



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 02:46 PM EDT

PDB ID : 2GTL / pdb\_00002gtl  
Title : Lumbricus Erythrocrutorin at 3.5Å resolution  
Authors : Royer Jr., W.E.; Sharma, H.; Strand, K.; Knapp, J.E.; Bhyravbhatla, B.  
Deposited on : 2006-04-28  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.015 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

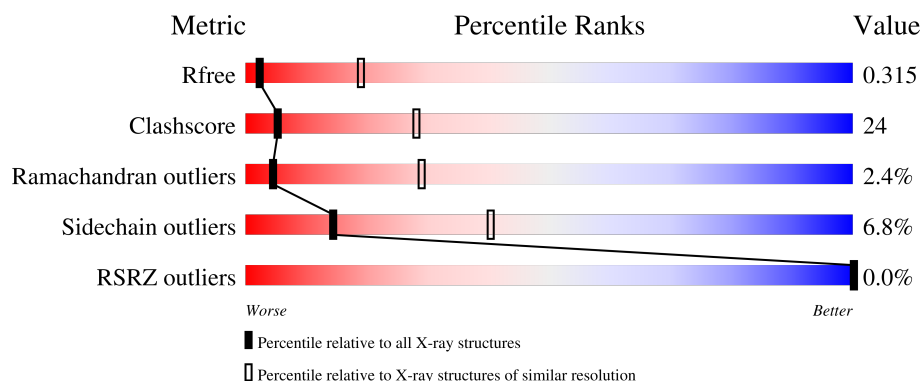
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                              |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------|
| 1   | A     | 151    | <div> <div>%</div> <div> <div></div> <div>47%</div> <div>44%</div> <div>5%</div> <div>• •</div> </div> </div> |
| 1   | E     | 151    | <div> <div>49%</div> <div>43%</div> <div>• • •</div> </div>                                                   |
| 1   | I     | 151    | <div> <div>48%</div> <div>43%</div> <div>5%</div> <div>• •</div> </div>                                       |
| 2   | B     | 145    | <div> <div>65%</div> <div>33%</div> <div>•</div> </div>                                                       |
| 2   | F     | 145    | <div> <div>62%</div> <div>37%</div> <div>•</div> </div>                                                       |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 2   | J     | 145    |  63% 35% .     |
| 3   | C     | 153    |  57% 35% 6% .  |
| 3   | G     | 153    |  58% 35% 5% .  |
| 3   | K     | 153    |  55% 37% 5% .  |
| 4   | D     | 140    |  56% 39% . .   |
| 4   | H     | 140    |  57% 38% . .   |
| 4   | L     | 140    |  59% 36% . .   |
| 5   | M     | 217    |  45% 43% 10% . |
| 6   | N     | 220    |  51% 38% 10% . |
| 7   | O     | 215    |  60% 37% . .   |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 19648 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 Extracellular globin 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1209  | 769 | 222 | 214 | 4 |         |         |       |
| 1   | E     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1209  | 769 | 222 | 214 | 4 |         |         |       |
| 1   | I     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1209  | 769 | 222 | 214 | 4 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 78      | LYS      | ASP    | conflict | UNP P13579 |
| E     | 78      | LYS      | ASP    | conflict | UNP P13579 |
| I     | 78      | LYS      | ASP    | conflict | UNP P13579 |

- Molecule 2 is a protein called Extracellular globin 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1148  | 720 | 212 | 213 | 3 |         |         |       |
| 2   | F     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1148  | 720 | 212 | 213 | 3 |         |         |       |
| 2   | J     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1148  | 720 | 212 | 213 | 3 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 66      | ASP      | GLU    | conflict | UNP P02218 |
| F     | 66      | ASP      | GLU    | conflict | UNP P02218 |
| J     | 66      | ASP      | GLU    | conflict | UNP P02218 |

- Molecule 3 is a protein called Extracellular globin-3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1185  | 755 | 210 | 217 | 3 |         |         |       |
| 3   | G     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1185  | 755 | 210 | 217 | 3 |         |         |       |
| 3   | K     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1185  | 755 | 210 | 217 | 3 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 49      | GLU      | ASP    | conflict | UNP P11069 |
| G     | 49      | GLU      | ASP    | conflict | UNP P11069 |
| K     | 49      | GLU      | ASP    | conflict | UNP P11069 |

- Molecule 4 is a protein called Hemoglobin chain d1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 725 | 198 | 202 | 4 |         |         |       |
| 4   | H     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 725 | 198 | 202 | 4 |         |         |       |
| 4   | L     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 725 | 198 | 202 | 4 |         |         |       |

- Molecule 5 is a protein called Hemoglobin linker chain L1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | M     | 217      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1705  | 1060 | 302 | 333 | 10 |         |         |       |

- Molecule 6 is a protein called Extracellular hemoglobin linker L2 subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 6   | N     | 220      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1722  | 1060 | 316 | 336 | 10 |         |         |       |

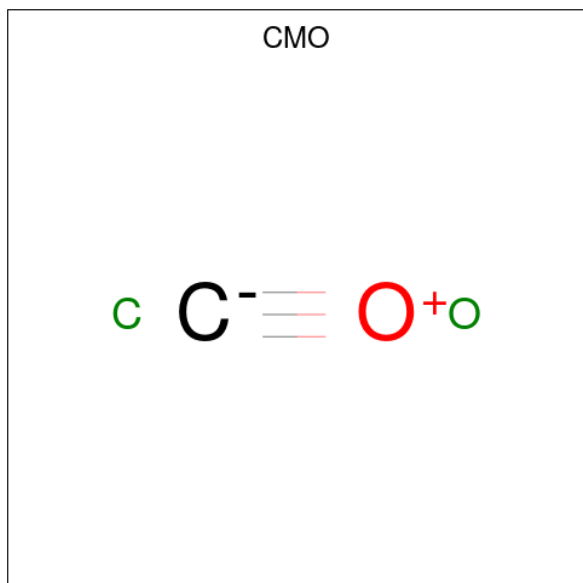
- Molecule 7 is a protein called Extracellular hemoglobin linker L3 subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 7   | O     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1663  | 1020 | 292 | 340 | 11 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| O     | 113     | CYS      | VAL    | conflict | UNP Q2I742 |

- Molecule 8 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



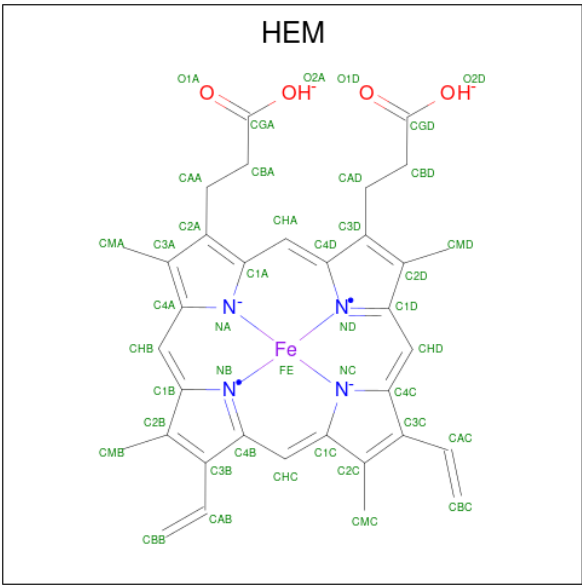
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 8   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 9   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 9   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 10  | M     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 10  | N     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 10  | O     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 11  | M     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

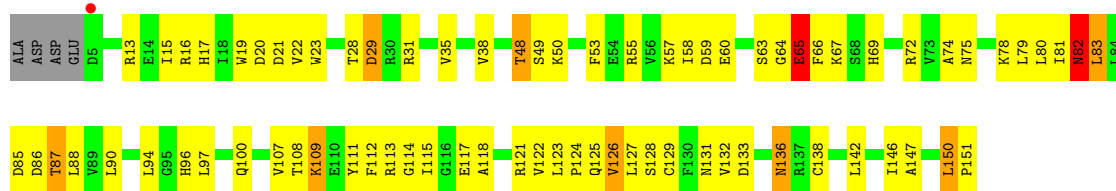


### 3 Residue-property plots

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

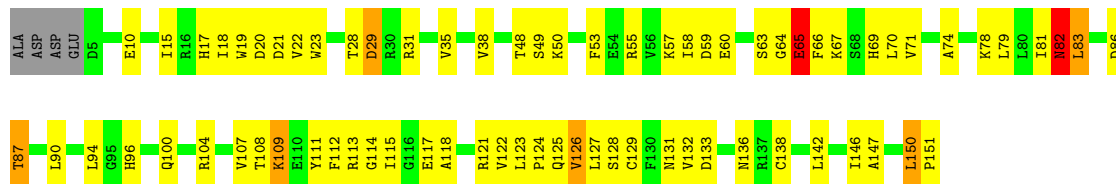
#### • Molecule 1: Extracellular globin 4

Chain A: 

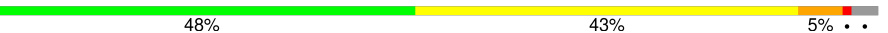


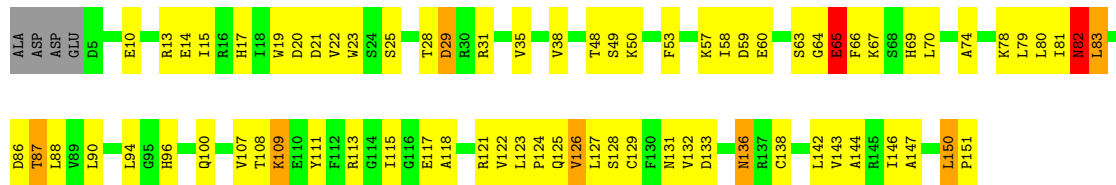
#### • Molecule 1: Extracellular globin 4

Chain E: 



#### • Molecule 1: Extracellular globin 4

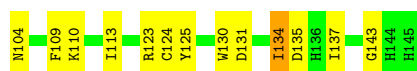
Chain I: 



#### • Molecule 2: Extracellular globin 2

Chain B: 





- Molecule 2: Extracellular globin 2

Chain F: 62% 37%



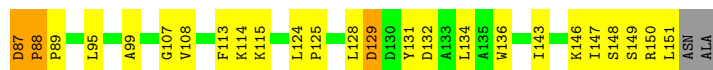
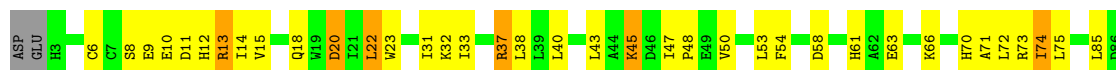
- Molecule 2: Extracellular globin 2

Chain J: 63% 35%



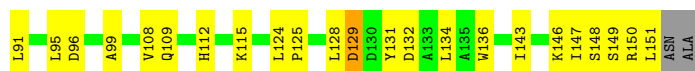
- Molecule 3: Extracellular globin-3

Chain C: 57% 35% 6%



- Molecule 3: Extracellular globin-3

Chain G: 58% 35% 5%



- Molecule 3: Extracellular globin-3

Chain K: 55% 37% 5%





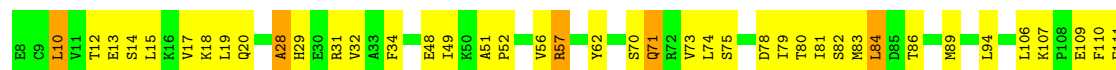
• Molecule 4: Hemoglobin chain d1



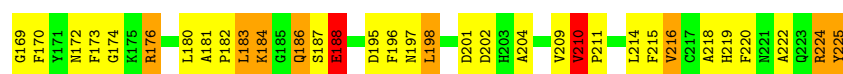
• Molecule 4: Hemoglobin chain d1



• Molecule 4: Hemoglobin chain d1

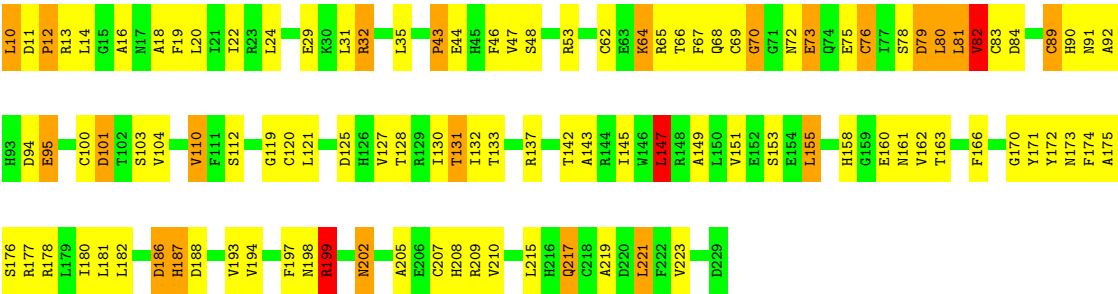


• Molecule 5: Hemoglobin linker chain L1



• Molecule 6: Extracellular hemoglobin linker L2 subunit





● Molecule 7: Extracellular hemoglobin linker L3 subunit



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 176.08Å 257.96Å 436.53Å<br>89.69° 97.15° 90.98°             | Depositor        |
| Resolution (Å)                                                          | 100.00 – 3.50<br>100.00 – 3.50                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (100.00-3.50)<br>63.7 (100.00-3.50)         | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.87 (at 3.33Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.288 , 0.297<br>0.310 , 0.315                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 45836 reflections (4.86%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 79.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.276                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 0.0                                                  | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | 0.015 for -h,k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.52                                                        | EDS              |
| Total number of atoms                                                   | 19648                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 68.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, CMO, 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     | 0.61         | 1/1237 (0.1%)  | 0.97        | 3/1670 (0.2%)   |
| 1   | E     | 0.58         | 0/1237         | 0.95        | 3/1670 (0.2%)   |
| 1   | I     | 0.58         | 0/1237         | 0.95        | 3/1670 (0.2%)   |
| 2   | B     | 0.60         | 0/1176         | 0.90        | 2/1587 (0.1%)   |
| 2   | F     | 0.60         | 0/1176         | 0.90        | 1/1587 (0.1%)   |
| 2   | J     | 0.57         | 0/1176         | 0.89        | 0/1587          |
| 3   | C     | 0.58         | 0/1209         | 0.93        | 5/1633 (0.3%)   |
| 3   | G     | 0.54         | 0/1209         | 0.91        | 5/1633 (0.3%)   |
| 3   | K     | 0.57         | 0/1209         | 0.92        | 5/1633 (0.3%)   |
| 4   | D     | 0.58         | 0/1159         | 0.90        | 4/1568 (0.3%)   |
| 4   | H     | 0.56         | 0/1159         | 0.88        | 4/1568 (0.3%)   |
| 4   | L     | 0.53         | 0/1159         | 0.87        | 4/1568 (0.3%)   |
| 5   | M     | 0.63         | 0/1745         | 1.03        | 10/2371 (0.4%)  |
| 6   | N     | 0.58         | 0/1752         | 0.98        | 6/2369 (0.3%)   |
| 7   | O     | 0.55         | 0/1699         | 0.98        | 6/2298 (0.3%)   |
| All | All   | 0.58         | 1/19539 (0.0%) | 0.94        | 61/26412 (0.2%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 48  | THR  | N-CA  | -5.58 | 1.39        | 1.46     |

All (61) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | I     | 65  | GLU  | N-CA-C | -7.94 | 102.61      | 111.82   |
| 1   | A     | 65  | GLU  | N-CA-C | -7.89 | 102.67      | 111.82   |
| 7   | O     | 73  | ASP  | CA-C-N | 7.75  | 127.68      | 119.85   |
| 7   | O     | 73  | ASP  | C-N-CA | 7.75  | 127.68      | 119.85   |
| 1   | E     | 65  | GLU  | N-CA-C | -7.68 | 102.91      | 111.82   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 138 | CYS  | N-CA-C  | 7.44  | 120.48      | 111.40   |
| 5   | M     | 61  | HIS  | N-CA-C  | 7.18  | 120.15      | 111.82   |
| 5   | M     | 141 | PHE  | CA-C-N  | 7.03  | 126.65      | 119.19   |
| 5   | M     | 141 | PHE  | C-N-CA  | 7.03  | 126.65      | 119.19   |
| 7   | O     | 121 | ARG  | CA-C-N  | 6.91  | 126.87      | 120.03   |
| 7   | O     | 121 | ARG  | C-N-CA  | 6.91  | 126.87      | 120.03   |
| 4   | H     | 138 | CYS  | N-CA-C  | 6.84  | 119.75      | 111.40   |
| 6   | N     | 80  | LEU  | N-CA-C  | -6.49 | 105.12      | 113.16   |
| 3   | K     | 13  | ARG  | N-CA-C  | -6.26 | 103.75      | 111.33   |
| 4   | D     | 28  | ALA  | CB-CA-C | -6.19 | 109.43      | 116.54   |
| 1   | A     | 109 | LYS  | N-CA-C  | -6.15 | 104.69      | 111.82   |
| 1   | E     | 109 | LYS  | N-CA-C  | -6.14 | 104.69      | 111.82   |
| 5   | M     | 222 | ALA  | N-CA-C  | 6.14  | 119.66      | 110.14   |
| 3   | C     | 13  | ARG  | N-CA-C  | -6.00 | 104.07      | 111.33   |
| 4   | L     | 28  | ALA  | CB-CA-C | -5.97 | 109.67      | 116.54   |
| 1   | I     | 109 | LYS  | N-CA-C  | -5.97 | 104.90      | 111.82   |
| 4   | H     | 28  | ALA  | CB-CA-C | -5.94 | 109.71      | 116.54   |
| 3   | G     | 47  | ILE  | CA-C-N  | 5.91  | 125.78      | 119.28   |
| 3   | G     | 47  | ILE  | C-N-CA  | 5.91  | 125.78      | 119.28   |
| 3   | G     | 13  | ARG  | N-CA-C  | -5.89 | 104.20      | 111.33   |
| 3   | K     | 47  | ILE  | CA-C-N  | 5.85  | 125.72      | 119.28   |
| 3   | K     | 47  | ILE  | C-N-CA  | 5.85  | 125.72      | 119.28   |
| 7   | O     | 17  | LEU  | N-CA-C  | -5.85 | 106.05      | 112.72   |
| 4   | H     | 86  | THR  | CA-C-N  | 5.80  | 125.00      | 118.97   |
| 4   | H     | 86  | THR  | C-N-CA  | 5.80  | 125.00      | 118.97   |
| 3   | K     | 88  | PRO  | N-CA-C  | 5.78  | 117.75      | 110.70   |
| 1   | I     | 150 | LEU  | N-CA-C  | 5.74  | 122.50      | 109.81   |
| 1   | E     | 150 | LEU  | N-CA-C  | 5.71  | 122.44      | 109.81   |
| 3   | C     | 88  | PRO  | N-CA-C  | 5.68  | 117.63      | 110.70   |
| 7   | O     | 16  | LYS  | N-CA-C  | -5.68 | 106.89      | 113.88   |
| 6   | N     | 101 | ASP  | N-CA-C  | -5.62 | 100.66      | 109.25   |
| 1   | A     | 150 | LEU  | N-CA-C  | 5.60  | 122.18      | 109.81   |
| 3   | C     | 47  | ILE  | CA-C-N  | 5.59  | 125.43      | 119.28   |
| 3   | C     | 47  | ILE  | C-N-CA  | 5.59  | 125.43      | 119.28   |
| 5   | M     | 160 | HIS  | N-CA-C  | 5.57  | 119.37      | 112.24   |
| 3   | G     | 22  | LEU  | N-CA-C  | 5.56  | 117.15      | 111.14   |
| 3   | C     | 22  | LEU  | N-CA-C  | 5.55  | 117.14      | 111.14   |
| 5   | M     | 119 | SER  | N-CA-C  | 5.54  | 122.60      | 110.80   |
| 4   | L     | 138 | CYS  | N-CA-C  | 5.44  | 119.88      | 112.04   |
| 6   | N     | 81  | LEU  | N-CA-C  | -5.40 | 106.56      | 114.39   |
| 4   | L     | 86  | THR  | CA-C-N  | 5.36  | 124.55      | 118.97   |
| 4   | L     | 86  | THR  | C-N-CA  | 5.36  | 124.55      | 118.97   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | D     | 86  | THR  | CA-C-N  | 5.31  | 124.49      | 118.97   |
| 4   | D     | 86  | THR  | C-N-CA  | 5.31  | 124.49      | 118.97   |
| 3   | G     | 88  | PRO  | N-CA-C  | 5.26  | 117.12      | 110.70   |
| 6   | N     | 147 | LEU  | N-CA-C  | 5.25  | 117.06      | 109.07   |
| 2   | B     | 134 | ILE  | N-CA-C  | -5.22 | 105.30      | 110.62   |
| 5   | M     | 210 | VAL  | N-CA-C  | -5.18 | 102.42      | 107.55   |
| 5   | M     | 102 | LEU  | N-CA-C  | -5.17 | 106.97      | 113.28   |
| 3   | K     | 22  | LEU  | N-CA-C  | 5.16  | 116.71      | 111.14   |
| 5   | M     | 22  | ASP  | N-CA-C  | -5.14 | 105.65      | 112.34   |
| 6   | N     | 76  | CYS  | N-CA-C  | 5.14  | 118.60      | 109.96   |
| 2   | F     | 53  | GLY  | N-CA-C  | -5.11 | 108.32      | 114.66   |
| 6   | N     | 217 | GLN  | N-CA-C  | 5.05  | 116.50      | 108.67   |
| 2   | B     | 143 | GLY  | N-CA-C  | -5.05 | 108.01      | 114.37   |
| 5   | M     | 104 | ILE  | CB-CA-C | -5.03 | 105.43      | 112.02   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1209  | 0        | 1194     | 79      | 0            |
| 1   | E     | 1209  | 0        | 1194     | 84      | 0            |
| 1   | I     | 1209  | 0        | 1194     | 85      | 0            |
| 2   | B     | 1148  | 0        | 1103     | 34      | 0            |
| 2   | F     | 1148  | 0        | 1103     | 40      | 0            |
| 2   | J     | 1148  | 0        | 1103     | 36      | 0            |
| 3   | C     | 1185  | 0        | 1191     | 57      | 0            |
| 3   | G     | 1185  | 0        | 1191     | 56      | 0            |
| 3   | K     | 1185  | 0        | 1191     | 55      | 0            |
| 4   | D     | 1129  | 0        | 1102     | 67      | 0            |
| 4   | H     | 1129  | 0        | 1102     | 72      | 0            |
| 4   | L     | 1129  | 0        | 1102     | 64      | 0            |
| 5   | M     | 1705  | 0        | 1547     | 94      | 0            |
| 6   | N     | 1722  | 0        | 1632     | 107     | 0            |
| 7   | O     | 1663  | 0        | 1479     | 87      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | A     | 2     | 0        | 0        | 0       | 0            |
| 8   | B     | 2     | 0        | 0        | 0       | 0            |
| 8   | C     | 2     | 0        | 0        | 0       | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | E     | 2     | 0        | 0        | 0       | 0            |
| 8   | F     | 2     | 0        | 0        | 0       | 0            |
| 8   | G     | 2     | 0        | 0        | 0       | 0            |
| 8   | H     | 2     | 0        | 0        | 0       | 0            |
| 8   | I     | 2     | 0        | 0        | 0       | 0            |
| 8   | J     | 2     | 0        | 0        | 0       | 0            |
| 8   | K     | 2     | 0        | 0        | 0       | 0            |
| 8   | L     | 2     | 0        | 0        | 0       | 0            |
| 9   | A     | 43    | 0        | 30       | 0       | 0            |
| 9   | B     | 43    | 0        | 30       | 0       | 0            |
| 9   | C     | 43    | 0        | 30       | 1       | 0            |
| 9   | D     | 43    | 0        | 30       | 3       | 0            |
| 9   | E     | 43    | 0        | 30       | 0       | 0            |
| 9   | F     | 43    | 0        | 30       | 0       | 0            |
| 9   | G     | 43    | 0        | 30       | 1       | 0            |
| 9   | H     | 43    | 0        | 30       | 3       | 0            |
| 9   | I     | 43    | 0        | 30       | 0       | 0            |
| 9   | J     | 43    | 0        | 30       | 0       | 0            |
| 9   | K     | 43    | 0        | 30       | 1       | 0            |
| 9   | L     | 43    | 0        | 30       | 3       | 0            |
| 10  | M     | 2     | 0        | 0        | 0       | 0            |
| 10  | N     | 1     | 0        | 0        | 0       | 0            |
| 10  | O     | 1     | 0        | 0        | 0       | 0            |
| 11  | M     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 19648 | 0        | 18788    | 933     | 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 24.

All (933) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 3:G:129:ASP:HB2  | 4:H:129:HIS:HB3 | 1.30                     | 1.12              |
| 4:L:83:MET:HE2   | 4:L:89:MET:HB3  | 1.33                     | 1.10              |
| 4:H:83:MET:HE2   | 4:H:89:MET:HB3  | 1.34                     | 1.07              |
| 4:D:83:MET:HE2   | 4:D:89:MET:HB3  | 1.35                     | 1.07              |
| 7:O:208:LEU:HD23 | 7:O:208:LEU:H   | 1.19                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:78:LYS:NZ    | 4:H:31:ARG:HH22  | 1.60                     | 0.98              |
| 4:D:128:THR:HG21 | 4:L:29:HIS:CE1   | 2.00                     | 0.96              |
| 6:N:66:THR:HG21  | 6:N:76:CYS:HB3   | 1.49                     | 0.94              |
| 1:A:35:VAL:HG21  | 1:A:74:ALA:HB2   | 1.50                     | 0.93              |
| 6:N:89:CYS:HB2   | 6:N:94:ASP:OD2   | 1.68                     | 0.92              |
| 1:I:35:VAL:HG21  | 1:I:74:ALA:HB2   | 1.52                     | 0.91              |
| 6:N:110:VAL:HG13 | 6:N:131:THR:HB   | 1.50                     | 0.91              |
| 1:E:35:VAL:HG21  | 1:E:74:ALA:HB2   | 1.54                     | 0.89              |
| 5:M:69:CYS:HB3   | 5:M:93:SER:OG    | 1.73                     | 0.89              |
| 4:D:128:THR:HG21 | 4:L:29:HIS:HE1   | 1.35                     | 0.88              |
| 1:I:14:GLU:CD    | 7:O:208:LEU:HD11 | 1.99                     | 0.88              |
| 7:O:209:SER:HB3  | 7:O:211:GLU:HG2  | 1.55                     | 0.87              |
| 7:O:204:ILE:HB   | 7:O:214:ALA:HB3  | 1.54                     | 0.87              |
| 1:I:14:GLU:OE2   | 7:O:208:LEU:HD11 | 1.76                     | 0.84              |
| 6:N:82:VAL:HG21  | 6:N:175:ALA:H    | 1.43                     | 0.83              |
| 3:K:74:ILE:HG23  | 3:K:75:LEU:H     | 1.44                     | 0.83              |
| 6:N:82:VAL:HG13  | 6:N:83:CYS:H     | 1.43                     | 0.83              |
| 2:B:110:LYS:HG3  | 2:B:134:ILE:HG21 | 1.62                     | 0.81              |
| 1:E:126:VAL:HG13 | 2:F:7:LEU:HD22   | 1.61                     | 0.81              |
| 3:G:74:ILE:HG23  | 3:G:75:LEU:H     | 1.46                     | 0.80              |
| 7:O:208:LEU:H    | 7:O:208:LEU:CD2  | 1.93                     | 0.80              |
| 3:C:74:ILE:HG23  | 3:C:75:LEU:H     | 1.46                     | 0.80              |
| 1:E:78:LYS:HZ1   | 4:H:31:ARG:HH22  | 1.26                     | 0.80              |
| 2:J:110:LYS:HG3  | 2:J:134:ILE:HG21 | 1.64                     | 0.79              |
| 2:F:51:VAL:HG21  | 2:F:64:HIS:HB2   | 1.65                     | 0.79              |
| 5:M:70:ARG:N     | 5:M:70:ARG:HD2   | 1.97                     | 0.79              |
| 2:F:110:LYS:HG3  | 2:F:134:ILE:HG21 | 1.64                     | 0.78              |
| 2:B:51:VAL:HG21  | 2:B:64:HIS:HB2   | 1.65                     | 0.77              |
| 2:J:51:VAL:HG21  | 2:J:64:HIS:HB2   | 1.67                     | 0.77              |
| 7:O:208:LEU:HD23 | 7:O:208:LEU:N    | 1.98                     | 0.77              |
| 1:E:67:LYS:HB3   | 4:H:89:MET:HE3   | 1.66                     | 0.77              |
| 7:O:138:PHE:C    | 7:O:140:PRO:HD2  | 2.10                     | 0.77              |
| 5:M:38:LEU:HD22  | 7:O:38:ARG:HH12  | 1.50                     | 0.76              |
| 5:M:115:ALA:HA   | 5:M:220:PHE:HB3  | 1.68                     | 0.76              |
| 4:D:128:THR:CG2  | 4:L:29:HIS:HE1   | 1.98                     | 0.76              |
| 4:H:84:LEU:HD11  | 4:H:142:ILE:HD11 | 1.67                     | 0.75              |
| 1:E:83:LEU:HD23  | 1:E:90:LEU:HA    | 1.69                     | 0.75              |
| 5:M:88:ASP:HB2   | 5:M:94:ASP:OD1   | 1.86                     | 0.75              |
| 4:L:84:LEU:HD11  | 4:L:142:ILE:HD11 | 1.69                     | 0.74              |
| 7:O:180:PRO:HD3  | 7:O:207:GLU:HG3  | 1.70                     | 0.73              |
| 1:A:83:LEU:HD23  | 1:A:90:LEU:HA    | 1.69                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:83:LEU:HD23  | 1:I:90:LEU:HA    | 1.69                     | 0.73              |
| 4:D:84:LEU:HD11  | 4:D:142:ILE:HD11 | 1.69                     | 0.72              |
| 7:O:188:LEU:HD12 | 7:O:189:VAL:H    | 1.54                     | 0.72              |
| 6:N:82:VAL:HG21  | 6:N:175:ALA:N    | 2.05                     | 0.72              |
| 5:M:148:ARG:HG3  | 5:M:148:ARG:HH11 | 1.55                     | 0.71              |
| 4:D:136:HIS:O    | 4:D:140:ASP:HB2  | 1.91                     | 0.71              |
| 1:A:126:VAL:HG23 | 1:A:127:LEU:HD23 | 1.73                     | 0.71              |
| 1:A:107:VAL:O    | 1:A:150:LEU:HD22 | 1.91                     | 0.71              |
| 1:E:126:VAL:HG23 | 1:E:127:LEU:HD23 | 1.73                     | 0.71              |
| 7:O:139:THR:N    | 7:O:140:PRO:HD2  | 2.06                     | 0.70              |
| 5:M:135:ALA:HB2  | 5:M:147:LEU:HB3  | 1.72                     | 0.70              |
| 5:M:20:HIS:O     | 5:M:24:LEU:HD13  | 1.91                     | 0.70              |
| 1:I:126:VAL:HG13 | 2:J:7:LEU:HD22   | 1.74                     | 0.69              |
| 3:K:129:ASP:HB2  | 4:L:129:HIS:HB3  | 1.74                     | 0.69              |
| 3:C:10:GLU:HB2   | 1:I:10:GLU:CD    | 2.17                     | 0.69              |
| 4:H:136:HIS:O    | 4:H:140:ASP:HB2  | 1.93                     | 0.69              |
| 1:I:126:VAL:HG23 | 1:I:127:LEU:HD23 | 1.74                     | 0.69              |
| 1:A:125:GLN:O    | 2:B:11:LYS:HE3   | 1.92                     | 0.69              |
| 1:I:78:LYS:NZ    | 4:L:31:ARG:HH22  | 1.91                     | 0.69              |
| 5:M:135:ALA:CB   | 5:M:147:LEU:HB3  | 2.23                     | 0.69              |
| 1:E:126:VAL:CG1  | 2:F:7:LEU:HD22   | 2.23                     | 0.69              |
| 6:N:162:VAL:HG12 | 6:N:163:THR:N    | 2.07                     | 0.69              |
| 1:I:107:VAL:O    | 1:I:150:LEU:HD22 | 1.93                     | 0.69              |
| 7:O:45:ARG:NH1   | 7:O:45:ARG:HB3   | 2.08                     | 0.68              |
| 6:N:10:LEU:HD23  | 6:N:12:PRO:HG2   | 1.76                     | 0.68              |
| 1:A:58:ILE:HG22  | 1:A:66:PHE:CE1   | 2.29                     | 0.68              |
| 2:F:18:ARG:HH22  | 2:F:124:CYS:HB2  | 1.57                     | 0.68              |
| 7:O:209:SER:CB   | 7:O:211:GLU:HG2  | 2.22                     | 0.68              |
| 1:I:58:ILE:HG22  | 1:I:66:PHE:CE1   | 2.29                     | 0.68              |
| 1:E:107:VAL:O    | 1:E:150:LEU:HD22 | 1.95                     | 0.67              |
| 4:H:20:GLN:HE21  | 4:H:135:TRP:HE1  | 1.41                     | 0.67              |
| 2:F:120:GLN:NE2  | 6:N:80:LEU:HD21  | 2.09                     | 0.67              |
| 4:L:136:HIS:O    | 4:L:140:ASP:HB2  | 1.93                     | 0.67              |
| 4:D:115:LEU:HB2  | 4:D:143:ILE:CD1  | 2.25                     | 0.67              |
| 6:N:162:VAL:HG12 | 6:N:163:THR:H    | 1.59                     | 0.67              |
| 2:B:87:GLU:HG2   | 3:C:66:LYS:HA    | 1.77                     | 0.66              |
| 2:B:18:ARG:HH22  | 2:B:124:CYS:HB2  | 1.60                     | 0.66              |
| 3:G:58:ASP:OD2   | 3:G:61:HIS:HB2   | 1.96                     | 0.66              |
| 2:J:18:ARG:HH22  | 2:J:124:CYS:HB2  | 1.59                     | 0.66              |
| 4:L:70:SER:O     | 4:L:74:LEU:HD23  | 1.95                     | 0.66              |
| 2:F:120:GLN:HE21 | 6:N:80:LEU:HD21  | 1.60                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:10:LEU:HD11  | 4:L:13:GLU:HG3   | 1.78                     | 0.66              |
| 1:A:13:ARG:HH22  | 3:G:10:GLU:CD    | 2.03                     | 0.66              |
| 3:C:22:LEU:HG    | 3:C:128:LEU:HD21 | 1.78                     | 0.66              |
| 4:D:20:GLN:HE21  | 4:D:135:TRP:HE1  | 1.43                     | 0.66              |
| 4:L:20:GLN:HE21  | 4:L:135:TRP:HE1  | 1.44                     | 0.66              |
| 6:N:132:ILE:HD12 | 6:N:147:LEU:HD12 | 1.78                     | 0.65              |
| 7:O:102:THR:HB   | 7:O:129:PHE:CE2  | 2.31                     | 0.65              |
| 1:E:58:ILE:HG22  | 1:E:66:PHE:CE1   | 2.31                     | 0.65              |
| 2:F:87:GLU:HG2   | 3:G:66:LYS:HA    | 1.77                     | 0.65              |
| 3:K:58:ASP:OD2   | 3:K:61:HIS:HB2   | 1.96                     | 0.65              |
| 4:D:70:SER:O     | 4:D:74:LEU:HD23  | 1.96                     | 0.65              |
| 1:E:10:GLU:CD    | 3:K:10:GLU:HB2   | 2.21                     | 0.65              |
| 4:H:10:LEU:HD11  | 4:H:13:GLU:HG3   | 1.77                     | 0.65              |
| 6:N:10:LEU:HD22  | 6:N:13:ARG:HB3   | 1.77                     | 0.65              |
| 5:M:28:LEU:HD23  | 5:M:28:LEU:C     | 2.22                     | 0.65              |
| 7:O:22:ASN:O     | 7:O:26:THR:HG23  | 1.96                     | 0.64              |
| 3:G:22:LEU:HG    | 3:G:128:LEU:HD21 | 1.80                     | 0.64              |
| 4:L:115:LEU:HB2  | 4:L:143:ILE:CD1  | 2.27                     | 0.64              |
| 6:N:198:ASN:O    | 6:N:199:ARG:HD2  | 1.98                     | 0.64              |
| 5:M:155:LEU:HD23 | 5:M:162:VAL:HA   | 1.78                     | 0.64              |
| 5:M:9:ARG:HH11   | 5:M:9:ARG:HB3    | 1.62                     | 0.64              |
| 4:D:10:LEU:HD11  | 4:D:13:GLU:HG3   | 1.78                     | 0.64              |
| 3:C:18:GLN:NE2   | 3:C:136:TRP:HE1  | 1.96                     | 0.64              |
| 3:C:58:ASP:OD2   | 3:C:61:HIS:HB2   | 1.96                     | 0.64              |
| 3:K:74:ILE:HG23  | 3:K:75:LEU:N     | 2.13                     | 0.64              |
| 3:C:48:PRO:C     | 3:C:50:VAL:H     | 2.05                     | 0.64              |
| 1:A:126:VAL:HG23 | 1:A:127:LEU:CD2  | 2.28                     | 0.64              |
| 6:N:10:LEU:HD13  | 6:N:13:ARG:HH21  | 1.62                     | 0.64              |
| 5:M:124:ASN:O    | 5:M:125:PRO:C    | 2.41                     | 0.63              |
| 1:E:126:VAL:HG23 | 1:E:127:LEU:CD2  | 2.29                     | 0.63              |
| 3:G:22:LEU:HB3   | 3:G:23:TRP:CE3   | 2.33                     | 0.63              |
| 4:H:115:LEU:HB2  | 4:H:143:ILE:CD1  | 2.28                     | 0.63              |
| 3:K:48:PRO:C     | 3:K:50:VAL:H     | 2.06                     | 0.63              |
| 6:N:82:VAL:HB    | 6:N:175:ALA:HB2  | 1.79                     | 0.63              |
| 2:F:74:ILE:HG23  | 3:G:72:LEU:HD13  | 1.80                     | 0.63              |
| 3:K:22:LEU:HG    | 3:K:128:LEU:HD21 | 1.80                     | 0.63              |
| 2:B:6:VAL:O      | 2:B:10:LEU:HD13  | 1.99                     | 0.63              |
| 1:I:126:VAL:HG23 | 1:I:127:LEU:CD2  | 2.29                     | 0.63              |
| 3:K:18:GLN:NE2   | 3:K:136:TRP:HE1  | 1.97                     | 0.62              |
| 5:M:20:HIS:O     | 5:M:23:TYR:HB3   | 1.99                     | 0.62              |
| 1:A:78:LYS:NZ    | 4:D:31:ARG:HH22  | 1.97                     | 0.62              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:113:ARG:O   | 1:A:117:GLU:HG3  | 2.00                     | 0.62              |
| 1:I:67:LYS:HB3  | 4:L:89:MET:HE3   | 1.82                     | 0.62              |
| 1:I:150:LEU:N   | 1:I:151:PRO:HD2  | 2.14                     | 0.62              |
| 3:K:22:LEU:HB3  | 3:K:23:TRP:CE3   | 2.34                     | 0.62              |
| 4:D:110:PHE:HA  | 4:D:113:ILE:HD12 | 1.81                     | 0.62              |
| 1:E:150:LEU:N   | 1:E:151:PRO:HD2  | 2.14                     | 0.62              |
| 3:G:22:LEU:HB3  | 3:G:23:TRP:CZ3   | 2.34                     | 0.62              |
| 4:H:70:SER:O    | 4:H:74:LEU:HD23  | 1.99                     | 0.62              |
| 3:K:22:LEU:HB3  | 3:K:23:TRP:CZ3   | 2.35                     | 0.62              |
| 6:N:82:VAL:HG13 | 6:N:83:CYS:N     | 2.12                     | 0.62              |
| 3:K:38:LEU:HD23 | 3:K:38:LEU:C     | 2.25                     | 0.62              |
| 1:E:10:GLU:HG3  | 3:K:10:GLU:HG3   | 1.80                     | 0.62              |
| 1:E:82:ASN:ND2  | 4:H:28:ALA:H     | 1.97                     | 0.62              |
| 3:G:74:ILE:HG23 | 3:G:75:LEU:N     | 2.14                     | 0.62              |
| 6:N:24:LEU:HD21 | 7:O:25:THR:OG1   | 2.00                     | 0.62              |
| 1:A:90:LEU:O    | 1:A:94:LEU:HB2   | 2.00                     | 0.62              |
| 3:C:22:LEU:HB3  | 3:C:23:TRP:CZ3   | 2.35                     | 0.62              |
| 6:N:66:THR:CG2  | 6:N:76:CYS:HB3   | 2.27                     | 0.62              |
| 7:O:196:ASN:O   | 7:O:197:PHE:HB2  | 2.00                     | 0.62              |
| 3:C:10:GLU:HG3  | 1:I:10:GLU:HG3   | 1.82                     | 0.61              |
| 3:C:22:LEU:HB3  | 3:C:23:TRP:CE3   | 2.35                     | 0.61              |
| 3:G:18:GLN:NE2  | 3:G:136:TRP:HE1  | 1.98                     | 0.61              |
| 4:H:20:GLN:NE2  | 4:H:135:TRP:HE1  | 1.98                     | 0.61              |
| 3:C:38:LEU:C    | 3:C:38:LEU:HD23  | 2.26                     | 0.61              |
| 1:I:113:ARG:O   | 1:I:117:GLU:HG3  | 2.01                     | 0.61              |
| 1:A:150:LEU:N   | 1:A:151:PRO:HD2  | 2.15                     | 0.61              |
| 1:E:90:LEU:O    | 1:E:94:LEU:HB2   | 2.01                     | 0.61              |
| 1:I:90:LEU:O    | 1:I:94:LEU:HB2   | 2.00                     | 0.61              |
| 5:M:78:HIS:ND1  | 5:M:80:LEU:HB2   | 2.15                     | 0.61              |
| 1:E:113:ARG:O   | 1:E:117:GLU:HG3  | 2.01                     | 0.61              |
| 4:L:110:PHE:HA  | 4:L:113:ILE:HD12 | 1.83                     | 0.61              |
| 5:M:64:GLU:O    | 5:M:65:HIS:HB2   | 2.01                     | 0.61              |
| 3:G:48:PRO:C    | 3:G:50:VAL:H     | 2.08                     | 0.60              |
| 6:N:181:LEU:HB2 | 6:N:193:VAL:CG1  | 2.31                     | 0.60              |
| 3:G:38:LEU:C    | 3:G:38:LEU:HD23  | 2.26                     | 0.60              |
| 7:O:77:ILE:C    | 7:O:77:ILE:HD12  | 2.25                     | 0.60              |
| 3:C:18:GLN:HE21 | 3:C:136:TRP:HE1  | 1.50                     | 0.60              |
| 2:J:6:VAL:O     | 2:J:10:LEU:HD13  | 2.02                     | 0.60              |
| 7:O:77:ILE:HD12 | 7:O:77:ILE:O     | 2.01                     | 0.60              |
| 3:C:48:PRO:C    | 3:C:50:VAL:N     | 2.58                     | 0.60              |
| 3:C:74:ILE:HG23 | 3:C:75:LEU:N     | 2.15                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:106:HIS:HD2  | 5:M:107:VAL:N    | 1.99                     | 0.60              |
| 3:C:10:GLU:HB2   | 1:I:10:GLU:OE1   | 2.02                     | 0.59              |
| 4:D:20:GLN:NE2   | 4:D:135:TRP:HE1  | 2.00                     | 0.59              |
| 3:K:18:GLN:HE21  | 3:K:136:TRP:HE1  | 1.50                     | 0.59              |
| 3:K:108:VAL:O    | 3:K:151:LEU:HD22 | 2.02                     | 0.59              |
| 1:E:66:PHE:O     | 1:E:69:HIS:HB3   | 2.02                     | 0.59              |
| 7:O:199:ARG:HA   | 7:O:218:PHE:O    | 2.03                     | 0.59              |
| 3:K:48:PRO:C     | 3:K:50:VAL:N     | 2.60                     | 0.59              |
| 4:D:109:GLU:O    | 4:D:113:ILE:HG13 | 2.03                     | 0.59              |
| 5:M:73:VAL:HG23  | 5:M:73:VAL:O     | 2.03                     | 0.59              |
| 5:M:78:HIS:CE1   | 5:M:80:LEU:HB2   | 2.37                     | 0.59              |
| 1:I:66:PHE:O     | 1:I:69:HIS:HB3   | 2.03                     | 0.59              |
| 7:O:188:LEU:HD12 | 7:O:189:VAL:N    | 2.16                     | 0.59              |
| 4:H:49:ILE:O     | 4:H:52:PRO:HD2   | 2.01                     | 0.59              |
| 6:N:78:SER:OG    | 6:N:80:LEU:HD23  | 2.03                     | 0.59              |
| 3:G:18:GLN:HE21  | 3:G:136:TRP:HE1  | 1.51                     | 0.58              |
| 3:G:129:ASP:OD2  | 3:G:129:ASP:N    | 2.36                     | 0.58              |
| 6:N:80:LEU:O     | 6:N:81:LEU:HD23  | 2.03                     | 0.58              |
| 2:B:5:GLY:H      | 2:B:8:GLU:CG     | 2.16                     | 0.58              |
| 1:E:28:THR:O     | 1:E:31:ARG:HG2   | 2.04                     | 0.58              |
| 4:L:10:LEU:CD1   | 4:L:13:GLU:H     | 2.16                     | 0.58              |
| 6:N:210:VAL:HG12 | 6:N:217:GLN:HA   | 1.85                     | 0.58              |
| 3:C:33:ILE:HG13  | 3:C:72:LEU:HD21  | 1.86                     | 0.58              |
| 4:H:109:GLU:O    | 4:H:113:ILE:HG13 | 2.04                     | 0.58              |
| 5:M:172:ASN:HD22 | 5:M:172:ASN:C    | 2.10                     | 0.58              |
| 6:N:43:PRO:HG2   | 6:N:44:GLU:H     | 1.68                     | 0.58              |
| 6:N:10:LEU:O     | 6:N:14:LEU:HD23  | 2.04                     | 0.58              |
| 4:H:110:PHE:HA   | 4:H:113:ILE:HD12 | 1.86                     | 0.58              |
| 3:C:108:VAL:O    | 3:C:151:LEU:HD22 | 2.04                     | 0.57              |
| 2:F:3:GLN:O      | 2:F:8:GLU:HG3    | 2.03                     | 0.57              |
| 2:J:3:GLN:O      | 2:J:8:GLU:HG3    | 2.04                     | 0.57              |
| 1:A:23:TRP:CZ3   | 1:A:74:ALA:HB1   | 2.39                     | 0.57              |
| 3:G:108:VAL:O    | 3:G:151:LEU:HD22 | 2.03                     | 0.57              |
| 4:D:49:ILE:O     | 4:D:52:PRO:HD2   | 2.04                     | 0.57              |
| 2:J:41:VAL:O     | 2:J:41:VAL:HG23  | 2.05                     | 0.57              |
| 5:M:202:ASP:OD1  | 5:M:224:ARG:HD2  | 2.04                     | 0.57              |
| 7:O:205:VAL:HG12 | 7:O:212:VAL:HA   | 1.86                     | 0.57              |
| 4:L:20:GLN:NE2   | 4:L:135:TRP:HE1  | 2.01                     | 0.57              |
| 4:L:109:GLU:O    | 4:L:113:ILE:HG13 | 2.04                     | 0.57              |
| 3:G:48:PRO:C     | 3:G:50:VAL:N     | 2.61                     | 0.57              |
| 1:A:28:THR:O     | 1:A:31:ARG:HG2   | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:128:THR:CG2  | 4:L:29:HIS:CE1   | 2.76                     | 0.57              |
| 4:H:10:LEU:CD1   | 4:H:13:GLU:H     | 2.17                     | 0.57              |
| 2:J:5:GLY:H      | 2:J:8:GLU:CG     | 2.17                     | 0.57              |
| 5:M:31:ILE:HG23  | 6:N:35:LEU:HD22  | 1.86                     | 0.57              |
| 2:B:110:LYS:HG3  | 2:B:134:ILE:CG2  | 2.34                     | 0.57              |
| 2:F:5:GLY:H      | 2:F:8:GLU:CG     | 2.17                     | 0.57              |
| 2:F:89:LEU:HD21  | 2:F:137:ILE:HG23 | 1.86                     | 0.57              |
| 6:N:10:LEU:C     | 6:N:12:PRO:HD2   | 2.30                     | 0.57              |
| 4:D:125:ARG:HG2  | 4:D:125:ARG:HH11 | 1.69                     | 0.57              |
| 1:E:78:LYS:HZ3   | 4:H:31:ARG:HH22  | 1.48                     | 0.57              |
| 5:M:172:ASN:HD22 | 5:M:173:PHE:N    | 2.03                     | 0.57              |
| 6:N:82:VAL:CG2   | 6:N:174:PHE:HB2  | 2.35                     | 0.57              |
| 6:N:181:LEU:HB2  | 6:N:193:VAL:HG13 | 1.87                     | 0.57              |
| 7:O:67:HIS:HB3   | 7:O:77:ILE:CD1   | 2.34                     | 0.57              |
| 2:B:3:GLN:O      | 2:B:8:GLU:HG3    | 2.04                     | 0.57              |
| 4:D:40:ARG:NH2   | 4:H:124:ASP:OD2  | 2.37                     | 0.56              |
| 6:N:10:LEU:HD13  | 6:N:13:ARG:NH2   | 2.20                     | 0.56              |
| 7:O:181:PRO:HG2  | 7:O:182:GLU:H    | 1.70                     | 0.56              |
| 1:I:125:GLN:O    | 2:J:11:LYS:HE3   | 2.04                     | 0.56              |
| 6:N:47:VAL:HG13  | 6:N:48:SER:N     | 2.20                     | 0.56              |
| 1:A:87:THR:HG21  | 3:G:134:LEU:H    | 1.71                     | 0.56              |
| 5:M:130:VAL:HG13 | 5:M:130:VAL:O    | 2.04                     | 0.56              |
| 6:N:147:LEU:N    | 6:N:147:LEU:HD23 | 2.20                     | 0.56              |
| 2:F:6:VAL:O      | 2:F:10:LEU:HD13  | 2.04                     | 0.56              |
| 4:D:10:LEU:CD1   | 4:D:13:GLU:H     | 2.17                     | 0.56              |
| 1:A:66:PHE:O     | 1:A:69:HIS:HB3   | 2.05                     | 0.56              |
| 1:E:147:ALA:HB2  | 1:E:150:LEU:HD12 | 1.88                     | 0.56              |
| 1:I:82:ASN:ND2   | 4:L:28:ALA:H     | 2.04                     | 0.56              |
| 3:C:129:ASP:OD2  | 3:C:129:ASP:N    | 2.39                     | 0.56              |
| 2:J:87:GLU:HG2   | 3:K:66:LYS:HA    | 1.88                     | 0.56              |
| 7:O:114:PHE:O    | 7:O:114:PHE:CD1  | 2.58                     | 0.56              |
| 2:B:41:VAL:HG23  | 2:B:41:VAL:O     | 2.06                     | 0.56              |
| 2:F:123:ARG:H    | 2:F:123:ARG:HD3  | 1.71                     | 0.56              |
| 2:B:8:GLU:CD     | 2:B:8:GLU:H      | 2.14                     | 0.55              |
| 4:D:115:LEU:HB2  | 4:D:143:ILE:HD11 | 1.87                     | 0.55              |
| 6:N:31:LEU:HD23  | 6:N:31:LEU:O     | 2.05                     | 0.55              |
| 4:H:125:ARG:HH11 | 4:H:125:ARG:HG2  | 1.71                     | 0.55              |
| 4:L:49:ILE:O     | 4:L:52:PRO:HD2   | 2.06                     | 0.55              |
| 5:M:57:LEU:HB2   | 7:O:57:LEU:HD13  | 1.87                     | 0.55              |
| 5:M:131:THR:O    | 5:M:149:ALA:HB1  | 2.07                     | 0.55              |
| 5:M:168:ARG:HG2  | 5:M:169:GLY:N    | 2.20                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:125:ARG:HG2  | 4:L:125:ARG:HH11 | 1.71                     | 0.55              |
| 6:N:130:ILE:HD11 | 6:N:193:VAL:HG21 | 1.88                     | 0.55              |
| 7:O:50:LEU:C     | 7:O:50:LEU:HD23  | 2.32                     | 0.55              |
| 6:N:16:ALA:C     | 6:N:18:ALA:H     | 2.14                     | 0.55              |
| 3:G:18:GLN:HE22  | 3:G:132:ASP:H    | 1.53                     | 0.55              |
| 3:K:33:ILE:HG13  | 3:K:72:LEU:HD21  | 1.89                     | 0.55              |
| 5:M:9:ARG:HB3    | 5:M:9:ARG:NH1    | 2.22                     | 0.55              |
| 7:O:139:THR:N    | 7:O:140:PRO:CD   | 2.69                     | 0.55              |
| 1:I:23:TRP:CZ3   | 1:I:74:ALA:HB1   | 2.42                     | 0.55              |
| 2:J:89:LEU:HD21  | 2:J:137:ILE:HG23 | 1.88                     | 0.55              |
| 7:O:112:VAL:HG22 | 7:O:113:CYS:N    | 2.22                     | 0.55              |
| 2:J:64:HIS:O     | 2:J:68:VAL:HG23  | 2.07                     | 0.55              |
| 7:O:93:GLU:C     | 7:O:95:GLU:H     | 2.15                     | 0.55              |
| 1:A:38:VAL:HA    | 1:A:122:VAL:HG21 | 1.89                     | 0.54              |
| 6:N:35:LEU:HA    | 7:O:35:LEU:HD11  | 1.89                     | 0.54              |
| 6:N:79:ASP:O     | 6:N:82:VAL:HG12  | 2.08                     | 0.54              |
| 6:N:198:ASN:O    | 6:N:198:ASN:CG   | 2.50                     | 0.54              |
| 1:A:67:LYS:HB3   | 4:D:89:MET:HE3   | 1.90                     | 0.54              |
| 1:I:28:THR:O     | 1:I:31:ARG:HG2   | 2.07                     | 0.54              |
| 7:O:21:THR:O     | 7:O:24:ILE:HG22  | 2.07                     | 0.54              |
| 1:E:38:VAL:HA    | 1:E:122:VAL:HG21 | 1.88                     | 0.54              |
| 1:E:78:LYS:HE2   | 4:H:31:ARG:NH1   | 2.23                     | 0.54              |
| 1:I:78:LYS:HZ1   | 4:L:31:ARG:HH22  | 1.54                     | 0.54              |
| 6:N:81:LEU:O     | 6:N:82:VAL:C     | 2.50                     | 0.54              |
| 2:B:89:LEU:HD21  | 2:B:137:ILE:HG23 | 1.90                     | 0.54              |
| 2:F:8:GLU:CD     | 2:F:8:GLU:H      | 2.15                     | 0.54              |
| 7:O:67:HIS:HB3   | 7:O:77:ILE:HD11  | 1.90                     | 0.54              |
| 1:A:83:LEU:HD11  | 4:D:71:GLN:HG2   | 1.90                     | 0.54              |
| 4:L:115:LEU:HB2  | 4:L:143:ILE:HD11 | 1.89                     | 0.54              |
| 1:E:23:TRP:CZ3   | 1:E:74:ALA:HB1   | 2.43                     | 0.54              |
| 2:F:64:HIS:O     | 2:F:68:VAL:HG23  | 2.07                     | 0.54              |
| 3:G:108:VAL:HG22 | 9:G:160:HEM:HBC2 | 1.90                     | 0.54              |
| 4:H:115:LEU:HB2  | 4:H:143:ILE:HD11 | 1.90                     | 0.54              |
| 1:I:38:VAL:HA    | 1:I:122:VAL:HG21 | 1.89                     | 0.54              |
| 2:J:56:THR:HA    | 2:J:61:PHE:CD2   | 2.43                     | 0.54              |
| 5:M:224:ARG:HG2  | 5:M:225:TYR:N    | 2.21                     | 0.54              |
| 3:C:148:SER:C    | 3:C:150:ARG:H    | 2.16                     | 0.54              |
| 2:B:123:ARG:HD3  | 2:B:123:ARG:H    | 1.73                     | 0.53              |
| 1:I:23:TRP:CD1   | 1:I:78:LYS:HZ2   | 2.25                     | 0.53              |
| 1:I:150:LEU:O    | 1:I:151:PRO:O    | 2.26                     | 0.53              |
| 5:M:143:ASN:O    | 5:M:144:ARG:HD3  | 2.07                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:178:ARG:NH2  | 6:N:180:ILE:HD11 | 2.23                     | 0.53              |
| 7:O:45:ARG:HB3   | 7:O:45:ARG:HH11  | 1.71                     | 0.53              |
| 1:E:78:LYS:HE2   | 4:H:31:ARG:HH12  | 1.73                     | 0.53              |
| 3:G:88:PRO:HG2   | 3:G:89:PRO:HD3   | 1.90                     | 0.53              |
| 2:B:56:THR:HA    | 2:B:61:PHE:CD2   | 2.44                     | 0.53              |
| 6:N:11:ASP:N     | 6:N:12:PRO:HD2   | 2.24                     | 0.53              |
| 7:O:45:ARG:HH11  | 7:O:45:ARG:CB    | 2.22                     | 0.53              |
| 7:O:146:VAL:HG21 | 7:O:178:ILE:HD13 | 1.89                     | 0.53              |
| 3:C:18:GLN:HE22  | 3:C:132:ASP:H    | 1.56                     | 0.53              |
| 1:E:53:PHE:HB2   | 1:E:58:ILE:HG21  | 1.91                     | 0.53              |
| 4:L:51:ALA:HB3   | 4:L:52:PRO:CD    | 2.39                     | 0.53              |
| 4:L:57:ARG:HG2   | 4:L:57:ARG:HH11  | 1.73                     | 0.53              |
| 5:M:110:SER:OG   | 5:M:131:THR:HB   | 2.08                     | 0.53              |
| 5:M:143:ASN:ND2  | 5:M:144:ARG:HE   | 2.06                     | 0.53              |
| 6:N:89:CYS:N     | 6:N:94:ASP:OD2   | 2.40                     | 0.53              |
| 7:O:158:GLU:O    | 7:O:158:GLU:HG3  | 2.09                     | 0.53              |
| 3:G:33:ILE:HG13  | 3:G:72:LEU:HD21  | 1.91                     | 0.53              |
| 3:K:18:GLN:HE22  | 3:K:132:ASP:H    | 1.57                     | 0.53              |
| 7:O:125:MET:HE1  | 7:O:204:ILE:HD11 | 1.90                     | 0.53              |
| 4:H:51:ALA:HB3   | 4:H:52:PRO:CD    | 2.39                     | 0.53              |
| 5:M:21:ILE:C     | 5:M:23:TYR:N     | 2.66                     | 0.53              |
| 7:O:100:LEU:C    | 7:O:100:LEU:HD23 | 2.34                     | 0.53              |
| 3:C:18:GLN:NE2   | 3:C:131:TYR:HA   | 2.24                     | 0.53              |
| 7:O:114:PHE:HD1  | 7:O:215:GLU:H    | 1.56                     | 0.53              |
| 6:N:82:VAL:HG21  | 6:N:174:PHE:HB2  | 1.90                     | 0.53              |
| 2:J:109:PHE:CE1  | 2:J:113:ILE:HD11 | 2.44                     | 0.52              |
| 1:A:150:LEU:O    | 1:A:151:PRO:O    | 2.27                     | 0.52              |
| 3:C:22:LEU:HD13  | 3:C:23:TRP:CH2   | 2.44                     | 0.52              |
| 4:D:51:ALA:HB3   | 4:D:52:PRO:CD    | 2.39                     | 0.52              |
| 1:E:23:TRP:CD1   | 1:E:78:LYS:HZ2   | 2.27                     | 0.52              |
| 3:G:18:GLN:NE2   | 3:G:131:TYR:HA   | 2.24                     | 0.52              |
| 5:M:195:ASP:HB3  | 5:M:197:ASN:ND2  | 2.25                     | 0.52              |
| 3:C:108:VAL:HG22 | 9:C:160:HEM:HBC2 | 1.91                     | 0.52              |
| 2:J:8:GLU:CD     | 2:J:8:GLU:H      | 2.16                     | 0.52              |
| 5:M:104:ILE:HG23 | 5:M:111:TYR:OH   | 2.09                     | 0.52              |
| 3:C:8:SER:N      | 3:C:11:ASP:HB2   | 2.25                     | 0.52              |
| 3:G:22:LEU:HD13  | 3:G:23:TRP:CH2   | 2.44                     | 0.52              |
| 3:G:148:SER:C    | 3:G:150:ARG:H    | 2.18                     | 0.52              |
| 7:O:185:GLY:O    | 7:O:206:HIS:HA   | 2.09                     | 0.52              |
| 1:E:71:VAL:HG11  | 4:H:79:ILE:HG23  | 1.90                     | 0.52              |
| 2:J:110:LYS:HG3  | 2:J:134:ILE:CG2  | 2.36                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:114:PHE:HD1  | 7:O:215:GLU:N    | 2.06                     | 0.52              |
| 7:O:161:VAL:HG12 | 7:O:163:MET:HG3  | 1.90                     | 0.52              |
| 1:A:147:ALA:HB2  | 1:A:150:LEU:HD12 | 1.92                     | 0.52              |
| 1:I:25:SER:HA    | 3:K:25:ASP:HB2   | 1.90                     | 0.52              |
| 1:I:126:VAL:CG1  | 2:J:7:LEU:HD22   | 2.39                     | 0.52              |
| 1:A:75:ASN:CG    | 4:D:79:ILE:HG12  | 2.35                     | 0.52              |
| 3:G:124:LEU:N    | 3:G:125:PRO:HD2  | 2.24                     | 0.52              |
| 5:M:148:ARG:HG3  | 5:M:148:ARG:NH1  | 2.23                     | 0.51              |
| 7:O:209:SER:O    | 7:O:210:GLU:CB   | 2.58                     | 0.51              |
| 1:E:123:LEU:N    | 1:E:124:PRO:HD2  | 2.25                     | 0.51              |
| 3:K:148:SER:C    | 3:K:150:ARG:H    | 2.17                     | 0.51              |
| 4:D:57:ARG:HH11  | 4:D:57:ARG:HG2   | 1.75                     | 0.51              |
| 2:F:56:THR:HA    | 2:F:61:PHE:CD2   | 2.45                     | 0.51              |
| 3:K:124:LEU:N    | 3:K:125:PRO:HD2  | 2.25                     | 0.51              |
| 4:L:56:VAL:O     | 4:L:57:ARG:C     | 2.53                     | 0.51              |
| 2:J:123:ARG:H    | 2:J:123:ARG:HD3  | 1.74                     | 0.51              |
| 1:E:15:ILE:C     | 1:E:17:HIS:N     | 2.67                     | 0.51              |
| 4:H:83:MET:CE    | 4:H:89:MET:HE2   | 2.41                     | 0.51              |
| 6:N:80:LEU:C     | 6:N:81:LEU:HD23  | 2.35                     | 0.51              |
| 1:I:53:PHE:HB2   | 1:I:58:ILE:HG21  | 1.92                     | 0.51              |
| 6:N:16:ALA:C     | 6:N:18:ALA:N     | 2.68                     | 0.51              |
| 6:N:82:VAL:CG2   | 6:N:175:ALA:N    | 2.73                     | 0.51              |
| 1:I:79:LEU:HD13  | 1:I:79:LEU:O     | 2.10                     | 0.51              |
| 4:L:83:MET:CE    | 4:L:89:MET:HE2   | 2.41                     | 0.51              |
| 3:C:87:ASP:C     | 3:C:89:PRO:HD2   | 2.36                     | 0.51              |
| 1:E:67:LYS:CB    | 4:H:89:MET:HE3   | 2.39                     | 0.51              |
| 1:I:123:LEU:N    | 1:I:124:PRO:HD2  | 2.25                     | 0.51              |
| 3:K:87:ASP:C     | 3:K:89:PRO:HD2   | 2.36                     | 0.51              |
| 6:N:18:ALA:C     | 6:N:20:LEU:N     | 2.67                     | 0.51              |
| 1:E:79:LEU:HD21  | 4:H:71:GLN:HG3   | 1.92                     | 0.51              |
| 3:K:18:GLN:NE2   | 3:K:131:TYR:HA   | 2.26                     | 0.51              |
| 7:O:180:PRO:HD3  | 7:O:207:GLU:CG   | 2.39                     | 0.51              |
| 5:M:170:PHE:CD1  | 5:M:170:PHE:C    | 2.89                     | 0.51              |
| 3:C:48:PRO:O     | 3:C:50:VAL:N     | 2.45                     | 0.50              |
| 4:D:56:VAL:O     | 4:D:57:ARG:C     | 2.53                     | 0.50              |
| 2:F:110:LYS:HG3  | 2:F:134:ILE:CG2  | 2.37                     | 0.50              |
| 6:N:46:PHE:CD1   | 6:N:46:PHE:C     | 2.88                     | 0.50              |
| 1:A:109:LYS:HD2  | 1:A:151:PRO:HD3  | 1.93                     | 0.50              |
| 2:F:41:VAL:HG23  | 2:F:41:VAL:O     | 2.10                     | 0.50              |
| 4:H:56:VAL:O     | 4:H:57:ARG:C     | 2.54                     | 0.50              |
| 1:I:109:LYS:HD2  | 1:I:151:PRO:HD3  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:94:LEU:HD21  | 4:L:142:ILE:HG23 | 1.93                     | 0.50              |
| 3:C:124:LEU:N    | 3:C:125:PRO:HD2  | 2.26                     | 0.50              |
| 2:F:76:ILE:O     | 2:F:79:LEU:HG    | 2.11                     | 0.50              |
| 3:K:8:SER:N      | 3:K:11:ASP:HB2   | 2.25                     | 0.50              |
| 5:M:106:HIS:CD2  | 5:M:107:VAL:N    | 2.79                     | 0.50              |
| 1:A:123:LEU:N    | 1:A:124:PRO:HD2  | 2.26                     | 0.50              |
| 3:K:88:PRO:HG2   | 3:K:89:PRO:HD3   | 1.94                     | 0.50              |
| 2:B:76:ILE:O     | 2:B:79:LEU:HG    | 2.10                     | 0.50              |
| 3:C:99:ALA:HA    | 3:C:147:ILE:O    | 2.12                     | 0.50              |
| 1:E:15:ILE:C     | 1:E:17:HIS:H     | 2.20                     | 0.50              |
| 1:E:60:GLU:O     | 1:E:63:SER:HB3   | 2.12                     | 0.50              |
| 3:K:11:ASP:O     | 3:K:14:ILE:HB    | 2.12                     | 0.50              |
| 5:M:115:ALA:HB2  | 5:M:128:ALA:HB2  | 1.94                     | 0.50              |
| 1:E:115:ILE:O    | 1:E:118:ALA:HB3  | 2.12                     | 0.50              |
| 1:I:14:GLU:OE2   | 7:O:208:LEU:HD21 | 2.12                     | 0.50              |
| 1:I:15:ILE:C     | 1:I:17:HIS:N     | 2.67                     | 0.50              |
| 5:M:115:ALA:O    | 5:M:125:PRO:HA   | 2.12                     | 0.50              |
| 5:M:172:ASN:C    | 5:M:172:ASN:ND2  | 2.67                     | 0.50              |
| 2:B:109:PHE:CE1  | 2:B:113:ILE:HD11 | 2.46                     | 0.50              |
| 4:H:57:ARG:HG2   | 4:H:57:ARG:HH11  | 1.76                     | 0.50              |
| 5:M:63:ASP:O     | 5:M:64:GLU:C     | 2.53                     | 0.50              |
| 2:F:102:PRO:C    | 2:F:104:ASN:N    | 2.70                     | 0.49              |
| 3:G:8:SER:N      | 3:G:11:ASP:HB2   | 2.27                     | 0.49              |
| 4:L:17:VAL:HG13  | 4:L:135:TRP:CE2  | 2.47                     | 0.49              |
| 7:O:100:LEU:HD23 | 7:O:101:PRO:N    | 2.27                     | 0.49              |
| 7:O:101:PRO:HG2  | 7:O:102:THR:H    | 1.77                     | 0.49              |
| 2:B:5:GLY:H      | 2:B:8:GLU:HG3    | 1.76                     | 0.49              |
| 4:H:94:LEU:HD21  | 4:H:142:ILE:HG23 | 1.93                     | 0.49              |
| 3:K:22:LEU:HD13  | 3:K:23:TRP:CH2   | 2.47                     | 0.49              |
| 5:M:114:LEU:HD12 | 5:M:126:ASP:O    | 2.11                     | 0.49              |
| 2:B:51:VAL:O     | 2:B:51:VAL:HG22  | 2.11                     | 0.49              |
| 1:E:78:LYS:HZ1   | 4:H:31:ARG:NH2   | 2.01                     | 0.49              |
| 3:K:72:LEU:O     | 3:K:73:ARG:C     | 2.56                     | 0.49              |
| 4:D:130:PHE:HD2  | 4:L:62:TYR:CE2   | 2.31                     | 0.49              |
| 1:I:23:TRP:NE1   | 1:I:78:LYS:HZ2   | 2.10                     | 0.49              |
| 3:K:108:VAL:HG22 | 9:K:160:HEM:HBC2 | 1.93                     | 0.49              |
| 5:M:36:ASN:C     | 5:M:38:LEU:H     | 2.20                     | 0.49              |
| 1:E:150:LEU:O    | 1:E:151:PRO:O    | 2.30                     | 0.49              |
| 2:F:109:PHE:CE1  | 2:F:113:ILE:HD11 | 2.48                     | 0.49              |
| 7:O:120:ARG:O    | 7:O:121:ARG:C    | 2.55                     | 0.49              |
| 7:O:121:ARG:N    | 7:O:122:PRO:CD   | 2.75                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:PHE:HB2   | 1:A:58:ILE:HG21  | 1.93                     | 0.49              |
| 3:C:9:GLU:HA     | 3:C:12:HIS:CE1   | 2.48                     | 0.49              |
| 2:F:51:VAL:HG22  | 2:F:51:VAL:O     | 2.13                     | 0.49              |
| 3:G:87:ASP:C     | 3:G:89:PRO:HD2   | 2.38                     | 0.49              |
| 5:M:210:VAL:HG12 | 5:M:215:PHE:O    | 2.12                     | 0.49              |
| 7:O:115:ASP:OD1  | 7:O:121:ARG:HA   | 2.12                     | 0.49              |
| 4:L:14:SER:OG    | 4:L:15:LEU:N     | 2.45                     | 0.49              |
| 4:D:94:LEU:HD21  | 4:D:142:ILE:HG23 | 1.94                     | 0.49              |
| 1:E:10:GLU:OE1   | 3:K:10:GLU:HB2   | 2.12                     | 0.49              |
| 1:E:109:LYS:HD2  | 1:E:151:PRO:HD3  | 1.95                     | 0.49              |
| 3:G:11:ASP:O     | 3:G:14:ILE:HB    | 2.13                     | 0.49              |
| 1:I:132:VAL:HG13 | 1:I:133:ASP:N    | 2.28                     | 0.49              |
| 6:N:53:ARG:HD2   | 7:O:58:GLU:OE1   | 2.13                     | 0.49              |
| 1:E:127:LEU:HD23 | 1:E:127:LEU:N    | 2.28                     | 0.49              |
| 1:I:147:ALA:HB2  | 1:I:150:LEU:HD12 | 1.94                     | 0.49              |
| 7:O:24:ILE:HG23  | 7:O:25:THR:N     | 2.28                     | 0.49              |
| 4:D:60:ASN:HD21  | 4:H:133:GLY:H    | 1.61                     | 0.48              |
| 7:O:93:GLU:O     | 7:O:95:GLU:N     | 2.46                     | 0.48              |
| 1:I:127:LEU:HD23 | 1:I:127:LEU:N    | 2.28                     | 0.48              |
| 1:A:87:THR:HG22  | 3:G:134:LEU:HG   | 1.96                     | 0.48              |
| 1:A:115:ILE:O    | 1:A:118:ALA:HB3  | 2.13                     | 0.48              |
| 3:C:70:HIS:O     | 3:C:74:ILE:HG22  | 2.12                     | 0.48              |
| 3:K:37:ARG:HH22  | 3:K:63:GLU:HB3   | 1.78                     | 0.48              |
| 3:K:48:PRO:O     | 3:K:50:VAL:N     | 2.46                     | 0.48              |
| 4:L:111:PHE:HB3  | 4:L:143:ILE:HG23 | 1.95                     | 0.48              |
| 3:C:37:ARG:HH22  | 3:C:63:GLU:HB3   | 1.79                     | 0.48              |
| 1:E:82:ASN:HD22  | 4:H:31:ARG:HD2   | 1.79                     | 0.48              |
| 3:G:32:LYS:HG2   | 3:G:75:LEU:HD12  | 1.95                     | 0.48              |
| 4:H:14:SER:O     | 4:H:17:VAL:N     | 2.46                     | 0.48              |
| 1:I:15:ILE:C     | 1:I:17:HIS:H     | 2.21                     | 0.48              |
| 1:I:28:THR:O     | 1:I:29:ASP:C     | 2.56                     | 0.48              |
| 7:O:114:PHE:O    | 7:O:214:ALA:HA   | 2.12                     | 0.48              |
| 1:A:23:TRP:CD1   | 1:A:78:LYS:HZ2   | 2.32                     | 0.48              |
| 4:D:83:MET:CE    | 4:D:89:MET:HE2   | 2.44                     | 0.48              |
| 1:E:147:ALA:CB   | 1:E:150:LEU:HD12 | 2.43                     | 0.48              |
| 5:M:181:ALA:HB1  | 5:M:182:PRO:HD2  | 1.95                     | 0.48              |
| 6:N:18:ALA:C     | 6:N:20:LEU:H     | 2.22                     | 0.48              |
| 6:N:137:ARG:NH2  | 6:N:142:THR:HB   | 2.28                     | 0.48              |
| 1:A:60:GLU:HB2   | 1:A:63:SER:HB3   | 1.96                     | 0.48              |
| 3:C:11:ASP:O     | 3:C:14:ILE:HB    | 2.13                     | 0.48              |
| 3:C:129:ASP:HA   | 4:D:16:LYS:HE3   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:142:LEU:O    | 1:I:146:ILE:HG13 | 2.14                     | 0.48              |
| 3:K:9:GLU:HA     | 3:K:12:HIS:CE1   | 2.49                     | 0.48              |
| 5:M:85:GLY:N     | 5:M:95:GLU:OE2   | 2.47                     | 0.48              |
| 6:N:75:GLU:OE1   | 6:N:90:HIS:HD2   | 1.96                     | 0.48              |
| 2:B:85:LEU:O     | 2:B:86:LYS:C     | 2.56                     | 0.48              |
| 4:H:111:PHE:HB3  | 4:H:143:ILE:HG23 | 1.96                     | 0.48              |
| 1:E:53:PHE:HB2   | 1:E:58:ILE:CG2   | 2.44                     | 0.48              |
| 1:E:108:THR:HG23 | 1:E:111:TYR:CE2  | 2.49                     | 0.48              |
| 1:I:115:ILE:O    | 1:I:118:ALA:HB3  | 2.13                     | 0.48              |
| 1:E:19:TRP:HE1   | 1:E:78:LYS:HD3   | 1.79                     | 0.47              |
| 3:G:70:HIS:O     | 3:G:74:ILE:HG22  | 2.14                     | 0.47              |
| 5:M:28:LEU:O     | 5:M:31:ILE:HB    | 2.15                     | 0.47              |
| 1:A:15:ILE:C     | 1:A:17:HIS:N     | 2.68                     | 0.47              |
| 2:B:64:HIS:O     | 2:B:68:VAL:HG23  | 2.15                     | 0.47              |
| 1:E:15:ILE:O     | 1:E:17:HIS:N     | 2.47                     | 0.47              |
| 3:G:37:ARG:HH22  | 3:G:63:GLU:HB3   | 1.79                     | 0.47              |
| 1:I:53:PHE:HB2   | 1:I:58:ILE:CG2   | 2.44                     | 0.47              |
| 1:I:60:GLU:HB2   | 1:I:63:SER:HB3   | 1.96                     | 0.47              |
| 2:J:51:VAL:HG22  | 2:J:51:VAL:O     | 2.15                     | 0.47              |
| 5:M:102:LEU:O    | 5:M:103:ASN:C    | 2.57                     | 0.47              |
| 5:M:117:TRP:HA   | 5:M:218:ALA:CB   | 2.44                     | 0.47              |
| 6:N:120:CYS:O    | 6:N:121:LEU:HG   | 2.13                     | 0.47              |
| 1:A:60:GLU:O     | 1:A:63:SER:HB3   | 2.14                     | 0.47              |
| 1:E:118:ALA:O    | 1:E:122:VAL:HG23 | 2.14                     | 0.47              |
| 1:I:29:ASP:OD2   | 3:K:30:LYS:HE3   | 2.14                     | 0.47              |
| 2:J:5:GLY:H      | 2:J:8:GLU:HG3    | 1.79                     | 0.47              |
| 2:B:102:PRO:C    | 2:B:104:ASN:N    | 2.71                     | 0.47              |
| 1:E:60:GLU:HB2   | 1:E:63:SER:HB3   | 1.95                     | 0.47              |
| 5:M:183:LEU:O    | 5:M:184:LYS:HB3  | 2.13                     | 0.47              |
| 5:M:196:PHE:CE2  | 5:M:204:ALA:HB2  | 2.49                     | 0.47              |
| 7:O:117:CYS:O    | 7:O:118:THR:C    | 2.57                     | 0.47              |
| 1:A:127:LEU:HD23 | 1:A:127:LEU:N    | 2.29                     | 0.47              |
| 3:K:12:HIS:HB2   | 3:K:85:LEU:HD13  | 1.97                     | 0.47              |
| 1:A:96:HIS:O     | 1:A:100:GLN:HG3  | 2.14                     | 0.47              |
| 7:O:120:ARG:N    | 7:O:120:ARG:HD2  | 2.29                     | 0.47              |
| 7:O:181:PRO:HD2  | 7:O:186:LEU:O    | 2.14                     | 0.47              |
| 1:A:23:TRP:CH2   | 1:A:74:ALA:HB1   | 2.50                     | 0.47              |
| 1:A:79:LEU:HD13  | 1:A:79:LEU:O     | 2.14                     | 0.47              |
| 4:D:51:ALA:HB3   | 4:D:52:PRO:HD3   | 1.97                     | 0.47              |
| 3:G:31:ILE:O     | 3:G:32:LYS:C     | 2.58                     | 0.47              |
| 3:G:88:PRO:HG2   | 3:G:89:PRO:CD    | 2.43                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:108:THR:HG23 | 1:I:111:TYR:CE2  | 2.50                     | 0.47              |
| 5:M:176:ARG:NH2  | 5:M:201:ASP:OD2  | 2.48                     | 0.47              |
| 5:M:210:VAL:HG13 | 5:M:210:VAL:O    | 2.15                     | 0.47              |
| 1:A:19:TRP:C     | 1:A:21:ASP:H     | 2.23                     | 0.47              |
| 1:A:19:TRP:HE1   | 1:A:78:LYS:HD3   | 1.79                     | 0.47              |
| 3:C:87:ASP:OD1   | 3:C:89:PRO:HG2   | 2.15                     | 0.47              |
| 3:G:48:PRO:O     | 3:G:50:VAL:N     | 2.48                     | 0.47              |
| 1:I:79:LEU:HD13  | 1:I:79:LEU:C     | 2.39                     | 0.47              |
| 2:J:76:ILE:O     | 2:J:79:LEU:HG    | 2.15                     | 0.47              |
| 3:K:88:PRO:N     | 3:K:89:PRO:HD2   | 2.30                     | 0.47              |
| 6:N:155:LEU:HD23 | 6:N:155:LEU:H    | 1.79                     | 0.47              |
| 1:A:15:ILE:C     | 1:A:17:HIS:H     | 2.23                     | 0.47              |
| 1:E:23:TRP:CH2   | 1:E:74:ALA:HB1   | 2.50                     | 0.47              |
| 2:F:28:ALA:O     | 2:F:29:PHE:C     | 2.58                     | 0.47              |
| 4:H:110:PHE:O    | 4:H:113:ILE:HB   | 2.15                     | 0.47              |
| 3:K:31:ILE:O     | 3:K:32:LYS:C     | 2.58                     | 0.47              |
| 6:N:10:LEU:CD2   | 6:N:12:PRO:HG2   | 2.43                     | 0.47              |
| 2:F:102:PRO:C    | 2:F:104:ASN:H    | 2.22                     | 0.47              |
| 1:I:118:ALA:O    | 1:I:122:VAL:HG23 | 2.15                     | 0.47              |
| 6:N:80:LEU:N     | 6:N:80:LEU:HD22  | 2.30                     | 0.47              |
| 2:B:28:ALA:O     | 2:B:29:PHE:C     | 2.56                     | 0.46              |
| 1:E:132:VAL:HG13 | 1:E:133:ASP:N    | 2.29                     | 0.46              |
| 3:G:88:PRO:N     | 3:G:89:PRO:HD2   | 2.30                     | 0.46              |
| 1:I:19:TRP:HE1   | 1:I:78:LYS:HD3   | 1.79                     | 0.46              |
| 5:M:152:SER:HA   | 5:M:163:SER:O    | 2.15                     | 0.46              |
| 1:A:53:PHE:HB2   | 1:A:58:ILE:CG2   | 2.45                     | 0.46              |
| 1:A:142:LEU:O    | 1:A:146:ILE:HG13 | 2.14                     | 0.46              |
| 3:C:88:PRO:HG2   | 3:C:89:PRO:HD3   | 1.96                     | 0.46              |
| 4:H:31:ARG:HB3   | 4:H:71:GLN:HE22  | 1.80                     | 0.46              |
| 6:N:208:HIS:HA   | 6:N:219:ALA:O    | 2.15                     | 0.46              |
| 7:O:203:HIS:CD2  | 7:O:215:GLU:HG3  | 2.49                     | 0.46              |
| 4:D:14:SER:OG    | 4:D:15:LEU:N     | 2.47                     | 0.46              |
| 4:D:118:LEU:O    | 4:D:122:LEU:HG   | 2.16                     | 0.46              |
| 4:H:118:LEU:O    | 4:H:122:LEU:HG   | 2.15                     | 0.46              |
| 5:M:121:GLU:O    | 5:M:122:ASP:C    | 2.58                     | 0.46              |
| 1:A:79:LEU:HD13  | 1:A:79:LEU:C     | 2.40                     | 0.46              |
| 4:D:73:VAL:O     | 4:D:74:LEU:C     | 2.59                     | 0.46              |
| 1:E:22:VAL:CG2   | 1:E:23:TRP:N     | 2.78                     | 0.46              |
| 1:E:23:TRP:NE1   | 1:E:78:LYS:HZ2   | 2.13                     | 0.46              |
| 5:M:71:GLY:HA3   | 5:M:91:ASP:OD1   | 2.15                     | 0.46              |
| 5:M:152:SER:OG   | 5:M:164:THR:HG23 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:68:GLN:OE1   | 7:O:69:CYS:N     | 2.48                     | 0.46              |
| 1:A:108:THR:HG23 | 1:A:111:TYR:CE2  | 2.50                     | 0.46              |
| 4:D:110:PHE:O    | 4:D:113:ILE:HB   | 2.15                     | 0.46              |
| 3:K:99:ALA:HA    | 3:K:147:ILE:O    | 2.16                     | 0.46              |
| 6:N:10:LEU:HD22  | 6:N:13:ARG:CB    | 2.42                     | 0.46              |
| 1:E:19:TRP:C     | 1:E:21:ASP:H     | 2.23                     | 0.46              |
| 4:L:51:ALA:HB3   | 4:L:52:PRO:HD3   | 1.97                     | 0.46              |
| 6:N:197:PHE:CD2  | 6:N:205:ALA:HB2  | 2.51                     | 0.46              |
| 1:E:28:THR:O     | 1:E:29:ASP:C     | 2.58                     | 0.46              |
| 1:E:69:HIS:O     | 1:E:70:LEU:C     | 2.59                     | 0.46              |
| 1:E:81:ILE:C     | 1:E:83:LEU:H     | 2.24                     | 0.46              |
| 2:F:85:LEU:O     | 2:F:86:LYS:C     | 2.58                     | 0.46              |
| 3:K:35:PHE:CE2   | 3:K:39:LEU:HD11  | 2.51                     | 0.46              |
| 5:M:183:LEU:O    | 5:M:184:LYS:CB   | 2.64                     | 0.46              |
| 6:N:64:LYS:O     | 6:N:65:ARG:HB2   | 2.15                     | 0.46              |
| 4:D:107:LYS:HB3  | 4:D:109:GLU:HG2  | 1.98                     | 0.46              |
| 4:H:14:SER:OG    | 4:H:15:LEU:N     | 2.49                     | 0.46              |
| 7:O:100:LEU:C    | 7:O:100:LEU:CD2  | 2.89                     | 0.46              |
| 3:C:72:LEU:O     | 3:C:73:ARG:C     | 2.59                     | 0.46              |
| 1:E:78:LYS:NZ    | 4:H:31:ARG:NH2   | 2.45                     | 0.46              |
| 3:G:45:LYS:HA    | 3:G:45:LYS:HE3   | 1.98                     | 0.46              |
| 3:G:99:ALA:HA    | 3:G:147:ILE:O    | 2.16                     | 0.46              |
| 4:L:110:PHE:O    | 4:L:113:ILE:HB   | 2.16                     | 0.46              |
| 6:N:162:VAL:CG1  | 6:N:163:THR:N    | 2.76                     | 0.46              |
| 1:A:23:TRP:NE1   | 1:A:78:LYS:HZ2   | 2.14                     | 0.46              |
| 1:A:57:LYS:HD2   | 1:A:65:GLU:HG3   | 1.98                     | 0.46              |
| 3:C:12:HIS:HB2   | 3:C:85:LEU:HD13  | 1.98                     | 0.46              |
| 4:D:18:LYS:NZ    | 4:D:82:SER:HA    | 2.31                     | 0.46              |
| 2:J:24:HIS:O     | 2:J:25:ASP:C     | 2.59                     | 0.46              |
| 2:J:28:ALA:O     | 2:J:29:PHE:C     | 2.58                     | 0.46              |
| 4:L:107:LYS:HB3  | 4:L:109:GLU:HG2  | 1.98                     | 0.46              |
| 5:M:114:LEU:HB2  | 6:N:73:GLU:HA    | 1.97                     | 0.46              |
| 5:M:149:ALA:HB3  | 5:M:180:LEU:HD13 | 1.98                     | 0.46              |
| 6:N:180:ILE:HG22 | 6:N:182:LEU:CD1  | 2.46                     | 0.46              |
| 2:F:5:GLY:H      | 2:F:8:GLU:HG3    | 1.80                     | 0.45              |
| 3:G:35:PHE:CE2   | 3:G:39:LEU:HD11  | 2.51                     | 0.45              |
| 4:H:49:ILE:C     | 4:H:51:ALA:N     | 2.73                     | 0.45              |
| 4:H:51:ALA:HB3   | 4:H:52:PRO:HD3   | 1.98                     | 0.45              |
| 4:H:107:LYS:HB3  | 4:H:109:GLU:HG2  | 1.98                     | 0.45              |
| 6:N:14:LEU:N     | 6:N:14:LEU:HD22  | 2.31                     | 0.45              |
| 6:N:147:LEU:CD2  | 6:N:171:TYR:HA   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:123:LEU:O    | 1:A:127:LEU:HD23 | 2.16                     | 0.45              |
| 4:D:49:ILE:C     | 4:D:51:ALA:N     | 2.73                     | 0.45              |
| 1:E:96:HIS:O     | 1:E:100:GLN:HG3  | 2.16                     | 0.45              |
| 3:G:12:HIS:O     | 3:G:13:ARG:C     | 2.59                     | 0.45              |
| 1:I:64:GLY:HA2   | 1:I:67:LYS:HB2   | 1.98                     | 0.45              |
| 1:I:94:LEU:HD12  | 1:I:94:LEU:HA    | 1.84                     | 0.45              |
| 6:N:133:THR:H    | 6:N:149:ALA:HA   | 1.80                     | 0.45              |
| 1:A:132:VAL:HG13 | 1:A:133:ASP:N    | 2.32                     | 0.45              |
| 3:G:9:GLU:HA     | 3:G:12:HIS:CE1   | 2.52                     | 0.45              |
| 1:I:81:ILE:C     | 1:I:83:LEU:H     | 2.24                     | 0.45              |
| 2:J:85:LEU:O     | 2:J:86:LYS:C     | 2.59                     | 0.45              |
| 6:N:10:LEU:HD23  | 6:N:12:PRO:CG    | 2.46                     | 0.45              |
| 6:N:101:ASP:CG   | 6:N:103:SER:HG   | 2.24                     | 0.45              |
| 3:C:88:PRO:N     | 3:C:89:PRO:HD2   | 2.31                     | 0.45              |
| 3:K:87:ASP:OD1   | 3:K:89:PRO:HG2   | 2.16                     | 0.45              |
| 6:N:62:CYS:HB3   | 6:N:66:THR:HB    | 1.99                     | 0.45              |
| 3:G:72:LEU:O     | 3:G:73:ARG:C     | 2.58                     | 0.45              |
| 1:I:19:TRP:C     | 1:I:21:ASP:H     | 2.24                     | 0.45              |
| 1:I:23:TRP:CH2   | 1:I:74:ALA:HB1   | 2.51                     | 0.45              |
| 7:O:93:GLU:C     | 7:O:95:GLU:N     | 2.73                     | 0.45              |
| 1:E:128:SER:O    | 1:E:129:CYS:HB2  | 2.16                     | 0.45              |
| 1:I:69:HIS:O     | 1:I:70:LEU:C     | 2.60                     | 0.45              |
| 4:L:75:SER:O     | 4:L:78:ASP:HB3   | 2.17                     | 0.45              |
| 4:H:17:VAL:HG13  | 4:H:135:TRP:CE2  | 2.52                     | 0.45              |
| 4:L:111:PHE:N    | 4:L:111:PHE:CD1  | 2.85                     | 0.45              |
| 5:M:176:ARG:HG2  | 5:M:176:ARG:HH11 | 1.82                     | 0.45              |
| 5:M:187:SER:O    | 5:M:188:GLU:C    | 2.60                     | 0.45              |
| 1:E:108:THR:H    | 1:E:111:TYR:HD2  | 1.63                     | 0.45              |
| 3:G:96:ASP:O     | 3:G:99:ALA:HB3   | 2.17                     | 0.45              |
| 3:K:129:ASP:OD2  | 3:K:129:ASP:N    | 2.37                     | 0.45              |
| 5:M:12:TYR:CD2   | 5:M:12:TYR:N     | 2.85                     | 0.45              |
| 5:M:219:HIS:ND1  | 5:M:219:HIS:C    | 2.75                     | 0.45              |
| 3:C:10:GLU:CD    | 1:I:13:ARG:HH22  | 2.25                     | 0.45              |
| 3:C:32:LYS:HG2   | 3:C:75:LEU:HD12  | 1.99                     | 0.45              |
| 4:D:10:LEU:HG    | 4:D:13:GLU:OE1   | 2.16                     | 0.45              |
| 1:E:123:LEU:HA   | 1:E:126:VAL:CG2  | 2.47                     | 0.45              |
| 5:M:196:PHE:C    | 5:M:198:LEU:H    | 2.25                     | 0.45              |
| 6:N:82:VAL:CG1   | 6:N:83:CYS:H     | 2.22                     | 0.45              |
| 6:N:84:ASP:HA    | 6:N:142:THR:OG1  | 2.16                     | 0.45              |
| 1:A:15:ILE:CD1   | 1:A:138:CYS:HB2  | 2.46                     | 0.44              |
| 1:A:131:ASN:C    | 1:A:131:ASN:HD22 | 2.25                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:111:PHE:HB3  | 4:D:143:ILE:HG23 | 1.98                     | 0.44              |
| 1:E:79:LEU:HD13  | 1:E:79:LEU:O     | 2.15                     | 0.44              |
| 4:H:111:PHE:CD1  | 4:H:111:PHE:N    | 2.85                     | 0.44              |
| 2:J:102:PRO:C    | 2:J:104:ASN:H    | 2.26                     | 0.44              |
| 7:O:161:VAL:CG1  | 7:O:163:MET:HG3  | 2.46                     | 0.44              |
| 1:A:108:THR:H    | 1:A:111:TYR:HD2  | 1.65                     | 0.44              |
| 2:B:92:LEU:O     | 2:B:93:GLN:C     | 2.58                     | 0.44              |
| 2:F:130:TRP:O    | 2:F:131:ASP:C    | 2.59                     | 0.44              |
| 1:I:14:GLU:CD    | 7:O:208:LEU:CD1  | 2.83                     | 0.44              |
| 2:J:84:THR:O     | 2:J:85:LEU:C     | 2.61                     | 0.44              |
| 3:K:148:SER:O    | 3:K:150:ARG:N    | 2.50                     | 0.44              |
| 6:N:70:GLY:N     | 6:N:91:ASN:HD21  | 2.15                     | 0.44              |
| 1:A:81:ILE:C     | 1:A:83:LEU:H     | 2.24                     | 0.44              |
| 1:A:123:LEU:HA   | 1:A:126:VAL:CG2  | 2.47                     | 0.44              |
| 3:C:148:SER:O    | 3:C:150:ARG:N    | 2.50                     | 0.44              |
| 1:I:60:GLU:O     | 1:I:63:SER:HB3   | 2.17                     | 0.44              |
| 3:K:70:HIS:O     | 3:K:74:ILE:HG22  | 2.16                     | 0.44              |
| 4:H:17:VAL:HG13  | 4:H:135:TRP:CZ2  | 2.53                     | 0.44              |
| 4:L:10:LEU:HD13  | 4:L:12:THR:H     | 1.82                     | 0.44              |
| 5:M:210:VAL:CG1  | 5:M:215:PHE:HB3  | 2.48                     | 0.44              |
| 6:N:147:LEU:HD23 | 6:N:171:TYR:HA   | 1.99                     | 0.44              |
| 4:D:10:LEU:HD11  | 4:D:13:GLU:H     | 1.83                     | 0.44              |
| 1:E:86:ASP:O     | 1:E:87:THR:C     | 2.61                     | 0.44              |
| 1:I:22:VAL:CG2   | 1:I:23:TRP:N     | 2.80                     | 0.44              |
| 4:L:17:VAL:HG13  | 4:L:135:TRP:CZ2  | 2.52                     | 0.44              |
| 4:L:134:ALA:O    | 4:L:138:CYS:HB2  | 2.18                     | 0.44              |
| 5:M:114:LEU:CB   | 6:N:73:GLU:HA    | 2.48                     | 0.44              |
| 5:M:132:ILE:HD13 | 5:M:149:ALA:HB2  | 1.99                     | 0.44              |
| 5:M:224:ARG:C    | 5:M:225:TYR:CD2  | 2.96                     | 0.44              |
| 6:N:29:GLU:O     | 6:N:32:ARG:HB2   | 2.18                     | 0.44              |
| 1:A:86:ASP:O     | 1:A:87:THR:C     | 2.61                     | 0.44              |
| 1:E:19:TRP:C     | 1:E:21:ASP:N     | 2.76                     | 0.44              |
| 1:E:131:ASN:C    | 1:E:131:ASN:HD22 | 2.25                     | 0.44              |
| 3:G:87:ASP:OD1   | 3:G:89:PRO:HG2   | 2.17                     | 0.44              |
| 4:H:60:ASN:HD21  | 4:L:133:GLY:H    | 1.63                     | 0.44              |
| 3:K:32:LYS:HG2   | 3:K:75:LEU:HD12  | 2.00                     | 0.44              |
| 3:K:150:ARG:O    | 3:K:151:LEU:HG   | 2.18                     | 0.44              |
| 1:A:19:TRP:C     | 1:A:21:ASP:N     | 2.75                     | 0.44              |
| 4:D:17:VAL:HG13  | 4:D:135:TRP:CE2  | 2.53                     | 0.44              |
| 1:E:123:LEU:O    | 1:E:127:LEU:HD23 | 2.18                     | 0.44              |
| 6:N:153:SER:O    | 6:N:155:LEU:HD22 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:24:ILE:C     | 7:O:26:THR:N     | 2.75                     | 0.44              |
| 1:A:15:ILE:O     | 1:A:17:HIS:N     | 2.51                     | 0.44              |
| 3:C:31:ILE:O     | 3:C:32:LYS:C     | 2.60                     | 0.44              |
| 4:D:31:ARG:HB3   | 4:D:71:GLN:HE22  | 1.83                     | 0.44              |
| 4:D:114:PHE:CZ   | 9:D:160:HEM:HAB  | 2.53                     | 0.44              |
| 4:H:10:LEU:HG    | 4:H:13:GLU:OE1   | 2.18                     | 0.44              |
| 3:K:113:PHE:O    | 3:K:114:LYS:C    | 2.60                     | 0.44              |
| 3:C:129:ASP:CA   | 4:D:16:LYS:HE3   | 2.48                     | 0.44              |
| 4:D:75:SER:O     | 4:D:78:ASP:HB3   | 2.18                     | 0.44              |
| 4:D:111:PHE:CD1  | 4:D:111:PHE:N    | 2.86                     | 0.44              |
| 1:E:79:LEU:HD13  | 1:E:79:LEU:C     | 2.43                     | 0.44              |
| 1:A:80:LEU:HD22  | 1:A:94:LEU:HD13  | 2.00                     | 0.43              |
| 1:A:147:ALA:CB   | 1:A:150:LEU:HD12 | 2.48                     | 0.43              |
| 3:K:95:LEU:HD21  | 3:K:143:ILE:HG23 | 2.00                     | 0.43              |
| 4:L:10:LEU:HG    | 4:L:13:GLU:OE1   | 2.18                     | 0.43              |
| 6:N:186:ASP:C    | 6:N:188:ASP:H    | 2.26                     | 0.43              |
| 1:A:22:VAL:CG2   | 1:A:23:TRP:N     | 2.81                     | 0.43              |
| 2:B:130:TRP:O    | 2:B:131:ASP:C    | 2.59                     | 0.43              |
| 2:F:73:ASP:O     | 2:F:74:ILE:C     | 2.59                     | 0.43              |
| 4:H:18:LYS:NZ    | 4:H:82:SER:HA    | 2.33                     | 0.43              |
| 4:H:79:ILE:O     | 4:H:80:THR:C     | 2.61                     | 0.43              |
| 1:I:15:ILE:O     | 1:I:17:HIS:N     | 2.50                     | 0.43              |
| 2:J:130:TRP:O    | 2:J:131:ASP:C    | 2.61                     | 0.43              |
| 3:K:12:HIS:O     | 3:K:13:ARG:C     | 2.58                     | 0.43              |
| 6:N:104:VAL:HG22 | 6:N:202:ASN:HD22 | 1.83                     | 0.43              |
| 6:N:173:ASN:C    | 6:N:173:ASN:HD22 | 2.27                     | 0.43              |
| 2:F:74:ILE:HG23  | 3:G:72:LEU:CD1   | 2.45                     | 0.43              |
| 2:J:102:PRO:C    | 2:J:104:ASN:N    | 2.72                     | 0.43              |
| 5:M:147:LEU:HD12 | 5:M:169:GLY:O    | 2.18                     | 0.43              |
| 6:N:162:VAL:CG1  | 6:N:163:THR:H    | 2.28                     | 0.43              |
| 2:B:102:PRO:C    | 2:B:104:ASN:H    | 2.25                     | 0.43              |
| 4:H:75:SER:O     | 4:H:78:ASP:HB3   | 2.19                     | 0.43              |
| 1:I:19:TRP:C     | 1:I:21:ASP:N     | 2.75                     | 0.43              |
| 1:I:57:LYS:HD2   | 1:I:65:GLU:HG3   | 1.99                     | 0.43              |
| 3:K:45:LYS:HE3   | 3:K:45:LYS:HA    | 1.99                     | 0.43              |
| 3:K:88:PRO:HG2   | 3:K:89:PRO:CD    | 2.48                     | 0.43              |
| 1:A:64:GLY:HA2   | 1:A:67:LYS:HB2   | 2.00                     | 0.43              |
| 4:D:114:PHE:CE2  | 9:D:160:HEM:HAB  | 2.53                     | 0.43              |
| 1:E:60:GLU:CB    | 1:E:63:SER:HB3   | 2.49                     | 0.43              |
| 1:I:131:ASN:C    | 1:I:131:ASN:HD22 | 2.25                     | 0.43              |
| 3:K:70:HIS:O     | 3:K:71:ALA:C     | 2.61                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:66:GLU:HG3   | 5:M:78:HIS:HA    | 2.00                     | 0.43              |
| 5:M:114:LEU:HD12 | 5:M:126:ASP:C    | 2.42                     | 0.43              |
| 7:O:45:ARG:HG3   | 7:O:46:LYS:N     | 2.34                     | 0.43              |
| 1:A:55:ARG:HD2   | 1:A:55:ARG:O     | 2.19                     | 0.43              |
| 2:B:73:ASP:O     | 2:B:74:ILE:C     | 2.61                     | 0.43              |
| 4:D:106:LEU:HD22 | 9:D:160:HEM:HBC2 | 2.00                     | 0.43              |
| 4:H:114:PHE:CE2  | 9:H:160:HEM:HAB  | 2.54                     | 0.43              |
| 1:I:143:VAL:O    | 1:I:144:ALA:C    | 2.62                     | 0.43              |
| 6:N:20:LEU:HD23  | 6:N:20:LEU:O     | 2.19                     | 0.43              |
| 6:N:207:CYS:HB2  | 6:N:221:LEU:HB3  | 2.00                     | 0.43              |
| 7:O:102:THR:HG22 | 7:O:108:PHE:CE2  | 2.53                     | 0.43              |
| 1:E:15:ILE:CD1   | 1:E:138:CYS:HB2  | 2.48                     | 0.43              |
| 1:I:96:HIS:O     | 1:I:100:GLN:HG3  | 2.18                     | 0.43              |
| 6:N:47:VAL:CG1   | 6:N:48:SER:N     | 2.81                     | 0.43              |
| 6:N:176:SER:HB2  | 6:N:178:ARG:HG3  | 2.01                     | 0.43              |
| 1:A:23:TRP:HZ3   | 1:A:74:ALA:HB1   | 1.81                     | 0.43              |
| 1:A:72:ARG:HD2   | 4:D:93:GLN:OE1   | 2.18                     | 0.43              |
| 1:A:128:SER:O    | 1:A:129:CYS:HB2  | 2.19                     | 0.43              |
| 4:H:49:ILE:C     | 4:H:51:ALA:H     | 2.27                     | 0.43              |
| 1:I:80:LEU:HD22  | 1:I:94:LEU:HD13  | 2.00                     | 0.43              |
| 1:I:136:ASN:HD22 | 1:I:136:ASN:HA   | 1.56                     | 0.43              |
| 5:M:182:PRO:HD2  | 5:M:211:PRO:HB3  | 2.01                     | 0.43              |
| 7:O:52:HIS:O     | 7:O:53:ARG:C     | 2.62                     | 0.43              |
| 2:B:24:HIS:O     | 2:B:25:ASP:C     | 2.61                     | 0.43              |
| 3:G:148:SER:O    | 3:G:150:ARG:N    | 2.51                     | 0.43              |
| 3:G:150:ARG:O    | 3:G:151:LEU:HG   | 2.19                     | 0.43              |
| 1:I:79:LEU:HD21  | 4:L:71:GLN:HG3   | 2.01                     | 0.43              |
| 1:I:86:ASP:O     | 1:I:87:THR:C     | 2.62                     | 0.43              |
| 1:I:108:THR:H    | 1:I:111:TYR:HD2  | 1.65                     | 0.43              |
| 6:N:53:ARG:NH1   | 7:O:58:GLU:OE2   | 2.52                     | 0.43              |
| 6:N:82:VAL:CB    | 6:N:175:ALA:HB2  | 2.49                     | 0.43              |
| 1:A:136:ASN:HD22 | 1:A:136:ASN:HA   | 1.56                     | 0.43              |
| 4:D:31:ARG:O     | 4:D:32:VAL:C     | 2.60                     | 0.43              |
| 2:J:73:ASP:O     | 2:J:74:ILE:C     | 2.62                     | 0.43              |
| 2:J:92:LEU:O     | 2:J:93:GLN:C     | 2.61                     | 0.43              |
| 5:M:146:TRP:CD1  | 5:M:146:TRP:H    | 2.36                     | 0.43              |
| 5:M:196:PHE:CD2  | 5:M:204:ALA:HB2  | 2.54                     | 0.43              |
| 6:N:128:THR:HB   | 6:N:221:LEU:HD11 | 2.01                     | 0.43              |
| 6:N:160:GLU:HB3  | 6:N:161:ASN:H    | 1.73                     | 0.43              |
| 1:E:142:LEU:O    | 1:E:146:ILE:HG13 | 2.18                     | 0.42              |
| 4:H:10:LEU:HD13  | 4:H:12:THR:H     | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:80:THR:O     | 4:H:84:LEU:HD13  | 2.19                     | 0.42              |
| 1:I:128:SER:O    | 1:I:129:CYS:HB2  | 2.19                     | 0.42              |
| 4:L:57:ARG:HG2   | 4:L:57:ARG:NH1   | 2.32                     | 0.42              |
| 4:L:114:PHE:CZ   | 9:L:160:HEM:HAB  | 2.54                     | 0.42              |
| 6:N:194:VAL:O    | 6:N:207:CYS:HA   | 2.19                     | 0.42              |
| 7:O:161:VAL:HG12 | 7:O:162:SER:N    | 2.34                     | 0.42              |
| 1:A:49:SER:O     | 1:A:50:LYS:C     | 2.62                     | 0.42              |
| 2:B:76:ILE:C     | 2:B:78:THR:H     | 2.27                     | 0.42              |
| 4:H:106:LEU:HD22 | 9:H:160:HEM:HBC2 | 2.01                     | 0.42              |
| 4:L:118:LEU:O    | 4:L:122:LEU:HG   | 2.18                     | 0.42              |
| 7:O:31:VAL:C     | 7:O:33:SER:N     | 2.76                     | 0.42              |
| 7:O:129:PHE:HE2  | 7:O:144:LEU:HD13 | 1.84                     | 0.42              |
| 7:O:209:SER:HB3  | 7:O:211:GLU:CG   | 2.39                     | 0.42              |
| 3:C:14:ILE:O     | 3:C:15:VAL:C     | 2.60                     | 0.42              |
| 2:F:75:ALA:HB1   | 2:F:137:ILE:HD13 | 2.02                     | 0.42              |
| 3:G:12:HIS:HB2   | 3:G:85:LEU:HD13  | 1.99                     | 0.42              |
| 5:M:38:LEU:HD22  | 7:O:38:ARG:NH1   | 2.26                     | 0.42              |
| 5:M:80:LEU:HA    | 5:M:143:ASN:ND2  | 2.35                     | 0.42              |
| 7:O:67:HIS:HB3   | 7:O:77:ILE:HD12  | 2.01                     | 0.42              |
| 2:B:123:ARG:HH21 | 5:M:214:LEU:HG   | 1.84                     | 0.42              |
| 3:C:113:PHE:O    | 3:C:114:LYS:C    | 2.62                     | 0.42              |
| 1:E:22:VAL:HG23  | 1:E:23:TRP:N     | 2.34                     | 0.42              |
| 1:E:55:ARG:HD2   | 1:E:55:ARG:O     | 2.19                     | 0.42              |
| 3:G:95:LEU:HD21  | 3:G:143:ILE:HG23 | 2.01                     | 0.42              |
| 5:M:90:ARG:NH1   | 7:O:113:CYS:HA   | 2.35                     | 0.42              |
| 5:M:172:ASN:ND2  | 5:M:174:GLY:H    | 2.17                     | 0.42              |
| 1:E:19:TRP:O     | 1:E:21:ASP:N     | 2.52                     | 0.42              |
| 2:F:24:HIS:O     | 2:F:25:ASP:C     | 2.61                     | 0.42              |
| 4:L:18:LYS:NZ    | 4:L:82:SER:HA    | 2.34                     | 0.42              |
| 5:M:131:THR:HG23 | 5:M:150:THR:OG1  | 2.20                     | 0.42              |
| 6:N:155:LEU:HD23 | 6:N:155:LEU:O    | 2.19                     | 0.42              |
| 1:A:19:TRP:O     | 1:A:21:ASP:N     | 2.53                     | 0.42              |
| 1:A:118:ALA:O    | 1:A:122:VAL:HG23 | 2.20                     | 0.42              |
| 2:B:8:GLU:O      | 2:B:12:VAL:HG23  | 2.20                     | 0.42              |
| 3:C:45:LYS:HE3   | 3:C:45:LYS:HA    | 2.00                     | 0.42              |
| 1:I:123:LEU:HA   | 1:I:126:VAL:CG2  | 2.48                     | 0.42              |
| 4:L:81:ILE:HA    | 4:L:84:LEU:HD13  | 2.01                     | 0.42              |
| 4:L:114:PHE:CE2  | 9:L:160:HEM:HAB  | 2.54                     | 0.42              |
| 6:N:151:VAL:HB   | 6:N:166:PHE:CE2  | 2.55                     | 0.42              |
| 1:A:60:GLU:CB    | 1:A:63:SER:HB3   | 2.49                     | 0.42              |
| 2:B:58:HIS:CE1   | 2:B:59:PRO:HG2   | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:12:HIS:O     | 3:C:13:ARG:C     | 2.60                     | 0.42              |
| 3:K:14:ILE:O     | 3:K:15:VAL:C     | 2.62                     | 0.42              |
| 4:L:49:ILE:C     | 4:L:51:ALA:N     | 2.76                     | 0.42              |
| 4:L:83:MET:CE    | 4:L:89:MET:HB3   | 2.25                     | 0.42              |
| 5:M:49:GLN:HE21  | 5:M:49:GLN:HB2   | 1.65                     | 0.42              |
| 5:M:75:GLU:OE1   | 5:M:90:ARG:HB2   | 2.20                     | 0.42              |
| 1:A:109:LYS:HB2  | 1:A:151:PRO:HD3  | 2.01                     | 0.42              |
| 4:D:107:LYS:HD2  | 4:D:107:LYS:N    | 2.34                     | 0.42              |
| 2:F:92:LEU:O     | 2:F:93:GLN:C     | 2.60                     | 0.42              |
| 3:G:14:ILE:O     | 3:G:15:VAL:C     | 2.62                     | 0.42              |
| 4:H:31:ARG:O     | 4:H:32:VAL:C     | 2.63                     | 0.42              |
| 4:L:10:LEU:HD12  | 4:L:13:GLU:H     | 1.85                     | 0.42              |
| 7:O:101:PRO:HB3  | 7:O:197:PHE:CD2  | 2.55                     | 0.42              |
| 1:A:82:ASN:ND2   | 4:D:31:ARG:CZ    | 2.82                     | 0.42              |
| 1:A:112:PHE:O    | 1:A:115:ILE:HG22 | 2.20                     | 0.42              |
| 3:C:88:PRO:HG2   | 3:C:89:PRO:CD    | 2.49                     | 0.42              |
| 4:D:10:LEU:HD13  | 4:D:12:THR:H     | 1.84                     | 0.42              |
| 4:D:49:ILE:C     | 4:D:51:ALA:H     | 2.27                     | 0.42              |
| 4:D:117:HIS:O    | 4:D:118:LEU:C    | 2.63                     | 0.42              |
| 2:F:70:GLY:O     | 2:F:73:ASP:HB3   | 2.20                     | 0.42              |
| 4:H:10:LEU:HD11  | 4:H:13:GLU:H     | 1.84                     | 0.42              |
| 1:I:60:GLU:CB    | 1:I:63:SER:HB3   | 2.50                     | 0.42              |
| 3:K:85:LEU:HA    | 3:K:91:LEU:HD22  | 2.02                     | 0.42              |
| 6:N:92:ALA:C     | 6:N:94:ASP:N     | 2.78                     | 0.42              |
| 6:N:112:SER:O    | 6:N:223:VAL:HA   | 2.20                     | 0.42              |
| 1:E:63:SER:OG    | 1:E:66:PHE:HB3   | 2.20                     | 0.42              |
| 2:F:84:THR:O     | 2:F:85:LEU:C     | 2.61                     | 0.42              |
| 3:G:70:HIS:O     | 3:G:71:ALA:C     | 2.63                     | 0.42              |
| 1:I:19:TRP:O     | 1:I:21:ASP:N     | 2.53                     | 0.42              |
| 1:I:147:ALA:CB   | 1:I:150:LEU:HD12 | 2.49                     | 0.42              |
| 5:M:119:SER:C    | 5:M:120:CYS:SG   | 3.03                     | 0.42              |
| 5:M:155:LEU:HD13 | 5:M:155:LEU:HA   | 1.91                     | 0.42              |
| 6:N:170:GLY:HA3  | 6:N:180:ILE:O    | 2.19                     | 0.42              |
| 3:C:20:ASP:C     | 3:C:22:LEU:N     | 2.78                     | 0.41              |
| 3:G:85:LEU:HA    | 3:G:91:LEU:HD22  | 2.02                     | 0.41              |
| 2:J:70:GLY:O     | 2:J:73:ASP:HB3   | 2.20                     | 0.41              |
| 5:M:183:LEU:HB2  | 5:M:186:GLN:NE2  | 2.35                     | 0.41              |
| 6:N:173:ASN:HD22 | 6:N:174:PHE:N    | 2.18                     | 0.41              |
| 7:O:48:GLY:O     | 7:O:51:ARG:HB3   | 2.20                     | 0.41              |
| 3:C:134:LEU:HD23 | 3:C:134:LEU:HA   | 1.92                     | 0.41              |
| 4:D:60:ASN:ND2   | 4:H:132:PHE:HB3  | 2.35                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:H:83:MET:CE   | 4:H:89:MET:HB3   | 2.26                     | 0.41              |
| 4:H:134:ALA:O   | 4:H:138:CYS:HB2  | 2.20                     | 0.41              |
| 4:L:73:VAL:O    | 4:L:74:LEU:C     | 2.63                     | 0.41              |
| 5:M:18:ASN:HD21 | 7:O:17:LEU:CB    | 2.33                     | 0.41              |
| 1:A:122:VAL:C   | 1:A:124:PRO:HD2  | 2.45                     | 0.41              |
| 4:D:19:LEU:O    | 4:D:22:ALA:HB3   | 2.20                     | 0.41              |
| 4:D:134:ALA:O   | 4:D:138:CYS:HB2  | 2.20                     | 0.41              |
| 3:G:63:GLU:H    | 3:G:63:GLU:CD    | 2.28                     | 0.41              |
| 3:G:109:GLN:O   | 3:G:112:HIS:HB2  | 2.20                     | 0.41              |
| 7:O:92:GLY:O    | 7:O:93:GLU:C     | 2.62                     | 0.41              |
| 2:F:76:ILE:C    | 2:F:78:THR:H     | 2.29                     | 0.41              |
| 4:L:14:SER:O    | 4:L:17:VAL:N     | 2.53                     | 0.41              |
| 6:N:19:PHE:C    | 6:N:22:ILE:HG22  | 2.45                     | 0.41              |
| 6:N:177:ARG:NH1 | 6:N:177:ARG:HG2  | 2.35                     | 0.41              |
| 7:O:83:CYS:O    | 7:O:139:THR:HB   | 2.20                     | 0.41              |
| 7:O:102:THR:HB  | 7:O:129:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:28:THR:O    | 1:A:29:ASP:C     | 2.62                     | 0.41              |
| 2:B:7:LEU:C     | 2:B:9:GLY:N      | 2.78                     | 0.41              |
| 2:B:87:GLU:OE2  | 3:C:66:LYS:HE3   | 2.20                     | 0.41              |
| 3:C:95:LEU:HD21 | 3:C:143:ILE:HG23 | 2.02                     | 0.41              |
| 4:D:125:ARG:HG2 | 4:D:125:ARG:NH1  | 2.34                     | 0.41              |
| 1:E:57:LYS:HD2  | 1:E:65:GLU:HG3   | 2.00                     | 0.41              |
| 1:E:122:VAL:C   | 1:E:124:PRO:HD2  | 2.45                     | 0.41              |
| 1:I:131:ASN:O   | 1:I:132:VAL:C    | 2.64                     | 0.41              |
| 6:N:155:LEU:H   | 6:N:155:LEU:CD2  | 2.33                     | 0.41              |
| 7:O:94:ASP:N    | 7:O:94:ASP:OD2   | 2.53                     | 0.41              |
| 1:A:13:ARG:NH2  | 3:G:10:GLU:CD    | 2.77                     | 0.41              |
| 4:H:14:SER:O    | 4:H:15:LEU:C     | 2.64                     | 0.41              |
| 4:H:19:LEU:O    | 4:H:22:ALA:HB3   | 2.21                     | 0.41              |
| 4:L:10:LEU:HD11 | 4:L:13:GLU:H     | 1.83                     | 0.41              |
| 6:N:64:LYS:HB3  | 6:N:64:LYS:NZ    | 2.35                     | 0.41              |
| 3:C:70:HIS:O    | 3:C:71:ALA:C     | 2.64                     | 0.41              |
| 4:D:17:VAL:HG13 | 4:D:135:TRP:CZ2  | 2.55                     | 0.41              |
| 4:H:69:HIS:O    | 4:H:70:SER:C     | 2.62                     | 0.41              |
| 4:H:114:PHE:CZ  | 9:H:160:HEM:HAB  | 2.55                     | 0.41              |
| 6:N:68:GLN:OE1  | 6:N:69:CYS:N     | 2.54                     | 0.41              |
| 1:A:50:LYS:HG2  | 1:A:58:ILE:HD12  | 2.02                     | 0.41              |
| 4:D:57:ARG:HG2  | 4:D:57:ARG:NH1   | 2.35                     | 0.41              |
| 4:D:81:ILE:HA   | 4:D:84:LEU:HD13  | 2.03                     | 0.41              |
| 1:E:83:LEU:HD11 | 4:H:71:GLN:HG2   | 2.03                     | 0.41              |
| 1:I:49:SER:O    | 1:I:50:LYS:C     | 2.64                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:63:SER:OG    | 1:I:66:PHE:HB3   | 2.20                     | 0.41              |
| 1:I:109:LYS:HB2  | 1:I:151:PRO:HD3  | 2.02                     | 0.41              |
| 2:B:70:GLY:O     | 2:B:73:ASP:HB3   | 2.21                     | 0.41              |
| 3:C:53:LEU:HD21  | 3:C:107:GLY:HA3  | 2.03                     | 0.41              |
| 4:D:69:HIS:O     | 4:D:70:SER:C     | 2.63                     | 0.41              |
| 1:E:17:HIS:O     | 1:E:18:ILE:C     | 2.64                     | 0.41              |
| 1:E:50:LYS:HG2   | 1:E:58:ILE:HD12  | 2.02                     | 0.41              |
| 4:H:57:ARG:HG2   | 4:H:57:ARG:NH1   | 2.36                     | 0.41              |
| 4:H:111:PHE:HD1  | 4:H:111:PHE:H    | 1.69                     | 0.41              |
| 1:I:15:ILE:CD1   | 1:I:138:CYS:HB2  | 2.51                     | 0.41              |
| 1:I:88:LEU:HD23  | 1:I:88:LEU:HA    | 1.92                     | 0.41              |
| 1:I:123:LEU:O    | 1:I:127:LEU:HD23 | 2.20                     | 0.41              |
| 2:J:76:ILE:C     | 2:J:78:THR:H     | 2.28                     | 0.41              |
| 3:K:40:LEU:O     | 3:K:43:LEU:HB3   | 2.21                     | 0.41              |
| 4:L:31:ARG:HB3   | 4:L:71:GLN:HE22  | 1.85                     | 0.41              |
| 4:L:34:PHE:CD1   | 4:L:34:PHE:C     | 2.99                     | 0.41              |
| 4:L:106:LEU:HD22 | 9:L:160:HEM:HBC2 | 2.02                     | 0.41              |
| 4:L:111:PHE:HD1  | 4:L:111:PHE:H    | 1.68                     | 0.41              |
| 6:N:66:THR:HG22  | 6:N:67:PHE:N     | 2.36                     | 0.41              |
| 6:N:209:ARG:HA   | 6:N:209:ARG:HD2  | 1.78                     | 0.41              |
| 1:A:88:LEU:HD23  | 1:A:88:LEU:HA    | 1.93                     | 0.41              |
| 1:A:97:LEU:HD23  | 1:A:146:ILE:CD1  | 2.50                     | 0.41              |
| 4:H:25:PHE:CE2   | 4:H:31:ARG:NE    | 2.89                     | 0.41              |
| 2:J:134:ILE:HD13 | 2:J:134:ILE:HA   | 1.97                     | 0.41              |
| 5:M:28:LEU:C     | 5:M:28:LEU:CD2   | 2.93                     | 0.41              |
| 7:O:209:SER:O    | 7:O:210:GLU:HB3  | 2.20                     | 0.41              |
| 1:A:16:ARG:NH2   | 1:A:85:ASP:CG    | 2.79                     | 0.40              |
| 1:A:63:SER:OG    | 1:A:66:PHE:HB3   | 2.21                     | 0.40              |
| 2:F:68:VAL:O     | 2:F:69:LEU:C     | 2.63                     | 0.40              |
| 2:F:111:THR:O    | 2:F:112:ALA:C    | 2.64                     | 0.40              |
| 4:H:73:VAL:O     | 4:H:74:LEU:C     | 2.64                     | 0.40              |
| 4:H:107:LYS:HD2  | 4:H:107:LYS:N    | 2.35                     | 0.40              |
| 3:K:109:GLN:O    | 3:K:112:HIS:HB2  | 2.21                     | 0.40              |
| 1:A:112:PHE:C    | 1:A:114:GLY:N    | 2.76                     | 0.40              |
| 3:C:150:ARG:O    | 3:C:151:LEU:HG   | 2.20                     | 0.40              |
| 4:D:79:ILE:O     | 4:D:80:THR:C     | 2.63                     | 0.40              |
| 1:E:64:GLY:HA2   | 1:E:67:LYS:HB2   | 2.02                     | 0.40              |
| 1:E:112:PHE:C    | 1:E:114:GLY:N    | 2.77                     | 0.40              |
| 2:F:127:ARG:O    | 2:F:128:GLU:C    | 2.64                     | 0.40              |
| 4:L:12:THR:C     | 4:L:14:SER:N     | 2.78                     | 0.40              |
| 4:L:31:ARG:O     | 4:L:32:VAL:C     | 2.65                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:L:49:ILE:C    | 4:L:51:ALA:H     | 2.29                     | 0.40              |
| 5:M:130:VAL:O   | 5:M:130:VAL:CG1  | 2.68                     | 0.40              |
| 6:N:145:ILE:HB  | 6:N:172:TYR:HB3  | 2.03                     | 0.40              |
| 6:N:147:LEU:N   | 6:N:147:LEU:CD2  | 2.83                     | 0.40              |
| 1:E:125:GLN:O   | 2:F:11:LYS:HE3   | 2.21                     | 0.40              |
| 1:I:78:LYS:HZ3  | 4:L:31:ARG:HH22  | 1.67                     | 0.40              |
| 2:J:105:TYR:O   | 2:J:106:PHE:C    | 2.64                     | 0.40              |
| 5:M:140:PHE:C   | 5:M:142:PRO:HD3  | 2.47                     | 0.40              |
| 6:N:19:PHE:HA   | 6:N:22:ILE:HG22  | 2.03                     | 0.40              |
| 6:N:69:CYS:O    | 6:N:70:GLY:C     | 2.64                     | 0.40              |
| 6:N:72:ASN:C    | 6:N:72:ASN:ND2   | 2.78                     | 0.40              |
| 7:O:39:LEU:O    | 7:O:40:ASP:C     | 2.64                     | 0.40              |
| 7:O:170:SER:OG  | 7:O:172:ALA:HB3  | 2.20                     | 0.40              |
| 1:E:49:SER:HB3  | 1:E:111:TYR:CD1  | 2.56                     | 0.40              |
| 1:E:104:ARG:HG2 | 1:E:104:ARG:HH11 | 1.86                     | 0.40              |
| 1:I:50:LYS:HG2  | 1:I:58:ILE:HD12  | 2.03                     | 0.40              |
| 1:I:123:LEU:C   | 1:I:125:GLN:H    | 2.28                     | 0.40              |
| 4:L:79:ILE:O    | 4:L:80:THR:C     | 2.63                     | 0.40              |
| 5:M:35:TYR:O    | 5:M:38:LEU:HB2   | 2.21                     | 0.40              |
| 3:C:40:LEU:O    | 3:C:43:LEU:HB3   | 2.21                     | 0.40              |
| 3:C:40:LEU:HD22 | 3:C:54:PHE:CE1   | 2.57                     | 0.40              |
| 4:D:12:THR:C    | 4:D:14:SER:N     | 2.79                     | 0.40              |
| 2:J:7:LEU:C     | 2:J:9:GLY:N      | 2.79                     | 0.40              |
| 2:J:58:HIS:CE1  | 2:J:59:PRO:HG2   | 2.57                     | 0.40              |
| 5:M:53:ARG:HG3  | 5:M:53:ARG:HH11  | 1.87                     | 0.40              |
| 5:M:66:GLU:HG2  | 5:M:77:ILE:C     | 2.46                     | 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     | 145/151 (96%)   | 119 (82%)  | 22 (15%)  | 4 (3%)   | 4           | 26 |
| 1   | E     | 145/151 (96%)   | 119 (82%)  | 22 (15%)  | 4 (3%)   | 4           | 26 |
| 1   | I     | 145/151 (96%)   | 120 (83%)  | 21 (14%)  | 4 (3%)   | 4           | 26 |
| 2   | B     | 143/145 (99%)   | 118 (82%)  | 24 (17%)  | 1 (1%)   | 18          | 51 |
| 2   | F     | 143/145 (99%)   | 120 (84%)  | 22 (15%)  | 1 (1%)   | 18          | 51 |
| 2   | J     | 143/145 (99%)   | 123 (86%)  | 18 (13%)  | 2 (1%)   | 9           | 38 |
| 3   | C     | 147/153 (96%)   | 122 (83%)  | 23 (16%)  | 2 (1%)   | 9           | 38 |
| 3   | G     | 147/153 (96%)   | 124 (84%)  | 21 (14%)  | 2 (1%)   | 9           | 38 |
| 3   | K     | 147/153 (96%)   | 124 (84%)  | 21 (14%)  | 2 (1%)   | 9           | 38 |
| 4   | D     | 138/140 (99%)   | 114 (83%)  | 21 (15%)  | 3 (2%)   | 5           | 30 |
| 4   | H     | 138/140 (99%)   | 114 (83%)  | 21 (15%)  | 3 (2%)   | 5           | 30 |
| 4   | L     | 138/140 (99%)   | 113 (82%)  | 23 (17%)  | 2 (1%)   | 9           | 38 |
| 5   | M     | 215/217 (99%)   | 178 (83%)  | 29 (14%)  | 8 (4%)   | 2           | 21 |
| 6   | N     | 218/220 (99%)   | 177 (81%)  | 28 (13%)  | 13 (6%)  | 1           | 12 |
| 7   | O     | 213/215 (99%)   | 171 (80%)  | 37 (17%)  | 5 (2%)   | 5           | 30 |
| All | All   | 2365/2419 (98%) | 1956 (83%) | 353 (15%) | 56 (2%)  | 4           | 29 |

All (56) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | THR  |
| 1   | E     | 29  | ASP  |
| 1   | E     | 87  | THR  |
| 1   | I     | 87  | THR  |
| 5   | M     | 123 | LEU  |
| 6   | N     | 82  | VAL  |
| 1   | A     | 29  | ASP  |
| 3   | C     | 149 | SER  |
| 3   | G     | 149 | SER  |
| 1   | I     | 29  | ASP  |
| 3   | K     | 149 | SER  |
| 6   | N     | 70  | GLY  |
| 6   | N     | 187 | HIS  |
| 7   | O     | 94  | ASP  |
| 3   | C     | 87  | ASP  |
| 4   | D     | 10  | LEU  |
| 4   | H     | 10  | LEU  |
| 4   | L     | 10  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 87  | LYS  |
| 5   | M     | 125 | PRO  |
| 6   | N     | 143 | ALA  |
| 6   | N     | 158 | HIS  |
| 7   | O     | 114 | PHE  |
| 7   | O     | 210 | GLU  |
| 2   | B     | 77  | SER  |
| 4   | D     | 103 | GLU  |
| 1   | E     | 20  | ASP  |
| 2   | F     | 77  | SER  |
| 3   | G     | 87  | ASP  |
| 4   | H     | 57  | ARG  |
| 1   | I     | 20  | ASP  |
| 2   | J     | 77  | SER  |
| 3   | K     | 87  | ASP  |
| 5   | M     | 186 | GLN  |
| 6   | N     | 79  | ASP  |
| 6   | N     | 186 | ASP  |
| 6   | N     | 199 | ARG  |
| 7   | O     | 113 | CYS  |
| 1   | A     | 20  | ASP  |
| 1   | A     | 82  | ASN  |
| 4   | D     | 57  | ARG  |
| 4   | H     | 103 | GLU  |
| 4   | L     | 57  | ARG  |
| 5   | M     | 119 | SER  |
| 5   | M     | 184 | LYS  |
| 5   | M     | 188 | GLU  |
| 6   | N     | 43  | PRO  |
| 6   | N     | 95  | GLU  |
| 6   | N     | 125 | ASP  |
| 1   | E     | 82  | ASN  |
| 1   | I     | 82  | ASN  |
| 2   | J     | 144 | HIS  |
| 6   | N     | 12  | PRO  |
| 6   | N     | 119 | GLY  |
| 5   | M     | 216 | VAL  |
| 7   | O     | 181 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 131/134 (98%)   | 123 (94%)  | 8 (6%)   | 17          | 43 |
| 1   | E     | 131/134 (98%)   | 123 (94%)  | 8 (6%)   | 17          | 43 |
| 1   | I     | 131/134 (98%)   | 123 (94%)  | 8 (6%)   | 17          | 43 |
| 2   | B     | 117/117 (100%)  | 111 (95%)  | 6 (5%)   | 21          | 48 |
| 2   | F     | 117/117 (100%)  | 111 (95%)  | 6 (5%)   | 21          | 48 |
| 2   | J     | 117/117 (100%)  | 111 (95%)  | 6 (5%)   | 21          | 48 |
| 3   | C     | 127/131 (97%)   | 119 (94%)  | 8 (6%)   | 16          | 42 |
| 3   | G     | 127/131 (97%)   | 119 (94%)  | 8 (6%)   | 16          | 42 |
| 3   | K     | 127/131 (97%)   | 119 (94%)  | 8 (6%)   | 16          | 42 |
| 4   | D     | 121/121 (100%)  | 115 (95%)  | 6 (5%)   | 22          | 48 |
| 4   | H     | 121/121 (100%)  | 115 (95%)  | 6 (5%)   | 22          | 48 |
| 4   | L     | 121/121 (100%)  | 115 (95%)  | 6 (5%)   | 22          | 48 |
| 5   | M     | 182/195 (93%)   | 153 (84%)  | 29 (16%) | 2           | 14 |
| 6   | N     | 186/193 (96%)   | 168 (90%)  | 18 (10%) | 8           | 30 |
| 7   | O     | 178/193 (92%)   | 170 (96%)  | 8 (4%)   | 24          | 50 |
| All | All   | 2034/2090 (97%) | 1895 (93%) | 139 (7%) | 14          | 40 |

All (139) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 48  | THR  |
| 1   | A     | 59  | ASP  |
| 1   | A     | 65  | GLU  |
| 1   | A     | 82  | ASN  |
| 1   | A     | 83  | LEU  |
| 1   | A     | 121 | ARG  |
| 1   | A     | 126 | VAL  |
| 1   | A     | 136 | ASN  |
| 2   | B     | 8   | GLU  |
| 2   | B     | 56  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 66  | ASP  |
| 2   | B     | 90  | ASP  |
| 2   | B     | 125 | TYR  |
| 2   | B     | 135 | ASP  |
| 3   | C     | 6   | CYS  |
| 3   | C     | 20  | ASP  |
| 3   | C     | 37  | ARG  |
| 3   | C     | 45  | LYS  |
| 3   | C     | 74  | ILE  |
| 3   | C     | 115 | LYS  |
| 3   | C     | 129 | ASP  |
| 3   | C     | 146 | LYS  |
| 4   | D     | 19  | LEU  |
| 4   | D     | 48  | GLU  |
| 4   | D     | 71  | GLN  |
| 4   | D     | 84  | LEU  |
| 4   | D     | 128 | THR  |
| 4   | D     | 138 | CYS  |
| 1   | E     | 48  | THR  |
| 1   | E     | 59  | ASP  |
| 1   | E     | 65  | GLU  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 83  | LEU  |
| 1   | E     | 121 | ARG  |
| 1   | E     | 126 | VAL  |
| 1   | E     | 136 | ASN  |
| 2   | F     | 8   | GLU  |
| 2   | F     | 56  | THR  |
| 2   | F     | 66  | ASP  |
| 2   | F     | 90  | ASP  |
| 2   | F     | 125 | TYR  |
| 2   | F     | 135 | ASP  |
| 3   | G     | 6   | CYS  |
| 3   | G     | 20  | ASP  |
| 3   | G     | 37  | ARG  |
| 3   | G     | 45  | LYS  |
| 3   | G     | 74  | ILE  |
| 3   | G     | 115 | LYS  |
| 3   | G     | 129 | ASP  |
| 3   | G     | 146 | LYS  |
| 4   | H     | 19  | LEU  |
| 4   | H     | 48  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 71  | GLN  |
| 4   | H     | 84  | LEU  |
| 4   | H     | 128 | THR  |
| 4   | H     | 138 | CYS  |
| 1   | I     | 48  | THR  |
| 1   | I     | 59  | ASP  |
| 1   | I     | 65  | GLU  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 83  | LEU  |
| 1   | I     | 121 | ARG  |
| 1   | I     | 126 | VAL  |
| 1   | I     | 136 | ASN  |
| 2   | J     | 8   | GLU  |
| 2   | J     | 56  | THR  |
| 2   | J     | 66  | ASP  |
| 2   | J     | 90  | ASP  |
| 2   | J     | 125 | TYR  |
| 2   | J     | 135 | ASP  |
| 3   | K     | 6   | CYS  |
| 3   | K     | 20  | ASP  |
| 3   | K     | 37  | ARG  |
| 3   | K     | 45  | LYS  |
| 3   | K     | 74  | ILE  |
| 3   | K     | 115 | LYS  |
| 3   | K     | 129 | ASP  |
| 3   | K     | 146 | LYS  |
| 4   | L     | 19  | LEU  |
| 4   | L     | 48  | GLU  |
| 4   | L     | 71  | GLN  |
| 4   | L     | 84  | LEU  |
| 4   | L     | 128 | THR  |
| 4   | L     | 138 | CYS  |
| 5   | M     | 9   | ARG  |
| 5   | M     | 10  | PHE  |
| 5   | M     | 12  | TYR  |
| 5   | M     | 19  | LEU  |
| 5   | M     | 38  | LEU  |
| 5   | M     | 80  | LEU  |
| 5   | M     | 95  | GLU  |
| 5   | M     | 103 | ASN  |
| 5   | M     | 112 | THR  |
| 5   | M     | 116 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 118 | THR  |
| 5   | M     | 121 | GLU  |
| 5   | M     | 124 | ASN  |
| 5   | M     | 131 | THR  |
| 5   | M     | 147 | LEU  |
| 5   | M     | 157 | GLU  |
| 5   | M     | 159 | ASP  |
| 5   | M     | 161 | THR  |
| 5   | M     | 163 | SER  |
| 5   | M     | 165 | THR  |
| 5   | M     | 176 | ARG  |
| 5   | M     | 183 | LEU  |
| 5   | M     | 188 | GLU  |
| 5   | M     | 198 | LEU  |
| 5   | M     | 209 | VAL  |
| 5   | M     | 210 | VAL  |
| 5   | M     | 216 | VAL  |
| 5   | M     | 224 | ARG  |
| 5   | M     | 225 | TYR  |
| 6   | N     | 10  | LEU  |
| 6   | N     | 32  | ARG  |
| 6   | N     | 64  | LYS  |
| 6   | N     | 73  | GLU  |
| 6   | N     | 82  | VAL  |
| 6   | N     | 89  | CYS  |
| 6   | N     | 95  | GLU  |
| 6   | N     | 100 | CYS  |
| 6   | N     | 110 | VAL  |
| 6   | N     | 127 | VAL  |
| 6   | N     | 131 | THR  |
| 6   | N     | 147 | LEU  |
| 6   | N     | 155 | LEU  |
| 6   | N     | 187 | HIS  |
| 6   | N     | 199 | ARG  |
| 6   | N     | 202 | ASN  |
| 6   | N     | 215 | LEU  |
| 6   | N     | 221 | LEU  |
| 7   | O     | 37  | ASP  |
| 7   | O     | 61  | SER  |
| 7   | O     | 114 | PHE  |
| 7   | O     | 173 | ASP  |
| 7   | O     | 176 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | O     | 183 | GLU  |
| 7   | O     | 208 | LEU  |
| 7   | O     | 210 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 69  | HIS  |
| 1   | A     | 82  | ASN  |
| 1   | A     | 96  | HIS  |
| 1   | A     | 125 | GLN  |
| 1   | A     | 131 | ASN  |
| 1   | A     | 136 | ASN  |
| 2   | B     | 52  | HIS  |
| 2   | B     | 115 | HIS  |
| 2   | B     | 120 | GLN  |
| 2   | B     | 145 | HIS  |
| 3   | C     | 12  | HIS  |
| 3   | C     | 16  | GLN  |
| 3   | C     | 18  | GLN  |
| 3   | C     | 51  | ASN  |
| 3   | C     | 61  | HIS  |
| 3   | C     | 70  | HIS  |
| 3   | C     | 76  | ASN  |
| 3   | C     | 83  | ASN  |
| 3   | C     | 100 | HIS  |
| 3   | C     | 126 | GLN  |
| 4   | D     | 20  | GLN  |
| 4   | D     | 46  | HIS  |
| 4   | D     | 117 | HIS  |
| 4   | D     | 141 | GLN  |
| 1   | E     | 69  | HIS  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 131 | ASN  |
| 1   | E     | 136 | ASN  |
| 2   | F     | 40  | GLN  |
| 2   | F     | 52  | HIS  |
| 2   | F     | 115 | HIS  |
| 2   | F     | 120 | GLN  |
| 2   | F     | 145 | HIS  |
| 3   | G     | 12  | HIS  |
| 3   | G     | 16  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 18  | GLN  |
| 3   | G     | 51  | ASN  |
| 3   | G     | 70  | HIS  |
| 3   | G     | 76  | ASN  |
| 3   | G     | 97  | HIS  |
| 3   | G     | 100 | HIS  |
| 3   | G     | 126 | GLN  |
| 4   | H     | 20  | GLN  |
| 4   | H     | 46  | HIS  |
| 4   | H     | 117 | HIS  |
| 4   | H     | 120 | HIS  |
| 4   | H     | 141 | GLN  |
| 1   | I     | 17  | HIS  |
| 1   | I     | 45  | HIS  |
| 1   | I     | 69  | HIS  |
| 1   | I     | 82  | ASN  |
| 1   | I     | 125 | GLN  |
| 1   | I     | 131 | ASN  |
| 1   | I     | 136 | ASN  |
| 2   | J     | 40  | GLN  |
| 2   | J     | 52  | HIS  |
| 2   | J     | 115 | HIS  |
| 2   | J     | 120 | GLN  |
| 2   | J     | 145 | HIS  |
| 3   | K     | 12  | HIS  |
| 3   | K     | 16  | GLN  |
| 3   | K     | 18  | GLN  |
| 3   | K     | 51  | ASN  |
| 3   | K     | 61  | HIS  |
| 3   | K     | 70  | HIS  |
| 3   | K     | 100 | HIS  |
| 3   | K     | 126 | GLN  |
| 4   | L     | 20  | GLN  |
| 4   | L     | 29  | HIS  |
| 4   | L     | 46  | HIS  |
| 4   | L     | 117 | HIS  |
| 4   | L     | 141 | GLN  |
| 5   | M     | 18  | ASN  |
| 5   | M     | 36  | ASN  |
| 5   | M     | 49  | GLN  |
| 5   | M     | 56  | ASN  |
| 5   | M     | 103 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 106 | HIS  |
| 5   | M     | 143 | ASN  |
| 5   | M     | 172 | ASN  |
| 6   | N     | 72  | ASN  |
| 6   | N     | 74  | GLN  |
| 6   | N     | 86  | HIS  |
| 6   | N     | 90  | HIS  |
| 6   | N     | 173 | ASN  |
| 6   | N     | 217 | GLN  |
| 7   | O     | 174 | 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 29 ligands modelled in this entry, 5 are monoatomic - leaving 24 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   | HEM  | F     | 160 | 2    | 50,50,50     | 1.29 | 5 (10%)     | 67,82,82    | 1.16 | 4 (5%)      |
| 9   | HEM  | D     | 160 | 4    | 50,50,50     | 1.26 | 5 (10%)     | 67,82,82    | 1.20 | 4 (5%)      |
| 9   | HEM  | E     | 160 | 1    | 50,50,50     | 1.37 | 6 (12%)     | 67,82,82    | 1.17 | 4 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | HEM  | H     | 160 | 4    | 50,50,50     | 1.36 | 6 (12%)  | 67,82,82    | 1.09 | 3 (4%)   |
| 9   | HEM  | L     | 160 | 4    | 50,50,50     | 1.24 | 4 (8%)   | 67,82,82    | 1.14 | 4 (5%)   |
| 8   | CMO  | E     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 8   | CMO  | C     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 9   | HEM  | C     | 160 | 3    | 50,50,50     | 1.30 | 5 (10%)  | 67,82,82    | 1.12 | 3 (4%)   |
| 8   | CMO  | I     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 8   | CMO  | K     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 9   | HEM  | B     | 160 | 2    | 50,50,50     | 1.31 | 5 (10%)  | 67,82,82    | 1.09 | 3 (4%)   |
| 8   | CMO  | F     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 9   | HEM  | I     | 160 | 1    | 50,50,50     | 1.36 | 5 (10%)  | 67,82,82    | 1.10 | 4 (5%)   |
| 8   | CMO  | D     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 8   | CMO  | G     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 9   | HEM  | G     | 160 | 3    | 50,50,50     | 1.22 | 5 (10%)  | 67,82,82    | 1.08 | 3 (4%)   |
| 9   | HEM  | K     | 160 | 3    | 50,50,50     | 1.18 | 5 (10%)  | 67,82,82    | 1.13 | 3 (4%)   |
| 8   | CMO  | H     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 8   | CMO  | J     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 8   | CMO  | L     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 9   | HEM  | A     | 160 | 1    | 50,50,50     | 1.30 | 5 (10%)  | 67,82,82    | 1.14 | 4 (5%)   |
| 8   | CMO  | B     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |
| 9   | HEM  | J     | 160 | 2    | 50,50,50     | 1.26 | 6 (12%)  | 67,82,82    | 1.08 | 2 (2%)   |
| 8   | CMO  | A     | 161 | -    | 0,1,1        | -    | -        | -           | -    | -        |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 9   | HEM  | B     | 160 | 2    | -       | 6/14/54/54 | -     |
| 9   | HEM  | F     | 160 | 2    | -       | 6/14/54/54 | -     |
| 9   | HEM  | D     | 160 | 4    | -       | 8/14/54/54 | -     |
| 9   | HEM  | C     | 160 | 3    | -       | 7/14/54/54 | -     |
| 9   | HEM  | K     | 160 | 3    | -       | 8/14/54/54 | -     |
| 9   | HEM  | E     | 160 | 1    | -       | 8/14/54/54 | -     |
| 9   | HEM  | H     | 160 | 4    | -       | 8/14/54/54 | -     |
| 9   | HEM  | I     | 160 | 1    | -       | 8/14/54/54 | -     |
| 9   | HEM  | L     | 160 | 4    | -       | 8/14/54/54 | -     |
| 9   | HEM  | G     | 160 | 3    | -       | 7/14/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 9   | HEM  | A     | 160 | 1    | -       | 8/14/54/54 | -     |
| 9   | HEM  | J     | 160 | 2    | -       | 6/14/54/54 | -     |

All (62) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | B     | 160 | HEM  | CAC-C3C | -4.11 | 1.36        | 1.47     |
| 9   | D     | 160 | HEM  | CAC-C3C | -4.06 | 1.36        | 1.47     |
| 9   | H     | 160 | HEM  | CAC-C3C | -3.84 | 1.37        | 1.47     |
| 9   | E     | 160 | HEM  | CAC-C3C | -3.80 | 1.37        | 1.47     |
| 9   | F     | 160 | HEM  | CAB-C3B | -3.70 | 1.37        | 1.47     |
| 9   | G     | 160 | HEM  | CAB-C3B | -3.66 | 1.37        | 1.47     |
| 9   | C     | 160 | HEM  | CAC-C3C | -3.59 | 1.37        | 1.47     |
| 9   | J     | 160 | HEM  | CAB-C3B | -3.51 | 1.38        | 1.47     |
| 9   | F     | 160 | HEM  | CAC-C3C | -3.45 | 1.38        | 1.47     |
| 9   | I     | 160 | HEM  | CAB-C3B | -3.41 | 1.38        | 1.47     |
| 9   | H     | 160 | HEM  | CAB-C3B | -3.41 | 1.38        | 1.47     |
| 9   | C     | 160 | HEM  | CAB-C3B | -3.40 | 1.38        | 1.47     |
| 9   | A     | 160 | HEM  | CAC-C3C | -3.40 | 1.38        | 1.47     |
| 9   | L     | 160 | HEM  | CAC-C3C | -3.35 | 1.38        | 1.47     |
| 9   | J     | 160 | HEM  | CAC-C3C | -3.33 | 1.38        | 1.47     |
| 9   | K     | 160 | HEM  | CAB-C3B | -3.32 | 1.38        | 1.47     |
| 9   | A     | 160 | HEM  | CAB-C3B | -3.25 | 1.38        | 1.47     |
| 9   | L     | 160 | HEM  | CAB-C3B | -3.25 | 1.38        | 1.47     |
| 9   | K     | 160 | HEM  | CAC-C3C | -3.17 | 1.38        | 1.47     |
| 9   | E     | 160 | HEM  | CAB-C3B | -3.09 | 1.39        | 1.47     |
| 9   | A     | 160 | HEM  | CBB-CAB | 3.06  | 1.45        | 1.30     |
| 9   | I     | 160 | HEM  | CBB-CAB | 3.02  | 1.44        | 1.30     |
| 9   | G     | 160 | HEM  | CAC-C3C | -2.96 | 1.39        | 1.47     |
| 9   | I     | 160 | HEM  | CAC-C3C | -2.96 | 1.39        | 1.47     |
| 9   | D     | 160 | HEM  | CBB-CAB | 2.96  | 1.44        | 1.30     |
| 9   | B     | 160 | HEM  | CAB-C3B | -2.96 | 1.39        | 1.47     |
| 9   | C     | 160 | HEM  | CBC-CAC | 2.95  | 1.44        | 1.30     |
| 9   | G     | 160 | HEM  | CBC-CAC | 2.95  | 1.44        | 1.30     |
| 9   | J     | 160 | HEM  | CBB-CAB | 2.94  | 1.44        | 1.30     |
| 9   | D     | 160 | HEM  | CAB-C3B | -2.91 | 1.39        | 1.47     |
| 9   | I     | 160 | HEM  | CBC-CAC | 2.90  | 1.44        | 1.30     |
| 9   | L     | 160 | HEM  | CBB-CAB | 2.87  | 1.44        | 1.30     |
| 9   | H     | 160 | HEM  | CBB-CAB | 2.81  | 1.43        | 1.30     |
| 9   | K     | 160 | HEM  | CBC-CAC | 2.80  | 1.43        | 1.30     |
| 9   | A     | 160 | HEM  | CBC-CAC | 2.78  | 1.43        | 1.30     |
| 9   | E     | 160 | HEM  | CBB-CAB | 2.77  | 1.43        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | L     | 160 | HEM  | CBC-CAC | 2.74  | 1.43        | 1.30     |
| 9   | F     | 160 | HEM  | C4D-ND  | -2.74 | 1.35        | 1.40     |
| 9   | G     | 160 | HEM  | CBB-CAB | 2.74  | 1.43        | 1.30     |
| 9   | B     | 160 | HEM  | CBB-CAB | 2.69  | 1.43        | 1.30     |
| 9   | F     | 160 | HEM  | CBC-CAC | 2.69  | 1.43        | 1.30     |
| 9   | H     | 160 | HEM  | CBC-CAC | 2.68  | 1.43        | 1.30     |
| 9   | B     | 160 | HEM  | CBC-CAC | 2.61  | 1.42        | 1.30     |
| 9   | F     | 160 | HEM  | CBB-CAB | 2.61  | 1.42        | 1.30     |
| 9   | D     | 160 | HEM  | CBC-CAC | 2.55  | 1.42        | 1.30     |
| 9   | K     | 160 | HEM  | CBB-CAB | 2.53  | 1.42        | 1.30     |
| 9   | C     | 160 | HEM  | C2A-C3A | -2.53 | 1.32        | 1.38     |
| 9   | J     | 160 | HEM  | CBC-CAC | 2.52  | 1.42        | 1.30     |
| 9   | E     | 160 | HEM  | CBC-CAC | 2.50  | 1.42        | 1.30     |
| 9   | K     | 160 | HEM  | C2A-C3A | -2.46 | 1.32        | 1.38     |
| 9   | G     | 160 | HEM  | C2A-C3A | -2.45 | 1.32        | 1.38     |
| 9   | J     | 160 | HEM  | C2A-C3A | -2.35 | 1.32        | 1.38     |
| 9   | E     | 160 | HEM  | FE-NB   | 2.32  | 2.02        | 1.94     |
| 9   | B     | 160 | HEM  | C4D-ND  | -2.31 | 1.36        | 1.40     |
| 9   | A     | 160 | HEM  | C2A-C3A | -2.30 | 1.32        | 1.38     |
| 9   | D     | 160 | HEM  | C2A-C3A | -2.29 | 1.32        | 1.38     |
| 9   | H     | 160 | HEM  | C4D-ND  | -2.23 | 1.36        | 1.40     |
| 9   | C     | 160 | HEM  | CBB-CAB | 2.21  | 1.41        | 1.30     |
| 9   | E     | 160 | HEM  | C2A-C3A | -2.19 | 1.33        | 1.38     |
| 9   | H     | 160 | HEM  | C3B-C2B | -2.09 | 1.32        | 1.37     |
| 9   | J     | 160 | HEM  | C4D-ND  | -2.05 | 1.36        | 1.40     |
| 9   | I     | 160 | HEM  | C2A-C3A | -2.00 | 1.33        | 1.38     |

All (41) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 9   | D     | 160 | HEM  | CMB-C2B-C1B | 3.17 | 129.98      | 125.03   |
| 9   | K     | 160 | HEM  | CMA-C3A-C4A | 2.97 | 129.95      | 125.42   |
| 9   | C     | 160 | HEM  | CMA-C3A-C4A | 2.87 | 129.79      | 125.42   |
| 9   | H     | 160 | HEM  | CMB-C2B-C1B | 2.85 | 129.49      | 125.03   |
| 9   | G     | 160 | HEM  | CMA-C3A-C4A | 2.74 | 129.59      | 125.42   |
| 9   | E     | 160 | HEM  | CMB-C2B-C1B | 2.71 | 129.27      | 125.03   |
| 9   | A     | 160 | HEM  | CMB-C2B-C1B | 2.70 | 129.26      | 125.03   |
| 9   | E     | 160 | HEM  | C3B-C4B-NB  | 2.62 | 111.35      | 109.47   |
| 9   | L     | 160 | HEM  | CMC-C2C-C1C | 2.60 | 129.31      | 124.73   |
| 9   | I     | 160 | HEM  | CMB-C2B-C1B | 2.57 | 129.04      | 125.03   |
| 9   | I     | 160 | HEM  | CAD-C3D-C4D | 2.53 | 129.11      | 124.70   |
| 9   | K     | 160 | HEM  | CAA-C2A-C1A | 2.51 | 129.84      | 124.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | L     | 160 | HEM  | CMB-C2B-C1B | 2.48  | 128.91      | 125.03   |
| 9   | D     | 160 | HEM  | CMC-C2C-C1C | 2.47  | 129.09      | 124.73   |
| 9   | E     | 160 | HEM  | CAD-C3D-C4D | 2.46  | 128.98      | 124.70   |
| 9   | B     | 160 | HEM  | CMD-C2D-C1D | 2.44  | 128.85      | 125.03   |
| 9   | C     | 160 | HEM  | C3B-C4B-NB  | 2.44  | 111.22      | 109.47   |
| 9   | C     | 160 | HEM  | CAA-C2A-C1A | 2.43  | 129.69      | 124.94   |
| 9   | G     | 160 | HEM  | CAA-C2A-C1A | 2.41  | 129.65      | 124.94   |
| 9   | A     | 160 | HEM  | CAD-C3D-C4D | 2.38  | 128.84      | 124.70   |
| 9   | F     | 160 | HEM  | CMA-C3A-C4A | 2.35  | 129.00      | 125.42   |
| 9   | F     | 160 | HEM  | C2B-C1B-NB  | 2.34  | 112.53      | 109.84   |
| 9   | E     | 160 | HEM  | CMB-C2B-C3B | -2.25 | 122.97      | 128.43   |
| 9   | B     | 160 | HEM  | C2B-C1B-NB  | 2.22  | 112.40      | 109.84   |
| 9   | G     | 160 | HEM  | C2A-C1A-NA  | 2.18  | 112.57      | 110.15   |
| 9   | J     | 160 | HEM  | CMA-C3A-C4A | 2.18  | 128.74      | 125.42   |
| 9   | B     | 160 | HEM  | CHA-C4D-C3D | -2.17 | 121.23      | 125.23   |
| 9   | J     | 160 | HEM  | CMD-C2D-C1D | 2.15  | 128.40      | 125.03   |
| 9   | L     | 160 | HEM  | CHA-C4D-C3D | -2.14 | 121.28      | 125.23   |
| 9   | F     | 160 | HEM  | CMD-C2D-C1D | 2.12  | 128.35      | 125.03   |
| 9   | I     | 160 | HEM  | C3B-C4B-NB  | 2.12  | 110.99      | 109.47   |
| 9   | L     | 160 | HEM  | CMA-C3A-C4A | 2.11  | 128.63      | 125.42   |
| 9   | H     | 160 | HEM  | CMA-C3A-C4A | 2.10  | 128.62      | 125.42   |
| 9   | D     | 160 | HEM  | CMA-C3A-C4A | 2.09  | 128.59      | 125.42   |
| 9   | A     | 160 | HEM  | C2A-C1A-NA  | 2.07  | 112.45      | 110.15   |
| 9   | D     | 160 | HEM  | CAC-C3C-C2C | -2.06 | 121.75      | 128.43   |
| 9   | I     | 160 | HEM  | CMB-C2B-C3B | -2.05 | 123.48      | 128.43   |
| 9   | A     | 160 | HEM  | C3B-C4B-NB  | 2.04  | 110.93      | 109.47   |
| 9   | F     | 160 | HEM  | CHA-C4D-C3D | -2.03 | 121.48      | 125.23   |
| 9   | K     | 160 | HEM  | CAD-C3D-C4D | 2.02  | 128.21      | 124.70   |
| 9   | H     | 160 | HEM  | C2B-C1B-NB  | 2.01  | 112.14      | 109.84   |

There are no chirality outliers.

All (88) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | A     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | A     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | A     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | A     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | B     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | D     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | E     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | E     | 160 | HEM  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | E     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | E     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | F     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | H     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | I     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | I     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | I     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | I     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | J     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | L     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | C     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | G     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | H     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | K     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 9   | L     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | B     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | D     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | D     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | F     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | H     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | H     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | J     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | L     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | L     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | D     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 9   | G     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | K     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | K     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | G     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | C     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 9   | C     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | G     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | K     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | L     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | C     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | D     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | I     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | A     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | B     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | E     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | H     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | F     | 160 | HEM  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | J     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 9   | L     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | D     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | A     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | H     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | I     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | A     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | F     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | E     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | F     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | J     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | B     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 9   | E     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | I     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | J     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | L     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | D     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | C     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | G     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | K     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | B     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | H     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 9   | A     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | F     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | K     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | C     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | D     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | G     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | J     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | C     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | G     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | K     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 9   | B     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | L     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | H     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | E     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | I     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 9   | K     | 160 | HEM  | C2C-C3C-CAC-CBC |

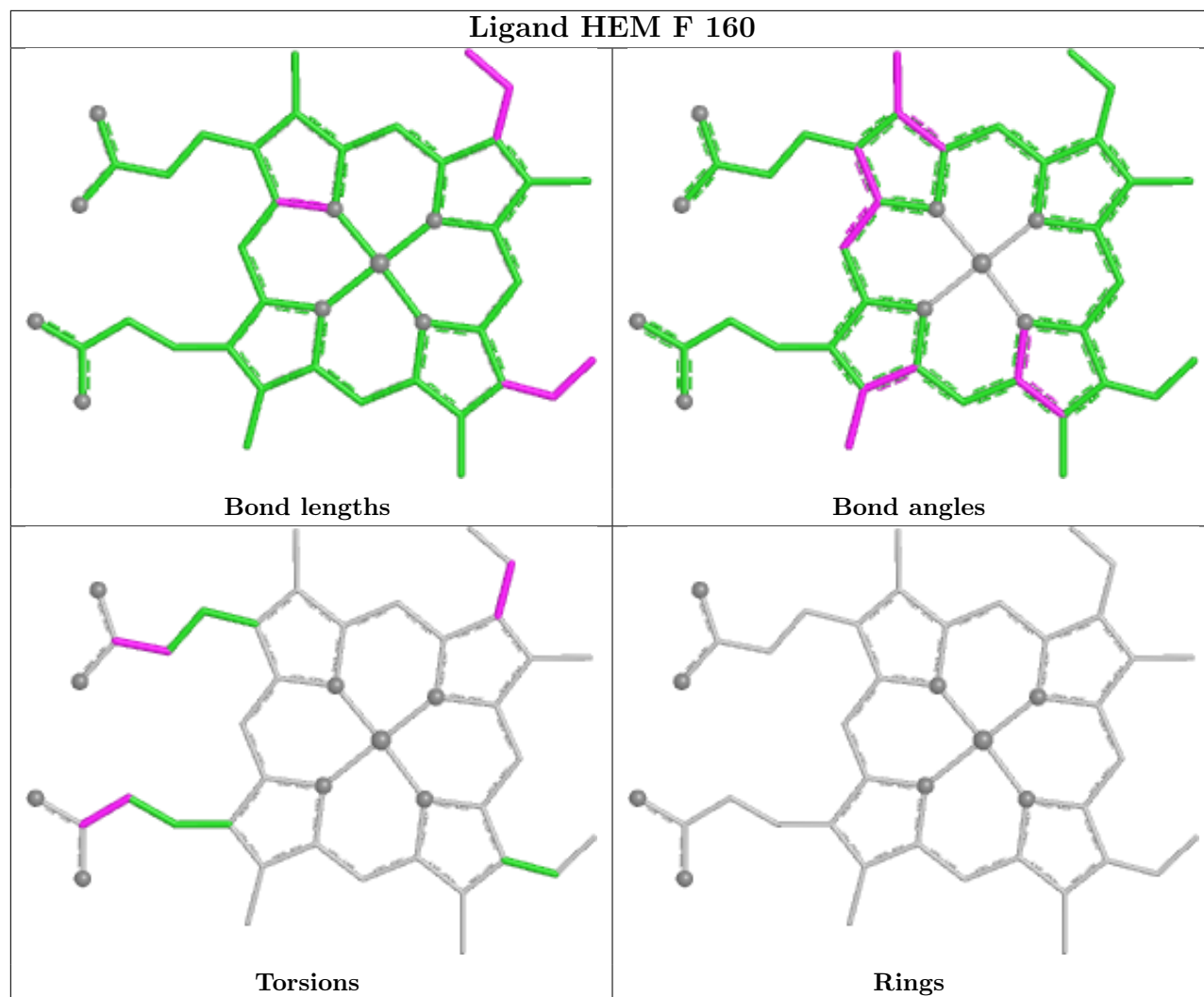
There are no ring outliers.

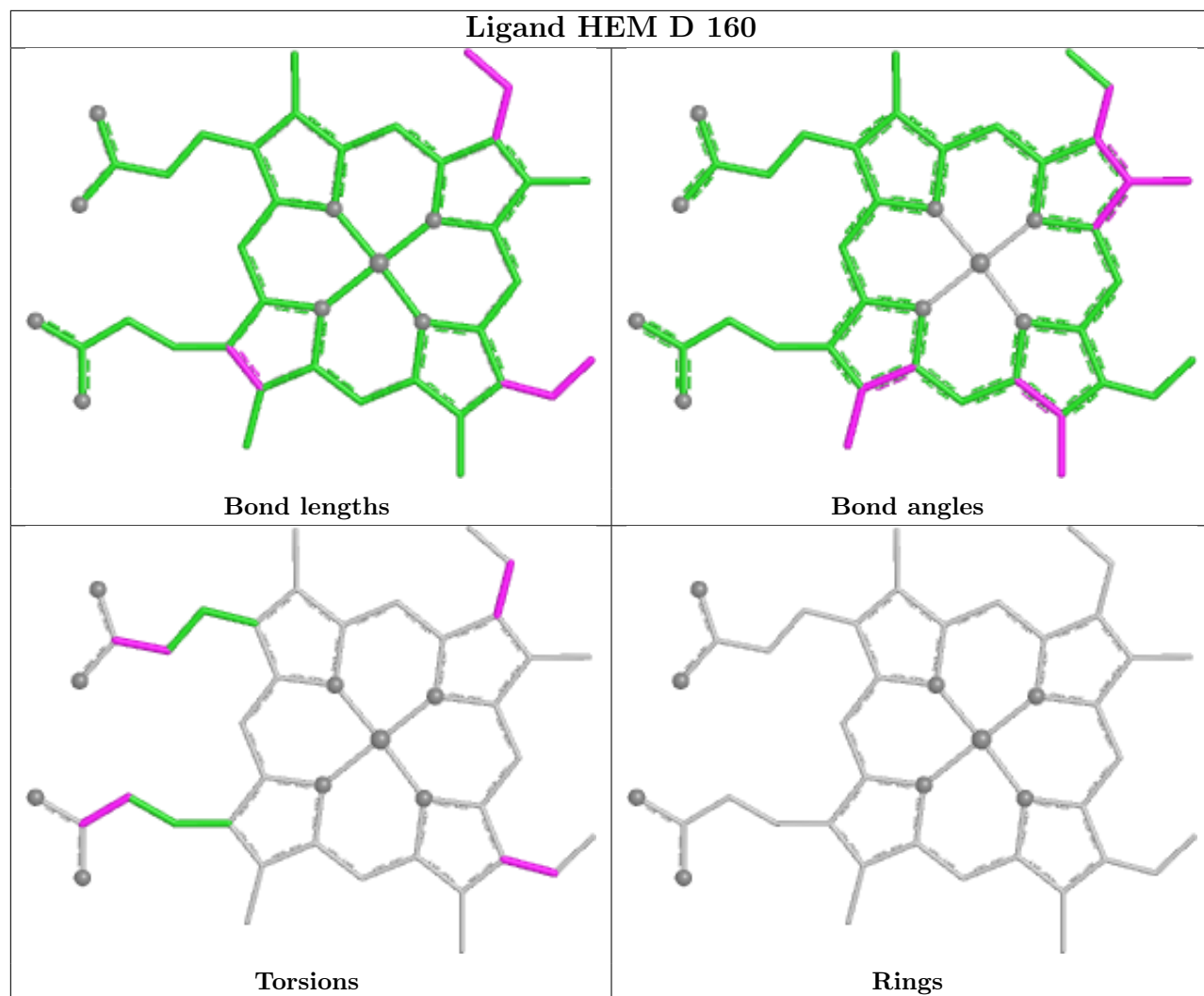
6 monomers are involved in 12 short contacts:

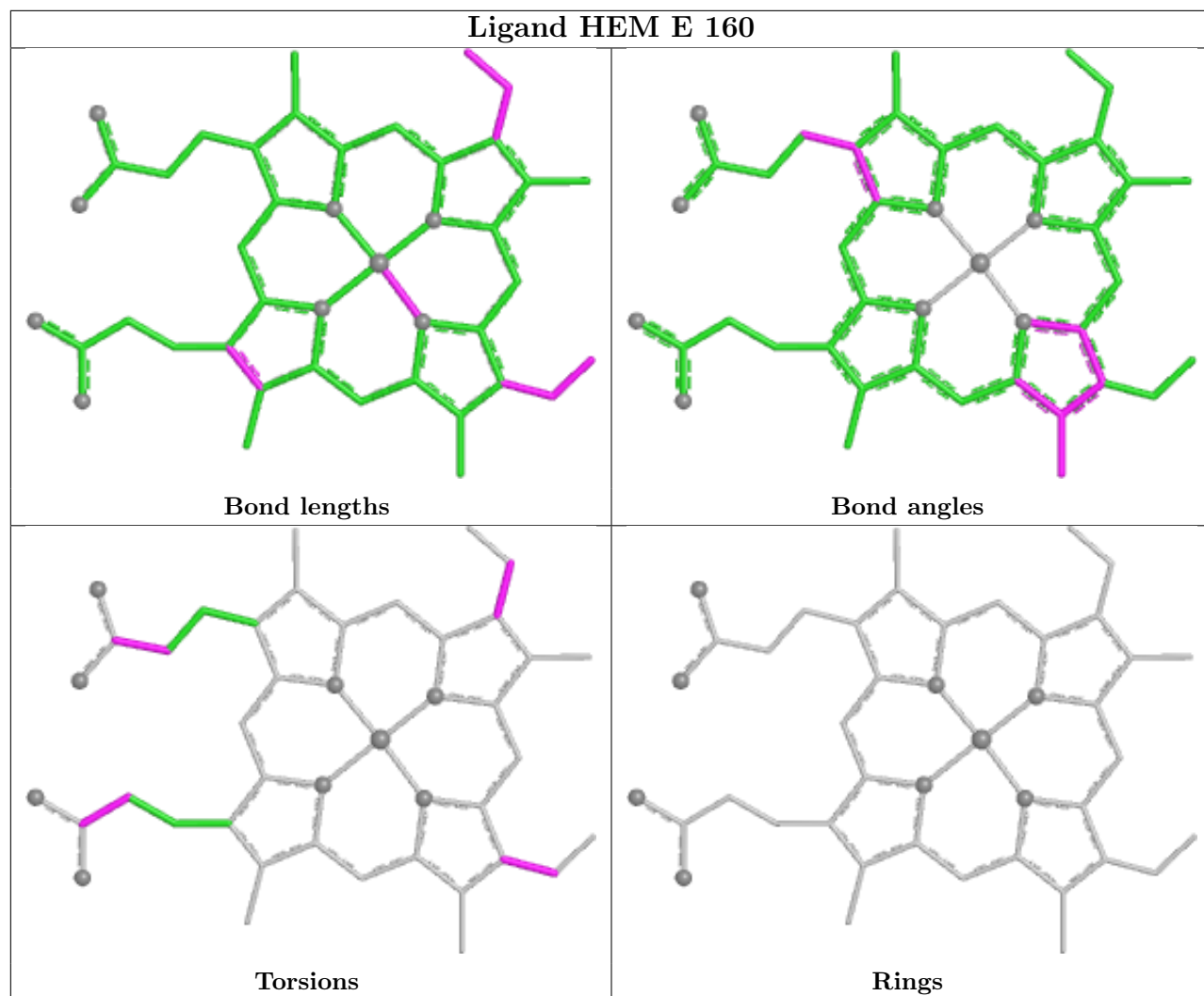
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | D     | 160 | HEM  | 3       | 0            |
| 9   | H     | 160 | HEM  | 3       | 0            |
| 9   | L     | 160 | HEM  | 3       | 0            |
| 9   | C     | 160 | HEM  | 1       | 0            |
| 9   | G     | 160 | HEM  | 1       | 0            |
| 9   | K     | 160 | HEM  | 1       | 0            |

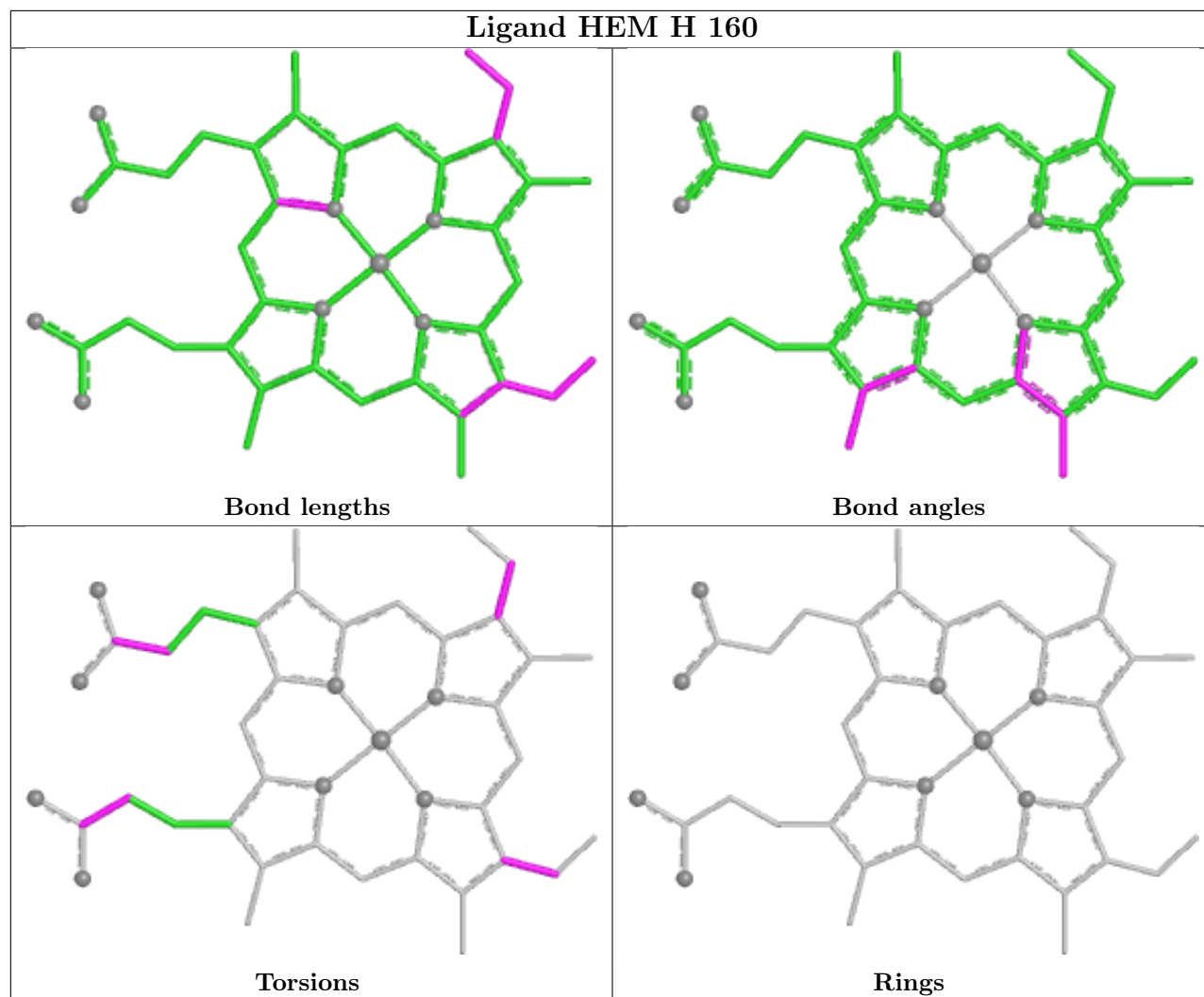
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

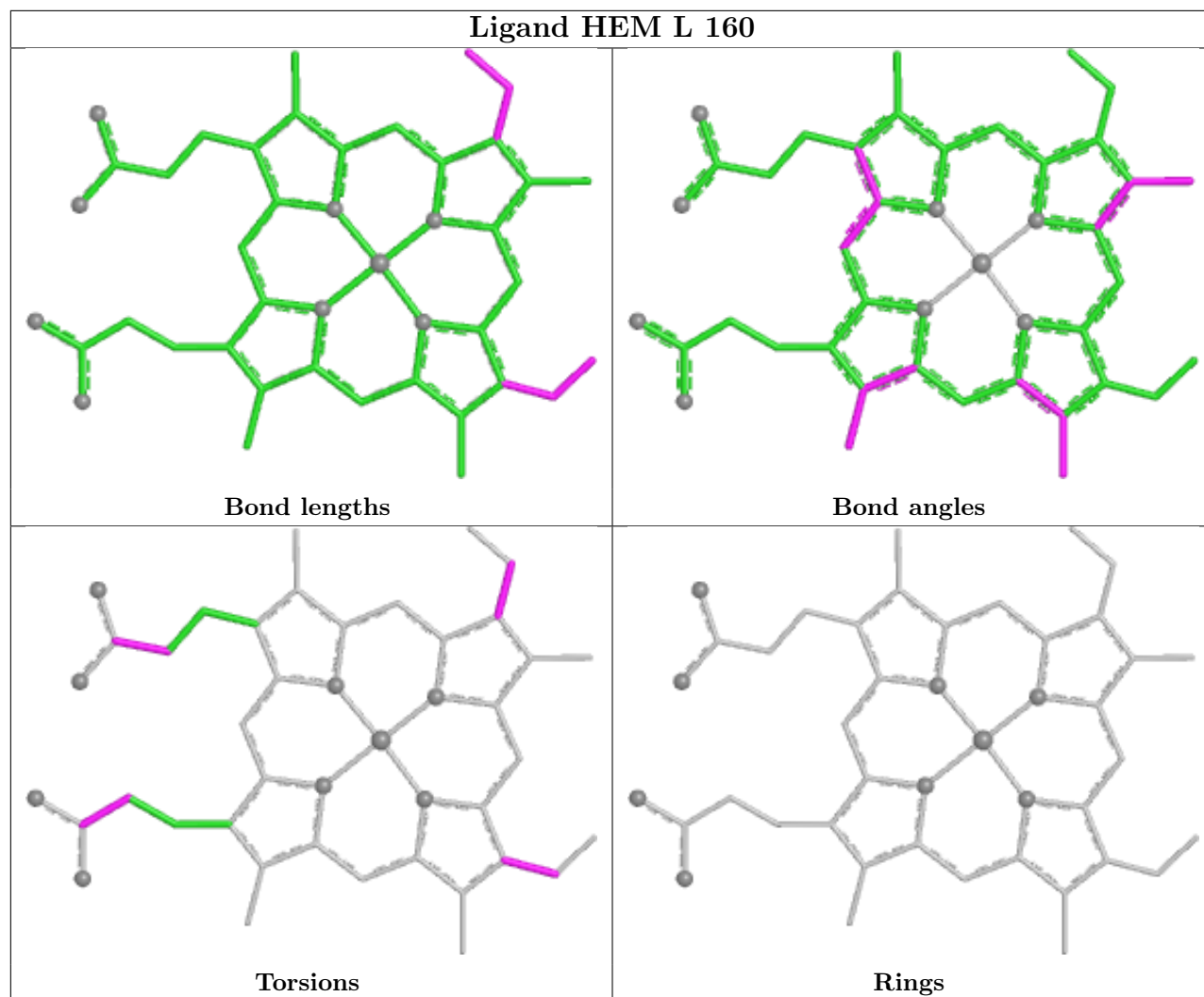


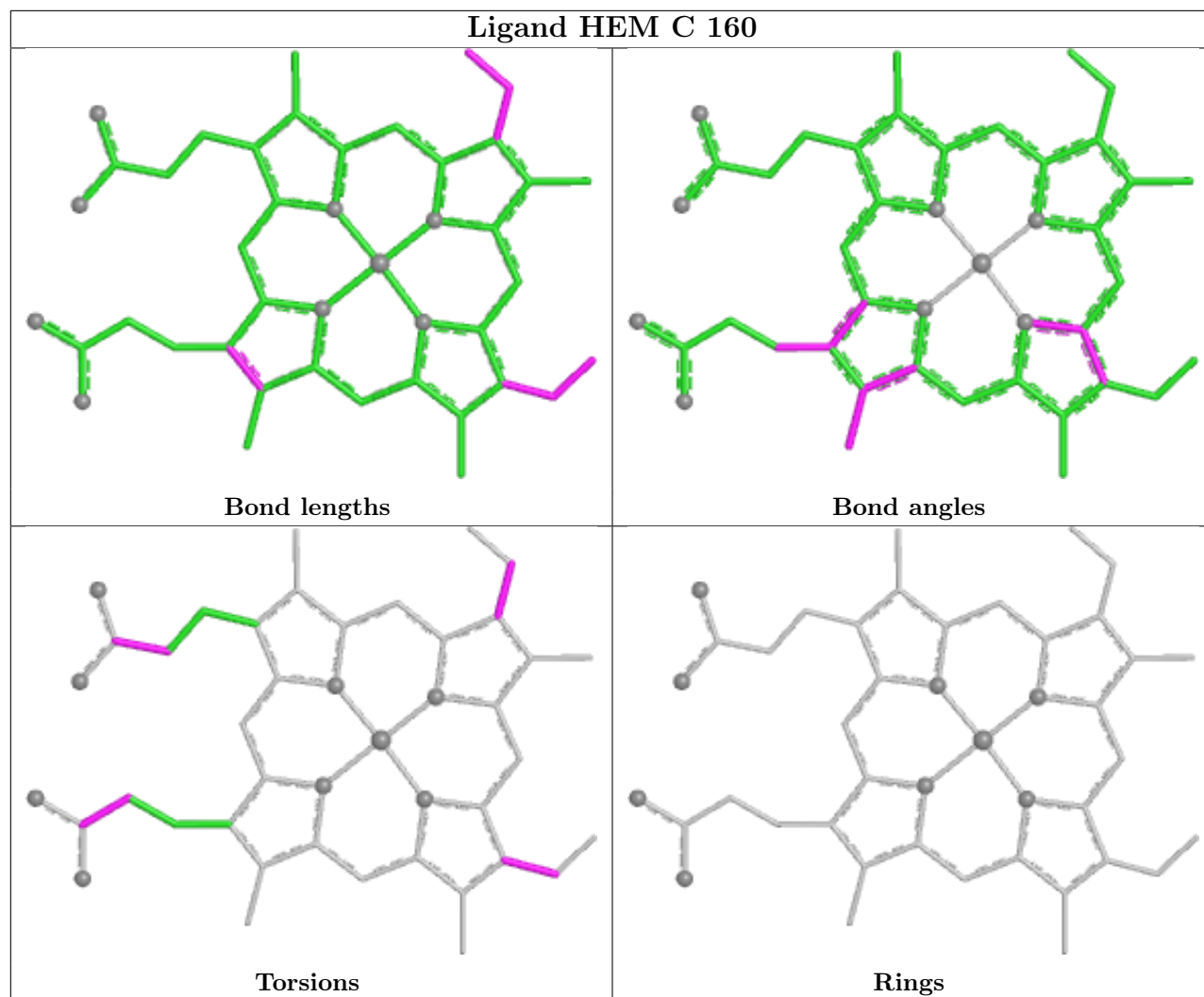


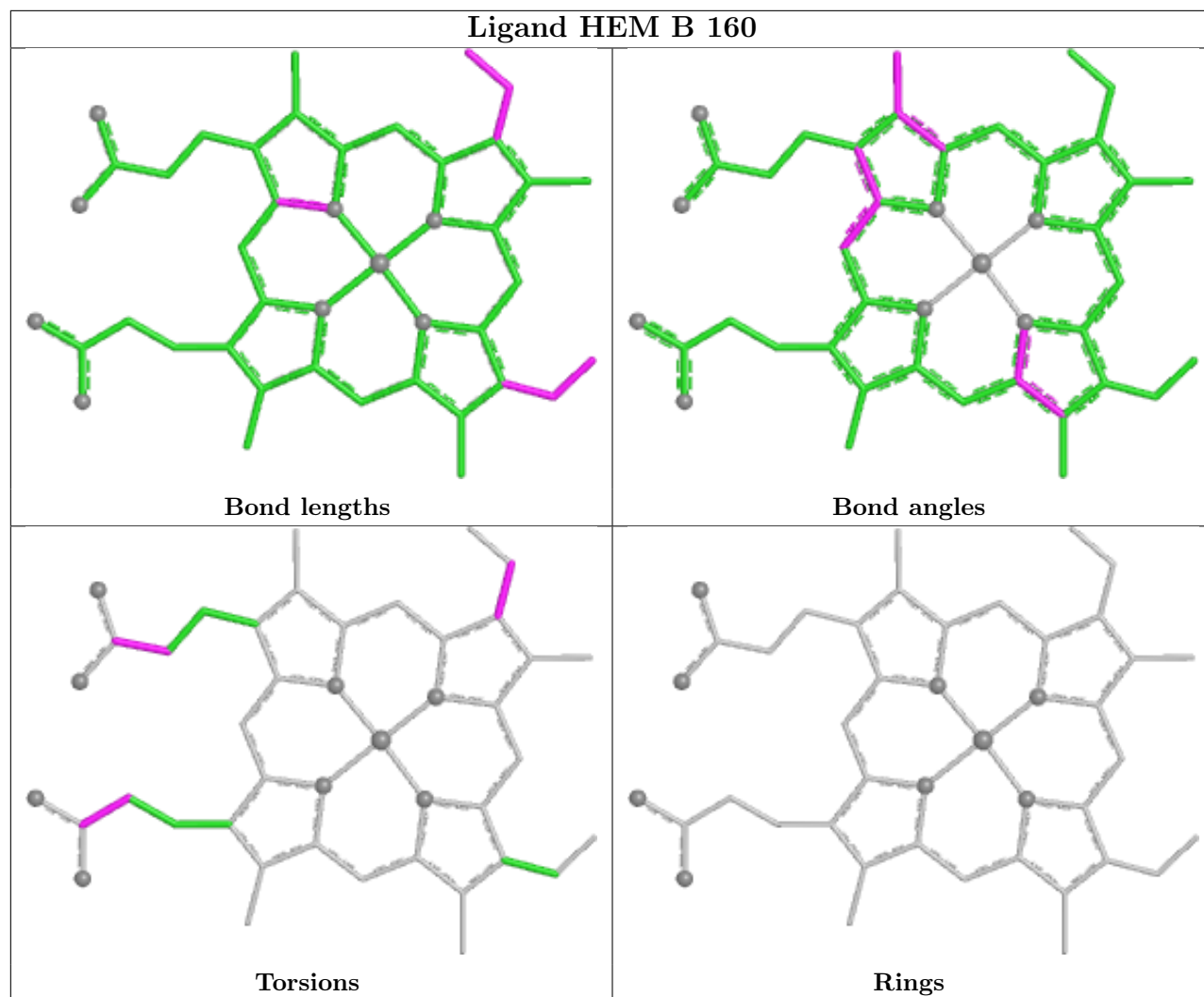




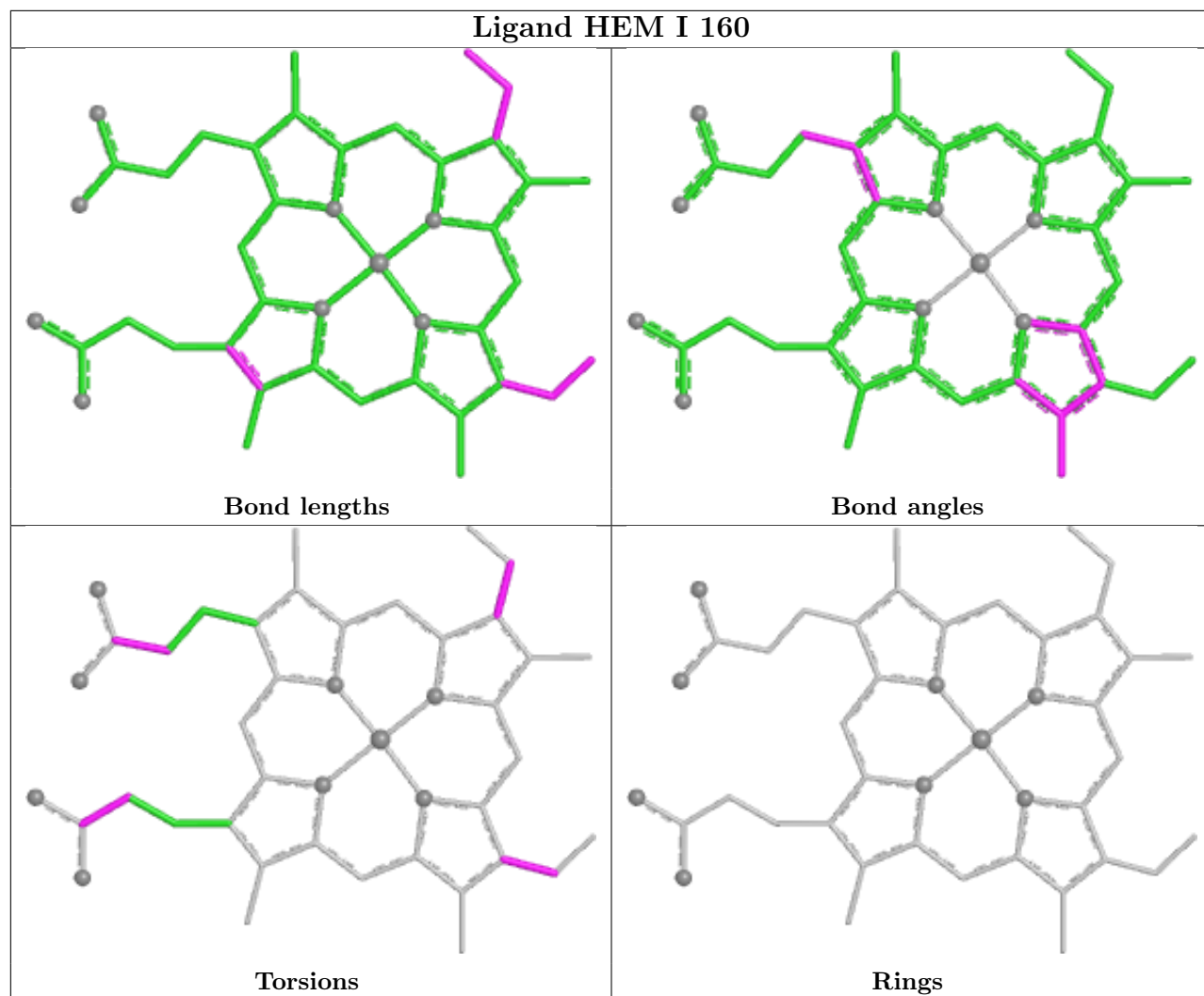




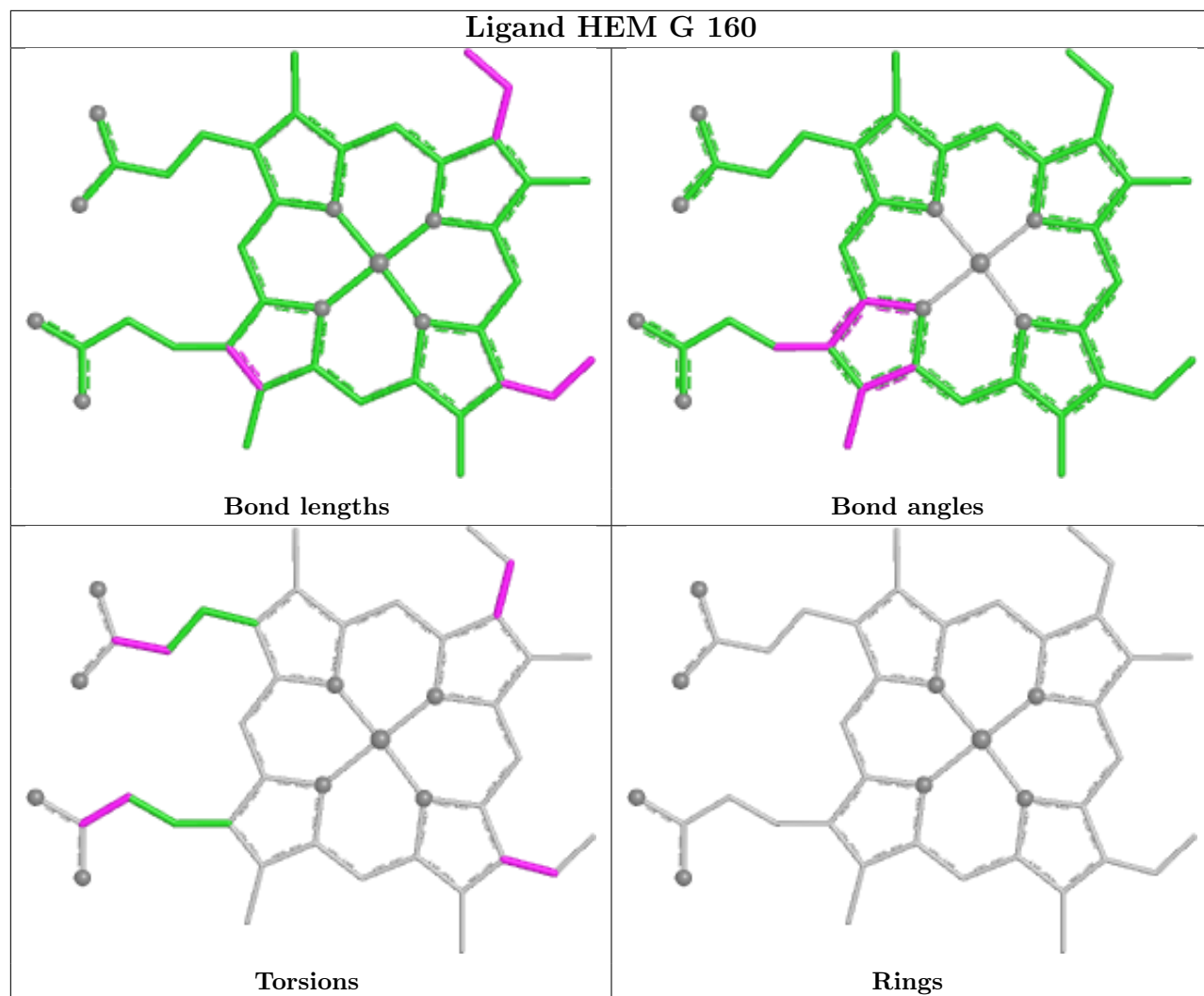


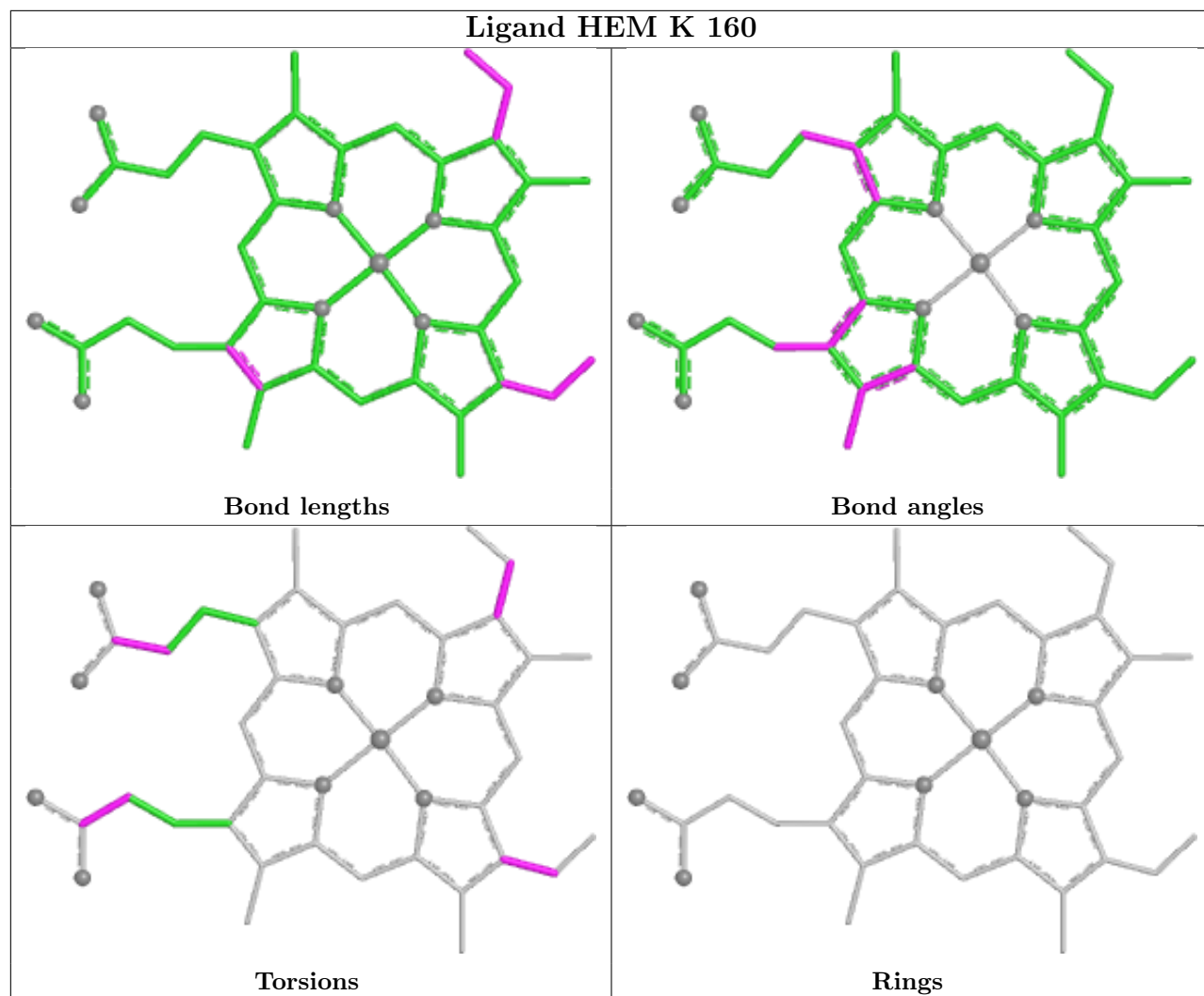


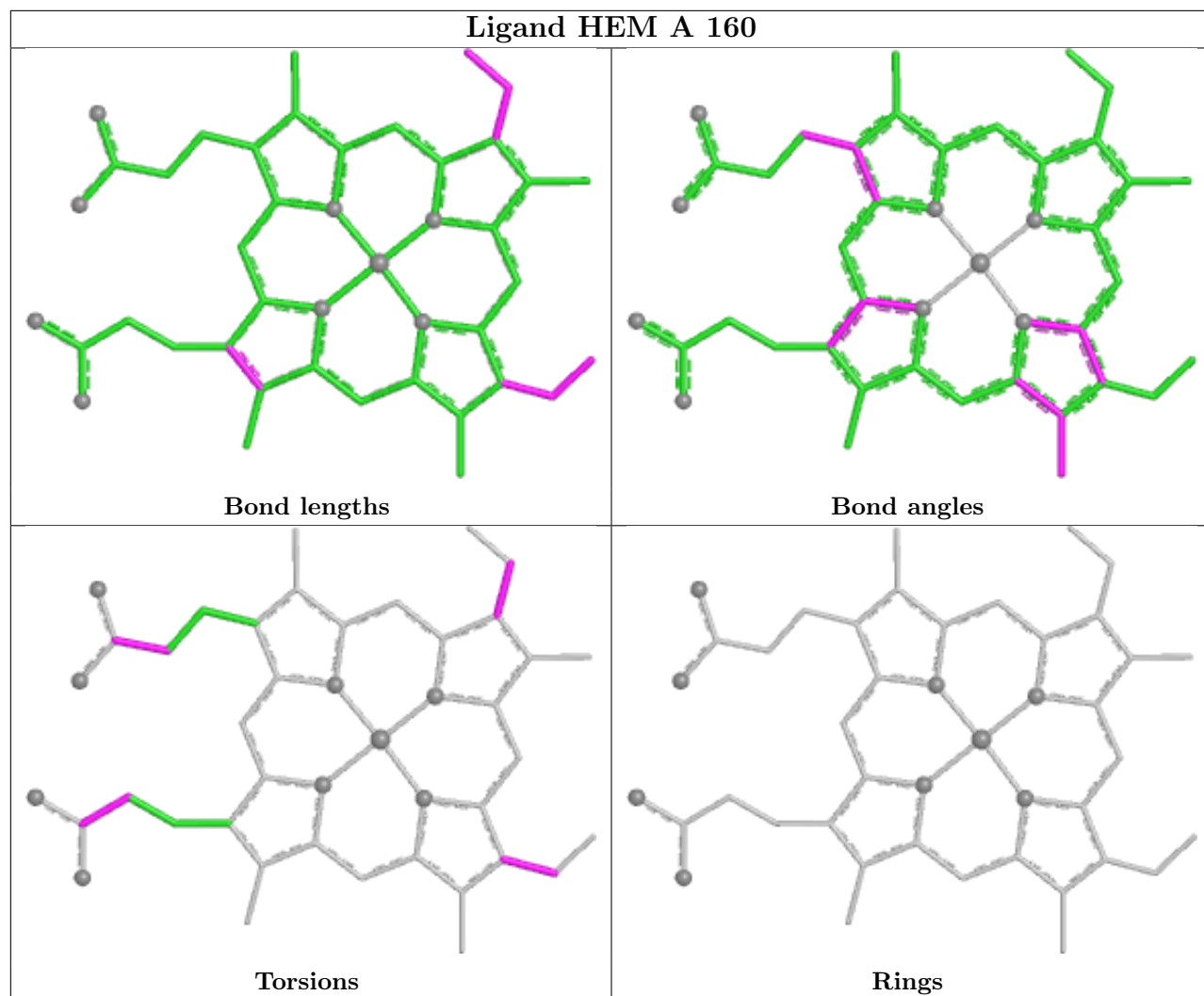
## Ligand HEM I 160

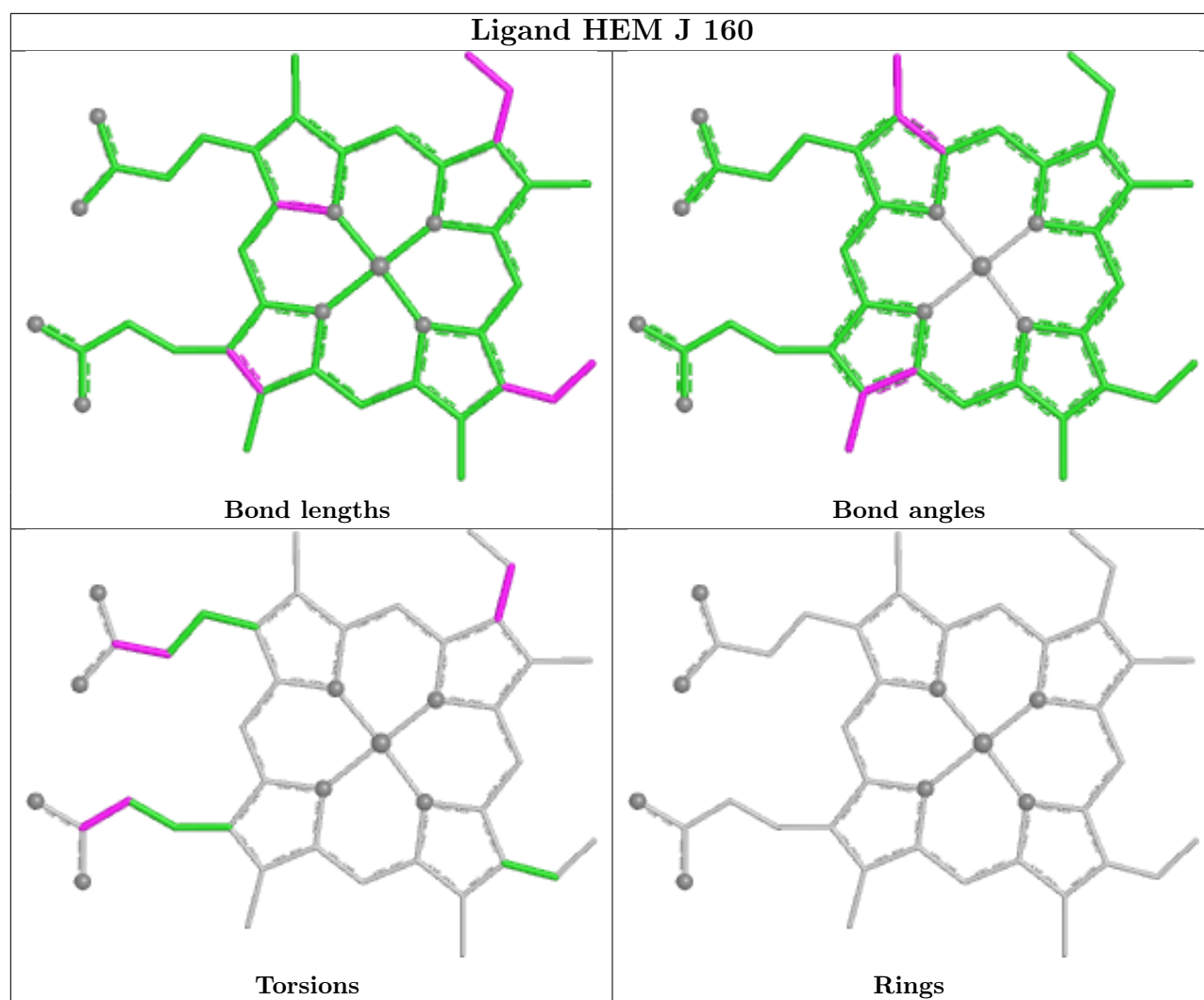












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 147/151 (97%)   | -0.31  | 1 (0%) 84 63   | 20, 66, 108, 122      | 0     |
| 1   | E     | 147/151 (97%)   | -0.40  | 0 100 100      | 31, 71, 113, 122      | 0     |
| 1   | I     | 147/151 (97%)   | -0.21  | 0 100 100      | 22, 69, 109, 122      | 0     |
| 2   | B     | 145/145 (100%)  | -0.37  | 0 100 100      | 10, 54, 102, 122      | 0     |
| 2   | F     | 145/145 (100%)  | -0.29  | 0 100 100      | 13, 49, 96, 116       | 0     |
| 2   | J     | 145/145 (100%)  | -0.29  | 0 100 100      | 25, 69, 114, 122      | 0     |
| 3   | C     | 149/153 (97%)   | -0.20  | 0 100 100      | 18, 62, 104, 122      | 0     |
| 3   | G     | 149/153 (97%)   | -0.32  | 0 100 100      | 15, 63, 111, 122      | 0     |
| 3   | K     | 149/153 (97%)   | -0.27  | 0 100 100      | 33, 85, 122, 122      | 0     |
| 4   | D     | 140/140 (100%)  | -0.42  | 0 100 100      | 33, 66, 107, 122      | 0     |
| 4   | H     | 140/140 (100%)  | -0.39  | 0 100 100      | 31, 69, 107, 122      | 0     |
| 4   | L     | 140/140 (100%)  | -0.42  | 0 100 100      | 31, 72, 108, 122      | 0     |
| 5   | M     | 217/217 (100%)  | -0.38  | 0 100 100      | 10, 48, 117, 122      | 0     |
| 6   | N     | 220/220 (100%)  | -0.39  | 0 100 100      | 9, 64, 120, 122       | 0     |
| 7   | O     | 215/215 (100%)  | -0.35  | 0 100 100      | 16, 69, 114, 122      | 0     |
| All | All   | 2395/2419 (99%) | -0.34  | 1 (0%) 100 100 | 9, 66, 114, 122       | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 5   | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

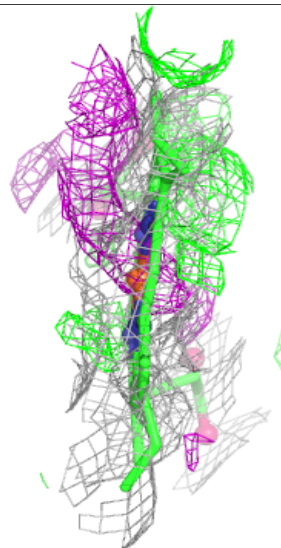
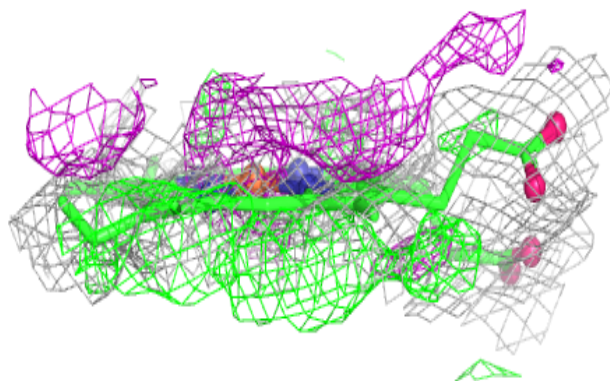
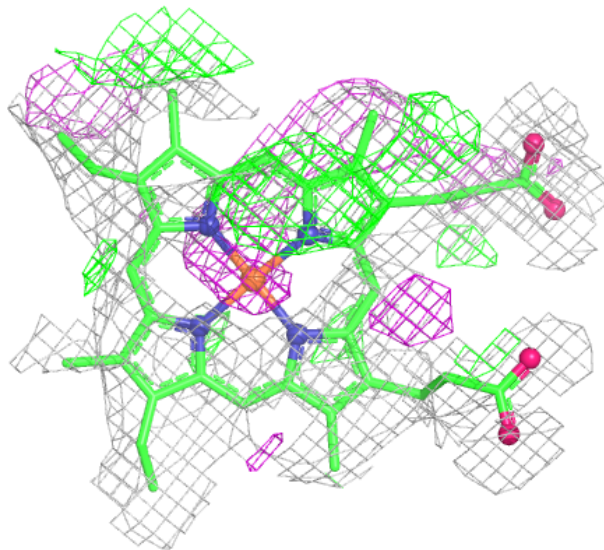
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8   | CMO  | C     | 161 | 2/2   | 0.96 | 0.16 | 46,46,46,46                 | 0     |
| 8   | CMO  | B     | 161 | 2/2   | 0.97 | 0.14 | 46,46,46,46                 | 0     |
| 9   | HEM  | G     | 160 | 43/43 | 0.97 | 0.12 | 66,66,66,66                 | 0     |
| 8   | CMO  | E     | 161 | 2/2   | 0.98 | 0.07 | 54,54,54,54                 | 0     |
| 8   | CMO  | L     | 161 | 2/2   | 0.98 | 0.10 | 72,72,72,72                 | 0     |
| 9   | HEM  | A     | 160 | 43/43 | 0.98 | 0.09 | 60,60,60,60                 | 0     |
| 9   | HEM  | B     | 160 | 43/43 | 0.98 | 0.10 | 26,26,26,26                 | 0     |
| 9   | HEM  | C     | 160 | 43/43 | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 9   | HEM  | D     | 160 | 43/43 | 0.98 | 0.09 | 38,38,38,38                 | 0     |
| 9   | HEM  | F     | 160 | 43/43 | 0.98 | 0.08 | 37,37,37,37                 | 0     |
| 8   | CMO  | A     | 161 | 2/2   | 0.98 | 0.10 | 82,82,82,82                 | 0     |
| 9   | HEM  | I     | 160 | 43/43 | 0.98 | 0.09 | 64,64,64,64                 | 0     |
| 9   | HEM  | J     | 160 | 43/43 | 0.98 | 0.09 | 54,54,54,54                 | 0     |
| 9   | HEM  | K     | 160 | 43/43 | 0.98 | 0.09 | 91,91,91,91                 | 0     |
| 8   | CMO  | H     | 161 | 2/2   | 0.99 | 0.09 | 68,68,68,68                 | 0     |
| 8   | CMO  | I     | 161 | 2/2   | 0.99 | 0.08 | 80,80,80,80                 | 0     |
| 9   | HEM  | E     | 160 | 43/43 | 0.99 | 0.08 | 71,71,71,71                 | 0     |
| 8   | CMO  | J     | 161 | 2/2   | 0.99 | 0.09 | 69,69,69,69                 | 0     |
| 8   | CMO  | K     | 161 | 2/2   | 0.99 | 0.08 | 69,69,69,69                 | 0     |
| 9   | HEM  | H     | 160 | 43/43 | 0.99 | 0.07 | 52,52,52,52                 | 0     |
| 8   | CMO  | D     | 161 | 2/2   | 0.99 | 0.09 | 74,74,74,74                 | 0     |
| 8   | CMO  | F     | 161 | 2/2   | 0.99 | 0.08 | 64,64,64,64                 | 0     |
| 8   | CMO  | G     | 161 | 2/2   | 0.99 | 0.10 | 38,38,38,38                 | 0     |
| 9   | HEM  | L     | 160 | 43/43 | 0.99 | 0.08 | 46,46,46,46                 | 0     |
| 10  | CA   | M     | 250 | 1/1   | 0.99 | 0.04 | 20,20,20,20                 | 0     |
| 10  | CA   | M     | 251 | 1/1   | 0.99 | 0.14 | 43,43,43,43                 | 0     |
| 10  | CA   | O     | 250 | 1/1   | 0.99 | 0.12 | 23,23,23,23                 | 0     |
| 11  | ZN   | M     | 252 | 1/1   | 0.99 | 0.05 | 58,58,58,58                 | 0     |
| 10  | CA   | N     | 250 | 1/1   | 1.00 | 0.09 | 15,15,15,15                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

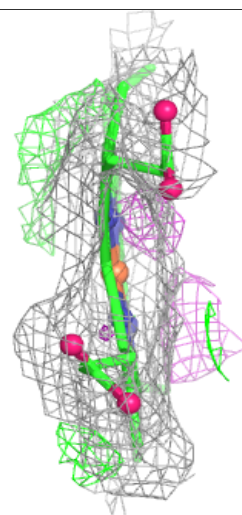
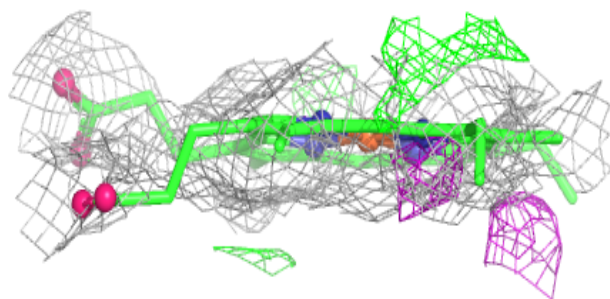
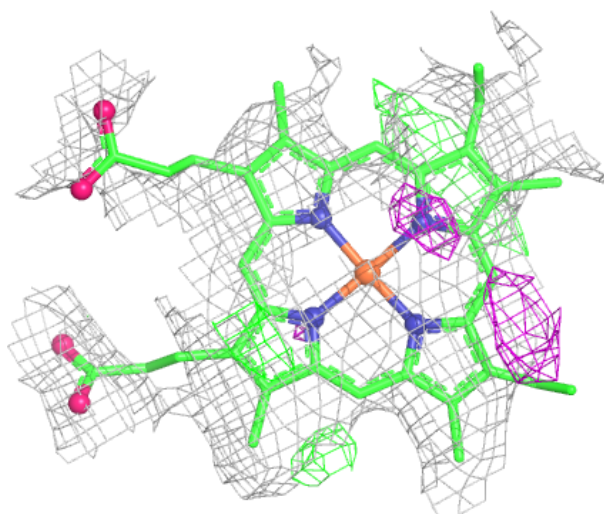
**Electron density around HEM G 160:**

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



**Electron density around HEM A 160:**

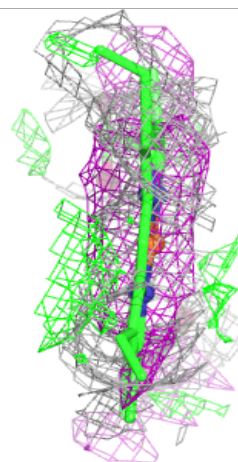
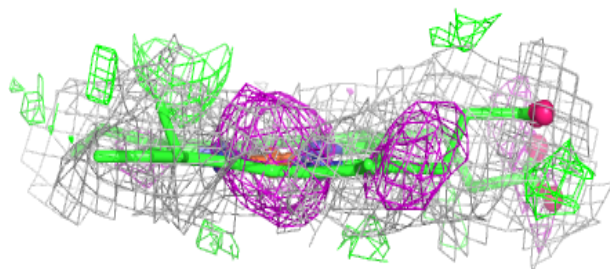
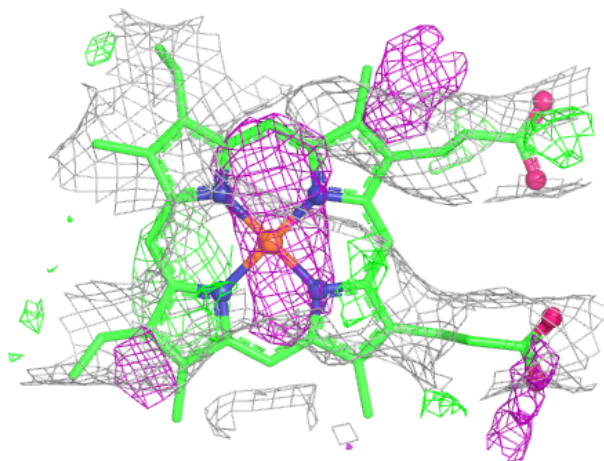
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





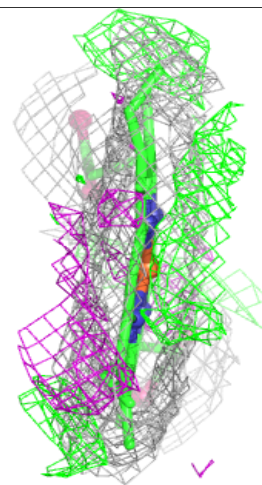
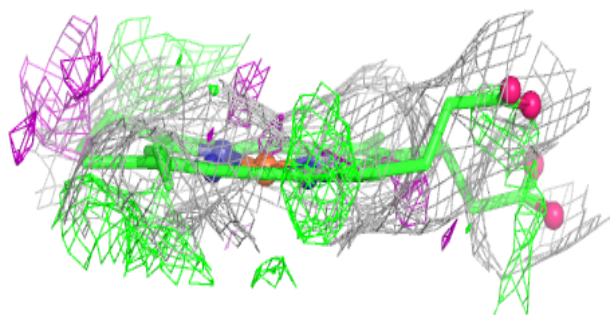
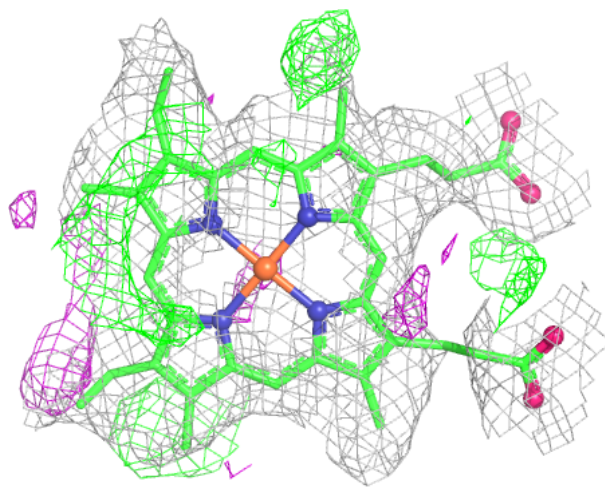
**Electron density around HEM B 160:**

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



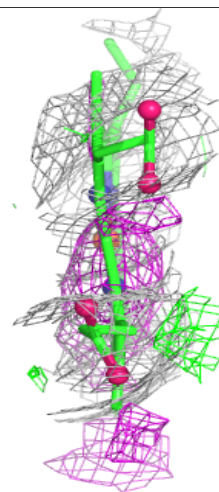
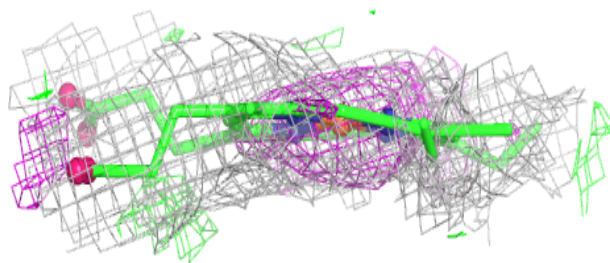
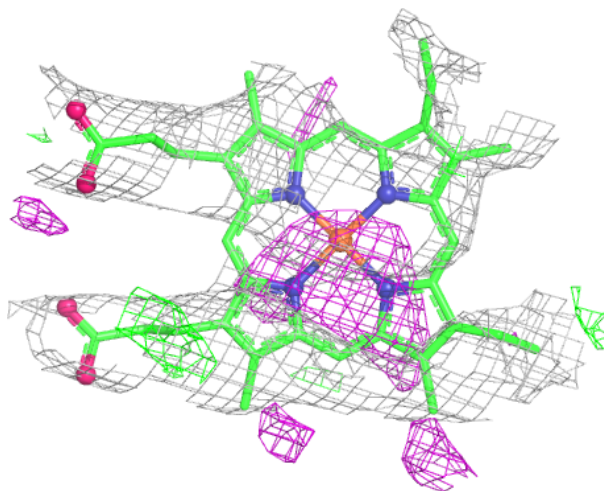
**Electron density around HEM C 160:**

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



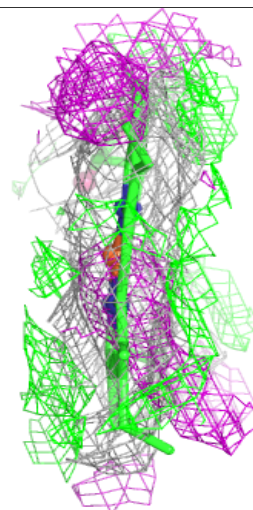
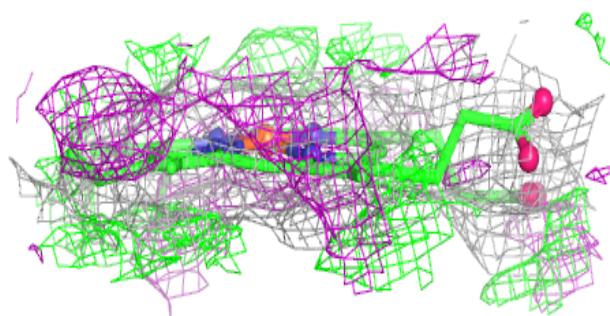
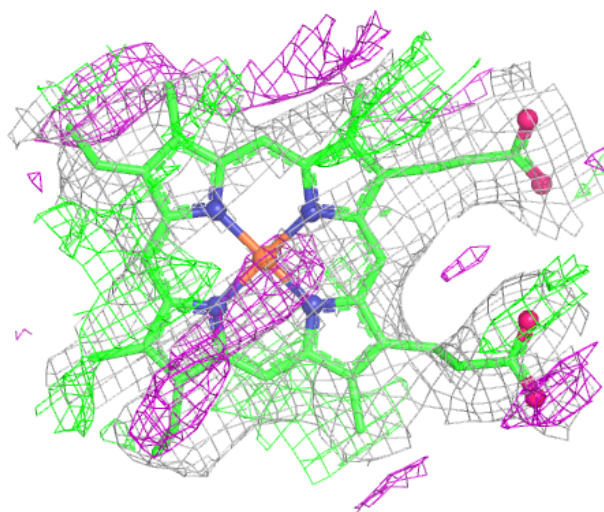
**Electron density around HEM D 160:**

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



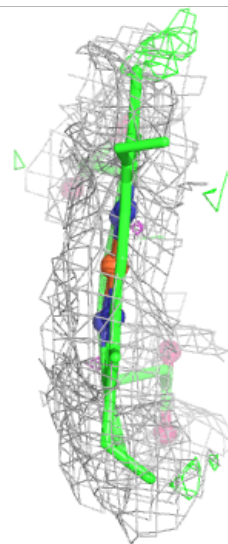
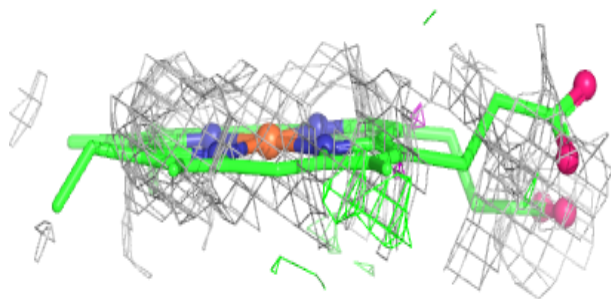
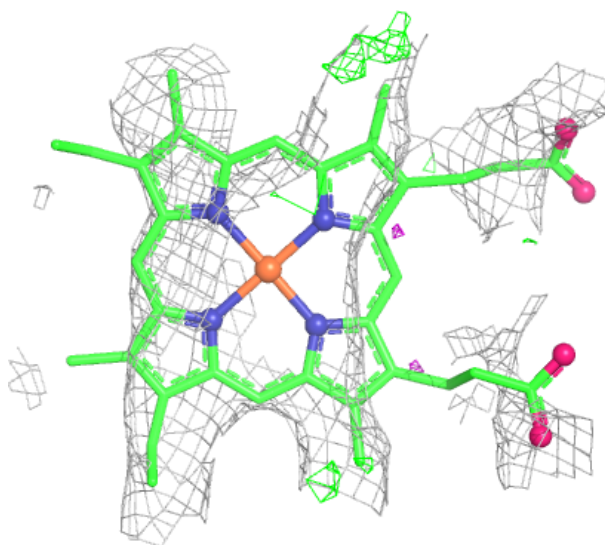
**Electron density around HEM F 160:**

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



**Electron density around HEM I 160:**

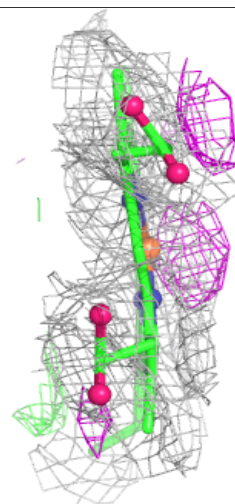
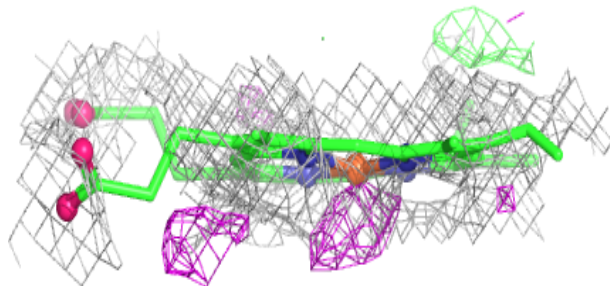
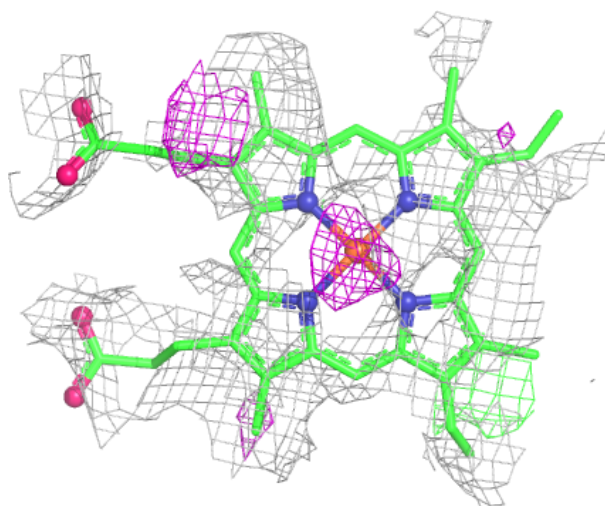
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





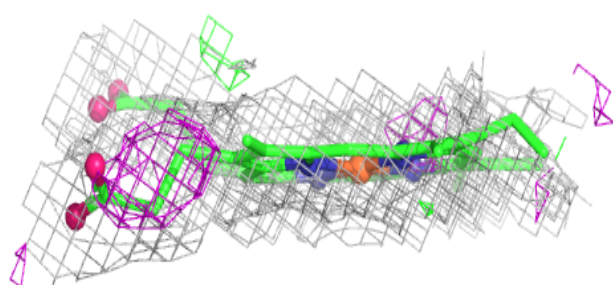
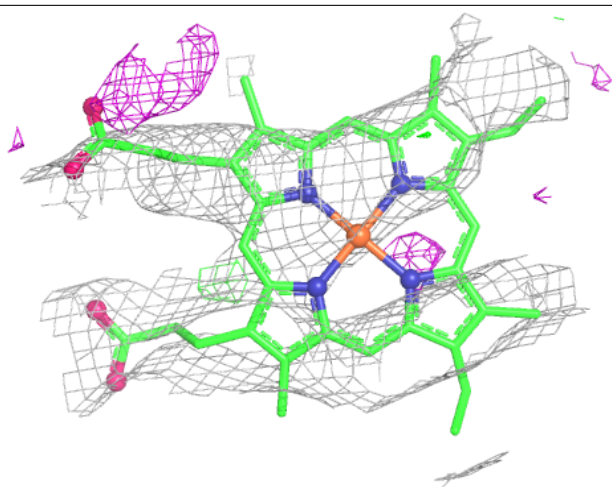
**Electron density around HEM J 160:**

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



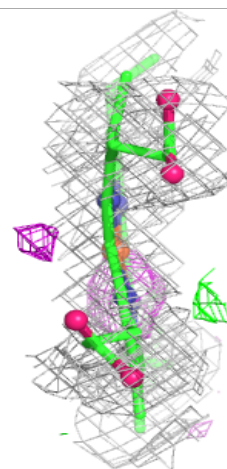
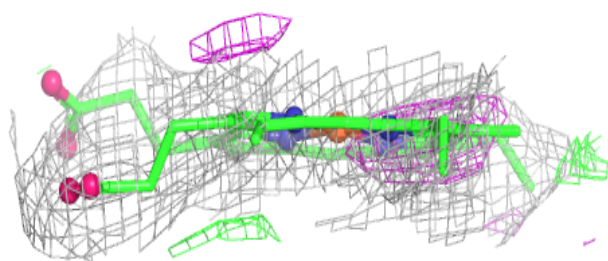
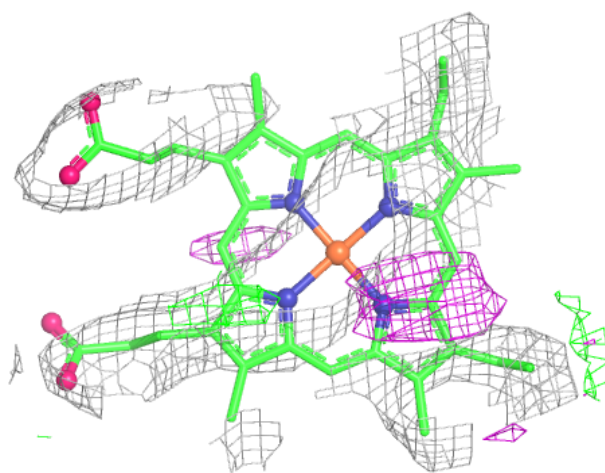
**Electron density around HEM K 160:**

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



**Electron density around HEM E 160:**

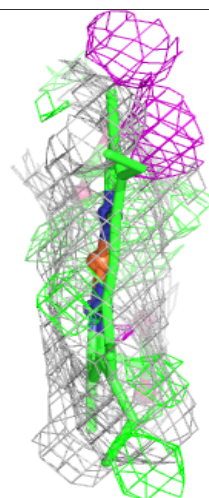
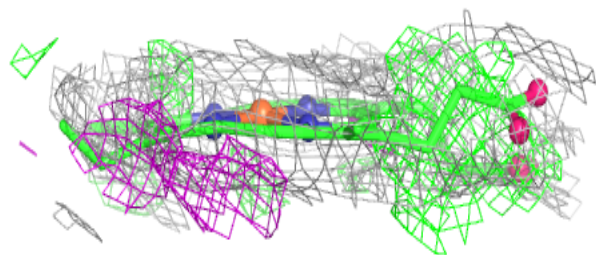
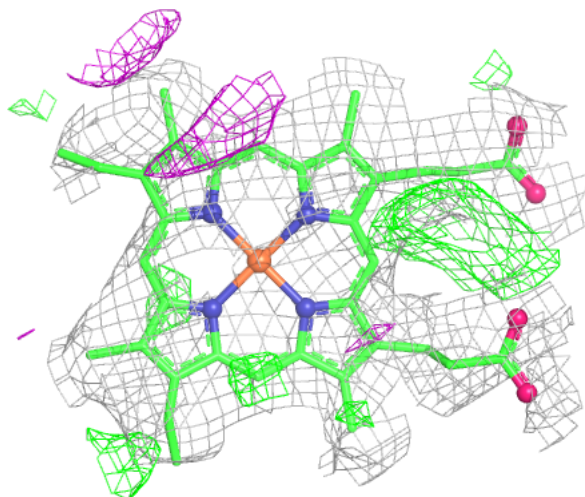
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





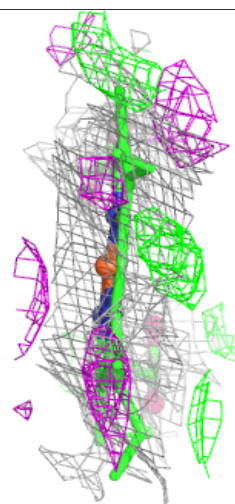
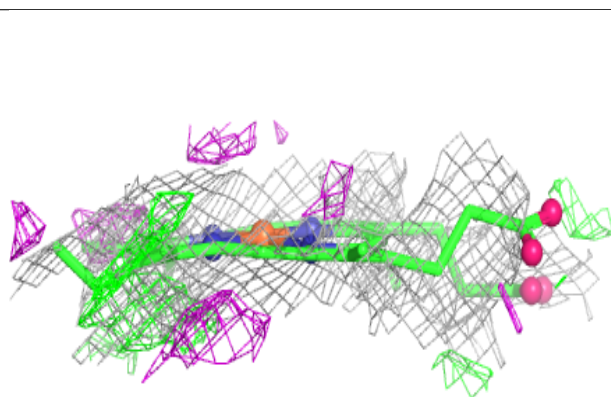
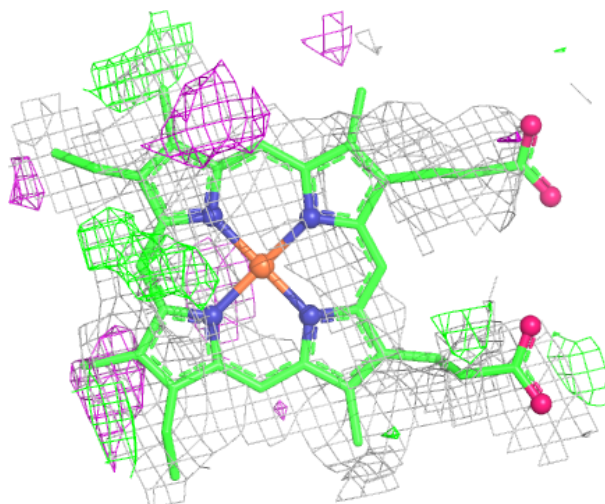
**Electron density around HEM H 160:**

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



**Electron density around HEM L 160:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.