:PRO:HD2 | 1.67 | 0.75 |
| 3:M:242:GLU:OE1 | 3:M:242:GLU:N | 2.18 | 0.75 |
| 3:C:186:MET:HG2 | 10:C:401:HEC:C4D | 2.17 | 0.74 |
| 3:M:2:SER:HG | 3:M:5:TRP:HD1 | 1.34 | 0.74 |
| 1:D:376:HIS:N | 1:D:458:THR:HG22 | 2.03 | 0.74 |
| 5:G:502:HEM:HBB2 | 5:G:502:HEM:HHC | 1.68 | 0.74 |
| 3:M:43:ALA:HA | 3:M:48:GLU:CB | 2.16 | 0.74 |
| 1:D:335:LEU:HB2 | 4:O:6:VAL:HG12 | 1.70 | 0.74 |
| 3:I:195:GLU:OE2 | 3:I:272:ARG:NH1 | 2.20 | 0.74 |
| 3:F:73:LEU:HB3 | 3:F:79:LEU:HD11 | 1.70 | 0.74 |
| 1:G:335:LEU:HB2 | 4:P:6:VAL:HG12 | 1.70 | 0.74 |
| 2:L:177:ASP:N | 2:L:177:ASP:OD1 | 2.21 | 0.74 |
| 3:F:189:TRP:HZ2 | 10:F:401:HEC:HMC2 | 1.51 | 0.73 |
| 3:F:189:TRP:CZ2 | 10:F:401:HEC:HMC2 | 2.24 | 0.73 |
| 2:B:57:ARG:NH2 | 2:B:97:PRO:O | 2.21 | 0.73 |
| 1:D:416:ASP:OD1 | 3:F:137:ARG:NH2 | 2.19 | 0.73 |
| 1:K:242:VAL:CG2 | 3:M:27:THR:HG21 | 2.18 | 0.73 |
| 3:I:82:TRP:CZ3 | 3:I:84:GLY:HA2 | 2.23 | 0.73 |
| 4:O:23:GLY:O | 4:O:27:PHE:HB2 | 1.89 | 0.73 |
| 5:A:502:HEM:HHC | 5:A:502:HEM:HBB2 | 1.69 | 0.73 |
| 3:F:66:LEU:H | 3:F:66:LEU:HD12 | 1.52 | 0.73 |
| 3:M:44:PHE:N | 3:M:47:ILE:O | 2.21 | 0.73 |
| 1:A:178:ASN:HD22 | 1:A:201:VAL:HG12 | 1.54 | 0.72 |
| 1:G:455:THR:O | 1:G:459:VAL:HG23 | 1.89 | 0.72 |
| 3:M:73:LEU:HD21 | 3:M:79:LEU:HD21 | 1.70 | 0.72 |
| 3:M:99:TRP:O | 3:M:103:VAL:HG23 | 1.89 | 0.72 |
| 1:G:115:LEU:HB3 | 1:G:117:PHE:CE2 | 2.24 | 0.72 |
| 3:F:167:TRP:CE2 | 3:F:182:ARG:HG2 | 2.25 | 0.72 |
| 3:I:36:THR:HG22 | 3:I:38:GLN:HB2 | 1.72 | 0.72 |
| 1:A:85:CYS:HB2 | 1:A:152:ARG:HB2 | 1.70 | 0.72 |
| 3:C:23:LEU:O | 3:C:27:THR:OG1 | 2.06 | 0.72 |
| 9:D:505:PO4:O3 | 3:F:72:TYR:OH | 2.06 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:1:MET:HB3 | 3:I:81:ASN:ND2 | 2.05 | 0.72 |
| 1:G:207:HIS:CD2 | 1:G:251:TYR:CE1 | 2.75 | 0.71 |
| 1:A:227:PRO:HB2 | 3:C:47:ILE:HD12 | 1.73 | 0.71 |
| 3:F:21:PHE:CE2 | 3:F:66:LEU:HD22 | 2.25 | 0.71 |
| 3:M:186:MET:HG2 | 10:M:402:HEC:C4D | 2.20 | 0.71 |
| 3:C:29:LYS:HG3 | 3:C:30:GLY:N | 2.04 | 0.71 |
| 1:K:85:CYS:HB2 | 1:K:152:ARG:HB2 | 1.72 | 0.71 |
| 3:C:66:LEU:O | 3:C:70:ILE:HD12 | 1.89 | 0.71 |
| 3:F:6:SER:HB2 | 3:F:81:ASN:ND2 | 2.04 | 0.71 |
| 1:D:234:VAL:HB | 3:F:49:GLU:CG | 2.18 | 0.71 |
| 3:I:189:TRP:HZ2 | 10:I:402:HEC:HMC2 | 1.54 | 0.71 |
| 3:C:86:LEU:HD12 | 3:C:87:PRO:HD2 | 1.72 | 0.71 |
| 1:K:457:ARG:HH11 | 1:K:460:GLN:HE21 | 1.38 | 0.71 |
| 5:K:502:HEM:HHC | 5:K:502:HEM:HBB2 | 1.71 | 0.71 |
| 1:D:10:SER:H | 1:D:82:GLN:HE22 | 1.39 | 0.70 |
| 2:E:57:ARG:NH2 | 2:E:97:PRO:O | 2.24 | 0.70 |
| 5:G:502:HEM:HBC2 | 5:G:502:HEM:HHD | 1.71 | 0.70 |
| 5:A:502:HEM:HBC2 | 5:A:502:HEM:HHD | 1.71 | 0.70 |
| 3:C:195:GLU:OE2 | 3:C:272:ARG:NH1 | 2.23 | 0.70 |
| 1:D:85:CYS:HB2 | 1:D:152:ARG:HB2 | 1.72 | 0.70 |
| 1:K:207:HIS:CD2 | 1:K:251:TYR:CE1 | 2.73 | 0.70 |
| 9:A:506:PO4:O3 | 3:C:72:TYR:OH | 2.06 | 0.70 |
| 3:F:50:TYR:HB3 | 3:F:52:ASN:HD21 | 1.57 | 0.70 |
| 1:G:238:ARG:NH2 | 3:I:30:GLY:O | 2.24 | 0.70 |
| 3:I:82:TRP:CH2 | 3:I:84:GLY:HA2 | 2.26 | 0.70 |
| 2:B:7:LEU:HA | 2:B:10:ASN:HD22 | 1.54 | 0.70 |
| 1:K:149:LEU:HD21 | 1:K:161:ASN:HD22 | 1.57 | 0.70 |
| 1:G:166:ALA:O | 1:G:170:THR:HG22 | 1.92 | 0.70 |
| 4:P:14:VAL:O | 4:P:18:VAL:HG23 | 1.90 | 0.70 |
| 1:A:76:THR:HG21 | 1:A:221:ILE:HG12 | 1.72 | 0.70 |
| 3:F:60:LEU:HD23 | 3:F:63:ILE:HD11 | 1.73 | 0.70 |
| 1:G:76:THR:HG21 | 1:G:221:ILE:HG12 | 1.72 | 0.70 |
| 1:K:235:TYR:HE2 | 1:K:292:MET:HB3 | 1.56 | 0.70 |
| 3:C:82:TRP:CH2 | 3:C:85:VAL:HG23 | 2.27 | 0.69 |
| 1:D:416:ASP:CG | 3:F:137:ARG:HH22 | 1.95 | 0.69 |
| 1:G:85:CYS:HB2 | 1:G:152:ARG:HB2 | 1.74 | 0.69 |
| 2:H:7:LEU:HA | 2:H:10:ASN:HD22 | 1.57 | 0.69 |
| 1:K:267:TRP:HA | 3:M:78:GLY:HA2 | 1.74 | 0.69 |
| 2:L:68:CYS:HB3 | 2:L:105:THR:HB | 1.73 | 0.69 |
| 1:D:156:HIS:CG | 3:F:42:HIS:CD2 | 2.78 | 0.69 |
| 1:K:10:SER:HB3 | 1:K:89:LEU:CD1 | 2.21 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:24:ILE:HD11 | 3:M:59:PHE:CE2 | 2.25 | 0.69 |
| 3:M:28:ARG:HE | 3:M:31:GLU:HG2 | 1.57 | 0.69 |
| 3:M:43:ALA:CA | 3:M:48:GLU:HB3 | 2.18 | 0.69 |
| 3:M:195:GLU:OE2 | 3:M:272:ARG:NH1 | 2.25 | 0.69 |
| 3:I:66:LEU:O | 3:I:70:ILE:HD12 | 1.92 | 0.69 |
| 3:C:167:TRP:CE2 | 3:C:182:ARG:HG2 | 2.27 | 0.69 |
| 1:K:267:TRP:HE1 | 2:L:36:GLN:HE22 | 1.41 | 0.69 |
| 1:K:467:TYR:O | 1:K:468:ASP:HB2 | 1.93 | 0.69 |
| 1:A:166:ALA:O | 1:A:170:THR:HG22 | 1.93 | 0.69 |
| 1:D:237:TYR:HD1 | 3:F:49:GLU:OE1 | 1.76 | 0.69 |
| 1:K:235:TYR:CE2 | 1:K:292:MET:HB3 | 2.28 | 0.69 |
| 3:I:76:TYR:C | 3:I:82:TRP:HZ3 | 1.96 | 0.68 |
| 3:F:62:PHE:CD1 | 3:F:66:LEU:HD11 | 2.28 | 0.68 |
| 3:M:79:LEU:H | 3:M:79:LEU:HD12 | 1.58 | 0.68 |
| 1:A:31:LEU:HD11 | 1:A:59:LEU:HD13 | 1.74 | 0.68 |
| 5:A:501:HEM:HBC2 | 5:A:501:HEM:HHD | 1.75 | 0.68 |
| 2:E:24:ILE:HG21 | 3:F:16:THR:HG21 | 1.74 | 0.68 |
| 3:I:189:TRP:CZ2 | 10:I:402:HEC:HMC2 | 2.29 | 0.68 |
| 3:I:242:GLU:OE1 | 3:I:242:GLU:N | 2.24 | 0.68 |
| 3:F:74:VAL:HA | 3:F:82:TRP:CZ2 | 2.28 | 0.68 |
| 3:F:186:MET:HG2 | 10:F:401:HEC:C4D | 2.24 | 0.68 |
| 1:K:76:THR:HG21 | 1:K:221:ILE:HG12 | 1.76 | 0.68 |
| 1:G:90:PHE:CD1 | 1:G:147:GLY:HA3 | 2.24 | 0.68 |
| 1:G:31:LEU:HD11 | 1:G:59:LEU:HD13 | 1.76 | 0.68 |
| 1:K:222:MET:HG3 | 1:K:314:LEU:HD21 | 1.76 | 0.68 |
| 1:G:376:HIS:N | 1:G:458:THR:HG22 | 2.09 | 0.67 |
| 1:K:463:LYS:CB | 1:K:464:PRO:HD3 | 2.24 | 0.67 |
| 1:G:237:TYR:CE2 | 1:G:241:ILE:HD11 | 2.29 | 0.67 |
| 3:F:121:SER:O | 3:F:125:VAL:HG23 | 1.94 | 0.67 |
| 3:F:40:MET:SD | 3:F:41:GLY:N | 2.68 | 0.67 |
| 1:D:76:THR:HG23 | 1:D:225:PHE:HE1 | 1.60 | 0.67 |
| 3:F:121:SER:O | 3:F:125:VAL:N | 2.28 | 0.67 |
| 3:C:62:PHE:O | 3:C:66:LEU:HD12 | 1.94 | 0.67 |
| 3:F:9:ILE:O | 3:F:13:THR:HG23 | 1.94 | 0.67 |
| 3:I:50:TYR:HB3 | 3:I:52:ASN:OD1 | 1.95 | 0.66 |
| 3:I:186:MET:HG2 | 10:I:402:HEC:C4D | 2.24 | 0.66 |
| 1:K:90:PHE:HD2 | 1:K:91:ALA:N | 1.94 | 0.66 |
| 1:D:166:ALA:O | 1:D:170:THR:HG22 | 1.96 | 0.66 |
| 2:L:157:MET:HE1 | 2:L:171:ASP:HB3 | 1.77 | 0.66 |
| 1:A:207:HIS:CD2 | 1:A:251:TYR:CD1 | 2.83 | 0.66 |
| 3:F:13:THR:O | 3:F:17:ILE:HG13 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:61:LEU:O | 3:M:65:THR:HG23 | 1.96 | 0.66 |
| 4:Q:24:PHE:HA | 4:Q:27:PHE:HB3 | 1.78 | 0.66 |
| 2:E:86:TYR:OH | 3:F:96:GLU:OE1 | 2.10 | 0.66 |
| 3:F:62:PHE:HD1 | 3:F:66:LEU:HD11 | 1.61 | 0.66 |
| 3:F:99:TRP:O | 3:F:103:VAL:HG23 | 1.96 | 0.65 |
| 1:G:463:LYS:HB2 | 1:G:464:PRO:HD3 | 1.76 | 0.65 |
| 3:M:6:SER:HA | 3:M:80:GLY:HA2 | 1.78 | 0.65 |
| 1:A:207:HIS:CD2 | 1:A:251:TYR:HE1 | 2.07 | 0.65 |
| 3:C:215:PRO:HB3 | 11:M:401:FC6:N24 | 2.12 | 0.65 |
| 1:G:149:LEU:HD21 | 1:G:161:ASN:HD22 | 1.62 | 0.65 |
| 1:D:149:LEU:HD21 | 1:D:161:ASN:HD22 | 1.61 | 0.65 |
| 1:D:207:HIS:CD2 | 1:D:251:TYR:CD1 | 2.85 | 0.65 |
| 1:D:416:ASP:OD1 | 3:F:137:ARG:NH1 | 2.30 | 0.65 |
| 3:F:36:THR:O | 3:F:38:GLN:NE2 | 2.30 | 0.65 |
| 1:G:238:ARG:HH12 | 3:I:30:GLY:C | 2.00 | 0.65 |
| 1:A:10:SER:H | 1:A:82:GLN:HE22 | 1.44 | 0.65 |
| 1:A:421:TYR:O | 2:B:82:ARG:NH2 | 2.30 | 0.65 |
| 1:K:421:TYR:O | 2:L:82:ARG:NH2 | 2.30 | 0.65 |
| 2:B:140:TYR:CZ | 10:B:301:HEC:HBB2 | 2.30 | 0.65 |
| 1:D:376:HIS:H | 1:D:458:THR:CG2 | 2.10 | 0.65 |
| 1:K:84:THR:HA | 3:M:45:ASP:HB2 | 1.78 | 0.65 |
| 1:K:237:TYR:CE2 | 1:K:241:ILE:HD11 | 2.32 | 0.65 |
| 1:K:463:LYS:HB2 | 1:K:464:PRO:HD3 | 1.79 | 0.65 |
| 3:M:189:TRP:HZ2 | 10:M:402:HEC:HMC2 | 1.62 | 0.65 |
| 2:E:8:GLU:OE2 | 3:F:42:HIS:NE2 | 2.31 | 0.64 |
| 2:H:7:LEU:HD13 | 2:H:13:LEU:HD22 | 1.77 | 0.64 |
| 2:H:177:ASP:OD1 | 2:H:177:ASP:N | 2.30 | 0.64 |
| 3:M:117:TYR:CE1 | 3:M:131:ALA:HB2 | 2.32 | 0.64 |
| 1:G:267:TRP:HE1 | 2:H:36:GLN:HE22 | 1.45 | 0.64 |
| 2:H:86:TYR:OH | 3:I:96:GLU:OE1 | 2.06 | 0.64 |
| 1:K:465:ALA:O | 1:K:467:TYR:N | 2.30 | 0.64 |
| 2:E:62:ARG:NH1 | 2:E:63:GLU:OE2 | 2.28 | 0.64 |
| 4:N:23:GLY:O | 4:N:27:PHE:HB2 | 1.97 | 0.64 |
| 2:E:128:PRO:HD2 | 2:E:129:ARG:HH21 | 1.61 | 0.64 |
| 4:O:4:ASP:H | 4:O:7:VAL:HG22 | 1.62 | 0.64 |
| 1:D:355:ALA:O | 1:D:359:ILE:HG12 | 1.97 | 0.64 |
| 3:M:62:PHE:CD1 | 3:M:66:LEU:HD11 | 2.33 | 0.64 |
| 3:M:177:SER:OG | 3:M:182:ARG:NH1 | 2.30 | 0.64 |
| 1:A:170:THR:HG21 | 1:A:212:PHE:CD2 | 2.33 | 0.63 |
| 3:C:1:MET:HB3 | 3:C:81:ASN:OD1 | 1.98 | 0.63 |
| 3:M:189:TRP:CZ2 | 10:M:402:HEC:HMC2 | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:274:VAL:HG21 | 3:I:73:LEU:CD2 | 2.27 | 0.63 |
| 1:K:10:SER:HB3 | 1:K:89:LEU:HD12 | 1.79 | 0.63 |
| 1:K:233:PRO:HG2 | 3:M:50:TYR:CZ | 2.34 | 0.63 |
| 3:C:25:PHE:HE1 | 3:C:59:PHE:HZ | 1.46 | 0.63 |
| 1:D:376:HIS:H | 1:D:458:THR:HG22 | 1.61 | 0.63 |
| 1:G:336:SER:O | 1:G:339:THR:OG1 | 2.12 | 0.63 |
| 1:G:376:HIS:H | 1:G:458:THR:HG22 | 1.63 | 0.63 |
| 4:Q:14:VAL:O | 4:Q:18:VAL:HG23 | 1.99 | 0.63 |
| 1:K:166:ALA:O | 1:K:170:THR:HG22 | 1.99 | 0.63 |
| 1:G:178:ASN:HD22 | 1:G:201:VAL:HG12 | 1.64 | 0.63 |
| 1:G:207:HIS:CD2 | 1:G:251:TYR:CD1 | 2.86 | 0.63 |
| 1:G:242:VAL:HG21 | 3:I:54:LEU:HD21 | 1.80 | 0.63 |
| 3:M:63:ILE:HA | 3:M:66:LEU:HD12 | 1.80 | 0.63 |
| 1:A:222:MET:HG3 | 1:A:314:LEU:HD21 | 1.80 | 0.63 |
| 1:A:340:ASP:H | 1:A:406:GLN:HE22 | 1.47 | 0.63 |
| 1:K:235:TYR:HE2 | 1:K:292:MET:CB | 2.12 | 0.63 |
| 3:C:109:LYS:HG2 | 3:C:110:TYR:CD2 | 2.33 | 0.62 |
| 1:D:421:TYR:O | 2:E:82:ARG:NH2 | 2.32 | 0.62 |
| 3:F:128:ASP:OD2 | 3:F:130:GLN:N | 2.31 | 0.62 |
| 1:K:90:PHE:CD1 | 1:K:147:GLY:HA3 | 2.34 | 0.62 |
| 1:K:207:HIS:CD2 | 1:K:251:TYR:CD1 | 2.87 | 0.62 |
| 1:K:343:ILE:HG12 | 5:K:502:HEM:HBA2 | 1.80 | 0.62 |
| 3:M:1:MET:HB3 | 3:M:81:ASN:OD1 | 1.99 | 0.62 |
| 1:D:76:THR:HG21 | 1:D:221:ILE:HG12 | 1.80 | 0.62 |
| 3:M:94:THR:OG1 | 3:M:97:LYS:HG3 | 1.99 | 0.62 |
| 2:E:177:ASP:OD1 | 2:E:177:ASP:N | 2.31 | 0.62 |
| 2:H:157:MET:HE1 | 2:H:171:ASP:HB3 | 1.80 | 0.62 |
| 3:M:133:LYS:HE3 | 3:M:137:ARG:HH21 | 1.64 | 0.62 |
| 1:A:149:LEU:HD21 | 1:A:161:ASN:HD22 | 1.65 | 0.62 |
| 2:B:157:MET:HE1 | 2:B:171:ASP:HB3 | 1.81 | 0.62 |
| 1:A:76:THR:HG23 | 1:A:225:PHE:HE1 | 1.64 | 0.62 |
| 3:F:29:LYS:CD | 3:F:30:GLY:H | 2.13 | 0.62 |
| 1:G:170:THR:HG21 | 1:G:212:PHE:CD2 | 2.35 | 0.62 |
| 1:K:235:TYR:CE2 | 1:K:292:MET:CB | 2.82 | 0.62 |
| 1:K:455:THR:O | 1:K:459:VAL:HG23 | 2.00 | 0.62 |
| 1:D:178:ASN:HD22 | 1:D:201:VAL:HG12 | 1.65 | 0.62 |
| 3:M:28:ARG:HA | 3:M:31:GLU:OE2 | 1.99 | 0.62 |
| 3:M:62:PHE:HE1 | 3:M:66:LEU:HD21 | 1.65 | 0.62 |
| 2:B:116:TYR:HE2 | 3:C:145:ILE:HG21 | 1.64 | 0.62 |
| 1:G:253:TRP:CH2 | 2:H:28:THR:HG21 | 2.34 | 0.62 |
| 1:K:31:LEU:HD11 | 1:K:59:LEU:HD13 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:267:TRP:HE1 | 2:B:36:GLN:HE22 | 1.48 | 0.61 |
| 4:O:14:VAL:O | 4:O:18:VAL:HG23 | 2.00 | 0.61 |
| 3:F:62:PHE:O | 3:F:66:LEU:HD12 | 2.01 | 0.61 |
| 5:G:501:HEM:HBC2 | 5:G:501:HEM:HHD | 1.82 | 0.61 |
| 1:A:281:ALA:HB3 | 1:A:282:PRO:HD3 | 1.81 | 0.61 |
| 2:E:140:TYR:CZ | 10:E:301:HEC:HBB2 | 2.34 | 0.61 |
| 3:F:29:LYS:HD2 | 3:F:30:GLY:H | 1.64 | 0.61 |
| 1:G:236:SER:HA | 3:I:52:ASN:HB2 | 1.82 | 0.61 |
| 3:C:109:LYS:HG2 | 3:C:110:TYR:CE2 | 2.34 | 0.61 |
| 1:A:63:ALA:O | 1:A:67:ALA:HB3 | 2.01 | 0.61 |
| 1:A:218:PHE:HA | 1:A:221:ILE:HG13 | 1.82 | 0.61 |
| 3:C:99:TRP:O | 3:C:103:VAL:HG23 | 2.00 | 0.61 |
| 1:D:343:ILE:HG12 | 5:D:502:HEM:HBA2 | 1.83 | 0.61 |
| 4:Q:24:PHE:O | 4:Q:28:ILE:HG13 | 2.01 | 0.61 |
| 2:B:177:ASP:N | 2:B:177:ASP:OD1 | 2.33 | 0.60 |
| 3:F:83:LYS:NZ | 3:F:91:GLY:O | 2.17 | 0.60 |
| 2:H:39:VAL:HG23 | 2:H:40:ASN:ND2 | 2.16 | 0.60 |
| 1:A:237:TYR:CE2 | 1:A:241:ILE:HD11 | 2.35 | 0.60 |
| 3:I:39:THR:HG22 | 3:I:40:MET:O | 2.01 | 0.60 |
| 2:H:140:TYR:CZ | 10:H:301:HEC:HBB2 | 2.35 | 0.60 |
| 3:I:97:LYS:O | 3:I:101:ARG:HG3 | 2.01 | 0.60 |
| 1:A:228:LYS:NZ | 3:C:45:ASP:OD1 | 2.31 | 0.60 |
| 2:B:62:ARG:NH1 | 2:B:63:GLU:OE2 | 2.31 | 0.60 |
| 11:C:403:FC6:N24 | 3:M:215:PRO:HB3 | 2.17 | 0.60 |
| 3:I:24:ILE:HD12 | 3:I:59:PHE:HE2 | 1.66 | 0.60 |
| 3:I:36:THR:CG2 | 3:I:38:GLN:HB2 | 2.31 | 0.60 |
| 3:F:195:GLU:OE2 | 3:F:272:ARG:NH1 | 2.35 | 0.60 |
| 1:K:76:THR:HG23 | 1:K:225:PHE:HE1 | 1.66 | 0.60 |
| 1:D:63:ALA:O | 1:D:67:ALA:HB3 | 2.01 | 0.60 |
| 3:F:187:PRO:HG2 | 3:F:189:TRP:CZ2 | 2.37 | 0.60 |
| 1:K:178:ASN:HD22 | 1:K:201:VAL:HG12 | 1.67 | 0.60 |
| 1:A:291:MET:SD | 4:N:24:PHE:CZ | 2.95 | 0.60 |
| 3:C:61:LEU:O | 3:C:65:THR:HG23 | 2.02 | 0.60 |
| 3:C:271:ILE:HG12 | 10:C:401:HEC:HMB2 | 1.84 | 0.60 |
| 1:G:63:ALA:O | 1:G:67:ALA:HB3 | 2.01 | 0.60 |
| 1:K:235:TYR:CD1 | 1:K:236:SER:N | 2.70 | 0.60 |
| 1:D:252:ILE:HD11 | 2:E:22:VAL:HG22 | 1.84 | 0.60 |
| 3:F:74:VAL:HA | 3:F:82:TRP:HZ2 | 1.67 | 0.60 |
| 1:G:281:ALA:HB3 | 1:G:282:PRO:HD3 | 1.84 | 0.60 |
| 1:G:468:ASP:OD1 | 1:G:470:ALA:N | 2.35 | 0.60 |
| 3:I:178:ILE:HG12 | 10:I:403:HEC:HMB2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:319:MET:HB2 | 4:Q:21:LEU:HD21 | 1.84 | 0.60 |
| 3:C:59:PHE:CE1 | 3:C:63:ILE:HD11 | 2.37 | 0.59 |
| 1:D:417:GLY:N | 3:F:110:TYR:CE2 | 2.70 | 0.59 |
| 1:A:346:VAL:HG22 | 5:A:501:HEM:C2D | 2.37 | 0.59 |
| 3:I:86:LEU:HD12 | 3:I:87:PRO:CD | 2.31 | 0.59 |
| 1:D:238:ARG:HH12 | 3:F:30:GLY:C | 2.05 | 0.59 |
| 1:D:31:LEU:HD11 | 1:D:59:LEU:HD13 | 1.85 | 0.59 |
| 3:C:62:PHE:CD1 | 3:C:66:LEU:HD11 | 2.38 | 0.59 |
| 11:F:403:FC6:N24 | 3:I:215:PRO:HB3 | 2.17 | 0.59 |
| 1:G:227:PRO:HB2 | 3:I:47:ILE:HD12 | 1.82 | 0.59 |
| 2:L:140:TYR:CZ | 10:L:301:HEC:HBB2 | 2.38 | 0.59 |
| 3:I:4:PHE:CD1 | 3:I:4:PHE:C | 2.75 | 0.59 |
| 1:A:370:PHE:CE2 | 1:A:459:VAL:HG13 | 2.37 | 0.59 |
| 1:G:343:ILE:HG12 | 5:G:502:HEM:HBA2 | 1.85 | 0.59 |
| 3:I:89:TYR:CD1 | 3:I:93:TRP:CD1 | 2.91 | 0.59 |
| 2:B:193:GLN:HA | 2:B:193:GLN:HE21 | 1.66 | 0.59 |
| 3:F:89:TYR:C | 3:F:97:LYS:HZ3 | 2.05 | 0.59 |
| 3:I:127:GLN:HE21 | 3:I:127:GLN:HA | 1.68 | 0.59 |
| 1:K:230:ALA:O | 1:K:300:LYS:NZ | 2.33 | 0.59 |
| 3:C:93:TRP:HE1 | 3:C:98:GLN:HE21 | 1.51 | 0.58 |
| 3:I:99:TRP:O | 3:I:103:VAL:HG23 | 2.03 | 0.58 |
| 2:L:62:ARG:NH1 | 2:L:63:GLU:OE2 | 2.35 | 0.58 |
| 3:F:60:LEU:O | 3:F:63:ILE:HG12 | 2.02 | 0.58 |
| 3:I:63:ILE:O | 3:I:67:VAL:HG23 | 2.02 | 0.58 |
| 3:F:271:ILE:HG12 | 10:F:401:HEC:HMB2 | 1.85 | 0.58 |
| 1:A:17:PHE:CZ | 1:A:99:PHE:HA | 2.39 | 0.58 |
| 1:K:457:ARG:HH11 | 1:K:460:GLN:NE2 | 2.01 | 0.58 |
| 5:K:501:HEM:HHH | 5:K:501:HEM:HBC2 | 1.83 | 0.58 |
| 3:M:24:ILE:CG1 | 3:M:59:PHE:HE2 | 2.16 | 0.58 |
| 1:K:10:SER:N | 1:K:82:GLN:HE22 | 2.02 | 0.58 |
| 1:K:63:ALA:O | 1:K:67:ALA:HB3 | 2.04 | 0.58 |
| 3:C:29:LYS:HG3 | 3:C:30:GLY:H | 1.66 | 0.58 |
| 3:F:82:TRP:CD1 | 3:F:82:TRP:C | 2.77 | 0.58 |
| 1:G:347:HIS:HA | 1:G:350:ALA:HB3 | 1.84 | 0.58 |
| 3:I:137:ARG:HG2 | 3:I:137:ARG:HH11 | 1.68 | 0.58 |
| 3:M:207:LYS:HD3 | 3:M:222:LEU:HD21 | 1.86 | 0.58 |
| 1:D:218:PHE:HA | 1:D:221:ILE:HG13 | 1.85 | 0.58 |
| 1:D:253:TRP:CZ3 | 3:F:13:THR:HG22 | 2.39 | 0.58 |
| 3:C:178:ILE:HG12 | 10:C:402:HEC:HMB2 | 1.86 | 0.58 |
| 3:F:40:MET:N | 3:F:49:GLU:O | 2.37 | 0.58 |
| 1:D:253:TRP:CH2 | 2:E:28:THR:HG21 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:222:MET:HG3 | 1:G:314:LEU:HD21 | 1.85 | 0.57 |
| 1:G:218:PHE:HA | 1:G:221:ILE:HG13 | 1.87 | 0.57 |
| 3:M:63:ILE:O | 3:M:67:VAL:HG23 | 2.04 | 0.57 |
| 1:A:13:VAL:HA | 1:A:16:GLN:HE21 | 1.70 | 0.57 |
| 1:K:235:TYR:HD1 | 1:K:236:SER:N | 2.03 | 0.57 |
| 1:G:10:SER:N | 1:G:82:GLN:HE22 | 2.02 | 0.57 |
| 1:D:359:ILE:HD12 | 1:D:451:MET:HE3 | 1.85 | 0.57 |
| 3:I:117:TYR:CZ | 3:I:131:ALA:HB2 | 2.40 | 0.57 |
| 3:C:128:ASP:OD2 | 3:C:131:ALA:N | 2.32 | 0.57 |
| 1:D:57:ARG:NH2 | 5:D:502:HEM:O2D | 2.37 | 0.57 |
| 3:M:24:ILE:HD11 | 3:M:59:PHE:HZ | 1.66 | 0.57 |
| 3:M:110:TYR:HA | 3:M:113:ILE:HG13 | 1.86 | 0.57 |
| 3:I:74:VAL:O | 3:I:82:TRP:CZ2 | 2.58 | 0.57 |
| 1:K:347:HIS:HA | 1:K:350:ALA:HB3 | 1.85 | 0.57 |
| 3:C:25:PHE:CE1 | 3:C:59:PHE:HZ | 2.23 | 0.57 |
| 1:D:242:VAL:HG22 | 3:F:27:THR:HG21 | 1.86 | 0.57 |
| 1:D:410:TRP:O | 2:E:82:ARG:NH1 | 2.37 | 0.57 |
| 4:Q:27:PHE:C | 4:Q:27:PHE:CD2 | 2.78 | 0.57 |
| 1:A:453:TYR:O | 1:A:457:ARG:HG2 | 2.05 | 0.57 |
| 3:F:63:ILE:HA | 3:F:66:LEU:CD1 | 2.34 | 0.57 |
| 1:K:242:VAL:HG21 | 3:M:54:LEU:HD21 | 1.87 | 0.57 |
| 4:P:24:PHE:HE1 | 4:P:28:ILE:HD11 | 1.69 | 0.57 |
| 3:C:89:TYR:CE1 | 3:C:93:TRP:CD1 | 2.93 | 0.56 |
| 3:F:79:LEU:O | 3:F:82:TRP:HB3 | 2.04 | 0.56 |
| 1:K:218:PHE:HA | 1:K:221:ILE:HG13 | 1.85 | 0.56 |
| 1:G:342:THR:O | 1:G:346:VAL:HG23 | 2.05 | 0.56 |
| 5:D:501:HEM:HBC2 | 5:D:501:HEM:HHD | 1.87 | 0.56 |
| 3:F:35:THR:O | 3:F:52:ASN:OD1 | 2.24 | 0.56 |
| 3:I:4:PHE:HD1 | 3:I:4:PHE:O | 1.87 | 0.56 |
| 3:M:62:PHE:CE1 | 3:M:66:LEU:HD21 | 2.40 | 0.56 |
| 1:A:347:HIS:HA | 1:A:350:ALA:HB3 | 1.88 | 0.56 |
| 2:E:6:LYS:HD3 | 2:E:8:GLU:OE2 | 2.06 | 0.56 |
| 1:A:411:ARG:NH1 | 4:N:4:ASP:OD2 | 2.39 | 0.56 |
| 1:D:233:PRO:HG2 | 3:F:50:TYR:CZ | 2.41 | 0.56 |
| 1:G:115:LEU:HD23 | 1:G:117:PHE:HE2 | 1.70 | 0.56 |
| 1:G:291:MET:SD | 4:P:24:PHE:HZ | 2.28 | 0.56 |
| 1:A:211:GLY:O | 1:A:215:THR:HB | 2.06 | 0.56 |
| 3:I:140:ALA:O | 3:I:144:SER:OG | 2.18 | 0.56 |
| 1:K:235:TYR:CE1 | 1:K:236:SER:HB2 | 2.41 | 0.56 |
| 1:K:237:TYR:HB2 | 3:M:49:GLU:HG3 | 1.87 | 0.56 |
| 2:E:157:MET:HE1 | 2:E:171:ASP:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:20:LEU:HD22 | 3:M:62:PHE:HZ | 1.70 | 0.56 |
| 1:A:359:ILE:HD11 | 1:A:448:MET:CE | 2.36 | 0.56 |
| 3:C:89:TYR:CD2 | 3:C:101:ARG:NH1 | 2.74 | 0.56 |
| 3:F:123:GLU:O | 3:F:126:ALA:HB3 | 2.06 | 0.56 |
| 1:D:281:ALA:HB3 | 1:D:282:PRO:HD3 | 1.87 | 0.56 |
| 1:K:170:THR:HG21 | 1:K:212:PHE:CD2 | 2.41 | 0.56 |
| 1:A:57:ARG:NH1 | 5:A:502:HEM:O2A | 2.39 | 0.55 |
| 1:A:253:TRP:CH2 | 2:B:28:THR:HG21 | 2.40 | 0.55 |
| 1:D:222:MET:HG3 | 1:D:314:LEU:HD21 | 1.87 | 0.55 |
| 1:D:245:TRP:CZ2 | 2:E:7:LEU:HD11 | 2.32 | 0.55 |
| 3:C:94:THR:OG1 | 3:C:97:LYS:HG3 | 2.06 | 0.55 |
| 1:D:347:HIS:HA | 1:D:350:ALA:HB3 | 1.87 | 0.55 |
| 1:K:281:ALA:HB3 | 1:K:282:PRO:HD3 | 1.88 | 0.55 |
| 1:D:8:ALA:HA | 1:D:469:ALA:O | 2.06 | 0.55 |
| 3:I:38:GLN:CD | 3:I:39:THR:H | 2.09 | 0.55 |
| 3:I:89:TYR:CE1 | 3:I:93:TRP:CD1 | 2.95 | 0.55 |
| 3:I:116:LYS:O | 3:I:120:MET:HG3 | 2.06 | 0.55 |
| 3:M:8:TYR:HE2 | 3:M:12:LEU:HD12 | 1.71 | 0.55 |
| 1:K:457:ARG:NH1 | 1:K:460:GLN:NE2 | 2.55 | 0.55 |
| 3:F:24:ILE:HG13 | 3:F:59:PHE:HE1 | 1.71 | 0.55 |
| 1:G:352:GLY:O | 1:G:356:MET:HG3 | 2.06 | 0.55 |
| 3:F:63:ILE:HA | 3:F:66:LEU:HD13 | 1.88 | 0.55 |
| 3:F:83:LYS:HD2 | 3:F:92:GLY:HA3 | 1.89 | 0.55 |
| 1:G:376:HIS:H | 1:G:458:THR:CG2 | 2.19 | 0.55 |
| 1:G:421:TYR:O | 2:H:82:ARG:NH2 | 2.40 | 0.55 |
| 1:K:376:HIS:N | 1:K:458:THR:HG22 | 2.22 | 0.55 |
| 1:A:359:ILE:HD11 | 1:A:448:MET:HE1 | 1.88 | 0.55 |
| 1:D:211:GLY:O | 1:D:215:THR:HB | 2.07 | 0.55 |
| 1:D:235:TYR:CE1 | 1:D:236:SER:HB2 | 2.42 | 0.55 |
| 1:G:242:VAL:HG22 | 3:I:27:THR:HG21 | 1.89 | 0.55 |
| 1:A:233:PRO:CG | 3:C:50:TYR:CE2 | 2.89 | 0.55 |
| 3:C:81:ASN:O | 3:C:83:LYS:HD3 | 2.07 | 0.55 |
| 1:A:252:ILE:HD11 | 2:B:22:VAL:HG22 | 1.89 | 0.54 |
| 3:C:63:ILE:O | 3:C:67:VAL:HG23 | 2.07 | 0.54 |
| 2:E:42:PRO:HG3 | 2:E:93:VAL:HG11 | 1.89 | 0.54 |
| 3:F:111:GLY:N | 3:F:112:PRO:HD2 | 2.22 | 0.54 |
| 1:G:230:ALA:O | 1:G:300:LYS:NZ | 2.34 | 0.54 |
| 1:K:264:LEU:HD12 | 1:K:265:PRO:HD2 | 1.89 | 0.54 |
| 3:M:28:ARG:O | 3:M:31:GLU:HB2 | 2.07 | 0.54 |
| 3:M:105:GLN:HB3 | 3:M:109:LYS:NZ | 2.22 | 0.54 |
| 1:A:376:HIS:HB2 | 1:A:458:THR:HG22 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:237:TYR:OH | 2:E:8:GLU:OE1 | 2.25 | 0.54 |
| 2:E:6:LYS:O | 2:E:7:LEU:HG | 2.06 | 0.54 |
| 3:F:177:SER:OG | 3:F:182:ARG:NH1 | 2.36 | 0.54 |
| 3:I:74:VAL:O | 3:I:82:TRP:CH2 | 2.60 | 0.54 |
| 1:K:17:PHE:CZ | 1:K:99:PHE:HA | 2.42 | 0.54 |
| 2:L:37:ASP:O | 2:L:41:GLU:HG3 | 2.07 | 0.54 |
| 3:C:50:TYR:HD1 | 3:C:52:ASN:HD21 | 1.56 | 0.54 |
| 3:I:76:TYR:CE1 | 3:I:86:LEU:HD22 | 2.42 | 0.54 |
| 3:M:59:PHE:CE1 | 3:M:63:ILE:HD11 | 2.42 | 0.54 |
| 1:D:238:ARG:NH2 | 3:F:30:GLY:O | 2.40 | 0.54 |
| 1:D:352:GLY:O | 1:D:356:MET:HG3 | 2.08 | 0.54 |
| 4:N:14:VAL:O | 4:N:18:VAL:HG23 | 2.07 | 0.54 |
| 3:C:207:LYS:HD3 | 3:C:222:LEU:HD21 | 1.89 | 0.54 |
| 2:H:70:SER:HA | 2:H:101:GLY:HA3 | 1.89 | 0.54 |
| 1:K:340:ASP:H | 1:K:406:GLN:HE22 | 1.55 | 0.54 |
| 3:M:37:ASP:C | 3:M:38:GLN:NE2 | 2.61 | 0.54 |
| 1:D:13:VAL:HA | 1:D:16:GLN:HE21 | 1.73 | 0.54 |
| 3:F:63:ILE:O | 3:F:67:VAL:HG23 | 2.06 | 0.54 |
| 1:K:10:SER:H | 1:K:82:GLN:HE22 | 1.54 | 0.54 |
| 1:K:331:THR:OG1 | 9:K:506:PO4:O2 | 2.22 | 0.54 |
| 2:L:6:LYS:O | 2:L:7:LEU:HG | 2.07 | 0.54 |
| 3:M:187:PRO:HG2 | 3:M:189:TRP:CZ2 | 2.43 | 0.54 |
| 3:C:206:ARG:NH1 | 3:C:262:SER:O | 2.40 | 0.54 |
| 3:F:97:LYS:HE2 | 3:F:101:ARG:HH12 | 1.73 | 0.54 |
| 1:K:13:VAL:HA | 1:K:16:GLN:HE21 | 1.72 | 0.54 |
| 1:K:211:GLY:O | 1:K:215:THR:HB | 2.08 | 0.54 |
| 3:M:62:PHE:CE1 | 3:M:66:LEU:HD11 | 2.43 | 0.54 |
| 1:A:342:THR:O | 1:A:346:VAL:HG23 | 2.07 | 0.54 |
| 1:D:170:THR:HG21 | 1:D:212:PHE:CD2 | 2.43 | 0.54 |
| 1:D:233:PRO:HB3 | 3:F:48:GLU:HG3 | 1.89 | 0.54 |
| 1:D:234:VAL:O | 3:F:50:TYR:N | 2.41 | 0.54 |
| 2:H:39:VAL:HG23 | 2:H:40:ASN:HD22 | 1.73 | 0.54 |
| 3:M:37:ASP:O | 3:M:38:GLN:NE2 | 2.41 | 0.54 |
| 1:D:267:TRP:HE1 | 2:E:36:GLN:HE22 | 1.56 | 0.54 |
| 2:B:128:PRO:HD2 | 2:B:129:ARG:HH21 | 1.73 | 0.54 |
| 2:E:70:SER:HA | 2:E:101:GLY:HA3 | 1.90 | 0.54 |
| 3:F:66:LEU:O | 3:F:70:ILE:HG12 | 2.07 | 0.54 |
| 1:G:64:VAL:HG11 | 5:G:502:HEM:C4C | 2.43 | 0.54 |
| 3:M:66:LEU:O | 3:M:70:ILE:HG13 | 2.07 | 0.54 |
| 3:I:177:SER:HA | 3:I:182:ARG:HD2 | 1.91 | 0.53 |
| 3:M:186:MET:HG2 | 10:M:402:HEC:C1D | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:12:LEU:O | 3:C:16:THR:OG1 | 2.26 | 0.53 |
| 3:F:37:ASP:OD2 | 3:F:50:TYR:CD1 | 2.62 | 0.53 |
| 1:D:10:SER:N | 1:D:82:GLN:HE22 | 2.04 | 0.53 |
| 1:D:17:PHE:CZ | 1:D:99:PHE:HA | 2.43 | 0.53 |
| 1:D:371:GLY:HA3 | 1:D:467:TYR:CD1 | 2.43 | 0.53 |
| 1:G:17:PHE:CZ | 1:G:99:PHE:HA | 2.43 | 0.53 |
| 3:F:76:TYR:CZ | 3:F:86:LEU:HD13 | 2.44 | 0.53 |
| 1:G:76:THR:HG23 | 1:G:225:PHE:HE1 | 1.73 | 0.53 |
| 1:G:370:PHE:CE2 | 1:G:459:VAL:HG13 | 2.43 | 0.53 |
| 1:D:446:ALA:O | 1:D:450:VAL:HG23 | 2.08 | 0.53 |
| 1:A:352:GLY:O | 1:A:356:MET:HG3 | 2.08 | 0.53 |
| 1:D:340:ASP:H | 1:D:406:GLN:HE22 | 1.55 | 0.53 |
| 3:F:60:LEU:HA | 3:F:63:ILE:CD1 | 2.37 | 0.53 |
| 3:I:167:TRP:CD2 | 3:I:182:ARG:HG2 | 2.44 | 0.53 |
| 3:M:24:ILE:HD13 | 3:M:24:ILE:C | 2.28 | 0.53 |
| 1:A:239:LEU:HD23 | 1:A:289:ASN:HD22 | 1.74 | 0.53 |
| 2:H:193:GLN:HE21 | 2:H:193:GLN:HA | 1.74 | 0.53 |
| 1:D:340:ASP:H | 1:D:406:GLN:NE2 | 2.07 | 0.53 |
| 2:E:86:TYR:HE2 | 3:F:99:TRP:CE3 | 2.27 | 0.53 |
| 3:F:120:MET:CE | 3:F:124:GLU:HB3 | 2.39 | 0.53 |
| 3:M:39:THR:HG22 | 3:M:40:MET:O | 2.09 | 0.53 |
| 1:G:82:GLN:NE2 | 1:G:89:LEU:H | 2.07 | 0.53 |
| 2:L:128:PRO:HD2 | 2:L:129:ARG:HH21 | 1.74 | 0.53 |
| 1:G:291:MET:SD | 4:P:24:PHE:CZ | 3.02 | 0.52 |
| 1:A:340:ASP:H | 1:A:406:GLN:NE2 | 2.07 | 0.52 |
| 1:D:261:TYR:HA | 3:F:95:GLN:OE1 | 2.09 | 0.52 |
| 3:F:8:TYR:O | 3:F:12:LEU:HD12 | 2.09 | 0.52 |
| 1:G:152:ARG:NH2 | 2:H:9:LYS:O | 2.42 | 0.52 |
| 3:I:61:LEU:O | 3:I:65:THR:HG23 | 2.08 | 0.52 |
| 1:K:253:TRP:CH2 | 2:L:28:THR:HG21 | 2.44 | 0.52 |
| 1:G:239:LEU:HD23 | 1:G:289:ASN:HD22 | 1.74 | 0.52 |
| 1:D:10:SER:H | 1:D:82:GLN:NE2 | 2.08 | 0.52 |
| 3:F:45:ASP:CG | 3:F:46:GLY:H | 2.13 | 0.52 |
| 3:I:8:TYR:O | 3:I:12:LEU:HD12 | 2.10 | 0.52 |
| 1:K:82:GLN:CG | 1:K:89:LEU:HG | 2.39 | 0.52 |
| 1:K:238:ARG:NH2 | 3:M:51:ASP:OD1 | 2.41 | 0.52 |
| 1:K:330:LYS:HB2 | 9:K:506:PO4:O1 | 2.10 | 0.52 |
| 2:L:193:GLN:HA | 2:L:193:GLN:HE21 | 1.74 | 0.52 |
| 1:G:236:SER:CA | 3:I:52:ASN:HB2 | 2.39 | 0.52 |
| 3:I:177:SER:OG | 3:I:182:ARG:NH1 | 2.40 | 0.52 |
| 3:M:2:SER:OG | 3:M:5:TRP:HD1 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:62:ASN:HD21 | 1:D:125:GLU:HG3 | 1.74 | 0.52 |
| 1:G:274:VAL:HG21 | 3:I:73:LEU:HD21 | 1.89 | 0.52 |
| 3:M:11:LEU:HD23 | 3:M:12:LEU:N | 2.24 | 0.52 |
| 1:D:346:VAL:HG22 | 5:D:501:HEM:C2D | 2.44 | 0.52 |
| 1:G:267:TRP:HA | 3:I:78:GLY:HA2 | 1.92 | 0.52 |
| 3:I:17:ILE:HG23 | 3:I:66:LEU:CD2 | 2.40 | 0.52 |
| 3:M:97:LYS:O | 3:M:101:ARG:HG3 | 2.09 | 0.52 |
| 2:E:24:ILE:HG21 | 3:F:16:THR:CG2 | 2.39 | 0.52 |
| 3:F:114:PHE:HB3 | 3:F:289:ASP:OD2 | 2.09 | 0.52 |
| 3:F:178:ILE:HG12 | 10:F:402:HEC:HMB2 | 1.91 | 0.52 |
| 2:E:152:ASP:HA | 2:E:155:LYS:HE3 | 1.92 | 0.52 |
| 3:F:29:LYS:CD | 3:F:30:GLY:N | 2.73 | 0.52 |
| 3:F:34:GLY:O | 3:F:36:THR:OG1 | 2.26 | 0.52 |
| 1:K:227:PRO:CB | 3:M:47:ILE:HG21 | 2.39 | 0.52 |
| 1:G:359:ILE:HD11 | 1:G:448:MET:HE1 | 1.92 | 0.51 |
| 1:K:321:THR:HG22 | 5:K:501:HEM:HAB | 1.93 | 0.51 |
| 2:H:63:GLU:HB3 | 10:H:301:HEC:HBB1 | 1.90 | 0.51 |
| 3:I:25:PHE:HE1 | 3:I:59:PHE:HZ | 1.58 | 0.51 |
| 3:F:40:MET:HB2 | 3:F:49:GLU:HB2 | 1.92 | 0.51 |
| 1:K:352:GLY:O | 1:K:356:MET:HG3 | 2.09 | 0.51 |
| 1:A:64:VAL:HG11 | 5:A:502:HEM:C4C | 2.45 | 0.51 |
| 1:D:207:HIS:CD2 | 1:D:251:TYR:HE1 | 2.07 | 0.51 |
| 3:M:8:TYR:HE2 | 3:M:12:LEU:CD1 | 2.23 | 0.51 |
| 2:B:152:ASP:HA | 2:B:155:LYS:HE3 | 1.92 | 0.51 |
| 1:D:301:LEU:HD21 | 1:D:311:VAL:HG21 | 1.93 | 0.51 |
| 2:E:193:GLN:HE21 | 2:E:193:GLN:HA | 1.74 | 0.51 |
| 3:F:75:LEU:HD22 | 3:F:86:LEU:HD12 | 1.92 | 0.51 |
| 1:G:395:TYR:CZ | 1:G:437:ARG:HD2 | 2.46 | 0.51 |
| 2:H:128:PRO:HD2 | 2:H:129:ARG:HH21 | 1.75 | 0.51 |
| 3:M:73:LEU:HG | 3:M:79:LEU:HD11 | 1.92 | 0.51 |
| 3:M:116:LYS:O | 3:M:120:MET:HG3 | 2.11 | 0.51 |
| 3:C:62:PHE:CE1 | 3:C:66:LEU:HD11 | 2.46 | 0.51 |
| 3:F:77:PRO:HG3 | 3:F:93:TRP:O | 2.10 | 0.51 |
| 3:I:56:ARG:O | 3:I:59:PHE:HB3 | 2.09 | 0.51 |
| 3:I:117:TYR:CE1 | 3:I:131:ALA:HB2 | 2.46 | 0.51 |
| 1:A:355:ALA:O | 1:A:359:ILE:HG12 | 2.11 | 0.51 |
| 3:C:59:PHE:CZ | 3:C:63:ILE:HD11 | 2.45 | 0.51 |
| 3:F:206:ARG:NH1 | 3:F:262:SER:O | 2.42 | 0.51 |
| 3:I:4:PHE:C | 3:I:4:PHE:HD1 | 2.14 | 0.51 |
| 3:I:73:LEU:HB3 | 3:I:79:LEU:CD1 | 2.37 | 0.51 |
| 4:P:24:PHE:CE1 | 4:P:28:ILE:HD11 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:37:ASP:CB | 3:F:38:GLN:HA | 2.28 | 0.51 |
| 1:G:10:SER:H | 1:G:82:GLN:NE2 | 2.03 | 0.51 |
| 1:G:252:ILE:HD11 | 2:H:22:VAL:HG22 | 1.93 | 0.51 |
| 1:G:355:ALA:O | 1:G:359:ILE:HG12 | 2.11 | 0.51 |
| 1:G:375:MET:CE | 1:G:458:THR:HG21 | 2.41 | 0.51 |
| 2:L:7:LEU:HD12 | 2:L:7:LEU:O | 2.11 | 0.51 |
| 3:M:11:LEU:HD23 | 3:M:12:LEU:HG | 1.93 | 0.51 |
| 2:B:157:MET:HE2 | 2:B:172:ILE:HA | 1.91 | 0.51 |
| 3:I:89:TYR:HA | 3:I:101:ARG:NH2 | 2.26 | 0.51 |
| 3:M:81:ASN:O | 3:M:83:LYS:HD3 | 2.10 | 0.51 |
| 3:M:121:SER:O | 3:M:125:VAL:HG23 | 2.10 | 0.51 |
| 3:M:177:SER:HA | 3:M:182:ARG:HD2 | 1.92 | 0.51 |
| 3:C:74:VAL:O | 3:C:82:TRP:CH2 | 2.64 | 0.51 |
| 1:D:82:GLN:NE2 | 1:D:89:LEU:H | 2.09 | 0.51 |
| 3:F:24:ILE:HG13 | 3:F:59:PHE:CE1 | 2.46 | 0.51 |
| 3:F:89:TYR:HD1 | 3:F:93:TRP:HD1 | 1.57 | 0.51 |
| 1:K:154:VAL:HG21 | 3:M:44:PHE:CE2 | 2.46 | 0.51 |
| 3:M:21:PHE:CE2 | 3:M:66:LEU:HD13 | 2.46 | 0.51 |
| 1:A:115:LEU:HB3 | 1:A:117:PHE:CE2 | 2.46 | 0.50 |
| 2:B:70:SER:HA | 2:B:101:GLY:HA3 | 1.91 | 0.50 |
| 2:E:140:TYR:CE1 | 10:E:301:HEC:HBB2 | 2.46 | 0.50 |
| 3:C:215:PRO:HG3 | 11:M:401:FC6:N25 | 2.27 | 0.50 |
| 1:G:235:TYR:CE1 | 1:G:236:SER:HB2 | 2.47 | 0.50 |
| 1:K:350:ALA:HB1 | 5:K:502:HEM:CAC | 2.41 | 0.50 |
| 5:K:501:HEM:HMB1 | 5:K:501:HEM:HBB2 | 1.92 | 0.50 |
| 2:L:6:LYS:HD3 | 2:L:8:GLU:OE2 | 2.11 | 0.50 |
| 3:M:179:LEU:HD22 | 3:M:283:GLN:HB2 | 1.94 | 0.50 |
| 3:F:167:TRP:CD2 | 3:F:182:ARG:HG2 | 2.46 | 0.50 |
| 1:K:313:SER:HB2 | 1:K:356:MET:HB2 | 1.93 | 0.50 |
| 2:B:62:ARG:HG3 | 2:B:63:GLU:N | 2.27 | 0.50 |
| 3:C:50:TYR:CB | 3:C:52:ASN:ND2 | 2.74 | 0.50 |
| 1:D:416:ASP:OD1 | 3:F:137:ARG:CZ | 2.59 | 0.50 |
| 1:K:359:ILE:HD12 | 1:K:384:HIS:HE1 | 1.75 | 0.50 |
| 3:C:167:TRP:CD2 | 3:C:182:ARG:HG2 | 2.46 | 0.50 |
| 1:K:82:GLN:HE21 | 1:K:88:THR:HA | 1.76 | 0.50 |
| 3:C:28:ARG:O | 3:C:28:ARG:HG2 | 2.12 | 0.50 |
| 1:A:370:PHE:C | 1:A:465:ALA:HB1 | 2.31 | 0.50 |
| 3:M:23:LEU:O | 3:M:27:THR:OG1 | 2.28 | 0.50 |
| 1:A:169:LEU:HD11 | 2:B:15:THR:HG23 | 1.94 | 0.50 |
| 1:D:156:HIS:CD2 | 3:F:42:HIS:CD2 | 2.92 | 0.50 |
| 2:E:39:VAL:HG23 | 2:E:40:ASN:ND2 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:211:GLY:O | 1:G:215:THR:HB | 2.11 | 0.50 |
| 2:H:148:LEU:HD11 | 2:H:187:ALA:HB2 | 1.94 | 0.50 |
| 1:K:235:TYR:CE1 | 3:M:52:ASN:ND2 | 2.79 | 0.50 |
| 1:A:82:GLN:NE2 | 1:A:89:LEU:H | 2.09 | 0.50 |
| 1:D:239:LEU:HD23 | 1:D:289:ASN:HD22 | 1.76 | 0.50 |
| 3:F:131:ALA:O | 3:F:134:MET:HB3 | 2.12 | 0.50 |
| 1:G:156:HIS:CD2 | 3:I:42:HIS:CD2 | 3.00 | 0.50 |
| 1:K:169:LEU:HD11 | 2:L:15:THR:HG23 | 1.94 | 0.50 |
| 1:K:342:THR:O | 1:K:346:VAL:HG23 | 2.11 | 0.50 |
| 3:M:133:LYS:HE3 | 3:M:137:ARG:NH2 | 2.27 | 0.50 |
| 2:B:6:LYS:O | 2:B:7:LEU:HG | 2.12 | 0.49 |
| 1:A:10:SER:N | 1:A:82:GLN:HE22 | 2.10 | 0.49 |
| 1:A:94:LEU:O | 1:A:98:THR:HG23 | 2.12 | 0.49 |
| 3:M:37:ASP:C | 3:M:38:GLN:HE21 | 2.16 | 0.49 |
| 1:A:238:ARG:NH2 | 3:C:30:GLY:O | 2.45 | 0.49 |
| 3:F:1:MET:HB3 | 3:F:81:ASN:ND2 | 2.27 | 0.49 |
| 1:G:120:SER:OG | 2:H:97:PRO:HG2 | 2.13 | 0.49 |
| 3:I:239:GLN:OE1 | 3:I:239:GLN:N | 2.26 | 0.49 |
| 1:K:10:SER:O | 1:K:89:LEU:HD11 | 2.12 | 0.49 |
| 1:K:64:VAL:HG11 | 5:K:502:HEM:C4C | 2.47 | 0.49 |
| 1:K:235:TYR:CD2 | 1:K:292:MET:HB2 | 2.47 | 0.49 |
| 1:G:346:VAL:HG22 | 5:G:501:HEM:C2D | 2.47 | 0.49 |
| 1:G:359:ILE:HD12 | 1:G:384:HIS:HE1 | 1.77 | 0.49 |
| 3:I:21:PHE:O | 3:I:24:ILE:HG22 | 2.12 | 0.49 |
| 1:K:238:ARG:HG3 | 3:M:51:ASP:OD2 | 2.12 | 0.49 |
| 2:L:63:GLU:HB3 | 10:L:301:HEC:HBB1 | 1.93 | 0.49 |
| 4:O:2:PHE:CE2 | 4:O:4:ASP:HB2 | 2.48 | 0.49 |
| 3:F:29:LYS:HD3 | 3:F:30:GLY:N | 2.27 | 0.49 |
| 3:F:66:LEU:HD12 | 3:F:66:LEU:N | 2.23 | 0.49 |
| 1:K:8:ALA:HA | 1:K:469:ALA:HA | 1.93 | 0.49 |
| 2:L:86:TYR:HE2 | 3:M:99:TRP:CE3 | 2.30 | 0.49 |
| 3:M:28:ARG:NH1 | 3:M:59:PHE:CE1 | 2.80 | 0.49 |
| 4:O:4:ASP:H | 4:O:7:VAL:CG2 | 2.25 | 0.49 |
| 3:I:76:TYR:C | 3:I:82:TRP:CZ3 | 2.83 | 0.49 |
| 3:M:122:VAL:HG22 | 3:M:292:HIS:CD2 | 2.46 | 0.49 |
| 1:A:15:ARG:HG2 | 1:A:370:PHE:CZ | 2.48 | 0.49 |
| 1:D:455:THR:C | 1:D:459:VAL:HG23 | 2.33 | 0.49 |
| 1:G:238:ARG:O | 1:G:242:VAL:HG23 | 2.12 | 0.49 |
| 3:I:271:ILE:HG12 | 10:I:402:HEC:HMB2 | 1.93 | 0.49 |
| 3:M:28:ARG:HG3 | 3:M:31:GLU:CD | 2.32 | 0.49 |
| 3:F:2:SER:HG | 3:F:5:TRP:HD1 | 1.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:6:SER:CB | 3:F:81:ASN:HD22 | 2.14 | 0.49 |
| 1:G:155:LYS:HE3 | 2:H:9:LYS:NZ | 2.27 | 0.49 |
| 2:E:43:VAL:HG13 | 2:E:46:MET:HB2 | 1.95 | 0.49 |
| 3:F:89:TYR:HD1 | 3:F:93:TRP:CD1 | 2.31 | 0.49 |
| 3:F:229:TYR:HE1 | 3:F:239:GLN:HA | 1.77 | 0.49 |
| 3:M:21:PHE:O | 3:M:24:ILE:HG22 | 2.13 | 0.49 |
| 2:B:43:VAL:HG13 | 2:B:46:MET:HB2 | 1.93 | 0.48 |
| 1:D:313:SER:HB2 | 1:D:356:MET:HB2 | 1.94 | 0.48 |
| 3:F:6:SER:HG | 3:F:81:ASN:H | 1.51 | 0.48 |
| 1:G:15:ARG:HG2 | 1:G:370:PHE:CZ | 2.48 | 0.48 |
| 2:H:88:VAL:HG12 | 2:H:90:GLY:H | 1.78 | 0.48 |
| 3:I:89:TYR:CD1 | 3:I:93:TRP:HD1 | 2.30 | 0.48 |
| 3:C:114:PHE:CE1 | 3:C:134:MET:HE1 | 2.48 | 0.48 |
| 3:C:122:VAL:HG22 | 3:C:292:HIS:CD2 | 2.47 | 0.48 |
| 1:D:238:ARG:O | 1:D:242:VAL:HG23 | 2.13 | 0.48 |
| 1:D:416:ASP:C | 3:F:110:TYR:CE2 | 2.86 | 0.48 |
| 3:F:26:ALA:O | 3:F:29:LYS:HG3 | 2.13 | 0.48 |
| 3:F:54:LEU:H | 3:F:54:LEU:HD22 | 1.78 | 0.48 |
| 1:G:169:LEU:HD11 | 2:H:15:THR:HG23 | 1.95 | 0.48 |
| 1:G:468:ASP:OD1 | 1:G:469:ALA:N | 2.45 | 0.48 |
| 2:L:70:SER:HA | 2:L:101:GLY:HA3 | 1.93 | 0.48 |
| 3:C:73:LEU:HB3 | 3:C:79:LEU:HD11 | 1.94 | 0.48 |
| 1:D:342:THR:O | 1:D:346:VAL:HG23 | 2.12 | 0.48 |
| 1:G:125:GLU:H | 1:G:125:GLU:HG2 | 1.36 | 0.48 |
| 3:M:62:PHE:O | 3:M:66:LEU:HG | 2.13 | 0.48 |
| 1:A:418:THR:OG1 | 3:C:137:ARG:HD2 | 2.13 | 0.48 |
| 2:B:39:VAL:HG23 | 2:B:40:ASN:ND2 | 2.27 | 0.48 |
| 3:C:166:ARG:HH21 | 10:C:401:HEC:HAD2 | 1.79 | 0.48 |
| 3:F:89:TYR:CD2 | 3:F:101:ARG:NH1 | 2.82 | 0.48 |
| 1:G:359:ILE:HD12 | 1:G:384:HIS:CE1 | 2.48 | 0.48 |
| 2:H:140:TYR:CE1 | 10:H:301:HEC:HBB2 | 2.48 | 0.48 |
| 1:D:84:THR:O | 3:F:44:PHE:HD2 | 1.95 | 0.48 |
| 1:D:233:PRO:CG | 3:F:50:TYR:CE2 | 2.90 | 0.48 |
| 1:G:57:ARG:NH1 | 5:G:502:HEM:O2A | 2.46 | 0.48 |
| 3:M:28:ARG:HG3 | 3:M:31:GLU:OE2 | 2.13 | 0.48 |
| 1:A:384:HIS:CE1 | 1:A:451:MET:HB2 | 2.49 | 0.48 |
| 3:C:184:ALA:HB1 | 10:C:401:HEC:HMD1 | 1.96 | 0.48 |
| 3:F:123:GLU:O | 3:F:127:GLN:HG3 | 2.14 | 0.48 |
| 3:I:179:LEU:HD23 | 3:I:291:VAL:HG11 | 1.96 | 0.48 |
| 3:M:37:ASP:OD1 | 3:M:38:GLN:N | 2.46 | 0.48 |
| 1:D:415:ASP:O | 3:F:110:TYR:CE2 | 2.67 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:416:ASP:CA | 3:F:110:TYR:HE2 | 2.26 | 0.48 |
| 1:G:159:VAL:HA | 1:G:162:TRP:CD2 | 2.49 | 0.48 |
| 1:K:233:PRO:CG | 3:M:50:TYR:CZ | 2.97 | 0.48 |
| 1:K:340:ASP:H | 1:K:406:GLN:NE2 | 2.12 | 0.48 |
| 1:G:384:HIS:CE1 | 1:G:451:MET:HB2 | 2.49 | 0.48 |
| 2:L:62:ARG:HH22 | 2:L:184:GLU:CD | 2.17 | 0.48 |
| 2:B:161:ARG:HA | 2:B:165:VAL:O | 2.14 | 0.48 |
| 1:D:159:VAL:HA | 1:D:162:TRP:CD2 | 2.49 | 0.48 |
| 3:F:40:MET:SD | 3:F:42:HIS:ND1 | 2.87 | 0.48 |
| 3:F:179:LEU:HD23 | 3:F:291:VAL:HG11 | 1.94 | 0.48 |
| 3:M:255:ALA:HA | 3:M:258:TRP:CD2 | 2.49 | 0.48 |
| 2:B:63:GLU:HB3 | 10:B:301:HEC:HBB1 | 1.96 | 0.48 |
| 1:K:376:HIS:H | 1:K:458:THR:CG2 | 2.27 | 0.48 |
| 1:A:310:LEU:O | 1:A:313:SER:HB3 | 2.13 | 0.47 |
| 3:C:189:TRP:O | 3:C:193:ILE:HG22 | 2.14 | 0.47 |
| 3:M:111:GLY:N | 3:M:112:PRO:CD | 2.77 | 0.47 |
| 3:M:178:ILE:HG12 | 10:M:403:HEC:HMB2 | 1.96 | 0.47 |
| 1:A:416:ASP:OD2 | 3:C:137:ARG:NH1 | 2.47 | 0.47 |
| 1:D:76:THR:HG21 | 1:D:221:ILE:CG1 | 2.44 | 0.47 |
| 1:G:315:ALA:HB2 | 4:P:24:PHE:CE1 | 2.48 | 0.47 |
| 3:I:122:VAL:HG22 | 3:I:292:HIS:CD2 | 2.50 | 0.47 |
| 3:F:14:LEU:HD23 | 3:F:17:ILE:HD12 | 1.96 | 0.47 |
| 1:K:57:ARG:NH2 | 5:K:502:HEM:O2D | 2.47 | 0.47 |
| 1:K:227:PRO:HB3 | 3:M:47:ILE:HG21 | 1.95 | 0.47 |
| 1:K:346:VAL:HG22 | 5:K:501:HEM:C2D | 2.49 | 0.47 |
| 3:M:44:PHE:O | 3:M:47:ILE:N | 2.47 | 0.47 |
| 1:A:346:VAL:HG22 | 5:A:501:HEM:C3D | 2.49 | 0.47 |
| 1:D:346:VAL:HG22 | 5:D:501:HEM:C3D | 2.49 | 0.47 |
| 1:K:376:HIS:H | 1:K:458:THR:HG22 | 1.80 | 0.47 |
| 2:B:137:MET:HB2 | 10:B:301:HEC:C1D | 2.44 | 0.47 |
| 2:E:62:ARG:HH22 | 2:E:184:GLU:CD | 2.18 | 0.47 |
| 3:I:187:PRO:HG2 | 3:I:189:TRP:CZ2 | 2.49 | 0.47 |
| 1:K:359:ILE:HD11 | 1:K:448:MET:CE | 2.44 | 0.47 |
| 1:A:236:SER:HA | 3:C:52:ASN:HB2 | 1.97 | 0.47 |
| 2:H:152:ASP:HA | 2:H:155:LYS:HE3 | 1.95 | 0.47 |
| 2:L:86:TYR:OH | 3:M:96:GLU:OE1 | 2.17 | 0.47 |
| 3:C:270:THR:HG23 | 3:C:275:ARG:HG2 | 1.97 | 0.47 |
| 1:D:228:LYS:HA | 3:F:47:ILE:HD11 | 1.95 | 0.47 |
| 1:D:230:ALA:O | 1:D:300:LYS:NZ | 2.38 | 0.47 |
| 1:D:412:ALA:HA | 4:O:2:PHE:CD2 | 2.50 | 0.47 |
| 1:G:94:LEU:O | 1:G:98:THR:HG23 | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:250:VAL:HG11 | 1:G:278:ILE:HG22 | 1.97 | 0.47 |
| 1:G:253:TRP:CH2 | 3:I:13:THR:HA | 2.49 | 0.47 |
| 1:G:310:LEU:O | 1:G:313:SER:HB3 | 2.14 | 0.47 |
| 1:G:359:ILE:HD11 | 1:G:448:MET:CE | 2.43 | 0.47 |
| 1:K:81:VAL:HG23 | 1:K:161:ASN:ND2 | 2.29 | 0.47 |
| 1:K:226:VAL:HB | 1:K:227:PRO:HD3 | 1.96 | 0.47 |
| 1:K:359:ILE:HD11 | 1:K:448:MET:HE1 | 1.95 | 0.47 |
| 1:K:446:ALA:O | 1:K:450:VAL:HG23 | 2.15 | 0.47 |
| 2:L:161:ARG:HA | 2:L:165:VAL:O | 2.15 | 0.47 |
| 3:M:166:ARG:NH2 | 3:M:250:PRO:HG3 | 2.30 | 0.47 |
| 1:A:128:TRP:CG | 1:A:129:PRO:HD3 | 2.49 | 0.47 |
| 1:G:233:PRO:CG | 3:I:50:TYR:CE2 | 2.93 | 0.47 |
| 1:K:82:GLN:CD | 1:K:89:LEU:HG | 2.35 | 0.47 |
| 1:K:453:TYR:O | 1:K:457:ARG:HG2 | 2.15 | 0.47 |
| 2:L:62:ARG:HG3 | 2:L:63:GLU:N | 2.29 | 0.47 |
| 3:F:68:PHE:HD1 | 3:F:68:PHE:O | 1.98 | 0.47 |
| 3:F:120:MET:HE2 | 3:F:120:MET:HB3 | 1.83 | 0.47 |
| 2:H:62:ARG:NH1 | 2:H:63:GLU:OE2 | 2.48 | 0.47 |
| 3:M:184:ALA:HB1 | 10:M:402:HEC:HMD1 | 1.97 | 0.47 |
| 4:P:23:GLY:O | 4:P:27:PHE:HB2 | 2.14 | 0.47 |
| 1:A:376:HIS:CB | 1:A:458:THR:HG22 | 2.44 | 0.47 |
| 1:D:253:TRP:HZ3 | 3:F:13:THR:HG22 | 1.79 | 0.47 |
| 3:I:73:LEU:CD1 | 3:I:79:LEU:HG | 2.45 | 0.47 |
| 3:I:189:TRP:O | 3:I:193:ILE:HG22 | 2.15 | 0.47 |
| 1:K:252:ILE:HD11 | 2:L:22:VAL:HG22 | 1.97 | 0.47 |
| 1:K:463:LYS:HB2 | 1:K:464:PRO:CD | 2.45 | 0.47 |
| 1:A:76:THR:HG21 | 1:A:221:ILE:CG1 | 2.43 | 0.46 |
| 1:K:287:MET:HG3 | 1:K:288:ILE:N | 2.30 | 0.46 |
| 2:L:140:TYR:CE1 | 10:L:301:HEC:HBB2 | 2.50 | 0.46 |
| 3:M:157:PHE:HA | 3:M:158:PRO:HD3 | 1.81 | 0.46 |
| 1:D:350:ALA:HB1 | 5:D:502:HEM:CAC | 2.45 | 0.46 |
| 3:F:215:PRO:HB3 | 11:I:401:FC6:N24 | 2.30 | 0.46 |
| 3:C:179:LEU:HD22 | 3:C:283:GLN:HB2 | 1.97 | 0.46 |
| 1:D:124:ALA:HB2 | 1:D:205:TYR:CE2 | 2.51 | 0.46 |
| 2:E:63:GLU:HB3 | 10:E:301:HEC:HBB1 | 1.97 | 0.46 |
| 1:G:13:VAL:HA | 1:G:16:GLN:HE21 | 1.79 | 0.46 |
| 3:I:24:ILE:HD13 | 3:I:24:ILE:C | 2.35 | 0.46 |
| 1:K:156:HIS:ND1 | 2:L:8:GLU:OE2 | 2.49 | 0.46 |
| 1:A:242:VAL:HG21 | 3:C:54:LEU:HD21 | 1.98 | 0.46 |
| 3:F:32:SER:HB3 | 3:F:36:THR:OG1 | 2.14 | 0.46 |
| 1:G:350:ALA:HB1 | 5:G:502:HEM:CAC | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:57:TRP:CG | 3:M:58:TRP:N | 2.83 | 0.46 |
| 4:Q:20:PHE:C | 4:Q:20:PHE:CD2 | 2.88 | 0.46 |
| 3:F:133:LYS:HD2 | 3:F:133:LYS:HA | 1.76 | 0.46 |
| 11:F:403:FC6:C21 | 3:I:215:PRO:HG3 | 2.45 | 0.46 |
| 2:H:161:ARG:HA | 2:H:165:VAL:O | 2.15 | 0.46 |
| 4:P:13:THR:O | 4:P:17:MET:HG2 | 2.16 | 0.46 |
| 1:A:238:ARG:HH22 | 3:C:30:GLY:C | 2.17 | 0.46 |
| 1:D:57:ARG:NH1 | 5:D:502:HEM:O2A | 2.48 | 0.46 |
| 3:F:86:LEU:HG | 3:F:87:PRO:CD | 2.39 | 0.46 |
| 3:I:6:SER:HB2 | 3:I:81:ASN:ND2 | 2.24 | 0.46 |
| 4:Q:21:LEU:HD13 | 4:Q:21:LEU:HA | 1.60 | 0.46 |
| 3:C:50:TYR:HB3 | 3:C:52:ASN:ND2 | 2.31 | 0.46 |
| 1:D:415:ASP:O | 3:F:110:TYR:HE2 | 1.98 | 0.46 |
| 3:I:89:TYR:CZ | 3:I:101:ARG:HD2 | 2.50 | 0.46 |
| 1:K:174:LEU:HD21 | 1:K:208:ASN:HB3 | 1.97 | 0.46 |
| 3:M:236:CYS:O | 3:M:244:MET:HG3 | 2.15 | 0.46 |
| 3:F:17:ILE:HA | 3:F:20:LEU:HG | 1.98 | 0.46 |
| 1:G:227:PRO:HB2 | 3:I:47:ILE:HG23 | 1.96 | 0.46 |
| 1:K:228:LYS:CA | 3:M:47:ILE:HD11 | 2.45 | 0.46 |
| 3:M:2:SER:OG | 3:M:5:TRP:CD1 | 2.66 | 0.46 |
| 1:A:66:PHE:O | 1:A:70:GLY:HA3 | 2.16 | 0.46 |
| 2:B:113:GLY:O | 2:B:193:GLN:NE2 | 2.49 | 0.46 |
| 1:K:42:PRO:HG3 | 2:L:136:LYS:HD2 | 1.97 | 0.46 |
| 3:M:105:GLN:HB3 | 3:M:109:LYS:HZ1 | 1.81 | 0.46 |
| 3:C:85:VAL:HG12 | 3:C:85:VAL:O | 2.15 | 0.46 |
| 1:D:226:VAL:HB | 1:D:227:PRO:HD3 | 1.97 | 0.46 |
| 3:F:57:TRP:HZ3 | 3:F:61:LEU:HD12 | 1.80 | 0.46 |
| 2:H:137:MET:HB2 | 10:H:301:HEC:CHD | 2.46 | 0.46 |
| 1:K:196:ALA:HB3 | 2:L:39:VAL:HB | 1.97 | 0.46 |
| 1:K:234:VAL:N | 3:M:48:GLU:O | 2.49 | 0.46 |
| 1:K:359:ILE:HD12 | 1:K:384:HIS:CE1 | 2.50 | 0.46 |
| 1:A:57:ARG:NH1 | 5:A:502:HEM:HAA1 | 2.31 | 0.45 |
| 1:A:250:VAL:CG2 | 3:C:20:LEU:HD11 | 2.46 | 0.45 |
| 2:B:125:LEU:HD21 | 10:B:301:HEC:HMB2 | 1.98 | 0.45 |
| 1:D:455:THR:HG22 | 1:D:459:VAL:CG2 | 2.46 | 0.45 |
| 2:E:86:TYR:HE2 | 3:F:99:TRP:CZ3 | 2.33 | 0.45 |
| 3:F:207:LYS:HA | 3:F:212:LEU:O | 2.15 | 0.45 |
| 1:G:321:THR:HG22 | 5:G:501:HEM:HAB | 1.98 | 0.45 |
| 2:L:72:MET:HE3 | 2:L:100:TRP:CD2 | 2.50 | 0.45 |
| 1:A:242:VAL:HG22 | 3:C:27:THR:HG21 | 1.98 | 0.45 |
| 1:A:264:LEU:HD12 | 1:A:265:PRO:HD2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:8:TYR:CE2 | 3:F:12:LEU:HD13 | 2.52 | 0.45 |
| 3:I:24:ILE:HD12 | 3:I:59:PHE:CE2 | 2.48 | 0.45 |
| 3:I:98:GLN:O | 3:I:101:ARG:HB2 | 2.17 | 0.45 |
| 1:A:350:ALA:HB1 | 5:A:502:HEM:CAC | 2.47 | 0.45 |
| 3:F:122:VAL:HG22 | 3:F:292:HIS:NE2 | 2.30 | 0.45 |
| 2:H:137:MET:HB2 | 10:H:301:HEC:C1D | 2.47 | 0.45 |
| 3:I:140:ALA:HA | 3:I:144:SER:HB3 | 1.99 | 0.45 |
| 1:A:250:VAL:HG11 | 1:A:278:ILE:HG22 | 1.99 | 0.45 |
| 1:D:128:TRP:CG | 1:D:129:PRO:HD3 | 2.51 | 0.45 |
| 2:H:62:ARG:HH22 | 2:H:184:GLU:CD | 2.20 | 0.45 |
| 1:K:12:LYS:HA | 1:K:15:ARG:NH1 | 2.31 | 0.45 |
| 1:K:317:TYR:HB2 | 1:K:353:TRP:CE3 | 2.51 | 0.45 |
| 2:B:57:ARG:NH1 | 2:B:99:LEU:HD12 | 2.31 | 0.45 |
| 1:D:174:LEU:HD21 | 1:D:208:ASN:HB3 | 1.98 | 0.45 |
| 1:D:379:GLY:O | 1:D:383:THR:HG23 | 2.17 | 0.45 |
| 1:D:414:ASN:HD21 | 1:D:420:THR:HG23 | 1.81 | 0.45 |
| 1:D:416:ASP:HA | 3:F:110:TYR:HE2 | 1.81 | 0.45 |
| 1:G:156:HIS:HD2 | 3:I:42:HIS:CD2 | 2.33 | 0.45 |
| 1:K:224:TYR:HE1 | 3:M:45:ASP:OD2 | 2.00 | 0.45 |
| 3:M:167:TRP:CD2 | 3:M:182:ARG:HG2 | 2.50 | 0.45 |
| 1:A:82:GLN:HE21 | 1:A:88:THR:HA | 1.82 | 0.45 |
| 1:A:152:ARG:NH2 | 2:B:9:LYS:O | 2.50 | 0.45 |
| 3:C:4:PHE:CD2 | 3:C:4:PHE:C | 2.89 | 0.45 |
| 3:C:177:SER:OG | 3:C:182:ARG:NH1 | 2.45 | 0.45 |
| 1:D:237:TYR:CE2 | 1:D:241:ILE:HD11 | 2.51 | 0.45 |
| 1:D:376:HIS:CG | 1:D:457:ARG:HB2 | 2.51 | 0.45 |
| 3:F:28:ARG:O | 3:F:28:ARG:HD3 | 2.16 | 0.45 |
| 3:F:236:CYS:O | 3:F:244:MET:HG3 | 2.17 | 0.45 |
| 3:I:184:ALA:HB1 | 10:I:402:HEC:HMD1 | 1.99 | 0.45 |
| 1:K:346:VAL:HG22 | 5:K:501:HEM:C3D | 2.52 | 0.45 |
| 1:A:233:PRO:HG2 | 3:C:50:TYR:CZ | 2.51 | 0.45 |
| 1:D:287:MET:HG3 | 1:D:288:ILE:N | 2.31 | 0.45 |
| 1:K:115:LEU:HB3 | 1:K:117:PHE:CE2 | 2.51 | 0.45 |
| 1:K:308:ARG:NH1 | 1:K:382:ASN:HD21 | 2.14 | 0.45 |
| 3:M:73:LEU:CD2 | 3:M:79:LEU:HD11 | 2.46 | 0.45 |
| 1:A:336:SER:O | 1:A:339:THR:OG1 | 2.17 | 0.45 |
| 2:B:109:LEU:O | 2:B:112:VAL:HG22 | 2.17 | 0.45 |
| 2:B:140:TYR:CE1 | 10:B:301:HEC:HBB2 | 2.51 | 0.45 |
| 1:D:158:TYR:HB2 | 3:F:44:PHE:CD2 | 2.51 | 0.45 |
| 3:F:67:VAL:O | 3:F:71:LEU:HD13 | 2.17 | 0.45 |
| 3:F:135:GLY:HA3 | 3:F:297:TYR:HB2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:233:PRO:HG2 | 3:M:50:TYR:CE2 | 2.51 | 0.45 |
| 1:K:301:LEU:HD21 | 1:K:311:VAL:HG21 | 1.98 | 0.45 |
| 1:A:253:TRP:CH2 | 3:C:13:THR:HA | 2.52 | 0.45 |
| 3:C:31:GLU:HG3 | 3:C:53:PRO:HB3 | 1.99 | 0.45 |
| 1:D:82:GLN:HE21 | 1:D:89:LEU:H | 1.65 | 0.45 |
| 1:G:309:PHE:CE2 | 1:G:359:ILE:HG21 | 2.52 | 0.45 |
| 1:A:73:LEU:HD12 | 1:A:73:LEU:HA | 1.81 | 0.45 |
| 1:A:159:VAL:HA | 1:A:162:TRP:CD2 | 2.52 | 0.45 |
| 1:D:81:VAL:HG23 | 1:D:161:ASN:ND2 | 2.32 | 0.45 |
| 2:E:137:MET:HB2 | 10:E:301:HEC:C1D | 2.47 | 0.45 |
| 1:G:212:PHE:HA | 1:G:216:ALA:HB3 | 1.99 | 0.45 |
| 3:I:186:MET:HG2 | 10:I:402:HEC:C1D | 2.44 | 0.45 |
| 3:M:270:THR:HG23 | 3:M:275:ARG:HG2 | 1.98 | 0.45 |
| 1:G:82:GLN:HE21 | 1:G:89:LEU:H | 1.65 | 0.44 |
| 1:G:128:TRP:CG | 1:G:129:PRO:HD3 | 2.52 | 0.44 |
| 3:I:255:ALA:HA | 3:I:258:TRP:CD2 | 2.51 | 0.44 |
| 1:K:235:TYR:CE2 | 1:K:292:MET:HB2 | 2.51 | 0.44 |
| 1:K:355:ALA:O | 1:K:359:ILE:HG12 | 2.16 | 0.44 |
| 3:M:40:MET:HG2 | 3:M:51:ASP:HB2 | 1.98 | 0.44 |
| 3:M:43:ALA:CB | 3:M:48:GLU:HB3 | 2.46 | 0.44 |
| 1:A:238:ARG:O | 1:A:242:VAL:HG23 | 2.18 | 0.44 |
| 1:A:291:MET:SD | 4:N:24:PHE:HZ | 2.40 | 0.44 |
| 2:B:88:VAL:HG12 | 2:B:90:GLY:H | 1.82 | 0.44 |
| 1:D:115:LEU:HB3 | 1:D:117:PHE:CE2 | 2.51 | 0.44 |
| 1:D:267:TRP:HB2 | 3:F:78:GLY:O | 2.17 | 0.44 |
| 1:D:443:ILE:O | 1:D:446:ALA:HB3 | 2.17 | 0.44 |
| 5:D:501:HEM:HMB1 | 5:D:501:HEM:HBB2 | 1.98 | 0.44 |
| 3:F:4:PHE:CD1 | 3:F:4:PHE:C | 2.90 | 0.44 |
| 1:K:411:ARG:NH1 | 4:Q:4:ASP:OD2 | 2.51 | 0.44 |
| 3:M:205:VAL:HG21 | 10:M:402:HEC:HMB3 | 1.99 | 0.44 |
| 3:C:36:THR:HG22 | 3:C:38:GLN:HG2 | 1.99 | 0.44 |
| 2:E:109:LEU:O | 2:E:112:VAL:HG22 | 2.18 | 0.44 |
| 3:F:68:PHE:HA | 3:F:71:LEU:HD22 | 1.99 | 0.44 |
| 10:F:401:HEC:HMC1 | 10:F:401:HEC:HBC3 | 1.99 | 0.44 |
| 3:I:121:SER:O | 3:I:125:VAL:HG23 | 2.16 | 0.44 |
| 9:K:506:PO4:P | 3:M:72:TYR:OH | 2.75 | 0.44 |
| 10:C:402:HEC:HBC3 | 10:C:402:HEC:HMC1 | 1.98 | 0.44 |
| 1:D:11:TYR:CD1 | 1:D:369:VAL:HA | 2.53 | 0.44 |
| 1:D:64:VAL:HG11 | 5:D:502:HEM:C4C | 2.53 | 0.44 |
| 3:F:73:LEU:HB3 | 3:F:79:LEU:CD1 | 2.43 | 0.44 |
| 1:G:82:GLN:HE21 | 1:G:88:THR:HA | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:90:PHE:CD1 | 1:K:147:GLY:CA | 3.01 | 0.44 |
| 3:M:56:ARG:O | 3:M:59:PHE:HB3 | 2.17 | 0.44 |
| 1:A:207:HIS:CD2 | 1:A:251:TYR:HD1 | 2.33 | 0.44 |
| 1:A:226:VAL:HB | 1:A:227:PRO:HD3 | 1.99 | 0.44 |
| 2:B:62:ARG:HH22 | 2:B:184:GLU:CD | 2.20 | 0.44 |
| 1:D:174:LEU:HD12 | 1:D:204:TRP:CZ2 | 2.52 | 0.44 |
| 3:F:38:GLN:CA | 3:F:38:GLN:HE21 | 2.29 | 0.44 |
| 3:F:89:TYR:CD1 | 3:F:93:TRP:HD1 | 2.36 | 0.44 |
| 3:F:121:SER:C | 3:F:125:VAL:HG23 | 2.37 | 0.44 |
| 1:G:367:PRO:HD3 | 1:G:375:MET:HE3 | 1.99 | 0.44 |
| 1:K:384:HIS:CE1 | 1:K:451:MET:HB2 | 2.52 | 0.44 |
| 2:L:152:ASP:HA | 2:L:155:LYS:HE3 | 1.98 | 0.44 |
| 3:M:38:GLN:O | 3:M:50:TYR:CE2 | 2.71 | 0.44 |
| 1:A:305:PRO:HB2 | 1:A:381:ILE:HG22 | 1.98 | 0.44 |
| 1:G:76:THR:HG21 | 1:G:221:ILE:CG1 | 2.45 | 0.44 |
| 1:G:261:TYR:HA | 3:I:95:GLN:OE1 | 2.18 | 0.44 |
| 1:G:264:LEU:HD12 | 1:G:265:PRO:HD2 | 1.99 | 0.44 |
| 1:G:377:SER:H | 1:G:454:ASN:HD21 | 1.66 | 0.44 |
| 2:L:148:LEU:HD11 | 2:L:187:ALA:HB2 | 2.00 | 0.44 |
| 1:D:331:THR:O | 4:O:6:VAL:HG13 | 2.18 | 0.44 |
| 1:G:340:ASP:H | 1:G:406:GLN:HE22 | 1.65 | 0.44 |
| 2:L:129:ARG:HD3 | 2:L:135:SER:O | 2.18 | 0.44 |
| 4:Q:4:ASP:H | 4:Q:7:VAL:HB | 1.82 | 0.44 |
| 1:A:39:LEU:HD23 | 1:A:39:LEU:HA | 1.88 | 0.44 |
| 3:C:121:SER:O | 3:C:125:VAL:HG23 | 2.18 | 0.44 |
| 3:C:242:GLU:CD | 3:C:242:GLU:H | 2.20 | 0.44 |
| 5:G:501:HEM:HMB1 | 5:G:501:HEM:HBB2 | 1.99 | 0.44 |
| 1:A:81:VAL:HG23 | 1:A:161:ASN:ND2 | 2.33 | 0.44 |
| 3:C:157:PHE:HA | 3:C:158:PRO:HD3 | 1.83 | 0.44 |
| 2:E:80:THR:HA | 2:E:84:GLY:O | 2.18 | 0.44 |
| 3:F:88:GLY:O | 3:F:89:TYR:HD2 | 2.01 | 0.44 |
| 1:G:108:LEU:HD12 | 1:G:108:LEU:HA | 1.80 | 0.44 |
| 1:G:305:PRO:HB2 | 1:G:381:ILE:HG22 | 2.00 | 0.44 |
| 1:K:76:THR:HG21 | 1:K:221:ILE:CG1 | 2.46 | 0.44 |
| 3:M:189:TRP:O | 3:M:193:ILE:HG22 | 2.16 | 0.44 |
| 3:F:82:TRP:C | 3:F:82:TRP:HD1 | 2.19 | 0.43 |
| 1:K:11:TYR:CD1 | 1:K:369:VAL:HA | 2.53 | 0.43 |
| 3:M:140:ALA:HA | 3:M:144:SER:HB3 | 2.00 | 0.43 |
| 3:C:140:ALA:O | 3:C:144:SER:OG | 2.21 | 0.43 |
| 1:D:170:THR:HB | 2:E:22:VAL:HG21 | 1.99 | 0.43 |
| 1:D:182:ILE:HD12 | 2:E:163:LEU:HG | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:111:ARG:HH22 | 2:E:199:LEU:HD13 | 1.83 | 0.43 |
| 2:E:161:ARG:HA | 2:E:165:VAL:O | 2.19 | 0.43 |
| 1:K:379:GLY:O | 1:K:383:THR:HG23 | 2.17 | 0.43 |
| 2:L:51:ALA:HB1 | 2:L:153:THR:HG21 | 1.99 | 0.43 |
| 4:P:4:ASP:H | 4:P:7:VAL:HB | 1.83 | 0.43 |
| 1:A:235:TYR:CD1 | 1:A:236:SER:HB2 | 2.54 | 0.43 |
| 1:A:350:ALA:HB1 | 5:A:502:HEM:C3C | 2.54 | 0.43 |
| 1:D:321:THR:HG22 | 5:D:501:HEM:HAB | 2.00 | 0.43 |
| 1:K:235:TYR:CD2 | 1:K:292:MET:CB | 3.01 | 0.43 |
| 1:K:376:HIS:HB3 | 1:K:454:ASN:ND2 | 2.32 | 0.43 |
| 1:K:377:SER:H | 1:K:454:ASN:HD21 | 1.67 | 0.43 |
| 2:B:6:LYS:HD2 | 2:B:6:LYS:HA | 1.61 | 0.43 |
| 3:C:74:VAL:O | 3:C:82:TRP:HH2 | 2.02 | 0.43 |
| 1:D:264:LEU:HD12 | 1:D:265:PRO:HD2 | 1.99 | 0.43 |
| 1:D:384:HIS:HE1 | 1:D:451:MET:HE3 | 1.83 | 0.43 |
| 3:F:83:LYS:HD2 | 3:F:91:GLY:O | 2.17 | 0.43 |
| 3:F:114:PHE:CD1 | 3:F:289:ASP:HB3 | 2.53 | 0.43 |
| 1:G:35:ILE:HB | 1:G:53:PHE:CE1 | 2.54 | 0.43 |
| 3:I:121:SER:OG | 3:I:123:GLU:HG2 | 2.19 | 0.43 |
| 3:M:38:GLN:HB2 | 3:M:39:THR:H | 1.64 | 0.43 |
| 4:O:20:PHE:C | 4:O:20:PHE:CD2 | 2.92 | 0.43 |
| 4:O:26:TYR:N | 4:O:26:TYR:CD2 | 2.86 | 0.43 |
| 1:D:207:HIS:CD2 | 1:D:251:TYR:HD1 | 2.36 | 0.43 |
| 1:D:463:LYS:H | 1:D:463:LYS:HG2 | 1.59 | 0.43 |
| 1:G:354:VAL:O | 1:G:358:SER:OG | 2.30 | 0.43 |
| 1:K:124:ALA:HB2 | 1:K:205:TYR:CE2 | 2.52 | 0.43 |
| 1:K:305:PRO:O | 1:K:308:ARG:HB2 | 2.18 | 0.43 |
| 2:L:42:PRO:HG3 | 2:L:93:VAL:HG11 | 2.00 | 0.43 |
| 3:M:89:TYR:HA | 3:M:101:ARG:NH2 | 2.33 | 0.43 |
| 4:P:4:ASP:OD1 | 4:P:5:ASN:N | 2.48 | 0.43 |
| 1:D:92:PRO:O | 1:D:95:ALA:HB3 | 2.18 | 0.43 |
| 1:D:238:ARG:NH1 | 3:F:30:GLY:O | 2.52 | 0.43 |
| 3:I:205:VAL:HG21 | 10:I:402:HEC:HMB3 | 2.01 | 0.43 |
| 1:K:233:PRO:CG | 3:M:50:TYR:CE2 | 3.02 | 0.43 |
| 1:K:309:PHE:CE2 | 1:K:359:ILE:HG21 | 2.54 | 0.43 |
| 1:K:446:ALA:HA | 1:K:449:LEU:HD12 | 2.00 | 0.43 |
| 3:M:60:LEU:HD13 | 3:M:61:LEU:N | 2.34 | 0.43 |
| 1:A:410:TRP:O | 2:B:82:ARG:NH1 | 2.52 | 0.43 |
| 1:A:457:ARG:HH11 | 1:A:457:ARG:HD2 | 1.67 | 0.43 |
| 3:C:206:ARG:HG2 | 3:C:212:LEU:HB2 | 2.01 | 0.43 |
| 3:F:120:MET:HE1 | 3:F:124:GLU:HB3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:258:TRP:CZ3 | 3:F:267:LEU:HD21 | 2.54 | 0.43 |
| 1:G:346:VAL:HG22 | 5:G:501:HEM:C3D | 2.53 | 0.43 |
| 1:G:371:GLY:HA3 | 1:G:465:ALA:HB1 | 1.99 | 0.43 |
| 3:I:57:TRP:CG | 3:I:58:TRP:N | 2.86 | 0.43 |
| 3:M:77:PRO:HG3 | 3:M:93:TRP:O | 2.19 | 0.43 |
| 3:C:20:LEU:HD23 | 3:C:20:LEU:HA | 1.78 | 0.43 |
| 3:C:45:ASP:CG | 3:C:46:GLY:H | 2.22 | 0.43 |
| 3:C:50:TYR:HB2 | 3:C:52:ASN:HD22 | 1.84 | 0.43 |
| 1:D:108:LEU:HD12 | 1:D:108:LEU:HA | 1.81 | 0.43 |
| 1:D:350:ALA:HB1 | 5:D:502:HEM:C3C | 2.54 | 0.43 |
| 1:D:376:HIS:CE1 | 1:D:457:ARG:HG3 | 2.54 | 0.43 |
| 3:F:58:TRP:CH2 | 3:F:62:PHE:HD2 | 2.37 | 0.43 |
| 1:G:207:HIS:CD2 | 1:G:251:TYR:HD1 | 2.36 | 0.43 |
| 3:I:85:VAL:HG12 | 3:I:85:VAL:O | 2.19 | 0.43 |
| 1:K:128:TRP:CG | 1:K:129:PRO:HD3 | 2.54 | 0.43 |
| 1:K:159:VAL:HA | 1:K:162:TRP:CD2 | 2.54 | 0.43 |
| 1:A:55:ARG:HH21 | 2:B:63:GLU:CD | 2.22 | 0.43 |
| 1:A:343:ILE:HG12 | 5:A:502:HEM:HBA2 | 2.01 | 0.43 |
| 2:E:51:ALA:HB1 | 2:E:153:THR:HG21 | 2.01 | 0.43 |
| 3:F:37:ASP:HB2 | 3:F:38:GLN:NE2 | 2.34 | 0.43 |
| 3:F:206:ARG:HG2 | 3:F:212:LEU:HB2 | 2.00 | 0.43 |
| 1:G:228:LYS:NZ | 3:I:45:ASP:OD1 | 2.46 | 0.43 |
| 3:I:24:ILE:CD1 | 3:I:59:PHE:HE2 | 2.31 | 0.43 |
| 3:I:229:TYR:HE1 | 3:I:239:GLN:HA | 1.83 | 0.43 |
| 3:I:279:MET:HB2 | 10:I:403:HEC:C4D | 2.48 | 0.43 |
| 1:K:463:LYS:CB | 1:K:464:PRO:CD | 2.95 | 0.43 |
| 3:M:279:MET:HB2 | 10:M:403:HEC:C4D | 2.48 | 0.43 |
| 1:A:266:ASP:OD2 | 3:C:95:GLN:HG2 | 2.19 | 0.43 |
| 1:A:319:MET:HG3 | 1:A:320:SER:N | 2.34 | 0.43 |
| 1:A:327:MET:HE2 | 1:A:327:MET:HB2 | 1.86 | 0.43 |
| 3:C:264:LEU:O | 3:C:268:GLN:HG3 | 2.19 | 0.43 |
| 1:D:158:TYR:HE2 | 3:F:49:GLU:OE2 | 2.02 | 0.43 |
| 1:D:260:HIS:HB2 | 1:D:333:ASN:OD1 | 2.19 | 0.43 |
| 1:D:335:LEU:HD13 | 4:O:7:VAL:HA | 2.00 | 0.43 |
| 1:G:446:ALA:O | 1:G:450:VAL:HG23 | 2.19 | 0.43 |
| 3:I:24:ILE:CD1 | 3:I:59:PHE:CE2 | 3.02 | 0.43 |
| 1:K:125:GLU:H | 1:K:125:GLU:HG2 | 1.42 | 0.43 |
| 2:L:140:TYR:OH | 10:L:301:HEC:HMC2 | 2.19 | 0.43 |
| 1:A:195:GLY:HA2 | 2:B:92:SER:HB2 | 2.00 | 0.42 |
| 1:D:308:ARG:NH1 | 1:D:382:ASN:HD21 | 2.17 | 0.42 |
| 2:E:116:TYR:HE2 | 3:F:145:ILE:HG21 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:60:LEU:HA | 3:F:60:LEU:HD23 | 1.74 | 0.42 |
| 3:F:279:MET:HB2 | 10:F:402:HEC:C4D | 2.49 | 0.42 |
| 3:I:50:TYR:CB | 3:I:52:ASN:OD1 | 2.64 | 0.42 |
| 3:I:63:ILE:HD13 | 3:I:63:ILE:N | 2.34 | 0.42 |
| 3:I:206:ARG:HG2 | 3:I:212:LEU:HB2 | 2.01 | 0.42 |
| 1:A:196:ALA:HB3 | 2:B:39:VAL:HB | 2.02 | 0.42 |
| 2:E:62:ARG:HG3 | 2:E:63:GLU:N | 2.34 | 0.42 |
| 3:F:103:VAL:HG12 | 3:F:107:ASP:OD2 | 2.19 | 0.42 |
| 1:G:235:TYR:CD1 | 1:G:236:SER:HB2 | 2.53 | 0.42 |
| 3:C:59:PHE:CD1 | 3:C:63:ILE:HD11 | 2.53 | 0.42 |
| 3:C:177:SER:HA | 3:C:182:ARG:HD2 | 2.02 | 0.42 |
| 1:D:13:VAL:HA | 1:D:16:GLN:NE2 | 2.35 | 0.42 |
| 1:D:349:GLY:O | 1:D:353:TRP:HB3 | 2.20 | 0.42 |
| 3:F:179:LEU:HD22 | 3:F:283:GLN:HB2 | 2.00 | 0.42 |
| 2:H:7:LEU:HA | 2:H:10:ASN:ND2 | 2.30 | 0.42 |
| 2:H:80:THR:HA | 2:H:84:GLY:O | 2.19 | 0.42 |
| 3:I:24:ILE:HD11 | 3:I:59:PHE:CD2 | 2.54 | 0.42 |
| 3:I:94:THR:OG1 | 3:I:97:LYS:HG3 | 2.19 | 0.42 |
| 3:I:179:LEU:HD22 | 3:I:283:GLN:HB2 | 2.01 | 0.42 |
| 1:K:305:PRO:HA | 1:K:308:ARG:HB2 | 2.01 | 0.42 |
| 1:A:125:GLU:H | 1:A:125:GLU:HG2 | 1.30 | 0.42 |
| 1:A:218:PHE:CZ | 1:A:354:VAL:HG13 | 2.54 | 0.42 |
| 1:A:235:TYR:CE1 | 1:A:236:SER:HB2 | 2.53 | 0.42 |
| 1:A:301:LEU:HD21 | 1:A:311:VAL:HG21 | 2.01 | 0.42 |
| 1:A:454:ASN:O | 1:A:458:THR:HG23 | 2.19 | 0.42 |
| 1:D:317:TYR:HB2 | 1:D:353:TRP:CE3 | 2.55 | 0.42 |
| 1:G:226:VAL:HB | 1:G:227:PRO:HD3 | 2.01 | 0.42 |
| 3:I:75:LEU:HD22 | 3:I:86:LEU:HB2 | 2.01 | 0.42 |
| 3:I:157:PHE:HA | 3:I:158:PRO:HD3 | 1.81 | 0.42 |
| 1:A:317:TYR:HB2 | 1:A:353:TRP:CE3 | 2.54 | 0.42 |
| 1:A:395:TYR:CZ | 1:A:437:ARG:HD2 | 2.55 | 0.42 |
| 3:F:144:SER:O | 3:F:148:GLY:N | 2.52 | 0.42 |
| 2:H:116:TYR:HE2 | 3:I:145:ILE:HG21 | 1.83 | 0.42 |
| 1:K:227:PRO:HB2 | 3:M:47:ILE:HG12 | 2.02 | 0.42 |
| 10:F:402:HEC:HBC3 | 10:F:402:HEC:HMC1 | 2.00 | 0.42 |
| 1:G:208:ASN:OD1 | 1:G:252:ILE:HA | 2.20 | 0.42 |
| 3:I:297:TYR:CZ | 3:I:301:LEU:HD11 | 2.55 | 0.42 |
| 1:K:228:LYS:NZ | 3:M:46:GLY:HA3 | 2.33 | 0.42 |
| 1:K:279:LEU:O | 1:K:282:PRO:HD2 | 2.19 | 0.42 |
| 3:M:68:PHE:CA | 3:M:71:LEU:HD12 | 2.36 | 0.42 |
| 3:M:90:GLU:O | 3:M:97:LYS:NZ | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:232:THR:HB | 10:C:401:HEC:HBB1 | 2.02 | 0.42 |
| 1:D:279:LEU:O | 1:D:282:PRO:HD2 | 2.19 | 0.42 |
| 1:D:457:ARG:HD2 | 1:D:457:ARG:HA | 1.84 | 0.42 |
| 1:G:58:PRO:HA | 1:G:61:THR:HB | 2.01 | 0.42 |
| 1:G:375:MET:HG3 | 1:G:381:ILE:HD11 | 2.01 | 0.42 |
| 2:H:24:ILE:HG21 | 3:I:16:THR:HG23 | 2.01 | 0.42 |
| 1:K:349:GLY:O | 1:K:353:TRP:HB3 | 2.19 | 0.42 |
| 4:N:4:ASP:OD1 | 4:N:5:ASN:N | 2.48 | 0.42 |
| 3:C:89:TYR:CD1 | 3:C:93:TRP:CD1 | 3.07 | 0.42 |
| 1:D:309:PHE:CE2 | 1:D:359:ILE:HG21 | 2.55 | 0.42 |
| 1:K:254:ALA:O | 1:K:257:HIS:ND1 | 2.52 | 0.42 |
| 4:Q:4:ASP:OD1 | 4:Q:5:ASN:N | 2.50 | 0.42 |
| 1:A:308:ARG:NH1 | 1:A:382:ASN:HD21 | 2.18 | 0.42 |
| 1:D:62:ASN:ND2 | 1:D:125:GLU:HG3 | 2.35 | 0.42 |
| 1:D:253:TRP:CH2 | 3:F:13:THR:HA | 2.54 | 0.42 |
| 1:D:305:PRO:HB2 | 1:D:381:ILE:HG22 | 2.02 | 0.42 |
| 3:M:271:ILE:HG12 | 10:M:402:HEC:HMB2 | 2.02 | 0.42 |
| 1:A:375:MET:HA | 1:A:375:MET:HE2 | 2.02 | 0.42 |
| 2:B:80:THR:HA | 2:B:84:GLY:O | 2.20 | 0.42 |
| 3:C:50:TYR:HB2 | 3:C:52:ASN:ND2 | 2.35 | 0.42 |
| 3:C:177:SER:HB2 | 10:C:402:HEC:HMA2 | 2.02 | 0.42 |
| 1:D:307:LEU:HD12 | 1:D:307:LEU:HA | 1.94 | 0.42 |
| 2:E:56:GLY:HA2 | 2:E:59:LEU:HD12 | 2.01 | 0.42 |
| 3:F:270:THR:HG23 | 3:F:275:ARG:HG2 | 2.01 | 0.42 |
| 1:G:57:ARG:NH2 | 5:G:502:HEM:O2D | 2.52 | 0.42 |
| 1:G:81:VAL:HA | 1:G:84:THR:HG22 | 2.02 | 0.42 |
| 1:G:340:ASP:H | 1:G:406:GLN:NE2 | 2.18 | 0.42 |
| 1:A:466:GLU:OE1 | 1:A:466:GLU:HA | 2.20 | 0.41 |
| 2:B:193:GLN:HA | 2:B:193:GLN:NE2 | 2.34 | 0.41 |
| 3:F:189:TRP:O | 3:F:193:ILE:HG22 | 2.19 | 0.41 |
| 1:K:208:ASN:OD1 | 1:K:252:ILE:HA | 2.20 | 0.41 |
| 1:A:57:ARG:NH2 | 5:A:502:HEM:O2D | 2.53 | 0.41 |
| 2:B:42:PRO:HG3 | 2:B:93:VAL:HG11 | 2.02 | 0.41 |
| 3:C:22:TRP:CE3 | 3:C:23:LEU:HA | 2.54 | 0.41 |
| 3:C:35:THR:O | 3:C:52:ASN:OD1 | 2.37 | 0.41 |
| 1:D:82:GLN:HE21 | 1:D:88:THR:HA | 1.85 | 0.41 |
| 3:F:240:GLY:O | 3:F:253:ASN:HB3 | 2.20 | 0.41 |
| 1:K:263:ALA:HB3 | 2:L:100:TRP:CH2 | 2.54 | 0.41 |
| 2:B:137:MET:HA | 2:B:138:PRO:HD3 | 1.95 | 0.41 |
| 3:C:212:LEU:HD23 | 3:C:212:LEU:HA | 1.85 | 0.41 |
| 1:G:182:ILE:HD12 | 2:H:163:LEU:HG | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:411:ARG:NH1 | 4:P:4:ASP:OD2 | 2.51 | 0.41 |
| 1:K:13:VAL:HA | 1:K:16:GLN:NE2 | 2.34 | 0.41 |
| 3:M:136:ALA:HB2 | 3:M:297:TYR:CE1 | 2.54 | 0.41 |
| 1:A:108:LEU:HA | 1:A:108:LEU:HD12 | 1.78 | 0.41 |
| 1:G:10:SER:HB2 | 1:G:88:THR:HG23 | 2.02 | 0.41 |
| 1:G:218:PHE:CD2 | 1:G:221:ILE:HD12 | 2.56 | 0.41 |
| 1:G:319:MET:HG3 | 1:G:320:SER:N | 2.35 | 0.41 |
| 3:I:24:ILE:HD13 | 3:I:24:ILE:O | 2.20 | 0.41 |
| 3:M:9:ILE:HD12 | 3:M:80:GLY:HA2 | 2.02 | 0.41 |
| 1:A:12:LYS:HA | 1:A:15:ARG:NH1 | 2.34 | 0.41 |
| 1:D:94:LEU:O | 1:D:98:THR:HG23 | 2.19 | 0.41 |
| 2:E:137:MET:HB2 | 10:E:301:HEC:CHD | 2.50 | 0.41 |
| 3:F:17:ILE:HA | 3:F:20:LEU:CG | 2.50 | 0.41 |
| 3:F:89:TYR:HB3 | 3:F:97:LYS:NZ | 2.35 | 0.41 |
| 1:G:159:VAL:HA | 1:G:162:TRP:CG | 2.55 | 0.41 |
| 1:K:17:PHE:O | 1:K:21:THR:OG1 | 2.33 | 0.41 |
| 1:K:115:LEU:HD23 | 1:K:117:PHE:HE2 | 1.86 | 0.41 |
| 3:M:24:ILE:CD1 | 3:M:59:PHE:HE2 | 2.33 | 0.41 |
| 1:D:305:PRO:HA | 1:D:308:ARG:HB2 | 2.03 | 0.41 |
| 3:F:37:ASP:HB3 | 3:F:38:GLN:CA | 2.32 | 0.41 |
| 3:F:111:GLY:N | 3:F:112:PRO:CD | 2.83 | 0.41 |
| 1:G:218:PHE:CZ | 1:G:354:VAL:HG13 | 2.56 | 0.41 |
| 2:H:7:LEU:O | 2:H:7:LEU:HG | 2.20 | 0.41 |
| 2:H:125:LEU:HD21 | 10:H:301:HEC:HMB2 | 2.02 | 0.41 |
| 1:K:66:PHE:O | 1:K:70:GLY:HA3 | 2.20 | 0.41 |
| 1:K:84:THR:O | 3:M:44:PHE:CE2 | 2.74 | 0.41 |
| 1:K:193:TYR:CE1 | 1:K:201:VAL:HG11 | 2.55 | 0.41 |
| 1:K:218:PHE:CD2 | 1:K:221:ILE:HD12 | 2.55 | 0.41 |
| 3:C:40:MET:HE3 | 3:C:40:MET:HB2 | 1.99 | 0.41 |
| 1:D:235:TYR:CD1 | 1:D:236:SER:HB2 | 2.56 | 0.41 |
| 2:E:148:LEU:HD11 | 2:E:187:ALA:HB2 | 2.02 | 0.41 |
| 3:F:40:MET:CB | 3:F:49:GLU:HB2 | 2.50 | 0.41 |
| 3:F:122:VAL:HA | 3:F:125:VAL:HG23 | 2.03 | 0.41 |
| 3:F:139:PHE:CD1 | 3:F:143:CYS:HB2 | 2.56 | 0.41 |
| 1:G:64:VAL:HG21 | 5:G:502:HEM:C2C | 2.55 | 0.41 |
| 1:G:66:PHE:O | 1:G:70:GLY:HA3 | 2.21 | 0.41 |
| 1:G:174:LEU:HD21 | 1:G:208:ASN:HB3 | 2.02 | 0.41 |
| 1:G:294:LEU:HD11 | 1:G:307:LEU:HD11 | 2.03 | 0.41 |
| 3:M:215:PRO:CD | 3:M:264:LEU:HD12 | 2.51 | 0.41 |
| 2:B:128:PRO:HD3 | 2:B:139:SER:HA | 2.03 | 0.41 |
| 1:D:237:TYR:O | 1:D:241:ILE:HD12 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:85:VAL:HG12 | 3:F:85:VAL:O | 2.21 | 0.41 |
| 3:M:24:ILE:CD1 | 3:M:59:PHE:CE2 | 3.01 | 0.41 |
| 1:A:58:PRO:HA | 1:A:61:THR:HB | 2.03 | 0.41 |
| 1:A:431:HIS:HD2 | 2:B:136:LYS:NZ | 2.18 | 0.41 |
| 1:D:195:GLY:HA2 | 2:E:92:SER:HB2 | 2.02 | 0.41 |
| 3:F:89:TYR:HB3 | 3:F:97:LYS:HZ3 | 1.86 | 0.41 |
| 3:F:134:MET:HG2 | 3:F:293:LEU:HD13 | 2.03 | 0.41 |
| 3:F:157:PHE:HA | 3:F:158:PRO:HD3 | 1.80 | 0.41 |
| 3:F:271:ILE:CD1 | 10:F:401:HEC:HMB2 | 2.51 | 0.41 |
| 1:G:233:PRO:HB3 | 3:I:48:GLU:HG3 | 2.03 | 0.41 |
| 1:G:290:GLY:O | 1:G:293:THR:HB | 2.21 | 0.41 |
| 1:G:418:THR:OG1 | 3:I:137:ARG:NH1 | 2.54 | 0.41 |
| 2:H:96:HIS:HA | 2:H:97:PRO:HA | 1.87 | 0.41 |
| 3:I:6:SER:CB | 3:I:81:ASN:HD22 | 2.25 | 0.41 |
| 10:I:403:HEC:HMC1 | 10:I:403:HEC:HBC3 | 2.03 | 0.41 |
| 2:L:96:HIS:HA | 2:L:97:PRO:HA | 1.88 | 0.41 |
| 3:M:61:LEU:HD12 | 3:M:61:LEU:HA | 1.91 | 0.41 |
| 3:M:166:ARG:HH21 | 10:M:402:HEC:HAD2 | 1.85 | 0.41 |
| 3:M:207:LYS:HA | 3:M:212:LEU:O | 2.21 | 0.41 |
| 4:N:20:PHE:CD2 | 4:N:20:PHE:C | 2.95 | 0.41 |
| 1:A:82:GLN:HE21 | 1:A:89:LEU:H | 1.67 | 0.41 |
| 1:A:218:PHE:CD2 | 1:A:221:ILE:HD12 | 2.56 | 0.41 |
| 3:C:21:PHE:O | 3:C:24:ILE:HG22 | 2.21 | 0.41 |
| 3:C:255:ALA:HA | 3:C:258:TRP:CD2 | 2.56 | 0.41 |
| 3:F:128:ASP:OD2 | 3:F:128:ASP:C | 2.58 | 0.41 |
| 1:G:317:TYR:HB2 | 1:G:353:TRP:CE3 | 2.56 | 0.41 |
| 2:H:74:ARG:HA | 2:H:75:PRO:HD3 | 1.88 | 0.41 |
| 2:H:137:MET:HA | 2:H:138:PRO:HD3 | 1.98 | 0.41 |
| 1:K:457:ARG:HD2 | 1:K:457:ARG:HA | 1.76 | 0.41 |
| 3:M:212:LEU:HD23 | 3:M:212:LEU:HA | 1.86 | 0.41 |
| 1:A:81:VAL:HA | 1:A:84:THR:HG22 | 2.03 | 0.40 |
| 3:C:166:ARG:NH2 | 3:C:250:PRO:HG3 | 2.37 | 0.40 |
| 11:C:403:FC6:N25 | 3:M:215:PRO:HG3 | 2.36 | 0.40 |
| 3:F:14:LEU:O | 3:F:17:ILE:HB | 2.21 | 0.40 |
| 3:F:255:ALA:HA | 3:F:258:TRP:CD2 | 2.56 | 0.40 |
| 3:F:282:GLN:HB3 | 3:F:286:LEU:HD12 | 2.03 | 0.40 |
| 1:K:267:TRP:CA | 3:M:78:GLY:HA2 | 2.48 | 0.40 |
| 1:K:350:ALA:HB1 | 5:K:502:HEM:C3C | 2.57 | 0.40 |
| 3:M:8:TYR:HA | 3:M:11:LEU:HD22 | 2.02 | 0.40 |
| 1:A:77:SER:O | 1:A:81:VAL:HG12 | 2.21 | 0.40 |
| 1:A:174:LEU:HD21 | 1:A:208:ASN:HB3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:291:MET:HE2 | 1:A:291:MET:HB2 | 1.76 | 0.40 |
| 1:A:386:TRP:O | 1:A:390:ILE:HG12 | 2.21 | 0.40 |
| 1:D:237:TYR:O | 1:D:240:SER:HB2 | 2.21 | 0.40 |
| 2:E:96:HIS:HA | 2:E:97:PRO:HA | 1.90 | 0.40 |
| 3:F:239:GLN:O | 3:F:239:GLN:HG3 | 2.20 | 0.40 |
| 3:I:69:GLY:O | 3:I:73:LEU:HD23 | 2.21 | 0.40 |
| 1:K:57:ARG:NH1 | 5:K:502:HEM:O2A | 2.54 | 0.40 |
| 4:Q:27:PHE:CD2 | 4:Q:27:PHE:O | 2.73 | 0.40 |
| 1:A:13:VAL:HA | 1:A:16:GLN:NE2 | 2.33 | 0.40 |
| 1:A:288:ILE:HD12 | 3:C:58:TRP:CD1 | 2.56 | 0.40 |
| 1:A:331:THR:O | 4:N:6:VAL:HG13 | 2.21 | 0.40 |
| 1:A:351:LEU:O | 1:A:355:ALA:HB3 | 2.21 | 0.40 |
| 2:B:48:PRO:HG3 | 2:B:166:PRO:HD2 | 2.03 | 0.40 |
| 3:C:57:TRP:CG | 3:C:58:TRP:N | 2.89 | 0.40 |
| 2:E:125:LEU:HD21 | 10:E:301:HEC:HMB2 | 2.02 | 0.40 |
| 1:G:11:TYR:CD1 | 1:G:369:VAL:HA | 2.56 | 0.40 |
| 1:G:235:TYR:O | 1:G:289:ASN:ND2 | 2.54 | 0.40 |
| 1:G:349:GLY:O | 1:G:353:TRP:HB3 | 2.22 | 0.40 |
| 1:G:453:TYR:O | 1:G:457:ARG:HG2 | 2.20 | 0.40 |
| 1:K:90:PHE:C | 1:K:90:PHE:CD2 | 2.95 | 0.40 |
| 3:M:60:LEU:O | 3:M:60:LEU:HD22 | 2.21 | 0.40 |
| 1:A:279:LEU:O | 1:A:282:PRO:HD2 | 2.22 | 0.40 |
| 3:C:47:ILE:H | 3:C:47:ILE:HG12 | 1.69 | 0.40 |
| 1:D:236:SER:OG | 1:D:239:LEU:HB2 | 2.21 | 0.40 |
| 1:D:254:ALA:O | 1:D:257:HIS:ND1 | 2.55 | 0.40 |
| 1:D:395:TYR:CZ | 1:D:437:ARG:HD2 | 2.57 | 0.40 |
| 3:F:61:LEU:O | 3:F:65:THR:HG23 | 2.20 | 0.40 |
| 1:G:256:PRO:HB2 | 1:G:272:GLY:HA3 | 2.03 | 0.40 |
| 1:G:379:GLY:O | 1:G:383:THR:HG23 | 2.22 | 0.40 |
| 3:M:76:TYR:CE1 | 3:M:86:LEU:HD22 | 2.57 | 0.40 |
| 1:A:294:LEU:HD11 | 1:A:307:LEU:HD11 | 2.04 | 0.40 |
| 2:B:132:VAL:HA | 2:B:133:PRO:HD2 | 1.89 | 0.40 |
| 1:D:253:TRP:CH2 | 3:F:13:THR:HG22 | 2.55 | 0.40 |
| 3:F:140:ALA:HA | 3:F:144:SER:HB3 | 2.04 | 0.40 |
| 1:G:386:TRP:O | 1:G:390:ILE:HG12 | 2.21 | 0.40 |
| 1:K:15:ARG:HG3 | 1:K:369:VAL:HG12 | 2.03 | 0.40 |
| 2:L:109:LEU:O | 2:L:112:VAL:HG22 | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 464/474 (98%) | 442 (95%) | 20 (4%) | 2 (0%) | 30 | 64 |
| 1 | D | 461/474 (97%) | 443 (96%) | 17 (4%) | 1 (0%) | 44 | 75 |
| 1 | G | 463/474 (98%) | 443 (96%) | 19 (4%) | 1 (0%) | 44 | 75 |
| 1 | K | 463/474 (98%) | 442 (96%) | 19 (4%) | 2 (0%) | 30 | 64 |
| 2 | B | 195/203 (96%) | 187 (96%) | 8 (4%) | 0 | 100 | 100 |
| 2 | E | 195/203 (96%) | 187 (96%) | 8 (4%) | 0 | 100 | 100 |
| 2 | H | 195/203 (96%) | 187 (96%) | 8 (4%) | 0 | 100 | 100 |
| 2 | L | 195/203 (96%) | 187 (96%) | 8 (4%) | 0 | 100 | 100 |
| 3 | C | 301/311 (97%) | 286 (95%) | 15 (5%) | 0 | 100 | 100 |
| 3 | F | 301/311 (97%) | 286 (95%) | 15 (5%) | 0 | 100 | 100 |
| 3 | I | 301/311 (97%) | 287 (95%) | 14 (5%) | 0 | 100 | 100 |
| 3 | M | 301/311 (97%) | 284 (94%) | 14 (5%) | 3 (1%) | 13 | 47 |
| 4 | N | 27/36 (75%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 4 | O | 27/36 (75%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 4 | P | 27/36 (75%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 4 | Q | 27/36 (75%) | 27 (100%) | 0 | 0 | 100 | 100 |
| All | All | 3943/4096 (96%) | 3769 (96%) | 165 (4%) | 9 (0%) | 44 | 75 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 466 | GLU |
| 1 | A | 468 | ASP |
| 1 | G | 465 | ALA |
| 1 | K | 466 | GLU |
| 1 | K | 468 | ASP |
| 3 | M | 38 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | M | 42 | HIS |
| 3 | M | 37 | ASP |
| 1 | D | 463 | LYS |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | A | 374/379 (99%) | 343 (92%) | 31 (8%) | 9 | 35 |
| 1 | D | 371/379 (98%) | 339 (91%) | 32 (9%) | 8 | 33 |
| 1 | G | 373/379 (98%) | 340 (91%) | 33 (9%) | 8 | 32 |
| 1 | K | 373/379 (98%) | 339 (91%) | 34 (9%) | 7 | 29 |
| 2 | B | 166/172 (96%) | 154 (93%) | 12 (7%) | 12 | 41 |
| 2 | E | 166/172 (96%) | 155 (93%) | 11 (7%) | 14 | 45 |
| 2 | H | 166/172 (96%) | 152 (92%) | 14 (8%) | 9 | 34 |
| 2 | L | 166/172 (96%) | 155 (93%) | 11 (7%) | 14 | 45 |
| 3 | C | 227/234 (97%) | 212 (93%) | 15 (7%) | 14 | 45 |
| 3 | F | 227/234 (97%) | 197 (87%) | 30 (13%) | 3 | 16 |
| 3 | I | 227/234 (97%) | 200 (88%) | 27 (12%) | 4 | 19 |
| 3 | M | 227/234 (97%) | 203 (89%) | 24 (11%) | 5 | 24 |
| 4 | N | 22/28 (79%) | 22 (100%) | 0 | 100 | 100 |
| 4 | O | 22/28 (79%) | 22 (100%) | 0 | 100 | 100 |
| 4 | P | 22/28 (79%) | 21 (96%) | 1 (4%) | 23 | 56 |
| 4 | Q | 22/28 (79%) | 19 (86%) | 3 (14%) | 3 | 15 |
| All | All | 3151/3252 (97%) | 2873 (91%) | 278 (9%) | 8 | 32 |

All (278) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 50 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 57 | ARG |
| 1 | A | 59 | LEU |
| 1 | A | 64 | VAL |
| 1 | A | 73 | LEU |
| 1 | A | 87 | THR |
| 1 | A | 104 | LEU |
| 1 | A | 107 | LEU |
| 1 | A | 108 | LEU |
| 1 | A | 119 | SER |
| 1 | A | 125 | GLU |
| 1 | A | 154 | VAL |
| 1 | A | 159 | VAL |
| 1 | A | 167 | PHE |
| 1 | A | 174 | LEU |
| 1 | A | 192 | LEU |
| 1 | A | 200 | MET |
| 1 | A | 243 | HIS |
| 1 | A | 251 | TYR |
| 1 | A | 271 | LEU |
| 1 | A | 275 | MET |
| 1 | A | 278 | ILE |
| 1 | A | 289 | ASN |
| 1 | A | 294 | LEU |
| 1 | A | 313 | SER |
| 1 | A | 319 | MET |
| 1 | A | 372 | ARG |
| 1 | A | 373 | GLU |
| 1 | A | 427 | LEU |
| 1 | A | 454 | ASN |
| 1 | A | 458 | THR |
| 2 | B | 6 | LYS |
| 2 | B | 13 | LEU |
| 2 | B | 16 | LEU |
| 2 | B | 17 | PHE |
| 2 | B | 22 | VAL |
| 2 | B | 27 | LEU |
| 2 | B | 62 | ARG |
| 2 | B | 92 | SER |
| 2 | B | 112 | VAL |
| 2 | B | 127 | ASN |
| 2 | B | 129 | ARG |
| 2 | B | 177 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 8 | TYR |
| 3 | C | 16 | THR |
| 3 | C | 27 | THR |
| 3 | C | 40 | MET |
| 3 | C | 47 | ILE |
| 3 | C | 48 | GLU |
| 3 | C | 62 | PHE |
| 3 | C | 130 | GLN |
| 3 | C | 163 | GLN |
| 3 | C | 175 | LYS |
| 3 | C | 179 | LEU |
| 3 | C | 182 | ARG |
| 3 | C | 201 | VAL |
| 3 | C | 239 | GLN |
| 3 | C | 264 | LEU |
| 1 | D | 50 | TRP |
| 1 | D | 57 | ARG |
| 1 | D | 59 | LEU |
| 1 | D | 64 | VAL |
| 1 | D | 73 | LEU |
| 1 | D | 87 | THR |
| 1 | D | 93 | LYS |
| 1 | D | 104 | LEU |
| 1 | D | 107 | LEU |
| 1 | D | 108 | LEU |
| 1 | D | 119 | SER |
| 1 | D | 125 | GLU |
| 1 | D | 154 | VAL |
| 1 | D | 159 | VAL |
| 1 | D | 167 | PHE |
| 1 | D | 174 | LEU |
| 1 | D | 192 | LEU |
| 1 | D | 200 | MET |
| 1 | D | 243 | HIS |
| 1 | D | 248 | ILE |
| 1 | D | 251 | TYR |
| 1 | D | 271 | LEU |
| 1 | D | 275 | MET |
| 1 | D | 278 | ILE |
| 1 | D | 289 | ASN |
| 1 | D | 294 | LEU |
| 1 | D | 319 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 372 | ARG |
| 1 | D | 373 | GLU |
| 1 | D | 427 | LEU |
| 1 | D | 456 | TRP |
| 1 | D | 467 | TYR |
| 2 | E | 13 | LEU |
| 2 | E | 16 | LEU |
| 2 | E | 17 | PHE |
| 2 | E | 22 | VAL |
| 2 | E | 27 | LEU |
| 2 | E | 62 | ARG |
| 2 | E | 92 | SER |
| 2 | E | 112 | VAL |
| 2 | E | 127 | ASN |
| 2 | E | 129 | ARG |
| 2 | E | 177 | ASP |
| 3 | F | 4 | PHE |
| 3 | F | 8 | TYR |
| 3 | F | 12 | LEU |
| 3 | F | 16 | THR |
| 3 | F | 20 | LEU |
| 3 | F | 21 | PHE |
| 3 | F | 24 | ILE |
| 3 | F | 27 | THR |
| 3 | F | 28 | ARG |
| 3 | F | 29 | LYS |
| 3 | F | 35 | THR |
| 3 | F | 36 | THR |
| 3 | F | 38 | GLN |
| 3 | F | 40 | MET |
| 3 | F | 54 | LEU |
| 3 | F | 62 | PHE |
| 3 | F | 63 | ILE |
| 3 | F | 68 | PHE |
| 3 | F | 71 | LEU |
| 3 | F | 82 | TRP |
| 3 | F | 121 | SER |
| 3 | F | 134 | MET |
| 3 | F | 137 | ARG |
| 3 | F | 145 | ILE |
| 3 | F | 163 | GLN |
| 3 | F | 175 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | F | 179 | LEU |
| 3 | F | 182 | ARG |
| 3 | F | 201 | VAL |
| 3 | F | 264 | LEU |
| 1 | G | 6 | SER |
| 1 | G | 50 | TRP |
| 1 | G | 57 | ARG |
| 1 | G | 59 | LEU |
| 1 | G | 64 | VAL |
| 1 | G | 73 | LEU |
| 1 | G | 87 | THR |
| 1 | G | 104 | LEU |
| 1 | G | 107 | LEU |
| 1 | G | 108 | LEU |
| 1 | G | 122 | GLU |
| 1 | G | 125 | GLU |
| 1 | G | 154 | VAL |
| 1 | G | 159 | VAL |
| 1 | G | 167 | PHE |
| 1 | G | 174 | LEU |
| 1 | G | 192 | LEU |
| 1 | G | 200 | MET |
| 1 | G | 243 | HIS |
| 1 | G | 248 | ILE |
| 1 | G | 251 | TYR |
| 1 | G | 271 | LEU |
| 1 | G | 275 | MET |
| 1 | G | 278 | ILE |
| 1 | G | 289 | ASN |
| 1 | G | 294 | LEU |
| 1 | G | 313 | SER |
| 1 | G | 319 | MET |
| 1 | G | 372 | ARG |
| 1 | G | 373 | GLU |
| 1 | G | 427 | LEU |
| 1 | G | 454 | ASN |
| 1 | G | 467 | TYR |
| 2 | H | 7 | LEU |
| 2 | H | 13 | LEU |
| 2 | H | 16 | LEU |
| 2 | H | 17 | PHE |
| 2 | H | 22 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | H | 27 | LEU |
| 2 | H | 44 | GLU |
| 2 | H | 62 | ARG |
| 2 | H | 92 | SER |
| 2 | H | 112 | VAL |
| 2 | H | 127 | ASN |
| 2 | H | 129 | ARG |
| 2 | H | 169 | GLU |
| 2 | H | 177 | ASP |
| 3 | I | 4 | PHE |
| 3 | I | 8 | TYR |
| 3 | I | 12 | LEU |
| 3 | I | 16 | THR |
| 3 | I | 20 | LEU |
| 3 | I | 24 | ILE |
| 3 | I | 27 | THR |
| 3 | I | 37 | ASP |
| 3 | I | 38 | GLN |
| 3 | I | 40 | MET |
| 3 | I | 47 | ILE |
| 3 | I | 49 | GLU |
| 3 | I | 62 | PHE |
| 3 | I | 63 | ILE |
| 3 | I | 66 | LEU |
| 3 | I | 73 | LEU |
| 3 | I | 86 | LEU |
| 3 | I | 108 | GLU |
| 3 | I | 127 | GLN |
| 3 | I | 133 | LYS |
| 3 | I | 137 | ARG |
| 3 | I | 163 | GLN |
| 3 | I | 175 | LYS |
| 3 | I | 179 | LEU |
| 3 | I | 182 | ARG |
| 3 | I | 201 | VAL |
| 3 | I | 264 | LEU |
| 1 | K | 50 | TRP |
| 1 | K | 57 | ARG |
| 1 | K | 59 | LEU |
| 1 | K | 64 | VAL |
| 1 | K | 73 | LEU |
| 1 | K | 87 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 89 | LEU |
| 1 | K | 90 | PHE |
| 1 | K | 104 | LEU |
| 1 | K | 107 | LEU |
| 1 | K | 108 | LEU |
| 1 | K | 125 | GLU |
| 1 | K | 154 | VAL |
| 1 | K | 159 | VAL |
| 1 | K | 167 | PHE |
| 1 | K | 174 | LEU |
| 1 | K | 192 | LEU |
| 1 | K | 200 | MET |
| 1 | K | 235 | TYR |
| 1 | K | 243 | HIS |
| 1 | K | 251 | TYR |
| 1 | K | 271 | LEU |
| 1 | K | 275 | MET |
| 1 | K | 278 | ILE |
| 1 | K | 289 | ASN |
| 1 | K | 294 | LEU |
| 1 | K | 313 | SER |
| 1 | K | 319 | MET |
| 1 | K | 372 | ARG |
| 1 | K | 373 | GLU |
| 1 | K | 427 | LEU |
| 1 | K | 454 | ASN |
| 1 | K | 466 | GLU |
| 1 | K | 467 | TYR |
| 2 | L | 13 | LEU |
| 2 | L | 16 | LEU |
| 2 | L | 17 | PHE |
| 2 | L | 22 | VAL |
| 2 | L | 27 | LEU |
| 2 | L | 62 | ARG |
| 2 | L | 92 | SER |
| 2 | L | 112 | VAL |
| 2 | L | 127 | ASN |
| 2 | L | 129 | ARG |
| 2 | L | 177 | ASP |
| 3 | M | 8 | TYR |
| 3 | M | 11 | LEU |
| 3 | M | 20 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | M | 24 | ILE |
| 3 | M | 27 | THR |
| 3 | M | 29 | LYS |
| 3 | M | 35 | THR |
| 3 | M | 38 | GLN |
| 3 | M | 40 | MET |
| 3 | M | 44 | PHE |
| 3 | M | 60 | LEU |
| 3 | M | 62 | PHE |
| 3 | M | 68 | PHE |
| 3 | M | 71 | LEU |
| 3 | M | 75 | LEU |
| 3 | M | 130 | GLN |
| 3 | M | 145 | ILE |
| 3 | M | 163 | GLN |
| 3 | M | 175 | LYS |
| 3 | M | 179 | LEU |
| 3 | M | 182 | ARG |
| 3 | M | 201 | VAL |
| 3 | M | 239 | GLN |
| 3 | M | 264 | LEU |
| 4 | P | 21 | LEU |
| 4 | Q | 20 | PHE |
| 4 | Q | 21 | LEU |
| 4 | Q | 27 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | GLN |
| 1 | A | 62 | ASN |
| 1 | A | 82 | GLN |
| 1 | A | 103 | GLN |
| 1 | A | 161 | ASN |
| 1 | A | 178 | ASN |
| 1 | A | 243 | HIS |
| 1 | A | 289 | ASN |
| 1 | A | 374 | GLN |
| 1 | A | 382 | ASN |
| 1 | A | 406 | GLN |
| 1 | A | 414 | ASN |
| 1 | A | 431 | HIS |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 454 | ASN |
| 1 | A | 460 | GLN |
| 2 | B | 10 | ASN |
| 2 | B | 29 | GLN |
| 2 | B | 36 | GLN |
| 2 | B | 40 | ASN |
| 2 | B | 127 | ASN |
| 2 | B | 193 | GLN |
| 3 | C | 52 | ASN |
| 3 | C | 98 | GLN |
| 3 | C | 105 | GLN |
| 3 | C | 141 | ASN |
| 3 | C | 163 | GLN |
| 3 | C | 231 | GLN |
| 3 | C | 266 | GLN |
| 3 | C | 292 | HIS |
| 1 | D | 16 | GLN |
| 1 | D | 62 | ASN |
| 1 | D | 82 | GLN |
| 1 | D | 103 | GLN |
| 1 | D | 161 | ASN |
| 1 | D | 178 | ASN |
| 1 | D | 243 | HIS |
| 1 | D | 289 | ASN |
| 1 | D | 374 | GLN |
| 1 | D | 382 | ASN |
| 1 | D | 406 | GLN |
| 1 | D | 414 | ASN |
| 1 | D | 431 | HIS |
| 1 | D | 460 | GLN |
| 2 | E | 10 | ASN |
| 2 | E | 29 | GLN |
| 2 | E | 36 | GLN |
| 2 | E | 40 | ASN |
| 2 | E | 127 | ASN |
| 2 | E | 193 | GLN |
| 3 | F | 38 | GLN |
| 3 | F | 42 | HIS |
| 3 | F | 52 | ASN |
| 3 | F | 81 | ASN |
| 3 | F | 163 | GLN |
| 3 | F | 266 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 16 | GLN |
| 1 | G | 62 | ASN |
| 1 | G | 82 | GLN |
| 1 | G | 103 | GLN |
| 1 | G | 156 | HIS |
| 1 | G | 161 | ASN |
| 1 | G | 178 | ASN |
| 1 | G | 289 | ASN |
| 1 | G | 374 | GLN |
| 1 | G | 382 | ASN |
| 1 | G | 406 | GLN |
| 1 | G | 414 | ASN |
| 1 | G | 431 | HIS |
| 1 | G | 454 | ASN |
| 2 | H | 10 | ASN |
| 2 | H | 29 | GLN |
| 2 | H | 36 | GLN |
| 2 | H | 40 | ASN |
| 2 | H | 127 | ASN |
| 2 | H | 193 | GLN |
| 3 | I | 42 | HIS |
| 3 | I | 81 | ASN |
| 3 | I | 105 | GLN |
| 3 | I | 127 | GLN |
| 3 | I | 141 | ASN |
| 3 | I | 163 | GLN |
| 3 | I | 266 | GLN |
| 3 | I | 268 | GLN |
| 3 | I | 276 | ASN |
| 3 | I | 292 | HIS |
| 1 | K | 16 | GLN |
| 1 | K | 62 | ASN |
| 1 | K | 82 | GLN |
| 1 | K | 103 | GLN |
| 1 | K | 161 | ASN |
| 1 | K | 178 | ASN |
| 1 | K | 243 | HIS |
| 1 | K | 289 | ASN |
| 1 | K | 374 | GLN |
| 1 | K | 382 | ASN |
| 1 | K | 406 | GLN |
| 1 | K | 414 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 431 | HIS |
| 1 | K | 454 | ASN |
| 1 | K | 460 | GLN |
| 2 | L | 10 | ASN |
| 2 | L | 29 | GLN |
| 2 | L | 36 | GLN |
| 2 | L | 40 | ASN |
| 2 | L | 71 | GLN |
| 2 | L | 127 | ASN |
| 2 | L | 193 | GLN |
| 3 | M | 38 | GLN |
| 3 | M | 141 | ASN |
| 3 | M | 163 | GLN |
| 3 | M | 266 | GLN |
| 3 | M | 268 | GLN |
| 3 | M | 292 | 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](#)

Of 44 ligands modelled in this entry, 12 are monoatomic - leaving 32 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 9 | PO4 | K | 506 | - | 4,4,4 | 1.14 | 0 | 6,6,6 | 0.88 | 0 |
| 11 | FC6 | I | 401 | - | 12,12,12 | 2.74 | 6 (50%) | - | | |
| 5 | HEM | D | 501 | 8,7,1 | 41,50,50 | 1.99 | 6 (14%) | 45,82,82 | 1.59 | 5 (11%) |
| 11 | FC6 | C | 403 | - | 12,12,12 | 2.64 | 6 (50%) | - | | |
| 5 | HEM | G | 502 | 7,1 | 41,50,50 | 2.01 | 6 (14%) | 45,82,82 | 1.85 | 9 (20%) |
| 8 | PEO | A | 505 | 5,6 | 1,1,1 | 0.43 | 0 | - | | |
| 11 | FC6 | F | 403 | - | 12,12,12 | 2.71 | 6 (50%) | - | | |
| 5 | HEM | K | 501 | 8,7,1 | 41,50,50 | 1.97 | 6 (14%) | 45,82,82 | 1.59 | 5 (11%) |
| 8 | PEO | G | 505 | 5,6 | 1,1,1 | 0.51 | 0 | - | | |
| 10 | HEC | F | 401 | 3 | 32,50,50 | 2.33 | 11 (34%) | 24,82,82 | 2.73 | 9 (37%) |
| 9 | PO4 | A | 506 | - | 4,4,4 | 1.03 | 0 | 6,6,6 | 0.35 | 0 |
| 11 | FC6 | M | 401 | - | 12,12,12 | 2.66 | 6 (50%) | - | | |
| 5 | HEM | K | 502 | 7,1 | 41,50,50 | 1.97 | 5 (12%) | 45,82,82 | 1.82 | 10 (22%) |
| 10 | HEC | I | 403 | 3 | 32,50,50 | 2.27 | 11 (34%) | 24,82,82 | 2.89 | 12 (50%) |
| 9 | PO4 | D | 505 | - | 4,4,4 | 0.94 | 0 | 6,6,6 | 0.39 | 0 |
| 5 | HEM | A | 502 | 7,1 | 41,50,50 | 1.96 | 6 (14%) | 45,82,82 | 1.74 | 6 (13%) |
| 10 | HEC | L | 301 | 2 | 32,50,50 | 2.13 | 11 (34%) | 24,82,82 | 2.64 | 10 (41%) |
| 5 | HEM | A | 501 | 8,7,1 | 41,50,50 | 1.95 | 6 (14%) | 45,82,82 | 1.67 | 7 (15%) |
| 8 | PEO | K | 507 | 5,6 | 1,1,1 | 0.46 | 0 | - | | |
| 10 | HEC | M | 403 | 3 | 32,50,50 | 2.30 | 10 (31%) | 24,82,82 | 2.85 | 13 (54%) |
| 10 | HEC | M | 402 | 3 | 32,50,50 | 2.20 | 10 (31%) | 24,82,82 | 2.91 | 11 (45%) |
| 5 | HEM | D | 502 | 7,1 | 41,50,50 | 1.98 | 6 (14%) | 45,82,82 | 1.82 | 8 (17%) |
| 10 | HEC | B | 301 | 2 | 32,50,50 | 2.11 | 11 (34%) | 24,82,82 | 2.73 | 8 (33%) |
| 5 | HEM | G | 501 | 8,7,1 | 41,50,50 | 1.94 | 7 (17%) | 45,82,82 | 1.69 | 8 (17%) |
| 8 | PEO | D | 506 | 5,6 | 1,1,1 | 0.46 | 0 | - | | |
| 10 | HEC | I | 402 | 3 | 32,50,50 | 2.33 | 11 (34%) | 24,82,82 | 2.87 | 12 (50%) |
| 10 | HEC | F | 402 | 3 | 32,50,50 | 2.47 | 11 (34%) | 24,82,82 | 2.64 | 9 (37%) |
| 9 | PO4 | G | 506 | - | 4,4,4 | 0.98 | 0 | 6,6,6 | 0.49 | 0 |
| 10 | HEC | H | 301 | 2 | 32,50,50 | 2.19 | 11 (34%) | 24,82,82 | 2.73 | 8 (33%) |
| 10 | HEC | C | 402 | 3 | 32,50,50 | 2.30 | 11 (34%) | 24,82,82 | 2.91 | 14 (58%) |
| 10 | HEC | C | 401 | 3 | 32,50,50 | 2.30 | 12 (37%) | 24,82,82 | 2.85 | 12 (50%) |
| 10 | HEC | E | 301 | 2 | 32,50,50 | 2.20 | 12 (37%) | 24,82,82 | 2.48 | 9 (37%) |

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 |
|-----|------|-------|-----|-------|---------|------------|-------|
| 5 | HEM | D | 501 | 8,7,1 | - | 2/12/54/54 | - |
| 5 | HEM | G | 502 | 7,1 | - | 1/12/54/54 | - |
| 5 | HEM | K | 501 | 8,7,1 | - | 2/12/54/54 | - |
| 10 | HEC | F | 401 | 3 | - | 2/10/54/54 | - |
| 5 | HEM | K | 502 | 7,1 | - | 1/12/54/54 | - |
| 10 | HEC | I | 403 | 3 | - | 2/10/54/54 | - |
| 10 | HEC | L | 301 | 2 | - | 4/10/54/54 | - |
| 5 | HEM | A | 502 | 7,1 | - | 3/12/54/54 | - |
| 5 | HEM | A | 501 | 8,7,1 | - | 4/12/54/54 | - |
| 10 | HEC | M | 403 | 3 | - | 2/10/54/54 | - |
| 10 | HEC | M | 402 | 3 | - | 2/10/54/54 | - |
| 5 | HEM | D | 502 | 7,1 | - | 3/12/54/54 | - |
| 10 | HEC | B | 301 | 2 | - | 4/10/54/54 | - |
| 5 | HEM | G | 501 | 8,7,1 | - | 2/12/54/54 | - |
| 10 | HEC | I | 402 | 3 | - | 2/10/54/54 | - |
| 10 | HEC | F | 402 | 3 | - | 3/10/54/54 | - |
| 10 | HEC | H | 301 | 2 | - | 4/10/54/54 | - |
| 10 | HEC | C | 402 | 3 | - | 2/10/54/54 | - |
| 10 | HEC | C | 401 | 3 | - | 2/10/54/54 | - |
| 10 | HEC | E | 301 | 2 | - | 4/10/54/54 | - |

All (204) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5 | D | 501 | HEM | C3D-C2D | 8.21 | 1.54 | 1.36 |
| 5 | K | 501 | HEM | C3D-C2D | 8.09 | 1.54 | 1.36 |
| 5 | G | 502 | HEM | C3D-C2D | 8.05 | 1.53 | 1.36 |
| 5 | A | 501 | HEM | C3D-C2D | 7.87 | 1.53 | 1.36 |
| 5 | D | 502 | HEM | C3D-C2D | 7.86 | 1.53 | 1.36 |
| 5 | K | 502 | HEM | C3D-C2D | 7.83 | 1.53 | 1.36 |
| 5 | G | 501 | HEM | C3D-C2D | 7.75 | 1.53 | 1.36 |
| 5 | A | 502 | HEM | C3D-C2D | 7.75 | 1.53 | 1.36 |
| 10 | F | 402 | HEC | C2B-C3B | 7.14 | 1.48 | 1.40 |
| 10 | F | 402 | HEC | C3C-C2C | 7.14 | 1.48 | 1.40 |
| 10 | H | 301 | HEC | C3C-C2C | 6.93 | 1.48 | 1.40 |
| 10 | I | 402 | HEC | C3C-C2C | 6.90 | 1.48 | 1.40 |
| 10 | I | 403 | HEC | C3C-C2C | 6.76 | 1.47 | 1.40 |
| 10 | M | 403 | HEC | C3C-C2C | 6.74 | 1.47 | 1.40 |
| 10 | F | 401 | HEC | C3C-C2C | 6.66 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10 | E | 301 | HEC | C3C-C2C | 6.61 | 1.47 | 1.40 |
| 10 | M | 402 | HEC | C3C-C2C | 6.53 | 1.47 | 1.40 |
| 10 | C | 402 | HEC | C3C-C2C | 6.45 | 1.47 | 1.40 |
| 10 | L | 301 | HEC | C3C-C2C | 6.41 | 1.47 | 1.40 |
| 10 | C | 402 | HEC | C2B-C3B | 6.36 | 1.47 | 1.40 |
| 10 | M | 403 | HEC | C2B-C3B | 6.29 | 1.47 | 1.40 |
| 10 | I | 402 | HEC | C2B-C3B | 6.27 | 1.47 | 1.40 |
| 10 | C | 401 | HEC | C3C-C2C | 6.27 | 1.47 | 1.40 |
| 10 | B | 301 | HEC | C3C-C2C | 6.21 | 1.47 | 1.40 |
| 10 | I | 403 | HEC | C2B-C3B | 6.01 | 1.47 | 1.40 |
| 10 | F | 401 | HEC | C2B-C3B | 5.93 | 1.46 | 1.40 |
| 10 | C | 401 | HEC | C2B-C3B | 5.77 | 1.46 | 1.40 |
| 10 | M | 402 | HEC | C2B-C3B | 5.62 | 1.46 | 1.40 |
| 10 | E | 301 | HEC | C2B-C3B | 5.61 | 1.46 | 1.40 |
| 5 | A | 502 | HEM | C3C-C2C | -5.40 | 1.32 | 1.40 |
| 5 | G | 502 | HEM | C3C-C2C | -5.28 | 1.33 | 1.40 |
| 10 | B | 301 | HEC | C2B-C3B | 5.25 | 1.46 | 1.40 |
| 10 | H | 301 | HEC | C2B-C3B | 5.24 | 1.46 | 1.40 |
| 10 | L | 301 | HEC | C2B-C3B | 5.06 | 1.46 | 1.40 |
| 5 | D | 502 | HEM | C3C-C2C | -5.06 | 1.33 | 1.40 |
| 5 | K | 502 | HEM | C3C-C2C | -5.01 | 1.33 | 1.40 |
| 5 | A | 501 | HEM | C3C-C2C | -5.01 | 1.33 | 1.40 |
| 5 | G | 501 | HEM | C3C-C2C | -4.88 | 1.33 | 1.40 |
| 5 | K | 501 | HEM | C3C-C2C | -4.80 | 1.33 | 1.40 |
| 10 | C | 401 | HEC | C3C-C4C | 4.68 | 1.51 | 1.43 |
| 5 | D | 501 | HEM | C3C-C2C | -4.65 | 1.33 | 1.40 |
| 11 | F | 403 | FC6 | C24-FE2 | -4.56 | 1.80 | 1.93 |
| 11 | I | 401 | FC6 | C22-FE2 | -4.52 | 1.80 | 1.93 |
| 11 | C | 403 | FC6 | C24-FE2 | -4.46 | 1.80 | 1.93 |
| 11 | I | 401 | FC6 | C24-FE2 | -4.40 | 1.80 | 1.93 |
| 10 | F | 401 | HEC | C3C-C4C | 4.27 | 1.50 | 1.43 |
| 11 | F | 403 | FC6 | C22-FE2 | -4.25 | 1.81 | 1.93 |
| 11 | M | 401 | FC6 | C11-FE2 | -4.13 | 1.81 | 1.93 |
| 11 | C | 403 | FC6 | C26-FE2 | -3.97 | 1.82 | 1.93 |
| 5 | D | 501 | HEM | C3C-CAC | 3.90 | 1.55 | 1.47 |
| 11 | C | 403 | FC6 | C21-FE2 | -3.86 | 1.82 | 1.93 |
| 11 | I | 401 | FC6 | C21-FE2 | -3.85 | 1.82 | 1.93 |
| 10 | F | 402 | HEC | C3C-C4C | 3.84 | 1.50 | 1.43 |
| 11 | F | 403 | FC6 | C21-FE2 | -3.83 | 1.82 | 1.93 |
| 11 | M | 401 | FC6 | C21-FE2 | -3.78 | 1.82 | 1.93 |
| 11 | M | 401 | FC6 | C22-FE2 | -3.77 | 1.82 | 1.93 |
| 11 | M | 401 | FC6 | C24-FE2 | -3.74 | 1.82 | 1.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10 | I | 402 | HEC | C3C-C4C | 3.72 | 1.49 | 1.43 |
| 5 | D | 502 | HEM | C3C-CAC | 3.71 | 1.55 | 1.47 |
| 5 | G | 501 | HEM | C3C-CAC | 3.70 | 1.55 | 1.47 |
| 5 | K | 502 | HEM | C3C-CAC | 3.67 | 1.55 | 1.47 |
| 10 | M | 402 | HEC | C3C-C4C | 3.66 | 1.49 | 1.43 |
| 11 | I | 401 | FC6 | C23-FE2 | -3.63 | 1.83 | 1.93 |
| 5 | K | 501 | HEM | C3C-CAC | 3.63 | 1.55 | 1.47 |
| 5 | G | 502 | HEM | C3C-CAC | 3.60 | 1.55 | 1.47 |
| 11 | M | 401 | FC6 | C26-FE2 | -3.55 | 1.83 | 1.93 |
| 11 | F | 403 | FC6 | C23-FE2 | -3.54 | 1.83 | 1.93 |
| 10 | C | 402 | HEC | C3C-C4C | 3.54 | 1.49 | 1.43 |
| 5 | A | 501 | HEM | C3C-CAC | 3.48 | 1.54 | 1.47 |
| 10 | L | 301 | HEC | C2A-C3A | 3.43 | 1.47 | 1.37 |
| 5 | A | 502 | HEM | C3C-CAC | 3.41 | 1.54 | 1.47 |
| 10 | F | 402 | HEC | C2A-C3A | 3.40 | 1.47 | 1.37 |
| 10 | C | 401 | HEC | C3D-C2D | 3.40 | 1.47 | 1.37 |
| 10 | F | 402 | HEC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 10 | H | 301 | HEC | C2A-C3A | 3.38 | 1.47 | 1.37 |
| 10 | H | 301 | HEC | C3D-C2D | 3.38 | 1.47 | 1.37 |
| 10 | C | 402 | HEC | C2A-C3A | 3.38 | 1.47 | 1.37 |
| 10 | M | 403 | HEC | C3C-C4C | 3.37 | 1.49 | 1.43 |
| 10 | I | 403 | HEC | C3C-C4C | 3.37 | 1.49 | 1.43 |
| 10 | L | 301 | HEC | C3D-C2D | 3.36 | 1.47 | 1.37 |
| 10 | F | 401 | HEC | C3D-C2D | 3.35 | 1.47 | 1.37 |
| 11 | I | 401 | FC6 | C11-FE2 | -3.35 | 1.83 | 1.93 |
| 11 | C | 403 | FC6 | C23-FE2 | -3.34 | 1.83 | 1.93 |
| 10 | E | 301 | HEC | C3D-C2D | 3.33 | 1.47 | 1.37 |
| 11 | C | 403 | FC6 | C22-FE2 | -3.32 | 1.83 | 1.93 |
| 11 | M | 401 | FC6 | C23-FE2 | -3.31 | 1.84 | 1.93 |
| 10 | F | 401 | HEC | C2A-C3A | 3.29 | 1.47 | 1.37 |
| 10 | I | 402 | HEC | C3D-C2D | 3.28 | 1.47 | 1.37 |
| 10 | M | 403 | HEC | C3D-C2D | 3.26 | 1.47 | 1.37 |
| 10 | E | 301 | HEC | C2A-C3A | 3.26 | 1.47 | 1.37 |
| 10 | I | 403 | HEC | C2A-C3A | 3.23 | 1.47 | 1.37 |
| 10 | M | 403 | HEC | C2A-C3A | 3.22 | 1.47 | 1.37 |
| 11 | F | 403 | FC6 | C11-FE2 | -3.21 | 1.84 | 1.93 |
| 10 | I | 402 | HEC | C2A-C3A | 3.21 | 1.47 | 1.37 |
| 10 | B | 301 | HEC | C3C-C4C | 3.20 | 1.48 | 1.43 |
| 11 | F | 403 | FC6 | C26-FE2 | -3.20 | 1.84 | 1.93 |
| 10 | H | 301 | HEC | C3C-C4C | 3.17 | 1.48 | 1.43 |
| 10 | B | 301 | HEC | C2A-C3A | 3.16 | 1.47 | 1.37 |
| 10 | C | 402 | HEC | C3D-C2D | 3.15 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10 | I | 403 | HEC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 10 | M | 402 | HEC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 10 | L | 301 | HEC | C3C-C4C | 3.07 | 1.48 | 1.43 |
| 10 | C | 401 | HEC | C2A-C3A | 3.07 | 1.46 | 1.37 |
| 5 | K | 501 | HEM | CAB-C3B | 3.06 | 1.55 | 1.47 |
| 10 | B | 301 | HEC | C3D-C2D | 3.05 | 1.46 | 1.37 |
| 11 | C | 403 | FC6 | C11-FE2 | -3.04 | 1.84 | 1.93 |
| 5 | D | 501 | HEM | CAB-C3B | 3.02 | 1.55 | 1.47 |
| 10 | E | 301 | HEC | C3C-C4C | 3.00 | 1.48 | 1.43 |
| 5 | A | 501 | HEM | CAB-C3B | 2.99 | 1.55 | 1.47 |
| 5 | G | 501 | HEM | CAB-C3B | 2.97 | 1.55 | 1.47 |
| 10 | M | 402 | HEC | C2A-C3A | 2.96 | 1.46 | 1.37 |
| 10 | I | 403 | HEC | C2A-C1A | 2.92 | 1.49 | 1.42 |
| 5 | D | 502 | HEM | CAB-C3B | 2.91 | 1.55 | 1.47 |
| 10 | F | 402 | HEC | C4D-CHA | 2.90 | 1.49 | 1.41 |
| 10 | M | 403 | HEC | C2A-C1A | 2.89 | 1.49 | 1.42 |
| 10 | F | 401 | HEC | C1D-CHD | 2.89 | 1.49 | 1.41 |
| 10 | F | 402 | HEC | C2A-C1A | 2.89 | 1.49 | 1.42 |
| 10 | C | 402 | HEC | C2A-C1A | 2.86 | 1.49 | 1.42 |
| 5 | K | 502 | HEM | CAB-C3B | 2.85 | 1.55 | 1.47 |
| 11 | I | 401 | FC6 | C26-FE2 | -2.85 | 1.85 | 1.93 |
| 10 | C | 402 | HEC | C4D-CHA | 2.85 | 1.48 | 1.41 |
| 10 | F | 402 | HEC | C1D-CHD | 2.78 | 1.48 | 1.41 |
| 10 | F | 401 | HEC | C2A-C1A | 2.77 | 1.48 | 1.42 |
| 5 | G | 502 | HEM | CAB-C3B | 2.76 | 1.55 | 1.47 |
| 5 | G | 502 | HEM | FE-NB | 2.75 | 2.10 | 1.96 |
| 10 | F | 402 | HEC | C3A-C4A | 2.73 | 1.48 | 1.42 |
| 10 | M | 403 | HEC | C4D-CHA | 2.73 | 1.48 | 1.41 |
| 10 | F | 401 | HEC | C4D-CHA | 2.72 | 1.48 | 1.41 |
| 10 | C | 401 | HEC | C4B-C3B | 2.71 | 1.48 | 1.43 |
| 10 | L | 301 | HEC | C4D-CHA | 2.68 | 1.48 | 1.41 |
| 10 | C | 401 | HEC | C2A-C1A | 2.68 | 1.48 | 1.42 |
| 10 | I | 403 | HEC | C4D-CHA | 2.67 | 1.48 | 1.41 |
| 5 | K | 502 | HEM | FE-NB | 2.66 | 2.10 | 1.96 |
| 5 | A | 502 | HEM | CAB-C3B | 2.64 | 1.54 | 1.47 |
| 10 | C | 401 | HEC | C4D-CHA | 2.64 | 1.48 | 1.41 |
| 10 | C | 401 | HEC | C1D-CHD | 2.61 | 1.48 | 1.41 |
| 10 | I | 402 | HEC | C4D-CHA | 2.61 | 1.48 | 1.41 |
| 10 | E | 301 | HEC | C2A-C1A | 2.55 | 1.48 | 1.42 |
| 10 | I | 402 | HEC | C2A-C1A | 2.55 | 1.48 | 1.42 |
| 10 | E | 301 | HEC | C4D-CHA | 2.53 | 1.48 | 1.41 |
| 10 | M | 402 | HEC | C4D-CHA | 2.52 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 10 | L | 301 | HEC | C2A-C1A | 2.51 | 1.48 | 1.42 |
| 10 | M | 402 | HEC | C1D-CHD | 2.50 | 1.47 | 1.41 |
| 10 | I | 402 | HEC | C4B-C3B | 2.47 | 1.47 | 1.43 |
| 10 | F | 402 | HEC | C1B-CHB | 2.47 | 1.47 | 1.41 |
| 10 | M | 403 | HEC | C3A-C4A | 2.46 | 1.48 | 1.42 |
| 10 | M | 403 | HEC | C1B-CHB | 2.46 | 1.47 | 1.41 |
| 10 | I | 402 | HEC | C1D-CHD | 2.45 | 1.47 | 1.41 |
| 10 | I | 403 | HEC | C1D-CHD | 2.45 | 1.47 | 1.41 |
| 10 | C | 402 | HEC | C3A-C4A | 2.40 | 1.48 | 1.42 |
| 10 | F | 401 | HEC | C1B-CHB | 2.39 | 1.47 | 1.41 |
| 10 | E | 301 | HEC | C4B-C3B | 2.38 | 1.47 | 1.43 |
| 10 | H | 301 | HEC | C4D-CHA | 2.38 | 1.47 | 1.41 |
| 10 | F | 401 | HEC | C3A-C4A | 2.37 | 1.47 | 1.42 |
| 10 | E | 301 | HEC | C3A-C4A | 2.37 | 1.47 | 1.42 |
| 10 | B | 301 | HEC | C1B-CHB | 2.37 | 1.47 | 1.41 |
| 10 | M | 402 | HEC | C2A-C1A | 2.35 | 1.47 | 1.42 |
| 10 | B | 301 | HEC | C4B-C3B | 2.34 | 1.47 | 1.43 |
| 10 | C | 402 | HEC | C1D-CHD | 2.32 | 1.47 | 1.41 |
| 10 | H | 301 | HEC | C4B-C3B | 2.32 | 1.47 | 1.43 |
| 10 | H | 301 | HEC | C3A-C4A | 2.31 | 1.47 | 1.42 |
| 10 | H | 301 | HEC | C1D-CHD | 2.31 | 1.47 | 1.41 |
| 10 | L | 301 | HEC | C1B-CHB | 2.31 | 1.47 | 1.41 |
| 10 | B | 301 | HEC | C2A-C1A | 2.29 | 1.47 | 1.42 |
| 10 | B | 301 | HEC | C1D-CHD | 2.28 | 1.47 | 1.41 |
| 10 | M | 402 | HEC | C4B-C3B | 2.28 | 1.47 | 1.43 |
| 10 | I | 403 | HEC | C1B-CHB | 2.26 | 1.47 | 1.41 |
| 10 | M | 402 | HEC | C1B-CHB | 2.26 | 1.47 | 1.41 |
| 10 | M | 403 | HEC | C1D-CHD | 2.26 | 1.47 | 1.41 |
| 10 | I | 403 | HEC | C3A-C4A | 2.25 | 1.47 | 1.42 |
| 10 | E | 301 | HEC | C1D-CHD | 2.24 | 1.47 | 1.41 |
| 10 | B | 301 | HEC | C4D-CHA | 2.23 | 1.47 | 1.41 |
| 5 | K | 501 | HEM | FE-NB | 2.23 | 2.07 | 1.96 |
| 10 | E | 301 | HEC | C1B-CHB | 2.23 | 1.47 | 1.41 |
| 5 | D | 502 | HEM | FE-NB | 2.22 | 2.07 | 1.96 |
| 10 | C | 401 | HEC | C3A-C4A | 2.20 | 1.47 | 1.42 |
| 5 | A | 502 | HEM | CAA-C2A | 2.19 | 1.55 | 1.52 |
| 10 | L | 301 | HEC | C1D-CHD | 2.19 | 1.47 | 1.41 |
| 5 | G | 502 | HEM | CAA-C2A | 2.19 | 1.55 | 1.52 |
| 10 | H | 301 | HEC | C2A-C1A | 2.17 | 1.47 | 1.42 |
| 5 | G | 501 | HEM | FE-NB | 2.16 | 2.07 | 1.96 |
| 10 | C | 402 | HEC | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 10 | I | 402 | HEC | C1B-CHB | 2.14 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10 | C | 401 | HEC | C1C-CHC | 2.13 | 1.46 | 1.41 |
| 10 | I | 403 | HEC | C4B-C3B | 2.13 | 1.46 | 1.43 |
| 10 | L | 301 | HEC | C4B-C3B | 2.13 | 1.46 | 1.43 |
| 5 | D | 502 | HEM | CAA-C2A | 2.13 | 1.55 | 1.52 |
| 5 | G | 501 | HEM | FE-ND | 2.12 | 2.07 | 1.96 |
| 10 | B | 301 | HEC | C3A-C4A | 2.12 | 1.47 | 1.42 |
| 5 | A | 502 | HEM | C3B-C2B | -2.11 | 1.33 | 1.37 |
| 10 | L | 301 | HEC | C3A-C4A | 2.10 | 1.47 | 1.42 |
| 10 | F | 401 | HEC | C4B-C3B | 2.10 | 1.46 | 1.43 |
| 10 | E | 301 | HEC | C1C-CHC | 2.09 | 1.46 | 1.41 |
| 10 | C | 402 | HEC | C4B-C3B | 2.07 | 1.46 | 1.43 |
| 10 | I | 402 | HEC | C3A-C4A | 2.07 | 1.47 | 1.42 |
| 5 | K | 501 | HEM | CMB-C2B | 2.07 | 1.55 | 1.50 |
| 10 | C | 401 | HEC | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 10 | F | 402 | HEC | C4B-C3B | 2.06 | 1.46 | 1.43 |
| 5 | A | 501 | HEM | FE-ND | 2.04 | 2.07 | 1.96 |
| 5 | D | 501 | HEM | FE-ND | 2.04 | 2.07 | 1.96 |
| 5 | G | 501 | HEM | CMB-C2B | 2.04 | 1.55 | 1.50 |
| 10 | H | 301 | HEC | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 5 | D | 501 | HEM | CMB-C2B | 2.03 | 1.55 | 1.50 |
| 5 | A | 501 | HEM | CMB-C2B | 2.01 | 1.55 | 1.50 |

All (185) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10 | B | 301 | HEC | CBA-CAA-C2A | -7.72 | 99.59 | 112.60 |
| 10 | M | 403 | HEC | C1D-C2D-C3D | -7.23 | 101.97 | 107.00 |
| 10 | C | 402 | HEC | C1D-C2D-C3D | -6.91 | 102.19 | 107.00 |
| 10 | I | 403 | HEC | C1D-C2D-C3D | -6.88 | 102.21 | 107.00 |
| 10 | H | 301 | HEC | CBA-CAA-C2A | -6.74 | 101.24 | 112.60 |
| 10 | I | 402 | HEC | C1D-C2D-C3D | -6.72 | 102.32 | 107.00 |
| 5 | G | 502 | HEM | C4D-ND-C1D | 6.59 | 111.88 | 105.07 |
| 5 | K | 501 | HEM | C4D-ND-C1D | 6.53 | 111.81 | 105.07 |
| 10 | M | 402 | HEC | C1D-C2D-C3D | -6.52 | 102.46 | 107.00 |
| 5 | D | 501 | HEM | C4D-ND-C1D | 6.52 | 111.81 | 105.07 |
| 10 | M | 402 | HEC | CBD-CAD-C3D | -6.52 | 101.50 | 112.62 |
| 10 | E | 301 | HEC | C1D-C2D-C3D | -6.49 | 102.48 | 107.00 |
| 10 | B | 301 | HEC | C1D-C2D-C3D | -6.47 | 102.50 | 107.00 |
| 10 | H | 301 | HEC | C1D-C2D-C3D | -6.35 | 102.58 | 107.00 |
| 5 | G | 501 | HEM | C4D-ND-C1D | 6.23 | 111.50 | 105.07 |
| 10 | L | 301 | HEC | C1D-C2D-C3D | -6.21 | 102.68 | 107.00 |
| 5 | A | 501 | HEM | C4D-ND-C1D | 6.19 | 111.47 | 105.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | D | 502 | HEM | C4D-ND-C1D | 6.18 | 111.46 | 105.07 |
| 5 | K | 502 | HEM | C4D-ND-C1D | 6.15 | 111.42 | 105.07 |
| 10 | C | 401 | HEC | CBD-CAD-C3D | -6.14 | 102.15 | 112.62 |
| 10 | C | 401 | HEC | C1D-C2D-C3D | -6.12 | 102.74 | 107.00 |
| 10 | F | 402 | HEC | C1D-C2D-C3D | -5.96 | 102.85 | 107.00 |
| 10 | L | 301 | HEC | CBA-CAA-C2A | -5.93 | 102.61 | 112.60 |
| 10 | F | 401 | HEC | C1D-C2D-C3D | -5.93 | 102.87 | 107.00 |
| 10 | F | 402 | HEC | CMC-C2C-C3C | 5.85 | 132.70 | 125.82 |
| 10 | F | 402 | HEC | C2B-C3B-C4B | -5.69 | 100.21 | 106.35 |
| 5 | A | 502 | HEM | C4D-ND-C1D | 5.64 | 110.90 | 105.07 |
| 10 | E | 301 | HEC | CBA-CAA-C2A | -5.56 | 103.23 | 112.60 |
| 10 | F | 401 | HEC | CBD-CAD-C3D | -5.48 | 103.26 | 112.62 |
| 10 | I | 403 | HEC | CMC-C2C-C3C | 5.40 | 132.17 | 125.82 |
| 10 | C | 402 | HEC | C2B-C3B-C4B | -5.39 | 100.53 | 106.35 |
| 10 | M | 402 | HEC | CAA-CBA-CGA | -5.35 | 98.75 | 113.76 |
| 10 | I | 403 | HEC | C2B-C3B-C4B | -5.31 | 100.62 | 106.35 |
| 10 | F | 401 | HEC | CMC-C2C-C3C | 5.16 | 131.89 | 125.82 |
| 10 | M | 403 | HEC | CMC-C2C-C3C | 5.09 | 131.81 | 125.82 |
| 10 | M | 403 | HEC | C2B-C3B-C4B | -5.06 | 100.89 | 106.35 |
| 10 | F | 401 | HEC | C2B-C3B-C4B | -5.01 | 100.94 | 106.35 |
| 10 | C | 401 | HEC | C4C-C3C-C2C | -4.98 | 100.97 | 106.35 |
| 10 | I | 402 | HEC | CBD-CAD-C3D | -4.98 | 104.12 | 112.62 |
| 10 | I | 402 | HEC | CMC-C2C-C3C | 4.73 | 131.38 | 125.82 |
| 10 | C | 401 | HEC | C2B-C3B-C4B | -4.57 | 101.42 | 106.35 |
| 10 | C | 402 | HEC | CMC-C2C-C3C | 4.55 | 131.17 | 125.82 |
| 10 | L | 301 | HEC | CMC-C2C-C3C | 4.54 | 131.16 | 125.82 |
| 10 | H | 301 | HEC | CMC-C2C-C3C | 4.45 | 131.05 | 125.82 |
| 10 | M | 402 | HEC | CMC-C2C-C3C | 4.44 | 131.05 | 125.82 |
| 10 | I | 402 | HEC | CAA-CBA-CGA | -4.35 | 101.56 | 113.76 |
| 10 | I | 402 | HEC | C2B-C3B-C4B | -4.33 | 101.68 | 106.35 |
| 10 | C | 402 | HEC | CBA-CAA-C2A | -4.28 | 105.39 | 112.60 |
| 10 | I | 403 | HEC | CAD-CBD-CGD | -4.28 | 101.77 | 113.76 |
| 10 | I | 402 | HEC | C4C-C3C-C2C | -4.26 | 101.75 | 106.35 |
| 10 | M | 402 | HEC | C2B-C3B-C4B | -4.25 | 101.77 | 106.35 |
| 5 | K | 502 | HEM | C4C-CHD-C1D | 4.19 | 128.09 | 122.56 |
| 5 | D | 502 | HEM | C4C-CHD-C1D | 4.09 | 127.95 | 122.56 |
| 10 | C | 401 | HEC | CAA-CBA-CGA | -4.03 | 102.47 | 113.76 |
| 5 | G | 502 | HEM | C4C-CHD-C1D | 3.98 | 127.81 | 122.56 |
| 5 | A | 502 | HEM | C4C-CHD-C1D | 3.87 | 127.67 | 122.56 |
| 10 | F | 401 | HEC | CAA-CBA-CGA | -3.83 | 103.01 | 113.76 |
| 10 | M | 403 | HEC | CAD-CBD-CGD | -3.72 | 103.32 | 113.76 |
| 5 | A | 501 | HEM | CAD-CBD-CGD | -3.68 | 105.69 | 113.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10 | C | 402 | HEC | CAD-CBD-CGD | -3.65 | 103.53 | 113.76 |
| 10 | L | 301 | HEC | C2B-C3B-C4B | -3.64 | 102.42 | 106.35 |
| 10 | E | 301 | HEC | CMC-C2C-C3C | 3.63 | 130.09 | 125.82 |
| 10 | H | 301 | HEC | C2B-C3B-C4B | -3.54 | 102.53 | 106.35 |
| 5 | G | 502 | HEM | CBA-CAA-C2A | -3.53 | 106.60 | 112.62 |
| 10 | B | 301 | HEC | CMC-C2C-C3C | 3.53 | 129.97 | 125.82 |
| 10 | E | 301 | HEC | C2B-C3B-C4B | -3.47 | 102.61 | 106.35 |
| 10 | F | 401 | HEC | C4C-C3C-C2C | -3.44 | 102.63 | 106.35 |
| 10 | I | 403 | HEC | CBA-CAA-C2A | -3.42 | 106.84 | 112.60 |
| 5 | G | 501 | HEM | C4C-CHD-C1D | 3.41 | 127.06 | 122.56 |
| 5 | D | 502 | HEM | CBA-CAA-C2A | -3.33 | 106.94 | 112.62 |
| 5 | G | 501 | HEM | CAD-CBD-CGD | -3.33 | 106.44 | 113.60 |
| 5 | D | 501 | HEM | CAD-CBD-CGD | -3.33 | 106.45 | 113.60 |
| 10 | C | 402 | HEC | C4C-C3C-C2C | -3.30 | 102.79 | 106.35 |
| 10 | C | 401 | HEC | CMB-C2B-C3B | 3.29 | 129.69 | 125.82 |
| 10 | L | 301 | HEC | C3B-C4B-NB | 3.27 | 117.11 | 110.94 |
| 5 | G | 501 | HEM | CBA-CAA-C2A | -3.27 | 107.05 | 112.62 |
| 5 | K | 501 | HEM | CAD-CBD-CGD | -3.26 | 106.58 | 113.60 |
| 10 | B | 301 | HEC | C3B-C4B-NB | 3.26 | 117.10 | 110.94 |
| 10 | L | 301 | HEC | CMA-C3A-C2A | 3.23 | 131.03 | 124.94 |
| 10 | M | 403 | HEC | C4C-C3C-C2C | -3.23 | 102.86 | 106.35 |
| 10 | B | 301 | HEC | C2B-C3B-C4B | -3.22 | 102.88 | 106.35 |
| 5 | A | 501 | HEM | C4C-CHD-C1D | 3.21 | 126.80 | 122.56 |
| 5 | A | 502 | HEM | CBA-CAA-C2A | -3.21 | 107.14 | 112.62 |
| 10 | H | 301 | HEC | C3B-C4B-NB | 3.20 | 116.98 | 110.94 |
| 10 | H | 301 | HEC | CMA-C3A-C2A | 3.18 | 130.93 | 124.94 |
| 10 | M | 403 | HEC | CAA-CBA-CGA | -3.17 | 104.88 | 113.76 |
| 10 | I | 403 | HEC | C3B-C4B-NB | 3.15 | 116.90 | 110.94 |
| 10 | F | 402 | HEC | C3B-C4B-NB | 3.12 | 116.83 | 110.94 |
| 10 | C | 402 | HEC | C3B-C4B-NB | 3.11 | 116.83 | 110.94 |
| 10 | I | 403 | HEC | C4C-C3C-C2C | -3.09 | 103.02 | 106.35 |
| 10 | M | 402 | HEC | C4C-C3C-C2C | -3.07 | 103.04 | 106.35 |
| 10 | L | 301 | HEC | C4C-C3C-C2C | -3.07 | 103.04 | 106.35 |
| 10 | F | 401 | HEC | C3B-C4B-NB | 3.04 | 116.69 | 110.94 |
| 10 | E | 301 | HEC | C3B-C4B-NB | 2.97 | 116.55 | 110.94 |
| 10 | E | 301 | HEC | C4C-C3C-C2C | -2.95 | 103.17 | 106.35 |
| 10 | F | 402 | HEC | C4C-C3C-C2C | -2.94 | 103.18 | 106.35 |
| 5 | D | 502 | HEM | C4B-CHC-C1C | 2.90 | 126.39 | 122.56 |
| 10 | I | 402 | HEC | CMA-C3A-C2A | 2.86 | 130.34 | 124.94 |
| 5 | G | 502 | HEM | CMA-C3A-C4A | -2.85 | 124.09 | 128.46 |
| 10 | H | 301 | HEC | C4C-C3C-C2C | -2.83 | 103.30 | 106.35 |
| 10 | C | 402 | HEC | CAA-CBA-CGA | -2.81 | 105.87 | 113.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10 | M | 403 | HEC | CBA-CAA-C2A | -2.81 | 107.87 | 112.60 |
| 10 | B | 301 | HEC | CMA-C3A-C2A | 2.80 | 130.23 | 124.94 |
| 10 | C | 402 | HEC | CMA-C3A-C2A | 2.79 | 130.20 | 124.94 |
| 10 | M | 403 | HEC | C3B-C4B-NB | 2.78 | 116.19 | 110.94 |
| 10 | F | 402 | HEC | CBA-CAA-C2A | -2.75 | 107.96 | 112.60 |
| 10 | M | 403 | HEC | CMB-C2B-C3B | 2.75 | 129.06 | 125.82 |
| 10 | C | 402 | HEC | CMB-C2B-C3B | 2.75 | 129.06 | 125.82 |
| 5 | K | 502 | HEM | CMA-C3A-C4A | -2.74 | 124.25 | 128.46 |
| 10 | B | 301 | HEC | C4C-C3C-C2C | -2.72 | 103.41 | 106.35 |
| 10 | I | 402 | HEC | CMB-C2B-C3B | 2.71 | 129.00 | 125.82 |
| 5 | K | 502 | HEM | CBA-CAA-C2A | -2.70 | 108.01 | 112.62 |
| 10 | C | 401 | HEC | CMC-C2C-C3C | 2.68 | 128.97 | 125.82 |
| 5 | A | 502 | HEM | C4B-CHC-C1C | 2.66 | 126.08 | 122.56 |
| 5 | D | 502 | HEM | C3B-C2B-C1B | 2.66 | 108.46 | 106.49 |
| 5 | G | 502 | HEM | C4B-CHC-C1C | 2.65 | 126.06 | 122.56 |
| 10 | I | 402 | HEC | C3B-C4B-NB | 2.62 | 115.89 | 110.94 |
| 5 | G | 501 | HEM | CAA-CBA-CGA | -2.61 | 106.43 | 113.76 |
| 5 | K | 501 | HEM | C4C-CHD-C1D | 2.61 | 126.00 | 122.56 |
| 10 | C | 401 | HEC | C3B-C4B-NB | 2.60 | 115.86 | 110.94 |
| 10 | M | 402 | HEC | C3B-C4B-NB | 2.59 | 115.84 | 110.94 |
| 10 | M | 403 | HEC | CMD-C2D-C3D | 2.59 | 129.82 | 124.94 |
| 5 | K | 502 | HEM | C4B-CHC-C1C | 2.58 | 125.96 | 122.56 |
| 10 | I | 403 | HEC | O1D-CGD-CBD | -2.57 | 114.82 | 123.08 |
| 10 | C | 402 | HEC | CMD-C2D-C3D | 2.57 | 129.78 | 124.94 |
| 5 | D | 501 | HEM | C4C-CHD-C1D | 2.55 | 125.92 | 122.56 |
| 10 | M | 403 | HEC | O1D-CGD-CBD | -2.52 | 115.00 | 123.08 |
| 10 | E | 301 | HEC | CMA-C3A-C2A | 2.51 | 129.67 | 124.94 |
| 5 | A | 502 | HEM | CHD-C1D-ND | 2.50 | 127.15 | 124.43 |
| 5 | D | 502 | HEM | C1B-NB-C4B | 2.48 | 107.64 | 105.07 |
| 10 | M | 402 | HEC | CMA-C3A-C2A | 2.46 | 129.59 | 124.94 |
| 10 | C | 401 | HEC | CMA-C3A-C2A | 2.45 | 129.57 | 124.94 |
| 10 | C | 402 | HEC | CBD-CAD-C3D | -2.45 | 108.44 | 112.62 |
| 5 | D | 502 | HEM | CHD-C1D-ND | 2.45 | 127.09 | 124.43 |
| 5 | K | 502 | HEM | C1B-NB-C4B | 2.43 | 107.59 | 105.07 |
| 5 | G | 502 | HEM | C1B-NB-C4B | 2.41 | 107.57 | 105.07 |
| 5 | D | 501 | HEM | C1B-NB-C4B | 2.41 | 107.56 | 105.07 |
| 10 | I | 403 | HEC | CMA-C3A-C2A | 2.40 | 129.47 | 124.94 |
| 10 | I | 402 | HEC | CMC-C2C-C1C | -2.37 | 124.82 | 128.46 |
| 5 | K | 502 | HEM | C3B-C2B-C1B | 2.32 | 108.21 | 106.49 |
| 10 | I | 403 | HEC | CMD-C2D-C3D | 2.31 | 129.29 | 124.94 |
| 5 | A | 501 | HEM | O1A-CGA-CBA | -2.31 | 115.67 | 123.08 |
| 5 | A | 501 | HEM | CMA-C3A-C4A | -2.30 | 124.93 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | G | 501 | HEM | CMD-C2D-C1D | 2.28 | 128.51 | 125.04 |
| 10 | I | 403 | HEC | CAA-CBA-CGA | -2.28 | 107.38 | 113.76 |
| 10 | C | 402 | HEC | O1D-CGD-CBD | -2.28 | 115.77 | 123.08 |
| 5 | K | 501 | HEM | C1B-NB-C4B | 2.27 | 107.42 | 105.07 |
| 10 | F | 401 | HEC | CMC-C2C-C1C | -2.27 | 124.98 | 128.46 |
| 10 | E | 301 | HEC | CMD-C2D-C3D | 2.27 | 129.22 | 124.94 |
| 10 | C | 401 | HEC | CMD-C2D-C3D | 2.26 | 129.21 | 124.94 |
| 10 | B | 301 | HEC | CMD-C2D-C3D | 2.26 | 129.20 | 124.94 |
| 5 | D | 501 | HEM | CBA-CAA-C2A | -2.26 | 108.76 | 112.62 |
| 10 | M | 402 | HEC | CMB-C2B-C3B | 2.25 | 128.47 | 125.82 |
| 10 | M | 402 | HEC | O1D-CGD-CBD | -2.25 | 115.85 | 123.08 |
| 10 | F | 401 | HEC | CMA-C3A-C2A | 2.25 | 129.18 | 124.94 |
| 10 | L | 301 | HEC | CMD-C2D-C3D | 2.25 | 129.18 | 124.94 |
| 5 | G | 502 | HEM | CHD-C1D-ND | 2.25 | 126.87 | 124.43 |
| 10 | E | 301 | HEC | CMB-C2B-C3B | 2.24 | 128.46 | 125.82 |
| 10 | H | 301 | HEC | CMD-C2D-C3D | 2.24 | 129.17 | 124.94 |
| 5 | D | 502 | HEM | CMA-C3A-C4A | -2.23 | 125.03 | 128.46 |
| 5 | A | 502 | HEM | O1A-CGA-CBA | -2.23 | 115.92 | 123.08 |
| 5 | A | 501 | HEM | CHD-C1D-ND | 2.22 | 126.84 | 124.43 |
| 5 | G | 502 | HEM | C3B-C2B-C1B | 2.20 | 108.12 | 106.49 |
| 5 | A | 501 | HEM | CAA-CBA-CGA | -2.19 | 107.61 | 113.76 |
| 10 | L | 301 | HEC | CBD-CAD-C3D | -2.19 | 108.89 | 112.62 |
| 10 | I | 403 | HEC | CBD-CAD-C3D | -2.16 | 108.93 | 112.62 |
| 10 | I | 402 | HEC | CMD-C2D-C3D | 2.14 | 128.97 | 124.94 |
| 10 | F | 402 | HEC | CAD-CBD-CGD | -2.13 | 107.79 | 113.76 |
| 5 | K | 502 | HEM | CAD-CBD-CGD | -2.12 | 109.05 | 113.60 |
| 5 | K | 502 | HEM | CHD-C1D-ND | 2.11 | 126.73 | 124.43 |
| 10 | F | 402 | HEC | CMC-C2C-C1C | -2.11 | 125.22 | 128.46 |
| 10 | F | 402 | HEC | CMB-C2B-C3B | 2.10 | 128.29 | 125.82 |
| 5 | G | 501 | HEM | C1B-NB-C4B | 2.10 | 107.25 | 105.07 |
| 10 | C | 401 | HEC | CAD-CBD-CGD | -2.08 | 107.92 | 113.76 |
| 10 | I | 402 | HEC | CAD-CBD-CGD | -2.08 | 107.92 | 113.76 |
| 10 | M | 402 | HEC | CAD-CBD-CGD | -2.08 | 107.92 | 113.76 |
| 5 | G | 501 | HEM | CAD-C3D-C4D | 2.08 | 128.29 | 124.66 |
| 10 | M | 403 | HEC | CBD-CAD-C3D | -2.08 | 109.08 | 112.62 |
| 10 | C | 401 | HEC | O1D-CGD-CBD | -2.06 | 116.45 | 123.08 |
| 5 | K | 501 | HEM | CBA-CAA-C2A | -2.05 | 109.12 | 112.62 |
| 5 | K | 502 | HEM | CHC-C4B-C3B | 2.05 | 127.71 | 124.57 |
| 10 | L | 301 | HEC | CMB-C2B-C3B | 2.04 | 128.22 | 125.82 |
| 10 | M | 403 | HEC | CMA-C3A-C2A | 2.04 | 128.78 | 124.94 |
| 5 | G | 502 | HEM | CHC-C4B-C3B | 2.02 | 127.66 | 124.57 |
| 10 | C | 402 | HEC | C3C-C4C-NC | 2.01 | 114.74 | 110.94 |

There are no chirality outliers.

All (51) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | A | 502 | HEM | C4B-C3B-CAB-CBB |
| 5 | D | 502 | HEM | C4B-C3B-CAB-CBB |
| 5 | G | 502 | HEM | C4B-C3B-CAB-CBB |
| 5 | K | 502 | HEM | C4B-C3B-CAB-CBB |
| 10 | L | 301 | HEC | C2A-CAA-CBA-CGA |
| 5 | D | 501 | HEM | CAD-CBD-CGD-O2D |
| 10 | C | 401 | HEC | CAA-CBA-CGA-O1A |
| 10 | E | 301 | HEC | CAD-CBD-CGD-O1D |
| 10 | F | 401 | HEC | CAA-CBA-CGA-O1A |
| 10 | B | 301 | HEC | CAD-CBD-CGD-O1D |
| 10 | L | 301 | HEC | CAD-CBD-CGD-O2D |
| 10 | B | 301 | HEC | CAD-CBD-CGD-O2D |
| 10 | I | 402 | HEC | CAA-CBA-CGA-O1A |
| 10 | I | 402 | HEC | CAA-CBA-CGA-O2A |
| 10 | L | 301 | HEC | CAD-CBD-CGD-O1D |
| 10 | M | 402 | HEC | CAA-CBA-CGA-O2A |
| 10 | E | 301 | HEC | CAD-CBD-CGD-O2D |
| 10 | M | 402 | HEC | CAA-CBA-CGA-O1A |
| 10 | H | 301 | HEC | CAD-CBD-CGD-O1D |
| 10 | H | 301 | HEC | CAD-CBD-CGD-O2D |
| 5 | A | 501 | HEM | CAD-CBD-CGD-O2D |
| 5 | D | 501 | HEM | CAD-CBD-CGD-O1D |
| 5 | D | 502 | HEM | CAD-CBD-CGD-O2D |
| 10 | F | 401 | HEC | CAA-CBA-CGA-O2A |
| 5 | A | 501 | HEM | CAD-CBD-CGD-O1D |
| 5 | A | 502 | HEM | CAD-CBD-CGD-O2D |
| 5 | G | 501 | HEM | CAD-CBD-CGD-O1D |
| 5 | D | 502 | HEM | CAD-CBD-CGD-O1D |
| 10 | C | 402 | HEC | CAD-CBD-CGD-O2D |
| 5 | G | 501 | HEM | CAD-CBD-CGD-O2D |
| 10 | C | 401 | HEC | CAA-CBA-CGA-O2A |
| 10 | C | 402 | HEC | CAD-CBD-CGD-O1D |
| 10 | M | 403 | HEC | CAD-CBD-CGD-O2D |
| 5 | A | 502 | HEM | CAD-CBD-CGD-O1D |
| 10 | H | 301 | HEC | CAA-CBA-CGA-O1A |
| 10 | I | 403 | HEC | CAD-CBD-CGD-O2D |
| 10 | B | 301 | HEC | CAA-CBA-CGA-O1A |
| 5 | K | 501 | HEM | CAD-CBD-CGD-O2D |
| 5 | K | 501 | HEM | CAD-CBD-CGD-O1D |
| 10 | F | 402 | HEC | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 10 | M | 403 | HEC | CAD-CBD-CGD-O1D |
| 10 | I | 403 | HEC | CAD-CBD-CGD-O1D |
| 10 | F | 402 | HEC | CAD-CBD-CGD-O1D |
| 10 | B | 301 | HEC | CAA-CBA-CGA-O2A |
| 5 | A | 501 | HEM | CAA-CBA-CGA-O2A |
| 10 | H | 301 | HEC | CAA-CBA-CGA-O2A |
| 10 | E | 301 | HEC | CAA-CBA-CGA-O2A |
| 10 | E | 301 | HEC | CAA-CBA-CGA-O1A |
| 10 | F | 402 | HEC | CAA-CBA-CGA-O2A |
| 5 | A | 501 | HEM | CAA-CBA-CGA-O1A |
| 10 | L | 301 | HEC | CAA-CBA-CGA-O2A |

There are no ring outliers.

28 monomers are involved in 129 short contacts:

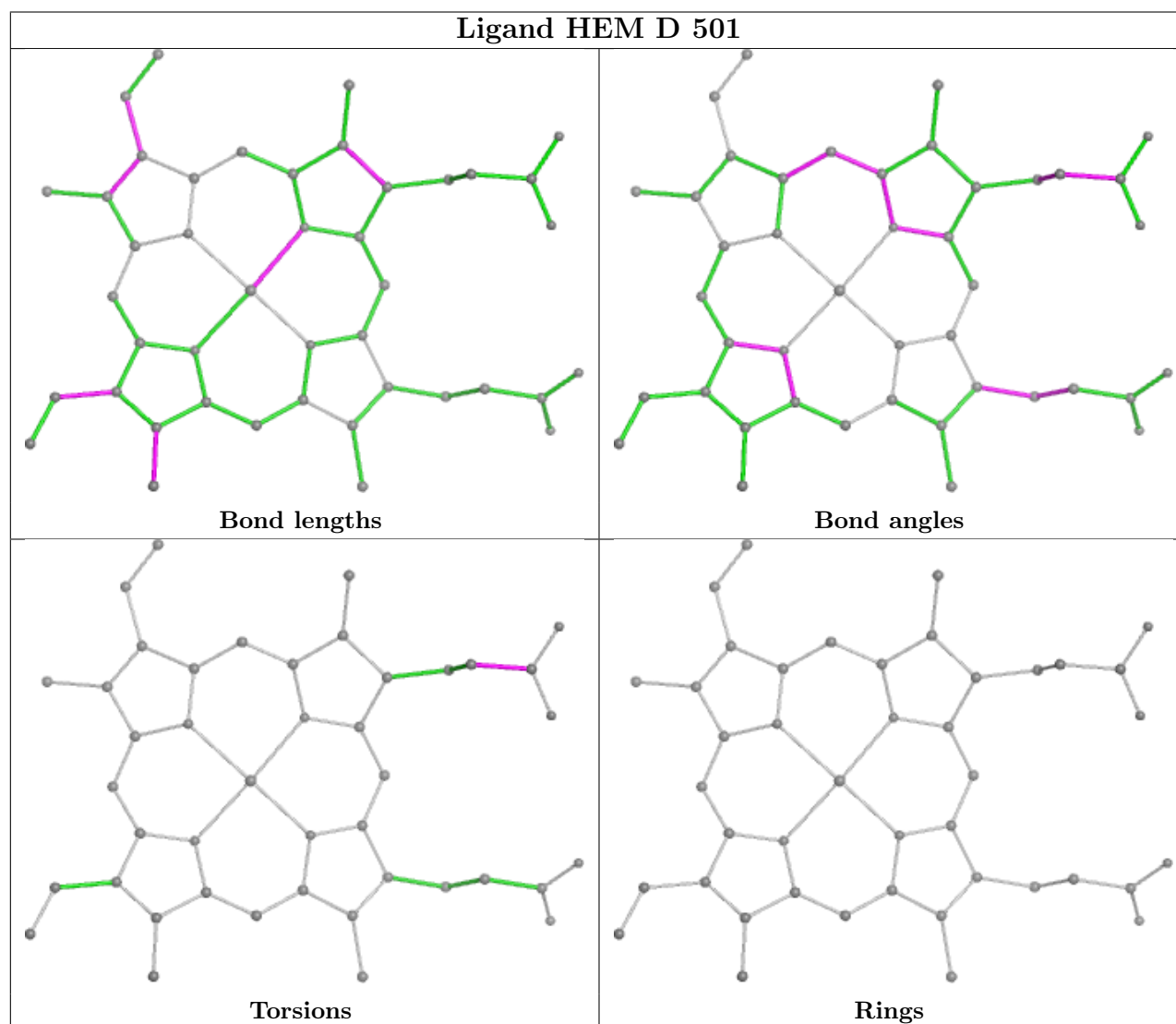
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9 | K | 506 | PO4 | 4 | 0 |
| 11 | I | 401 | FC6 | 1 | 0 |
| 5 | D | 501 | HEM | 5 | 0 |
| 11 | C | 403 | FC6 | 2 | 0 |
| 5 | G | 502 | HEM | 8 | 0 |
| 11 | F | 403 | FC6 | 2 | 0 |
| 5 | K | 501 | HEM | 5 | 0 |
| 10 | F | 401 | HEC | 7 | 0 |
| 9 | A | 506 | PO4 | 1 | 0 |
| 11 | M | 401 | FC6 | 2 | 0 |
| 5 | K | 502 | HEM | 8 | 0 |
| 10 | I | 403 | HEC | 3 | 0 |
| 9 | D | 505 | PO4 | 1 | 0 |
| 5 | A | 502 | HEM | 9 | 0 |
| 10 | L | 301 | HEC | 4 | 0 |
| 5 | A | 501 | HEM | 3 | 0 |
| 10 | M | 403 | HEC | 2 | 0 |
| 10 | M | 402 | HEC | 9 | 0 |
| 5 | D | 502 | HEM | 8 | 0 |
| 10 | B | 301 | HEC | 5 | 0 |
| 5 | G | 501 | HEM | 5 | 0 |
| 10 | I | 402 | HEC | 8 | 0 |
| 10 | F | 402 | HEC | 3 | 0 |
| 9 | G | 506 | PO4 | 1 | 0 |
| 10 | H | 301 | HEC | 6 | 0 |
| 10 | C | 402 | HEC | 3 | 0 |

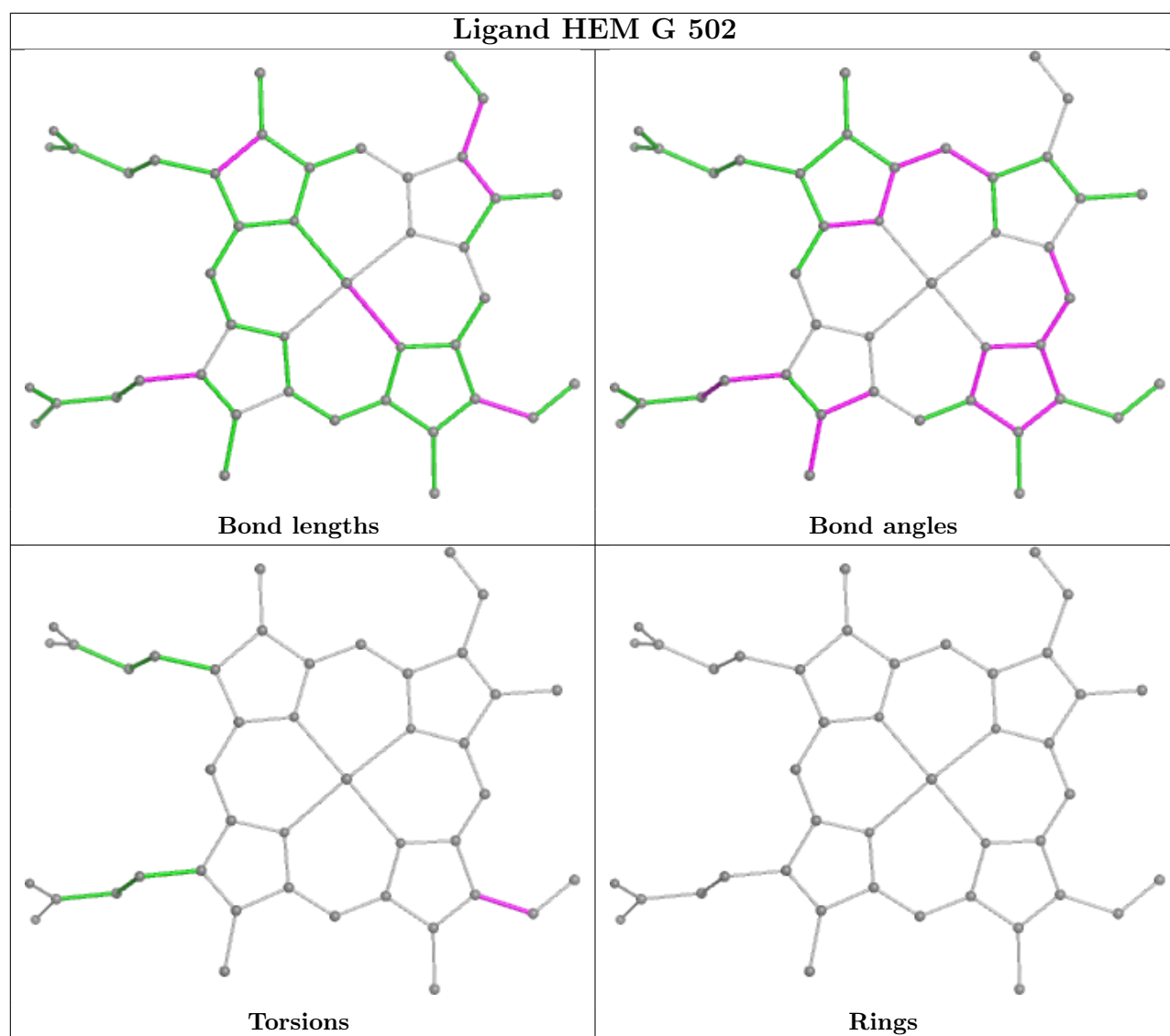
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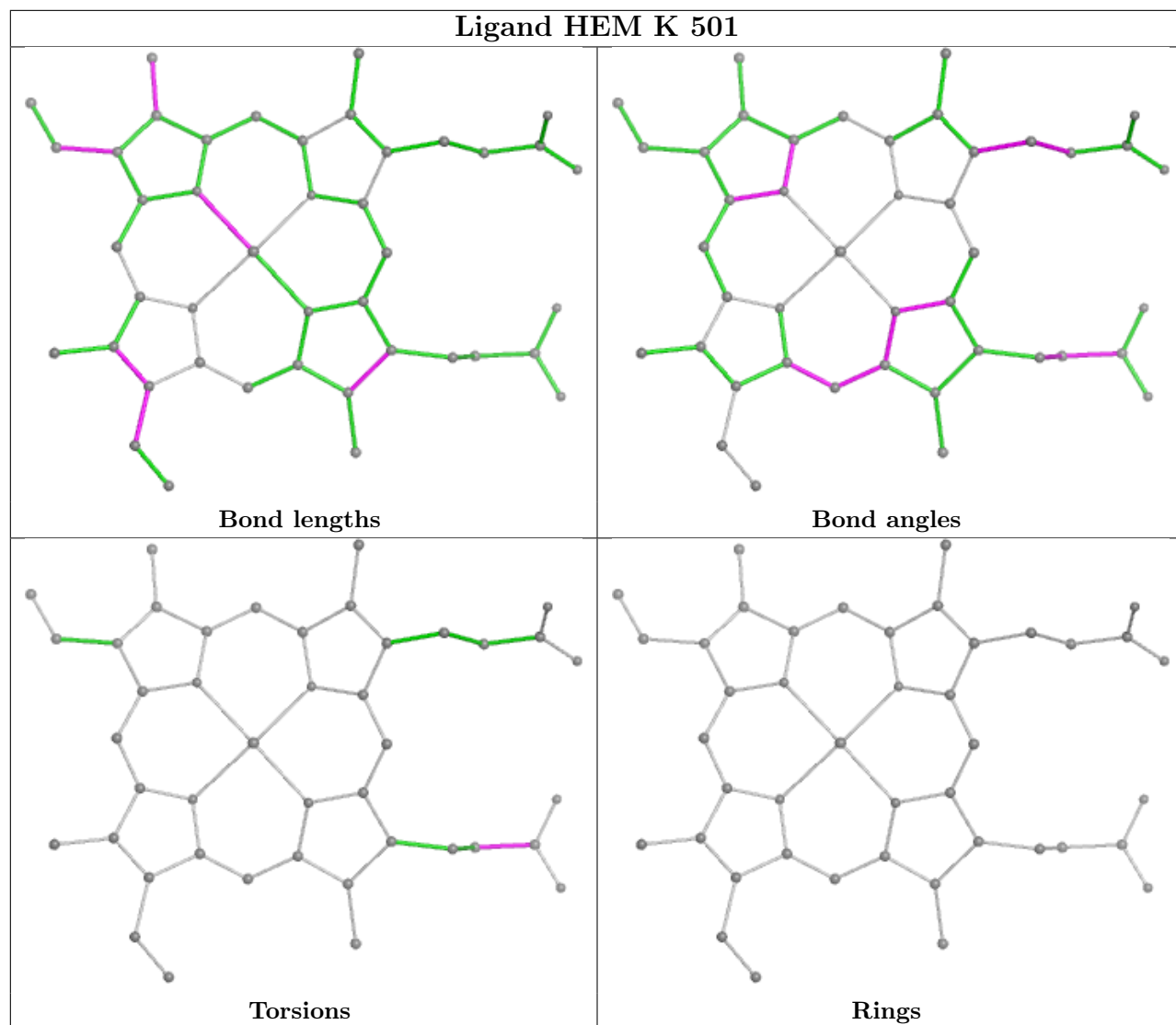
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 10 | C | 401 | HEC | 8 | 0 |
| 10 | E | 301 | HEC | 6 | 0 |

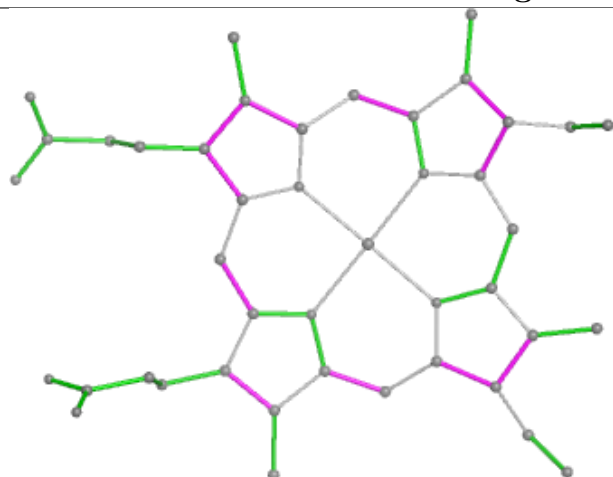
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



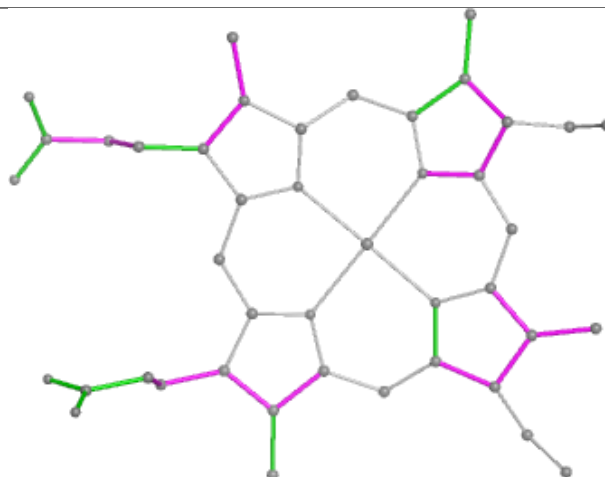




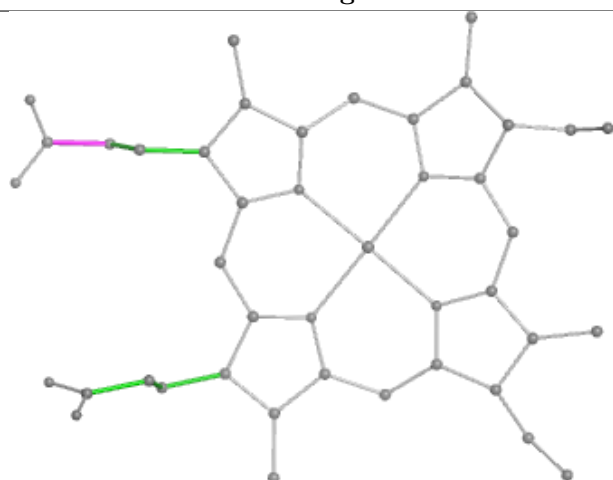
Ligand HEC F 401



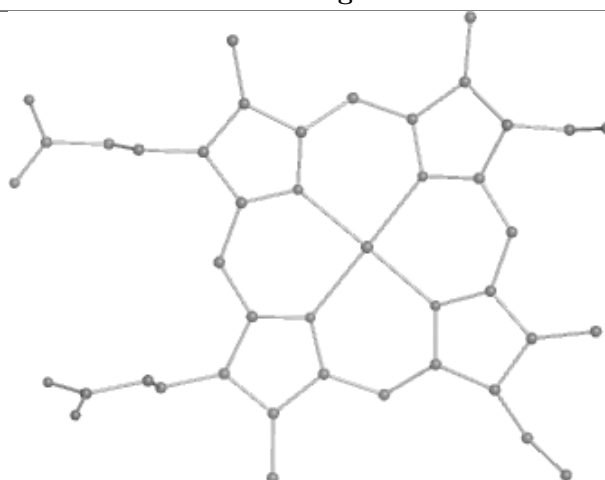
Bond lengths



Bond angles

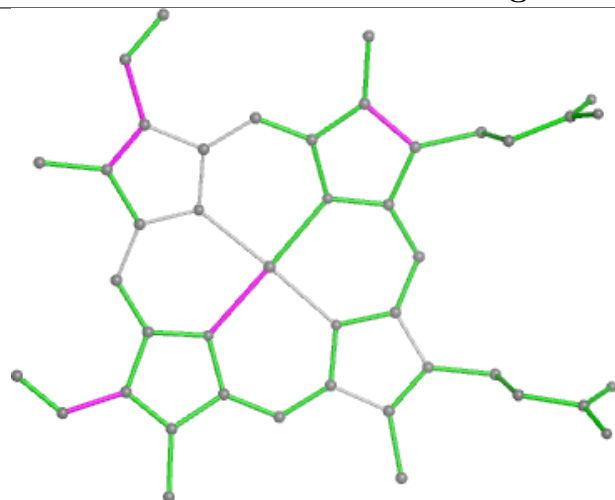


Torsions

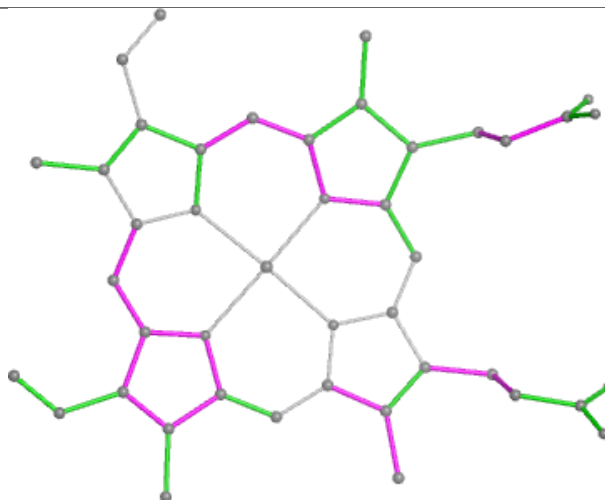


Rings

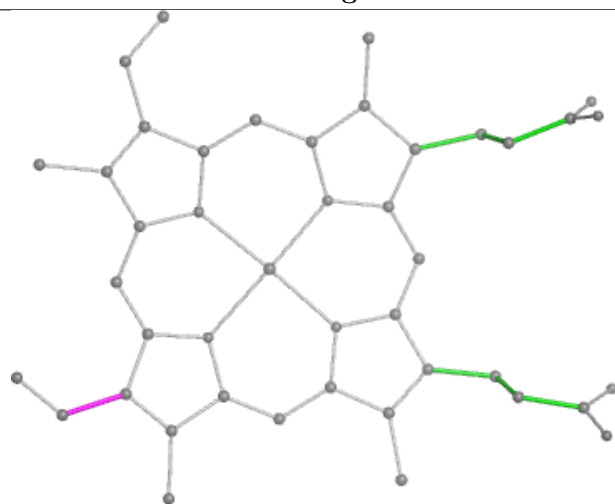
Ligand HEM K 502



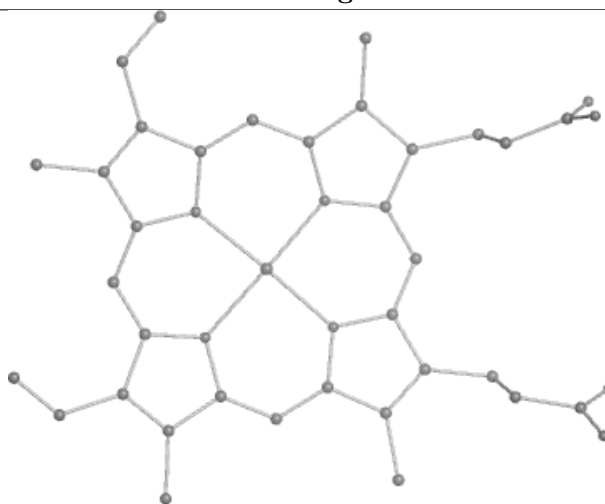
Bond lengths



Bond angles

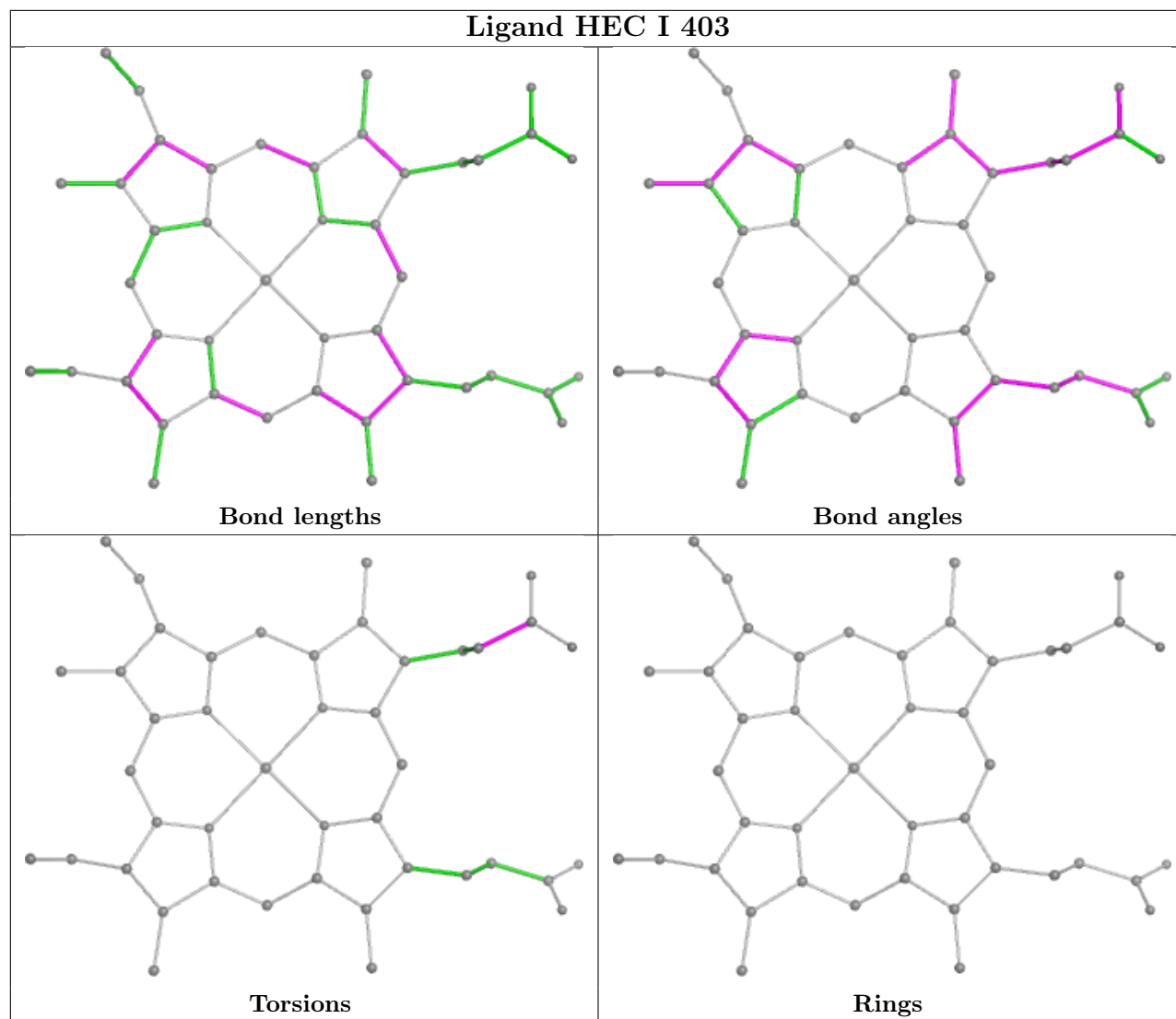


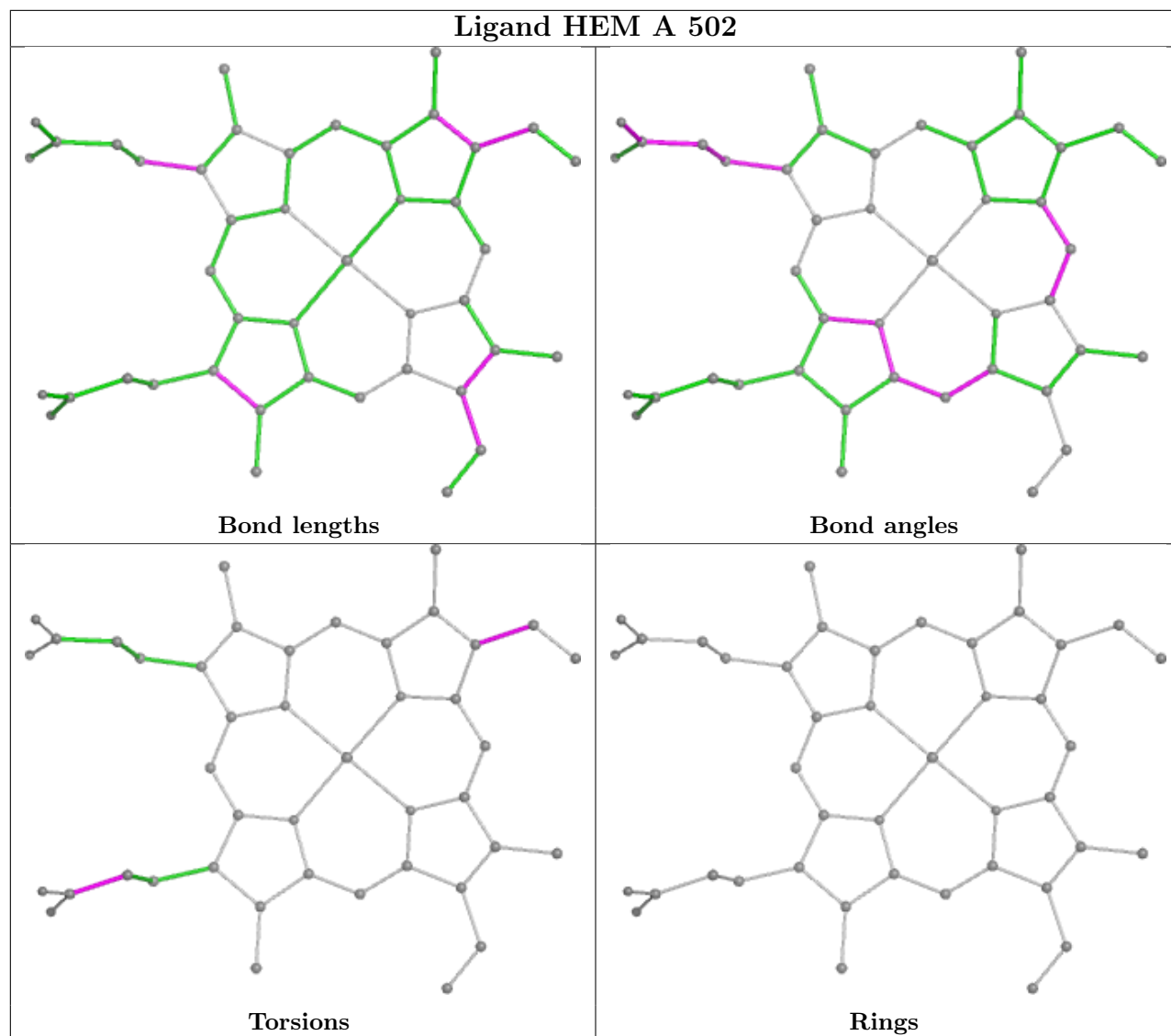
Torsions



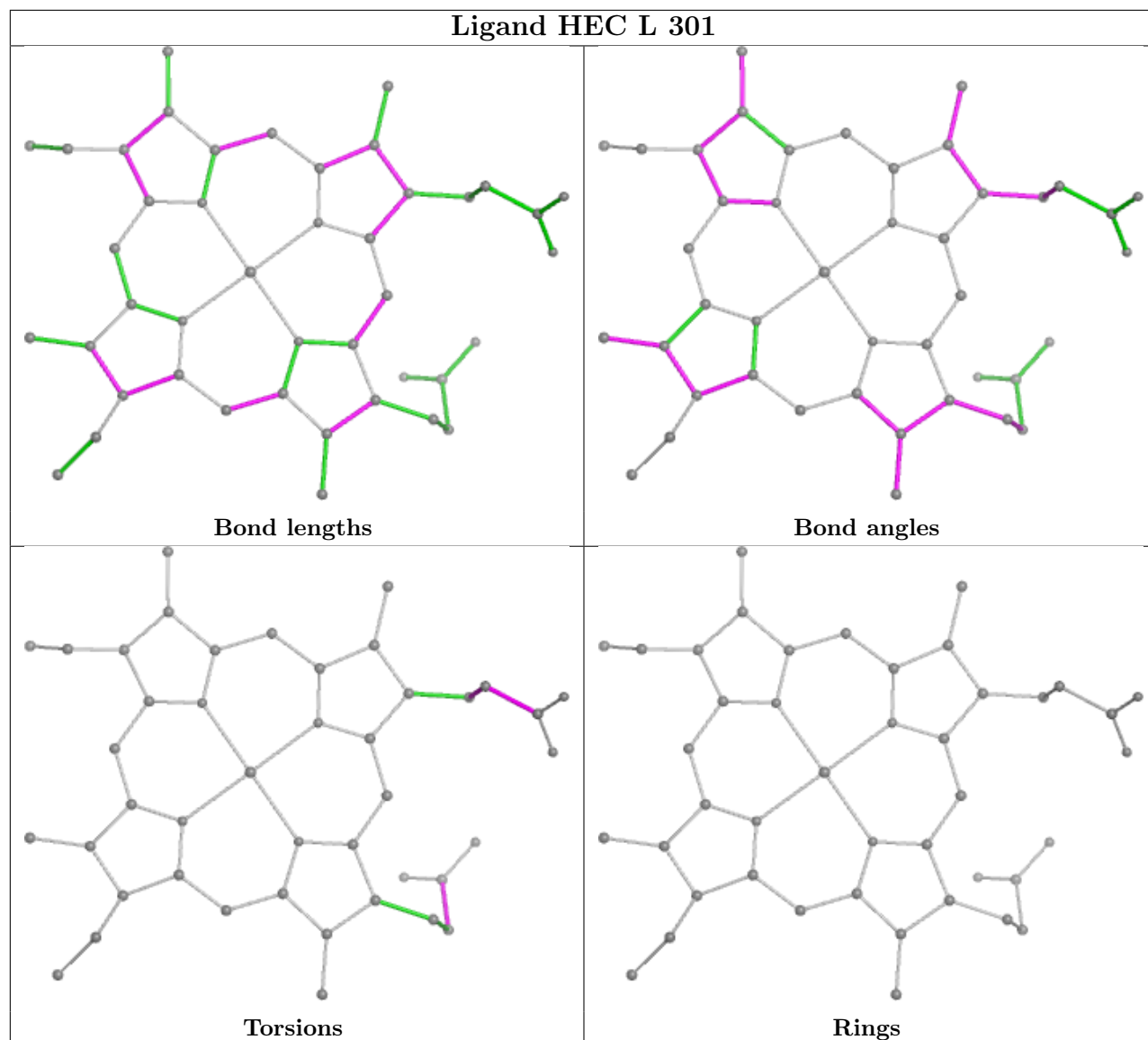
Rings

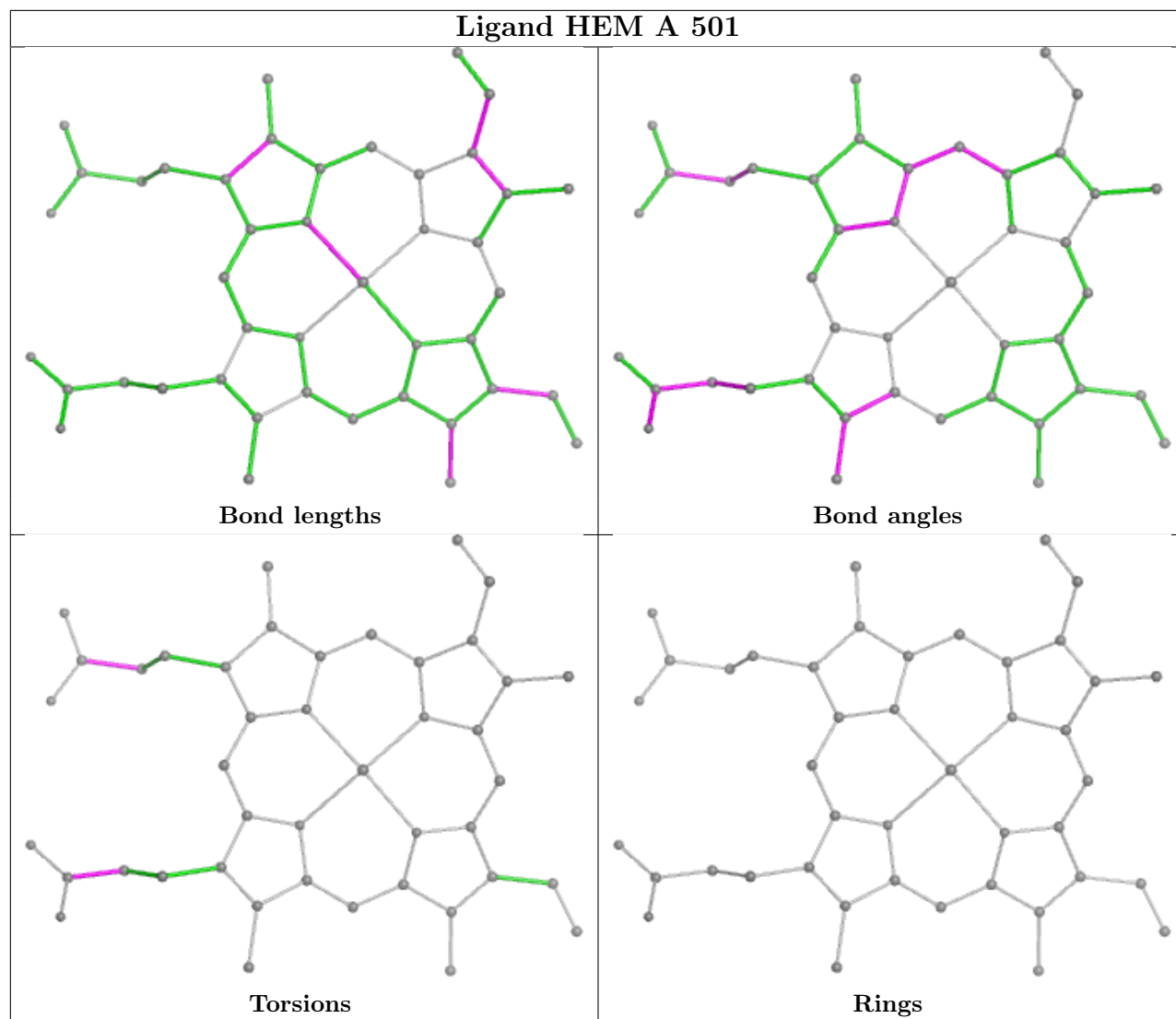
Ligand HEC I 403

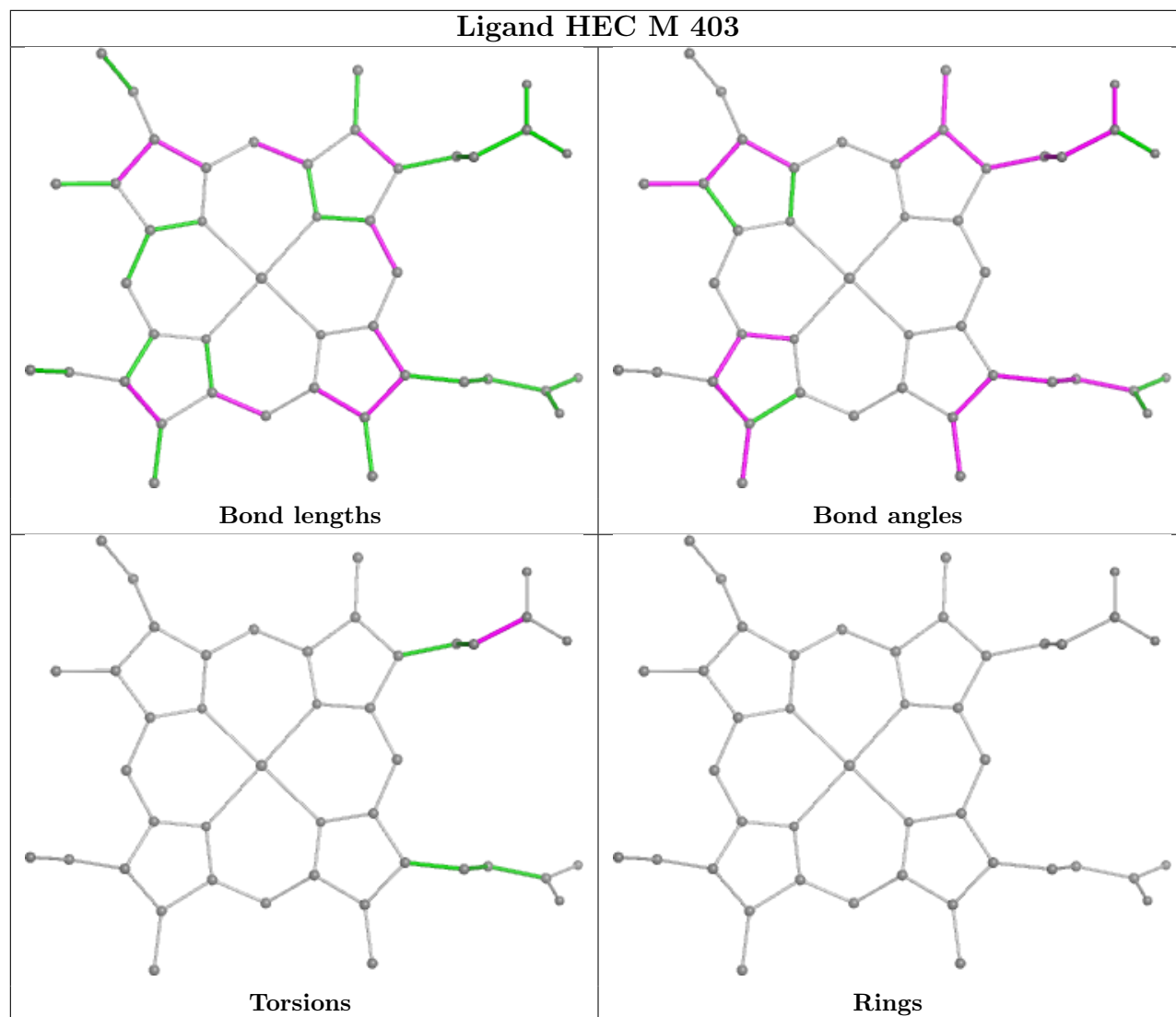


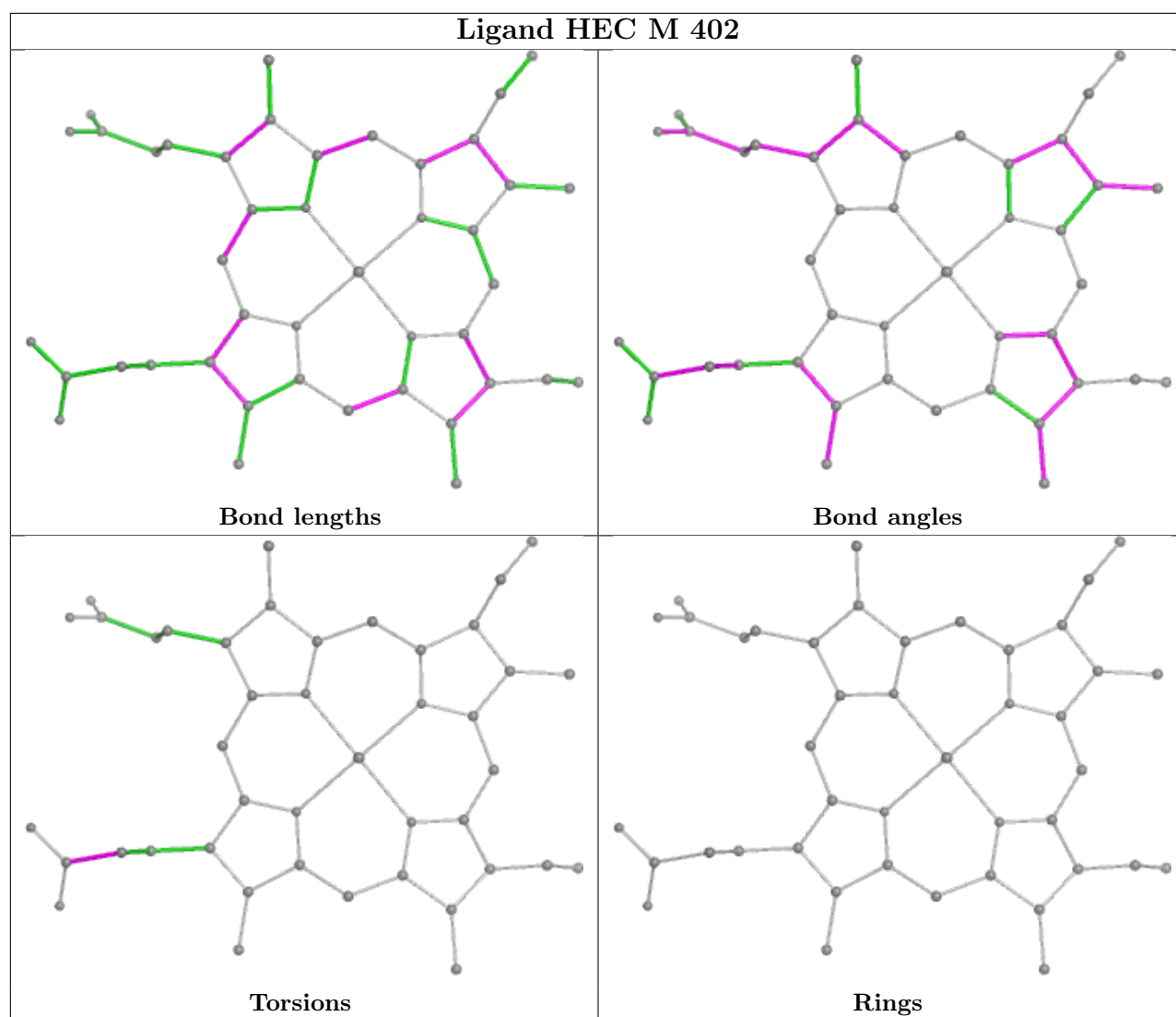


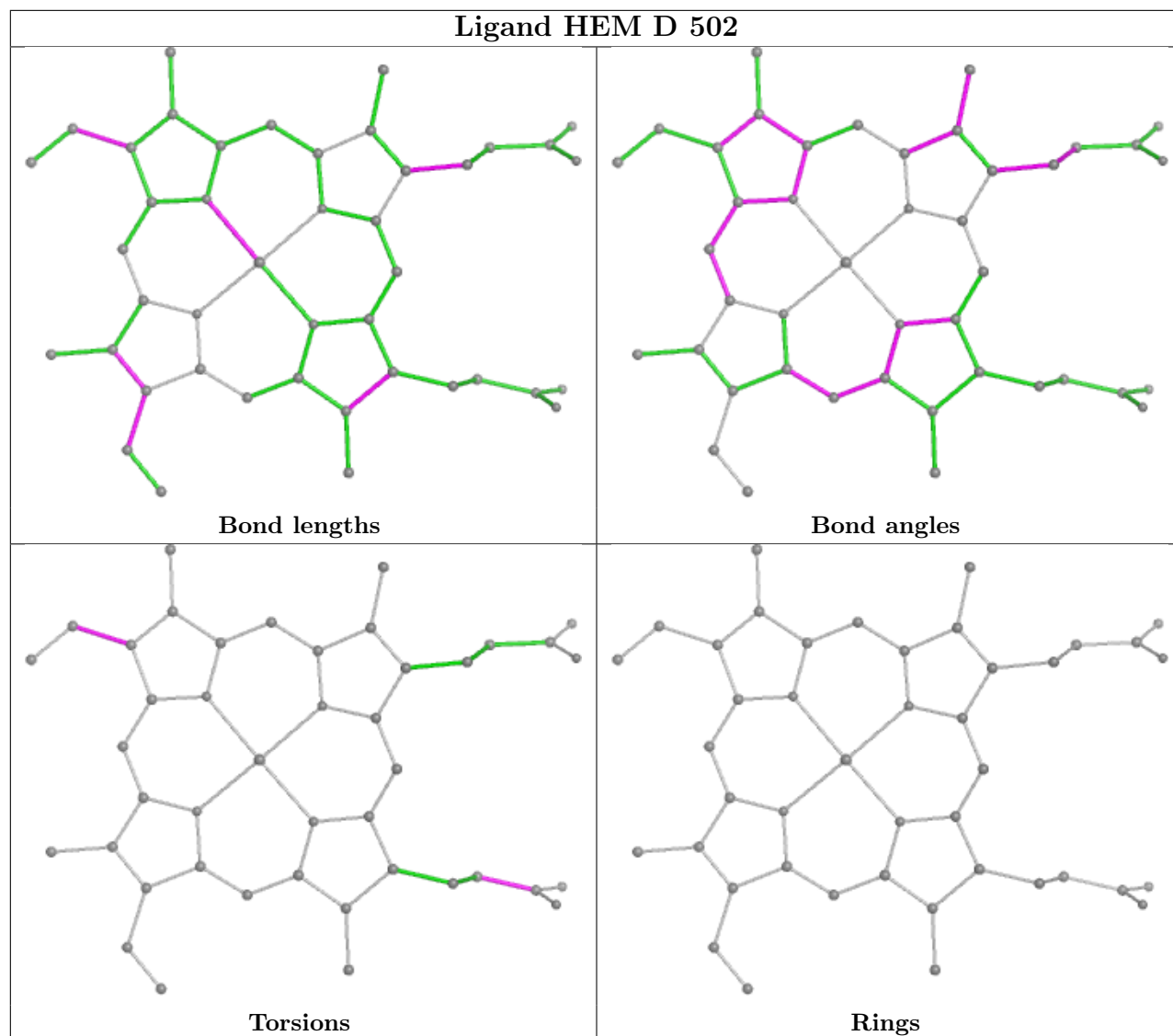
Ligand HEC L 301

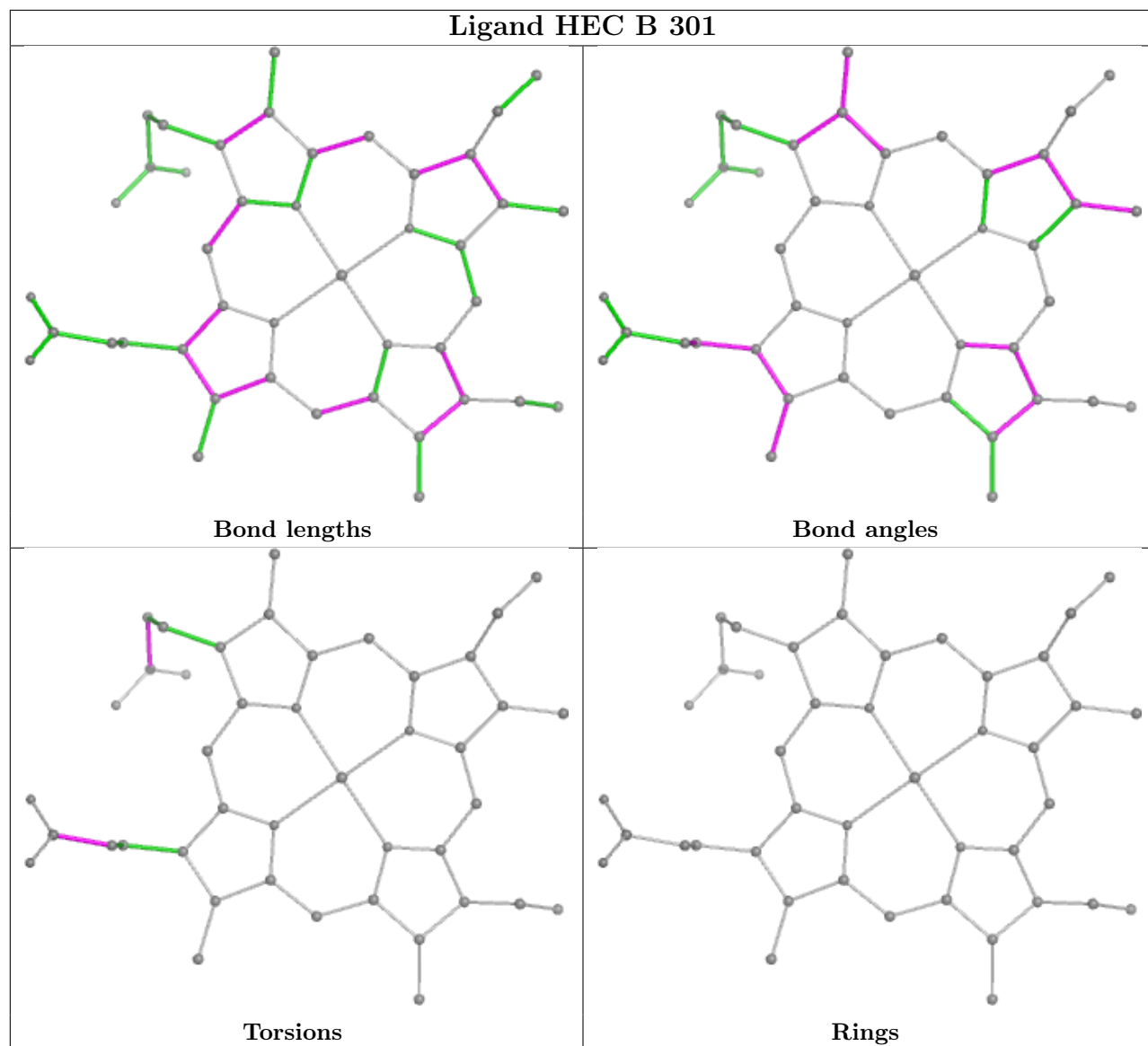


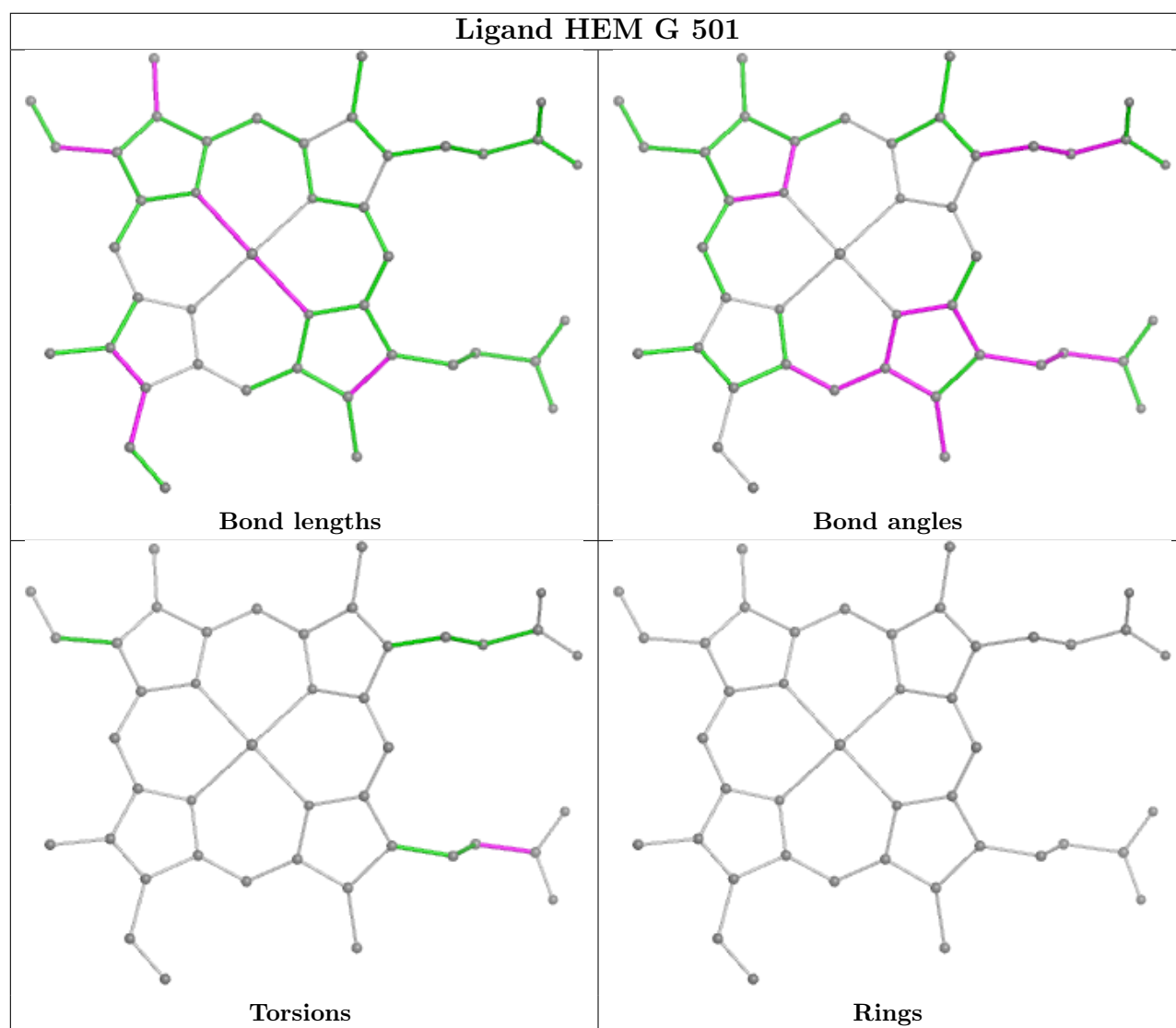




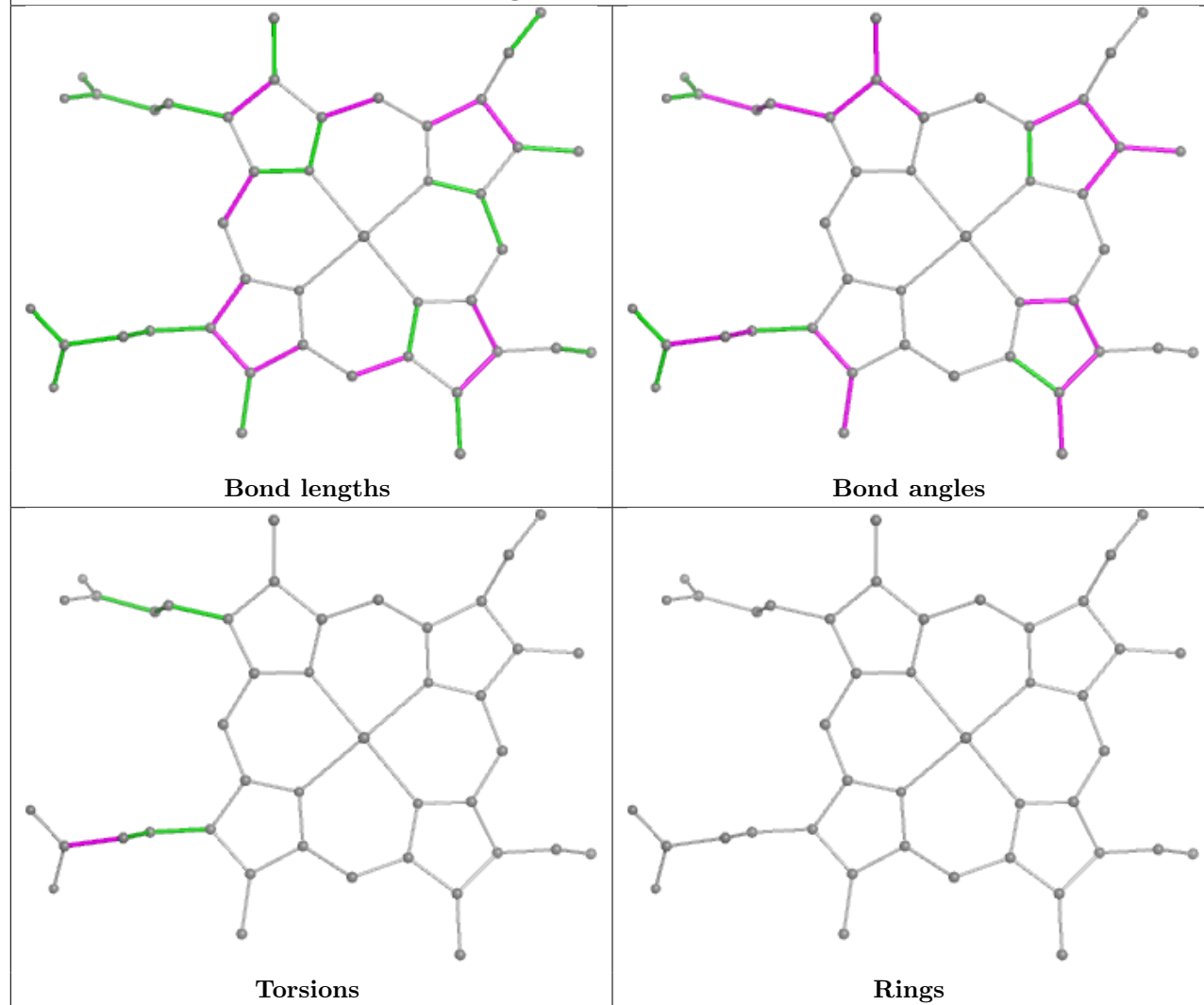




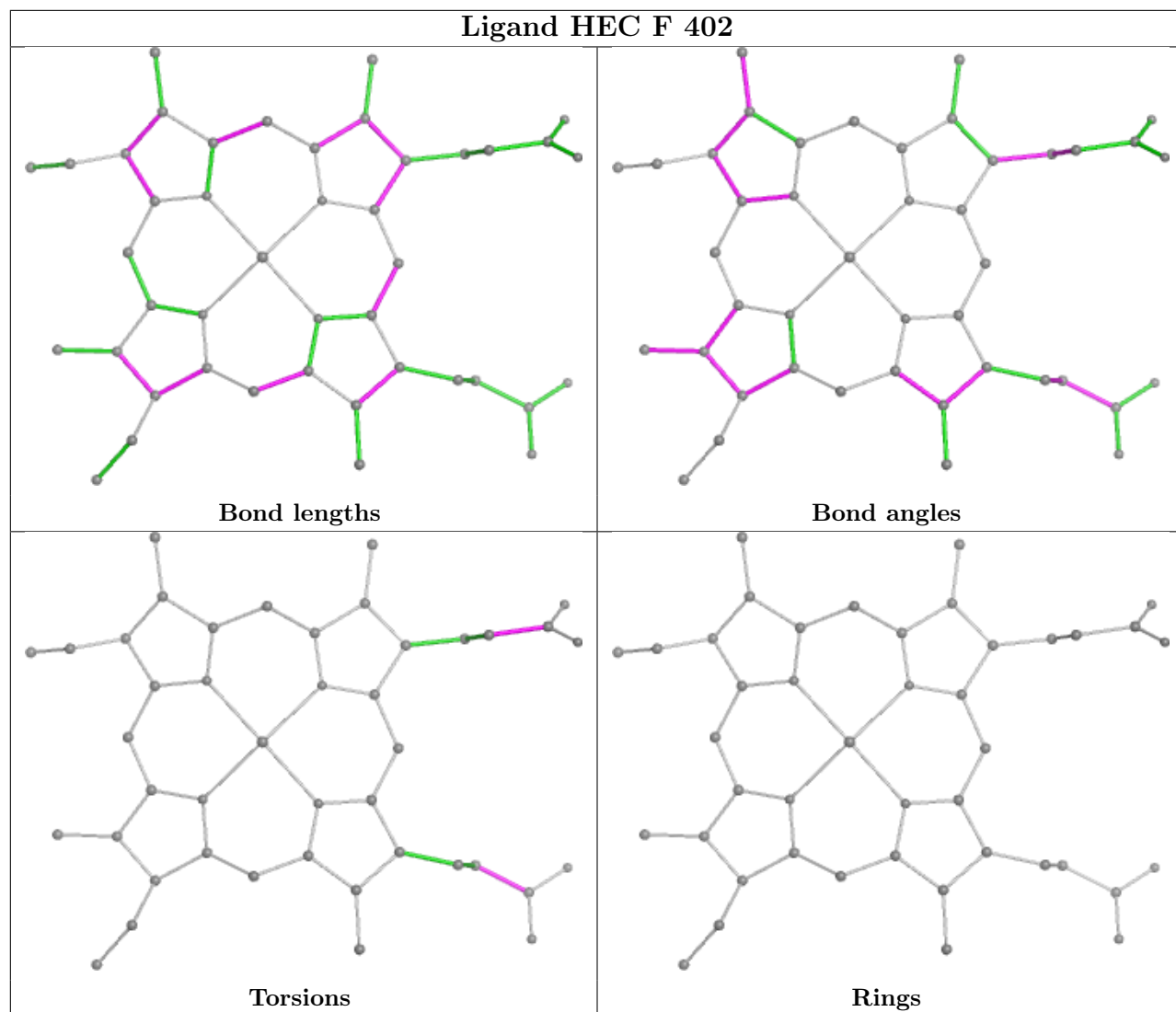


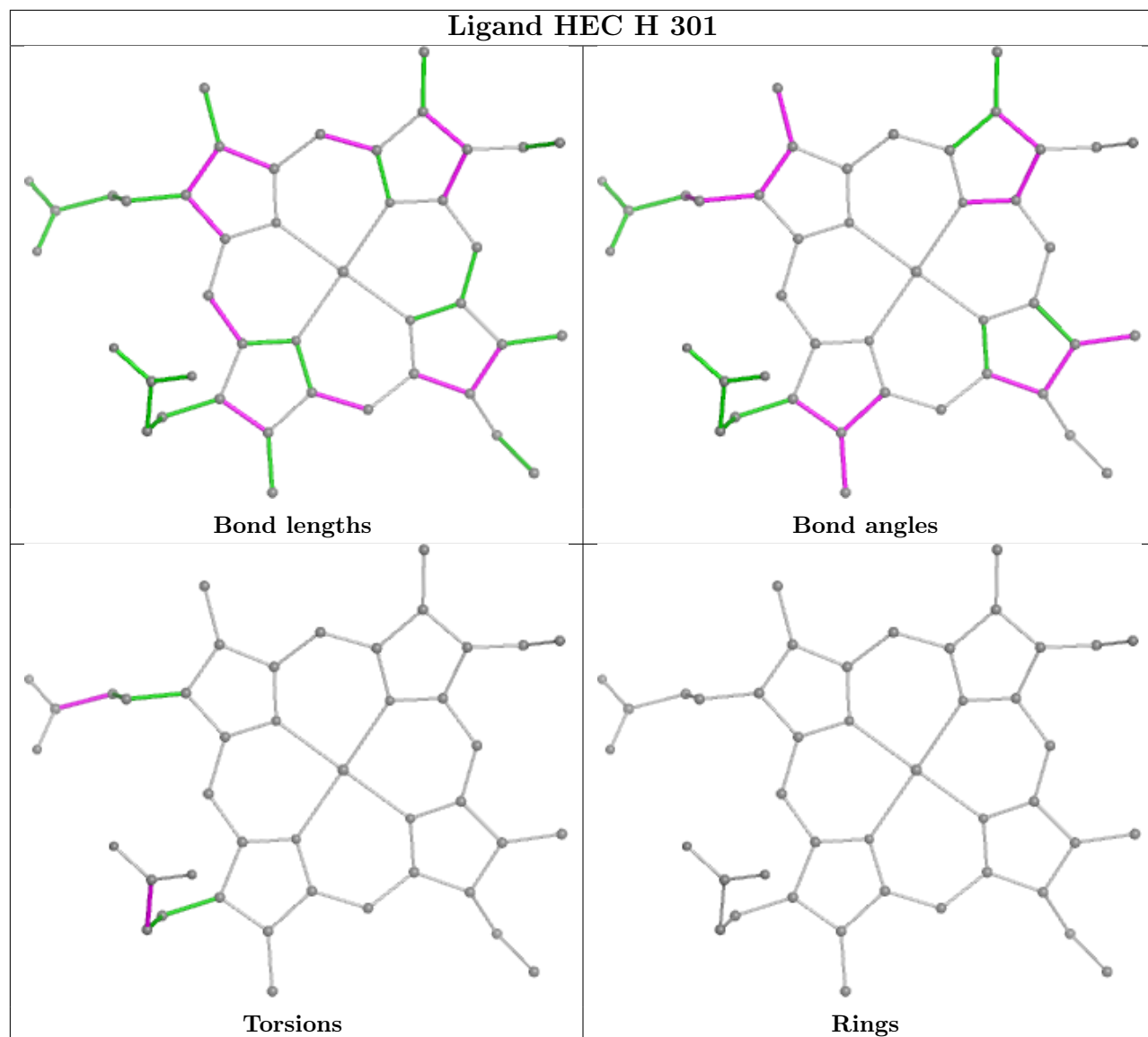


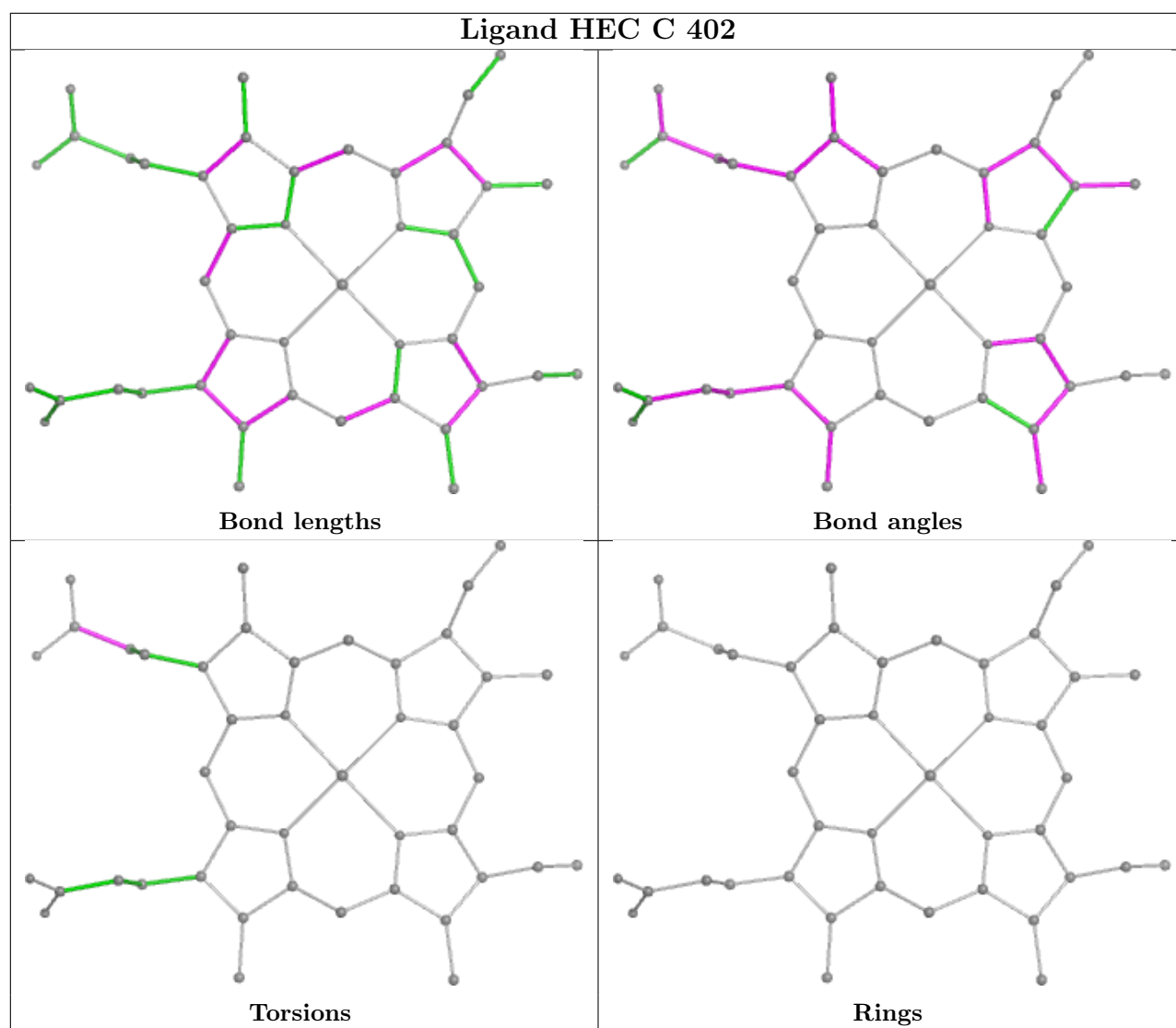
Ligand HEC I 402

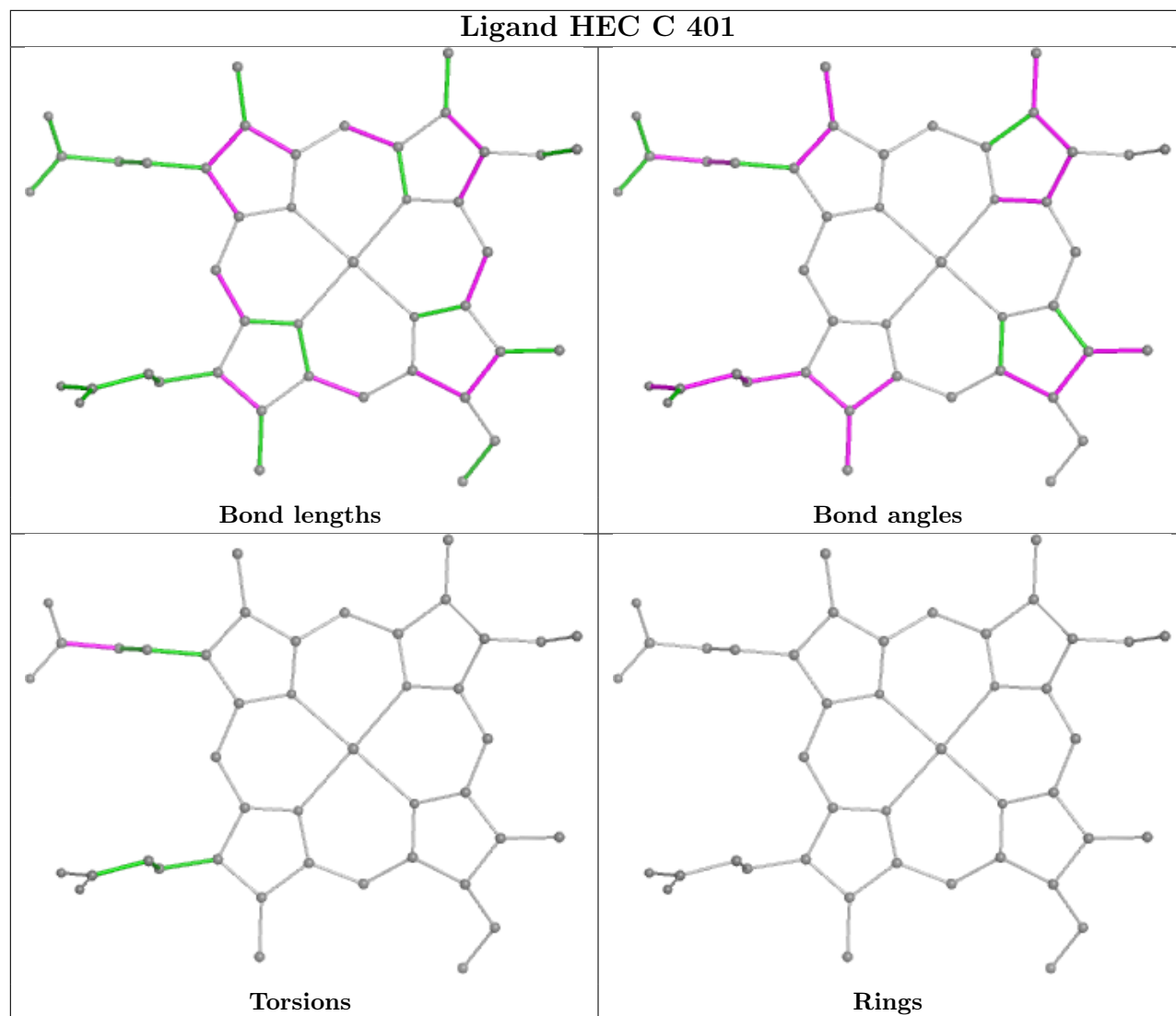


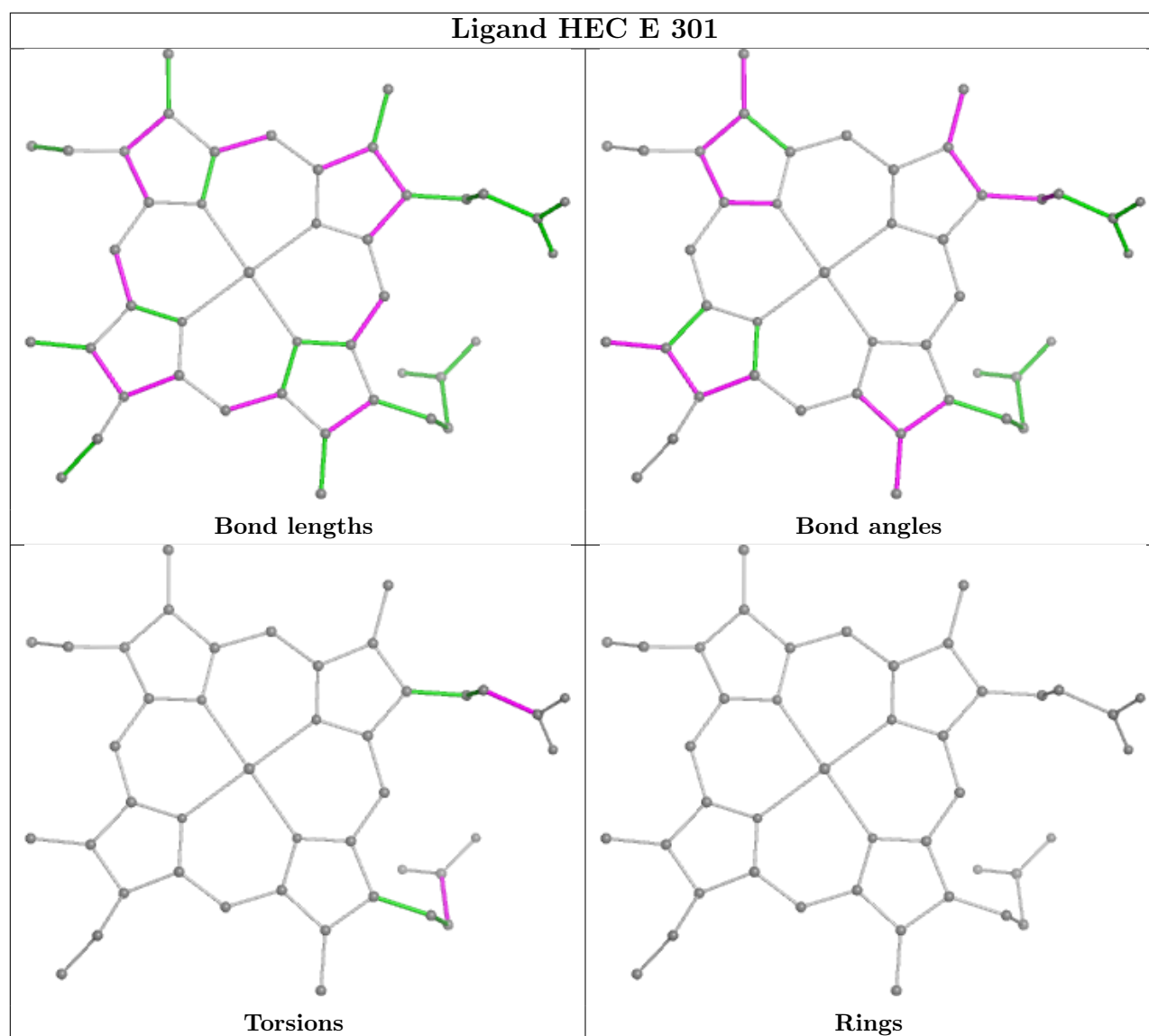
Ligand HEC F 402











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, 95th 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 ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 466/474 (98%) | -0.87 | 3 (0%) 85 76 | 45, 76, 129, 206 | 0 |
| 1 | D | 463/474 (97%) | -0.44 | 1 (0%) 92 87 | 76, 153, 234, 310 | 0 |
| 1 | G | 465/474 (98%) | -0.77 | 4 (0%) 81 68 | 55, 90, 142, 254 | 0 |
| 1 | K | 465/474 (98%) | -0.37 | 2 (0%) 89 81 | 61, 145, 226, 280 | 0 |
| 2 | B | 197/203 (97%) | -0.98 | 0 100 100 | 42, 70, 126, 169 | 0 |
| 2 | E | 197/203 (97%) | -0.49 | 0 100 100 | 68, 138, 213, 279 | 0 |
| 2 | H | 197/203 (97%) | -0.86 | 0 100 100 | 54, 83, 146, 202 | 0 |
| 2 | L | 197/203 (97%) | -0.58 | 0 100 100 | 52, 110, 215, 322 | 0 |
| 3 | C | 303/311 (97%) | -0.79 | 0 100 100 | 41, 83, 138, 192 | 0 |
| 3 | F | 303/311 (97%) | -0.15 | 5 (1%) 69 53 | 72, 173, 260, 419 | 0 |
| 3 | I | 303/311 (97%) | -0.68 | 0 100 100 | 52, 106, 166, 215 | 0 |
| 3 | M | 303/311 (97%) | -0.57 | 2 (0%) 84 73 | 43, 85, 243, 322 | 0 |
| 4 | N | 29/36 (80%) | -0.33 | 0 100 100 | 65, 92, 167, 174 | 0 |
| 4 | O | 29/36 (80%) | -0.20 | 0 100 100 | 148, 172, 249, 263 | 0 |
| 4 | P | 29/36 (80%) | -0.33 | 0 100 100 | 91, 109, 173, 191 | 0 |
| 4 | Q | 29/36 (80%) | 0.21 | 0 100 100 | 119, 142, 186, 199 | 0 |
| All | All | 3975/4096 (97%) | -0.60 | 17 (0%) 89 81 | 41, 107, 219, 419 | 0 |

All (17) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | F | 43 | ALA | 3.3 |
| 1 | A | 465 | ALA | 2.9 |
| 3 | F | 2 | SER | 2.9 |
| 3 | M | 50 | TYR | 2.8 |
| 3 | F | 49 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | K | 470 | ALA | 2.6 |
| 1 | A | 461 | ALA | 2.6 |
| 1 | D | 470 | ALA | 2.5 |
| 1 | G | 470 | ALA | 2.4 |
| 1 | G | 465 | ALA | 2.3 |
| 1 | A | 462 | ALA | 2.3 |
| 3 | F | 3 | THR | 2.2 |
| 3 | F | 40 | MET | 2.2 |
| 1 | G | 468 | ASP | 2.1 |
| 3 | M | 82 | TRP | 2.0 |
| 1 | G | 461 | ALA | 2.0 |
| 1 | K | 461 | ALA | 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 monosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 9 | PO4 | D | 505 | 5/5 | 0.59 | 0.11 | 180,183,183,185 | 0 |
| 9 | PO4 | K | 506 | 5/5 | 0.80 | 0.09 | 138,141,143,150 | 0 |
| 9 | PO4 | G | 506 | 5/5 | 0.82 | 0.10 | 130,132,139,152 | 0 |
| 11 | FC6 | F | 403 | 13/13 | 0.85 | 0.33 | 53,61,87,101 | 13 |
| 7 | CA | D | 504 | 1/1 | 0.89 | 0.10 | 151,151,151,151 | 0 |
| 7 | CA | K | 505 | 1/1 | 0.91 | 0.08 | 136,136,136,136 | 0 |
| 9 | PO4 | A | 506 | 5/5 | 0.91 | 0.07 | 60,68,75,88 | 0 |
| 8 | PEO | K | 507 | 2/2 | 0.92 | 0.09 | 131,131,131,131 | 0 |
| 11 | FC6 | I | 401 | 13/13 | 0.93 | 0.18 | 78,94,143,158 | 13 |
| 7 | CA | A | 504 | 1/1 | 0.94 | 0.06 | 99,99,99,99 | 0 |
| 10 | HEC | C | 402 | 43/43 | 0.94 | 0.12 | 36,54,72,160 | 0 |

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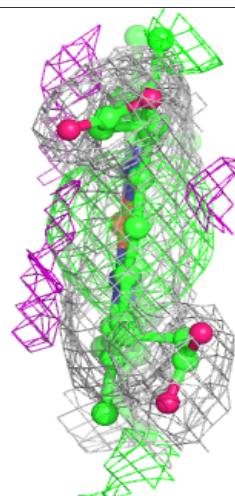
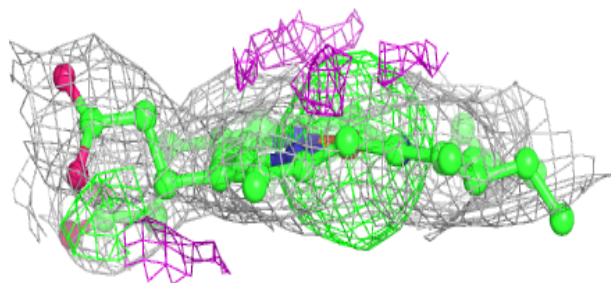
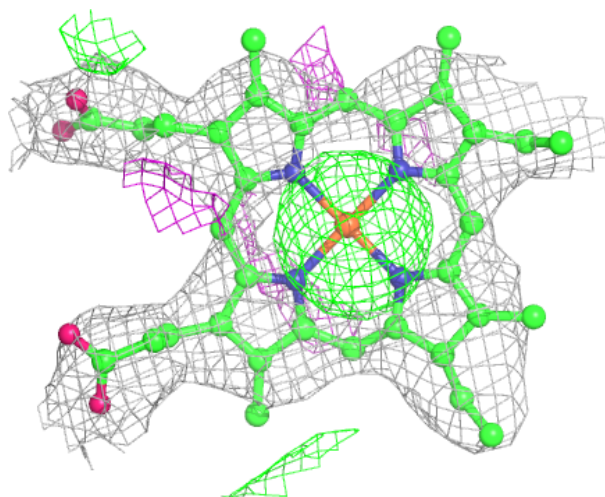
Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6 | CU | A | 503 | 1/1 | 0.95 | 0.19 | 133,133,133,133 | 0 |
| 7 | CA | A | 507 | 1/1 | 0.95 | 0.18 | 84,84,84,84 | 0 |
| 6 | CU | K | 503 | 1/1 | 0.96 | 0.05 | 133,133,133,133 | 0 |
| 7 | CA | G | 504 | 1/1 | 0.96 | 0.06 | 87,87,87,87 | 0 |
| 10 | HEC | B | 301 | 43/43 | 0.96 | 0.10 | 39,55,69,119 | 0 |
| 8 | PEO | D | 506 | 2/2 | 0.97 | 0.06 | 145,145,145,147 | 0 |
| 7 | CA | D | 507 | 1/1 | 0.97 | 0.05 | 96,96,96,96 | 0 |
| 5 | HEM | K | 501 | 43/43 | 0.97 | 0.13 | 119,135,151,154 | 0 |
| 10 | HEC | F | 402 | 43/43 | 0.97 | 0.12 | 117,134,147,154 | 0 |
| 5 | HEM | D | 501 | 43/43 | 0.97 | 0.10 | 93,119,136,143 | 0 |
| 8 | PEO | A | 505 | 2/2 | 0.97 | 0.07 | 74,74,74,74 | 0 |
| 5 | HEM | G | 502 | 43/43 | 0.98 | 0.07 | 54,66,77,86 | 0 |
| 6 | CU | D | 503 | 1/1 | 0.98 | 0.03 | 118,118,118,118 | 0 |
| 5 | HEM | D | 502 | 43/43 | 0.98 | 0.08 | 89,110,124,130 | 0 |
| 10 | HEC | C | 401 | 43/43 | 0.98 | 0.08 | 44,57,66,73 | 0 |
| 8 | PEO | G | 505 | 2/2 | 0.98 | 0.05 | 80,80,80,83 | 0 |
| 10 | HEC | F | 401 | 43/43 | 0.98 | 0.09 | 85,103,116,121 | 0 |
| 5 | HEM | K | 502 | 43/43 | 0.98 | 0.10 | 95,108,128,130 | 0 |
| 10 | HEC | H | 301 | 43/43 | 0.98 | 0.08 | 42,53,70,79 | 0 |
| 10 | HEC | I | 402 | 43/43 | 0.98 | 0.08 | 38,54,77,91 | 0 |
| 10 | HEC | I | 403 | 43/43 | 0.98 | 0.09 | 50,61,69,85 | 0 |
| 10 | HEC | M | 402 | 43/43 | 0.98 | 0.07 | 33,42,54,63 | 0 |
| 10 | HEC | M | 403 | 43/43 | 0.98 | 0.08 | 35,51,64,84 | 0 |
| 11 | FC6 | C | 403 | 13/13 | 0.98 | 0.10 | 60,75,98,101 | 13 |
| 7 | CA | G | 507 | 1/1 | 0.98 | 0.04 | 72,72,72,72 | 0 |
| 7 | CA | K | 504 | 1/1 | 0.98 | 0.03 | 95,95,95,95 | 0 |
| 11 | FC6 | M | 401 | 13/13 | 0.98 | 0.11 | 43,60,98,98 | 13 |
| 5 | HEM | A | 501 | 43/43 | 0.99 | 0.07 | 45,63,72,76 | 0 |
| 10 | HEC | E | 301 | 43/43 | 0.99 | 0.07 | 62,73,96,102 | 0 |
| 5 | HEM | A | 502 | 43/43 | 0.99 | 0.08 | 41,54,79,83 | 0 |
| 10 | HEC | L | 301 | 43/43 | 0.99 | 0.08 | 49,65,78,78 | 0 |
| 5 | HEM | G | 501 | 43/43 | 0.99 | 0.06 | 57,72,84,93 | 0 |
| 6 | CU | G | 503 | 1/1 | 1.00 | 0.04 | 74,74,74,74 | 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.

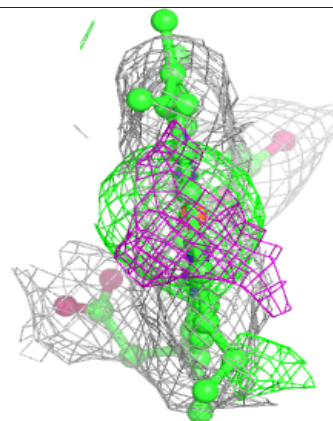
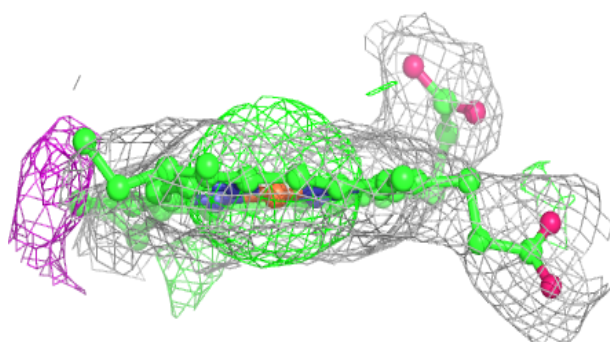
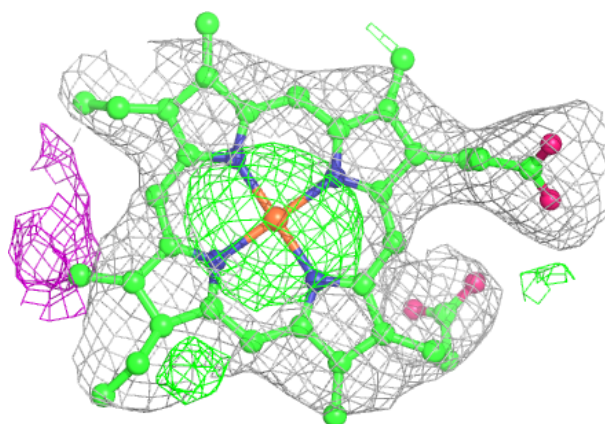
Electron density around HEC C 402:

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



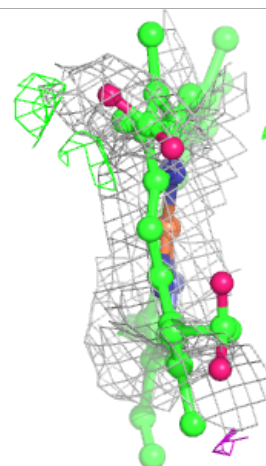
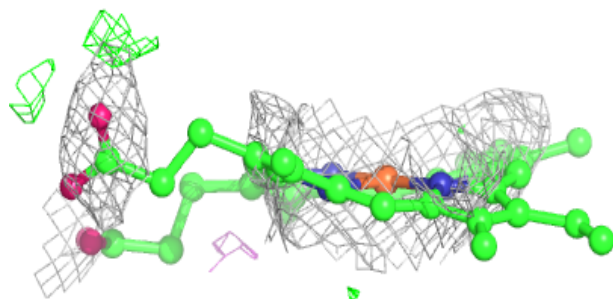
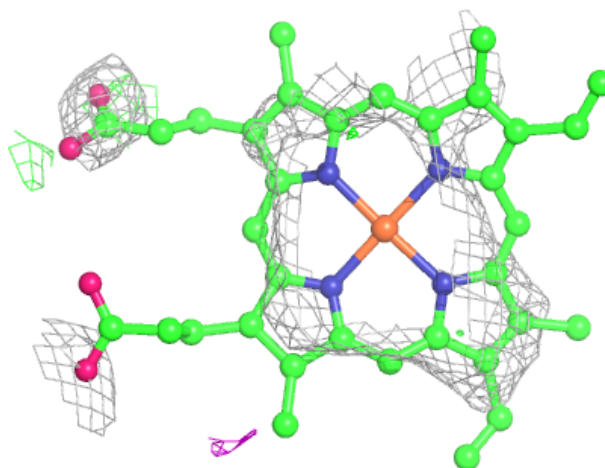
Electron density around HEC B 301:

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and green (positive)



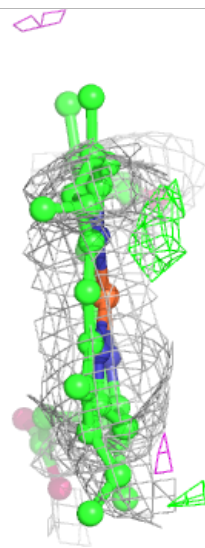
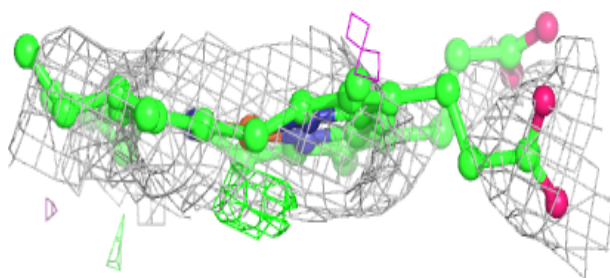
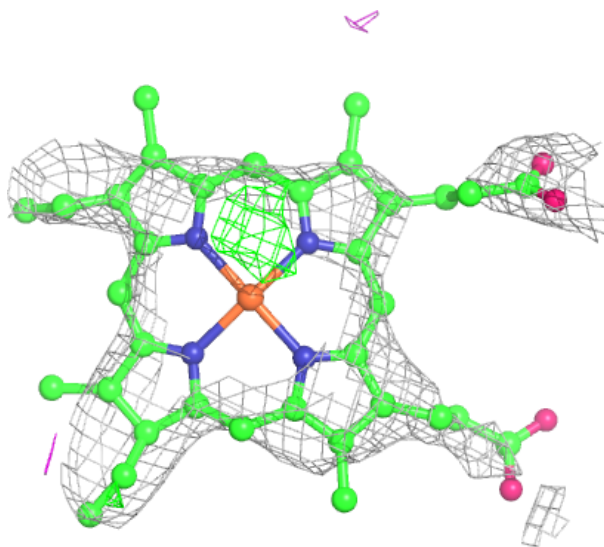
Electron density around HEM K 501:

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and green (positive)



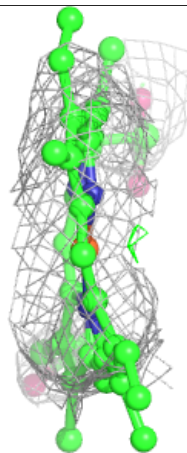
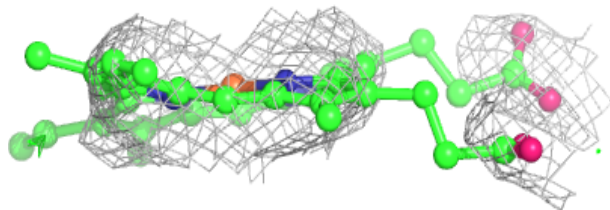
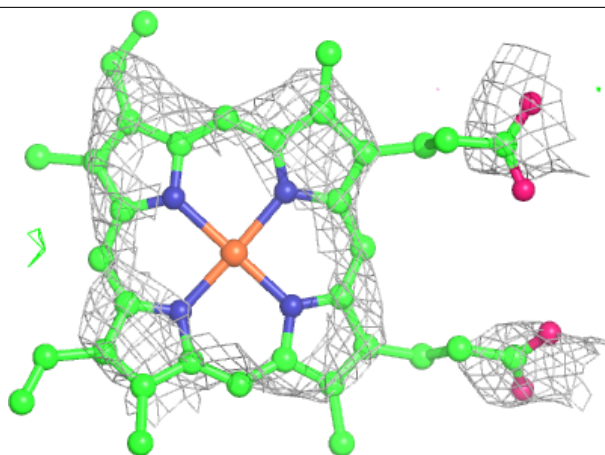
Electron density around HEC F 402:

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



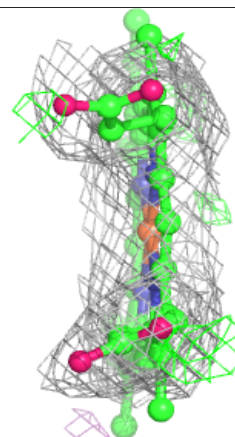
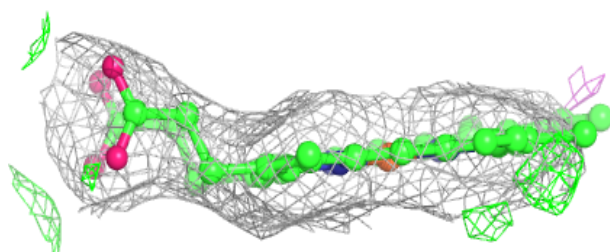
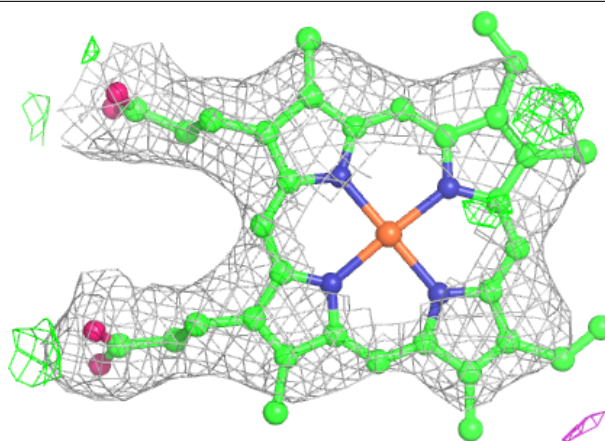
Electron density around HEM D 501:

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



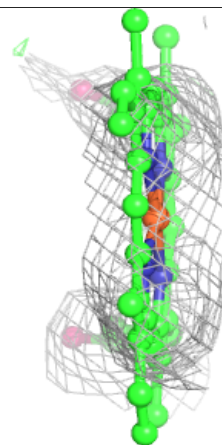
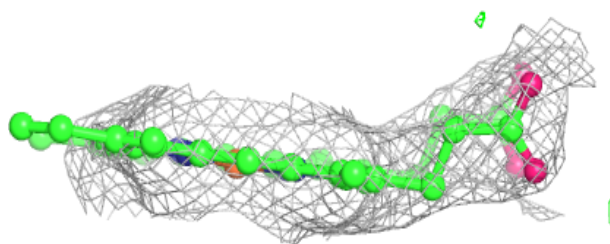
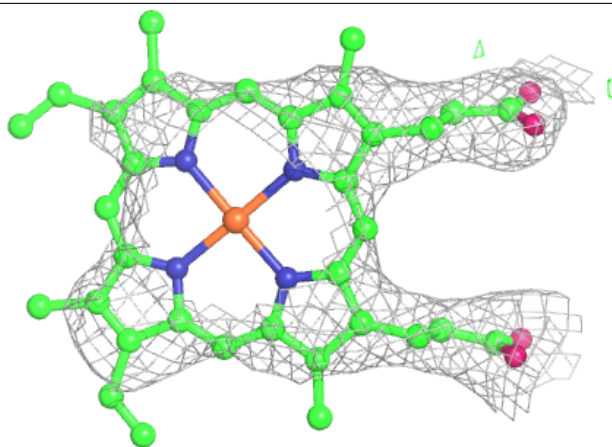
Electron density around HEM G 502:

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and green (positive)



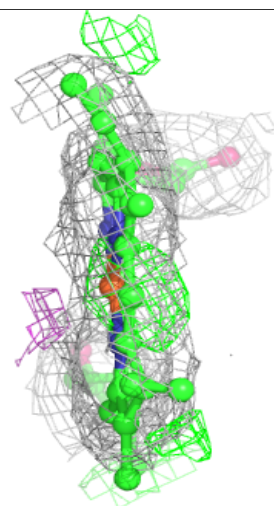
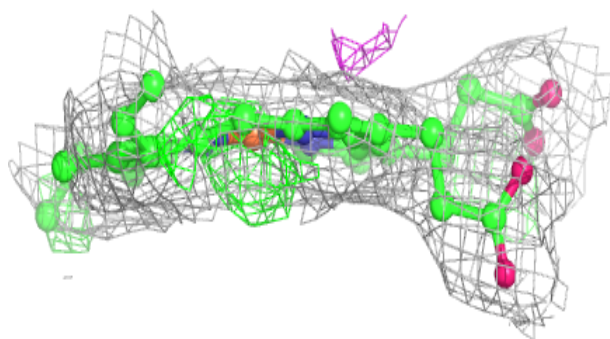
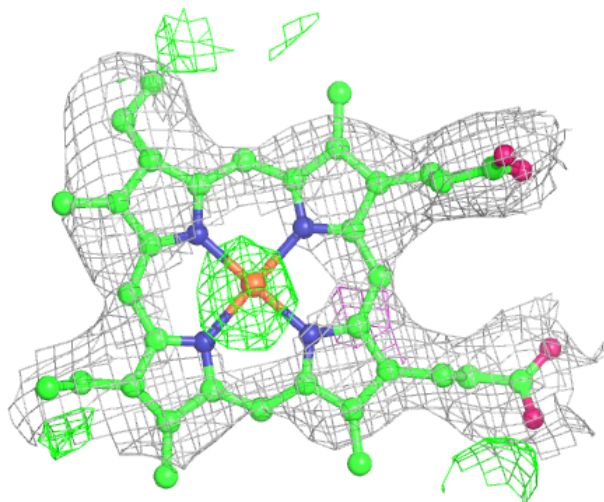
Electron density around HEM D 502:

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and green (positive)



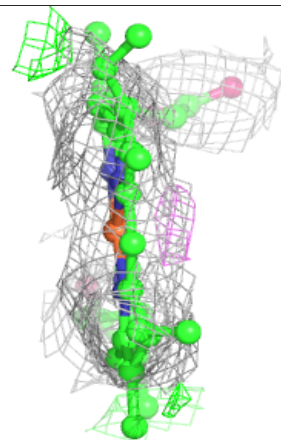
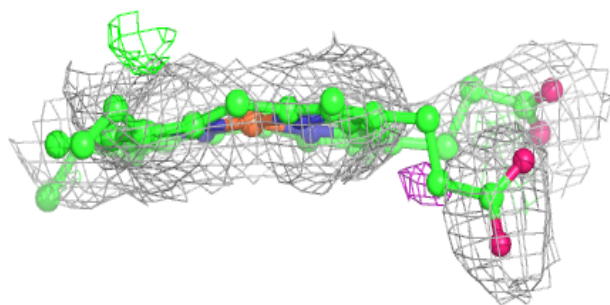
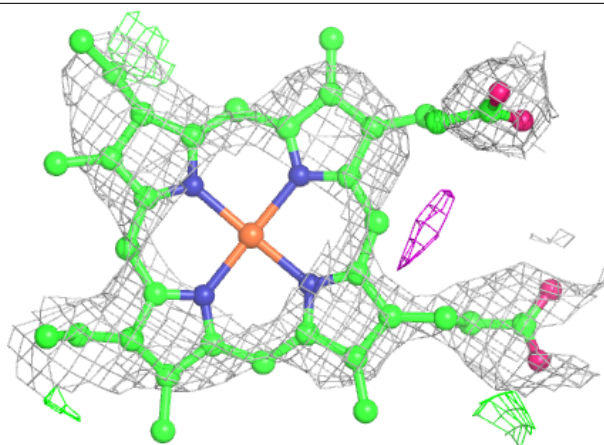
Electron density around HEC C 401:

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and green (positive)



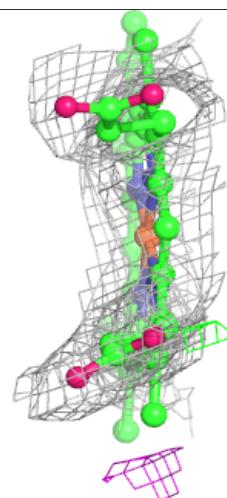
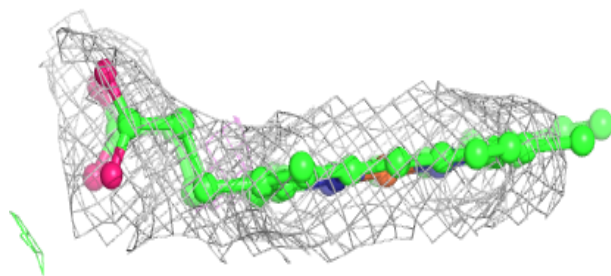
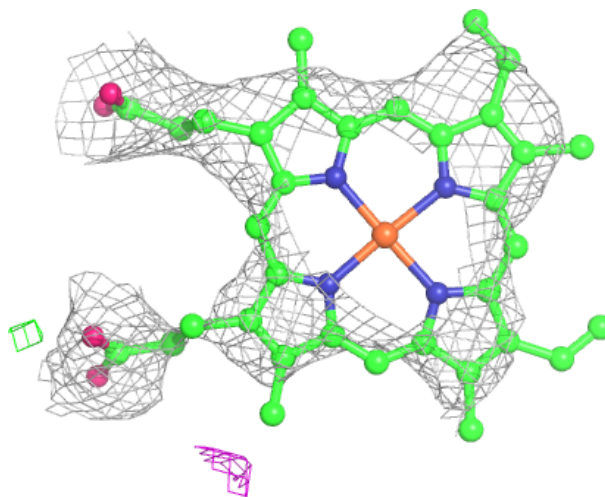
Electron density around HEC F 401:

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



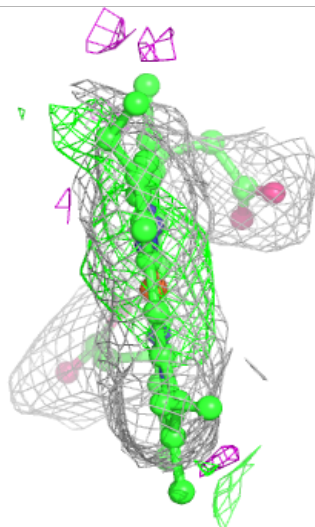
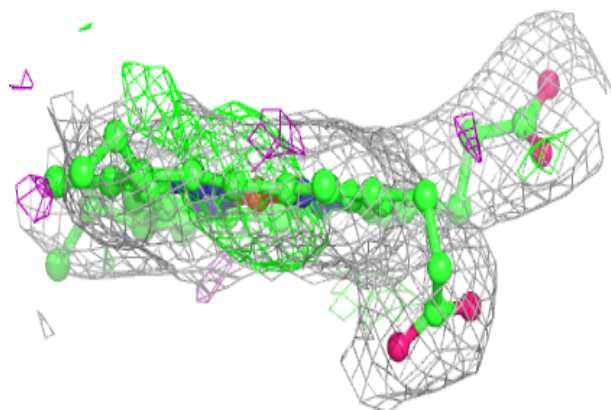
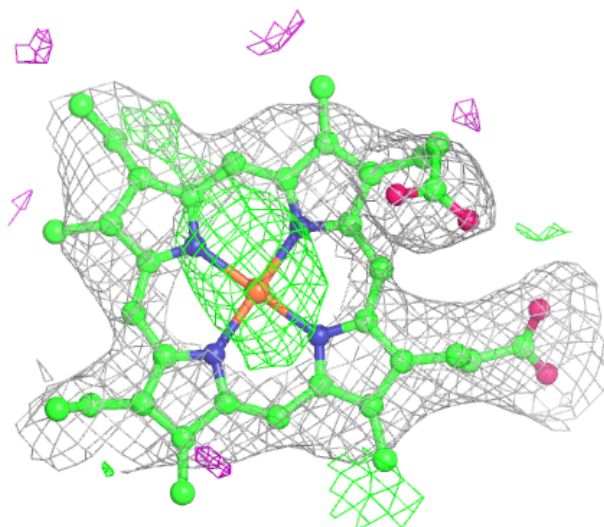
Electron density around HEM K 502:

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and green (positive)



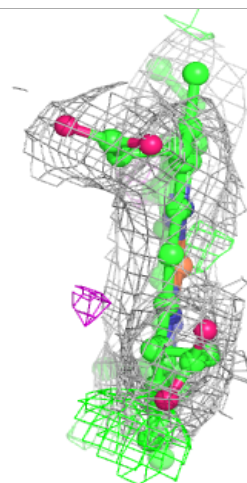
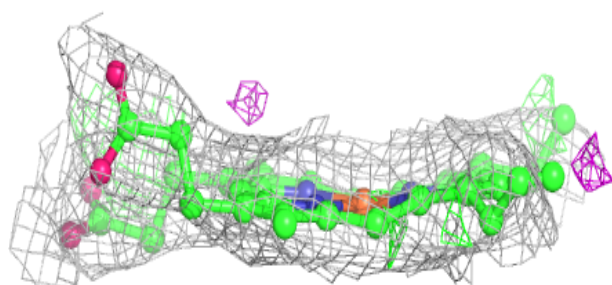
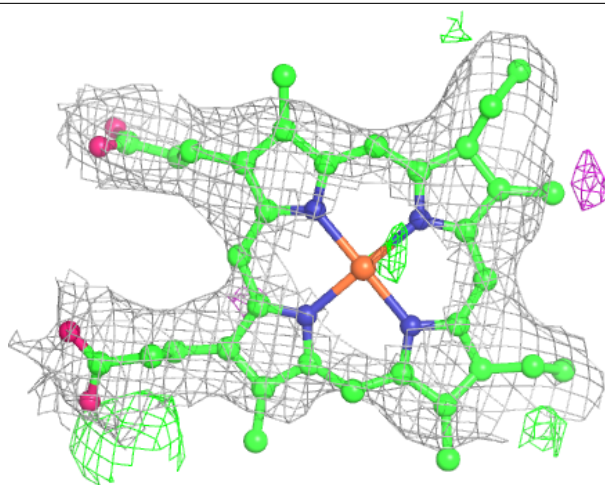
Electron density around HEC H 301:

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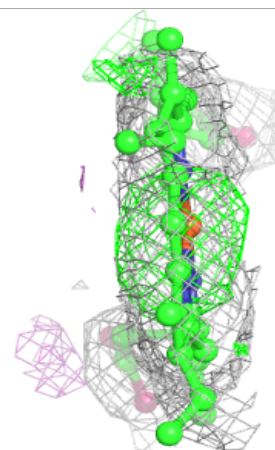
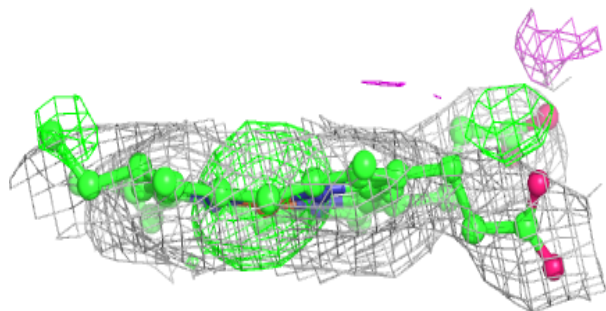
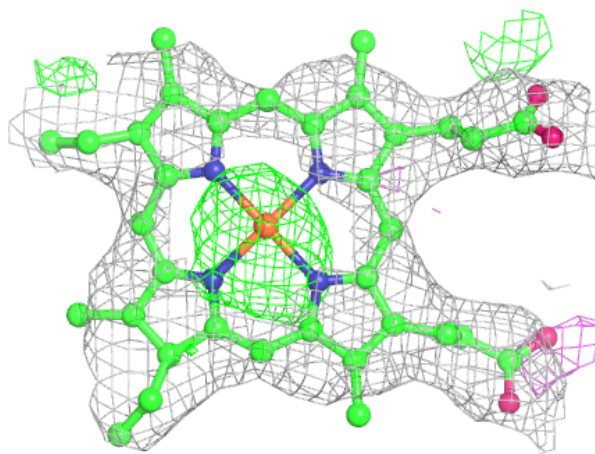
Electron density around HEC I 402:

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and green (positive)



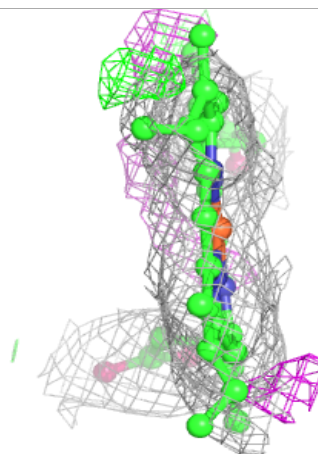
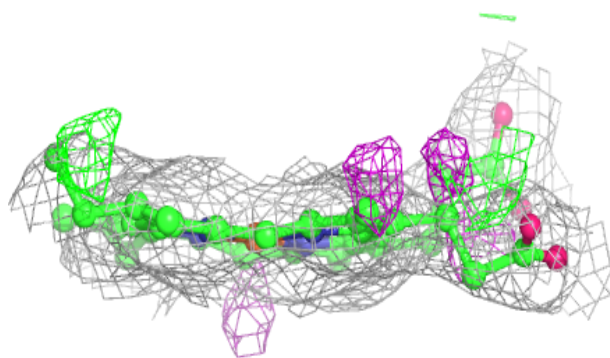
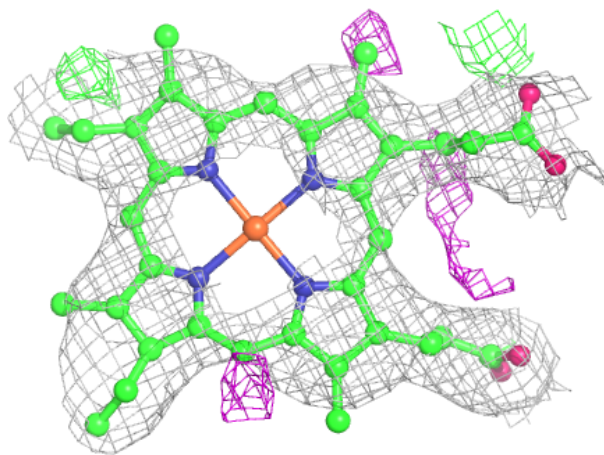
Electron density around HEC I 403:

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



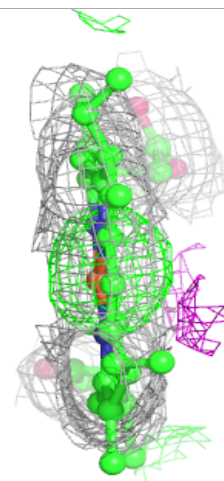
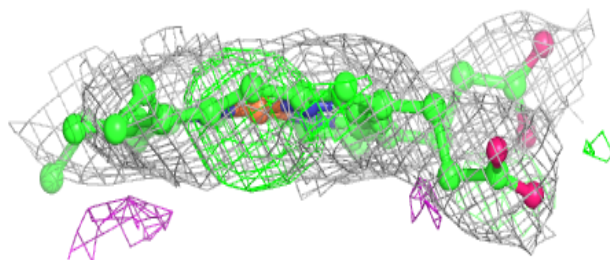
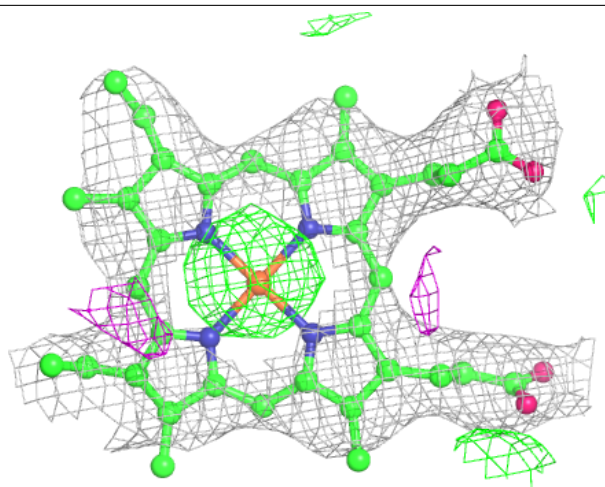
Electron density around HEC M 402:

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



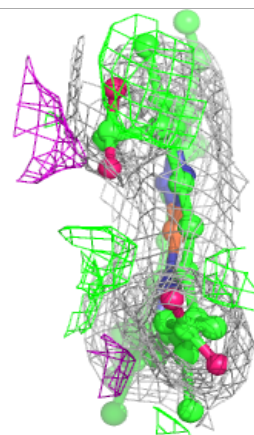
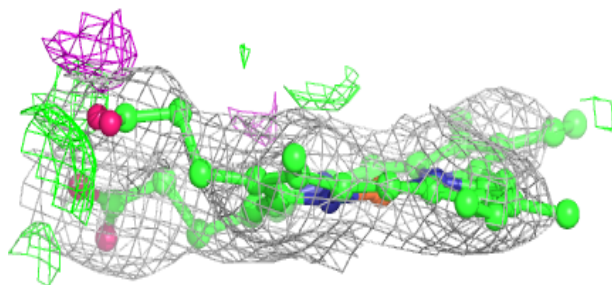
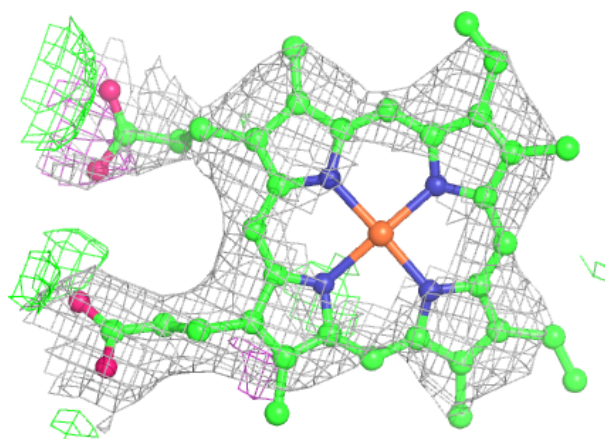
Electron density around HEC M 403:

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



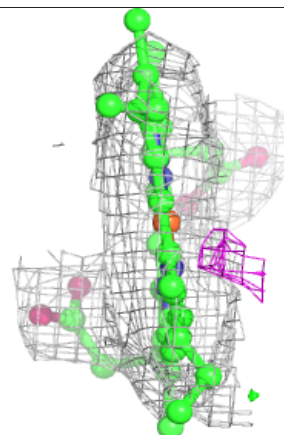
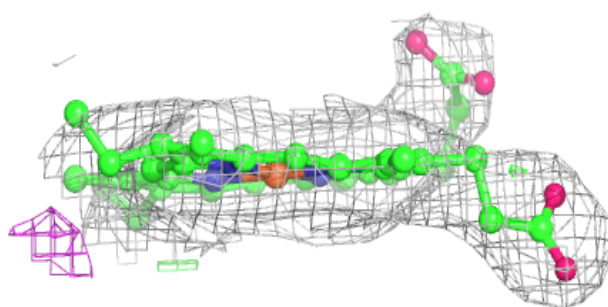
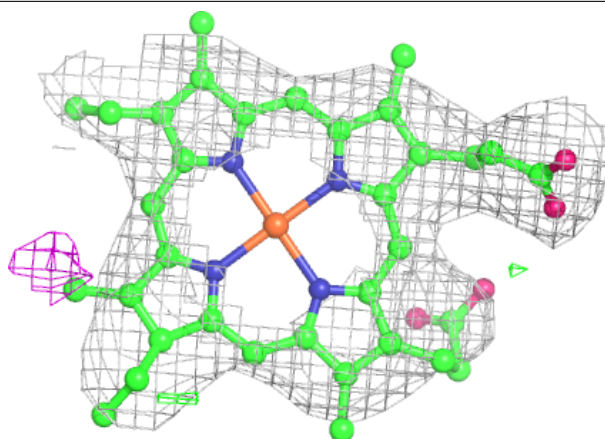
Electron density around HEM A 501:

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

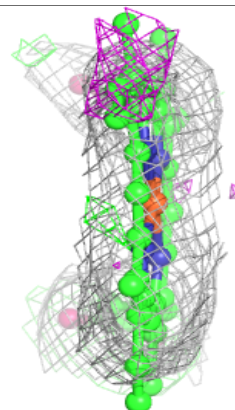
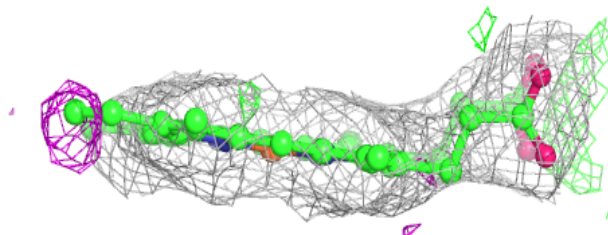
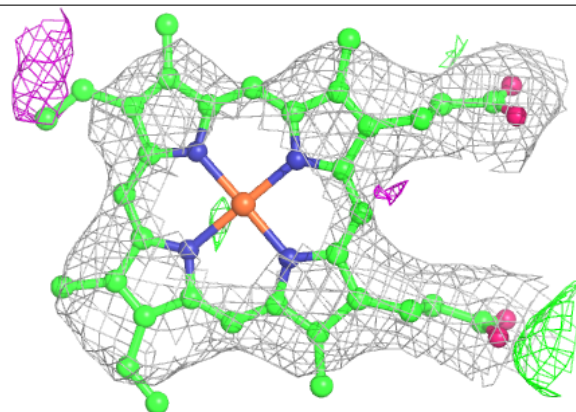


Electron density around HEC E 301:

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

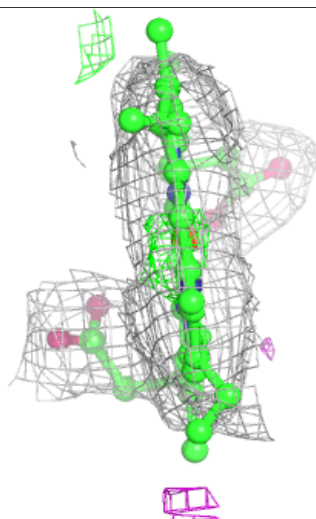
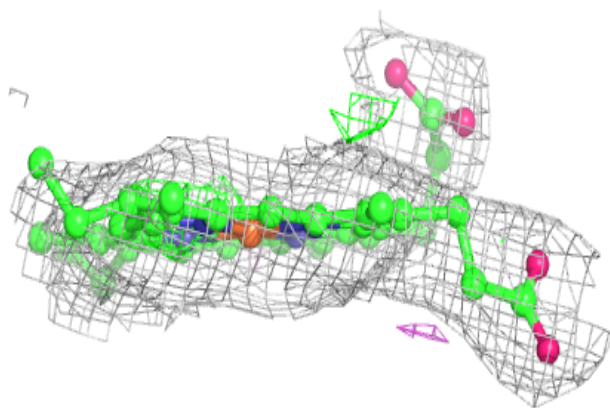
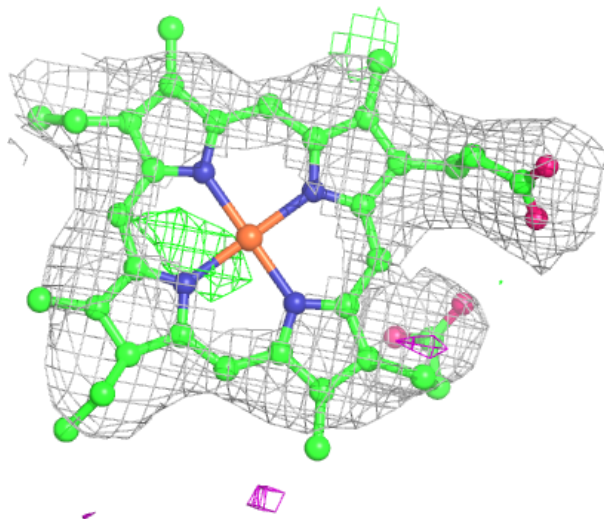
**Electron density around HEM A 502:**

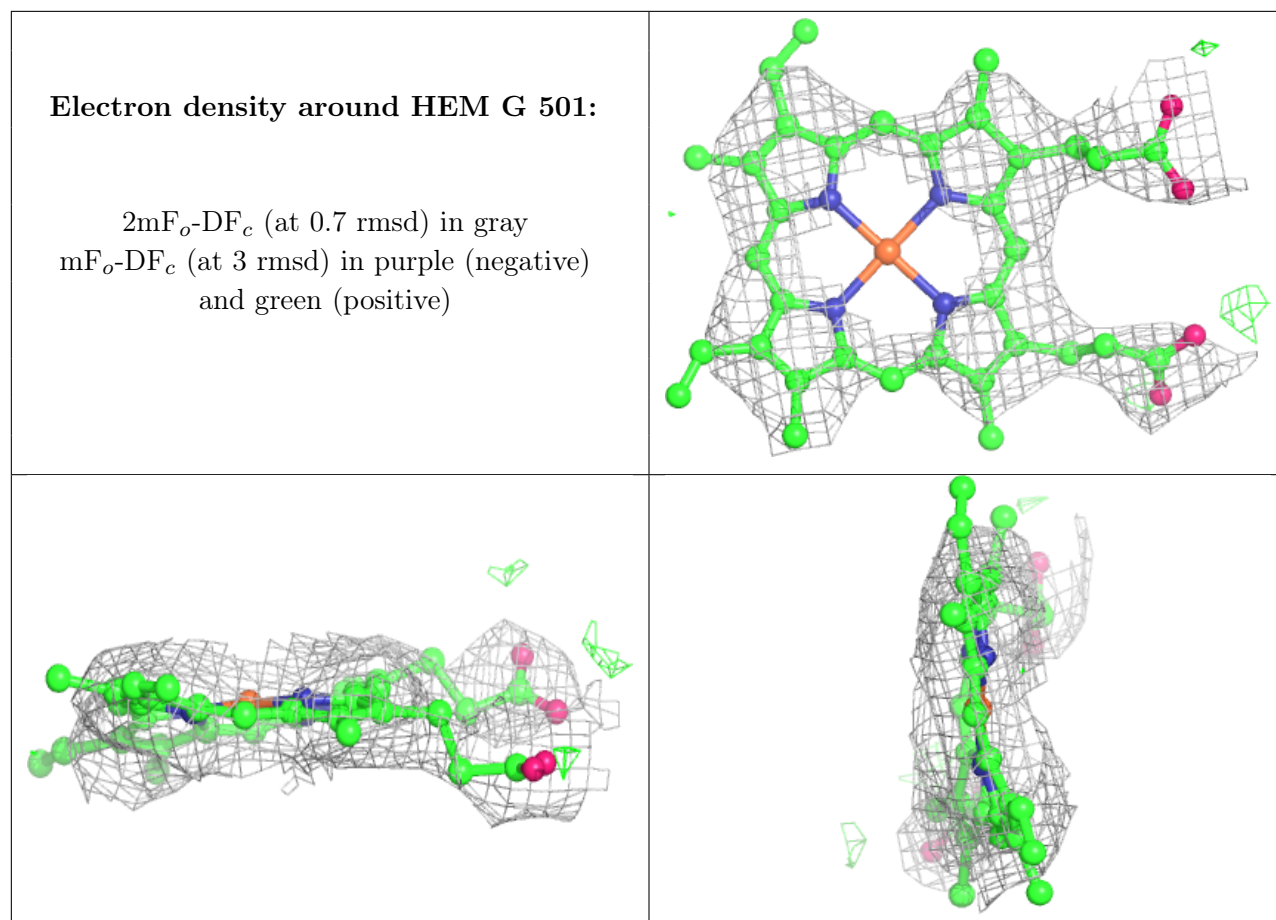
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC L 301:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.